Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 05:30 PM JST

PDB ID	:	6JLL
Title	:	XFEL structure of cyanobacterial photosystem II (2F state, dataset1)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2019-03-06
Resolution	:	2.15 Å(reported)

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

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

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

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

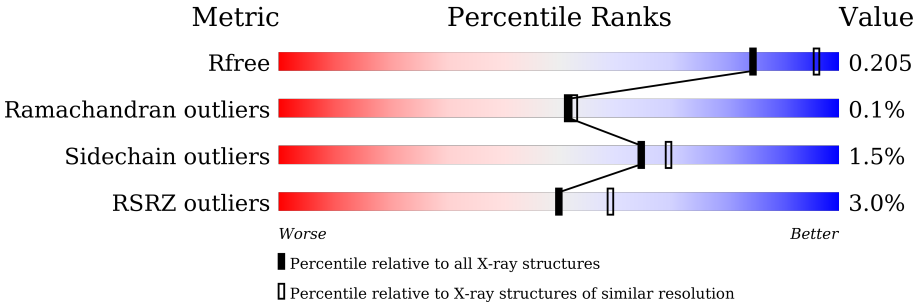
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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}	130704	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	%, 97%
1	a	344	3%, 96%
2	B	505	%, 99%
2	b	505	5%, 99%
3	C	455	%, 98%
3	c	455	%, 99%
4	D	342	99%

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Mol	Chain	Length	Quality of chain
4	d	342	%, 99%
5	E	84	10%, 95%
5	e	84	12%, 95%
6	F	44	7%, 77%, 23%
6	f	44	5%, 70%, 27%
7	H	65	5%, 97%
7	h	65	3%, 98%
8	I	38	8%, 97%
8	i	38	5%, 95%
9	J	39	8%, 97%
9	j	39	10%, 97%
10	K	37	97%
10	k	37	95%, 5%
11	L	37	3%, 97%
11	l	37	3%, 100%
12	M	36	6%, 92%, 6%
12	m	36	89%, 6%, 6%
13	O	244	%, 98%
13	o	244	2%, 98%
14	T	32	3%, 88%, 6%, 6%
14	t	32	88%, 6%, 6%
15	U	104	91%, 7%
15	u	104	91%, 7%
16	V	137	100%
16	v	137	%, 100%

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Mol	Chain	Length	Quality of chain
17	Y	30	23% 93%
17	y	30	7% 90% 7%
18	X	40	10% 98%
18	x	40	10% 95% 5%
19	Z	62	11% 95% 5%
19	z	62	16% 94% 6%
20	R	34	53% 85% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	410	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	b	626	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 55675 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
			Total	C	N	O	S			
1	A	334	3014	1963	496	537	18	0	54	0
1	a	334	3010	1964	494	534	18	0	56	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	504	4021	2639	667	702	13	0	10	0
2	b	503	4022	2644	664	701	13	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	451	3553	2322	592	626	13	0	14	0
3	c	455	3641	2382	606	639	14	0	20	0

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	81	668	436	107	125	0	2	0
5	e	81	670	439	107	124	0	2	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	34	275	187	45	42	1	0	0	0
6	f	32	257	175	43	38	1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	38	272	182	42	47	1	0	0	0
9	j	39	280	187	43	48	2	0	0	0

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	243	1903	1191	315	392	5	0	8	0
			Total	C	N	O	S			
13	o	243	1891	1183	315	388	5	0	5	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	264	185	36	41	2	0	1	0
			Total	C	N	O	S			
14	t	30	264	185	36	41	2	0	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1085	689	181	211	4	0	2	0
			Total	C	N	O	S			
16	v	137	1077	684	178	211	4	0	1	0

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

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

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

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

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

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

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

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

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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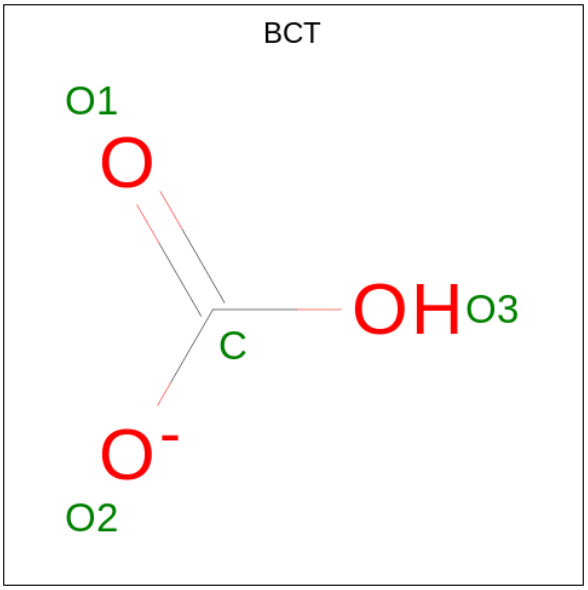
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
22	a	2	4	4	0	2
			Total	Cl		
22	v	1	1	1	0	0

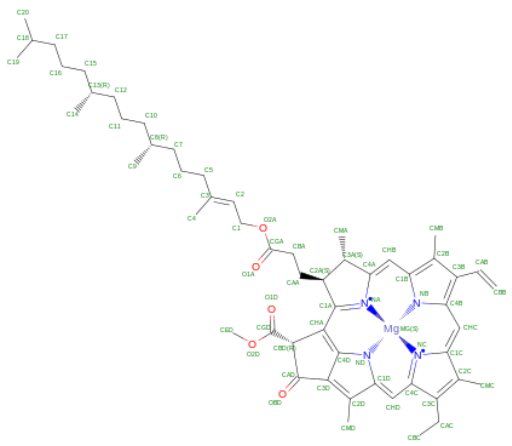
- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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

CLA



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

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

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

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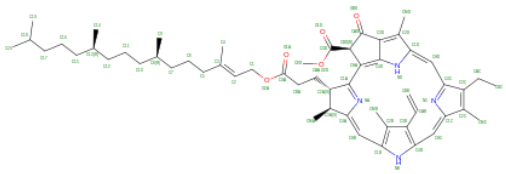
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
24	c	1	65	55	1	4	5	0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

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

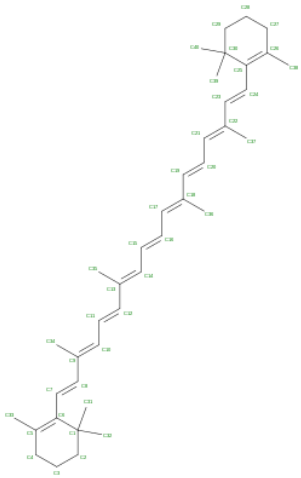
PHO



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

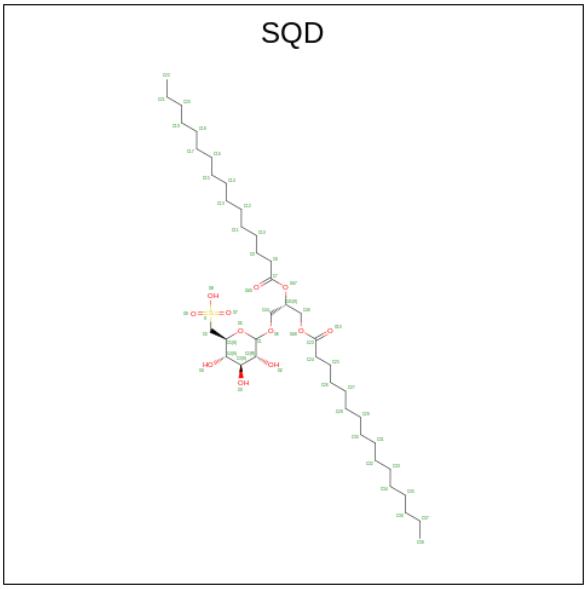
- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR



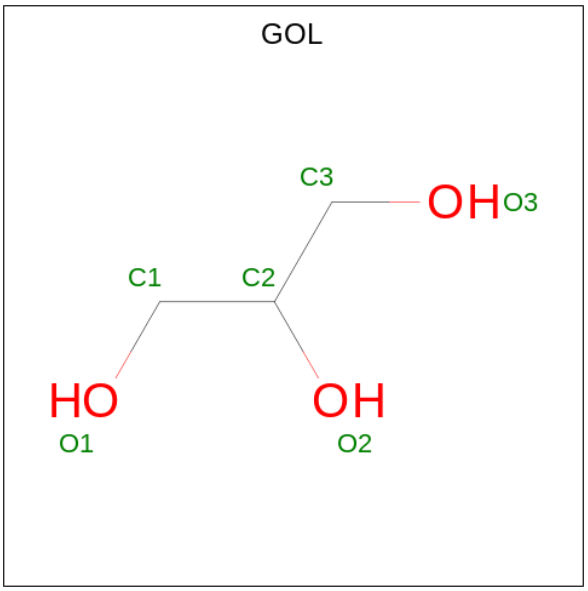
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
26	A	1	40	40	0	0
26	B	1	40	40	0	0
26	B	1	40	40	0	0
26	B	1	40	40	0	0
26	C	1	40	40	0	0
26	C	1	40	40	0	0
26	D	1	40	40	0	0
26	H	1	40	40	0	0
26	K	1	40	40	0	0
26	T	1	40	40	0	0
26	Y	1	40	40	0	0
26	a	1	40	40	0	0
26	b	1	40	40	0	0
26	b	1	40	40	0	0
26	b	1	40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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
			Total	C	O	S		
27	B	1	54	41	12	1	0	0
			Total	C	O	S		
27	F	1	43	30	12	1	0	0
			Total	C	O	S		
27	a	1	54	41	12	1	0	0
			Total	C	O	S		
27	a	1	54	41	12	1	0	0
			Total	C	O	S		
27	b	1	54	41	12	1	0	0
			Total	C	O	S		
27	f	1	43	30	12	1	0	0

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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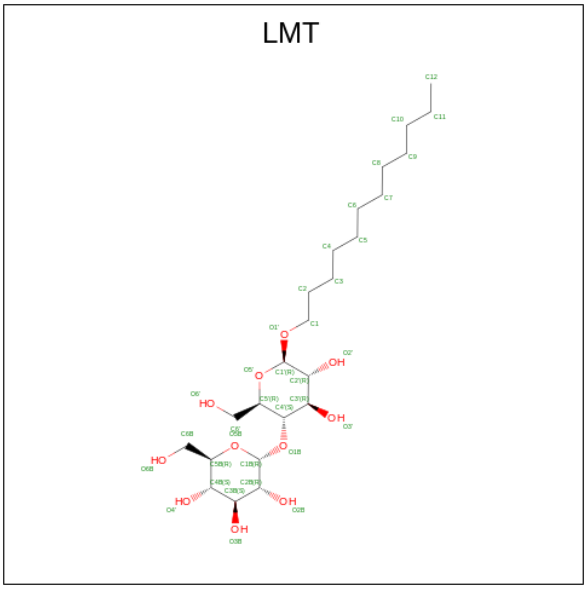
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	T	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	V	1	6	3	3	0	0
28	a	1	6	3	3	0	0
28	a	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	b	1	6	3	3	0	0
28	c	1	6	3	3	0	0
28	c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

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



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

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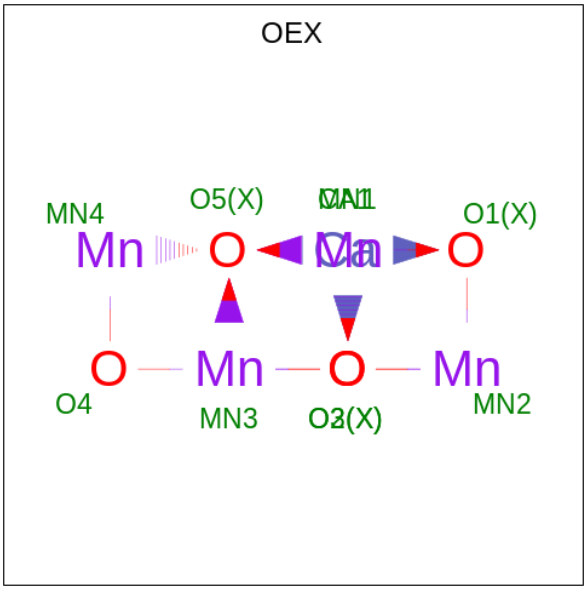
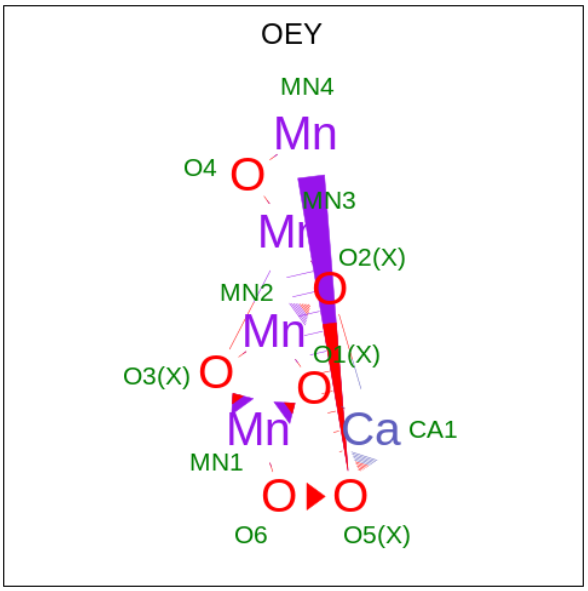
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	f	1	35	24	11	0	0
			Total	C	O		
29	m	1	35	24	11	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



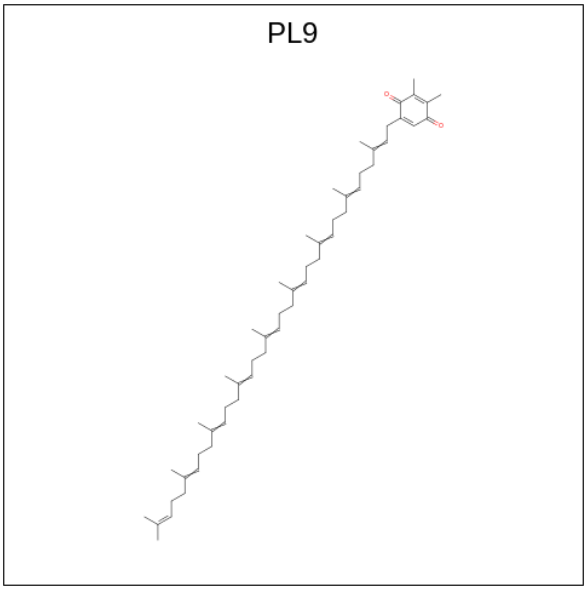
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
30	A	1	10	1	4	5	0	1
			Total	Ca	Mn	O		
30	a	1	10	1	4	5	0	1

- Molecule 31 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: $CaMn_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
31	A	1	11	1	4	6	0	1
			Total	Ca	Mn	O		
31	a	1	11	1	4	6	0	1

- Molecule 32 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 (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



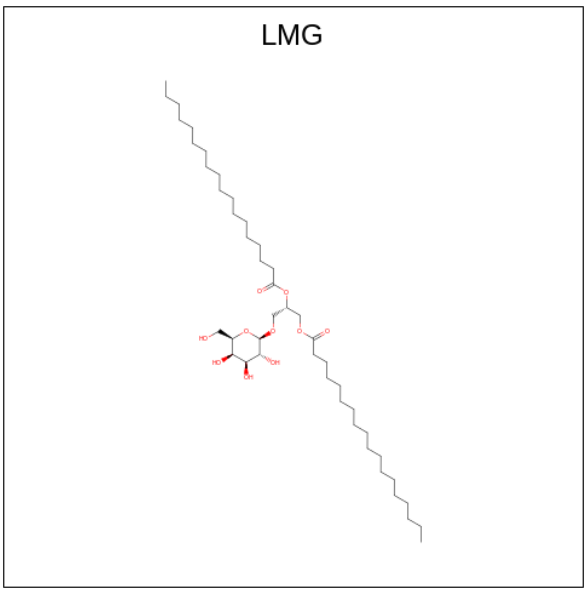
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 110 106 4	0	1
32	D	1	Total C O 110 106 4	0	1
32	a	1	Total C O 110 106 4	0	1
32	d	1	Total C O 110 106 4	0	1

- Molecule 33 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 28 23 5	0	0
33	B	1	Total C O 33 28 5	0	0
33	C	1	Total C O 34 29 5	0	0
33	D	2	Total C O 57 51 6	0	0
33	I	1	Total C O 40 35 5	0	0
33	J	1	Total C 10 10	0	0
33	M	1	Total C 10 10	0	0
33	X	1	Total C O 18 16 2	0	0
33	a	1	Total C O 30 25 5	0	0
33	b	1	Total C O 33 28 5	0	0
33	c	1	Total C O 32 27 5	0	0
33	d	3	Total C O 71 63 8	0	0
33	i	1	Total C O 40 35 5	0	0
33	j	1	Total C 10 10	0	0
33	m	1	Total C 10 10	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: $C_{45}H_{86}O_{10}$).

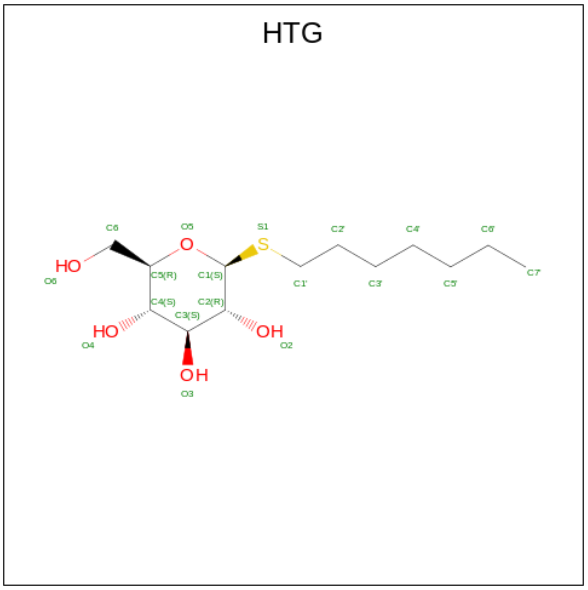


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	A	1	51	41	10	0	0
34	B	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	C	1	51	41	10	0	0
34	D	1	51	41	10	0	0
34	Z	1	37	27	10	0	0
34	a	1	51	41	10	0	0
34	b	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	c	1	51	41	10	0	0
34	j	1	51	41	10	0	0
34	z	1	39	29	10	0	0

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



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

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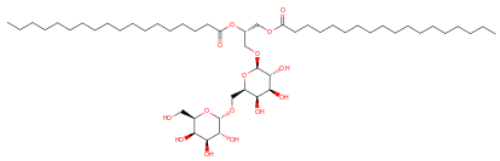
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
36	B	1	19	13	5	1	0	0
			Total	C	O	S		
36	B	1	19	13	5	1	0	0
			Total	C	O	S		
36	C	1	19	13	5	1	0	0
			Total	C	O	S		
36	C	1	19	13	5	1	0	0
			Total	C	O	S		
36	H	1	16	10	5	1	0	0
			Total	C	O	S		
36	V	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	b	1	19	13	5	1	0	0
			Total	C	O	S		
36	c	1	19	13	5	1	0	0
			Total	C	O	S		
36	c	1	19	13	5	1	0	0
			Total	C	O	S		
36	d	1	16	10	5	1	0	0

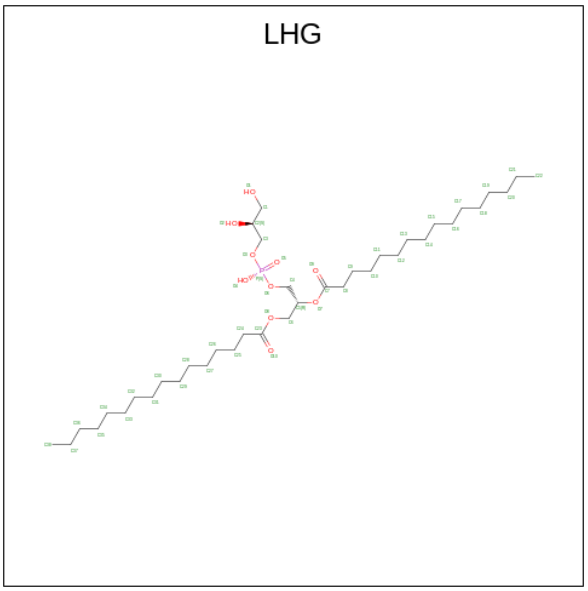
- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



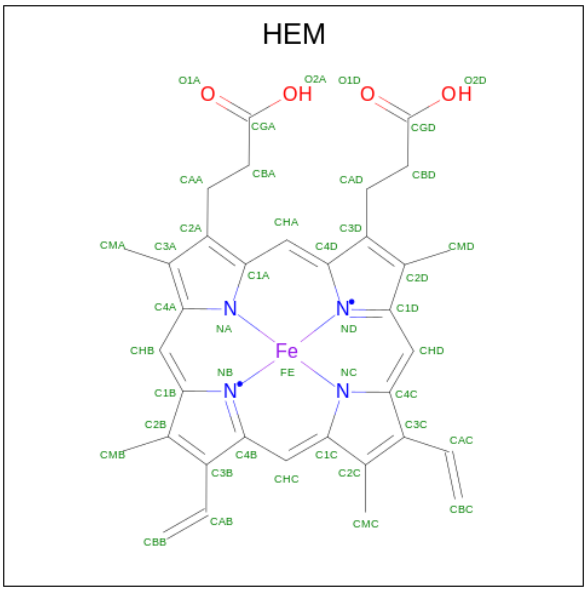
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
37	C	1	62	47	15	0	0
37	C	1	62	47	15	0	0
37	C	1	62	47	15	0	0
37	D	1	52	42	10	0	0
37	H	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	c	1	62	47	15	0	0
37	e	1	62	47	15	0	0
37	h	1	62	47	15	0	0

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



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	A	161	173	173	0	14
			Total	O		
41	B	290	294	294	0	4
			Total	O		
41	C	228	232	232	0	4

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	D	146	Total O 150 150	0	5
41	E	30	Total O 30 30	0	0
41	F	9	Total O 9 9	0	0
41	H	48	Total O 49 49	0	1
41	I	5	Total O 5 5	0	0
41	J	10	Total O 10 10	0	0
41	K	9	Total O 9 9	0	0
41	L	13	Total O 14 14	0	1
41	M	23	Total O 23 23	0	0
41	O	178	Total O 180 180	0	2
41	T	17	Total O 18 18	0	1
41	U	77	Total O 77 77	0	0
41	V	117	Total O 119 119	0	2
41	Y	4	Total O 4 4	0	0
41	X	6	Total O 6 6	0	0
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 162 162	0	12
41	b	266	Total O 269 269	0	3
41	c	200	Total O 205 205	0	5
41	d	129	Total O 132 132	0	3
41	e	19	Total O 19 19	0	0

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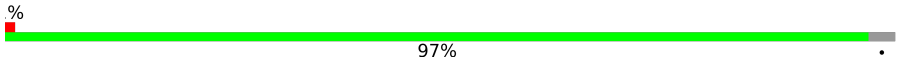
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	f	8	Total O 8 8	0	0
41	h	44	Total O 44 44	0	0
41	i	5	Total O 5 5	0	0
41	j	6	Total O 6 6	0	0
41	k	7	Total O 7 7	0	0
41	l	9	Total O 9 9	0	0
41	m	11	Total O 11 11	0	0
41	o	155	Total O 155 155	0	0
41	t	11	Total O 11 11	0	0
41	u	93	Total O 93 93	0	0
41	v	81	Total O 82 82	0	1
41	y	2	Total O 2 2	0	0
41	x	6	Total O 6 6	0	0

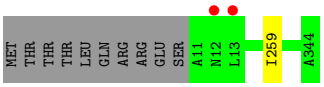
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

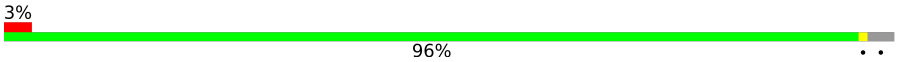
Chain A:





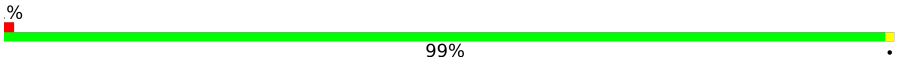
• Molecule 1: Photosystem II protein D1

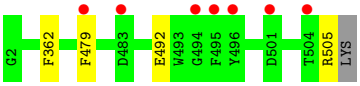
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

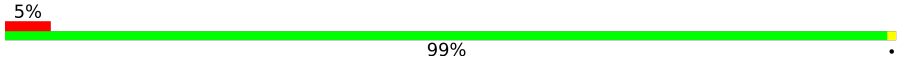
Chain B:

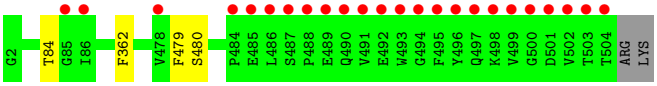




• Molecule 2: Photosystem II CP47 reaction center protein

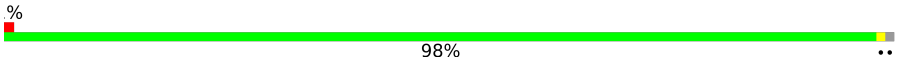
Chain b:





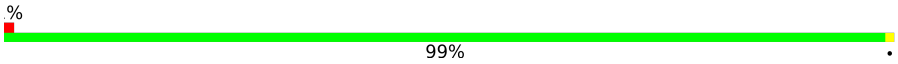
• Molecule 3: Photosystem II CP43 reaction center protein

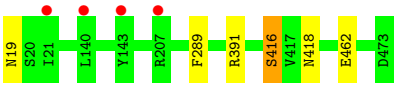
Chain C:



• Molecule 3: Photosystem II CP43 reaction center protein

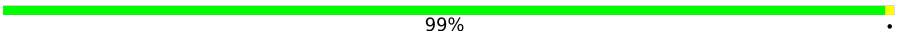
Chain c:

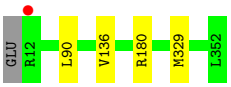




• Molecule 4: Photosystem II D2 protein

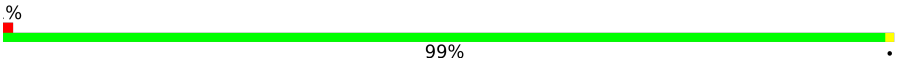
Chain D:

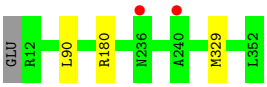




• Molecule 4: Photosystem II D2 protein

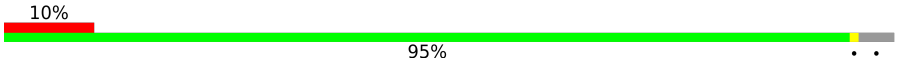
Chain d:

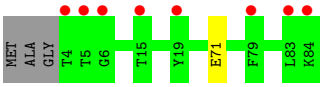




• Molecule 5: Cytochrome b559 subunit alpha

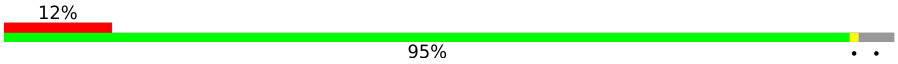
Chain E:

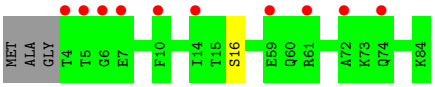




• Molecule 5: Cytochrome b559 subunit alpha

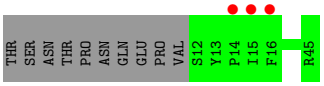
Chain e:





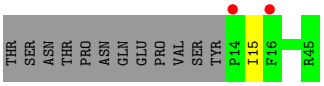
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



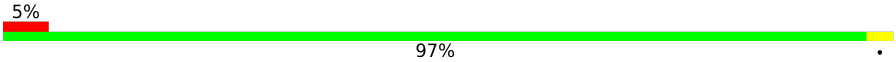
• Molecule 6: Cytochrome b559 subunit beta

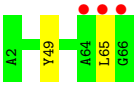
Chain f:



• Molecule 7: Photosystem II reaction center protein H

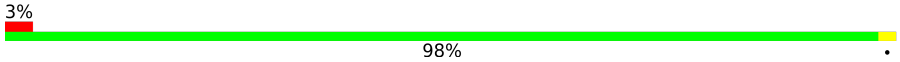
Chain H:

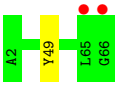




• Molecule 7: Photosystem II reaction center protein H

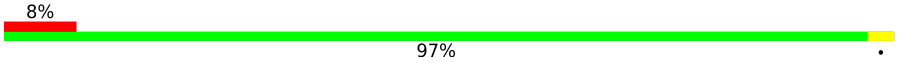
Chain h:

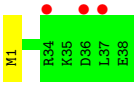




• Molecule 8: Photosystem II reaction center protein I

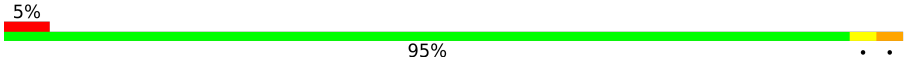
Chain I:

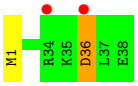




• Molecule 8: Photosystem II reaction center protein I

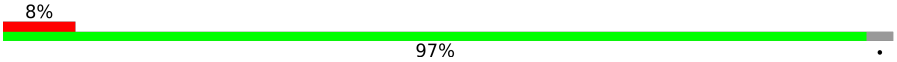
Chain i:

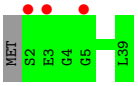




• Molecule 9: Photosystem II reaction center protein J

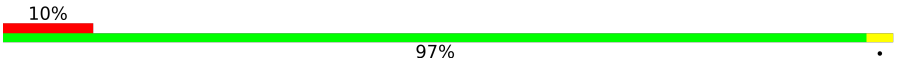
Chain J:

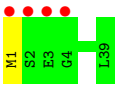




• Molecule 9: Photosystem II reaction center protein J

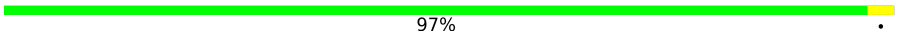
Chain j:



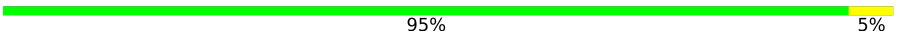


• Molecule 10: Photosystem II reaction center protein K

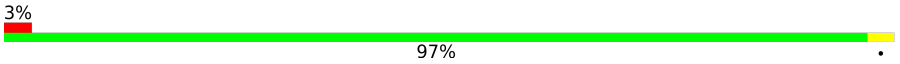
Chain K:



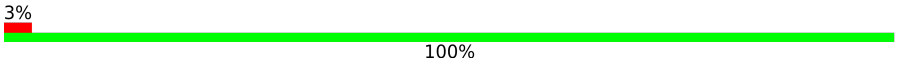
• Molecule 10: Photosystem II reaction center protein K

Chain k: 

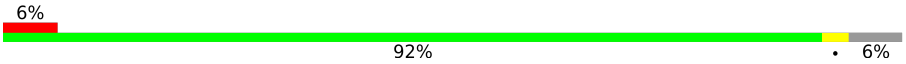
• Molecule 11: Photosystem II reaction center protein L

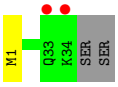
Chain L: 

• Molecule 11: Photosystem II reaction center protein L

Chain l: 

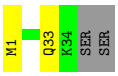
• Molecule 12: Photosystem II reaction center protein M

Chain M: 

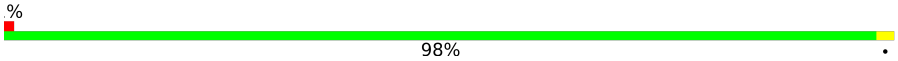


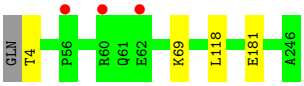
• Molecule 12: Photosystem II reaction center protein M

Chain m:

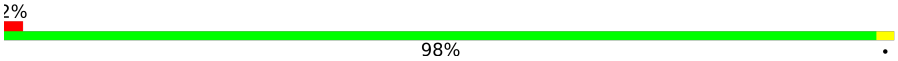


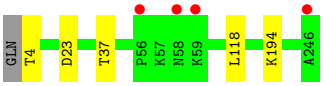
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 



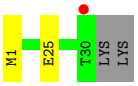
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 



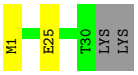
• Molecule 14: Photosystem II reaction center protein T

Chain T:



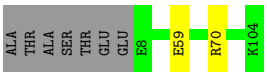
• Molecule 14: Photosystem II reaction center protein T

Chain t:



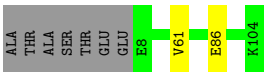
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



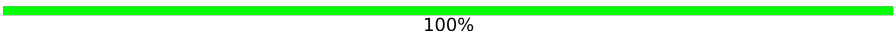
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



• Molecule 16: Cytochrome c-550

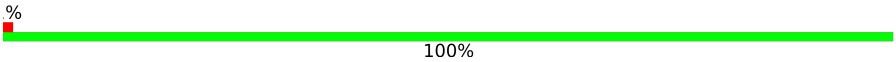
Chain V:



There are no outlier residues recorded for this chain.

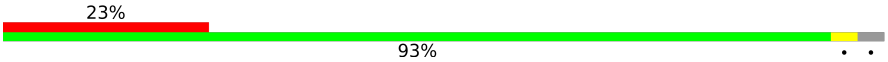
• Molecule 16: Cytochrome c-550

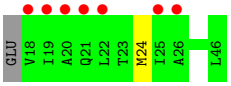
Chain v:



• Molecule 17: Photosystem II reaction center protein Ycf12

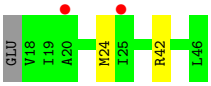
Chain Y:





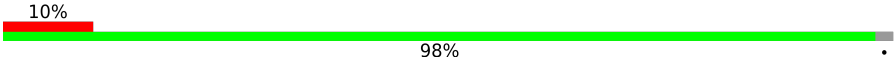
• Molecule 17: Photosystem II reaction center protein Ycf12

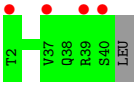
Chain y:



• Molecule 18: Photosystem II reaction center protein X

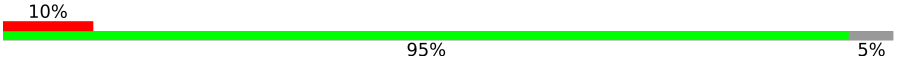
Chain X:

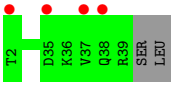




• Molecule 18: Photosystem II reaction center protein X

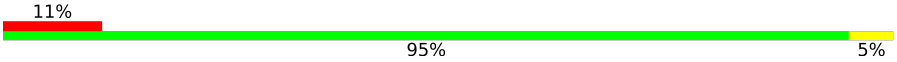
Chain x:

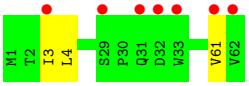




• Molecule 19: Photosystem II reaction center protein Z

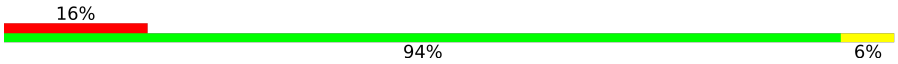
Chain Z:

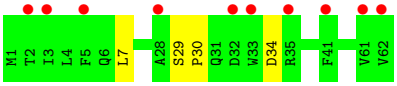




• Molecule 19: Photosystem II reaction center protein Z

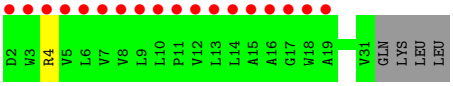
Chain z:





• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 178.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.15) 99.9 (178.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.156 , 0.203 0.159 , 0.205	Depositor DCC
R_{free} test set	26822 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 76.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	55675	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: PL9, OEY, CLA, BCT, GOL, OEX, HEM, LMT, HTG, PHO, FME, LHG, MG, BCR, DGD, CL, SQD, UNL, FE2, CA, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	0/3115	0.55	0/4242
1	a	0.44	0/3117	0.54	0/4245
2	B	0.44	0/4191	0.53	0/5709
2	b	0.42	0/4198	0.52	0/5720
3	C	0.39	0/3678	0.51	0/5007
3	c	0.38	0/3774	0.51	0/5135
4	D	0.48	0/2952	0.55	0/4021
4	d	0.45	0/2952	0.54	0/4021
5	E	0.34	0/693	0.49	0/944
5	e	0.33	0/695	0.49	0/948
6	F	0.41	0/284	0.51	0/387
6	f	0.40	0/265	0.52	0/360
7	H	0.36	0/535	0.55	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.35	0/311	0.49	0/419
8	i	0.34	0/311	0.45	0/419
9	J	0.33	0/278	0.41	0/376
9	j	0.35	0/286	0.45	0/386
10	K	0.34	0/303	0.50	0/416
10	k	0.34	0/303	0.50	0/416
11	L	0.44	0/319	0.48	0/433
11	l	0.43	0/319	0.46	0/433
12	M	0.48	0/270	0.57	0/368
12	m	0.43	0/262	0.54	0/357
13	O	0.38	0/1958	0.56	0/2654
13	o	0.37	0/1937	0.54	0/2625
14	T	0.49	0/266	0.54	0/362
14	t	0.49	0/266	0.52	0/362
15	U	0.38	0/785	0.53	0/1064
15	u	0.39	0/785	0.52	0/1064
16	V	0.39	0/1109	0.50	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.35	0/1098	0.50	0/1488
17	Y	0.35	0/216	0.50	0/289
17	y	0.30	0/216	0.43	0/289
18	X	0.34	0/290	0.45	0/392
18	x	0.30	0/284	0.46	0/384
19	Z	0.31	0/490	0.43	0/669
19	z	0.28	0/490	0.44	0/669
20	R	0.23	0/245	0.37	0/338
All	All	0.41	0/44370	0.52	0/60354

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/344 (112%)	380 (99%)	3 (1%)	1 (0%)	41	37
1	a	384/344 (112%)	378 (98%)	5 (1%)	1 (0%)	41	37
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	461/455 (101%)	450 (98%)	9 (2%)	2 (0%)	34	29
3	c	473/455 (104%)	459 (97%)	12 (2%)	2 (0%)	34	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
4	d	355/342 (104%)	345 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	81 (100%)	0	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	1
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	245 (98%)	4 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	3
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5429/5384 (101%)	5309 (98%)	111 (2%)	9 (0%)	51	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	i	36	ASP
19	z	30	PRO
1	a	259	ILE
1	A	259	ILE
19	Z	61	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/279 (112%)	311 (100%)	0	100	100
1	a	311/279 (112%)	309 (99%)	2 (1%)	86	90
2	B	412/403 (102%)	408 (99%)	4 (1%)	76	81
2	b	413/403 (102%)	409 (99%)	4 (1%)	76	81
3	C	361/356 (101%)	356 (99%)	5 (1%)	67	72
3	c	371/356 (104%)	363 (98%)	8 (2%)	52	55
4	D	290/277 (105%)	286 (99%)	4 (1%)	67	72
4	d	290/277 (105%)	287 (99%)	3 (1%)	76	81
5	E	74/73 (101%)	73 (99%)	1 (1%)	67	72
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	31
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	33
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	61
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	42
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	32
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	37
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	11
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	44
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	37
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	53
13	o	211/207 (102%)	206 (98%)	5 (2%)	49	51
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	9
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	9
15	U	84/89 (94%)	82 (98%)	2 (2%)	49	51
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	51
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	118 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	24
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	5
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	31
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	15
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	29
All	All	4504/4403 (102%)	4434 (98%)	70 (2%)	65	67

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
2	B	479	PHE
2	B	492	GLU
2	B	505	ARG
3	C	29	GLU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	418	ASN
4	D	90	LEU
4	D	136	VAL
4	D	180	ARG
4	D	329	MET
5	E	71	GLU
7	H	49	TYR
7	H	65	LEU
10	K	17	ILE
11	L	13	ASN
13	O	4	THR
13	O	69	LYS
13	O	118	LEU
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	59	GLU
15	U	70	ARG
17	Y	24	MET
19	Z	3	ILE
19	Z	4	LEU
20	R	4	ARG
1	a	12	ASN
1	a	305	SER
2	b	84	THR
2	b	362	PHE
2	b	479	PHE
2	b	480	SER
3	c	19	ASN
3	c	289	PHE
3	c	391	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN

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Mol	Chain	Res	Type
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	180	ARG
4	d	329	MET
5	e	16	SER
6	f	15	ILE
7	h	49	TYR
8	i	36	ASP
9	j	1	MET
10	k	10	LYS
10	k	17	ILE
12	m	33	GLN
13	o	4	THR
13	o	23	ASP
13	o	37	THR
13	o	118	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	61	VAL
15	u	86	GLU
17	y	24	MET
17	y	42	ARG
19	z	7	LEU
19	z	29	SER
19	z	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	53	ASN
2	B	331	ASN
2	B	490	GLN
3	C	201	ASN
4	D	61	HIS
4	D	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN

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Mol	Chain	Res	Type
19	Z	58	ASN
1	a	12	ASN
1	a	315	ASN
2	b	53	ASN
2	b	331	ASN
3	c	373	ASN
4	d	61	HIS
4	d	83	ASN
4	d	332	GLN
13	o	130	GLN
19	z	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	t	1	14	8,9,10	0.79	0	7,9,11	2.41	4 (57%)
12	FME	m	1	12	8,9,10	0.66	0	7,9,11	1.33	1 (14%)
8	FME	i	1	8	8,9,10	0.60	0	7,9,11	1.21	1 (14%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.26	1 (14%)
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.30	1 (14%)
12	FME	M	1	12	8,9,10	0.67	0	7,9,11	1.39	2 (28%)

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
14	FME	t	1	14	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-3.87	116.87	122.82
14	t	1	FME	C-CA-N	2.86	114.89	109.73
14	T	1	FME	O-C-CA	-2.50	118.22	124.78
14	t	1	FME	O-C-CA	-2.43	118.40	124.78
14	t	1	FME	O1-CN-N	-2.33	119.13	125.27
12	m	1	FME	O-C-CA	-2.30	118.76	124.78
8	I	1	FME	O-C-CA	-2.28	118.79	124.78
12	M	1	FME	CA-N-CN	-2.28	119.31	122.82
12	M	1	FME	O-C-CA	-2.07	119.36	124.78
8	i	1	FME	O-C-CA	-2.04	119.43	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 266 ligands modelled in this entry, 24 are monoatomic and 18 are unknown - leaving 224 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	GOL	B	629	-	5,5,5	0.36	0	5,5,5	0.33	0
38	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.07	3 (6%)
26	BCR	t	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.62	14 (25%)
28	GOL	V	202	-	5,5,5	0.37	0	5,5,5	0.28	0
24	CLA	B	614	-	65,73,73	2.06	15 (23%)	76,113,113	2.58	27 (35%)
27	SQD	A	416	-	53,54,54	1.03	3 (5%)	62,65,65	1.18	6 (9%)
27	SQD	F	103	-	42,43,54	1.15	3 (7%)	51,54,65	1.64	11 (21%)
28	GOL	o	301	-	5,5,5	0.37	0	5,5,5	0.27	0
34	LMG	A	422	-	51,51,55	0.94	2 (3%)	59,59,63	1.13	5 (8%)
34	LMG	b	630	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
36	HTG	H	101	-	16,16,19	1.12	2 (12%)	20,21,24	1.22	1 (5%)
29	LMT	A	417	-	36,36,36	0.61	1 (2%)	47,47,47	1.25	3 (6%)
26	BCR	D	404	-	41,41,41	1.02	1 (2%)	56,56,56	1.80	11 (19%)
23	BCT	A	404[A]	21	2,3,3	0.63	0	2,3,3	1.09	0
34	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.13	4 (8%)
28	GOL	V	204	-	5,5,5	0.38	0	5,5,5	0.26	0
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)
24	CLA	b	626	-	65,73,73	2.05	17 (26%)	76,113,113	2.74	28 (36%)
28	GOL	A	413	-	5,5,5	0.34	0	5,5,5	0.25	0
32	PL9	d	405[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.55	13 (19%)
28	GOL	V	203	-	5,5,5	0.35	0	5,5,5	0.43	0
36	HTG	b	608	-	19,19,19	1.03	2 (10%)	23,24,24	1.48	2 (8%)
26	BCR	C	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.49	9 (16%)
26	BCR	C	514	-	41,41,41	1.03	1 (2%)	56,56,56	1.55	10 (17%)
29	LMT	M	103	-	36,36,36	0.52	1 (2%)	47,47,47	0.99	3 (6%)
34	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	0.98	3 (5%)
28	GOL	b	605	-	5,5,5	0.37	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	b	616	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	27 (35%)
24	CLA	b	624	-	65,73,73	2.03	15 (23%)	76,113,113	2.88	29 (38%)
27	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.41	7 (13%)
27	SQD	A	412	-	53,54,54	0.97	3 (5%)	62,65,65	1.53	11 (17%)
34	LMG	c	523	-	51,51,55	0.96	2 (3%)	59,59,63	1.22	8 (13%)
29	LMT	b	631	-	25,25,36	0.52	0	30,30,47	0.67	0
31	OEY	a	418[B]	3,1,41	0,16,16	-	-	-		
36	HTG	B	633	-	19,19,19	1.01	2 (10%)	23,24,24	1.43	2 (8%)
26	BCR	b	627	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	5 (8%)
24	CLA	b	617	41	65,73,73	1.96	16 (24%)	76,113,113	2.82	25 (32%)
24	CLA	c	506	-	65,73,73	2.06	17 (26%)	76,113,113	2.66	25 (32%)
24	CLA	C	507	41	65,73,73	2.02	15 (23%)	76,113,113	2.71	27 (35%)
34	LMG	B	622	-	51,51,55	0.93	2 (3%)	59,59,63	1.08	4 (6%)
24	CLA	C	504	41	65,73,73	2.06	17 (26%)	76,113,113	2.84	28 (36%)
24	CLA	c	515	3	65,73,73	2.03	16 (24%)	76,113,113	2.66	25 (32%)
38	LHG	D	407	-	48,48,48	0.86	2 (4%)	51,54,54	1.09	5 (9%)
26	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.47	9 (16%)
24	CLA	C	511	3	65,73,73	2.07	15 (23%)	76,113,113	2.70	28 (36%)
23	BCT	A	404[B]	21	2,3,3	0.63	0	2,3,3	1.02	0
27	SQD	b	601	-	53,54,54	1.04	3 (5%)	62,65,65	1.55	9 (14%)
24	CLA	c	508	41	65,73,73	2.07	17 (26%)	76,113,113	2.85	31 (40%)
38	LHG	d	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.98	2 (3%)
24	CLA	d	401	41	65,73,73	2.08	17 (26%)	76,113,113	2.77	30 (39%)
28	GOL	v	202	-	5,5,5	0.35	0	5,5,5	0.25	0
37	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	6 (7%)
32	PL9	d	405[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.61	16 (23%)
24	CLA	C	510	-	65,73,73	2.10	16 (24%)	76,113,113	2.65	28 (36%)
28	GOL	A	414	-	5,5,5	0.46	0	5,5,5	0.53	0
28	GOL	C	525	-	5,5,5	0.39	0	5,5,5	0.67	0
28	GOL	C	524	-	5,5,5	0.38	0	5,5,5	0.77	0
24	CLA	d	403	-	65,73,73	2.04	17 (26%)	76,113,113	2.82	28 (36%)
37	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	0.98	5 (6%)
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.10	2 (3%)
24	CLA	B	610	-	65,73,73	2.04	16 (24%)	76,113,113	2.69	27 (35%)
26	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.56	11 (19%)
28	GOL	V	205	-	5,5,5	0.34	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	b	621	-	65,73,73	2.00	15 (23%)	76,113,113	2.77	27 (35%)
24	CLA	b	618	-	65,73,73	2.12	16 (24%)	76,113,113	2.64	29 (38%)
28	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.55	0
25	PHO	a	420[A]	-	51,69,69	1.85	8 (15%)	47,99,99	1.96	10 (21%)
38	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.84	3 (5%)
28	GOL	v	203	-	5,5,5	0.40	0	5,5,5	0.26	0
29	LMT	a	404	-	36,36,36	0.48	1 (2%)	47,47,47	1.20	3 (6%)
36	HTG	C	523	-	19,19,19	1.03	2 (10%)	23,24,24	1.81	4 (17%)
28	GOL	b	603	-	5,5,5	0.43	0	5,5,5	0.47	0
24	CLA	c	505	-	65,73,73	2.04	16 (24%)	76,113,113	2.66	26 (34%)
24	CLA	b	622	-	65,73,73	2.09	16 (24%)	76,113,113	2.67	29 (38%)
39	HEM	F	102	6,5	41,50,50	1.25	4 (9%)	45,82,82	1.95	9 (20%)
26	BCR	b	629	-	41,41,41	1.08	1 (2%)	56,56,56	1.22	6 (10%)
37	DGD	H	103	-	63,63,67	0.88	3 (4%)	77,77,81	1.05	7 (9%)
39	HEM	V	206	16	41,50,50	1.40	6 (14%)	45,82,82	1.73	9 (20%)
28	GOL	T	102	-	5,5,5	0.39	0	5,5,5	0.26	0
36	HTG	d	411	-	16,16,19	1.13	2 (12%)	20,21,24	1.90	2 (10%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.94	1 (2%)
26	BCR	a	413	-	41,41,41	1.04	1 (2%)	56,56,56	1.17	7 (12%)
36	HTG	c	524	-	19,19,19	1.04	2 (10%)	23,24,24	1.53	2 (8%)
37	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	0.96	2 (2%)
24	CLA	c	517	-	65,73,73	2.03	16 (24%)	76,113,113	2.76	29 (38%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.05	4 (7%)
38	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.07	3 (5%)
24	CLA	A	406	41	65,73,73	2.03	15 (23%)	76,113,113	2.89	31 (40%)
25	PHO	a	411	-	51,69,69	1.86	9 (17%)	47,99,99	1.67	8 (17%)
30	OEX	a	417[A]	3,1,41	0,15,15	-	-	-		
24	CLA	d	402	-	65,73,73	2.03	16 (24%)	76,113,113	2.77	27 (35%)
24	CLA	B	609	-	65,73,73	2.05	17 (26%)	76,113,113	2.70	29 (38%)
29	LMT	B	635	-	25,25,36	0.51	0	30,30,47	0.87	1 (3%)
26	BCR	T	103	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	16 (28%)
26	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.61	8 (14%)
25	PHO	a	420[B]	-	51,69,69	1.86	8 (15%)	47,99,99	1.81	9 (19%)
24	CLA	a	410	41	65,73,73	2.03	15 (23%)	76,113,113	2.80	29 (38%)
32	PL9	a	416[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.91	20 (29%)
36	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.57	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
26	BCR	B	620	-	41,41,41	1.06	1 (2%)	56,56,56	1.52	8 (14%)
26	BCR	d	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.56	10 (17%)
23	BCT	a	419[A]	-	2,3,3	0.66	0	2,3,3	0.85	0
24	CLA	B	603	-	65,73,73	2.08	16 (24%)	76,113,113	2.84	30 (39%)
26	BCR	k	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.45	10 (17%)
26	BCR	K	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.55	13 (23%)
36	HTG	b	609	-	19,19,19	1.06	2 (10%)	23,24,24	1.23	3 (13%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.14	0
32	PL9	D	405[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.65	20 (29%)
24	CLA	b	611	41	65,73,73	2.08	15 (23%)	76,113,113	2.76	25 (32%)
26	BCR	c	527	-	41,41,41	1.04	1 (2%)	56,56,56	1.56	9 (16%)
36	HTG	B	625	-	19,19,19	1.07	2 (10%)	23,24,24	1.87	4 (17%)
28	GOL	O	301	-	5,5,5	0.37	0	5,5,5	0.41	0
24	CLA	c	509	-	65,73,73	2.00	15 (23%)	76,113,113	2.64	26 (34%)
31	OEY	A	419[B]	3,1,41	0,16,16	-	-	-		
28	GOL	B	631	-	5,5,5	0.37	0	5,5,5	0.30	0
34	LMG	Z	101	-	37,37,55	0.95	2 (5%)	45,45,63	1.38	6 (13%)
38	LHG	a	422	-	41,41,48	1.02	2 (4%)	44,47,54	0.95	3 (6%)
36	HTG	b	632	-	19,19,19	0.77	1 (5%)	23,24,24	1.29	2 (8%)
24	CLA	B	612	-	65,73,73	1.99	16 (24%)	76,113,113	2.84	27 (35%)
28	GOL	t	102	-	5,5,5	0.47	0	5,5,5	0.16	0
37	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.97	4 (5%)
24	CLA	C	509	-	65,73,73	2.14	16 (24%)	76,113,113	2.75	28 (36%)
29	LMT	T	104	-	25,25,36	0.50	0	30,30,47	0.93	1 (3%)
24	CLA	a	412	-	65,73,73	2.05	15 (23%)	76,113,113	2.79	30 (39%)
29	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.13	3 (6%)
24	CLA	c	511	41	65,73,73	2.04	16 (24%)	76,113,113	2.72	24 (31%)
37	DGD	c	521	-	63,63,67	0.87	2 (3%)	77,77,81	1.08	6 (7%)
24	CLA	B	611	41	65,73,73	2.11	17 (26%)	76,113,113	2.69	30 (39%)
27	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.45	10 (16%)
28	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.26	0
36	HTG	c	525	-	19,19,19	1.02	2 (10%)	23,24,24	1.47	2 (8%)
24	CLA	B	616	-	65,73,73	1.99	16 (24%)	76,113,113	2.78	29 (38%)
37	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	0.92	4 (5%)
28	GOL	T	101	-	5,5,5	0.50	0	5,5,5	0.19	0
24	CLA	B	604	-	65,73,73	2.09	17 (26%)	76,113,113	2.77	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	LMT	m	102	-	36,36,36	0.45	0	47,47,47	1.01	3 (6%)
24	CLA	b	620	41	65,73,73	2.07	16 (24%)	76,113,113	2.73	27 (35%)
28	GOL	V	201	35	5,5,5	0.36	0	5,5,5	0.24	0
32	PL9	a	416[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.85	20 (29%)
24	CLA	C	512	-	65,73,73	2.03	16 (24%)	76,113,113	2.75	26 (34%)
28	GOL	A	415	-	5,5,5	0.41	0	5,5,5	0.21	0
34	LMG	D	412	40	51,51,55	0.89	2 (3%)	59,59,63	1.00	3 (5%)
23	BCT	a	419[B]	21	2,3,3	0.66	0	2,3,3	0.74	0
26	BCR	b	628	-	41,41,41	0.96	1 (2%)	56,56,56	1.34	9 (16%)
39	HEM	e	102	6,5	41,50,50	1.28	5 (12%)	45,82,82	1.77	9 (20%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	8 (14%)
26	BCR	H	102	-	41,41,41	1.10	1 (2%)	56,56,56	1.44	9 (16%)
28	GOL	b	607	-	5,5,5	0.37	0	5,5,5	0.31	0
28	GOL	v	201	-	5,5,5	0.34	0	5,5,5	0.25	0
26	BCR	A	411	-	41,41,41	1.04	1 (2%)	56,56,56	1.21	5 (8%)
32	PL9	D	405[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.71	20 (29%)
24	CLA	c	514	-	65,73,73	2.07	16 (24%)	76,113,113	2.74	29 (38%)
25	PHO	A	409[A]	-	51,69,69	1.88	8 (15%)	47,99,99	1.82	9 (19%)
24	CLA	C	501	-	65,73,73	2.03	16 (24%)	76,113,113	2.73	25 (32%)
34	LMG	j	101	40	51,51,55	0.92	2 (3%)	59,59,63	0.94	4 (6%)
24	CLA	b	623	-	65,73,73	2.08	16 (24%)	76,113,113	2.66	26 (34%)
36	HTG	b	633	-	19,19,19	1.16	2 (10%)	23,24,24	1.91	4 (17%)
27	SQD	a	414	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	12 (19%)
24	CLA	B	605	-	65,73,73	2.01	16 (24%)	76,113,113	2.85	26 (34%)
28	GOL	a	402	-	5,5,5	0.37	0	5,5,5	0.28	0
24	CLA	B	606	-	65,73,73	2.00	15 (23%)	76,113,113	2.84	27 (35%)
26	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.39	8 (14%)
24	CLA	D	402	-	65,73,73	1.98	17 (26%)	76,113,113	2.84	28 (36%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.09	5 (6%)
24	CLA	a	409	-	65,73,73	2.07	16 (24%)	76,113,113	2.76	32 (42%)
24	CLA	b	615	-	65,73,73	2.02	15 (23%)	76,113,113	2.90	24 (31%)
26	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.51	11 (19%)
27	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.22	4 (6%)
28	GOL	f	101	35	5,5,5	0.32	0	5,5,5	0.36	0
28	GOL	a	401	-	5,5,5	0.48	0	5,5,5	0.50	0
24	CLA	B	607	-	65,73,73	2.05	17 (26%)	76,113,113	2.82	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	c	507	-	65,73,73	2.05	16 (24%)	76,113,113	2.74	25 (32%)
24	CLA	C	502	-	65,73,73	2.02	16 (24%)	76,113,113	2.69	27 (35%)
28	GOL	B	626	-	5,5,5	0.43	0	5,5,5	0.33	0
36	HTG	B	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.24	1 (4%)
38	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.05	4 (7%)
24	CLA	c	516	-	65,73,73	2.04	16 (24%)	76,113,113	2.79	27 (35%)
24	CLA	B	617	-	65,73,73	2.04	16 (24%)	76,113,113	2.70	28 (36%)
24	CLA	C	506	-	65,73,73	2.05	16 (24%)	76,113,113	2.68	27 (35%)
25	PHO	A	409[B]	-	51,69,69	1.91	8 (15%)	47,99,99	1.75	9 (19%)
32	PL9	A	420[A]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
28	GOL	B	636	-	5,5,5	0.40	0	5,5,5	0.53	0
29	LMT	a	421	-	36,36,36	0.46	0	47,47,47	0.83	1 (2%)
24	CLA	C	508	-	65,73,73	2.10	16 (24%)	76,113,113	2.75	28 (36%)
24	CLA	c	513	-	65,73,73	2.11	16 (24%)	76,113,113	2.70	27 (35%)
28	GOL	c	502	-	5,5,5	0.41	0	5,5,5	0.51	0
24	CLA	B	602	41	65,73,73	2.07	14 (21%)	76,113,113	2.76	24 (31%)
25	PHO	A	408	-	51,69,69	1.82	8 (15%)	47,99,99	1.69	7 (14%)
36	HTG	b	602	-	19,19,19	0.92	1 (5%)	23,24,24	1.18	2 (8%)
39	HEM	v	205	16	41,50,50	1.29	6 (14%)	45,82,82	1.77	9 (20%)
24	CLA	C	513	-	65,73,73	2.06	16 (24%)	76,113,113	2.71	28 (36%)
30	OEX	A	418[A]	3,1,41	0,15,15	-	-	-		
24	CLA	C	503	-	65,73,73	2.06	16 (24%)	76,113,113	2.68	24 (31%)
24	CLA	A	405	-	65,73,73	2.04	15 (23%)	76,113,113	2.67	26 (34%)
24	CLA	A	410	-	65,73,73	2.07	16 (24%)	76,113,113	2.71	32 (42%)
34	LMG	a	415	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	4 (6%)
36	HTG	V	207	-	19,19,19	1.05	2 (10%)	23,24,24	1.25	3 (13%)
24	CLA	b	613	-	65,73,73	2.01	16 (24%)	76,113,113	2.75	30 (39%)
24	CLA	B	615	-	65,73,73	2.01	16 (24%)	76,113,113	2.86	28 (36%)
24	CLA	B	608	41	65,73,73	2.03	16 (24%)	76,113,113	2.74	30 (39%)
24	CLA	A	407	41	65,73,73	2.01	16 (24%)	76,113,113	2.77	29 (38%)
28	GOL	b	604	-	5,5,5	0.36	0	5,5,5	0.25	0
24	CLA	c	512	-	65,73,73	2.08	16 (24%)	76,113,113	2.69	29 (38%)
28	GOL	c	501	-	5,5,5	0.32	0	5,5,5	0.31	0
29	LMT	f	103	-	36,36,36	0.46	0	47,47,47	0.83	1 (2%)
34	LMG	c	522	-	51,51,55	0.91	2 (3%)	59,59,63	1.13	5 (8%)
24	CLA	b	612	-	65,73,73	2.05	17 (26%)	76,113,113	2.79	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	b	619	-	65,73,73	2.03	15 (23%)	76,113,113	2.77	27 (35%)
37	DGD	D	406	-	52,52,67	1.00	3 (5%)	60,60,81	1.16	4 (6%)
24	CLA	b	625	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	27 (35%)
32	PL9	A	420[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.76	22 (32%)
29	LMT	F	101	-	36,36,36	0.48	0	47,47,47	0.92	1 (2%)
29	LMT	M	104	-	36,36,36	0.46	0	47,47,47	0.87	1 (2%)
29	LMT	D	401	-	36,36,36	0.43	0	47,47,47	0.99	1 (2%)
36	HTG	B	624	-	19,19,19	0.83	1 (5%)	23,24,24	1.48	3 (13%)
24	CLA	B	613	-	65,73,73	2.04	16 (24%)	76,113,113	2.88	28 (36%)
24	CLA	D	403	-	65,73,73	2.06	17 (26%)	76,113,113	2.77	28 (36%)
36	HTG	B	632	-	19,19,19	1.09	2 (10%)	23,24,24	1.36	3 (13%)
38	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	4 (7%)
24	CLA	b	614	-	65,73,73	2.05	16 (24%)	76,113,113	2.76	26 (34%)
28	GOL	B	627	-	5,5,5	0.33	0	5,5,5	0.44	0
24	CLA	c	510	-	65,73,73	2.05	16 (24%)	76,113,113	2.73	27 (35%)
24	CLA	C	505	-	65,73,73	2.03	16 (24%)	76,113,113	2.64	24 (31%)
38	LHG	d	407	-	48,48,48	0.90	2 (4%)	51,54,54	1.02	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	629	-	-	1/4/4/4	-
38	LHG	E	101	-	-	20/46/46/53	-
26	BCR	t	101	-	-	2/29/63/63	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
24	CLA	B	614	-	1/1/15/20	3/37/115/115	-
27	SQD	A	416	-	-	15/49/69/69	0/1/1/1
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
28	GOL	o	301	-	-	0/4/4/4	-
34	LMG	A	422	-	-	20/46/66/70	0/1/1/1
34	LMG	b	630	-	-	10/46/66/70	0/1/1/1
36	HTG	H	101	-	-	0/7/27/30	0/1/1/1
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	z	101	-	-	14/34/54/70	0/1/1/1
28	GOL	V	204	-	-	1/4/4/4	-
37	DGD	e	101	-	-	27/51/91/95	0/2/2/2
24	CLA	b	626	-	1/1/15/20	9/37/115/115	-
28	GOL	A	413	-	-	1/4/4/4	-
32	PL9	d	405[A]	-	-	8/53/73/73	0/1/1/1
28	GOL	V	203	-	-	2/4/4/4	-
36	HTG	b	608	-	-	1/10/30/30	0/1/1/1
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
29	LMT	M	103	-	-	9/21/61/61	0/2/2/2
34	LMG	C	519	-	-	13/46/66/70	0/1/1/1
28	GOL	b	605	-	-	1/4/4/4	-
24	CLA	b	616	-	1/1/15/20	9/37/115/115	-
24	CLA	b	624	-	1/1/15/20	19/37/115/115	-
27	SQD	f	102	-	-	14/38/58/69	0/1/1/1
27	SQD	A	412	-	-	8/49/69/69	0/1/1/1
34	LMG	c	523	-	-	3/46/66/70	0/1/1/1
29	LMT	b	631	-	-	4/17/37/61	0/1/1/2
36	HTG	B	633	-	-	0/10/30/30	0/1/1/1
26	BCR	b	627	-	-	2/29/63/63	0/2/2/2
24	CLA	b	617	41	1/1/15/20	0/37/115/115	-
24	CLA	c	506	-	-	4/37/115/115	-
24	CLA	C	507	41	1/1/15/20	7/37/115/115	-
34	LMG	B	622	-	-	9/46/66/70	0/1/1/1
24	CLA	C	504	41	1/1/15/20	5/37/115/115	-
24	CLA	c	515	3	1/1/15/20	6/37/115/115	-
38	LHG	D	407	-	-	13/53/53/53	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	CLA	C	511	3	1/1/15/20	3/37/115/115	-
27	SQD	b	601	-	-	22/49/69/69	0/1/1/1
24	CLA	c	508	41	1/1/15/20	5/37/115/115	-
38	LHG	d	408	-	-	11/53/53/53	-
24	CLA	d	401	41	1/1/15/20	6/37/115/115	-
28	GOL	v	202	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	C	516	-	-	15/51/91/95	0/2/2/2
32	PL9	d	405[B]	-	-	5/53/73/73	0/1/1/1
24	CLA	C	510	-	1/1/15/20	8/37/115/115	-
28	GOL	A	414	-	-	2/4/4/4	-
28	GOL	C	525	-	-	0/4/4/4	-
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	d	403	-	1/1/15/20	3/37/115/115	-
37	DGD	C	517	-	-	17/51/91/95	0/2/2/2
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
24	CLA	B	610	-	1/1/15/20	3/37/115/115	-
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	V	205	-	-	2/4/4/4	-
24	CLA	b	621	-	-	3/37/115/115	-
24	CLA	b	618	-	-	2/37/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-
25	PHO	a	420[A]	-	-	1/37/103/103	0/5/6/6
38	LHG	D	408	-	-	12/53/53/53	-
28	GOL	v	203	-	-	2/4/4/4	-
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
36	HTG	C	523	-	-	3/10/30/30	0/1/1/1
28	GOL	b	603	-	-	0/4/4/4	-
24	CLA	c	505	-	1/1/15/20	2/37/115/115	-
24	CLA	b	622	-	1/1/15/20	1/37/115/115	-
39	HEM	F	102	6,5	-	7/12/54/54	-
26	BCR	b	629	-	-	0/29/63/63	0/2/2/2
37	DGD	H	103	-	-	13/51/91/95	0/2/2/2
39	HEM	V	206	16	-	4/12/54/54	-
28	GOL	T	102	-	-	2/4/4/4	-
36	HTG	d	411	-	-	1/7/27/30	0/1/1/1
29	LMT	M	101	-	-	4/21/61/61	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
36	HTG	c	524	-	-	3/10/30/30	0/1/1/1
37	DGD	c	520	-	-	18/51/91/95	0/2/2/2
24	CLA	c	517	-	-	4/37/115/115	-
38	LHG	L	101	-	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	D	409	-	-	12/53/53/53	-
24	CLA	A	406	41	1/1/15/20	6/37/115/115	-
25	PHO	a	411	-	-	4/37/103/103	0/5/6/6
24	CLA	d	402	-	1/1/15/20	3/37/115/115	-
24	CLA	B	609	-	-	1/37/115/115	-
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
26	BCR	T	103	-	-	3/29/63/63	0/2/2/2
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
25	PHO	a	420[B]	-	-	3/37/103/103	0/5/6/6
24	CLA	a	410	41	-	6/37/115/115	-
32	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
36	HTG	C	522	-	-	0/10/30/30	0/1/1/1
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/15/20	5/37/115/115	-
26	BCR	k	101	-	-	2/29/63/63	0/2/2/2
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
36	HTG	b	609	-	-	0/10/30/30	0/1/1/1
28	GOL	B	630	-	-	4/4/4/4	-
32	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
24	CLA	b	611	41	1/1/15/20	17/37/115/115	-
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
36	HTG	B	625	-	-	4/10/30/30	0/1/1/1
28	GOL	O	301	-	-	2/4/4/4	-
24	CLA	c	509	-	1/1/15/20	2/37/115/115	-
28	GOL	B	631	-	-	1/4/4/4	-
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
38	LHG	a	422	-	-	19/46/46/53	-
36	HTG	b	632	-	-	3/10/30/30	0/1/1/1
24	CLA	B	612	-	1/1/15/20	0/37/115/115	-
28	GOL	t	102	-	-	0/4/4/4	-
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2
24	CLA	C	509	-	1/1/15/20	11/37/115/115	-
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
24	CLA	a	412	-	1/1/15/20	9/37/115/115	-
29	LMT	C	521	-	-	11/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	511	41	1/1/15/20	4/37/115/115	-
37	DGD	c	521	-	-	15/51/91/95	0/2/2/2
24	CLA	B	611	41	1/1/15/20	4/37/115/115	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
28	GOL	b	606	-	-	2/4/4/4	-
36	HTG	c	525	-	-	0/10/30/30	0/1/1/1
24	CLA	B	616	-	1/1/15/20	10/37/115/115	-
37	DGD	C	518	-	-	11/51/91/95	0/2/2/2
28	GOL	T	101	-	-	2/4/4/4	-
24	CLA	B	604	-	1/1/15/20	6/37/115/115	-
29	LMT	m	102	-	-	7/21/61/61	0/2/2/2
24	CLA	b	620	41	1/1/15/20	6/37/115/115	-
28	GOL	V	201	35	-	2/4/4/4	-
32	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
24	CLA	C	512	-	1/1/15/20	8/37/115/115	-
28	GOL	A	415	-	-	2/4/4/4	-
34	LMG	D	412	40	-	7/46/66/70	0/1/1/1
26	BCR	b	628	-	-	1/29/63/63	0/2/2/2
39	HEM	e	102	6,5	-	7/12/54/54	-
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
26	BCR	H	102	-	-	1/29/63/63	0/2/2/2
28	GOL	b	607	-	-	3/4/4/4	-
28	GOL	v	201	-	-	2/4/4/4	-
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
32	PL9	D	405[B]	-	-	7/53/73/73	0/1/1/1
24	CLA	c	514	-	1/1/15/20	9/37/115/115	-
25	PHO	A	409[A]	-	-	0/37/103/103	0/5/6/6
24	CLA	C	501	-	1/1/15/20	5/37/115/115	-
34	LMG	j	101	40	-	11/46/66/70	0/1/1/1
24	CLA	b	623	-	1/1/15/20	2/37/115/115	-
36	HTG	b	633	-	-	5/10/30/30	0/1/1/1
27	SQD	a	414	-	-	14/49/69/69	0/1/1/1
24	CLA	B	605	-	1/1/15/20	6/37/115/115	-
28	GOL	a	402	-	-	2/4/4/4	-
24	CLA	B	606	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	D	402	-	1/1/15/20	1/37/115/115	-
37	DGD	c	519	-	-	14/51/91/95	0/2/2/2
24	CLA	a	409	-	1/1/15/20	4/37/115/115	-
24	CLA	b	615	-	1/1/15/20	4/37/115/115	-
26	BCR	c	518	-	-	2/29/63/63	0/2/2/2
27	SQD	a	405	-	-	17/49/69/69	0/1/1/1
28	GOL	f	101	35	-	3/4/4/4	-
28	GOL	a	401	-	-	0/4/4/4	-
24	CLA	B	607	-	1/1/15/20	4/37/115/115	-
24	CLA	c	507	-	-	4/37/115/115	-
24	CLA	C	502	-	1/1/15/20	8/37/115/115	-
28	GOL	B	626	-	-	1/4/4/4	-
36	HTG	B	623	-	-	4/10/30/30	0/1/1/1
38	LHG	d	406	-	-	10/53/53/53	-
24	CLA	c	516	-	1/1/15/20	9/37/115/115	-
24	CLA	B	617	-	1/1/15/20	6/37/115/115	-
24	CLA	C	506	-	1/1/15/20	8/37/115/115	-
25	PHO	A	409[B]	-	-	1/37/103/103	0/5/6/6
32	PL9	A	420[A]	-	-	10/53/73/73	0/1/1/1
28	GOL	B	636	-	-	0/4/4/4	-
29	LMT	a	421	-	-	4/21/61/61	0/2/2/2
24	CLA	C	508	-	1/1/15/20	5/37/115/115	-
24	CLA	c	513	-	1/1/15/20	11/37/115/115	-
28	GOL	c	502	-	-	1/4/4/4	-
24	CLA	B	602	41	1/1/15/20	12/37/115/115	-
25	PHO	A	408	-	-	4/37/103/103	0/5/6/6
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
39	HEM	v	205	16	-	4/12/54/54	-
24	CLA	C	513	-	1/1/15/20	7/37/115/115	-
24	CLA	C	503	-	1/1/15/20	2/37/115/115	-
24	CLA	A	405	-	1/1/15/20	7/37/115/115	-
24	CLA	A	410	-	1/1/15/20	7/37/115/115	-
34	LMG	a	415	-	-	16/46/66/70	0/1/1/1
36	HTG	V	207	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	613	-	1/1/15/20	5/37/115/115	-
24	CLA	B	615	-	1/1/15/20	15/37/115/115	-
24	CLA	B	608	41	1/1/15/20	6/37/115/115	-
24	CLA	A	407	41	-	2/37/115/115	-
28	GOL	b	604	-	-	0/4/4/4	-
24	CLA	c	512	-	1/1/15/20	4/37/115/115	-
28	GOL	c	501	-	-	0/4/4/4	-
29	LMT	f	103	-	-	10/21/61/61	0/2/2/2
34	LMG	c	522	-	-	15/46/66/70	0/1/1/1
24	CLA	b	612	-	1/1/15/20	3/37/115/115	-
24	CLA	b	619	-	1/1/15/20	4/37/115/115	-
37	DGD	D	406	-	-	21/47/67/95	0/1/1/2
24	CLA	b	625	-	1/1/15/20	4/37/115/115	-
32	PL9	A	420[B]	-	-	10/53/73/73	0/1/1/1
29	LMT	F	101	-	-	3/21/61/61	0/2/2/2
29	LMT	M	104	-	-	7/21/61/61	0/2/2/2
29	LMT	D	401	-	-	8/21/61/61	0/2/2/2
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
24	CLA	B	613	-	1/1/15/20	3/37/115/115	-
24	CLA	D	403	-	1/1/15/20	7/37/115/115	-
36	HTG	B	632	-	-	3/10/30/30	0/1/1/1
38	LHG	l	101	-	-	15/53/53/53	-
24	CLA	b	614	-	1/1/15/20	6/37/115/115	-
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	c	510	-	1/1/15/20	15/37/115/115	-
24	CLA	C	505	-	1/1/15/20	5/37/115/115	-
38	LHG	d	407	-	-	10/53/53/53	-

All (1349) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	622	CLA	C3B-C2B	6.68	1.49	1.40
24	B	613	CLA	C3B-C2B	6.54	1.49	1.40
24	C	509	CLA	C3B-C2B	6.51	1.49	1.40
24	B	603	CLA	C3B-C2B	6.46	1.49	1.40
25	A	409[A]	PHO	C3B-C2B	6.46	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	409[B]	PHO	C3B-C2B	6.45	1.49	1.40
24	C	504	CLA	C3B-C2B	6.40	1.49	1.40
24	b	614	CLA	C3B-C2B	6.36	1.49	1.40
24	B	614	CLA	C3B-C2B	6.28	1.49	1.40
24	c	512	CLA	C3B-C2B	6.28	1.49	1.40
24	c	513	CLA	C3B-C2B	6.27	1.49	1.40
24	B	617	CLA	C3B-C2B	6.26	1.49	1.40
24	B	605	CLA	C3B-C2B	6.25	1.49	1.40
24	b	624	CLA	C3B-C2B	6.25	1.49	1.40
24	c	515	CLA	C3B-C2B	6.22	1.49	1.40
24	C	508	CLA	C3B-C2B	6.22	1.49	1.40
24	c	510	CLA	C3B-C2B	6.21	1.49	1.40
24	b	616	CLA	C3B-C2B	6.21	1.49	1.40
24	A	406	CLA	C3B-C2B	6.20	1.49	1.40
24	c	508	CLA	C3B-C2B	6.18	1.48	1.40
24	C	510	CLA	C3B-C2B	6.18	1.48	1.40
24	b	621	CLA	C3B-C2B	6.17	1.48	1.40
24	d	401	CLA	C3B-C2B	6.15	1.48	1.40
25	a	420[B]	PHO	C3B-C2B	6.15	1.48	1.40
24	b	623	CLA	C3B-C2B	6.09	1.48	1.40
25	a	420[A]	PHO	C3B-C2B	6.09	1.48	1.40
24	b	611	CLA	C3B-C2B	6.08	1.48	1.40
24	b	626	CLA	C3B-C2B	6.08	1.48	1.40
24	B	607	CLA	C3B-C2B	6.06	1.48	1.40
24	c	514	CLA	C3B-C2B	6.03	1.48	1.40
24	D	402	CLA	C3B-C2B	6.01	1.48	1.40
24	C	511	CLA	C3B-C2B	5.98	1.48	1.40
24	a	409	CLA	C3B-C2B	5.98	1.48	1.40
24	c	511	CLA	C3B-C2B	5.94	1.48	1.40
24	b	620	CLA	C3B-C2B	5.92	1.48	1.40
24	B	605	CLA	C1D-ND	5.90	1.45	1.37
24	c	506	CLA	C3B-C2B	5.88	1.48	1.40
24	A	410	CLA	C3B-C2B	5.88	1.48	1.40
24	d	402	CLA	C3B-C2B	5.88	1.48	1.40
24	B	615	CLA	C3B-C2B	5.87	1.48	1.40
24	C	505	CLA	C3B-C2B	5.87	1.48	1.40
24	D	403	CLA	C3B-C2B	5.81	1.48	1.40
24	b	611	CLA	C3C-C2C	5.81	1.49	1.36
24	c	505	CLA	C3B-C2B	5.80	1.48	1.40
24	B	602	CLA	C3B-C2B	5.79	1.48	1.40
24	d	403	CLA	C3B-C2B	5.79	1.48	1.40
24	b	613	CLA	C3B-C2B	5.78	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C3B-C2B	5.74	1.48	1.40
24	C	513	CLA	C3B-C2B	5.74	1.48	1.40
24	B	604	CLA	C3C-C2C	5.73	1.48	1.36
25	A	409[B]	PHO	C3D-C2D	5.69	1.49	1.39
24	b	623	CLA	C3C-C2C	5.68	1.48	1.36
24	A	405	CLA	C3B-C2B	5.67	1.48	1.40
24	C	512	CLA	C3B-C2B	5.66	1.48	1.40
24	b	625	CLA	C3B-C2B	5.66	1.48	1.40
24	B	608	CLA	C3B-C2B	5.65	1.48	1.40
24	B	604	CLA	C3B-C2B	5.63	1.48	1.40
24	b	620	CLA	C3C-C2C	5.61	1.48	1.36
24	C	502	CLA	C3B-C2B	5.60	1.48	1.40
25	A	408	PHO	C3B-C2B	5.60	1.48	1.40
24	b	615	CLA	C3C-C2C	5.60	1.48	1.36
24	D	403	CLA	C1D-ND	5.59	1.44	1.37
24	c	507	CLA	C3B-C2B	5.59	1.48	1.40
24	a	410	CLA	C3B-C2B	5.57	1.48	1.40
24	B	611	CLA	C3B-C2B	5.57	1.48	1.40
25	a	420[A]	PHO	C3D-C2D	5.57	1.49	1.39
25	a	411	PHO	C3D-C2D	5.56	1.49	1.39
24	A	407	CLA	C3B-C2B	5.56	1.48	1.40
25	a	411	PHO	C3B-C2B	5.56	1.48	1.40
24	b	612	CLA	C3B-C2B	5.55	1.48	1.40
24	B	603	CLA	C3C-C2C	5.55	1.48	1.36
24	B	611	CLA	C3C-C2C	5.54	1.48	1.36
24	a	412	CLA	C3B-C2B	5.54	1.48	1.40
24	B	612	CLA	C3B-C2B	5.54	1.48	1.40
24	B	609	CLA	C3B-C2B	5.52	1.48	1.40
24	c	516	CLA	C3B-C2B	5.52	1.48	1.40
24	c	509	CLA	C3B-C2B	5.51	1.48	1.40
24	c	514	CLA	C3C-C2C	5.51	1.48	1.36
24	b	615	CLA	C3B-C2B	5.51	1.48	1.40
24	b	617	CLA	C3B-C2B	5.49	1.48	1.40
24	C	507	CLA	C3B-C2B	5.49	1.48	1.40
24	B	602	CLA	C3C-C2C	5.49	1.48	1.36
24	C	506	CLA	C3B-C2B	5.47	1.48	1.40
24	a	409	CLA	C1D-ND	5.47	1.44	1.37
24	a	410	CLA	CHC-C1C	5.47	1.49	1.35
24	C	509	CLA	C1D-ND	5.46	1.44	1.37
24	A	406	CLA	C1D-ND	5.45	1.44	1.37
24	C	503	CLA	C1D-ND	5.44	1.44	1.37
24	b	623	CLA	C1D-ND	5.44	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3C-C2C	5.44	1.48	1.36
24	b	623	CLA	O2D-CGD	5.44	1.46	1.33
24	C	501	CLA	C3B-C2B	5.43	1.47	1.40
24	B	611	CLA	C1D-ND	5.42	1.44	1.37
24	C	510	CLA	C3C-C2C	5.41	1.48	1.36
24	c	517	CLA	C3C-C2C	5.41	1.48	1.36
24	b	625	CLA	C1D-ND	5.40	1.44	1.37
24	c	513	CLA	C1D-ND	5.39	1.44	1.37
24	b	612	CLA	C3C-C2C	5.38	1.48	1.36
25	A	409[A]	PHO	C3D-C2D	5.37	1.49	1.39
24	C	507	CLA	C3C-C2C	5.36	1.48	1.36
24	b	618	CLA	C3C-C2C	5.36	1.48	1.36
24	B	606	CLA	O2D-CGD	5.36	1.46	1.33
24	d	401	CLA	C3C-C2C	5.35	1.48	1.36
24	b	616	CLA	C3C-C2C	5.35	1.48	1.36
24	C	509	CLA	C3C-C2C	5.34	1.48	1.36
24	c	516	CLA	C3C-C2C	5.33	1.48	1.36
24	B	616	CLA	CHC-C1C	5.32	1.48	1.35
24	C	502	CLA	C1D-ND	5.32	1.44	1.37
24	A	405	CLA	CHC-C1C	5.32	1.48	1.35
24	C	506	CLA	C1D-ND	5.31	1.44	1.37
24	C	510	CLA	C1D-ND	5.31	1.44	1.37
24	d	401	CLA	C1D-ND	5.31	1.44	1.37
24	C	503	CLA	CHC-C1C	5.31	1.48	1.35
25	a	420[B]	PHO	C3D-C2D	5.31	1.48	1.39
24	b	618	CLA	C1D-ND	5.30	1.44	1.37
24	c	507	CLA	CHC-C1C	5.30	1.48	1.35
24	C	501	CLA	CHC-C1C	5.29	1.48	1.35
24	B	602	CLA	C1D-ND	5.29	1.44	1.37
24	A	406	CLA	C3C-C2C	5.28	1.48	1.36
24	c	517	CLA	C3B-C2B	5.27	1.47	1.40
24	B	610	CLA	CHC-C1C	5.27	1.48	1.35
24	B	610	CLA	C3C-C2C	5.26	1.47	1.36
24	c	510	CLA	C3C-C2C	5.26	1.47	1.36
24	B	608	CLA	C3C-C2C	5.26	1.47	1.36
24	C	512	CLA	C3C-C2C	5.25	1.47	1.36
24	C	513	CLA	C3C-C2C	5.25	1.47	1.36
24	C	503	CLA	C3C-C2C	5.25	1.47	1.36
24	C	502	CLA	C3C-C2C	5.25	1.47	1.36
24	c	508	CLA	O2D-CGD	5.25	1.46	1.33
24	c	516	CLA	CHC-C1C	5.25	1.48	1.35
24	C	505	CLA	CHC-C1C	5.24	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C1D-ND	5.23	1.44	1.37
24	C	501	CLA	C1D-ND	5.23	1.44	1.37
24	C	503	CLA	C3B-C2B	5.23	1.47	1.40
24	A	407	CLA	CHC-C1C	5.23	1.48	1.35
24	a	412	CLA	O2D-CGD	5.22	1.45	1.33
24	B	604	CLA	CHC-C1C	5.22	1.48	1.35
24	c	512	CLA	C3C-C2C	5.22	1.47	1.36
24	c	506	CLA	C3C-C2C	5.22	1.47	1.36
24	A	407	CLA	C3C-C2C	5.21	1.47	1.36
24	B	616	CLA	O2D-CGD	5.21	1.45	1.33
24	C	505	CLA	C3C-C2C	5.21	1.47	1.36
24	a	409	CLA	C3C-C2C	5.20	1.47	1.36
24	D	403	CLA	C3C-C2C	5.20	1.47	1.36
24	B	602	CLA	CHC-C1C	5.20	1.48	1.35
24	B	609	CLA	C3C-C2C	5.19	1.47	1.36
26	b	629	BCR	C23-C22	-5.19	1.34	1.45
24	a	412	CLA	C3C-C2C	5.19	1.47	1.36
24	B	614	CLA	O2D-CGD	5.18	1.45	1.33
24	c	514	CLA	C1D-ND	5.18	1.44	1.37
24	c	517	CLA	C1D-ND	5.18	1.44	1.37
24	c	506	CLA	O2D-CGD	5.17	1.45	1.33
24	B	606	CLA	C1D-ND	5.17	1.44	1.37
24	c	511	CLA	C3C-C2C	5.16	1.47	1.36
25	A	408	PHO	C3D-C2D	5.16	1.48	1.39
24	b	611	CLA	C1D-ND	5.16	1.44	1.37
24	C	511	CLA	C3C-C2C	5.16	1.47	1.36
25	A	409[B]	PHO	O2D-CGD	5.15	1.45	1.33
24	c	515	CLA	C3C-C2C	5.15	1.47	1.36
24	b	612	CLA	CHC-C1C	5.14	1.48	1.35
24	d	403	CLA	C3C-C2C	5.14	1.47	1.36
24	c	506	CLA	CHC-C1C	5.14	1.48	1.35
24	C	507	CLA	CHC-C1C	5.14	1.48	1.35
24	B	603	CLA	CHC-C1C	5.14	1.48	1.35
24	c	510	CLA	C1D-ND	5.14	1.44	1.37
24	C	512	CLA	CHC-C1C	5.14	1.48	1.35
24	c	513	CLA	C3C-C2C	5.13	1.47	1.36
24	C	504	CLA	C3C-C2C	5.13	1.47	1.36
24	c	507	CLA	C3C-C2C	5.13	1.47	1.36
24	b	618	CLA	CHC-C1C	5.12	1.48	1.35
24	c	508	CLA	C3C-C2C	5.12	1.47	1.36
24	b	626	CLA	O2D-CGD	5.11	1.45	1.33
24	b	622	CLA	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C3B-C2B	5.11	1.47	1.40
24	C	508	CLA	O2D-CGD	5.11	1.45	1.33
25	A	409[A]	PHO	O2D-CGD	5.11	1.45	1.33
24	C	504	CLA	C1D-ND	5.11	1.44	1.37
24	b	619	CLA	O2D-CGD	5.11	1.45	1.33
24	B	612	CLA	O2D-CGD	5.11	1.45	1.33
24	A	405	CLA	C3C-C2C	5.10	1.47	1.36
24	B	607	CLA	C3C-C2C	5.10	1.47	1.36
24	c	509	CLA	CHC-C1C	5.10	1.48	1.35
24	a	412	CLA	C1D-ND	5.10	1.44	1.37
24	b	614	CLA	C3C-C2C	5.10	1.47	1.36
24	C	513	CLA	C1D-ND	5.10	1.44	1.37
25	a	411	PHO	O2D-CGD	5.10	1.45	1.33
24	C	502	CLA	CHC-C1C	5.10	1.48	1.35
26	B	620	BCR	C23-C22	-5.10	1.35	1.45
24	c	517	CLA	CHC-C1C	5.09	1.48	1.35
24	B	612	CLA	C3C-C2C	5.09	1.47	1.36
24	c	512	CLA	C1D-ND	5.09	1.44	1.37
24	c	505	CLA	C1D-ND	5.09	1.44	1.37
24	b	622	CLA	C3C-C2C	5.09	1.47	1.36
24	b	611	CLA	CHC-C1C	5.09	1.48	1.35
24	b	620	CLA	CHC-C1C	5.09	1.48	1.35
24	b	619	CLA	CHC-C1C	5.09	1.48	1.35
24	b	621	CLA	C3C-C2C	5.08	1.47	1.36
24	b	624	CLA	C3C-C2C	5.08	1.47	1.36
24	A	410	CLA	C1D-ND	5.08	1.44	1.37
24	A	410	CLA	O2D-CGD	5.08	1.45	1.33
24	B	615	CLA	C3C-C2C	5.08	1.47	1.36
24	B	607	CLA	O2D-CGD	5.08	1.45	1.33
24	B	616	CLA	C1D-ND	5.07	1.44	1.37
24	C	507	CLA	C1D-ND	5.07	1.44	1.37
24	B	606	CLA	C3C-C2C	5.07	1.47	1.36
24	b	615	CLA	CHC-C1C	5.07	1.48	1.35
24	b	619	CLA	C3C-C2C	5.07	1.47	1.36
24	A	410	CLA	CHC-C1C	5.06	1.48	1.35
24	c	513	CLA	O2D-CGD	5.06	1.45	1.33
24	B	609	CLA	C1D-ND	5.06	1.44	1.37
24	d	403	CLA	O2D-CGD	5.06	1.45	1.33
24	d	401	CLA	O2D-CGD	5.06	1.45	1.33
24	b	617	CLA	C3C-C2C	5.06	1.47	1.36
24	b	615	CLA	O2D-CGD	5.06	1.45	1.33
24	B	605	CLA	C3C-C2C	5.06	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	C3B-C2B	5.06	1.47	1.40
24	b	624	CLA	O2D-CGD	5.06	1.45	1.33
24	C	509	CLA	CHC-C1C	5.05	1.47	1.35
24	b	618	CLA	O2D-CGD	5.05	1.45	1.33
24	B	617	CLA	O2D-CGD	5.05	1.45	1.33
24	C	509	CLA	O2D-CGD	5.04	1.45	1.33
24	C	513	CLA	CHC-C1C	5.04	1.47	1.35
24	c	508	CLA	C1D-ND	5.04	1.44	1.37
24	C	510	CLA	CHC-C1C	5.04	1.47	1.35
24	B	613	CLA	CHC-C1C	5.04	1.47	1.35
24	B	614	CLA	C1D-ND	5.04	1.44	1.37
24	d	402	CLA	CHC-C1C	5.04	1.47	1.35
24	C	505	CLA	O2D-CGD	5.03	1.45	1.33
24	b	622	CLA	C1D-ND	5.03	1.44	1.37
24	B	606	CLA	CHC-C1C	5.03	1.47	1.35
24	b	614	CLA	C1D-ND	5.03	1.44	1.37
25	a	420[B]	PHO	O2D-CGD	5.02	1.45	1.33
24	b	620	CLA	C1D-ND	5.02	1.44	1.37
24	B	617	CLA	CHC-C1C	5.02	1.47	1.35
24	c	512	CLA	CHC-C1C	5.02	1.47	1.35
24	B	612	CLA	CHC-C1C	5.01	1.47	1.35
24	C	504	CLA	CHC-C1C	5.01	1.47	1.35
24	B	608	CLA	C1D-ND	5.01	1.43	1.37
24	c	516	CLA	O2D-CGD	5.00	1.45	1.33
24	c	513	CLA	CHC-C1C	5.00	1.47	1.35
24	C	512	CLA	C1D-ND	5.00	1.43	1.37
24	D	403	CLA	CHC-C1C	5.00	1.47	1.35
24	c	509	CLA	C3C-C2C	5.00	1.47	1.36
24	B	608	CLA	CHC-C1C	5.00	1.47	1.35
24	C	501	CLA	C3C-C2C	5.00	1.47	1.36
24	b	620	CLA	O2D-CGD	5.00	1.45	1.33
25	a	411	PHO	OBD-CAD	4.99	1.29	1.22
24	b	625	CLA	C3C-C2C	4.99	1.47	1.36
24	c	512	CLA	O2D-CGD	4.99	1.45	1.33
25	a	420[A]	PHO	O2D-CGD	4.99	1.45	1.33
24	c	515	CLA	CHC-C1C	4.98	1.47	1.35
24	d	403	CLA	C1D-ND	4.98	1.43	1.37
24	b	624	CLA	C1D-ND	4.98	1.43	1.37
24	B	607	CLA	CHC-C1C	4.98	1.47	1.35
24	d	402	CLA	C3C-C2C	4.97	1.47	1.36
25	A	408	PHO	OBD-CAD	4.97	1.29	1.22
24	B	617	CLA	C3C-C2C	4.97	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	505	CLA	O2D-CGD	4.97	1.45	1.33
24	C	513	CLA	O2D-CGD	4.96	1.45	1.33
24	b	621	CLA	O2D-CGD	4.96	1.45	1.33
24	c	510	CLA	CHC-C1C	4.96	1.47	1.35
24	C	508	CLA	CHC-C1C	4.96	1.47	1.35
24	B	610	CLA	C3B-C2B	4.96	1.47	1.40
25	A	408	PHO	O2D-CGD	4.96	1.45	1.33
24	a	412	CLA	CHC-C1C	4.96	1.47	1.35
24	A	410	CLA	C3C-C2C	4.96	1.47	1.36
26	C	514	BCR	C23-C22	-4.95	1.35	1.45
24	C	506	CLA	O2D-CGD	4.95	1.45	1.33
24	d	403	CLA	CHC-C1C	4.95	1.47	1.35
24	D	402	CLA	C3C-C2C	4.94	1.47	1.36
24	b	617	CLA	CHC-C1C	4.94	1.47	1.35
24	c	514	CLA	CHC-C1C	4.94	1.47	1.35
24	C	511	CLA	O2D-CGD	4.93	1.45	1.33
24	c	505	CLA	C3C-C2C	4.93	1.47	1.36
24	C	510	CLA	O2D-CGD	4.93	1.45	1.33
24	c	515	CLA	C1D-ND	4.93	1.43	1.37
24	b	611	CLA	O2D-CGD	4.92	1.45	1.33
24	C	506	CLA	C3C-C2C	4.92	1.47	1.36
26	k	101	BCR	C23-C22	-4.92	1.35	1.45
24	b	616	CLA	CHC-C1C	4.92	1.47	1.35
24	b	624	CLA	CHC-C1C	4.91	1.47	1.35
24	C	508	CLA	C1D-ND	4.91	1.43	1.37
24	b	613	CLA	C3C-C2C	4.91	1.47	1.36
24	b	619	CLA	C1D-ND	4.91	1.43	1.37
24	c	511	CLA	CHC-C1C	4.90	1.47	1.35
24	C	506	CLA	CHC-C1C	4.90	1.47	1.35
24	B	603	CLA	O2D-CGD	4.89	1.45	1.33
24	C	511	CLA	C1D-ND	4.88	1.43	1.37
26	d	404	BCR	C23-C22	-4.88	1.35	1.45
24	B	614	CLA	C3C-C2C	4.88	1.47	1.36
26	T	103	BCR	C23-C22	-4.88	1.35	1.45
24	b	613	CLA	CHC-C1C	4.87	1.47	1.35
24	b	623	CLA	CHC-C1C	4.87	1.47	1.35
24	c	508	CLA	CHC-C1C	4.87	1.47	1.35
24	c	516	CLA	C1D-ND	4.86	1.43	1.37
24	B	606	CLA	C3B-C2B	4.86	1.47	1.40
24	c	507	CLA	C1D-ND	4.86	1.43	1.37
24	a	410	CLA	O2D-CGD	4.85	1.45	1.33
24	c	505	CLA	CHC-C1C	4.85	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C1D-ND	4.85	1.43	1.37
24	c	511	CLA	O2D-CGD	4.85	1.45	1.33
24	D	403	CLA	O2D-CGD	4.85	1.45	1.33
24	b	625	CLA	CHC-C1C	4.85	1.47	1.35
24	b	621	CLA	CHC-C1C	4.85	1.47	1.35
24	B	616	CLA	C3C-C2C	4.84	1.47	1.36
24	B	617	CLA	C1D-ND	4.84	1.43	1.37
24	c	514	CLA	O2D-CGD	4.83	1.45	1.33
24	B	610	CLA	O2D-CGD	4.83	1.45	1.33
24	B	615	CLA	CHC-C1C	4.83	1.47	1.35
24	b	613	CLA	O2D-CGD	4.83	1.45	1.33
24	B	602	CLA	O2D-CGD	4.83	1.45	1.33
24	c	517	CLA	O2D-CGD	4.82	1.45	1.33
24	a	410	CLA	C3C-C2C	4.82	1.47	1.36
24	a	410	CLA	C1D-ND	4.81	1.43	1.37
24	b	626	CLA	C1D-ND	4.81	1.43	1.37
24	b	626	CLA	C3C-C2C	4.81	1.47	1.36
24	C	501	CLA	O2D-CGD	4.81	1.44	1.33
24	C	502	CLA	O2D-CGD	4.81	1.44	1.33
24	b	614	CLA	O2D-CGD	4.81	1.44	1.33
26	y	101	BCR	C23-C22	-4.80	1.35	1.45
26	K	101	BCR	C23-C22	-4.80	1.35	1.45
24	B	613	CLA	O2D-CGD	4.80	1.44	1.33
24	c	510	CLA	O2D-CGD	4.80	1.44	1.33
24	c	509	CLA	C1D-ND	4.79	1.43	1.37
24	B	615	CLA	C1D-ND	4.79	1.43	1.37
26	c	527	BCR	C23-C22	-4.79	1.35	1.45
24	B	611	CLA	O2D-CGD	4.78	1.44	1.33
24	a	409	CLA	O2D-CGD	4.78	1.44	1.33
24	C	511	CLA	CHC-C1C	4.78	1.47	1.35
24	B	608	CLA	O2D-CGD	4.78	1.44	1.33
24	B	610	CLA	C1D-ND	4.78	1.43	1.37
24	c	507	CLA	O2D-CGD	4.77	1.44	1.33
24	B	605	CLA	CHC-C1C	4.77	1.47	1.35
24	b	626	CLA	CHC-C1C	4.75	1.47	1.35
26	h	101	BCR	C23-C22	-4.75	1.35	1.45
24	B	607	CLA	C1D-ND	4.75	1.43	1.37
24	B	609	CLA	O2D-CGD	4.74	1.44	1.33
24	B	609	CLA	CHC-C1C	4.73	1.47	1.35
24	c	511	CLA	C1D-ND	4.73	1.43	1.37
24	b	614	CLA	CHC-C1C	4.73	1.47	1.35
24	b	622	CLA	CHC-C1C	4.72	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	O2D-CGD	4.72	1.44	1.33
26	t	101	BCR	C23-C22	-4.72	1.35	1.45
24	A	405	CLA	C1D-ND	4.72	1.43	1.37
24	c	509	CLA	O2D-CGD	4.72	1.44	1.33
24	C	504	CLA	O2D-CGD	4.71	1.44	1.33
24	B	602	CLA	O2A-CGA	4.71	1.47	1.33
24	A	407	CLA	O2D-CGD	4.70	1.44	1.33
24	b	612	CLA	O2D-CGD	4.70	1.44	1.33
24	A	407	CLA	C1D-ND	4.69	1.43	1.37
24	b	625	CLA	O2D-CGD	4.69	1.44	1.33
24	b	621	CLA	C1D-ND	4.68	1.43	1.37
24	B	603	CLA	C1D-ND	4.68	1.43	1.37
24	B	611	CLA	CHC-C1C	4.68	1.47	1.35
24	B	604	CLA	O2D-CGD	4.68	1.44	1.33
24	b	618	CLA	CHD-C1D	4.68	1.47	1.38
24	b	617	CLA	O2D-CGD	4.67	1.44	1.33
24	C	507	CLA	O2D-CGD	4.66	1.44	1.33
24	B	605	CLA	O2D-CGD	4.66	1.44	1.33
26	H	102	BCR	C23-C22	-4.65	1.35	1.45
24	B	604	CLA	C1D-ND	4.65	1.43	1.37
24	A	407	CLA	CHD-C1D	4.64	1.47	1.38
24	a	409	CLA	CHC-C1C	4.64	1.46	1.35
24	A	405	CLA	O2D-CGD	4.64	1.44	1.33
24	d	401	CLA	CHC-C1C	4.64	1.46	1.35
24	B	612	CLA	C1D-ND	4.64	1.43	1.37
26	Y	101	BCR	C23-C22	-4.64	1.36	1.45
24	d	402	CLA	O2D-CGD	4.63	1.44	1.33
24	c	506	CLA	C1D-ND	4.62	1.43	1.37
24	B	613	CLA	C3C-C2C	4.62	1.46	1.36
24	b	615	CLA	C1D-ND	4.61	1.43	1.37
24	c	515	CLA	O2D-CGD	4.61	1.44	1.33
24	b	612	CLA	CHD-C1D	4.61	1.47	1.38
24	b	616	CLA	O2D-CGD	4.60	1.44	1.33
27	a	405	SQD	O48-C23	4.60	1.46	1.33
24	a	409	CLA	CHD-C1D	4.59	1.47	1.38
26	A	411	BCR	C23-C22	-4.59	1.36	1.45
24	B	611	CLA	CHD-C1D	4.58	1.47	1.38
24	C	510	CLA	CHD-C1D	4.57	1.47	1.38
26	C	515	BCR	C23-C22	-4.56	1.36	1.45
27	A	416	SQD	O48-C23	4.56	1.46	1.33
24	D	402	CLA	CHC-C1C	4.54	1.46	1.35
24	B	614	CLA	CHC-C1C	4.54	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	O2D-CGD	4.53	1.44	1.33
24	C	506	CLA	CHD-C1D	4.53	1.47	1.38
24	c	512	CLA	O2A-CGA	4.53	1.46	1.33
24	B	610	CLA	O2A-CGA	4.53	1.46	1.33
24	C	505	CLA	C1D-ND	4.53	1.43	1.37
37	D	406	DGD	O1G-C1A	4.52	1.46	1.33
26	c	518	BCR	C23-C22	-4.52	1.36	1.45
24	C	503	CLA	O2D-CGD	4.50	1.44	1.33
26	a	413	BCR	C23-C22	-4.50	1.36	1.45
27	f	102	SQD	O47-C7	4.49	1.47	1.34
24	b	619	CLA	CHD-C1D	4.46	1.47	1.38
24	B	607	CLA	CHD-C1D	4.46	1.47	1.38
24	A	406	CLA	CHC-C1C	4.46	1.46	1.35
24	c	511	CLA	O2A-CGA	4.45	1.46	1.33
25	a	420[B]	PHO	OBD-CAD	4.45	1.28	1.22
24	D	402	CLA	O2D-CGD	4.45	1.44	1.33
24	b	625	CLA	O2A-CGA	4.45	1.46	1.33
24	C	509	CLA	O2A-CGA	4.45	1.46	1.33
34	z	101	LMG	O8-C28	4.45	1.46	1.33
24	A	406	CLA	O2D-CGD	4.45	1.44	1.33
27	F	103	SQD	O47-C7	4.44	1.46	1.34
24	c	507	CLA	CHD-C1D	4.44	1.47	1.38
24	C	508	CLA	CHD-C1D	4.43	1.47	1.38
24	B	609	CLA	CHD-C1D	4.43	1.47	1.38
24	B	609	CLA	O2A-CGA	4.43	1.46	1.33
34	C	520	LMG	O7-C10	4.43	1.46	1.34
34	C	519	LMG	O8-C28	4.42	1.46	1.33
24	b	616	CLA	CHD-C1D	4.42	1.47	1.38
26	B	619	BCR	C23-C22	-4.42	1.36	1.45
24	b	611	CLA	O2A-CGA	4.41	1.46	1.33
24	c	515	CLA	CHD-C1D	4.41	1.46	1.38
26	D	404	BCR	C23-C22	-4.40	1.36	1.45
24	c	513	CLA	O2A-CGA	4.40	1.46	1.33
24	c	513	CLA	CHD-C1D	4.40	1.46	1.38
37	e	101	DGD	O2G-C1B	4.39	1.46	1.34
24	D	402	CLA	C1D-ND	4.38	1.43	1.37
24	B	606	CLA	O2A-CGA	4.38	1.46	1.33
24	b	625	CLA	CHD-C1D	4.37	1.46	1.38
24	c	512	CLA	CHD-C1D	4.37	1.46	1.38
27	a	405	SQD	O47-C7	4.36	1.46	1.34
26	b	627	BCR	C23-C22	-4.36	1.36	1.45
24	c	509	CLA	CHD-C1D	4.36	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C1D-ND	4.36	1.43	1.37
38	E	101	LHG	O8-C23	4.35	1.46	1.33
24	B	610	CLA	CHD-C1D	4.35	1.46	1.38
27	B	621	SQD	O47-C7	4.35	1.46	1.34
24	A	406	CLA	O2A-CGA	4.35	1.46	1.33
24	C	511	CLA	CHD-C1D	4.34	1.46	1.38
24	c	514	CLA	CHD-C1D	4.34	1.46	1.38
24	C	507	CLA	O2A-CGA	4.34	1.46	1.33
24	b	611	CLA	CHD-C1D	4.34	1.46	1.38
24	B	617	CLA	CHD-C1D	4.34	1.46	1.38
24	b	626	CLA	O2A-CGA	4.33	1.46	1.33
24	c	516	CLA	O2A-CGA	4.33	1.46	1.33
24	b	622	CLA	CHD-C1D	4.33	1.46	1.38
24	C	503	CLA	CHD-C1D	4.32	1.46	1.38
37	D	406	DGD	O2G-C1B	4.32	1.46	1.34
24	C	513	CLA	CHD-C1D	4.32	1.46	1.38
24	B	611	CLA	OBD-CAD	4.31	1.29	1.22
26	B	618	BCR	C23-C22	-4.31	1.36	1.45
25	A	409[B]	PHO	OBD-CAD	4.31	1.28	1.22
24	C	506	CLA	O2A-CGA	4.31	1.45	1.33
24	A	410	CLA	CHD-C1D	4.30	1.46	1.38
24	C	512	CLA	O2A-CGA	4.30	1.45	1.33
24	d	402	CLA	CHD-C1D	4.30	1.46	1.38
24	B	617	CLA	O2A-CGA	4.30	1.45	1.33
34	A	422	LMG	O7-C10	4.29	1.46	1.34
24	c	510	CLA	CHD-C1D	4.29	1.46	1.38
37	e	101	DGD	O1G-C1A	4.29	1.45	1.33
34	A	422	LMG	O8-C28	4.28	1.45	1.33
24	d	401	CLA	O2A-CGA	4.28	1.45	1.33
24	b	621	CLA	O2A-CGA	4.28	1.45	1.33
27	f	102	SQD	O48-C23	4.28	1.45	1.33
24	C	511	CLA	O2A-CGA	4.27	1.45	1.33
24	C	508	CLA	O2A-CGA	4.27	1.45	1.33
24	B	608	CLA	O2A-CGA	4.26	1.45	1.33
24	B	613	CLA	C1D-ND	4.26	1.43	1.37
24	D	403	CLA	CHD-C1D	4.26	1.46	1.38
24	d	402	CLA	C1D-ND	4.26	1.43	1.37
24	C	501	CLA	CHD-C1D	4.25	1.46	1.38
24	b	613	CLA	O2A-CGA	4.25	1.45	1.33
38	a	422	LHG	O8-C23	4.24	1.45	1.33
24	b	620	CLA	CHD-C1D	4.24	1.46	1.38
24	d	401	CLA	CHD-C1D	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	CLA	O2A-CGA	4.24	1.45	1.33
34	a	415	LMG	O8-C28	4.24	1.45	1.33
24	C	513	CLA	O2A-CGA	4.24	1.45	1.33
38	D	409	LHG	O7-C7	4.24	1.46	1.34
24	a	410	CLA	O2A-CGA	4.24	1.45	1.33
25	a	420[A]	PHO	O2A-CGA	4.24	1.45	1.33
24	a	409	CLA	CHD-C4C	4.24	1.48	1.39
24	c	505	CLA	CHD-C1D	4.23	1.46	1.38
34	c	523	LMG	O7-C10	4.23	1.46	1.34
24	C	512	CLA	CHD-C1D	4.23	1.46	1.38
24	B	614	CLA	C3D-C2D	4.22	1.50	1.39
24	c	506	CLA	O2A-CGA	4.22	1.45	1.33
24	d	402	CLA	O2A-CGA	4.22	1.45	1.33
25	A	409[A]	PHO	OBD-CAD	4.22	1.28	1.22
24	b	613	CLA	C1D-ND	4.22	1.43	1.37
37	h	102	DGD	O1G-C1A	4.21	1.45	1.33
24	C	503	CLA	O2A-CGA	4.21	1.45	1.33
24	c	517	CLA	O2A-CGA	4.21	1.45	1.33
37	c	521	DGD	O1G-C1A	4.21	1.45	1.33
24	b	615	CLA	CHD-C1D	4.21	1.46	1.38
37	C	517	DGD	O1G-C1A	4.21	1.45	1.33
34	c	523	LMG	O8-C28	4.20	1.45	1.33
38	d	408	LHG	O8-C23	4.20	1.45	1.33
27	b	601	SQD	O48-C23	4.20	1.45	1.33
24	C	501	CLA	O2A-CGA	4.20	1.45	1.33
27	b	601	SQD	O47-C7	4.20	1.46	1.34
24	a	412	CLA	CHD-C1D	4.19	1.46	1.38
26	b	628	BCR	C23-C22	-4.19	1.36	1.45
24	B	607	CLA	O2A-CGA	4.19	1.45	1.33
34	j	101	LMG	O7-C10	4.19	1.46	1.34
38	d	408	LHG	O7-C7	4.19	1.46	1.34
24	B	608	CLA	CHD-C1D	4.19	1.46	1.38
24	a	410	CLA	CHD-C1D	4.18	1.46	1.38
37	H	103	DGD	O1G-C1A	4.18	1.45	1.33
24	b	624	CLA	O2A-CGA	4.18	1.45	1.33
24	c	507	CLA	O2A-CGA	4.18	1.45	1.33
34	B	622	LMG	O8-C28	4.18	1.45	1.33
24	b	618	CLA	CHD-C4C	4.17	1.48	1.39
24	b	616	CLA	CHD-C4C	4.17	1.48	1.39
24	C	510	CLA	CHD-C4C	4.17	1.48	1.39
24	C	507	CLA	CHD-C1D	4.17	1.46	1.38
24	C	511	CLA	C3D-C2D	4.17	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	630	LMG	O8-C28	4.17	1.45	1.33
24	C	502	CLA	CHD-C1D	4.16	1.46	1.38
27	a	414	SQD	O48-C23	4.16	1.45	1.33
34	C	520	LMG	O8-C28	4.16	1.45	1.33
24	B	602	CLA	CHD-C1D	4.15	1.46	1.38
24	b	613	CLA	CHD-C1D	4.15	1.46	1.38
24	C	509	CLA	CHD-C1D	4.15	1.46	1.38
38	l	101	LHG	O8-C23	4.14	1.45	1.33
24	b	612	CLA	O2A-CGA	4.14	1.45	1.33
24	b	618	CLA	O2A-CGA	4.14	1.45	1.33
24	C	510	CLA	O2A-CGA	4.14	1.45	1.33
24	c	505	CLA	O2A-CGA	4.13	1.45	1.33
24	C	505	CLA	CHD-C1D	4.13	1.46	1.38
25	a	420[A]	PHO	OBD-CAD	4.13	1.28	1.22
24	c	508	CLA	CHD-C1D	4.13	1.46	1.38
38	E	101	LHG	O7-C7	4.13	1.46	1.34
24	d	403	CLA	CHD-C1D	4.13	1.46	1.38
34	c	522	LMG	O8-C28	4.13	1.45	1.33
24	d	403	CLA	O2A-CGA	4.13	1.45	1.33
24	c	507	CLA	OBD-CAD	4.13	1.29	1.22
24	B	610	CLA	C3D-C2D	4.12	1.50	1.39
24	B	613	CLA	O2A-CGA	4.12	1.45	1.33
25	A	409[A]	PHO	O2A-CGA	4.12	1.45	1.33
37	c	520	DGD	O1G-C1A	4.11	1.45	1.33
25	A	408	PHO	O2A-CGA	4.11	1.45	1.33
27	F	103	SQD	O48-C23	4.11	1.45	1.33
24	B	604	CLA	CHD-C1D	4.11	1.46	1.38
27	B	621	SQD	O48-C23	4.11	1.45	1.33
38	a	422	LHG	O7-C7	4.11	1.45	1.34
24	c	511	CLA	CHD-C1D	4.11	1.46	1.38
24	b	626	CLA	CHD-C1D	4.11	1.46	1.38
24	c	516	CLA	CHD-C1D	4.10	1.46	1.38
38	L	101	LHG	O8-C23	4.10	1.45	1.33
34	Z	101	LMG	O7-C10	4.10	1.45	1.34
24	C	503	CLA	CHD-C4C	4.10	1.48	1.39
24	C	504	CLA	CHD-C1D	4.10	1.46	1.38
24	B	616	CLA	O2A-CGA	4.10	1.45	1.33
36	b	633	HTG	C1'-S1	-4.09	1.76	1.81
24	c	517	CLA	CHD-C1D	4.09	1.46	1.38
24	B	611	CLA	C3D-C2D	4.09	1.50	1.39
24	B	603	CLA	OBD-CAD	4.09	1.29	1.22
24	B	611	CLA	CHD-C4C	4.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	CHD-C4C	4.08	1.48	1.39
24	b	616	CLA	O2A-CGA	4.08	1.45	1.33
37	C	516	DGD	O1G-C1A	4.08	1.45	1.33
24	C	509	CLA	CHD-C4C	4.08	1.48	1.39
24	C	511	CLA	CHD-C4C	4.07	1.48	1.39
24	b	623	CLA	CHD-C4C	4.07	1.48	1.39
25	a	420[B]	PHO	O2A-CGA	4.06	1.45	1.33
24	A	410	CLA	O2A-CGA	4.06	1.45	1.33
24	c	512	CLA	C3D-C2D	4.06	1.50	1.39
24	B	604	CLA	O2A-CGA	4.05	1.45	1.33
24	C	504	CLA	O2A-CGA	4.05	1.45	1.33
34	c	522	LMG	O7-C10	4.05	1.45	1.34
37	C	518	DGD	O1G-C1A	4.05	1.45	1.33
24	b	619	CLA	O2A-CGA	4.04	1.45	1.33
24	b	614	CLA	O2A-CGA	4.04	1.45	1.33
34	D	412	LMG	O8-C28	4.04	1.45	1.33
24	C	506	CLA	CHD-C4C	4.04	1.48	1.39
37	h	102	DGD	O2G-C1B	4.04	1.45	1.34
34	C	519	LMG	O7-C10	4.03	1.45	1.34
37	C	516	DGD	O2G-C1B	4.03	1.45	1.34
24	B	614	CLA	CHD-C1D	4.03	1.46	1.38
24	c	505	CLA	C3D-C2D	4.03	1.50	1.39
25	A	409[B]	PHO	O2A-CGA	4.03	1.45	1.33
24	b	619	CLA	CHD-C4C	4.02	1.48	1.39
24	c	506	CLA	CHD-C1D	4.02	1.46	1.38
24	B	603	CLA	O2A-CGA	4.02	1.45	1.33
24	B	608	CLA	CHD-C4C	4.02	1.48	1.39
24	c	517	CLA	CHD-C4C	4.02	1.48	1.39
34	j	101	LMG	O8-C28	4.02	1.45	1.33
24	B	613	CLA	CHD-C1D	4.02	1.46	1.38
24	B	612	CLA	CHD-C1D	4.02	1.46	1.38
24	b	614	CLA	CHD-C1D	4.02	1.46	1.38
24	A	405	CLA	CHD-C4C	4.01	1.48	1.39
24	c	514	CLA	CHD-C4C	4.01	1.48	1.39
24	b	618	CLA	OBD-CAD	4.01	1.29	1.22
34	B	622	LMG	O7-C10	4.01	1.45	1.34
24	D	402	CLA	CHD-C1D	4.01	1.46	1.38
37	c	521	DGD	O2G-C1B	4.01	1.45	1.34
24	b	626	CLA	C3D-C2D	4.01	1.50	1.39
24	c	510	CLA	CHD-C4C	4.01	1.48	1.39
24	c	506	CLA	C3D-C2D	4.01	1.50	1.39
24	b	620	CLA	O2A-CGA	4.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	412	CLA	O2A-CGA	4.00	1.45	1.33
24	b	611	CLA	C3D-C2D	4.00	1.50	1.39
24	A	406	CLA	C3D-C2D	4.00	1.50	1.39
24	C	512	CLA	C3D-C2D	4.00	1.50	1.39
24	b	620	CLA	OBD-CAD	4.00	1.29	1.22
24	D	402	CLA	O2A-CGA	4.00	1.45	1.33
24	C	513	CLA	CHD-C4C	4.00	1.48	1.39
34	z	101	LMG	O7-C10	3.99	1.45	1.34
24	c	513	CLA	CHD-C4C	3.99	1.48	1.39
24	C	501	CLA	CHD-C4C	3.99	1.48	1.39
24	c	510	CLA	O2A-CGA	3.98	1.45	1.33
24	b	622	CLA	C3D-C2D	3.98	1.50	1.39
24	B	603	CLA	CHD-C1D	3.98	1.46	1.38
27	A	416	SQD	O47-C7	3.98	1.45	1.34
24	c	516	CLA	C3D-C2D	3.98	1.50	1.39
37	C	518	DGD	O2G-C1B	3.97	1.45	1.34
24	B	607	CLA	CHD-C4C	3.97	1.48	1.39
24	C	504	CLA	C3D-C2D	3.97	1.50	1.39
39	V	206	HEM	C4D-ND	-3.96	1.33	1.40
24	a	410	CLA	OBD-CAD	3.96	1.29	1.22
38	D	409	LHG	O8-C23	3.96	1.44	1.33
24	D	403	CLA	O2A-CGA	3.96	1.44	1.33
27	a	414	SQD	O47-C7	3.96	1.45	1.34
24	C	505	CLA	O2A-CGA	3.96	1.44	1.33
24	C	506	CLA	C3D-C2D	3.95	1.49	1.39
27	A	412	SQD	O48-C23	3.95	1.44	1.33
24	C	512	CLA	CHD-C4C	3.95	1.48	1.39
24	C	504	CLA	CHD-C4C	3.95	1.48	1.39
24	c	508	CLA	CHD-C4C	3.94	1.48	1.39
24	a	412	CLA	OBD-CAD	3.94	1.29	1.22
24	b	623	CLA	CHD-C1D	3.94	1.46	1.38
24	b	621	CLA	CHD-C1D	3.93	1.46	1.38
24	c	511	CLA	C3D-C2D	3.93	1.49	1.39
24	B	610	CLA	OBD-CAD	3.93	1.29	1.22
38	d	407	LHG	O7-C7	3.93	1.45	1.34
24	A	407	CLA	O2A-CGA	3.93	1.44	1.33
34	b	630	LMG	O7-C10	3.93	1.45	1.34
24	C	509	CLA	OBD-CAD	3.93	1.29	1.22
24	D	403	CLA	CHD-C4C	3.92	1.48	1.39
24	b	615	CLA	O2A-CGA	3.92	1.44	1.33
38	D	408	LHG	O7-C7	3.92	1.45	1.34
24	c	514	CLA	OBD-CAD	3.92	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	l	101	LHG	O7-C7	3.91	1.45	1.34
24	b	624	CLA	CHD-C4C	3.91	1.48	1.39
24	c	508	CLA	O2A-CGA	3.91	1.44	1.33
38	d	407	LHG	O8-C23	3.91	1.44	1.33
24	b	625	CLA	C3D-C2D	3.91	1.49	1.39
34	a	415	LMG	O7-C10	3.91	1.45	1.34
36	B	632	HTG	C1'-S1	-3.91	1.76	1.81
24	a	412	CLA	CHD-C4C	3.91	1.48	1.39
24	B	615	CLA	O2A-CGA	3.90	1.44	1.33
24	d	402	CLA	CHD-C4C	3.90	1.48	1.39
24	C	508	CLA	CHD-C4C	3.90	1.48	1.39
34	D	412	LMG	O7-C10	3.90	1.45	1.34
24	A	405	CLA	C3D-C2D	3.90	1.49	1.39
24	b	612	CLA	OBD-CAD	3.89	1.29	1.22
37	H	103	DGD	O2G-C1B	3.89	1.45	1.34
24	b	624	CLA	C3D-C2D	3.89	1.49	1.39
24	d	401	CLA	CHD-C4C	3.89	1.48	1.39
24	A	405	CLA	O2A-CGA	3.89	1.44	1.33
24	C	509	CLA	C3D-C2D	3.88	1.49	1.39
24	A	407	CLA	CHD-C4C	3.88	1.48	1.39
24	C	507	CLA	C3D-C2D	3.88	1.49	1.39
24	b	611	CLA	CHD-C4C	3.88	1.48	1.39
24	B	609	CLA	C3D-C2D	3.88	1.49	1.39
24	B	615	CLA	CHD-C1D	3.88	1.45	1.38
24	B	606	CLA	C3D-C2D	3.87	1.49	1.39
24	C	503	CLA	C3D-C2D	3.87	1.49	1.39
24	C	502	CLA	C3D-C2D	3.87	1.49	1.39
37	c	520	DGD	O2G-C1B	3.87	1.45	1.34
25	a	420[A]	PHO	C3C-C2C	3.87	1.49	1.37
24	c	514	CLA	O2A-CGA	3.87	1.44	1.33
24	B	604	CLA	CHD-C4C	3.86	1.48	1.39
25	A	409[B]	PHO	C3C-C2C	3.86	1.49	1.37
24	c	509	CLA	CHD-C4C	3.86	1.48	1.39
24	B	602	CLA	C3D-C2D	3.86	1.49	1.39
25	A	409[A]	PHO	C3C-C2C	3.86	1.49	1.37
38	L	101	LHG	O7-C7	3.86	1.45	1.34
24	b	617	CLA	CHD-C1D	3.86	1.45	1.38
24	B	609	CLA	CHD-C4C	3.85	1.48	1.39
24	c	516	CLA	CHD-C4C	3.85	1.48	1.39
24	d	401	CLA	C3D-C2D	3.85	1.49	1.39
38	D	407	LHG	O8-C23	3.85	1.44	1.33
24	b	625	CLA	CHD-C4C	3.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	O2A-CGA	3.85	1.44	1.33
24	c	508	CLA	C3D-C2D	3.84	1.49	1.39
24	b	612	CLA	CHD-C4C	3.84	1.48	1.39
24	B	605	CLA	CHD-C1D	3.84	1.45	1.38
24	b	620	CLA	CHD-C4C	3.84	1.48	1.39
36	B	623	HTG	C1'-S1	-3.83	1.76	1.81
24	B	610	CLA	CHD-C4C	3.83	1.48	1.39
24	A	405	CLA	CHD-C1D	3.83	1.45	1.38
24	c	513	CLA	C3D-C2D	3.83	1.49	1.39
24	B	606	CLA	CHD-C1D	3.83	1.45	1.38
24	b	620	CLA	C3D-C2D	3.83	1.49	1.39
24	C	513	CLA	C3D-C2D	3.83	1.49	1.39
24	b	619	CLA	C3D-C2D	3.83	1.49	1.39
24	b	624	CLA	CHD-C1D	3.83	1.45	1.38
24	C	511	CLA	OBD-CAD	3.83	1.29	1.22
24	c	509	CLA	O2A-CGA	3.82	1.44	1.33
24	B	603	CLA	CHD-C4C	3.82	1.48	1.39
27	A	412	SQD	O47-C7	3.82	1.45	1.34
24	c	515	CLA	CHD-C4C	3.82	1.47	1.39
24	C	508	CLA	C3D-C2D	3.82	1.49	1.39
24	C	502	CLA	CHD-C4C	3.81	1.47	1.39
24	d	401	CLA	OBD-CAD	3.81	1.29	1.22
24	b	612	CLA	C3D-C2D	3.81	1.49	1.39
37	c	519	DGD	O1G-C1A	3.81	1.44	1.33
24	b	619	CLA	OBD-CAD	3.81	1.29	1.22
24	B	614	CLA	O2A-CGA	3.80	1.44	1.33
24	c	513	CLA	OBD-CAD	3.80	1.29	1.22
24	d	402	CLA	C3D-C2D	3.80	1.49	1.39
24	c	506	CLA	CHD-C4C	3.79	1.47	1.39
24	b	623	CLA	O2A-CGA	3.79	1.44	1.33
24	B	606	CLA	OBD-CAD	3.79	1.29	1.22
24	a	410	CLA	CHD-C4C	3.79	1.47	1.39
24	c	505	CLA	CHD-C4C	3.79	1.47	1.39
24	b	618	CLA	C3D-C2D	3.79	1.49	1.39
24	b	622	CLA	O2A-CGA	3.78	1.44	1.33
24	A	410	CLA	OBD-CAD	3.78	1.29	1.22
24	a	412	CLA	C3D-C2D	3.78	1.49	1.39
24	B	604	CLA	C3D-C2D	3.78	1.49	1.39
24	a	409	CLA	OBD-CAD	3.78	1.29	1.22
24	A	406	CLA	CHD-C4C	3.78	1.47	1.39
24	B	615	CLA	CHD-C4C	3.77	1.47	1.39
24	C	507	CLA	CHD-C4C	3.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	CHD-C4C	3.77	1.47	1.39
24	b	626	CLA	CHD-C4C	3.76	1.47	1.39
24	b	617	CLA	CHD-C4C	3.76	1.47	1.39
24	C	510	CLA	C3D-C2D	3.76	1.49	1.39
25	a	420[B]	PHO	C3C-C2C	3.76	1.48	1.37
24	B	612	CLA	C3D-C2D	3.75	1.49	1.39
38	d	406	LHG	O8-C23	3.75	1.44	1.33
24	C	501	CLA	C3D-C2D	3.75	1.49	1.39
24	c	507	CLA	CHD-C4C	3.75	1.47	1.39
24	c	516	CLA	OBD-CAD	3.75	1.28	1.22
24	A	406	CLA	CHD-C1D	3.75	1.45	1.38
24	B	615	CLA	C3D-C2D	3.75	1.49	1.39
24	c	512	CLA	CHD-C4C	3.75	1.47	1.39
24	C	508	CLA	OBD-CAD	3.74	1.28	1.22
36	B	625	HTG	C1'-S1	-3.74	1.76	1.81
24	B	616	CLA	CHD-C1D	3.74	1.45	1.38
24	c	515	CLA	C3D-C2D	3.74	1.49	1.39
24	b	615	CLA	C3D-C2D	3.74	1.49	1.39
24	b	623	CLA	C3D-C2D	3.74	1.49	1.39
24	B	602	CLA	CHD-C4C	3.74	1.47	1.39
24	A	410	CLA	C3D-C2D	3.74	1.49	1.39
24	B	606	CLA	CHD-C4C	3.74	1.47	1.39
24	B	613	CLA	OBD-CAD	3.73	1.28	1.22
24	D	403	CLA	C3D-C2D	3.73	1.49	1.39
24	D	402	CLA	CHD-C4C	3.73	1.47	1.39
24	b	616	CLA	C3D-C2D	3.73	1.49	1.39
24	C	504	CLA	OBD-CAD	3.73	1.28	1.22
24	B	611	CLA	O2A-CGA	3.73	1.44	1.33
24	b	625	CLA	OBD-CAD	3.73	1.28	1.22
24	A	410	CLA	CHD-C4C	3.72	1.47	1.39
24	B	603	CLA	C3D-C2D	3.72	1.49	1.39
37	c	519	DGD	O2G-C1B	3.72	1.44	1.34
38	D	408	LHG	O8-C23	3.72	1.44	1.33
24	c	517	CLA	C3D-C2D	3.72	1.49	1.39
24	b	615	CLA	CHD-C4C	3.72	1.47	1.39
37	C	517	DGD	O2G-C1B	3.72	1.44	1.34
24	C	512	CLA	OBD-CAD	3.71	1.28	1.22
24	B	602	CLA	OBD-CAD	3.71	1.28	1.22
24	B	617	CLA	C3D-C2D	3.71	1.49	1.39
24	b	617	CLA	O2A-CGA	3.71	1.44	1.33
36	V	207	HTG	C1'-S1	-3.70	1.76	1.81
24	c	509	CLA	OBD-CAD	3.70	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	OBD-CAD	3.70	1.28	1.22
36	b	609	HTG	C1'-S1	-3.70	1.76	1.81
24	b	613	CLA	OBD-CAD	3.68	1.28	1.22
36	b	608	HTG	C1'-S1	-3.68	1.76	1.81
24	B	604	CLA	OBD-CAD	3.68	1.28	1.22
24	b	622	CLA	CHD-C4C	3.68	1.47	1.39
24	c	510	CLA	C3D-C2D	3.67	1.49	1.39
24	b	613	CLA	C3D-C2D	3.66	1.49	1.39
24	d	403	CLA	OBD-CAD	3.66	1.28	1.22
24	B	615	CLA	OBD-CAD	3.65	1.28	1.22
24	d	403	CLA	CHD-C4C	3.65	1.47	1.39
25	a	411	PHO	C3C-C2C	3.65	1.48	1.37
24	b	626	CLA	OBD-CAD	3.65	1.28	1.22
24	D	403	CLA	OBD-CAD	3.64	1.28	1.22
24	c	507	CLA	C3D-C2D	3.64	1.49	1.39
24	B	609	CLA	OBD-CAD	3.64	1.28	1.22
24	c	509	CLA	C3D-C2D	3.64	1.49	1.39
24	B	614	CLA	OBD-CAD	3.63	1.28	1.22
24	b	624	CLA	OBD-CAD	3.63	1.28	1.22
36	d	411	HTG	C1'-S1	-3.63	1.76	1.81
39	V	206	HEM	C1B-NB	-3.62	1.34	1.40
24	c	515	CLA	OBD-CAD	3.62	1.28	1.22
24	A	407	CLA	C3D-C2D	3.62	1.49	1.39
24	d	403	CLA	C3D-C2D	3.62	1.49	1.39
24	b	614	CLA	C3D-C2D	3.61	1.49	1.39
24	b	621	CLA	C3D-C2D	3.61	1.49	1.39
24	B	605	CLA	O2A-CGA	3.61	1.43	1.33
24	b	621	CLA	CHD-C4C	3.61	1.47	1.39
24	D	402	CLA	C3D-C2D	3.61	1.49	1.39
24	C	501	CLA	OBD-CAD	3.61	1.28	1.22
24	B	612	CLA	O2A-CGA	3.61	1.43	1.33
24	b	615	CLA	OBD-CAD	3.61	1.28	1.22
24	d	402	CLA	OBD-CAD	3.61	1.28	1.22
25	A	408	PHO	C3C-C2C	3.60	1.48	1.37
24	b	613	CLA	CHD-C4C	3.59	1.47	1.39
24	c	511	CLA	OBD-CAD	3.59	1.28	1.22
36	c	524	HTG	C1'-S1	-3.58	1.76	1.81
36	C	523	HTG	C1'-S1	-3.58	1.76	1.81
24	a	410	CLA	C3D-C2D	3.57	1.48	1.39
24	c	514	CLA	C3D-C2D	3.57	1.48	1.39
24	b	611	CLA	OBD-CAD	3.57	1.28	1.22
36	B	633	HTG	C1'-S1	-3.57	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	CHD-C4C	3.57	1.47	1.39
24	b	616	CLA	OBD-CAD	3.57	1.28	1.22
24	b	617	CLA	C3D-C2D	3.54	1.48	1.39
24	c	512	CLA	OBD-CAD	3.54	1.28	1.22
24	B	616	CLA	CHD-C4C	3.53	1.47	1.39
24	B	607	CLA	C3D-C2D	3.53	1.48	1.39
36	c	525	HTG	C1'-S1	-3.53	1.76	1.81
24	B	608	CLA	C3D-C2D	3.53	1.48	1.39
24	B	613	CLA	C3D-C2D	3.52	1.48	1.39
24	B	617	CLA	OBD-CAD	3.52	1.28	1.22
38	D	407	LHG	O7-C7	3.51	1.44	1.34
36	H	101	HTG	C1'-S1	-3.51	1.76	1.81
24	B	614	CLA	CHD-C4C	3.51	1.47	1.39
38	d	406	LHG	O7-C7	3.50	1.44	1.34
24	C	503	CLA	OBD-CAD	3.50	1.28	1.22
24	A	407	CLA	OBD-CAD	3.50	1.28	1.22
39	e	102	HEM	C4D-ND	-3.50	1.34	1.40
24	A	405	CLA	OBD-CAD	3.49	1.28	1.22
24	B	617	CLA	CHD-C4C	3.49	1.47	1.39
24	c	506	CLA	OBD-CAD	3.49	1.28	1.22
24	b	614	CLA	CHD-C4C	3.49	1.47	1.39
24	b	622	CLA	OBD-CAD	3.49	1.28	1.22
24	a	409	CLA	O2A-CGA	3.48	1.43	1.33
24	B	605	CLA	CHD-C4C	3.47	1.47	1.39
25	A	409[B]	PHO	CHA-CBD	-3.47	1.48	1.52
24	C	510	CLA	OBD-CAD	3.46	1.28	1.22
24	B	616	CLA	C3D-C2D	3.44	1.48	1.39
24	b	621	CLA	OBD-CAD	3.43	1.28	1.22
39	F	102	HEM	C4D-ND	-3.42	1.34	1.40
24	B	613	CLA	C1C-C2C	3.42	1.51	1.44
36	C	522	HTG	C1'-S1	-3.41	1.77	1.81
24	B	612	CLA	OBD-CAD	3.41	1.28	1.22
36	b	602	HTG	C1'-S1	-3.41	1.77	1.81
24	c	517	CLA	OBD-CAD	3.40	1.28	1.22
24	C	505	CLA	C3D-C2D	3.40	1.48	1.39
24	b	614	CLA	OBD-CAD	3.40	1.28	1.22
24	a	409	CLA	C3D-C2D	3.39	1.48	1.39
39	v	205	HEM	C1B-NB	-3.39	1.34	1.40
24	C	513	CLA	OBD-CAD	3.39	1.28	1.22
25	a	411	PHO	O2A-CGA	3.39	1.43	1.33
24	B	607	CLA	OBD-CAD	3.36	1.28	1.22
24	c	505	CLA	OBD-CAD	3.33	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	OBD-CAD	3.33	1.28	1.22
24	c	508	CLA	OBD-CAD	3.30	1.28	1.22
24	D	402	CLA	OBD-CAD	3.29	1.28	1.22
24	b	617	CLA	OBD-CAD	3.27	1.28	1.22
25	a	411	PHO	CHA-CBD	-3.27	1.48	1.52
25	A	409[A]	PHO	CHA-CBD	-3.26	1.48	1.52
24	A	406	CLA	OBD-CAD	3.25	1.28	1.22
24	B	613	CLA	CHD-C4C	3.23	1.46	1.39
39	e	102	HEM	C1B-NB	-3.23	1.34	1.40
24	C	507	CLA	OBD-CAD	3.23	1.28	1.22
24	B	608	CLA	OBD-CAD	3.22	1.28	1.22
24	C	502	CLA	OBD-CAD	3.22	1.28	1.22
24	b	623	CLA	OBD-CAD	3.20	1.28	1.22
24	C	506	CLA	OBD-CAD	3.19	1.28	1.22
25	a	420[B]	PHO	CHA-CBD	-3.19	1.48	1.52
24	B	605	CLA	C3D-C2D	3.17	1.47	1.39
39	v	205	HEM	C4D-ND	-3.16	1.34	1.40
24	C	505	CLA	OBD-CAD	3.15	1.27	1.22
36	B	624	HTG	C1'-S1	-3.15	1.77	1.81
24	D	402	CLA	C4C-C3C	3.12	1.50	1.45
24	B	613	CLA	C1B-NB	-3.12	1.32	1.35
24	c	507	CLA	C1C-C2C	3.12	1.50	1.44
39	F	102	HEM	C1B-NB	-3.09	1.35	1.40
24	B	604	CLA	C1C-C2C	3.00	1.50	1.44
24	c	511	CLA	C4D-CHA	2.99	1.49	1.38
24	B	606	CLA	C1C-C2C	2.99	1.50	1.44
24	B	614	CLA	C4C-C3C	2.98	1.50	1.45
27	A	416	SQD	C6-S	-2.96	1.66	1.77
24	A	410	CLA	C1C-C2C	2.96	1.50	1.44
24	C	503	CLA	C1C-C2C	2.95	1.50	1.44
27	f	102	SQD	C6-S	-2.93	1.66	1.77
24	B	614	CLA	C1C-C2C	2.92	1.50	1.44
39	V	206	HEM	FE-NB	2.91	2.11	1.96
24	a	409	CLA	C1C-C2C	2.89	1.50	1.44
39	v	205	HEM	FE-NB	2.89	2.11	1.96
24	C	507	CLA	C4D-CHA	2.89	1.48	1.38
24	b	622	CLA	C4D-CHA	2.86	1.48	1.38
24	b	614	CLA	C4D-CHA	2.86	1.48	1.38
24	C	508	CLA	C4C-C3C	2.83	1.49	1.45
24	b	625	CLA	C4D-CHA	2.83	1.48	1.38
24	A	405	CLA	C4C-C3C	2.82	1.49	1.45
24	C	507	CLA	C1C-C2C	2.82	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C4B-CHC	2.82	1.48	1.41
39	e	102	HEM	FE-NB	2.81	2.10	1.96
24	c	505	CLA	C4D-CHA	2.81	1.48	1.38
24	c	508	CLA	C1C-C2C	2.81	1.50	1.44
25	a	420[A]	PHO	CHA-CBD	-2.80	1.49	1.52
24	A	410	CLA	C4B-CHC	2.80	1.48	1.41
25	A	408	PHO	CHA-CBD	-2.79	1.49	1.52
24	B	615	CLA	C1C-C2C	2.79	1.50	1.44
24	b	613	CLA	C1C-C2C	2.78	1.50	1.44
24	A	406	CLA	C4D-CHA	2.78	1.48	1.38
24	b	614	CLA	C1B-CHB	2.78	1.48	1.41
24	b	626	CLA	C4D-CHA	2.78	1.48	1.38
24	a	409	CLA	C4C-C3C	2.78	1.49	1.45
24	B	611	CLA	C4D-CHA	2.78	1.48	1.38
24	d	403	CLA	C1C-C2C	2.77	1.49	1.44
24	B	605	CLA	C4D-CHA	2.77	1.48	1.38
24	b	618	CLA	C4D-CHA	2.77	1.48	1.38
24	B	614	CLA	C4D-CHA	2.77	1.48	1.38
36	b	632	HTG	C1'-S1	-2.77	1.77	1.81
24	c	506	CLA	C4D-CHA	2.77	1.48	1.38
24	C	510	CLA	C4D-CHA	2.76	1.48	1.38
24	C	511	CLA	C4C-C3C	2.76	1.49	1.45
24	B	612	CLA	C1C-C2C	2.76	1.49	1.44
24	d	401	CLA	C1B-CHB	2.75	1.48	1.41
24	b	614	CLA	C1C-C2C	2.75	1.49	1.44
24	C	509	CLA	C4C-C3C	2.75	1.49	1.45
24	b	617	CLA	C4B-CHC	2.75	1.48	1.41
27	F	103	SQD	C6-S	-2.74	1.67	1.77
24	B	617	CLA	C4D-CHA	2.74	1.48	1.38
24	B	608	CLA	C4B-CHC	2.74	1.48	1.41
24	c	517	CLA	C1C-C2C	2.74	1.49	1.44
27	a	405	SQD	C6-S	-2.74	1.67	1.77
24	b	618	CLA	C1B-CHB	2.72	1.48	1.41
24	c	513	CLA	C4D-CHA	2.72	1.48	1.38
24	b	612	CLA	C4C-C3C	2.71	1.49	1.45
29	A	417	LMT	O1'-C1'	2.71	1.44	1.40
24	C	504	CLA	C4D-CHA	2.71	1.48	1.38
24	b	617	CLA	C3D-C4D	-2.71	1.38	1.44
24	B	607	CLA	C4C-C3C	2.71	1.49	1.45
24	C	510	CLA	C1B-CHB	2.71	1.48	1.41
24	B	611	CLA	C4C-C3C	2.70	1.49	1.45
24	C	511	CLA	C4D-CHA	2.70	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	410	CLA	C1B-CHB	2.70	1.48	1.41
24	a	410	CLA	C1C-C2C	2.69	1.49	1.44
24	B	615	CLA	C1B-CHB	2.69	1.48	1.41
27	A	412	SQD	C6-S	-2.69	1.67	1.77
24	d	403	CLA	C4B-CHC	2.69	1.48	1.41
24	c	513	CLA	C1B-CHB	2.69	1.48	1.41
24	A	405	CLA	C4D-CHA	2.68	1.47	1.38
24	b	621	CLA	C4D-CHA	2.68	1.47	1.38
24	C	509	CLA	C4D-CHA	2.68	1.47	1.38
39	F	102	HEM	FE-NB	2.68	2.10	1.96
24	C	503	CLA	C4B-CHC	2.67	1.48	1.41
24	b	617	CLA	C4D-CHA	2.67	1.47	1.38
24	b	626	CLA	C1B-CHB	2.67	1.48	1.41
24	c	509	CLA	C4C-C3C	2.66	1.49	1.45
24	C	513	CLA	C4D-CHA	2.66	1.47	1.38
24	C	506	CLA	C4C-C3C	2.66	1.49	1.45
24	c	514	CLA	C1B-CHB	2.66	1.48	1.41
24	b	616	CLA	C1C-C2C	2.66	1.49	1.44
24	b	623	CLA	C4C-C3C	2.66	1.49	1.45
24	C	509	CLA	C1B-CHB	2.66	1.48	1.41
27	B	621	SQD	C6-S	-2.65	1.67	1.77
24	d	402	CLA	C4C-C3C	2.65	1.49	1.45
24	c	511	CLA	C1C-C2C	2.65	1.49	1.44
24	B	615	CLA	C4C-C3C	2.64	1.49	1.45
24	C	506	CLA	C4D-CHA	2.64	1.47	1.38
24	c	509	CLA	C1B-CHB	2.64	1.48	1.41
24	B	615	CLA	C4D-CHA	2.64	1.47	1.38
24	B	613	CLA	C4B-CHC	2.64	1.48	1.41
24	B	607	CLA	C4D-CHA	2.63	1.47	1.38
24	B	603	CLA	C4C-C3C	2.63	1.49	1.45
24	B	612	CLA	C4B-CHC	2.63	1.48	1.41
24	B	606	CLA	C4B-CHC	2.63	1.48	1.41
24	c	506	CLA	C1C-C2C	2.63	1.49	1.44
27	a	414	SQD	C6-S	-2.62	1.67	1.77
27	b	601	SQD	C6-S	-2.62	1.67	1.77
24	C	512	CLA	C4D-CHA	2.62	1.47	1.38
24	C	508	CLA	C4D-CHA	2.61	1.47	1.38
24	B	604	CLA	C1B-NB	-2.61	1.32	1.35
24	c	516	CLA	C4D-CHA	2.61	1.47	1.38
24	B	608	CLA	C4D-CHA	2.61	1.47	1.38
24	C	508	CLA	C1C-C2C	2.61	1.49	1.44
24	A	410	CLA	C4D-CHA	2.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	516	CLA	C1C-C2C	2.60	1.49	1.44
24	c	513	CLA	C1C-C2C	2.60	1.49	1.44
34	Z	101	LMG	O8-C28	2.60	1.46	1.33
24	c	514	CLA	C4C-C3C	2.60	1.49	1.45
24	B	605	CLA	C1C-C2C	2.60	1.49	1.44
24	C	505	CLA	C4D-CHA	2.59	1.47	1.38
24	b	618	CLA	C4B-CHC	2.59	1.48	1.41
24	b	619	CLA	C4D-CHA	2.59	1.47	1.38
24	B	605	CLA	C1B-CHB	2.59	1.48	1.41
24	d	403	CLA	C1B-CHB	2.59	1.48	1.41
32	A	420[B]	PL9	C6-C5	2.58	1.48	1.35
24	D	402	CLA	C3D-C4D	-2.58	1.38	1.44
32	a	416[A]	PL9	C6-C5	2.58	1.48	1.35
24	c	507	CLA	C4B-CHC	2.58	1.48	1.41
24	C	506	CLA	C1B-CHB	2.58	1.48	1.41
24	b	616	CLA	C4D-CHA	2.58	1.47	1.38
24	b	622	CLA	C1B-CHB	2.58	1.48	1.41
24	B	613	CLA	C1B-CHB	2.58	1.48	1.41
32	a	416[B]	PL9	C6-C5	2.57	1.48	1.35
24	B	612	CLA	C4D-CHA	2.57	1.47	1.38
24	c	517	CLA	C4B-CHC	2.57	1.48	1.41
24	C	502	CLA	C4D-CHA	2.57	1.47	1.38
24	a	412	CLA	C1B-CHB	2.57	1.48	1.41
24	B	610	CLA	C4D-CHA	2.57	1.47	1.38
24	b	612	CLA	C1C-C2C	2.57	1.49	1.44
24	B	612	CLA	C1B-CHB	2.57	1.48	1.41
25	a	420[B]	PHO	C3A-C2A	-2.57	1.52	1.54
24	C	505	CLA	C4B-CHC	2.57	1.48	1.41
24	D	403	CLA	C1C-C2C	2.56	1.49	1.44
24	B	616	CLA	C4D-CHA	2.56	1.47	1.38
24	C	501	CLA	C4B-CHC	2.56	1.48	1.41
24	B	604	CLA	C4B-CHC	2.56	1.48	1.41
24	c	514	CLA	C4D-CHA	2.56	1.47	1.38
24	a	412	CLA	C4D-CHA	2.56	1.47	1.38
32	D	405[A]	PL9	C6-C5	2.56	1.48	1.35
24	b	615	CLA	C1B-CHB	2.56	1.48	1.41
24	c	508	CLA	C4D-CHA	2.55	1.47	1.38
24	b	622	CLA	C4C-C3C	2.55	1.49	1.45
24	B	617	CLA	C3D-C4D	-2.55	1.38	1.44
32	A	420[A]	PL9	C6-C5	2.55	1.48	1.35
24	B	609	CLA	C4D-CHA	2.55	1.47	1.38
24	B	602	CLA	C4D-CHA	2.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	101	HTG	C1-S1	-2.55	1.76	1.80
24	C	511	CLA	C1B-CHB	2.55	1.48	1.41
24	C	512	CLA	C1C-C2C	2.55	1.49	1.44
24	B	608	CLA	C4C-C3C	2.55	1.49	1.45
24	c	505	CLA	C4C-C3C	2.55	1.49	1.45
24	c	515	CLA	C4D-CHA	2.55	1.47	1.38
24	A	407	CLA	C4B-CHC	2.55	1.48	1.41
24	d	402	CLA	C1B-CHB	2.55	1.48	1.41
24	C	505	CLA	C3D-C4D	-2.55	1.38	1.44
24	B	616	CLA	C1C-C2C	2.55	1.49	1.44
24	c	507	CLA	C4C-C3C	2.54	1.49	1.45
24	b	619	CLA	C1B-CHB	2.54	1.48	1.41
24	b	621	CLA	C1B-CHB	2.54	1.48	1.41
24	A	410	CLA	C4C-C3C	2.54	1.49	1.45
24	C	505	CLA	C1C-C2C	2.54	1.49	1.44
24	b	615	CLA	C1C-C2C	2.54	1.49	1.44
24	b	622	CLA	C1C-C2C	2.54	1.49	1.44
24	B	602	CLA	C1B-CHB	2.53	1.48	1.41
32	d	405[A]	PL9	C6-C5	2.53	1.48	1.35
24	C	513	CLA	C4B-CHC	2.53	1.48	1.41
24	C	501	CLA	C4D-CHA	2.53	1.47	1.38
24	b	623	CLA	C1B-CHB	2.53	1.48	1.41
24	C	501	CLA	C1C-C2C	2.53	1.49	1.44
24	c	508	CLA	C1B-CHB	2.53	1.48	1.41
24	C	509	CLA	C4B-CHC	2.52	1.48	1.41
24	c	516	CLA	C4B-CHC	2.52	1.48	1.41
24	C	513	CLA	C1C-C2C	2.52	1.49	1.44
24	C	507	CLA	C4B-CHC	2.52	1.48	1.41
24	b	611	CLA	C4D-CHA	2.52	1.47	1.38
24	C	510	CLA	C3D-C4D	-2.52	1.38	1.44
24	B	610	CLA	C3D-C4D	-2.52	1.38	1.44
24	B	605	CLA	OBD-CAD	2.52	1.26	1.22
24	A	405	CLA	C1C-C2C	2.51	1.49	1.44
24	b	624	CLA	C1C-C2C	2.51	1.49	1.44
24	b	623	CLA	C4D-CHA	2.51	1.47	1.38
24	D	403	CLA	C1B-CHB	2.51	1.48	1.41
24	B	604	CLA	C4D-CHA	2.51	1.47	1.38
24	b	615	CLA	C4D-CHA	2.51	1.47	1.38
32	D	405[B]	PL9	C6-C5	2.51	1.48	1.35
24	b	613	CLA	C4D-CHA	2.51	1.47	1.38
24	d	402	CLA	C4D-CHA	2.50	1.47	1.38
32	d	405[B]	PL9	C6-C5	2.50	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C1B-CHB	2.50	1.47	1.41
24	b	620	CLA	C4C-C3C	2.50	1.49	1.45
24	C	504	CLA	C1B-CHB	2.50	1.47	1.41
24	D	402	CLA	C1B-CHB	2.49	1.47	1.41
24	c	505	CLA	C1B-CHB	2.49	1.47	1.41
24	c	511	CLA	C4C-C3C	2.49	1.49	1.45
24	A	407	CLA	C1C-C2C	2.49	1.49	1.44
24	B	607	CLA	C1C-C2C	2.49	1.49	1.44
24	d	403	CLA	C4C-C3C	2.49	1.49	1.45
24	c	517	CLA	C4D-CHA	2.48	1.47	1.38
24	C	509	CLA	C1C-C2C	2.48	1.49	1.44
24	b	620	CLA	C4B-CHC	2.48	1.47	1.41
24	c	512	CLA	C4D-CHA	2.48	1.47	1.38
24	A	407	CLA	C4D-CHA	2.48	1.47	1.38
24	C	512	CLA	C1B-CHB	2.48	1.47	1.41
39	V	206	HEM	C3B-C4B	2.47	1.49	1.44
24	a	412	CLA	C1C-C2C	2.47	1.49	1.44
24	B	613	CLA	C4D-CHA	2.47	1.47	1.38
24	a	410	CLA	C4D-CHA	2.47	1.47	1.38
24	B	617	CLA	C4B-CHC	2.47	1.47	1.41
24	c	510	CLA	C3D-C4D	-2.47	1.38	1.44
24	B	609	CLA	C4B-NB	-2.47	1.33	1.35
24	c	511	CLA	C1B-CHB	2.46	1.47	1.41
24	B	610	CLA	C1B-CHB	2.46	1.47	1.41
24	b	614	CLA	C4C-C3C	2.46	1.49	1.45
24	B	602	CLA	C4B-CHC	2.46	1.47	1.41
24	b	615	CLA	C4B-CHC	2.46	1.47	1.41
24	b	612	CLA	C4D-CHA	2.46	1.47	1.38
24	d	403	CLA	C4D-CHA	2.45	1.47	1.38
24	B	603	CLA	C4D-CHA	2.45	1.47	1.38
39	F	102	HEM	CHB-C1B	2.45	1.41	1.35
24	c	507	CLA	C4D-CHA	2.45	1.47	1.38
24	C	513	CLA	C4C-C3C	2.45	1.49	1.45
24	c	515	CLA	C1B-CHB	2.44	1.47	1.41
24	B	611	CLA	C1B-CHB	2.44	1.47	1.41
24	D	402	CLA	C1C-C2C	2.44	1.49	1.44
24	A	405	CLA	C3D-C4D	-2.43	1.38	1.44
36	c	524	HTG	C1-S1	-2.43	1.77	1.80
24	d	402	CLA	C3D-C4D	-2.43	1.38	1.44
24	B	609	CLA	C1B-CHB	2.43	1.47	1.41
24	b	616	CLA	C1B-CHB	2.43	1.47	1.41
24	C	504	CLA	C1C-C2C	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	C1B-CHB	2.43	1.47	1.41
36	b	633	HTG	C1-S1	-2.43	1.77	1.80
24	c	509	CLA	C4D-CHA	2.43	1.47	1.38
24	C	502	CLA	C4C-C3C	2.43	1.49	1.45
24	C	511	CLA	C1C-C2C	2.43	1.49	1.44
24	C	502	CLA	C1C-C2C	2.43	1.49	1.44
24	b	614	CLA	C4B-CHC	2.42	1.47	1.41
24	C	503	CLA	C4D-CHA	2.41	1.47	1.38
24	b	613	CLA	C4B-CHC	2.41	1.47	1.41
24	C	506	CLA	C3D-C4D	-2.41	1.38	1.44
24	a	412	CLA	C4B-CHC	2.41	1.47	1.41
24	C	502	CLA	C1B-CHB	2.41	1.47	1.41
24	c	512	CLA	C1B-CHB	2.41	1.47	1.41
24	D	403	CLA	C4D-CHA	2.41	1.47	1.38
24	a	409	CLA	C4D-CHA	2.41	1.47	1.38
24	B	608	CLA	C1C-C2C	2.41	1.49	1.44
24	B	615	CLA	C4B-CHC	2.41	1.47	1.41
24	b	617	CLA	C1B-CHB	2.41	1.47	1.41
24	c	510	CLA	C4D-CHA	2.41	1.47	1.38
24	b	620	CLA	C1B-CHB	2.40	1.47	1.41
24	c	509	CLA	C1C-C2C	2.40	1.49	1.44
24	C	508	CLA	C3D-C4D	-2.40	1.38	1.44
24	B	609	CLA	C1C-C2C	2.40	1.49	1.44
24	c	510	CLA	C1B-CHB	2.40	1.47	1.41
24	c	511	CLA	C4B-CHC	2.40	1.47	1.41
36	V	207	HTG	C1-S1	-2.40	1.77	1.80
24	B	606	CLA	C4D-CHA	2.40	1.46	1.38
24	b	620	CLA	C4D-CHA	2.40	1.46	1.38
24	C	512	CLA	C4B-CHC	2.39	1.47	1.41
24	c	507	CLA	C3D-C4D	-2.39	1.38	1.44
24	B	603	CLA	C1C-C2C	2.39	1.49	1.44
24	B	611	CLA	C4B-CHC	2.39	1.47	1.41
24	b	611	CLA	C4B-CHC	2.39	1.47	1.41
24	b	624	CLA	C1B-CHB	2.39	1.47	1.41
24	B	615	CLA	C3D-C4D	-2.38	1.38	1.44
24	B	604	CLA	C1B-CHB	2.38	1.47	1.41
24	b	617	CLA	C1C-C2C	2.38	1.49	1.44
24	b	625	CLA	C1B-CHB	2.37	1.47	1.41
24	b	623	CLA	C1C-C2C	2.37	1.49	1.44
24	B	605	CLA	C4C-C3C	2.37	1.49	1.45
24	b	615	CLA	C3D-C4D	-2.36	1.38	1.44
24	B	613	CLA	C4C-C3C	2.36	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C4B-CHC	2.36	1.47	1.41
36	b	608	HTG	C1-S1	-2.36	1.77	1.80
24	b	623	CLA	C3D-C4D	-2.36	1.38	1.44
24	c	517	CLA	C3D-C4D	-2.36	1.38	1.44
24	a	409	CLA	C3D-C4D	-2.36	1.38	1.44
25	a	411	PHO	C3A-C2A	-2.36	1.52	1.54
24	C	502	CLA	C4B-CHC	2.35	1.47	1.41
24	b	619	CLA	C3D-C4D	-2.35	1.38	1.44
24	d	402	CLA	C1B-NB	-2.35	1.33	1.35
24	B	609	CLA	C4C-C3C	2.35	1.49	1.45
24	C	513	CLA	C3D-C4D	-2.35	1.38	1.44
24	c	506	CLA	C4B-CHC	2.35	1.47	1.41
24	c	506	CLA	C3D-C4D	-2.35	1.38	1.44
25	A	409[A]	PHO	C3A-C2A	-2.35	1.52	1.54
24	C	510	CLA	C4B-CHC	2.35	1.47	1.41
24	B	610	CLA	C4B-CHC	2.35	1.47	1.41
24	B	614	CLA	C1B-CHB	2.34	1.47	1.41
24	d	401	CLA	C1C-C2C	2.34	1.49	1.44
24	b	622	CLA	C4B-CHC	2.34	1.47	1.41
24	B	616	CLA	C3D-C4D	-2.34	1.38	1.44
24	a	410	CLA	C1B-CHB	2.34	1.47	1.41
25	a	420[A]	PHO	C3A-C2A	-2.34	1.52	1.54
24	c	512	CLA	C3D-C4D	-2.34	1.38	1.44
24	C	503	CLA	C4C-C3C	2.33	1.49	1.45
24	A	405	CLA	C4B-CHC	2.33	1.47	1.41
37	h	102	DGD	O5D-C1E	2.33	1.44	1.40
24	c	506	CLA	C1B-CHB	2.33	1.47	1.41
24	c	507	CLA	C1B-CHB	2.33	1.47	1.41
24	B	604	CLA	C3D-C4D	-2.33	1.38	1.44
24	B	608	CLA	C1B-CHB	2.33	1.47	1.41
24	C	505	CLA	C4C-C3C	2.33	1.49	1.45
36	d	411	HTG	C1-S1	-2.33	1.77	1.80
24	a	409	CLA	C1B-CHB	2.33	1.47	1.41
24	d	401	CLA	C3D-C4D	-2.33	1.38	1.44
24	B	603	CLA	C3D-C4D	-2.32	1.38	1.44
24	c	508	CLA	C4C-C3C	2.32	1.49	1.45
24	B	604	CLA	C4C-C3C	2.32	1.49	1.45
24	B	603	CLA	C4B-CHC	2.32	1.47	1.41
24	b	618	CLA	C1C-C2C	2.32	1.49	1.44
36	B	632	HTG	C1-S1	-2.32	1.77	1.80
24	a	412	CLA	C4C-C3C	2.32	1.49	1.45
24	B	602	CLA	C1C-C2C	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	C1B-NB	-2.31	1.33	1.35
24	C	510	CLA	C1C-C2C	2.31	1.49	1.44
24	c	509	CLA	C4B-CHC	2.31	1.47	1.41
24	c	513	CLA	C4C-C3C	2.31	1.49	1.45
24	B	607	CLA	C3D-C4D	-2.30	1.39	1.44
24	D	403	CLA	C4C-C3C	2.30	1.49	1.45
24	A	406	CLA	C1B-CHB	2.30	1.47	1.41
24	b	618	CLA	C3D-C4D	-2.30	1.39	1.44
24	b	617	CLA	C1B-NB	-2.29	1.33	1.35
24	d	401	CLA	C4D-CHA	2.29	1.46	1.38
36	c	525	HTG	C1-S1	-2.29	1.77	1.80
24	B	610	CLA	C4C-C3C	2.29	1.49	1.45
24	B	612	CLA	C4C-C3C	2.29	1.49	1.45
24	b	613	CLA	C1B-CHB	2.29	1.47	1.41
24	c	508	CLA	C3D-C4D	-2.29	1.39	1.44
36	b	609	HTG	C1-S1	-2.28	1.77	1.80
24	D	402	CLA	C4D-CHA	2.28	1.46	1.38
24	c	513	CLA	C4B-CHC	2.28	1.47	1.41
24	d	402	CLA	C4B-CHC	2.28	1.47	1.41
24	c	508	CLA	C4B-CHC	2.28	1.47	1.41
24	A	410	CLA	C3D-C4D	-2.28	1.39	1.44
24	b	612	CLA	C4B-CHC	2.28	1.47	1.41
24	B	616	CLA	C1B-CHB	2.28	1.47	1.41
24	c	513	CLA	C3D-C4D	-2.28	1.39	1.44
24	B	610	CLA	C1C-C2C	2.27	1.49	1.44
24	a	409	CLA	C4B-CHC	2.27	1.47	1.41
24	b	619	CLA	C4B-CHC	2.27	1.47	1.41
24	C	501	CLA	C1B-CHB	2.27	1.47	1.41
24	B	607	CLA	C1B-CHB	2.27	1.47	1.41
24	b	618	CLA	C4C-C3C	2.27	1.48	1.45
24	b	624	CLA	C4D-CHA	2.27	1.46	1.38
24	C	503	CLA	C3D-C4D	-2.27	1.39	1.44
24	D	402	CLA	C4B-CHC	2.27	1.47	1.41
24	B	606	CLA	C3D-C4D	-2.26	1.39	1.44
24	D	403	CLA	C4B-CHC	2.26	1.47	1.41
24	B	605	CLA	C4B-CHC	2.26	1.47	1.41
24	b	621	CLA	C4C-C3C	2.26	1.48	1.45
24	b	626	CLA	C1C-NC	-2.26	1.34	1.37
24	C	507	CLA	C1B-CHB	2.26	1.47	1.41
24	B	611	CLA	C3D-C4D	-2.26	1.39	1.44
24	b	626	CLA	C4B-CHC	2.26	1.47	1.41
37	D	406	DGD	O3G-C1D	2.25	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	C3D-C4D	-2.24	1.39	1.44
24	B	603	CLA	C1B-CHB	2.24	1.47	1.41
39	V	206	HEM	CHB-C1B	2.24	1.40	1.35
24	C	510	CLA	C4C-C3C	2.24	1.48	1.45
24	B	607	CLA	C4B-CHC	2.23	1.47	1.41
24	C	501	CLA	C3D-C4D	-2.23	1.39	1.44
24	b	625	CLA	C4B-CHC	2.23	1.47	1.41
24	C	503	CLA	C1B-CHB	2.23	1.47	1.41
36	C	522	HTG	C1-S1	-2.23	1.77	1.80
24	b	611	CLA	C1B-CHB	2.23	1.47	1.41
24	c	517	CLA	C4C-C3C	2.23	1.48	1.45
24	c	510	CLA	C4B-CHC	2.23	1.47	1.41
24	b	612	CLA	C1B-CHB	2.23	1.47	1.41
24	C	513	CLA	C1B-CHB	2.22	1.47	1.41
24	b	619	CLA	C1C-C2C	2.22	1.48	1.44
24	B	609	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	612	CLA	C3D-C4D	-2.22	1.39	1.44
24	b	613	CLA	C4C-C3C	2.21	1.48	1.45
39	V	206	HEM	C1D-ND	-2.21	1.34	1.38
24	b	613	CLA	C3D-C4D	-2.20	1.39	1.44
24	C	501	CLA	C4C-C3C	2.20	1.48	1.45
24	c	511	CLA	C3D-C4D	-2.20	1.39	1.44
39	e	102	HEM	C3B-C4B	2.20	1.49	1.44
24	b	620	CLA	C1C-C2C	2.20	1.48	1.44
24	b	616	CLA	C4B-CHC	2.20	1.47	1.41
24	C	502	CLA	C3D-C4D	-2.19	1.39	1.44
24	A	407	CLA	C4C-C3C	2.19	1.48	1.45
24	C	504	CLA	C1B-NB	-2.19	1.33	1.35
25	A	408	PHO	C3A-C2A	-2.19	1.52	1.54
24	b	624	CLA	C3D-C4D	-2.19	1.39	1.44
24	c	505	CLA	C1C-C2C	2.19	1.48	1.44
24	b	625	CLA	C3D-C4D	-2.18	1.39	1.44
24	b	616	CLA	C4C-C3C	2.18	1.48	1.45
25	a	411	PHO	CBD-CGD	-2.18	1.49	1.52
25	A	409[B]	PHO	C3A-C2A	-2.18	1.52	1.54
24	B	605	CLA	C1A-CHA	2.18	1.52	1.43
24	d	403	CLA	C3D-C4D	-2.18	1.39	1.44
24	C	508	CLA	C1B-CHB	2.17	1.47	1.41
24	b	614	CLA	C3D-C4D	-2.17	1.39	1.44
24	c	512	CLA	C1C-C2C	2.17	1.48	1.44
24	B	614	CLA	C4B-CHC	2.17	1.47	1.41
24	b	611	CLA	C3D-C4D	-2.17	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	CLA	C3D-C4D	-2.17	1.39	1.44
24	C	512	CLA	C4C-C3C	2.16	1.48	1.45
24	c	512	CLA	C4B-CHC	2.16	1.47	1.41
24	d	401	CLA	C4B-CHC	2.15	1.47	1.41
24	b	626	CLA	C4C-C3C	2.15	1.48	1.45
24	b	611	CLA	C1C-C2C	2.15	1.48	1.44
24	c	505	CLA	C3D-C4D	-2.15	1.39	1.44
24	c	516	CLA	C3D-C4D	-2.15	1.39	1.44
24	c	514	CLA	C1C-C2C	2.15	1.48	1.44
24	c	517	CLA	C1B-CHB	2.15	1.47	1.41
24	C	504	CLA	C4B-CHC	2.14	1.46	1.41
24	c	506	CLA	C1C-NC	-2.14	1.34	1.37
24	A	406	CLA	C4C-C3C	2.14	1.48	1.45
24	C	508	CLA	C4B-CHC	2.14	1.46	1.41
24	B	606	CLA	C1B-CHB	2.14	1.46	1.41
24	b	622	CLA	C1C-NC	-2.13	1.34	1.37
24	C	504	CLA	C4C-C3C	2.13	1.48	1.45
24	D	403	CLA	C3D-C4D	-2.13	1.39	1.44
24	d	401	CLA	C1C-NC	-2.13	1.34	1.37
24	c	516	CLA	C1B-CHB	2.13	1.46	1.41
24	c	510	CLA	C1C-C2C	2.13	1.48	1.44
29	a	404	LMT	O1'-C1'	2.13	1.43	1.40
24	c	508	CLA	C1B-NB	-2.13	1.33	1.35
36	B	625	HTG	C1-S1	-2.12	1.77	1.80
36	B	633	HTG	C1-S1	-2.12	1.77	1.80
32	D	405[B]	PL9	C2-C3	2.12	1.40	1.34
24	B	612	CLA	C3D-C4D	-2.11	1.39	1.44
24	b	616	CLA	C3D-C4D	-2.11	1.39	1.44
24	b	625	CLA	C1C-C2C	2.11	1.48	1.44
39	e	102	HEM	CHB-C1B	2.11	1.40	1.35
36	C	523	HTG	C1-S1	-2.11	1.77	1.80
24	C	506	CLA	C1C-C2C	2.11	1.48	1.44
24	B	617	CLA	C4C-C3C	2.11	1.48	1.45
24	c	512	CLA	C4C-C3C	2.11	1.48	1.45
24	c	514	CLA	C4B-CHC	2.10	1.46	1.41
24	C	506	CLA	C4B-CHC	2.10	1.46	1.41
24	b	624	CLA	C4B-CHC	2.10	1.46	1.41
24	A	406	CLA	C4B-CHC	2.10	1.46	1.41
24	b	625	CLA	C4C-C3C	2.09	1.48	1.45
37	H	103	DGD	O5D-C1E	2.09	1.43	1.40
24	A	406	CLA	C1C-C2C	2.09	1.48	1.44
39	v	205	HEM	C3B-C4B	2.08	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	410	CLA	C3D-C4D	-2.08	1.39	1.44
24	D	402	CLA	C1B-NB	-2.08	1.33	1.35
39	v	205	HEM	CHB-C1B	2.07	1.40	1.35
24	B	608	CLA	C1D-C2D	2.07	1.49	1.45
24	b	612	CLA	C1D-C2D	2.07	1.49	1.45
24	b	626	CLA	C1D-C2D	2.07	1.49	1.45
24	C	504	CLA	C3D-C4D	-2.07	1.39	1.44
24	C	509	CLA	C3D-C4D	-2.07	1.39	1.44
24	C	507	CLA	C4C-C3C	2.07	1.48	1.45
32	D	405[A]	PL9	C2-C3	2.06	1.40	1.34
24	b	620	CLA	C3D-C4D	-2.06	1.39	1.44
24	c	515	CLA	C1C-C2C	2.06	1.48	1.44
24	C	512	CLA	C3D-C4D	-2.06	1.39	1.44
24	d	403	CLA	C1D-C2D	2.05	1.49	1.45
24	b	626	CLA	C3D-C4D	-2.05	1.39	1.44
24	B	617	CLA	C1C-C2C	2.05	1.48	1.44
24	B	609	CLA	C4B-CHC	2.05	1.46	1.41
24	A	407	CLA	C1B-CHB	2.05	1.46	1.41
32	d	405[B]	PL9	C2-C3	2.05	1.40	1.34
24	c	516	CLA	C4C-C3C	2.05	1.48	1.45
32	d	405[A]	PL9	C2-C3	2.05	1.40	1.34
29	M	103	LMT	O1'-C1'	2.05	1.43	1.40
24	c	515	CLA	C3D-C4D	-2.05	1.39	1.44
24	d	401	CLA	C4C-C3C	2.04	1.48	1.45
38	d	406	LHG	O7-C5	-2.04	1.41	1.46
24	b	623	CLA	C4B-CHC	2.04	1.46	1.41
32	a	416[B]	PL9	C2-C3	2.04	1.40	1.34
24	b	621	CLA	C3D-C4D	-2.04	1.39	1.44
24	c	506	CLA	C4C-C3C	2.04	1.48	1.45
24	D	403	CLA	C1D-C2D	2.03	1.49	1.45
32	a	416[A]	PL9	C2-C3	2.03	1.40	1.34
24	c	505	CLA	C4B-CHC	2.03	1.46	1.41
24	c	515	CLA	C4B-CHC	2.02	1.46	1.41
24	a	410	CLA	C4C-C3C	2.02	1.48	1.45
24	C	511	CLA	C3D-C4D	-2.02	1.39	1.44
32	A	420[B]	PL9	C2-C3	2.01	1.39	1.34
24	B	616	CLA	C4C-C3C	2.01	1.48	1.45
24	c	515	CLA	C4C-C3C	2.01	1.48	1.45
24	c	510	CLA	C4C-C3C	2.01	1.48	1.45
24	B	611	CLA	C4B-NB	-2.01	1.33	1.35
24	B	611	CLA	C1D-C2D	2.01	1.49	1.45
39	v	205	HEM	C1D-C2D	2.00	1.48	1.44

All (2644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	C1D-ND-C4D	-10.41	98.94	106.33
24	a	410	CLA	C1D-ND-C4D	-10.25	99.06	106.33
24	B	613	CLA	C1D-ND-C4D	-10.11	99.15	106.33
24	B	606	CLA	C1D-ND-C4D	-9.96	99.26	106.33
24	C	503	CLA	C1D-ND-C4D	-9.86	99.33	106.33
24	A	407	CLA	C1D-ND-C4D	-9.75	99.41	106.33
24	d	403	CLA	C1D-ND-C4D	-9.74	99.41	106.33
24	B	616	CLA	C1D-ND-C4D	-9.73	99.42	106.33
24	a	412	CLA	C1D-ND-C4D	-9.71	99.44	106.33
24	B	612	CLA	C1D-ND-C4D	-9.66	99.47	106.33
24	c	507	CLA	C1D-ND-C4D	-9.64	99.49	106.33
24	B	608	CLA	C1D-ND-C4D	-9.59	99.52	106.33
24	D	403	CLA	C1D-ND-C4D	-9.57	99.54	106.33
24	b	621	CLA	C1D-ND-C4D	-9.55	99.55	106.33
24	B	602	CLA	C1D-ND-C4D	-9.54	99.56	106.33
24	b	619	CLA	C1D-ND-C4D	-9.49	99.59	106.33
24	B	603	CLA	C1D-ND-C4D	-9.47	99.61	106.33
24	c	515	CLA	C1D-ND-C4D	-9.45	99.62	106.33
24	c	517	CLA	C1D-ND-C4D	-9.42	99.64	106.33
24	A	406	CLA	C2D-C1D-ND	9.40	117.03	110.10
24	b	617	CLA	C1D-ND-C4D	-9.40	99.66	106.33
24	C	509	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	b	620	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	A	406	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	C	501	CLA	C1D-ND-C4D	-9.38	99.67	106.33
24	B	613	CLA	C2D-C1D-ND	9.34	116.98	110.10
24	C	512	CLA	C1D-ND-C4D	-9.33	99.71	106.33
24	D	402	CLA	C1D-ND-C4D	-9.26	99.76	106.33
24	d	401	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	b	624	CLA	C1D-ND-C4D	-9.24	99.77	106.33
24	c	514	CLA	C1D-ND-C4D	-9.19	99.81	106.33
24	b	613	CLA	C1D-ND-C4D	-9.18	99.81	106.33
24	C	511	CLA	C1D-ND-C4D	-9.16	99.83	106.33
24	c	508	CLA	C1D-ND-C4D	-9.13	99.85	106.33
24	B	604	CLA	C1D-ND-C4D	-9.11	99.86	106.33
24	A	410	CLA	C1D-ND-C4D	-9.10	99.87	106.33
24	B	615	CLA	C1D-ND-C4D	-9.09	99.88	106.33
24	C	513	CLA	C1D-ND-C4D	-9.05	99.91	106.33
24	c	510	CLA	C1D-ND-C4D	-9.04	99.91	106.33
24	B	607	CLA	C1D-ND-C4D	-9.04	99.92	106.33
24	c	513	CLA	C1D-ND-C4D	-9.01	99.93	106.33
24	b	612	CLA	C1D-ND-C4D	-9.01	99.94	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C1D-ND-C4D	-9.00	99.94	106.33
24	a	409	CLA	C1D-ND-C4D	-8.99	99.95	106.33
24	C	507	CLA	C1D-ND-C4D	-8.96	99.97	106.33
24	B	606	CLA	C2D-C1D-ND	8.95	116.70	110.10
24	c	516	CLA	C1D-ND-C4D	-8.93	99.99	106.33
24	b	625	CLA	C1D-ND-C4D	-8.92	100.00	106.33
24	b	616	CLA	C1D-ND-C4D	-8.92	100.00	106.33
24	b	611	CLA	C1D-ND-C4D	-8.91	100.00	106.33
24	C	504	CLA	C1D-ND-C4D	-8.91	100.00	106.33
24	B	605	CLA	C2D-C1D-ND	8.88	116.65	110.10
24	c	506	CLA	C1D-ND-C4D	-8.88	100.03	106.33
24	c	509	CLA	C1D-ND-C4D	-8.86	100.04	106.33
24	C	502	CLA	C1D-ND-C4D	-8.85	100.05	106.33
24	C	507	CLA	C2D-C1D-ND	8.80	116.59	110.10
24	b	618	CLA	C1D-ND-C4D	-8.76	100.11	106.33
24	b	626	CLA	C1D-ND-C4D	-8.73	100.14	106.33
24	d	402	CLA	C1D-ND-C4D	-8.68	100.17	106.33
24	b	615	CLA	C2D-C1D-ND	8.68	116.50	110.10
24	B	609	CLA	C1D-ND-C4D	-8.67	100.17	106.33
24	b	624	CLA	C2D-C1D-ND	8.65	116.48	110.10
24	B	612	CLA	C2D-C1D-ND	8.64	116.47	110.10
24	b	621	CLA	C2D-C1D-ND	8.64	116.47	110.10
24	a	412	CLA	C2D-C1D-ND	8.58	116.43	110.10
24	B	610	CLA	C1D-ND-C4D	-8.58	100.24	106.33
24	b	623	CLA	C1D-ND-C4D	-8.54	100.27	106.33
24	C	504	CLA	C2D-C1D-ND	8.54	116.39	110.10
24	C	505	CLA	C1D-ND-C4D	-8.52	100.28	106.33
24	a	410	CLA	C2D-C1D-ND	8.51	116.37	110.10
24	C	506	CLA	C1D-ND-C4D	-8.50	100.29	106.33
24	C	508	CLA	C1D-ND-C4D	-8.49	100.31	106.33
24	C	512	CLA	C2D-C1D-ND	8.46	116.34	110.10
24	b	622	CLA	C1D-ND-C4D	-8.46	100.33	106.33
24	d	403	CLA	C2D-C1D-ND	8.44	116.32	110.10
24	B	611	CLA	C1D-ND-C4D	-8.36	100.39	106.33
24	c	512	CLA	C1D-ND-C4D	-8.35	100.41	106.33
24	B	615	CLA	C2D-C1D-ND	8.34	116.25	110.10
24	c	505	CLA	C1D-ND-C4D	-8.32	100.43	106.33
24	B	617	CLA	C1D-ND-C4D	-8.29	100.44	106.33
24	B	608	CLA	C2D-C1D-ND	8.29	116.21	110.10
24	c	516	CLA	C2D-C1D-ND	8.28	116.21	110.10
24	c	511	CLA	C1D-ND-C4D	-8.27	100.46	106.33
24	C	510	CLA	C1D-ND-C4D	-8.25	100.47	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	C2D-C1D-ND	8.23	116.17	110.10
24	C	509	CLA	C2D-C1D-ND	8.13	116.09	110.10
24	B	616	CLA	C2D-C1D-ND	8.13	116.09	110.10
24	B	602	CLA	C2D-C1D-ND	8.13	116.09	110.10
24	A	407	CLA	C2D-C1D-ND	8.12	116.09	110.10
24	D	403	CLA	C2D-C1D-ND	8.10	116.08	110.10
24	B	607	CLA	C2D-C1D-ND	8.09	116.06	110.10
24	b	614	CLA	C1D-ND-C4D	-8.09	100.59	106.33
24	A	405	CLA	C1D-ND-C4D	-8.08	100.59	106.33
24	c	506	CLA	C2D-C1D-ND	8.07	116.05	110.10
24	C	511	CLA	C2D-C1D-ND	8.07	116.05	110.10
24	b	620	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	b	622	CLA	C2D-C1D-ND	8.04	116.03	110.10
24	C	503	CLA	C2D-C1D-ND	8.03	116.02	110.10
24	b	617	CLA	C2D-C1D-ND	8.03	116.02	110.10
24	c	508	CLA	C2D-C1D-ND	8.00	116.00	110.10
24	c	511	CLA	C2D-C1D-ND	7.93	115.95	110.10
24	d	401	CLA	C2D-C1D-ND	7.93	115.95	110.10
24	b	619	CLA	C2D-C1D-ND	7.93	115.94	110.10
24	C	502	CLA	C2D-C1D-ND	7.91	115.93	110.10
24	c	505	CLA	C2D-C1D-ND	7.90	115.93	110.10
24	C	501	CLA	C2D-C1D-ND	7.88	115.91	110.10
24	b	614	CLA	C2D-C1D-ND	7.88	115.91	110.10
24	B	603	CLA	C2D-C1D-ND	7.82	115.86	110.10
24	b	623	CLA	C2D-C1D-ND	7.80	115.85	110.10
24	C	513	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	B	614	CLA	C2D-C1D-ND	7.78	115.84	110.10
24	c	515	CLA	C2D-C1D-ND	7.75	115.81	110.10
24	b	625	CLA	C2D-C1D-ND	7.74	115.81	110.10
24	c	513	CLA	C2D-C1D-ND	7.74	115.81	110.10
24	B	605	CLA	CMD-C2D-C1D	7.73	138.34	124.71
24	c	517	CLA	C2D-C1D-ND	7.72	115.79	110.10
25	a	420[A]	PHO	O2D-CGD-CBD	7.69	120.74	111.00
24	b	611	CLA	C2D-C1D-ND	7.69	115.77	110.10
24	A	410	CLA	C2D-C1D-ND	7.68	115.77	110.10
24	D	402	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	B	609	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	b	626	CLA	C2D-C1D-ND	7.65	115.74	110.10
24	b	616	CLA	C2D-C1D-ND	7.62	115.72	110.10
24	C	508	CLA	C2D-C1D-ND	7.60	115.70	110.10
24	B	617	CLA	C2D-C1D-ND	7.59	115.70	110.10
24	B	610	CLA	C2D-C1D-ND	7.56	115.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	C2D-C1D-ND	7.45	115.59	110.10
24	c	510	CLA	C2D-C1D-ND	7.44	115.59	110.10
24	B	604	CLA	C2D-C1D-ND	7.44	115.59	110.10
24	c	512	CLA	C2D-C1D-ND	7.44	115.59	110.10
24	b	612	CLA	C2D-C1D-ND	7.37	115.54	110.10
24	B	614	CLA	C1D-ND-C4D	-7.34	101.12	106.33
24	c	514	CLA	C2D-C1D-ND	7.32	115.50	110.10
24	a	409	CLA	CMD-C2D-C1D	7.32	137.61	124.71
24	B	606	CLA	CHD-C4C-C3C	-7.30	114.11	124.84
24	C	506	CLA	C2D-C1D-ND	7.27	115.46	110.10
24	b	615	CLA	CHD-C4C-C3C	-7.18	114.29	124.84
24	b	612	CLA	C4A-NA-C1A	-7.13	103.50	106.71
24	B	611	CLA	C2D-C1D-ND	7.12	115.35	110.10
24	d	402	CLA	C2D-C1D-ND	7.11	115.34	110.10
25	A	408	PHO	O2D-CGD-CBD	7.07	119.95	111.00
24	b	617	CLA	CMD-C2D-C1D	7.04	137.13	124.71
24	b	618	CLA	C2D-C1D-ND	7.01	115.27	110.10
24	A	405	CLA	C2D-C1D-ND	7.01	115.27	110.10
36	d	411	HTG	C1'-S1-C1	7.01	113.20	100.09
24	d	403	CLA	CMD-C2D-C1D	6.98	137.01	124.71
24	B	616	CLA	CMD-C2D-C1D	6.95	136.96	124.71
25	a	411	PHO	O2D-CGD-CBD	6.89	119.72	111.00
24	c	511	CLA	O2D-CGD-CBD	6.87	123.48	111.27
24	D	402	CLA	C2C-C1C-NC	6.87	116.41	109.97
24	C	510	CLA	C2D-C1D-ND	6.86	115.16	110.10
24	C	505	CLA	C4A-NA-C1A	-6.84	103.63	106.71
24	a	409	CLA	C2D-C1D-ND	6.84	115.14	110.10
24	d	402	CLA	C4A-NA-C1A	-6.83	103.64	106.71
24	c	509	CLA	C2D-C1D-ND	6.83	115.14	110.10
24	D	402	CLA	CMD-C2D-C1D	6.79	136.68	124.71
24	b	625	CLA	CMD-C2D-C1D	6.75	136.60	124.71
24	c	517	CLA	CMD-C2D-C1D	6.74	136.60	124.71
24	c	510	CLA	CMD-C2D-C1D	6.74	136.59	124.71
24	b	611	CLA	O2D-CGD-CBD	6.71	123.19	111.27
24	C	510	CLA	CMD-C2D-C1D	6.70	136.51	124.71
24	B	613	CLA	CHD-C4C-C3C	-6.69	115.00	124.84
24	C	505	CLA	C2D-C1D-ND	6.69	115.03	110.10
24	B	616	CLA	CHD-C4C-C3C	-6.69	115.01	124.84
25	a	420[B]	PHO	O2D-CGD-CBD	6.69	119.47	111.00
24	c	514	CLA	CMD-C2D-C1D	6.68	136.49	124.71
24	d	402	CLA	C2C-C1C-NC	6.63	116.19	109.97
24	C	504	CLA	CMD-C2D-C1D	6.63	136.40	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
24	b	617	CLA	CHD-C1D-ND	-6.58	118.41	124.45
24	b	614	CLA	C2C-C1C-NC	6.57	116.13	109.97
24	b	615	CLA	CHD-C1D-ND	-6.57	118.42	124.45
24	B	603	CLA	CMD-C2D-C1D	6.57	136.29	124.71
24	C	513	CLA	CMD-C2D-C1D	6.56	136.28	124.71
24	B	614	CLA	C2C-C1C-NC	6.55	116.10	109.97
24	b	612	CLA	CMD-C2D-C1D	6.52	136.21	124.71
24	C	501	CLA	O2D-CGD-CBD	6.51	122.83	111.27
24	c	508	CLA	CMD-C2D-C1D	6.51	136.18	124.71
24	A	407	CLA	CHD-C1D-ND	-6.50	118.48	124.45
24	b	625	CLA	C4A-NA-C1A	-6.49	103.79	106.71
25	A	409[A]	PHO	O2D-CGD-CBD	6.49	119.22	111.00
24	c	507	CLA	CMD-C2D-C1D	6.49	136.15	124.71
24	d	402	CLA	CMD-C2D-C1D	6.48	136.13	124.71
26	D	404	BCR	C7-C8-C9	-6.46	116.48	126.23
24	b	615	CLA	CMD-C2D-C1D	6.45	136.09	124.71
24	B	605	CLA	C2C-C1C-NC	6.45	116.02	109.97
24	B	605	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
24	D	403	CLA	CMD-C2D-C1D	6.44	136.06	124.71
24	c	516	CLA	C4A-NA-C1A	-6.44	103.81	106.71
24	C	513	CLA	CHD-C1D-ND	-6.43	118.54	124.45
24	c	510	CLA	CHD-C1D-ND	-6.41	118.56	124.45
24	B	603	CLA	CHD-C1D-ND	-6.41	118.56	124.45
24	b	614	CLA	CMD-C2D-C1D	6.41	136.01	124.71
24	b	617	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	B	602	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
24	C	504	CLA	CHD-C1D-ND	-6.36	118.61	124.45
24	b	611	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
24	A	405	CLA	C4A-NA-C1A	-6.36	103.85	106.71
24	B	608	CLA	CHD-C1D-ND	-6.35	118.62	124.45
24	C	507	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
24	D	402	CLA	CHD-C1D-ND	-6.34	118.63	124.45
24	B	610	CLA	CMD-C2D-C1D	6.34	135.88	124.71
24	C	506	CLA	CMD-C2D-C1D	6.32	135.86	124.71
24	B	615	CLA	CMD-C2D-C1D	6.32	135.85	124.71
24	d	401	CLA	CMD-C2D-C1D	6.32	135.85	124.71
24	B	616	CLA	CHD-C1D-ND	-6.28	118.68	124.45
24	A	406	CLA	C2C-C1C-NC	6.28	115.86	109.97
24	C	509	CLA	CMD-C2D-C1D	6.27	135.77	124.71
24	b	624	CLA	CMD-C2D-C1D	6.27	135.77	124.71
24	d	402	CLA	CHD-C1D-ND	-6.27	118.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	CHD-C1D-ND	-6.27	118.69	124.45
24	b	620	CLA	CMD-C2D-C1D	6.27	135.76	124.71
24	c	516	CLA	CHD-C4C-C3C	-6.25	115.65	124.84
25	A	409[B]	PHO	O2D-CGD-CBD	6.25	118.92	111.00
24	C	503	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
24	A	405	CLA	CMD-C2D-C1D	6.25	135.72	124.71
24	b	616	CLA	C4A-NA-C1A	-6.25	103.90	106.71
24	B	617	CLA	CHD-C4C-C3C	-6.24	115.66	124.84
24	C	508	CLA	CMD-C2D-C1D	6.24	135.70	124.71
36	C	522	HTG	C1'-S1-C1	6.23	111.75	100.09
24	b	611	CLA	CMD-C2D-C1D	6.22	135.68	124.71
24	B	610	CLA	C4A-NA-C1A	-6.22	103.91	106.71
24	c	509	CLA	C4A-NA-C1A	-6.21	103.91	106.71
24	a	410	CLA	CHD-C1D-ND	-6.21	118.75	124.45
24	d	401	CLA	C2C-C1C-NC	6.21	115.79	109.97
24	B	607	CLA	CMD-C2D-C1D	6.21	135.65	124.71
24	D	403	CLA	CHD-C1D-ND	-6.20	118.75	124.45
24	C	512	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
24	B	604	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
24	c	511	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	b	612	CLA	CHD-C1D-ND	-6.18	118.78	124.45
24	c	505	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	B	602	CLA	O2D-CGD-CBD	6.18	122.24	111.27
24	b	621	CLA	CMD-C2D-C1D	6.17	135.59	124.71
24	b	618	CLA	C4A-NA-C1A	-6.16	103.94	106.71
24	d	403	CLA	CHD-C1D-ND	-6.15	118.80	124.45
24	b	626	CLA	O2D-CGD-CBD	6.15	122.19	111.27
24	C	507	CLA	CMD-C2D-C1D	6.14	135.54	124.71
24	b	624	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
24	c	508	CLA	CHD-C1D-ND	-6.14	118.81	124.45
24	b	619	CLA	C4A-NA-C1A	-6.14	103.95	106.71
24	B	603	CLA	C4A-NA-C1A	-6.12	103.95	106.71
24	b	619	CLA	CMD-C2D-C1D	6.11	135.49	124.71
24	b	625	CLA	CHD-C1D-ND	-6.11	118.84	124.45
24	c	507	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
24	c	511	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
24	b	616	CLA	CMD-C2D-C1D	6.10	135.47	124.71
24	c	506	CLA	C4A-NA-C1A	-6.10	103.97	106.71
24	b	615	CLA	C4A-NA-C1A	-6.09	103.97	106.71
24	d	403	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
24	c	513	CLA	CMD-C2D-C1D	6.09	135.45	124.71
24	B	611	CLA	CMD-C2D-C1D	6.09	135.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	624	CLA	O2D-CGD-CBD	6.09	122.08	111.27
24	B	611	CLA	C2C-C1C-NC	6.08	115.67	109.97
24	C	501	CLA	CMD-C2D-C1D	6.08	135.44	124.71
24	a	410	CLA	CMD-C2D-C1D	6.08	135.43	124.71
24	b	619	CLA	CHD-C1D-ND	-6.08	118.87	124.45
24	b	614	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
24	c	509	CLA	C2C-C1C-NC	6.07	115.66	109.97
24	c	517	CLA	CHD-C1D-ND	-6.07	118.88	124.45
24	C	505	CLA	CMD-C2D-C1D	6.07	135.41	124.71
24	B	608	CLA	CMD-C2D-C1D	6.06	135.40	124.71
24	c	506	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
24	D	402	CLA	C4A-NA-C1A	-6.06	103.98	106.71
24	B	617	CLA	O2D-CGD-CBD	6.05	122.02	111.27
24	a	410	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
24	C	503	CLA	CMD-C2D-C1D	6.04	135.36	124.71
24	B	609	CLA	CMD-C2D-C1D	6.03	135.35	124.71
24	B	604	CLA	O2D-CGD-CBD	6.03	121.98	111.27
24	b	625	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	C	503	CLA	CHD-C1D-ND	-6.01	118.93	124.45
24	c	516	CLA	O2D-CGD-CBD	6.00	121.93	111.27
24	C	502	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	c	507	CLA	C4A-NA-C1A	-5.99	104.02	106.71
24	b	616	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
24	d	401	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
24	B	617	CLA	CMD-C2D-C1D	5.96	135.21	124.71
24	b	613	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
24	b	626	CLA	CMD-C2D-C1D	5.96	135.21	124.71
24	C	506	CLA	C2C-C1C-NC	5.96	115.55	109.97
24	b	614	CLA	O2D-CGD-CBD	5.95	121.85	111.27
24	B	610	CLA	CHD-C1D-ND	-5.95	118.98	124.45
24	B	609	CLA	C2C-C1C-NC	5.95	115.55	109.97
24	c	517	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	C	505	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
24	C	512	CLA	O2D-CGD-CBD	5.92	121.79	111.27
24	B	616	CLA	C4A-NA-C1A	-5.92	104.04	106.71
24	c	513	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
24	b	623	CLA	C2C-C1C-NC	5.91	115.51	109.97
24	A	410	CLA	CMD-C2D-C1D	5.91	135.12	124.71
24	B	602	CLA	CMD-C2D-C1D	5.90	135.12	124.71
24	B	610	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
24	B	602	CLA	CHD-C1D-ND	-5.90	119.03	124.45
24	C	501	CLA	CHD-C4C-C3C	-5.89	116.18	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	412	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
24	B	607	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	C	502	CLA	CMD-C2D-C1D	5.86	135.04	124.71
24	b	624	CLA	CHD-C1D-ND	-5.86	119.07	124.45
24	C	511	CLA	C2C-C1C-NC	5.86	115.46	109.97
24	b	619	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
24	B	607	CLA	CHD-C1D-ND	-5.85	119.08	124.45
24	c	514	CLA	CHD-C1D-ND	-5.85	119.08	124.45
24	C	510	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	c	508	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
24	A	406	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
24	b	611	CLA	CHD-C1D-ND	-5.84	119.09	124.45
24	b	620	CLA	CHD-C1D-ND	-5.84	119.09	124.45
24	b	621	CLA	C2C-C1C-NC	5.84	115.44	109.97
24	b	621	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
24	A	410	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	b	618	CLA	CMD-C2D-C1D	5.83	134.98	124.71
24	b	624	CLA	C2C-C1C-NC	5.82	115.43	109.97
24	c	508	CLA	C2C-C1C-NC	5.82	115.42	109.97
24	b	622	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
24	B	612	CLA	CMD-C2D-C1D	5.81	134.95	124.71
24	A	407	CLA	CMD-C2D-C1D	5.81	134.95	124.71
24	C	507	CLA	CHD-C1D-ND	-5.80	119.13	124.45
24	c	512	CLA	C4A-NA-C1A	-5.79	104.10	106.71
24	C	504	CLA	O2D-CGD-CBD	5.79	121.56	111.27
24	C	509	CLA	CHD-C1D-ND	-5.78	119.14	124.45
36	c	524	HTG	C1'-S1-C1	5.77	110.89	100.09
24	B	603	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
24	B	615	CLA	O2D-CGD-CBD	5.76	121.51	111.27
24	a	412	CLA	CMD-C2D-C1D	5.76	134.86	124.71
24	c	514	CLA	C2C-C1C-NC	5.76	115.37	109.97
24	c	505	CLA	CMD-C2D-C1D	5.75	134.85	124.71
24	C	503	CLA	C4A-NA-C1A	-5.75	104.12	106.71
24	B	612	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	B	615	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
24	a	412	CLA	C2C-C1C-NC	5.74	115.35	109.97
24	d	403	CLA	C4A-NA-C1A	-5.73	104.13	106.71
24	B	615	CLA	C2C-C1C-NC	5.72	115.33	109.97
24	B	615	CLA	CHD-C1D-ND	-5.72	119.20	124.45
24	B	609	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
24	C	508	CLA	O2D-CGD-CBD	5.70	121.39	111.27
24	b	623	CLA	CMD-C2D-C1D	5.70	134.75	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	O2D-CGD-CBD	5.69	121.39	111.27
24	B	613	CLA	O2D-CGD-CBD	5.69	121.38	111.27
24	A	405	CLA	C2C-C1C-NC	5.69	115.30	109.97
26	Y	101	BCR	C33-C5-C6	-5.69	118.14	124.53
24	c	515	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
24	B	604	CLA	C4A-NA-C1A	-5.69	104.15	106.71
24	b	622	CLA	C2C-C1C-NC	5.68	115.29	109.97
24	b	626	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
24	c	512	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
24	b	616	CLA	CHD-C1D-ND	-5.67	119.24	124.45
24	c	515	CLA	CHD-C1D-ND	-5.67	119.24	124.45
24	C	511	CLA	CHD-C1D-ND	-5.67	119.24	124.45
24	C	509	CLA	C2C-C1C-NC	5.66	115.28	109.97
24	a	409	CLA	C2C-C1C-NC	5.66	115.28	109.97
24	a	412	CLA	CHD-C1D-ND	-5.66	119.25	124.45
24	B	614	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
24	c	512	CLA	C2C-C1C-NC	5.66	115.27	109.97
36	b	633	HTG	C1'-S1-C1	5.65	110.67	100.09
24	b	619	CLA	C2C-C1C-NC	5.65	115.27	109.97
24	c	512	CLA	CMD-C2D-C1D	5.65	134.68	124.71
24	B	604	CLA	CMD-C2D-C1D	5.65	134.67	124.71
24	B	614	CLA	CMD-C2D-C1D	5.65	134.67	124.71
24	C	508	CLA	C2C-C1C-NC	5.65	115.26	109.97
24	b	618	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
24	c	509	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
24	C	509	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
24	B	606	CLA	CMD-C2D-C1D	5.62	134.61	124.71
24	c	505	CLA	O2D-CGD-CBD	5.61	121.24	111.27
24	c	509	CLA	O2D-CGD-CBD	5.61	121.24	111.27
24	A	405	CLA	CHD-C1D-ND	-5.61	119.30	124.45
24	c	507	CLA	CHD-C1D-ND	-5.60	119.31	124.45
24	b	620	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
24	C	506	CLA	CHD-C1D-ND	-5.59	119.31	124.45
24	b	623	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
24	c	510	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
24	A	407	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
24	d	401	CLA	CHD-C1D-ND	-5.58	119.33	124.45
24	C	508	CLA	CHD-C1D-ND	-5.58	119.33	124.45
24	B	615	CLA	C4A-NA-C1A	-5.57	104.20	106.71
24	C	507	CLA	O2D-CGD-CBD	5.57	121.16	111.27
24	c	515	CLA	CMD-C2D-C1D	5.56	134.52	124.71
24	C	504	CLA	C2C-C1C-NC	5.56	115.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
24	B	612	CLA	CHD-C1D-ND	-5.55	119.36	124.45
24	c	516	CLA	CMD-C2D-C1D	5.55	134.49	124.71
24	C	505	CLA	C2C-C1C-NC	5.54	115.16	109.97
24	A	406	CLA	CMD-C2D-C1D	5.54	134.47	124.71
24	C	511	CLA	CMD-C2D-C1D	5.54	134.47	124.71
36	B	633	HTG	C1'-S1-C1	5.52	110.41	100.09
24	b	626	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	A	407	CLA	C4A-NA-C1A	-5.51	104.23	106.71
24	B	611	CLA	CHD-C1D-ND	-5.51	119.39	124.45
24	b	621	CLA	CHD-C1D-ND	-5.50	119.39	124.45
24	c	511	CLA	CMD-C2D-C1D	5.50	134.41	124.71
24	B	607	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	C	508	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	B	617	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	b	613	CLA	CHD-C1D-ND	-5.50	119.40	124.45
24	c	514	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
24	c	505	CLA	CHD-C4C-C3C	-5.49	116.76	124.84
24	B	613	CLA	CMD-C2D-C1D	5.49	134.39	124.71
24	A	406	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
24	c	513	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	c	517	CLA	C4A-NA-C1A	-5.48	104.24	106.71
24	b	625	CLA	C2C-C1C-NC	5.48	115.11	109.97
36	C	523	HTG	C1'-S1-C1	5.47	110.33	100.09
24	C	513	CLA	C4A-NA-C1A	-5.47	104.25	106.71
24	B	605	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
24	c	506	CLA	CHD-C1D-ND	-5.45	119.45	124.45
24	b	613	CLA	CMD-C2D-C1D	5.44	134.31	124.71
24	B	603	CLA	C2C-C1C-NC	5.44	115.07	109.97
24	B	604	CLA	C2C-C1C-NC	5.43	115.06	109.97
24	C	504	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
24	C	506	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
24	b	613	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	C	513	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
24	b	616	CLA	C2C-C1C-NC	5.41	115.04	109.97
36	B	625	HTG	C1'-S1-C1	5.40	110.20	100.09
24	A	406	CLA	CHD-C1D-ND	-5.40	119.49	124.45
24	C	510	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	D	403	CLA	CHD-C4C-C3C	-5.39	116.91	124.84
24	C	512	CLA	CHD-C1D-ND	-5.39	119.50	124.45
24	C	508	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
39	F	102	HEM	CHC-C4B-NB	5.38	130.27	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	609	CLA	CHD-C1D-ND	-5.37	119.52	124.45
24	c	509	CLA	CMD-C2D-C1D	5.37	134.18	124.71
24	a	410	CLA	C4A-NA-C1A	-5.36	104.30	106.71
24	B	607	CLA	O2D-CGD-CBD	5.36	120.79	111.27
24	B	613	CLA	C3C-C4C-NC	5.36	116.58	110.57
24	c	511	CLA	CHD-C1D-ND	-5.35	119.54	124.45
24	b	611	CLA	C4A-NA-C1A	-5.34	104.30	106.71
24	B	608	CLA	C2C-C1C-NC	5.34	114.97	109.97
24	b	612	CLA	O2D-CGD-CBD	5.34	120.76	111.27
24	C	502	CLA	C2C-C1C-NC	5.34	114.97	109.97
36	c	525	HTG	C1'-S1-C1	5.34	110.07	100.09
24	B	617	CLA	C2C-C1C-NC	5.33	114.97	109.97
24	C	501	CLA	CHD-C1D-ND	-5.33	119.56	124.45
24	B	605	CLA	CHD-C1D-ND	-5.32	119.56	124.45
24	b	626	CLA	C4A-NA-C1A	-5.32	104.31	106.71
36	b	608	HTG	C1'-S1-C1	5.32	110.05	100.09
24	D	402	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
24	a	409	CLA	C4A-NA-C1A	-5.32	104.31	106.71
24	b	618	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	b	618	CLA	CHD-C1D-ND	-5.30	119.58	124.45
27	f	102	SQD	O47-C7-C8	5.30	122.92	111.50
24	b	613	CLA	O2D-CGD-CBD	5.29	120.68	111.27
36	B	625	HTG	O5-C1-C2	5.29	116.97	110.31
24	b	612	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	D	403	CLA	C4A-NA-C1A	-5.27	104.34	106.71
24	c	513	CLA	CHD-C1D-ND	-5.27	119.61	124.45
24	B	608	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	c	512	CLA	CHD-C1D-ND	-5.26	119.62	124.45
24	c	510	CLA	C2C-C1C-NC	5.26	114.90	109.97
24	B	609	CLA	O2D-CGD-CBD	5.26	120.61	111.27
24	B	607	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
24	b	617	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	c	505	CLA	CHD-C1D-ND	-5.24	119.64	124.45
24	C	513	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	C	502	CLA	CHD-C1D-ND	-5.23	119.64	124.45
24	B	604	CLA	CHD-C1D-ND	-5.23	119.65	124.45
24	a	409	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
24	B	612	CLA	C4A-NA-C1A	-5.21	104.36	106.71
24	c	516	CLA	CHD-C1D-ND	-5.19	119.69	124.45
24	C	501	CLA	C2C-C1C-NC	5.17	114.81	109.97
24	C	512	CLA	CMD-C2D-C1D	5.16	133.80	124.71
24	C	502	CLA	C4A-NA-C1A	-5.16	104.39	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	C4A-NA-C1A	-5.15	104.39	106.71
24	B	605	CLA	O2D-CGD-CBD	5.14	120.41	111.27
24	B	613	CLA	CHD-C1D-ND	-5.14	119.73	124.45
24	D	403	CLA	C2C-C1C-NC	5.12	114.77	109.97
27	b	601	SQD	O6-C1-C2	5.12	116.30	108.30
24	C	505	CLA	O2D-CGD-CBD	5.12	120.37	111.27
24	A	410	CLA	CHD-C1D-ND	-5.12	119.75	124.45
24	C	510	CLA	CHD-C1D-ND	-5.12	119.75	124.45
24	C	504	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
24	b	620	CLA	O2D-CGD-CBD	5.11	120.36	111.27
24	c	515	CLA	C2C-C1C-NC	5.09	114.74	109.97
26	t	101	BCR	C33-C5-C6	-5.08	118.82	124.53
24	C	507	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
24	B	611	CLA	O2D-CGD-CBD	5.08	120.29	111.27
24	B	608	CLA	O2D-CGD-CBD	5.07	120.27	111.27
24	b	624	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
39	F	102	HEM	CAD-CBD-CGD	5.05	124.46	113.60
24	c	512	CLA	O2D-CGD-CBD	5.04	120.23	111.27
24	b	620	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	b	620	CLA	C4A-NA-C1A	-5.04	104.44	106.71
36	b	633	HTG	O5-C1-C2	5.03	116.64	110.31
27	F	103	SQD	O47-C7-C8	5.02	122.33	111.50
24	C	512	CLA	C2C-C1C-NC	5.02	114.67	109.97
24	b	617	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	b	621	CLA	C4A-NA-C1A	-5.01	104.45	106.71
24	B	614	CLA	C3C-C4C-NC	5.00	116.18	110.57
24	C	510	CLA	C4A-NA-C1A	-4.97	104.47	106.71
25	A	409[A]	PHO	C1-C2-C3	-4.97	117.45	126.04
24	c	506	CLA	CMD-C2D-C1D	4.94	133.42	124.71
27	A	412	SQD	O47-C7-C8	4.94	122.15	111.50
24	b	614	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
24	b	614	CLA	C4A-NA-C1A	-4.93	104.49	106.71
24	B	610	CLA	C2C-C1C-NC	4.93	114.59	109.97
24	b	612	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	c	516	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	B	611	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
24	b	626	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	B	606	CLA	O2D-CGD-CBD	4.90	119.97	111.27
25	a	420[B]	PHO	C1-C2-C3	-4.90	117.57	126.04
24	A	406	CLA	O2D-CGD-CBD	4.90	119.97	111.27
24	A	406	CLA	C1C-C2C-C3C	-4.90	101.81	106.96
26	B	620	BCR	C15-C14-C13	-4.90	120.32	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	506	CLA	C2C-C1C-NC	4.89	114.56	109.97
24	A	410	CLA	C2C-C1C-NC	4.89	114.56	109.97
24	d	403	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	b	624	CLA	C4A-NA-C1A	-4.89	104.51	106.71
24	b	615	CLA	C3D-C4D-ND	4.89	118.14	110.24
24	A	407	CLA	C2C-C1C-NC	4.88	114.54	109.97
24	B	613	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
27	B	621	SQD	O6-C1-C2	4.86	115.89	108.30
24	b	614	CLA	C3C-C4C-NC	4.86	116.02	110.57
24	B	606	CLA	CHD-C1D-ND	-4.86	119.99	124.45
24	d	403	CLA	C2C-C1C-NC	4.86	114.52	109.97
24	b	623	CLA	C4A-NA-C1A	-4.85	104.53	106.71
24	C	510	CLA	O2D-CGD-CBD	4.85	119.88	111.27
27	B	621	SQD	O47-C7-C8	4.84	121.94	111.50
24	C	503	CLA	C2C-C1C-NC	4.84	114.50	109.97
24	B	615	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	D	403	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
24	B	602	CLA	C2C-C1C-NC	4.83	114.50	109.97
24	b	615	CLA	C3C-C4C-NC	4.83	115.99	110.57
24	B	613	CLA	C2C-C1C-NC	4.83	114.50	109.97
24	C	507	CLA	C2C-C1C-NC	4.83	114.50	109.97
24	b	623	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
24	b	614	CLA	CHD-C1D-ND	-4.82	120.02	124.45
24	C	512	CLA	C4A-NA-C1A	-4.82	104.54	106.71
24	B	606	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	b	616	CLA	O2D-CGD-CBD	4.82	119.83	111.27
36	H	101	HTG	C1'-S1-C1	4.81	109.08	100.09
24	C	506	CLA	O2D-CGD-CBD	4.80	119.81	111.27
24	c	513	CLA	O2D-CGD-CBD	4.79	119.78	111.27
24	b	617	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	B	612	CLA	C3C-C4C-NC	4.78	115.94	110.57
24	b	613	CLA	C4A-NA-C1A	-4.78	104.56	106.71
24	b	615	CLA	C2C-C1C-NC	4.78	114.45	109.97
24	c	507	CLA	C2C-C1C-NC	4.78	114.45	109.97
25	a	420[A]	PHO	C1-C2-C3	-4.78	117.78	126.04
24	c	505	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	A	405	CLA	CHD-C4C-C3C	-4.78	117.82	124.84
24	b	622	CLA	C3C-C4C-NC	4.77	115.92	110.57
24	d	401	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
36	B	624	HTG	C1'-S1-C1	4.77	109.01	100.09
39	V	206	HEM	C1B-NB-C4B	4.77	110.00	105.07
24	B	607	CLA	C3D-C2D-C1D	-4.77	99.33	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C3C-C4C-NC	4.76	115.91	110.57
24	A	407	CLA	C3D-C4D-ND	4.76	117.94	110.24
27	a	414	SQD	O6-C1-C2	4.76	115.73	108.30
24	B	612	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
24	C	509	CLA	C1-C2-C3	-4.76	117.82	126.04
24	c	510	CLA	C4A-NA-C1A	-4.75	104.57	106.71
24	c	509	CLA	CHD-C1D-ND	-4.75	120.09	124.45
24	c	517	CLA	C2C-C1C-NC	4.74	114.42	109.97
36	b	632	HTG	C1'-S1-C1	4.74	108.97	100.09
24	a	410	CLA	C3D-C4D-ND	4.74	117.91	110.24
24	c	514	CLA	O2D-CGD-CBD	4.74	119.69	111.27
24	C	508	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
36	C	523	HTG	C1-O5-C5	4.73	121.30	112.58
24	C	501	CLA	C4A-NA-C1A	-4.73	104.58	106.71
27	b	601	SQD	O47-C7-C8	4.73	121.69	111.50
37	e	101	DGD	O6E-C5E-C4E	4.72	118.27	109.69
24	C	502	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
24	B	614	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
24	C	505	CLA	CHD-C1D-ND	-4.70	120.13	124.45
24	a	410	CLA	O2D-CGD-CBD	4.70	119.62	111.27
24	c	508	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	B	608	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
24	A	407	CLA	O2D-CGD-CBD	4.68	119.59	111.27
24	b	623	CLA	CHD-C1D-ND	-4.68	120.15	124.45
24	b	613	CLA	C3C-C4C-NC	4.68	115.82	110.57
24	C	506	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	b	621	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	d	402	CLA	CHD-C4C-C3C	-4.67	117.98	124.84
24	c	511	CLA	C3D-C2D-C1D	-4.66	99.46	105.83
24	C	513	CLA	C3D-C2D-C1D	-4.66	99.46	105.83
25	A	409[B]	PHO	C1-C2-C3	-4.66	117.97	126.04
24	c	506	CLA	O2D-CGD-CBD	4.66	119.55	111.27
24	B	616	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	B	603	CLA	O2D-CGD-CBD	4.66	119.54	111.27
24	a	412	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
26	T	103	BCR	C33-C5-C6	-4.65	119.31	124.53
24	b	625	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	A	410	CLA	C4A-NA-C1A	-4.65	104.62	106.71
24	B	610	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	606	CLA	C1D-CHD-C4C	-4.64	116.05	126.06
24	a	412	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	c	515	CLA	C3D-C4D-ND	4.64	117.74	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	617	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	b	611	CLA	C2C-C1C-NC	4.63	114.31	109.97
24	b	622	CLA	O2D-CGD-CBD	4.63	119.49	111.27
24	C	512	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
24	c	507	CLA	O2D-CGD-CBD	4.62	119.47	111.27
24	b	615	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
34	a	415	LMG	O7-C10-C11	4.61	121.44	111.50
37	C	516	DGD	O2G-C1B-C2B	4.61	121.44	111.50
24	c	511	CLA	C3C-C4C-NC	4.61	115.74	110.57
24	c	507	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	c	507	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	C	503	CLA	C3D-C4D-ND	4.60	117.68	110.24
24	D	402	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
34	A	422	LMG	O7-C10-C11	4.58	121.38	111.50
24	B	616	CLA	C2C-C1C-NC	4.57	114.25	109.97
24	b	619	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
34	c	523	LMG	O7-C10-C11	4.57	121.35	111.50
24	C	509	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	D	403	CLA	O2D-CGD-CBD	4.57	119.38	111.27
24	B	617	CLA	CHD-C1D-ND	-4.57	120.26	124.45
24	c	516	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	B	606	CLA	C3C-C4C-NC	4.55	115.67	110.57
24	b	620	CLA	C3D-C4D-ND	4.54	117.59	110.24
24	B	602	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
24	b	619	CLA	C3D-C4D-ND	4.54	117.58	110.24
24	c	509	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	b	612	CLA	C3D-C4D-ND	4.53	117.57	110.24
24	C	511	CLA	O2D-CGD-CBD	4.53	119.33	111.27
24	C	501	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	d	401	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
24	d	402	CLA	C3D-C4D-ND	4.53	117.56	110.24
24	b	620	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	c	506	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	c	513	CLA	C4A-NA-C1A	-4.52	104.67	106.71
24	C	505	CLA	C3C-C4C-NC	4.51	115.63	110.57
24	c	506	CLA	C3C-C4C-NC	4.51	115.63	110.57
24	B	603	CLA	C3D-C4D-ND	4.51	117.53	110.24
24	b	622	CLA	C4A-NA-C1A	-4.50	104.68	106.71
24	C	503	CLA	C3C-C4C-NC	4.50	115.62	110.57
24	A	407	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	B	606	CLA	C2C-C1C-NC	4.50	114.19	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	e	101	DGD	O2G-C1B-C2B	4.50	121.20	111.50
24	D	402	CLA	C3D-C4D-ND	4.50	117.51	110.24
24	b	613	CLA	C3D-C4D-ND	4.50	117.51	110.24
24	a	410	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	b	611	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
34	C	520	LMG	O7-C10-C11	4.49	121.17	111.50
24	b	616	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	b	614	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
24	C	507	CLA	C4A-NA-C1A	-4.48	104.69	106.71
24	c	512	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	B	602	CLA	C3D-C4D-ND	4.47	117.47	110.24
24	c	514	CLA	C3D-C4D-ND	4.47	117.47	110.24
24	c	517	CLA	C3D-C4D-ND	4.47	117.46	110.24
24	B	611	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
24	B	617	CLA	C3C-C4C-NC	4.46	115.58	110.57
24	c	509	CLA	C3D-C4D-ND	4.46	117.46	110.24
24	a	412	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
24	c	513	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
24	B	606	CLA	C3D-C4D-ND	4.46	117.45	110.24
24	B	604	CLA	C3D-C4D-ND	4.46	117.45	110.24
24	c	507	CLA	C3D-C4D-ND	4.46	117.45	110.24
24	C	502	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	B	611	CLA	C4A-NA-C1A	-4.45	104.70	106.71
24	c	517	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	B	616	CLA	C3C-C4C-NC	4.44	115.56	110.57
24	B	609	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
24	d	403	CLA	O2D-CGD-CBD	4.43	119.15	111.27
24	D	402	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
24	b	624	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	B	615	CLA	O2D-CGD-O1D	-4.43	115.18	123.84
24	C	503	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
24	A	410	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
26	b	627	BCR	C33-C5-C6	-4.42	119.57	124.53
24	b	626	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
24	B	609	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
24	c	505	CLA	C3C-C4C-NC	4.41	115.52	110.57
24	d	403	CLA	C3D-C4D-ND	4.41	117.37	110.24
24	B	613	CLA	C3D-C4D-ND	4.40	117.36	110.24
24	b	617	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
24	B	606	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	C	501	CLA	C3D-C4D-ND	4.40	117.36	110.24
24	C	504	CLA	C4A-NA-C1A	-4.40	104.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	c	521	DGD	O2G-C1B-C2B	4.39	120.97	111.50
24	D	403	CLA	C3D-C4D-ND	4.39	117.34	110.24
24	C	508	CLA	C3C-C4C-NC	4.39	115.49	110.57
24	C	511	CLA	C3D-C4D-ND	4.39	117.33	110.24
24	d	401	CLA	C3D-C4D-ND	4.39	117.33	110.24
24	C	506	CLA	C4A-NA-C1A	-4.39	104.73	106.71
24	B	604	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
39	v	205	HEM	CHC-C4B-NB	4.38	129.19	124.43
29	A	417	LMT	C1'-O5'-C5'	4.38	122.28	113.69
24	C	507	CLA	C3C-C4C-NC	4.38	115.48	110.57
36	B	632	HTG	C1'-S1-C1	4.37	108.27	100.09
26	B	618	BCR	C33-C5-C6	-4.37	119.62	124.53
24	b	617	CLA	C3D-C4D-ND	4.37	117.31	110.24
24	a	412	CLA	C3D-C4D-ND	4.37	117.30	110.24
24	c	508	CLA	C3C-C4C-NC	4.36	115.47	110.57
26	D	404	BCR	C33-C5-C6	-4.36	119.63	124.53
24	b	623	CLA	C3B-C4B-NB	4.36	114.85	109.21
24	A	406	CLA	C3B-C4B-NB	4.36	114.85	109.21
27	a	405	SQD	O8-S-C6	4.36	112.68	105.74
24	C	510	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
24	B	603	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
24	b	619	CLA	O2D-CGD-CBD	4.34	118.98	111.27
24	A	410	CLA	O2D-CGD-CBD	4.34	118.98	111.27
24	C	509	CLA	O2D-CGD-CBD	4.34	118.98	111.27
24	B	608	CLA	C3D-C4D-ND	4.34	117.25	110.24
24	B	612	CLA	C3D-C4D-ND	4.34	117.25	110.24
24	B	614	CLA	CHD-C1D-ND	-4.33	120.47	124.45
24	b	615	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	b	622	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
24	d	402	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
24	b	611	CLA	C3D-C4D-ND	4.33	117.24	110.24
24	A	405	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
24	C	512	CLA	C3D-C4D-ND	4.32	117.23	110.24
24	A	410	CLA	C3C-C4C-NC	4.32	115.42	110.57
24	b	612	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
24	C	511	CLA	C3B-C4B-NB	4.32	114.79	109.21
24	c	510	CLA	C3D-C4D-ND	4.32	117.22	110.24
24	B	616	CLA	C3D-C4D-ND	4.31	117.21	110.24
24	c	511	CLA	C4A-NA-C1A	-4.31	104.77	106.71
24	a	409	CLA	C3D-C4D-ND	4.30	117.20	110.24
24	C	502	CLA	C1-C2-C3	-4.30	118.61	126.04
36	B	623	HTG	C1'-S1-C1	4.30	108.13	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C4A-NA-C1A	-4.30	104.77	106.71
24	c	515	CLA	C4A-NA-C1A	-4.30	104.77	106.71
24	A	410	CLA	C3D-C4D-ND	4.30	117.19	110.24
24	c	517	CLA	O2D-CGD-CBD	4.30	118.90	111.27
24	B	604	CLA	O2D-CGD-O1D	-4.29	115.45	123.84
24	b	621	CLA	O2D-CGD-CBD	4.29	118.88	111.27
24	B	615	CLA	C3C-C4C-NC	4.28	115.38	110.57
24	a	409	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
24	C	509	CLA	C3D-C4D-ND	4.26	117.14	110.24
24	c	514	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	b	621	CLA	C3D-C4D-ND	4.26	117.12	110.24
24	d	401	CLA	O2D-CGD-CBD	4.26	118.83	111.27
24	B	610	CLA	C3D-C4D-ND	4.25	117.12	110.24
24	b	626	CLA	C3D-C4D-ND	4.25	117.12	110.24
24	c	508	CLA	C3D-C4D-ND	4.25	117.12	110.24
24	B	605	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	B	606	CLA	CMC-C2C-C1C	4.25	131.50	125.04
24	C	502	CLA	C3C-C4C-NC	4.25	115.33	110.57
24	d	403	CLA	C3C-C4C-NC	4.24	115.33	110.57
24	C	504	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
24	b	616	CLA	C3C-C4C-NC	4.24	115.33	110.57
24	B	605	CLA	C1D-CHD-C4C	-4.24	116.91	126.06
24	c	515	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
24	C	511	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
24	c	511	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
24	b	624	CLA	C1-C2-C3	-4.24	118.72	126.04
24	b	622	CLA	CMD-C2D-C1D	4.23	132.18	124.71
27	a	405	SQD	O47-C7-C8	4.23	120.62	111.50
24	C	512	CLA	C3C-C4C-NC	4.23	115.32	110.57
24	c	512	CLA	C3C-C4C-NC	4.23	115.31	110.57
24	B	613	CLA	C4A-NA-C1A	-4.23	104.81	106.71
26	y	101	BCR	C33-C5-C6	-4.22	119.78	124.53
24	b	618	CLA	C3D-C4D-ND	4.22	117.07	110.24
24	B	607	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
24	C	513	CLA	C3D-C4D-ND	4.22	117.06	110.24
24	a	410	CLA	C2C-C1C-NC	4.21	113.92	109.97
27	A	412	SQD	O6-C1-C2	4.21	114.88	108.30
24	a	409	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
24	B	602	CLA	C4A-NA-C1A	-4.21	104.81	106.71
24	B	610	CLA	O2D-CGD-CBD	4.21	118.75	111.27
24	b	624	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
39	e	102	HEM	CHC-C4B-NB	4.20	128.99	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	623	CLA	C3C-C4C-NC	4.20	115.28	110.57
24	C	504	CLA	CBC-CAC-C3C	-4.20	100.86	112.43
24	A	406	CLA	CBC-CAC-C3C	-4.20	100.86	112.43
26	c	527	BCR	C15-C14-C13	-4.19	121.33	127.31
24	C	501	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
24	c	510	CLA	O2D-CGD-CBD	4.18	118.69	111.27
24	A	405	CLA	C3D-C4D-ND	4.17	116.99	110.24
24	c	508	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
24	B	611	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	c	506	CLA	C3D-C4D-ND	4.17	116.98	110.24
24	C	506	CLA	C3D-C4D-ND	4.16	116.97	110.24
24	B	612	CLA	O2D-CGD-CBD	4.16	118.66	111.27
37	D	406	DGD	O2G-C1B-C2B	4.16	120.47	111.50
24	B	605	CLA	C3B-C4B-NB	4.16	114.59	109.21
26	T	103	BCR	C11-C10-C9	-4.16	121.37	127.31
24	b	624	CLA	C3D-C4D-ND	4.16	116.96	110.24
26	H	102	BCR	C38-C26-C25	-4.16	119.86	124.53
36	b	602	HTG	C1'-S1-C1	4.16	107.86	100.09
24	b	618	CLA	O2D-CGD-CBD	4.16	118.65	111.27
24	A	405	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
38	D	409	LHG	O7-C7-C8	4.15	120.45	111.50
24	B	604	CLA	C3C-C4C-NC	4.15	115.23	110.57
24	c	513	CLA	C3D-C4D-ND	4.15	116.95	110.24
24	b	613	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
24	B	617	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
24	b	616	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
24	B	614	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
24	b	625	CLA	C3D-C4D-ND	4.13	116.92	110.24
26	d	404	BCR	C24-C23-C22	-4.13	120.00	126.23
24	d	402	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
24	c	517	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
24	c	514	CLA	C3B-C4B-NB	4.12	114.54	109.21
32	d	405[B]	PL9	C42-C43-C44	-4.12	117.75	127.66
24	c	512	CLA	C3D-C4D-ND	4.12	116.89	110.24
24	b	617	CLA	C3C-C4C-NC	4.11	115.18	110.57
24	d	401	CLA	C3B-C4B-NB	4.10	114.52	109.21
24	b	622	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
24	b	615	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
24	b	626	CLA	CAC-C3C-C4C	4.10	130.12	124.81
24	B	609	CLA	C3D-C4D-ND	4.10	116.86	110.24
24	b	621	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	C	502	CLA	C3D-C4D-ND	4.09	116.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
24	c	516	CLA	C3D-C4D-ND	4.09	116.85	110.24
24	c	516	CLA	C3C-C4C-NC	4.08	115.15	110.57
24	C	503	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
24	c	508	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
24	B	602	CLA	C3C-C4C-NC	4.08	115.14	110.57
24	b	613	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
24	b	619	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
24	b	616	CLA	C3D-C4D-ND	4.07	116.83	110.24
24	c	513	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
24	a	410	CLA	C3C-C4C-NC	4.07	115.14	110.57
24	b	626	CLA	C3B-C4B-NB	4.06	114.46	109.21
24	B	603	CLA	C3C-C4C-NC	4.06	115.12	110.57
27	a	414	SQD	O47-C7-C8	4.05	120.23	111.50
24	b	626	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	B	615	CLA	C3D-C4D-ND	4.05	116.79	110.24
39	F	102	HEM	C1B-NB-C4B	4.05	109.25	105.07
24	b	622	CLA	CHD-C1D-ND	-4.05	120.73	124.45
24	C	505	CLA	C1D-CHD-C4C	-4.04	117.33	126.06
24	b	625	CLA	C3C-C4C-NC	4.04	115.10	110.57
24	c	513	CLA	C3C-C4C-NC	4.04	115.10	110.57
24	B	611	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	B	602	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
24	c	510	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	b	611	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
24	b	625	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
39	v	205	HEM	C1B-NB-C4B	4.03	109.24	105.07
24	b	621	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	b	618	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
24	C	510	CLA	C3D-C4D-ND	4.02	116.74	110.24
24	d	401	CLA	C3C-C4C-NC	4.02	115.08	110.57
24	c	516	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
24	C	510	CLA	C1-C2-C3	-4.01	119.11	126.04
24	c	514	CLA	C1-C2-C3	-4.01	119.11	126.04
29	a	404	LMT	C1'-O5'-C5'	4.01	121.56	113.69
24	C	510	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
24	c	515	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
24	B	616	CLA	C1D-CHD-C4C	-4.00	117.42	126.06
24	C	505	CLA	C3D-C4D-ND	4.00	116.71	110.24
24	C	510	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	B	604	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
24	B	602	CLA	C1D-CHD-C4C	-4.00	117.43	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C3D-C4D-ND	4.00	116.70	110.24
24	A	406	CLA	C3D-C4D-ND	4.00	116.70	110.24
24	C	509	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
24	B	607	CLA	C3D-C4D-ND	3.99	116.70	110.24
24	B	614	CLA	C3B-C4B-NB	3.99	114.36	109.21
24	b	611	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
24	b	612	CLA	C3C-C4C-NC	3.98	115.03	110.57
24	b	619	CLA	C3C-C4C-NC	3.98	115.03	110.57
39	e	102	HEM	CHD-C1D-ND	3.97	128.75	124.43
24	a	409	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
24	B	615	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
24	C	504	CLA	C3D-C4D-ND	3.96	116.65	110.24
29	A	417	LMT	O5'-C5'-C4'	3.96	118.10	109.75
24	B	609	CLA	C4A-NA-C1A	-3.95	104.93	106.71
24	D	402	CLA	C3C-C4C-NC	3.95	115.00	110.57
24	d	402	CLA	O2D-CGD-CBD	3.95	118.28	111.27
24	B	612	CLA	CMC-C2C-C1C	3.95	131.05	125.04
37	c	520	DGD	O2G-C1B-C2B	3.95	120.01	111.50
24	b	626	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
37	e	101	DGD	C3E-C4E-C5E	3.95	117.28	110.24
24	C	509	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	C	501	CLA	C3C-C4C-NC	3.94	114.99	110.57
38	D	407	LHG	O7-C7-C8	3.94	119.99	111.50
24	B	604	CLA	C3D-C2D-C1D	-3.94	100.46	105.83
24	b	620	CLA	C3C-C4C-NC	3.93	114.98	110.57
24	b	611	CLA	C3C-C4C-NC	3.93	114.98	110.57
24	d	401	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
24	B	612	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
24	C	511	CLA	C4A-NA-C1A	-3.93	104.94	106.71
29	a	404	LMT	O5'-C5'-C4'	3.93	118.04	109.75
24	C	513	CLA	C3C-C4C-NC	3.93	114.97	110.57
39	e	102	HEM	C1B-NB-C4B	3.92	109.13	105.07
24	C	502	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
24	b	618	CLA	C3C-C4C-NC	3.92	114.96	110.57
24	c	505	CLA	CAC-C3C-C4C	3.92	129.89	124.81
24	B	607	CLA	C1D-CHD-C4C	-3.91	117.61	126.06
24	c	511	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
34	Z	101	LMG	O7-C10-C11	3.91	119.92	111.50
24	d	402	CLA	C3C-C4C-NC	3.91	114.95	110.57
26	T	103	BCR	C15-C16-C17	-3.90	115.48	123.47
24	B	607	CLA	C3C-C4C-NC	3.90	114.94	110.57
24	c	509	CLA	C1D-CHD-C4C	-3.89	117.66	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	405[B]	PL9	C42-C43-C44	-3.89	118.29	127.66
24	A	406	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
24	C	511	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
24	c	514	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
32	a	416[B]	PL9	C7-C8-C9	-3.88	120.33	126.79
24	B	603	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
37	c	519	DGD	O2G-C1B-C2B	3.88	119.86	111.50
24	C	513	CLA	O2D-CGD-CBD	3.88	118.16	111.27
24	D	402	CLA	CMC-C2C-C1C	3.88	130.95	125.04
25	A	408	PHO	C1A-C2A-C3A	-3.88	99.15	102.84
26	y	101	BCR	C15-C14-C13	-3.88	121.78	127.31
24	C	506	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
24	B	611	CLA	CAA-C2A-C3A	-3.86	102.19	112.78
24	c	513	CLA	C3B-C4B-NB	3.86	114.20	109.21
24	B	609	CLA	C3C-C4C-NC	3.86	114.90	110.57
24	C	504	CLA	O2D-CGD-O1D	-3.85	116.30	123.84
24	C	506	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	B	604	CLA	CAA-C2A-C3A	-3.85	102.23	112.78
32	a	416[A]	PL9	C22-C23-C24	-3.85	118.39	127.66
24	b	614	CLA	CMC-C2C-C1C	3.85	130.90	125.04
24	a	412	CLA	C3C-C4C-NC	3.85	114.88	110.57
24	c	505	CLA	C3D-C4D-ND	3.85	116.46	110.24
24	D	402	CLA	C3B-C4B-NB	3.84	114.18	109.21
24	A	405	CLA	C3C-C4C-NC	3.84	114.88	110.57
24	c	517	CLA	C3C-C4C-NC	3.84	114.88	110.57
24	B	612	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
24	b	623	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
24	C	508	CLA	C3B-C4B-NB	3.83	114.16	109.21
24	b	613	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
24	C	504	CLA	C3C-C4C-NC	3.83	114.87	110.57
24	C	511	CLA	CAC-C3C-C4C	3.83	129.78	124.81
27	B	621	SQD	O7-S-C6	3.83	111.49	106.94
27	b	601	SQD	C3-C4-C5	3.83	117.06	110.24
24	C	512	CLA	C1D-CHD-C4C	-3.83	117.81	126.06
24	c	505	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
27	A	416	SQD	O48-C23-C24	3.82	123.91	111.91
32	a	416[A]	PL9	C32-C33-C34	-3.82	118.45	127.66
24	b	622	CLA	C3B-C4B-NB	3.82	114.15	109.21
24	B	606	CLA	CHD-C4C-NC	3.82	130.22	124.20
24	B	615	CLA	CAC-C3C-C4C	3.82	129.76	124.81
24	C	511	CLA	C3C-C4C-NC	3.81	114.85	110.57
24	D	403	CLA	C3C-C4C-NC	3.81	114.85	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
24	d	402	CLA	C1-C2-C3	-3.81	119.46	126.04
24	d	402	CLA	C3B-C4B-NB	3.81	114.13	109.21
24	b	623	CLA	C3D-C4D-ND	3.80	116.39	110.24
24	C	501	CLA	O2D-CGD-O1D	-3.80	116.40	123.84
38	E	101	LHG	O7-C7-C8	3.80	119.69	111.50
24	B	608	CLA	C3C-C4C-NC	3.80	114.83	110.57
24	c	512	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	c	510	CLA	C1-C2-C3	-3.80	119.47	126.04
24	C	513	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
24	b	623	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
24	a	412	CLA	C1-C2-C3	-3.80	119.48	126.04
24	B	613	CLA	CMC-C2C-C1C	3.79	130.81	125.04
24	B	617	CLA	C3D-C4D-ND	3.79	116.37	110.24
29	D	401	LMT	O1B-C4'-C3'	3.78	117.34	107.28
24	b	622	CLA	C3D-C4D-ND	3.78	116.36	110.24
24	b	624	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
26	C	515	BCR	C33-C5-C6	-3.77	120.29	124.53
24	C	507	CLA	C3D-C4D-ND	3.77	116.34	110.24
24	b	612	CLA	CAC-C3C-C4C	3.77	129.70	124.81
24	b	614	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	A	407	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
24	b	618	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
24	c	511	CLA	C3D-C4D-ND	3.76	116.32	110.24
36	b	609	HTG	C1'-S1-C1	3.76	107.12	100.09
24	D	402	CLA	CAC-C3C-C4C	3.75	129.68	124.81
32	a	416[A]	PL9	C7-C3-C4	3.75	119.92	116.88
24	c	509	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
24	C	510	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	b	622	CLA	CAC-C3C-C4C	3.74	129.66	124.81
24	c	512	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	B	610	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
24	b	617	CLA	C4A-NA-C1A	-3.74	105.03	106.71
24	C	506	CLA	CAC-C3C-C4C	3.74	129.66	124.81
24	c	515	CLA	O2D-CGD-CBD	3.73	117.90	111.27
24	b	616	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
24	d	403	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
27	A	416	SQD	O47-C7-C8	3.72	119.53	111.50
24	c	514	CLA	C3C-C4C-NC	3.72	114.75	110.57
24	C	505	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
24	B	610	CLA	C3C-C4C-NC	3.72	114.75	110.57
24	C	506	CLA	C1C-C2C-C3C	-3.72	103.04	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	519	LMG	O7-C10-C11	3.72	119.52	111.50
32	A	420[A]	PL9	C7-C3-C4	3.72	119.90	116.88
32	a	416[B]	PL9	C7-C3-C4	3.72	119.90	116.88
24	c	510	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
24	b	624	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
37	C	517	DGD	O2G-C1B-C2B	3.71	119.50	111.50
24	B	609	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
24	c	506	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
24	c	516	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
24	b	614	CLA	C3B-C4B-NB	3.71	114.00	109.21
26	C	514	BCR	C7-C8-C9	-3.70	120.65	126.23
38	l	101	LHG	O7-C7-C8	3.70	119.47	111.50
38	d	407	LHG	O7-C7-C8	3.68	119.44	111.50
24	B	613	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
24	B	608	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	c	513	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	C	513	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	a	409	CLA	CAA-C2A-C3A	-3.68	102.71	112.78
24	b	622	CLA	C1-C2-C3	-3.68	119.68	126.04
24	C	501	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
26	H	102	BCR	C16-C17-C18	-3.68	122.06	127.31
26	c	527	BCR	C16-C17-C18	-3.68	122.06	127.31
27	a	405	SQD	O48-C23-C24	3.67	123.43	111.91
26	C	515	BCR	C7-C8-C9	-3.67	120.69	126.23
24	B	607	CLA	C3B-C4B-NB	3.67	113.95	109.21
24	a	409	CLA	C1-C2-C3	-3.67	119.70	126.04
24	C	504	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
24	C	507	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
24	c	512	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
24	A	410	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
24	B	609	CLA	C3B-C4B-NB	3.65	113.94	109.21
27	a	414	SQD	C1-C2-C3	-3.65	102.39	110.00
24	D	403	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	b	625	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	B	614	CLA	C4A-NA-C1A	-3.65	105.06	106.71
24	b	616	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	C	511	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	a	412	CLA	C4A-NA-C1A	-3.65	105.07	106.71
24	c	515	CLA	C3C-C4C-NC	3.65	114.66	110.57
24	A	405	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
24	b	613	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	c	510	CLA	CBC-CAC-C3C	-3.64	102.40	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	C4A-NA-C1A	-3.64	105.07	106.71
32	a	416[A]	PL9	C15-C14-C16	3.63	121.39	115.27
24	A	407	CLA	C3C-C4C-NC	3.63	114.65	110.57
34	b	630	LMG	O7-C10-C11	3.63	119.33	111.50
32	a	416[A]	PL9	C7-C8-C9	-3.63	120.75	126.79
37	D	406	DGD	C1D-C2D-C3D	3.63	117.55	110.00
24	D	402	CLA	O2D-CGD-CBD	3.62	117.71	111.27
24	b	618	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	C	508	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
24	C	505	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	D	403	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
27	F	103	SQD	O5-C5-C4	3.61	116.26	109.69
24	b	612	CLA	CAA-C2A-C3A	-3.61	102.89	112.78
24	C	507	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	a	412	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
24	a	410	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
24	B	615	CLA	CMC-C2C-C1C	3.60	130.52	125.04
24	B	613	CLA	C4-C3-C5	3.60	121.33	115.27
25	a	411	PHO	O1D-CGD-CBD	-3.60	118.75	124.74
26	c	518	BCR	C7-C8-C9	-3.60	120.80	126.23
24	c	513	CLA	C1-C2-C3	-3.60	119.82	126.04
39	F	102	HEM	CBA-CAA-C2A	-3.59	106.49	112.62
24	C	509	CLA	C4A-NA-C1A	-3.59	105.09	106.71
34	c	522	LMG	O8-C28-C29	3.58	123.15	111.91
24	b	619	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
24	B	612	CLA	C1-C2-C3	-3.58	119.85	126.04
26	d	404	BCR	C33-C5-C6	-3.58	120.51	124.53
24	c	510	CLA	C3B-C4B-NB	3.58	113.83	109.21
24	b	622	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
26	h	101	BCR	C16-C17-C18	-3.57	122.21	127.31
37	h	102	DGD	O2G-C1B-C2B	3.56	119.18	111.50
24	A	405	CLA	O2D-CGD-CBD	3.56	117.60	111.27
24	A	407	CLA	C4-C3-C5	3.56	121.26	115.27
26	D	404	BCR	C24-C23-C22	-3.56	120.85	126.23
26	b	628	BCR	C29-C30-C25	3.56	115.96	110.48
26	b	627	BCR	C7-C8-C9	-3.56	120.86	126.23
24	c	515	CLA	C3B-C4B-NB	3.56	113.81	109.21
24	b	620	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
24	C	510	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
24	c	515	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
24	B	603	CLA	C1-C2-C3	-3.55	119.90	126.04
24	d	403	CLA	CAC-C3C-C4C	3.55	129.42	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	410	CLA	CAC-C3C-C4C	3.55	129.41	124.81
24	C	504	CLA	C3B-C4B-NB	3.55	113.80	109.21
34	c	522	LMG	O7-C10-C11	3.55	119.14	111.50
26	C	514	BCR	C15-C14-C13	-3.54	122.25	127.31
24	C	503	CLA	O2D-CGD-CBD	3.54	117.55	111.27
39	V	206	HEM	CHC-C4B-NB	3.53	128.27	124.43
24	D	402	CLA	C1-C2-C3	-3.53	119.94	126.04
24	B	603	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
24	b	617	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
34	z	101	LMG	O7-C10-C11	3.53	119.10	111.50
24	C	507	CLA	CMC-C2C-C1C	3.53	130.41	125.04
24	A	405	CLA	C3B-C4B-NB	3.52	113.77	109.21
39	v	205	HEM	C4D-ND-C1D	3.52	108.71	105.07
24	B	602	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
26	K	101	BCR	C15-C14-C13	-3.52	122.28	127.31
36	V	207	HTG	C1'-S1-C1	3.52	106.68	100.09
27	A	412	SQD	C45-O47-C7	-3.52	109.13	117.79
24	c	514	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
24	C	506	CLA	C3B-C4B-NB	3.51	113.75	109.21
26	c	518	BCR	C33-C5-C6	-3.51	120.58	124.53
24	C	509	CLA	C3B-C4B-NB	3.51	113.75	109.21
24	b	621	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
24	a	409	CLA	C3C-C4C-NC	3.51	114.51	110.57
24	b	617	CLA	CAA-C2A-C3A	-3.51	103.17	112.78
24	b	612	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
25	A	409[A]	PHO	C1A-C2A-C3A	-3.51	99.50	102.84
24	c	509	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
26	d	404	BCR	C38-C26-C25	-3.50	120.59	124.53
24	c	517	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	B	611	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
24	b	626	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
24	c	505	CLA	C3B-C4B-NB	3.49	113.73	109.21
24	b	615	CLA	CHD-C4C-NC	3.49	129.71	124.20
24	B	610	CLA	C3B-C4B-NB	3.49	113.72	109.21
24	B	611	CLA	C3B-C4B-NB	3.49	113.72	109.21
24	C	508	CLA	C1C-C2C-C3C	-3.48	103.29	106.96
24	D	403	CLA	C4-C3-C5	3.48	121.13	115.27
24	B	615	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
25	a	420[A]	PHO	C1A-C2A-C3A	-3.48	99.53	102.84
24	c	514	CLA	C4-C3-C5	3.48	121.12	115.27
32	a	416[B]	PL9	C32-C33-C34	-3.48	119.29	127.66
38	L	101	LHG	O7-C7-C8	3.47	118.99	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C3C-C4C-NC	3.47	114.47	110.57
24	d	401	CLA	C4A-NA-C1A	-3.47	105.14	106.71
24	D	403	CLA	CAC-C3C-C4C	3.47	129.31	124.81
24	c	505	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
24	b	613	CLA	C3B-C4B-NB	3.47	113.69	109.21
24	b	620	CLA	C1-C2-C3	-3.47	120.05	126.04
24	B	615	CLA	O2A-CGA-O1A	-3.47	114.85	123.59
24	C	508	CLA	CMB-C2B-C3B	3.46	131.16	124.68
24	c	515	CLA	C1-C2-C3	-3.46	120.06	126.04
26	t	101	BCR	C15-C16-C17	-3.46	116.39	123.47
25	a	420[A]	PHO	O2D-CGD-O1D	-3.45	117.09	123.84
24	C	502	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	D	403	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
24	d	402	CLA	CAC-C3C-C4C	3.45	129.28	124.81
24	c	508	CLA	C3B-C4B-NB	3.45	113.66	109.21
24	B	613	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
24	B	617	CLA	C3B-C4B-NB	3.44	113.66	109.21
24	C	512	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	b	623	CLA	C1-C2-C3	-3.44	120.09	126.04
24	B	613	CLA	C4C-C3C-C2C	-3.44	101.88	106.90
24	A	405	CLA	CAA-C2A-C3A	-3.44	103.36	112.78
24	B	607	CLA	CAC-C3C-C4C	3.44	129.27	124.81
34	D	412	LMG	O7-C10-C11	3.43	118.90	111.50
27	F	103	SQD	O6-C1-C2	3.43	113.66	108.30
24	A	405	CLA	CAC-C3C-C4C	3.43	129.26	124.81
26	k	101	BCR	C24-C23-C22	-3.43	121.05	126.23
24	c	510	CLA	C3C-C4C-NC	3.43	114.42	110.57
24	b	623	CLA	O2D-CGD-CBD	3.43	117.36	111.27
34	a	415	LMG	C8-O7-C10	-3.42	109.36	117.79
24	C	509	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
32	A	420[B]	PL9	C7-C3-C4	3.42	119.65	116.88
24	b	615	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
24	B	608	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
24	C	508	CLA	CAC-C3C-C4C	3.41	129.24	124.81
32	a	416[B]	PL9	C22-C23-C24	-3.41	119.44	127.66
24	A	406	CLA	CHC-C1C-C2C	-3.41	117.29	126.72
24	b	616	CLA	CMB-C2B-C3B	3.41	131.05	124.68
32	A	420[A]	PL9	C32-C33-C34	-3.41	119.46	127.66
24	b	625	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
32	A	420[B]	PL9	C37-C38-C39	-3.40	119.47	127.66
39	e	102	HEM	CAD-CBD-CGD	3.40	120.92	113.60
24	B	608	CLA	CAA-C2A-C3A	-3.40	103.47	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	521	LMT	C1'-O5'-C5'	3.40	120.36	113.69
24	c	508	CLA	C4-C3-C5	3.39	120.98	115.27
24	B	604	CLA	CMC-C2C-C1C	3.39	130.21	125.04
24	B	605	CLA	C4A-NA-C1A	-3.39	105.18	106.71
25	a	420[B]	PHO	C1A-C2A-C3A	-3.39	99.61	102.84
24	B	614	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
24	a	409	CLA	C3B-C4B-NB	3.39	113.59	109.21
24	b	612	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
24	b	621	CLA	C3B-C4B-NB	3.38	113.59	109.21
32	A	420[B]	PL9	C32-C33-C34	-3.38	119.51	127.66
24	b	613	CLA	CMC-C2C-C1C	3.38	130.19	125.04
26	d	404	BCR	C7-C8-C9	-3.38	121.12	126.23
24	B	611	CLA	CHC-C1C-C2C	-3.38	117.37	126.72
24	b	625	CLA	O2D-CGD-CBD	3.38	117.28	111.27
24	b	611	CLA	CHD-C4C-NC	3.38	129.53	124.20
26	B	619	BCR	C33-C5-C6	-3.38	120.74	124.53
24	b	614	CLA	C3D-C4D-ND	3.38	115.70	110.24
24	b	611	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
26	C	514	BCR	C33-C5-C6	-3.37	120.75	124.53
34	c	523	LMG	O6-C5-C4	3.37	115.81	109.69
24	B	617	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
24	C	512	CLA	C1-C2-C3	-3.36	120.23	126.04
24	b	611	CLA	C3B-C4B-NB	3.36	113.56	109.21
24	C	508	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
24	B	607	CLA	CMB-C2B-C3B	3.36	130.96	124.68
24	c	511	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
24	B	608	CLA	C3B-C4B-NB	3.34	113.53	109.21
24	A	407	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
24	B	610	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
24	B	603	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
29	C	521	LMT	O1B-C4'-C3'	3.33	116.15	107.28
32	d	405[A]	PL9	C42-C43-C44	-3.33	119.63	127.66
24	c	506	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
32	D	405[B]	PL9	C7-C8-C9	-3.33	121.25	126.79
24	B	614	CLA	C1-C2-C3	-3.33	120.29	126.04
24	B	611	CLA	C3C-C4C-NC	3.33	114.30	110.57
24	c	514	CLA	C4A-NA-C1A	-3.33	105.21	106.71
24	b	617	CLA	CBC-CAC-C3C	-3.33	103.26	112.43
26	Y	101	BCR	C15-C14-C13	-3.32	122.56	127.31
24	b	615	CLA	C4C-C3C-C2C	-3.32	102.05	106.90
24	C	506	CLA	CBC-CAC-C3C	-3.32	103.27	112.43
25	A	409[A]	PHO	CMB-C2B-C3B	3.32	130.89	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	CHD-C4C-NC	3.32	129.44	124.20
24	b	617	CLA	C3B-C4B-NB	3.32	113.50	109.21
26	K	101	BCR	C7-C8-C9	-3.32	121.22	126.23
24	b	622	CLA	O2A-CGA-O1A	-3.32	115.22	123.59
24	C	512	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	B	602	CLA	C3B-C4B-NB	3.31	113.49	109.21
32	a	416[B]	PL9	C15-C14-C16	3.31	120.84	115.27
32	a	416[A]	PL9	C17-C18-C19	-3.31	119.69	127.66
24	D	402	CLA	C1D-CHD-C4C	-3.31	118.93	126.06
24	c	506	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
24	c	507	CLA	CAC-C3C-C4C	3.30	129.09	124.81
24	a	412	CLA	C3B-C4B-NB	3.30	113.48	109.21
24	C	501	CLA	CMC-C2C-C1C	3.30	130.06	125.04
32	d	405[B]	PL9	C27-C28-C29	-3.30	119.72	127.66
24	B	602	CLA	CHD-C4C-NC	3.29	129.39	124.20
32	D	405[B]	PL9	C37-C38-C39	-3.29	119.74	127.66
24	b	617	CLA	CHD-C4C-NC	3.29	129.39	124.20
24	B	603	CLA	C3B-C4B-NB	3.29	113.46	109.21
27	F	103	SQD	O7-S-C6	3.29	110.84	106.94
24	B	612	CLA	C3B-C4B-NB	3.29	113.46	109.21
24	C	502	CLA	C3B-C4B-NB	3.28	113.46	109.21
26	D	404	BCR	C38-C26-C25	-3.28	120.84	124.53
27	A	412	SQD	O8-S-C6	3.28	110.97	105.74
27	f	102	SQD	C1-O5-C5	3.28	120.13	113.69
24	c	508	CLA	CMC-C2C-C1C	3.28	130.03	125.04
26	D	404	BCR	C28-C27-C26	-3.27	108.23	114.08
26	y	101	BCR	C16-C17-C18	-3.27	122.64	127.31
24	A	407	CLA	CBC-CAC-C3C	-3.27	103.42	112.43
24	c	516	CLA	C1-C2-C3	-3.27	120.39	126.04
24	B	615	CLA	C4-C3-C5	3.27	120.77	115.27
24	B	603	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
24	B	606	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
24	B	606	CLA	C4-C3-C5	3.26	120.76	115.27
24	c	507	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
24	c	517	CLA	C1-C2-C3	-3.25	120.41	126.04
24	b	618	CLA	C3B-C4B-NB	3.25	113.42	109.21
24	c	506	CLA	C3B-C4B-NB	3.25	113.42	109.21
27	a	414	SQD	O8-S-C6	3.25	110.92	105.74
32	D	405[B]	PL9	C40-C39-C41	3.25	120.74	115.27
24	b	616	CLA	CMC-C2C-C1C	3.25	129.99	125.04
24	B	613	CLA	C3B-C4B-NB	3.25	113.41	109.21
24	B	614	CLA	C3D-C4D-ND	3.25	115.49	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C38-C26-C25	-3.24	120.89	124.53
24	A	410	CLA	CMC-C2C-C1C	3.24	129.98	125.04
24	b	620	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
24	B	615	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	A	410	CLA	C1-C2-C3	-3.24	120.44	126.04
25	A	409[A]	PHO	C4-C3-C5	3.24	120.72	115.27
26	C	514	BCR	C16-C17-C18	-3.24	122.69	127.31
24	b	624	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	A	406	CLA	C4A-NA-C1A	-3.24	105.25	106.71
24	A	410	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
24	B	607	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
24	B	614	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
24	b	620	CLA	C3B-C4B-NB	3.23	113.38	109.21
24	b	617	CLA	CMC-C2C-C1C	3.23	129.95	125.04
24	b	622	CLA	O2A-CGA-CBA	3.23	122.04	111.91
26	k	101	BCR	C20-C21-C22	-3.22	122.71	127.31
27	a	414	SQD	O9-S-C6	3.22	110.77	106.94
24	d	403	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
24	c	515	CLA	CAC-C3C-C4C	3.22	128.99	124.81
39	V	206	HEM	CHB-C1B-NB	3.22	128.36	124.38
24	B	611	CLA	O2A-CGA-CBA	3.22	122.00	111.91
24	b	612	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
24	B	602	CLA	O2A-CGA-CBA	3.22	122.00	111.91
24	d	402	CLA	CHC-C1C-C2C	-3.22	117.83	126.72
24	C	511	CLA	CHC-C1C-C2C	-3.21	117.83	126.72
27	a	414	SQD	C44-O6-C1	-3.21	107.46	113.74
24	B	607	CLA	CMC-C2C-C1C	3.21	129.93	125.04
24	A	406	CLA	CHD-C4C-NC	3.21	129.26	124.20
26	k	101	BCR	C7-C8-C9	-3.21	121.39	126.23
24	C	506	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
24	C	508	CLA	C1-C2-C3	-3.21	120.50	126.04
24	c	508	CLA	C1-C2-C3	-3.21	120.50	126.04
24	c	506	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
32	D	405[A]	PL9	C42-C43-C44	-3.20	119.94	127.66
25	a	420[A]	PHO	C4-C3-C5	3.20	120.66	115.27
26	B	619	BCR	C29-C30-C25	3.20	115.41	110.48
37	H	103	DGD	O2G-C1B-C2B	3.20	118.40	111.50
32	A	420[A]	PL9	C20-C19-C21	3.20	120.66	115.27
24	b	620	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	B	614	CLA	O2D-CGD-CBD	3.20	116.95	111.27
34	B	622	LMG	O8-C28-C29	3.20	121.95	111.91
24	c	509	CLA	C4C-C3C-C2C	-3.20	102.23	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	420[A]	PHO	CMB-C2B-C3B	3.20	130.66	124.68
24	C	506	CLA	C4-C3-C5	3.20	120.65	115.27
24	D	402	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
36	B	624	HTG	C1-O5-C5	3.20	118.47	112.58
24	B	607	CLA	C1-C2-C3	-3.20	120.52	126.04
32	D	405[A]	PL9	C7-C8-C9	-3.20	121.47	126.79
24	b	624	CLA	C3B-C4B-NB	3.20	113.34	109.21
24	C	509	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
24	B	611	CLA	CAC-C3C-C4C	3.19	128.95	124.81
32	a	416[A]	PL9	C37-C38-C39	-3.19	119.98	127.66
39	v	205	HEM	CHD-C1D-ND	3.19	127.89	124.43
32	a	416[A]	PL9	C10-C9-C11	3.18	120.62	115.27
24	b	622	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	b	625	CLA	CAC-C3C-C4C	3.18	128.93	124.81
24	b	623	CLA	CHC-C1C-C2C	-3.17	117.94	126.72
26	B	619	BCR	C37-C22-C21	-3.17	118.48	122.92
24	c	516	CLA	CHD-C4C-NC	3.17	129.20	124.20
26	c	518	BCR	C15-C14-C13	-3.17	122.78	127.31
24	B	616	CLA	CMC-C2C-C1C	3.17	129.87	125.04
24	B	613	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
38	d	406	LHG	O8-C23-O10	-3.17	115.59	123.59
24	d	403	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	d	401	CLA	C2A-C1A-CHA	-3.17	118.32	123.86
32	a	416[A]	PL9	C27-C28-C29	-3.17	120.03	127.66
24	C	503	CLA	C1C-C2C-C3C	-3.17	103.63	106.96
32	d	405[A]	PL9	C37-C38-C39	-3.17	120.04	127.66
34	B	622	LMG	O7-C10-C11	3.16	118.31	111.50
24	C	502	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
25	A	409[B]	PHO	C1A-C2A-C3A	-3.16	99.84	102.84
32	a	416[A]	PL9	C20-C19-C21	3.16	120.58	115.27
24	C	512	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
32	A	420[A]	PL9	C37-C38-C39	-3.15	120.06	127.66
24	B	617	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
32	A	420[B]	PL9	C7-C8-C9	-3.15	121.55	126.79
24	B	613	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	b	623	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	b	612	CLA	C1C-C2C-C3C	-3.15	103.65	106.96
24	c	505	CLA	CHC-C1C-C2C	-3.14	118.02	126.72
32	a	416[B]	PL9	C37-C38-C39	-3.14	120.09	127.66
32	a	416[B]	PL9	C7-C3-C2	-3.14	119.17	123.30
32	D	405[A]	PL9	C37-C38-C39	-3.14	120.10	127.66
32	A	420[A]	PL9	C7-C8-C9	-3.14	121.57	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
24	b	613	CLA	CAC-C3C-C4C	3.13	128.88	124.81
24	C	504	CLA	CMC-C2C-C1C	3.13	129.81	125.04
26	B	619	BCR	C28-C27-C26	-3.13	108.48	114.08
24	d	403	CLA	C3B-C4B-NB	3.13	113.26	109.21
32	a	416[B]	PL9	C17-C18-C19	-3.13	120.12	127.66
24	C	510	CLA	C4-C3-C5	3.13	120.54	115.27
26	D	404	BCR	C29-C30-C25	3.13	115.30	110.48
32	A	420[B]	PL9	C20-C19-C21	3.13	120.53	115.27
24	B	605	CLA	C3D-C4D-ND	3.13	115.30	110.24
24	B	617	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
39	v	205	HEM	CHA-C4D-ND	3.13	128.24	124.38
24	B	612	CLA	CAC-C3C-C4C	3.13	128.87	124.81
24	c	517	CLA	CMC-C2C-C1C	3.12	129.79	125.04
39	e	102	HEM	CHB-C1B-NB	3.12	128.24	124.38
24	b	626	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
32	D	405[A]	PL9	C10-C9-C11	3.12	120.52	115.27
38	d	408	LHG	O7-C7-C8	3.12	118.22	111.50
24	C	505	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
24	C	508	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
24	d	401	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
24	B	610	CLA	CAC-C3C-C4C	3.11	128.85	124.81
24	c	514	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
24	b	615	CLA	C2A-C1A-CHA	-3.11	118.42	123.86
24	A	410	CLA	C4-C3-C5	3.11	120.50	115.27
24	c	507	CLA	CMC-C2C-C1C	3.11	129.77	125.04
34	C	519	LMG	O8-C28-C29	3.11	121.67	111.91
24	B	616	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
24	B	607	CLA	C4-C3-C5	3.11	120.50	115.27
24	b	611	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	b	615	CLA	C4-C3-C5	3.11	120.50	115.27
24	a	410	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
32	A	420[B]	PL9	C22-C23-C24	-3.10	120.19	127.66
24	B	616	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	b	620	CLA	CAC-C3C-C4C	3.10	128.83	124.81
24	c	505	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
24	B	610	CLA	CHD-C4C-NC	3.10	129.09	124.20
24	B	607	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
27	A	412	SQD	O9-S-C6	3.10	110.62	106.94
24	A	410	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
25	A	408	PHO	O1D-CGD-CBD	-3.10	119.58	124.74
24	B	617	CLA	C1-O2A-CGA	3.09	124.56	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	O2A-CGA-CBA	3.09	121.62	111.91
37	e	101	DGD	O5D-C1E-C2E	3.09	113.13	108.30
32	a	416[B]	PL9	C20-C19-C21	3.09	120.47	115.27
24	b	614	CLA	C1-C2-C3	-3.09	120.70	126.04
24	B	616	CLA	O2D-CGD-CBD	3.09	116.76	111.27
26	B	619	BCR	C2-C1-C6	3.09	115.24	110.48
37	c	519	DGD	C2G-O2G-C1B	-3.09	110.19	117.79
24	D	403	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	C	511	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
38	l	101	LHG	O8-C23-C24	3.09	121.59	111.91
37	C	518	DGD	O2G-C1B-C2B	3.09	118.15	111.50
26	A	411	BCR	C33-C5-C6	-3.09	121.06	124.53
34	Z	101	LMG	O6-C5-C4	3.08	115.30	109.69
24	C	504	CLA	CAC-C3C-C4C	3.08	128.81	124.81
27	F	103	SQD	O9-S-C6	3.08	110.60	106.94
24	b	619	CLA	C3B-C4B-NB	3.08	113.19	109.21
24	b	613	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	B	608	CLA	CAC-C3C-C4C	3.08	128.80	124.81
24	b	614	CLA	CAC-C3C-C4C	3.08	128.80	124.81
26	K	101	BCR	C20-C21-C22	-3.08	122.92	127.31
24	B	605	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
32	a	416[A]	PL9	C7-C3-C2	-3.08	119.26	123.30
24	d	401	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
32	a	416[A]	PL9	C42-C43-C44	-3.07	120.26	127.66
32	A	420[A]	PL9	C7-C3-C2	-3.07	119.26	123.30
24	b	625	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
26	C	514	BCR	C20-C21-C22	-3.07	122.93	127.31
24	b	621	CLA	CBC-CAC-C3C	-3.07	103.98	112.43
24	a	409	CLA	O2D-CGD-CBD	3.06	116.71	111.27
24	c	517	CLA	CHD-C4C-NC	3.06	129.03	124.20
29	T	104	LMT	C1'-O5'-C5'	3.06	119.70	113.69
32	d	405[A]	PL9	C27-C28-C29	-3.06	120.29	127.66
32	a	416[B]	PL9	C27-C28-C29	-3.06	120.29	127.66
37	h	102	DGD	O1G-C1A-O1A	-3.06	115.87	123.59
24	B	604	CLA	CHD-C4C-NC	3.06	129.02	124.20
26	t	101	BCR	C15-C14-C13	3.06	131.67	127.31
24	b	616	CLA	C4-C3-C5	3.06	120.41	115.27
24	B	614	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
24	b	611	CLA	CHC-C1C-C2C	-3.05	118.28	126.72
27	A	412	SQD	C1-O5-C5	-3.05	107.70	113.69
24	a	412	CLA	C4-C3-C5	3.05	120.40	115.27
36	C	523	HTG	O5-C5-C4	3.05	115.23	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	C4-C3-C5	3.05	120.40	115.27
26	Y	101	BCR	C10-C11-C12	-3.05	113.71	123.22
24	b	621	CLA	CAC-C3C-C4C	3.05	128.76	124.81
39	V	206	HEM	CBA-CAA-C2A	-3.04	107.43	112.62
24	C	507	CLA	CHD-C4C-NC	3.04	129.00	124.20
26	B	620	BCR	C32-C1-C6	-3.04	105.37	110.30
24	b	617	CLA	CHC-C1C-C2C	-3.04	118.31	126.72
24	B	613	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
24	A	406	CLA	CMB-C2B-C3B	3.04	130.36	124.68
39	e	102	HEM	CHA-C4D-ND	3.04	128.13	124.38
38	D	409	LHG	O8-C23-C24	3.04	121.44	111.91
24	c	509	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	a	412	CLA	CMC-C2C-C1C	3.04	129.66	125.04
32	a	416[B]	PL9	C42-C43-C44	-3.04	120.35	127.66
24	B	603	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
34	c	523	LMG	C3-C4-C5	3.03	115.65	110.24
24	B	608	CLA	CMC-C2C-C1C	3.03	129.65	125.04
24	b	618	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	B	606	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
37	h	102	DGD	O1G-C1A-C2A	3.03	121.41	111.91
24	B	610	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
24	B	614	CLA	C4-C3-C5	3.03	120.36	115.27
24	C	502	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
24	C	513	CLA	C1-C2-C3	-3.02	120.81	126.04
32	a	416[B]	PL9	C10-C9-C11	3.02	120.36	115.27
24	b	622	CLA	C4-C3-C5	3.02	120.36	115.27
24	c	509	CLA	CAC-C3C-C4C	3.02	128.73	124.81
24	b	621	CLA	C1-C2-C3	-3.02	120.82	126.04
26	K	101	BCR	C24-C23-C22	-3.02	121.67	126.23
24	b	621	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
24	B	602	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	C	513	CLA	CAC-C3C-C4C	3.02	128.73	124.81
24	C	508	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	b	626	CLA	O2A-CGA-CBA	3.02	121.37	111.91
24	b	625	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
24	B	607	CLA	CBC-CAC-C3C	-3.01	104.12	112.43
24	c	510	CLA	CHD-C4C-NC	3.01	128.95	124.20
24	C	512	CLA	CHD-C4C-NC	3.01	128.95	124.20
24	d	402	CLA	O2A-CGA-CBA	3.01	121.36	111.91
24	C	504	CLA	C4-C3-C5	3.01	120.33	115.27
24	a	410	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	C	512	CLA	C4C-C3C-C2C	-3.01	102.51	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	626	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
26	B	618	BCR	C7-C8-C9	-3.01	121.69	126.23
39	e	102	HEM	C4D-ND-C1D	3.01	108.18	105.07
24	B	612	CLA	CHD-C4C-NC	3.01	128.94	124.20
24	c	516	CLA	CMC-C2C-C1C	3.00	129.61	125.04
26	B	619	BCR	C31-C1-C6	-3.00	105.43	110.30
27	F	103	SQD	C44-O6-C1	-3.00	107.88	113.74
24	b	623	CLA	CAC-C3C-C4C	3.00	128.70	124.81
24	C	505	CLA	C3B-C4B-NB	3.00	113.08	109.21
24	a	412	CLA	CHD-C4C-NC	3.00	128.93	124.20
24	C	510	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
24	B	609	CLA	CBC-CAC-C3C	-2.99	104.18	112.43
24	B	604	CLA	C2A-C1A-CHA	-2.99	118.63	123.86
24	c	510	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	b	623	CLA	C4-C3-C5	2.99	120.30	115.27
24	d	402	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
24	c	507	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
24	B	613	CLA	C1-C2-C3	-2.99	120.88	126.04
24	a	409	CLA	CAA-C2A-C1A	-2.98	102.20	111.97
24	B	605	CLA	C4-C3-C5	2.98	120.29	115.27
32	d	405[B]	PL9	C40-C39-C41	2.98	120.29	115.27
24	c	512	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
38	E	101	LHG	O8-C23-C24	2.98	121.26	111.91
24	d	402	CLA	C1D-CHD-C4C	-2.98	119.63	126.06
24	b	625	CLA	CHD-C4C-NC	2.98	128.90	124.20
24	b	611	CLA	C4-C3-C5	2.98	120.28	115.27
24	A	406	CLA	CAA-C2A-C3A	-2.98	104.62	112.78
24	b	616	CLA	O2A-CGA-CBA	2.98	121.25	111.91
38	D	407	LHG	O8-C23-C24	2.98	121.25	111.91
24	B	604	CLA	C3B-C4B-NB	2.97	113.06	109.21
37	H	103	DGD	O1G-C1A-C2A	2.97	121.24	111.91
24	a	410	CLA	CHD-C4C-NC	2.97	128.89	124.20
24	B	612	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	B	604	CLA	O2A-CGA-O1A	-2.97	116.10	123.59
24	A	405	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
24	b	613	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
24	C	503	CLA	CMC-C2C-C1C	2.97	129.56	125.04
26	B	618	BCR	C16-C17-C18	-2.97	123.08	127.31
24	a	409	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
24	b	615	CLA	C3B-C4B-NB	2.97	113.05	109.21
32	A	420[B]	PL9	C7-C3-C2	-2.96	119.40	123.30
26	c	518	BCR	C16-C17-C18	-2.96	123.08	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	O2A-CGA-CBA	2.96	121.20	111.91
32	A	420[A]	PL9	C22-C23-C24	-2.96	120.53	127.66
24	c	509	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
24	B	617	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
24	B	615	CLA	O2A-CGA-CBA	2.95	121.17	111.91
24	d	401	CLA	CHD-C4C-NC	2.95	128.85	124.20
24	b	615	CLA	CAC-C3C-C2C	2.95	132.58	127.53
24	c	515	CLA	CHD-C4C-NC	2.95	128.85	124.20
24	C	506	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	C	511	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
24	c	512	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	a	412	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
24	c	515	CLA	CMB-C2B-C3B	2.95	130.19	124.68
25	A	409[B]	PHO	C4-C3-C5	2.95	120.23	115.27
24	C	510	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
24	A	410	CLA	C3B-C4B-NB	2.94	113.02	109.21
24	B	616	CLA	C3B-C4B-NB	2.94	113.02	109.21
24	B	610	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
27	b	601	SQD	O8-S-C6	2.94	110.42	105.74
24	C	504	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
24	C	501	CLA	CHD-C4C-NC	2.94	128.83	124.20
24	B	605	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	c	515	CLA	CMC-C2C-C1C	2.94	129.51	125.04
24	B	609	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
24	A	410	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
24	c	511	CLA	CMC-C2C-C1C	2.93	129.50	125.04
24	c	513	CLA	O2A-CGA-CBA	2.93	121.11	111.91
24	b	614	CLA	O2A-CGA-CBA	2.93	121.11	111.91
38	d	406	LHG	O8-C23-C24	2.93	121.11	111.91
24	B	609	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
37	c	521	DGD	O1G-C1A-C2A	2.93	121.10	111.91
24	a	412	CLA	CHC-C1C-C2C	-2.93	118.63	126.72
32	d	405[A]	PL9	C40-C39-C41	2.92	120.19	115.27
24	B	609	CLA	CMA-C3A-C4A	-2.92	103.92	111.77
24	b	612	CLA	C3B-C4B-NB	2.92	112.99	109.21
24	c	517	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	C	511	CLA	C4-C3-C5	2.92	120.18	115.27
24	A	410	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
24	B	614	CLA	CAC-C3C-C4C	2.92	128.59	124.81
24	a	409	CLA	C2A-C1A-CHA	-2.92	118.76	123.86
26	b	628	BCR	C37-C22-C21	-2.92	118.84	122.92
24	b	612	CLA	C4-C3-C5	2.92	120.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	405[B]	PL9	C10-C9-C11	2.92	120.17	115.27
32	A	420[A]	PL9	C27-C28-C29	-2.91	120.64	127.66
27	b	601	SQD	C44-O6-C1	-2.91	108.05	113.74
24	b	623	CLA	O2A-CGA-CBA	2.91	121.05	111.91
24	C	503	CLA	O2A-CGA-CBA	2.91	121.05	111.91
24	c	515	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
25	a	420[B]	PHO	C4-C3-C5	2.91	120.16	115.27
24	d	403	CLA	CHD-C4C-NC	2.91	128.78	124.20
24	D	402	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
24	C	513	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	c	512	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
24	c	511	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	b	619	CLA	CHC-C1C-C2C	-2.90	118.69	126.72
24	B	603	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	c	509	CLA	C3B-C4B-NB	2.90	112.96	109.21
24	C	506	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
27	F	103	SQD	O48-C23-C24	2.90	121.00	111.91
26	c	518	BCR	C3-C4-C5	-2.90	108.90	114.08
26	B	618	BCR	C15-C14-C13	-2.90	123.18	127.31
24	C	505	CLA	C1-O2A-CGA	2.90	124.04	116.44
25	a	420[B]	PHO	O2D-CGD-O1D	-2.90	118.18	123.84
24	B	609	CLA	O2A-CGA-CBA	2.89	120.99	111.91
27	f	102	SQD	O5-C5-C4	2.89	114.95	109.69
24	D	402	CLA	C4-C3-C5	2.89	120.14	115.27
24	B	617	CLA	CHD-C4C-NC	2.89	128.76	124.20
24	c	513	CLA	CHD-C4C-NC	2.89	128.76	124.20
27	F	103	SQD	C3-C4-C5	2.89	115.39	110.24
32	A	420[A]	PL9	C42-C43-C44	-2.89	120.70	127.66
24	b	614	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
24	c	514	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
24	C	501	CLA	CBC-CAC-C3C	-2.88	104.49	112.43
24	b	618	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
24	c	515	CLA	O2A-CGA-CBA	2.88	120.94	111.91
24	b	619	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	C	509	CLA	O2A-CGA-CBA	2.88	120.93	111.91
26	c	527	BCR	C33-C5-C6	-2.87	121.30	124.53
24	b	613	CLA	O2A-CGA-CBA	2.87	120.93	111.91
26	c	527	BCR	C11-C10-C9	-2.87	123.21	127.31
24	C	510	CLA	CAC-C3C-C4C	2.87	128.54	124.81
24	C	507	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	B	615	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
24	C	502	CLA	O2A-CGA-O1A	-2.87	116.34	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
36	V	207	HTG	C1-C2-C3	-2.87	104.92	110.59
24	b	616	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
26	B	620	BCR	C10-C11-C12	-2.87	114.27	123.22
24	C	509	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
24	d	401	CLA	CBC-CAC-C3C	-2.87	104.53	112.43
24	d	402	CLA	C2A-C1A-CHA	-2.86	118.85	123.86
24	B	605	CLA	CHD-C4C-NC	2.86	128.72	124.20
24	C	502	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
24	C	501	CLA	C3B-C4B-NB	2.86	112.91	109.21
24	A	407	CLA	CHD-C4C-NC	2.86	128.71	124.20
24	c	516	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
24	C	503	CLA	CHD-C4C-NC	2.86	128.71	124.20
38	a	422	LHG	O7-C7-C8	2.86	117.67	111.50
32	a	416[A]	PL9	C35-C34-C36	2.86	120.08	115.27
24	a	410	CLA	C3B-C4B-NB	2.86	112.91	109.21
32	D	405[B]	PL9	C22-C23-C24	-2.86	120.77	127.66
38	d	406	LHG	O7-C7-C8	2.86	117.66	111.50
24	D	403	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
24	b	618	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
24	b	625	CLA	C4-C3-C5	2.85	120.07	115.27
32	d	405[B]	PL9	C37-C38-C39	-2.85	120.79	127.66
24	C	510	CLA	CHD-C4C-NC	2.85	128.70	124.20
37	D	406	DGD	O1G-C1A-C2A	2.85	120.86	111.91
26	H	102	BCR	C24-C23-C22	-2.85	121.93	126.23
24	c	513	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	c	511	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
24	c	510	CLA	C4-C3-C5	2.85	120.06	115.27
24	b	616	CLA	CAC-C3C-C4C	2.85	128.50	124.81
32	a	416[A]	PL9	C53-C6-C1	2.85	120.81	114.99
24	B	610	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
24	c	512	CLA	CAC-C3C-C4C	2.85	128.50	124.81
32	a	416[B]	PL9	C53-C6-C1	2.85	120.81	114.99
26	T	103	BCR	C36-C18-C19	2.84	122.56	118.08
24	b	622	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
32	A	420[A]	PL9	C53-C6-C1	2.84	120.80	114.99
32	a	416[A]	PL9	C25-C24-C26	2.84	120.05	115.27
25	a	411	PHO	C1A-C2A-C3A	-2.84	100.14	102.84
26	T	103	BCR	C12-C13-C14	-2.84	114.58	118.94
24	c	506	CLA	CAC-C3C-C4C	2.84	128.49	124.81
32	D	405[A]	PL9	C40-C39-C41	2.84	120.04	115.27
24	b	619	CLA	CMC-C2C-C1C	2.84	129.36	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
24	B	606	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
24	c	514	CLA	CBC-CAC-C3C	-2.83	104.63	112.43
24	C	505	CLA	CAC-C3C-C4C	2.83	128.48	124.81
24	B	617	CLA	CBC-CAC-C3C	-2.83	104.63	112.43
24	C	512	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
24	C	504	CLA	CMB-C2B-C3B	2.82	129.96	124.68
24	B	612	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	C	514	BCR	C38-C26-C25	-2.82	121.36	124.53
24	b	617	CLA	C4-C3-C5	2.82	120.02	115.27
24	b	624	CLA	CHD-C4C-NC	2.82	128.65	124.20
24	B	609	CLA	CHD-C4C-NC	2.82	128.64	124.20
24	C	508	CLA	C4-C3-C5	2.82	120.01	115.27
24	c	505	CLA	CMC-C2C-C1C	2.82	129.33	125.04
24	a	410	CLA	C4-C3-C5	2.82	120.01	115.27
24	b	616	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
26	k	101	BCR	C11-C10-C9	-2.81	123.29	127.31
27	A	416	SQD	O48-C23-O10	-2.81	116.49	123.59
24	C	509	CLA	CAC-C3C-C4C	2.81	128.46	124.81
24	C	502	CLA	CHD-C4C-NC	2.81	128.63	124.20
38	D	409	LHG	O8-C23-O10	-2.81	116.50	123.59
24	c	508	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
27	A	412	SQD	O48-C23-C24	2.81	120.72	111.91
24	b	622	CLA	CMB-C2B-C3B	2.81	129.93	124.68
26	h	101	BCR	C38-C26-C25	-2.81	121.38	124.53
24	a	410	CLA	O2A-CGA-O1A	-2.80	116.51	123.59
24	A	407	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	b	616	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	A	405	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	B	605	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
32	A	420[B]	PL9	C53-C6-C1	2.80	120.71	114.99
39	F	102	HEM	CHB-C1B-NB	2.80	127.84	124.38
24	C	509	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	d	403	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
32	A	420[B]	PL9	C27-C28-C29	-2.79	120.94	127.66
24	b	616	CLA	CHD-C4C-NC	2.79	128.60	124.20
32	D	405[A]	PL9	C22-C23-C24	-2.79	120.94	127.66
24	D	403	CLA	CMC-C2C-C1C	2.79	129.29	125.04
32	D	405[B]	PL9	C17-C18-C19	-2.79	120.94	127.66
32	A	420[B]	PL9	C15-C14-C16	2.79	119.96	115.27
24	c	513	CLA	CMC-C2C-C1C	2.79	129.28	125.04
24	b	621	CLA	CMC-C2C-C1C	2.79	129.28	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	BCR	C29-C30-C25	2.78	114.76	110.48
24	B	614	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
32	D	405[A]	PL9	C27-C28-C29	-2.78	120.96	127.66
24	c	513	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
24	B	615	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
24	B	602	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
26	Y	101	BCR	C16-C17-C18	-2.78	123.34	127.31
24	c	508	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
24	b	615	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
24	a	409	CLA	O2A-CGA-CBA	2.78	120.62	111.91
24	b	621	CLA	CHD-C4C-NC	2.78	128.58	124.20
34	z	101	LMG	O8-C28-C29	2.78	120.62	111.91
24	C	511	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
24	B	611	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	c	511	CLA	C3B-C4B-NB	2.77	112.80	109.21
24	B	615	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	c	516	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	C	505	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	C	509	CLA	CMB-C2B-C3B	2.77	129.86	124.68
24	c	516	CLA	C3B-C4B-NB	2.77	112.79	109.21
24	b	616	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
24	c	508	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	B	605	CLA	C1-C2-C3	-2.77	121.26	126.04
24	C	513	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
24	c	508	CLA	CAC-C3C-C4C	2.76	128.40	124.81
32	d	405[A]	PL9	C53-C6-C1	2.76	120.64	114.99
24	c	507	CLA	C1-C2-C3	-2.76	121.27	126.04
24	C	511	CLA	O2A-CGA-CBA	2.76	120.57	111.91
32	D	405[A]	PL9	C25-C24-C26	2.76	119.91	115.27
24	A	407	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
24	d	403	CLA	CMC-C2C-C1C	2.76	129.24	125.04
32	d	405[B]	PL9	C7-C8-C9	-2.76	122.20	126.79
26	t	101	BCR	C28-C27-C26	-2.76	109.15	114.08
24	a	409	CLA	CMC-C2C-C1C	2.76	129.24	125.04
27	A	416	SQD	O8-S-C6	2.76	110.14	105.74
24	b	620	CLA	O2A-CGA-CBA	2.76	120.56	111.91
24	a	410	CLA	C1-C2-C3	-2.76	121.28	126.04
24	c	508	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
32	A	420[B]	PL9	C42-C43-C44	-2.75	121.03	127.66
39	V	206	HEM	CHD-C1D-ND	2.75	127.42	124.43
32	d	405[A]	PL9	C15-C14-C16	2.75	119.90	115.27
24	b	612	CLA	CHC-C1C-C2C	-2.75	119.11	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	416[B]	PL9	C25-C24-C26	2.75	119.90	115.27
24	A	405	CLA	CMB-C2B-C3B	2.75	129.83	124.68
32	a	416[A]	PL9	C40-C39-C41	2.75	119.89	115.27
24	b	619	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
27	b	601	SQD	O48-C23-C24	2.75	120.53	111.91
32	D	405[B]	PL9	C53-C6-C1	2.75	120.61	114.99
24	B	608	CLA	CHC-C1C-C2C	-2.75	119.13	126.72
37	H	103	DGD	C3G-O3G-C1D	-2.75	108.38	113.74
24	B	610	CLA	CBC-CAC-C3C	-2.74	104.86	112.43
32	a	416[B]	PL9	C40-C39-C41	2.74	119.88	115.27
32	d	405[B]	PL9	C25-C24-C26	2.74	119.88	115.27
24	b	624	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
24	c	513	CLA	CAC-C3C-C4C	2.74	128.37	124.81
24	B	603	CLA	CHD-C4C-NC	2.74	128.52	124.20
24	D	402	CLA	O2A-CGA-CBA	2.74	120.50	111.91
24	b	624	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
24	B	616	CLA	CAC-C3C-C4C	2.74	128.36	124.81
24	b	621	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
24	b	621	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	B	611	CLA	CMA-C3A-C4A	-2.74	104.42	111.77
24	b	617	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
24	c	515	CLA	C4-C3-C5	2.73	119.87	115.27
24	B	608	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	D	403	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	a	410	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
24	B	606	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
24	B	610	CLA	CMC-C2C-C1C	2.73	129.19	125.04
34	b	630	LMG	O8-C28-C29	2.73	120.47	111.91
36	d	411	HTG	C1-O5-C5	2.73	117.61	112.58
24	b	613	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
24	c	517	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
24	B	606	CLA	CED-O2D-CGD	2.73	122.10	115.94
38	L	101	LHG	O8-C23-C24	2.72	120.46	111.91
24	c	511	CLA	C4-C3-C5	2.72	119.85	115.27
24	c	507	CLA	O2A-CGA-CBA	2.72	120.45	111.91
25	a	411	PHO	CMA-C3A-C4A	-2.72	108.41	114.38
25	a	411	PHO	C1-O2A-CGA	2.72	123.58	116.44
24	a	412	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
24	c	513	CLA	C4-C3-C5	2.72	119.85	115.27
24	c	514	CLA	CHD-C4C-NC	2.72	128.49	124.20
32	D	405[B]	PL9	C27-C28-C29	-2.72	121.11	127.66
36	b	633	HTG	C1-O5-C5	2.72	117.59	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
24	d	403	CLA	C4-C3-C5	2.72	119.84	115.27
26	T	103	BCR	C35-C13-C12	2.72	122.36	118.08
24	b	618	CLA	CHD-C4C-NC	2.71	128.48	124.20
32	D	405[B]	PL9	C12-C13-C14	-2.71	121.12	127.66
24	b	618	CLA	O2A-CGA-CBA	2.71	120.42	111.91
32	A	420[A]	PL9	C45-C44-C46	2.71	119.83	115.27
24	b	618	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
26	d	404	BCR	C28-C27-C26	-2.71	109.23	114.08
24	C	511	CLA	CHD-C4C-NC	2.71	128.48	124.20
24	c	516	CLA	O2A-CGA-CBA	2.71	120.41	111.91
24	d	403	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
24	C	511	CLA	CMC-C2C-C1C	2.71	129.16	125.04
24	A	406	CLA	CMA-C3A-C4A	-2.71	104.50	111.77
24	a	409	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
24	D	402	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
24	B	603	CLA	CMB-C2B-C3B	2.71	129.74	124.68
32	A	420[A]	PL9	C15-C14-C16	2.71	119.82	115.27
24	c	517	CLA	C4-C3-C5	2.70	119.82	115.27
24	c	516	CLA	C4-C3-C5	2.70	119.82	115.27
24	b	624	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
32	d	405[A]	PL9	C20-C19-C21	2.70	119.82	115.27
24	b	624	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
32	A	420[B]	PL9	C25-C24-C26	2.70	119.82	115.27
29	B	635	LMT	C1'-O5'-C5'	2.70	118.99	113.69
24	C	513	CLA	O2A-CGA-CBA	2.70	120.38	111.91
24	B	606	CLA	C3B-C4B-NB	2.70	112.70	109.21
32	a	416[A]	PL9	C30-C29-C31	2.70	119.81	115.27
24	B	612	CLA	CMA-C3A-C4A	-2.70	104.52	111.77
24	D	403	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
26	b	629	BCR	C38-C26-C25	-2.70	121.50	124.53
24	C	506	CLA	C1-C2-C3	-2.70	121.38	126.04
24	A	410	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
24	b	625	CLA	CBC-CAC-C3C	-2.70	105.00	112.43
24	c	515	CLA	C4C-C3C-C2C	-2.70	102.97	106.90
32	A	420[A]	PL9	C25-C24-C26	2.70	119.81	115.27
24	A	406	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
24	B	608	CLA	C1-C2-C3	-2.69	121.38	126.04
24	c	506	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
24	C	501	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
24	C	509	CLA	C4-C3-C5	2.69	119.79	115.27
24	A	407	CLA	C4C-C3C-C2C	-2.69	102.98	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	506	CLA	CHD-C4C-NC	2.69	128.44	124.20
24	C	513	CLA	CMC-C2C-C1C	2.69	129.13	125.04
24	C	509	CLA	CHD-C4C-NC	2.68	128.43	124.20
34	Z	101	LMG	C1-O6-C5	2.68	118.95	113.69
24	C	502	CLA	CAC-C3C-C4C	2.68	128.29	124.81
26	b	627	BCR	C15-C14-C13	-2.68	123.48	127.31
26	t	101	BCR	C7-C8-C9	-2.68	122.19	126.23
24	B	604	CLA	O2A-CGA-CBA	2.68	120.32	111.91
37	C	516	DGD	O3G-C3G-C2G	-2.68	104.44	110.90
24	A	405	CLA	CAA-C2A-C1A	-2.68	103.20	111.97
39	V	206	HEM	CHA-C4D-ND	2.68	127.69	124.38
24	B	613	CLA	CHD-C4C-NC	2.68	128.42	124.20
24	A	406	CLA	C4-C3-C5	2.68	119.77	115.27
24	A	407	CLA	C3B-C4B-NB	2.67	112.67	109.21
39	F	102	HEM	CHD-C1D-ND	2.67	127.34	124.43
24	d	401	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
24	a	410	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	a	420[A]	PHO	CMA-C3A-C4A	-2.67	108.53	114.38
24	b	615	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
32	d	405[A]	PL9	C10-C9-C11	2.67	119.76	115.27
25	a	420[B]	PHO	CMB-C2B-C3B	2.67	129.67	124.68
32	a	416[B]	PL9	C35-C34-C36	2.67	119.76	115.27
24	b	613	CLA	CHC-C1C-C2C	-2.67	119.35	126.72
34	a	415	LMG	O8-C28-C29	2.67	120.27	111.91
24	c	507	CLA	CHD-C4C-NC	2.67	128.40	124.20
24	B	612	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
24	b	620	CLA	CHD-C4C-NC	2.66	128.40	124.20
24	C	501	CLA	C1-O2A-CGA	2.66	123.43	116.44
26	h	101	BCR	C11-C10-C9	-2.66	123.52	127.31
24	b	611	CLA	CMB-C2B-C3B	2.66	129.65	124.68
24	b	626	CLA	CHD-C4C-NC	2.66	128.39	124.20
36	B	625	HTG	C1-O5-C5	2.66	117.48	112.58
25	A	409[A]	PHO	O2D-CGD-O1D	-2.66	118.65	123.84
24	C	510	CLA	O2A-CGA-CBA	2.65	120.23	111.91
26	k	101	BCR	C10-C11-C12	-2.65	114.94	123.22
27	a	414	SQD	O48-C23-C24	2.65	120.23	111.91
32	d	405[B]	PL9	C20-C19-C21	2.65	119.73	115.27
38	d	407	LHG	C6-C5-C4	-2.65	105.52	111.79
24	A	407	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
24	C	508	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	C	503	CLA	CAC-C3C-C4C	2.65	128.25	124.81
26	K	101	BCR	C38-C26-C25	-2.65	121.55	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
24	c	511	CLA	CHD-C4C-NC	2.65	128.38	124.20
24	B	609	CLA	CMB-C2B-C3B	2.65	129.63	124.68
24	C	507	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	b	615	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
24	d	402	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
24	C	512	CLA	C4-C3-C5	2.65	119.72	115.27
24	b	621	CLA	CMA-C3A-C4A	-2.65	104.66	111.77
26	t	101	BCR	C7-C6-C5	-2.65	115.05	121.46
24	c	514	CLA	CMA-C3A-C4A	-2.64	104.67	111.77
32	D	405[B]	PL9	C51-C49-C50	2.64	120.44	114.60
26	h	101	BCR	C7-C8-C9	-2.64	122.25	126.23
24	C	509	CLA	CMC-C2C-C1C	2.64	129.06	125.04
27	b	601	SQD	O7-S-C6	2.64	110.08	106.94
26	t	101	BCR	C1-C6-C7	2.64	123.24	115.78
24	B	605	CLA	OBD-CAD-C3D	-2.64	122.17	128.52
24	A	410	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	A	406	CLA	CAA-CBA-CGA	2.64	120.96	113.25
26	y	101	BCR	C38-C26-C25	-2.64	121.57	124.53
38	D	407	LHG	O8-C23-O10	-2.63	116.94	123.59
24	C	509	CLA	C1-O2A-CGA	2.63	123.35	116.44
24	c	510	CLA	CMB-C2B-C3B	2.63	129.60	124.68
24	B	609	CLA	CMC-C2C-C1C	2.63	129.05	125.04
24	C	513	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
24	b	619	CLA	O2A-CGA-CBA	2.63	120.17	111.91
26	c	527	BCR	C28-C27-C26	-2.63	109.38	114.08
24	b	619	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
24	d	403	CLA	CAA-C2A-C3A	-2.63	105.58	112.78
24	b	613	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
24	b	618	CLA	CMB-C2B-C3B	2.63	129.60	124.68
24	a	410	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
24	c	517	CLA	O2A-CGA-CBA	2.63	120.15	111.91
24	C	502	CLA	O2A-CGA-CBA	2.63	120.15	111.91
24	a	410	CLA	CMC-C2C-C1C	2.63	129.04	125.04
24	c	512	CLA	CMC-C2C-C1C	2.63	129.04	125.04
24	B	611	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
27	B	621	SQD	O48-C23-C24	2.63	120.15	111.91
37	H	103	DGD	O1G-C1A-O1A	-2.62	116.97	123.59
24	d	402	CLA	CMC-C2C-C1C	2.62	129.03	125.04
24	b	625	CLA	C11-C10-C8	-2.62	107.44	115.92
24	C	513	CLA	C3B-C4B-NB	2.62	112.60	109.21
24	A	407	CLA	CMC-C2C-C1C	2.62	129.03	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
24	C	513	CLA	C4-C3-C5	2.62	119.68	115.27
32	A	420[B]	PL9	C45-C44-C46	2.62	119.68	115.27
24	C	510	CLA	CMB-C2B-C3B	2.62	129.58	124.68
24	B	611	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	b	622	CLA	CMC-C2C-C1C	2.62	129.03	125.04
36	C	523	HTG	O5-C1-C2	2.62	113.61	110.31
24	c	514	CLA	CMB-C2B-C3B	2.62	129.58	124.68
24	b	612	CLA	C1-C2-C3	-2.62	121.52	126.04
32	D	405[B]	PL9	C45-C44-C46	2.62	119.67	115.27
32	d	405[B]	PL9	C45-C44-C46	2.62	119.67	115.27
27	b	601	SQD	O47-C7-O49	-2.62	117.38	123.70
34	c	523	LMG	C8-O7-C10	-2.62	111.35	117.79
24	C	512	CLA	O2A-CGA-CBA	2.62	120.12	111.91
24	a	412	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
24	c	512	CLA	C1-C2-C3	-2.61	121.52	126.04
34	C	520	LMG	O8-C28-C29	2.61	120.11	111.91
24	b	616	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
39	v	205	HEM	CHB-C1B-NB	2.61	127.61	124.38
25	A	409[B]	PHO	CMB-C2B-C3B	2.61	129.57	124.68
24	c	516	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
32	A	420[B]	PL9	C12-C13-C14	-2.61	121.37	127.66
34	j	101	LMG	O7-C10-C11	2.61	117.13	111.50
24	C	501	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
37	C	517	DGD	O1G-C1A-C2A	2.61	120.10	111.91
32	A	420[A]	PL9	C30-C29-C31	2.61	119.66	115.27
36	b	609	HTG	C1-O5-C5	2.61	117.39	112.58
39	F	102	HEM	CBD-CAD-C3D	-2.61	105.38	112.63
24	a	409	CLA	CHD-C4C-NC	2.61	128.32	124.20
24	c	514	CLA	O2A-CGA-CBA	2.61	120.09	111.91
32	d	405[A]	PL9	C12-C13-C14	-2.61	121.38	127.66
26	C	515	BCR	C24-C23-C22	-2.61	122.30	126.23
24	A	410	CLA	CHD-C4C-NC	2.60	128.31	124.20
24	c	512	CLA	CAA-C2A-C3A	-2.60	105.65	112.78
24	B	608	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	C	501	CLA	C4-C3-C5	2.60	119.65	115.27
24	c	516	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
24	b	619	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
24	A	406	CLA	CED-O2D-CGD	2.60	121.81	115.94
24	c	517	CLA	CAC-C3C-C4C	2.60	128.18	124.81
32	A	420[B]	PL9	C10-C9-C11	2.60	119.64	115.27
24	B	614	CLA	O2A-CGA-CBA	2.60	120.05	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	101	BCR	C11-C10-C9	-2.60	123.61	127.31
24	c	508	CLA	CHD-C4C-NC	2.59	128.29	124.20
24	b	623	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
24	b	624	CLA	O2A-CGA-CBA	2.59	120.03	111.91
32	D	405[B]	PL9	C25-C24-C26	2.59	119.63	115.27
32	A	420[A]	PL9	C12-C13-C14	-2.59	121.43	127.66
26	T	103	BCR	C34-C9-C10	-2.59	119.30	122.92
24	b	614	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
24	b	619	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
24	b	626	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
24	B	609	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
24	B	605	CLA	CMC-C2C-C1C	2.58	128.97	125.04
26	k	101	BCR	C15-C14-C13	-2.58	123.63	127.31
27	f	102	SQD	O48-C23-C24	2.58	120.00	111.91
24	c	511	CLA	O1D-CGD-CBD	-2.58	119.21	124.48
32	D	405[B]	PL9	C20-C19-C21	2.58	119.61	115.27
24	c	512	CLA	C2A-C1A-CHA	-2.58	119.36	123.86
24	b	619	CLA	C4-C3-C5	2.58	119.60	115.27
24	C	504	CLA	CHD-C4C-NC	2.58	128.26	124.20
39	V	206	HEM	C4D-ND-C1D	2.58	107.73	105.07
24	c	517	CLA	C2A-C1A-CHA	-2.58	119.36	123.86
24	B	606	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
37	C	518	DGD	O1G-C1A-C2A	2.57	119.98	111.91
24	C	506	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
24	B	607	CLA	O2A-CGA-CBA	2.57	119.97	111.91
24	B	615	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
24	C	505	CLA	CHD-C4C-NC	2.57	128.25	124.20
29	M	103	LMT	O5'-C5'-C4'	2.57	115.17	109.75
24	a	412	CLA	O2A-CGA-CBA	2.57	119.96	111.91
24	c	508	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
39	V	206	HEM	CAD-CBD-CGD	2.57	119.12	113.60
26	h	101	BCR	C16-C15-C14	-2.56	118.22	123.47
24	B	616	CLA	CBC-CAC-C3C	-2.56	105.36	112.43
24	D	403	CLA	CHD-C4C-NC	2.56	128.24	124.20
34	A	422	LMG	C8-O7-C10	-2.56	111.49	117.79
24	b	614	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
32	D	405[A]	PL9	C53-C6-C1	2.56	120.22	114.99
26	h	101	BCR	C10-C11-C12	-2.56	115.23	123.22
24	B	604	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
24	A	407	CLA	C1-C2-C3	-2.56	121.62	126.04
24	B	607	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
38	a	422	LHG	O8-C23-C24	2.56	119.93	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	CMB-C2B-C3B	2.56	129.46	124.68
24	B	608	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
34	c	522	LMG	O8-C28-O10	-2.56	117.14	123.59
24	C	506	CLA	CHD-C4C-NC	2.56	128.23	124.20
24	B	616	CLA	CHC-C1C-C2C	-2.56	119.65	126.72
24	c	517	CLA	C3B-C4B-NB	2.55	112.51	109.21
26	b	629	BCR	C2-C1-C6	2.55	114.41	110.48
36	B	625	HTG	C1-C2-C3	2.55	115.63	110.59
24	C	503	CLA	C3B-C4B-NB	2.55	112.51	109.21
37	C	517	DGD	C2G-O2G-C1B	-2.55	111.51	117.79
39	e	102	HEM	CBD-CAD-C3D	-2.55	105.54	112.63
24	C	512	CLA	CMC-C2C-C1C	2.55	128.92	125.04
26	b	629	BCR	C24-C23-C22	-2.55	122.38	126.23
32	a	416[A]	PL9	C51-C49-C50	2.55	120.23	114.60
24	C	507	CLA	C1-C2-C3	-2.55	121.64	126.04
24	B	615	CLA	CHD-C4C-NC	2.55	128.21	124.20
24	c	506	CLA	O2A-CGA-CBA	2.54	119.89	111.91
24	c	516	CLA	CMB-C2B-C3B	2.54	129.43	124.68
24	A	407	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	a	410	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
24	D	403	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
24	b	620	CLA	C4-C3-C5	2.54	119.55	115.27
34	c	523	LMG	O8-C28-C29	2.54	119.88	111.91
24	d	403	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	B	611	CLA	CAA-CBA-CGA	-2.54	105.84	113.25
24	B	616	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
32	A	420[A]	PL9	C17-C18-C19	-2.54	121.56	127.66
24	c	511	CLA	O2A-CGA-CBA	2.53	119.86	111.91
27	A	412	SQD	O47-C7-O49	-2.53	117.58	123.70
24	B	612	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
32	d	405[B]	PL9	C15-C14-C16	2.53	119.53	115.27
24	C	501	CLA	CAC-C3C-C4C	2.53	128.09	124.81
32	D	405[A]	PL9	C20-C19-C21	2.53	119.53	115.27
24	c	512	CLA	CHD-C4C-NC	2.53	128.19	124.20
36	c	525	HTG	C1-O5-C5	2.53	117.24	112.58
24	c	507	CLA	C3B-C4B-NB	2.53	112.47	109.21
24	C	507	CLA	CHC-C1C-C2C	-2.52	119.74	126.72
24	b	625	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	B	602	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
37	c	519	DGD	O2G-C1B-O1B	-2.52	117.61	123.70
24	c	506	CLA	C1-C2-C3	-2.52	121.68	126.04
24	C	505	CLA	CMC-C2C-C1C	2.52	128.88	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	402	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
24	c	517	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
24	a	412	CLA	CMA-C3A-C2A	-2.52	103.67	113.83
24	B	604	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
24	B	607	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
24	A	405	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
24	b	619	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
24	B	617	CLA	CAC-C3C-C4C	2.51	128.07	124.81
24	B	611	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
24	C	513	CLA	CMB-C2B-C3B	2.51	129.38	124.68
24	B	613	CLA	CMB-C2B-C3B	2.51	129.38	124.68
24	C	503	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
24	b	621	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
24	A	405	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
27	f	102	SQD	O47-C7-O49	-2.51	117.64	123.70
27	a	414	SQD	C1-O5-C5	-2.51	108.77	113.69
24	c	509	CLA	C4-C3-C5	2.51	119.49	115.27
24	b	612	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	b	620	CLA	CAA-C2A-C3A	-2.51	105.92	112.78
32	d	405[B]	PL9	C10-C9-C11	2.51	119.49	115.27
24	C	505	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
32	d	405[B]	PL9	C53-C6-C1	2.50	120.11	114.99
24	a	412	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
24	C	513	CLA	CHD-C4C-NC	2.50	128.14	124.20
24	b	624	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
38	L	101	LHG	O8-C23-O10	-2.50	117.29	123.59
27	b	601	SQD	C1-C2-C3	-2.50	104.79	110.00
24	A	407	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
32	a	416[B]	PL9	C51-C49-C50	2.50	120.12	114.60
24	D	403	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
24	a	410	CLA	CAC-C3C-C4C	2.49	128.05	124.81
24	C	506	CLA	CMC-C2C-C1C	2.49	128.83	125.04
24	A	410	CLA	O2A-CGA-CBA	2.49	119.72	111.91
36	b	609	HTG	O5-C1-C2	2.49	113.44	110.31
26	y	101	BCR	C21-C20-C19	-2.49	115.45	123.22
24	A	410	CLA	CED-O2D-CGD	2.49	121.56	115.94
32	a	416[B]	PL9	C30-C29-C31	2.49	119.46	115.27
24	C	502	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
24	A	410	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
24	b	624	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
34	Z	101	LMG	C8-O7-C10	-2.48	111.67	117.79
26	c	527	BCR	C29-C30-C25	2.48	114.30	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	515	BCR	C15-C14-C13	-2.48	123.77	127.31
24	C	510	CLA	CMC-C2C-C1C	2.48	128.82	125.04
32	A	420[B]	PL9	C30-C29-C31	2.48	119.44	115.27
38	D	408	LHG	O8-C23-O10	-2.48	117.33	123.59
24	b	626	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	b	624	CLA	CMB-C2B-C3B	2.48	129.31	124.68
26	C	515	BCR	C21-C20-C19	-2.48	115.49	123.22
24	c	510	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
25	A	408	PHO	CMA-C3A-C4A	-2.48	108.95	114.38
24	c	512	CLA	C4-C3-C5	2.48	119.44	115.27
24	c	505	CLA	O2A-CGA-CBA	2.47	119.67	111.91
37	C	516	DGD	O1G-C1A-O1A	-2.47	117.35	123.59
24	A	407	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
24	C	507	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
24	c	510	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
24	b	626	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
24	b	613	CLA	CHD-C4C-NC	2.47	128.10	124.20
24	C	507	CLA	C3B-C4B-NB	2.47	112.40	109.21
24	B	609	CLA	CHB-C4A-NA	2.47	127.92	124.51
24	B	614	CLA	CHB-C4A-NA	2.47	127.92	124.51
34	B	622	LMG	O1-C7-C8	-2.47	104.95	110.90
37	e	101	DGD	O1G-C1A-C2A	2.47	119.65	111.91
24	b	623	CLA	CHD-C4C-NC	2.47	128.09	124.20
24	B	612	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
24	b	623	CLA	CMA-C3A-C4A	-2.46	105.15	111.77
26	B	620	BCR	C2-C1-C6	2.46	114.28	110.48
24	d	401	CLA	CMA-C3A-C2A	-2.46	103.90	113.83
24	B	611	CLA	CHD-C4C-NC	2.46	128.08	124.20
27	a	405	SQD	O48-C23-O10	-2.46	117.39	123.59
24	c	508	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
25	A	409[B]	PHO	O2D-CGD-O1D	-2.46	119.03	123.84
26	Y	101	BCR	C28-C27-C26	-2.46	109.69	114.08
24	C	503	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
26	a	413	BCR	C15-C14-C13	-2.45	123.81	127.31
24	B	608	CLA	CHD-C4C-NC	2.45	128.07	124.20
25	a	420[A]	PHO	CMC-C2C-C3C	2.45	129.57	124.94
26	b	628	BCR	C8-C7-C6	-2.45	120.31	127.20
24	c	510	CLA	CMC-C2C-C1C	2.45	128.77	125.04
24	b	614	CLA	CHD-C4C-NC	2.45	128.07	124.20
27	F	103	SQD	C1-C2-C3	-2.45	104.89	110.00
32	A	420[B]	PL9	C17-C18-C19	-2.45	121.77	127.66
26	c	518	BCR	C38-C26-C25	-2.45	121.78	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	514	BCR	C11-C10-C9	-2.45	123.82	127.31
24	c	512	CLA	O2A-CGA-CBA	2.44	119.58	111.91
24	b	615	CLA	C1-C2-C3	-2.44	121.82	126.04
26	T	103	BCR	C21-C20-C19	-2.44	115.59	123.22
24	c	517	CLA	CMB-C2B-C3B	2.44	129.24	124.68
26	t	101	BCR	C12-C13-C14	-2.44	115.20	118.94
24	c	517	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
27	a	414	SQD	C45-O47-C7	-2.44	111.79	117.79
24	B	615	CLA	C1-C2-C3	-2.44	121.83	126.04
24	b	611	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
24	c	507	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
24	b	614	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
26	K	101	BCR	C10-C11-C12	-2.44	115.61	123.22
24	c	507	CLA	C4-C3-C5	2.44	119.37	115.27
32	A	420[B]	PL9	C40-C39-C41	2.44	119.37	115.27
24	B	604	CLA	CMA-C3A-C2A	-2.44	104.00	113.83
24	b	623	CLA	CED-O2D-CGD	2.43	121.44	115.94
24	C	504	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
26	t	101	BCR	C21-C20-C19	-2.43	115.63	123.22
24	B	605	CLA	O2A-CGA-CBA	2.43	119.53	111.91
38	d	408	LHG	O8-C23-C24	2.43	119.53	111.91
24	b	626	CLA	C1-C2-C3	-2.43	121.84	126.04
24	b	626	CLA	C4-C3-C5	2.43	119.35	115.27
32	A	420[A]	PL9	C10-C9-C11	2.43	119.35	115.27
34	j	101	LMG	O6-C5-C4	2.43	114.10	109.69
24	C	507	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
24	c	517	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
24	c	516	CLA	CBA-CAA-C2A	-2.42	106.71	113.86
24	C	502	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
24	B	605	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	b	617	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
24	B	615	CLA	CMB-C2B-C3B	2.42	129.20	124.68
24	A	410	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
27	F	103	SQD	O47-C7-O49	-2.42	117.86	123.70
24	c	507	CLA	CHC-C1C-C2C	-2.42	120.03	126.72
37	C	516	DGD	C2G-O2G-C1B	-2.42	111.84	117.79
34	Z	101	LMG	C9-O8-C28	2.41	123.17	117.10
29	m	102	LMT	O5'-C5'-C4'	2.41	114.84	109.75
32	D	405[A]	PL9	C12-C13-C14	-2.41	121.85	127.66
24	d	403	CLA	O2A-CGA-CBA	2.41	119.47	111.91
27	A	412	SQD	C1-C2-C3	-2.41	104.97	110.00
24	a	412	CLA	C2A-C1A-CHA	-2.41	119.64	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
37	h	102	DGD	C2G-O2G-C1B	-2.41	111.86	117.79
24	c	510	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
25	A	408	PHO	C4-C3-C5	2.41	119.32	115.27
24	A	406	CLA	CHB-C4A-NA	2.41	127.84	124.51
39	V	206	HEM	O2D-CGD-CBD	2.41	121.76	114.03
24	b	618	CLA	C1-C2-C3	-2.41	121.88	126.04
24	B	611	CLA	C4-C3-C5	2.41	119.32	115.27
26	A	411	BCR	C24-C23-C22	-2.40	122.60	126.23
24	c	507	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
24	b	619	CLA	CED-O2D-CGD	2.40	121.38	115.94
24	a	410	CLA	CMB-C2B-C3B	2.40	129.17	124.68
24	b	625	CLA	CHA-C1A-NA	-2.40	120.90	126.40
24	c	505	CLA	CMB-C2B-C3B	2.40	129.17	124.68
24	B	614	CLA	CMC-C2C-C1C	2.40	128.69	125.04
32	D	405[A]	PL9	C15-C14-C16	2.40	119.31	115.27
24	b	612	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
24	B	607	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
24	D	402	CLA	CHD-C4C-NC	2.40	127.98	124.20
24	c	513	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
37	C	516	DGD	C3G-C2G-C1G	-2.40	106.12	111.79
24	C	512	CLA	CAC-C3C-C4C	2.40	127.92	124.81
24	a	412	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	B	603	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
24	B	614	CLA	OBD-CAD-C3D	-2.39	122.76	128.52
26	C	515	BCR	C28-C27-C26	-2.39	109.81	114.08
26	H	102	BCR	C29-C30-C25	2.39	114.16	110.48
24	C	510	CLA	C4-C3-C2	-2.39	117.55	123.68
26	b	628	BCR	C28-C27-C26	-2.39	109.81	114.08
24	C	502	CLA	C4-C3-C5	2.39	119.29	115.27
34	D	412	LMG	C9-C8-C7	-2.39	106.14	111.79
27	A	412	SQD	O48-C23-O10	-2.38	117.57	123.59
38	D	408	LHG	O7-C7-C8	2.38	116.64	111.50
24	B	603	CLA	CAC-C3C-C4C	2.38	127.90	124.81
24	a	409	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
24	b	617	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
24	c	510	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
27	A	412	SQD	C44-O6-C1	-2.38	109.10	113.74
37	e	101	DGD	C1E-O6E-C5E	2.38	118.35	113.69
32	D	405[A]	PL9	C45-C44-C46	2.37	119.26	115.27
24	B	617	CLA	O2A-CGA-CBA	2.37	119.36	111.91
24	D	402	CLA	CAA-C2A-C3A	-2.37	106.28	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	614	CLA	CED-O2D-CGD	2.37	121.30	115.94
24	A	405	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
32	D	405[A]	PL9	C17-C18-C19	-2.37	121.95	127.66
34	z	101	LMG	C8-O7-C10	-2.37	111.95	117.79
24	B	607	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	C	513	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
29	M	103	LMT	O1B-C1B-C2B	2.37	114.24	108.10
24	B	611	CLA	CMB-C2B-C3B	2.37	129.11	124.68
24	c	508	CLA	O2A-CGA-CBA	2.37	119.34	111.91
24	C	505	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	b	615	CLA	O2A-CGA-CBA	2.37	119.33	111.91
24	a	410	CLA	CAA-CBA-CGA	2.37	120.17	113.25
26	K	101	BCR	C16-C17-C18	-2.37	123.93	127.31
24	b	613	CLA	CMB-C2B-C3B	2.36	129.10	124.68
24	d	402	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	c	513	CLA	CMB-C2B-C3B	2.36	129.09	124.68
24	c	506	CLA	O2A-C1-C2	2.36	114.83	108.64
37	C	518	DGD	O3G-C3G-C2G	-2.36	105.21	110.90
24	B	603	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
32	d	405[B]	PL9	C12-C13-C14	-2.36	121.98	127.66
34	c	522	LMG	C8-O7-C10	-2.36	111.99	117.79
24	c	513	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
24	d	401	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
24	d	403	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
24	b	616	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
24	c	512	CLA	CMB-C2B-C3B	2.35	129.08	124.68
34	Z	101	LMG	C1-C2-C3	2.35	114.89	110.00
37	D	406	DGD	O6D-C5D-C6D	2.35	111.41	106.67
37	H	103	DGD	C3E-C4E-C5E	-2.35	106.05	110.24
24	C	513	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
24	B	602	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
26	b	628	BCR	C24-C23-C22	-2.35	122.69	126.23
24	A	406	CLA	C2A-C1A-CHA	-2.35	119.76	123.86
24	B	611	CLA	CGD-CBD-CAD	-2.34	103.14	110.73
38	d	406	LHG	O7-C7-O9	-2.34	118.04	123.70
25	a	411	PHO	CBA-CAA-C2A	-2.34	106.97	113.81
24	B	612	CLA	O2A-CGA-CBA	2.34	119.25	111.91
37	c	521	DGD	C2G-O2G-C1B	-2.34	112.03	117.79
26	K	101	BCR	C37-C22-C21	-2.34	119.65	122.92
24	C	504	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
24	B	611	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
32	a	416[A]	PL9	C45-C44-C46	2.34	119.20	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	101	BCR	C37-C22-C23	2.33	121.75	118.08
24	c	513	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
24	b	612	CLA	CHD-C4C-NC	2.33	127.88	124.20
26	K	101	BCR	C33-C5-C6	-2.33	121.91	124.53
26	a	413	BCR	C38-C26-C25	-2.33	121.91	124.53
24	A	410	CLA	CMA-C3A-C2A	-2.33	104.43	113.83
32	A	420[A]	PL9	C40-C39-C41	2.33	119.19	115.27
32	D	405[A]	PL9	C35-C34-C36	2.33	119.19	115.27
24	b	618	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	b	619	CLA	C1-O2A-CGA	2.33	122.55	116.44
24	a	409	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	B	620	BCR	C28-C27-C26	-2.33	109.92	114.08
26	d	404	BCR	C39-C30-C25	-2.33	106.53	110.30
34	A	422	LMG	O8-C28-C29	2.33	119.20	111.91
32	a	416[B]	PL9	C12-C13-C14	-2.33	122.06	127.66
26	b	628	BCR	C33-C5-C6	-2.33	121.92	124.53
24	B	613	CLA	O2A-CGA-CBA	2.32	119.20	111.91
24	b	618	CLA	CAC-C3C-C4C	2.32	127.83	124.81
24	b	617	CLA	C4C-C3C-C2C	-2.32	103.51	106.90
24	c	506	CLA	CMC-C2C-C1C	2.32	128.58	125.04
37	c	519	DGD	O3G-C3G-C2G	-2.32	105.30	110.90
24	a	409	CLA	CAC-C3C-C4C	2.32	127.82	124.81
24	B	608	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
24	C	501	CLA	C1-C2-C3	-2.32	122.03	126.04
24	a	409	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
24	a	410	CLA	O2A-CGA-CBA	2.32	119.17	111.91
24	A	407	CLA	CAA-CBA-CGA	2.32	120.02	113.25
26	d	404	BCR	C29-C28-C27	-2.31	106.20	111.38
24	d	403	CLA	CMB-C2B-C3B	2.31	129.01	124.68
24	a	412	CLA	CAC-C3C-C4C	2.31	127.81	124.81
24	B	604	CLA	C1-O2A-CGA	2.31	122.51	116.44
24	A	405	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
32	d	405[A]	PL9	C45-C44-C46	2.31	119.16	115.27
26	C	515	BCR	C11-C10-C9	-2.31	124.02	127.31
32	D	405[B]	PL9	C36-C37-C38	-2.31	104.30	111.88
26	K	101	BCR	C3-C4-C5	-2.31	109.96	114.08
24	A	410	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
26	a	413	BCR	C40-C30-C25	-2.31	106.56	110.30
24	d	403	CLA	CGD-CBD-CAD	-2.31	103.27	110.73
38	D	407	LHG	C5-O7-C7	-2.31	112.11	117.79
24	b	621	CLA	O2A-CGA-CBA	2.30	119.14	111.91
26	C	515	BCR	C37-C22-C23	2.30	121.71	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
24	b	620	CLA	CMB-C2B-C3B	2.30	128.98	124.68
24	B	616	CLA	C4-C3-C5	2.30	119.14	115.27
26	H	102	BCR	C37-C22-C21	-2.30	119.71	122.92
24	c	509	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
24	c	505	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
24	b	622	CLA	CED-O2D-CGD	2.29	121.12	115.94
32	D	405[A]	PL9	C32-C33-C34	-2.29	122.14	127.66
26	k	101	BCR	C2-C1-C6	2.29	114.01	110.48
24	b	618	CLA	C4-C3-C5	2.29	119.12	115.27
24	D	402	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
24	C	504	CLA	C1-O2A-CGA	2.29	122.45	116.44
24	A	405	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	c	518	BCR	C11-C10-C9	-2.29	124.05	127.31
24	c	511	CLA	CAC-C3C-C4C	2.28	127.77	124.81
26	B	618	BCR	C11-C10-C9	-2.28	124.05	127.31
26	y	101	BCR	C10-C11-C12	-2.28	116.09	123.22
24	c	507	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
24	B	603	CLA	C4-C3-C5	2.28	119.11	115.27
26	c	527	BCR	C35-C13-C14	-2.28	119.73	122.92
26	H	102	BCR	C7-C8-C9	-2.28	122.79	126.23
24	c	509	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
24	B	603	CLA	CMC-C2C-C1C	2.28	128.51	125.04
24	D	403	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
36	b	633	HTG	C1-C2-C3	2.28	115.08	110.59
24	c	516	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
24	b	626	CLA	CMB-C2B-C3B	2.28	128.94	124.68
24	b	625	CLA	O2A-CGA-CBA	2.27	119.05	111.91
24	C	507	CLA	CAC-C3C-C4C	2.27	127.76	124.81
24	b	622	CLA	CHD-C4C-NC	2.27	127.78	124.20
26	y	101	BCR	C24-C23-C22	-2.27	122.80	126.23
32	A	420[B]	PL9	C8-C7-C3	2.27	118.40	111.98
24	c	509	CLA	CMC-C2C-C1C	2.27	128.50	125.04
24	C	507	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
24	b	617	CLA	CAA-CBA-CGA	2.27	119.89	113.25
32	a	416[B]	PL9	C45-C44-C46	2.27	119.09	115.27
37	C	517	DGD	O2G-C1B-O1B	-2.27	118.22	123.70
24	c	509	CLA	CHD-C4C-NC	2.27	127.78	124.20
24	b	618	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
24	b	620	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
24	B	610	CLA	CMB-C2B-C1B	2.27	131.95	128.46
26	H	102	BCR	C31-C1-C6	-2.27	106.62	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	CHA-C1A-NA	-2.26	121.21	126.40
24	A	406	CLA	C4C-C3C-C2C	-2.26	103.60	106.90
34	b	630	LMG	O8-C28-O10	-2.26	117.88	123.59
24	B	606	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
27	B	621	SQD	C1-C2-C3	-2.26	105.28	110.00
24	b	626	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
24	C	503	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
25	A	409[B]	PHO	O2A-CGA-CBA	2.26	119.01	111.91
24	d	402	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
29	M	103	LMT	O5B-C5B-C4B	2.26	113.80	109.69
24	d	401	CLA	C1-O2A-CGA	2.26	122.37	116.44
32	A	420[B]	PL9	C35-C34-C36	2.26	119.07	115.27
25	A	409[A]	PHO	O2A-CGA-CBA	2.26	119.00	111.91
29	a	404	LMT	C1B-O1B-C4'	-2.26	112.38	117.96
24	B	610	CLA	C1-O2A-CGA	2.26	122.36	116.44
26	T	103	BCR	C29-C28-C27	-2.26	106.34	111.38
24	b	612	CLA	O2A-CGA-CBA	2.25	118.98	111.91
29	m	102	LMT	C1B-O5B-C5B	2.25	118.11	113.69
32	D	405[A]	PL9	C51-C49-C50	2.25	119.58	114.60
26	y	101	BCR	C35-C13-C14	-2.25	119.77	122.92
39	F	102	HEM	O2A-CGA-CBA	2.25	121.27	114.03
26	c	518	BCR	C21-C20-C19	-2.25	116.20	123.22
24	c	508	CLA	C11-C10-C8	-2.25	108.65	115.92
24	a	410	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
37	c	520	DGD	O1G-C1A-C2A	2.25	118.96	111.91
26	b	628	BCR	C38-C26-C25	-2.25	122.00	124.53
24	C	511	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
24	B	609	CLA	C1-C2-C3	-2.25	122.16	126.04
24	C	504	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
24	C	511	CLA	CMB-C2B-C3B	2.24	128.87	124.68
24	b	624	CLA	C4-C3-C2	-2.24	117.94	123.68
32	A	420[A]	PL9	C8-C7-C3	2.24	118.31	111.98
24	c	517	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	c	509	CLA	C1-O2A-CGA	2.23	122.31	116.44
32	d	405[B]	PL9	C30-C29-C31	2.23	119.03	115.27
24	c	505	CLA	OBD-CAD-C3D	-2.23	123.15	128.52
24	B	610	CLA	C1-C2-C3	-2.23	122.18	126.04
24	c	505	CLA	CHD-C4C-NC	2.23	127.72	124.20
24	b	618	CLA	CMC-C2C-C1C	2.23	128.44	125.04
27	a	414	SQD	O9-S-O7	-2.23	106.23	113.95
24	B	613	CLA	CMA-C3A-C2A	-2.23	104.83	113.83
24	b	624	CLA	C4-C3-C5	2.23	119.02	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	417	LMT	C6'-C5'-C4'	-2.23	106.84	113.33
24	c	506	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
32	D	405[B]	PL9	C7-C3-C4	2.23	118.69	116.88
24	B	603	CLA	C1-O2A-CGA	2.23	122.29	116.44
26	D	404	BCR	C21-C20-C19	-2.23	116.27	123.22
24	b	619	CLA	CAC-C3C-C4C	2.23	127.70	124.81
24	B	616	CLA	CED-O2D-CGD	2.23	120.97	115.94
39	v	205	HEM	O2A-CGA-CBA	2.23	121.18	114.03
36	b	632	HTG	C1-C2-C3	2.23	114.98	110.59
24	B	608	CLA	O2A-CGA-CBA	2.22	118.89	111.91
24	B	614	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
24	B	614	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
24	d	403	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
34	z	101	LMG	C7-O1-C1	-2.22	109.40	113.74
27	f	102	SQD	O7-S-C6	2.22	109.58	106.94
26	T	103	BCR	C16-C17-C18	-2.22	124.14	127.31
26	K	101	BCR	C2-C1-C6	2.22	113.90	110.48
26	B	618	BCR	C34-C9-C10	-2.22	119.82	122.92
24	c	509	CLA	C1-C2-C3	-2.21	122.21	126.04
24	c	512	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
24	B	602	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	A	410	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
25	a	420[A]	PHO	O2A-CGA-CBA	2.21	118.84	111.91
24	B	606	CLA	CAC-C3C-C4C	2.21	127.68	124.81
26	C	515	BCR	C15-C16-C17	-2.21	118.95	123.47
32	D	405[B]	PL9	C32-C33-C34	-2.21	122.34	127.66
27	B	621	SQD	O8-S-C6	2.21	109.26	105.74
24	C	503	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
32	d	405[A]	PL9	C22-C23-C24	-2.21	122.35	127.66
37	c	521	DGD	O2G-C1B-O1B	-2.21	118.37	123.70
32	A	420[A]	PL9	C35-C34-C36	2.21	118.98	115.27
24	B	613	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
38	D	408	LHG	O8-C23-C24	2.21	118.83	111.91
24	d	401	CLA	O2A-CGA-CBA	2.21	118.83	111.91
24	B	616	CLA	C2A-C1A-CHA	-2.20	120.00	123.86
26	D	404	BCR	C10-C11-C12	-2.20	116.34	123.22
27	B	621	SQD	C44-O6-C1	-2.20	109.43	113.74
24	D	402	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
24	b	621	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
24	B	616	CLA	C1-C2-C3	-2.20	122.23	126.04
37	C	518	DGD	C3G-C2G-C1G	-2.20	106.58	111.79
24	b	625	CLA	C6-C7-C8	-2.20	108.81	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	BCR	C21-C20-C19	-2.20	116.35	123.22
38	d	407	LHG	O8-C23-C24	2.20	118.81	111.91
26	Y	101	BCR	C24-C23-C22	-2.20	122.92	126.23
24	B	613	CLA	CHC-C1C-C2C	-2.19	120.65	126.72
37	C	516	DGD	O1G-C1A-C2A	2.19	118.79	111.91
24	c	506	CLA	CMB-C2B-C3B	2.19	128.78	124.68
32	A	420[B]	PL9	C51-C49-C50	2.19	119.44	114.60
24	c	514	CLA	CHB-C4A-NA	2.19	127.54	124.51
24	B	605	CLA	CAC-C3C-C4C	2.19	127.65	124.81
29	a	421	LMT	C1B-O1B-C4'	-2.19	112.54	117.96
32	D	405[B]	PL9	C15-C14-C16	2.19	118.95	115.27
26	B	618	BCR	C36-C18-C17	-2.19	119.86	122.92
27	B	621	SQD	O47-C7-O49	-2.19	118.42	123.70
25	a	420[B]	PHO	O2A-CGA-CBA	2.19	118.77	111.91
24	C	512	CLA	CBC-CAC-C3C	-2.19	106.41	112.43
24	B	615	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
26	a	413	BCR	C33-C5-C6	-2.19	122.07	124.53
26	T	103	BCR	C1-C6-C7	2.18	121.95	115.78
24	b	614	CLA	C6-C7-C8	-2.18	108.86	115.92
26	y	101	BCR	C37-C22-C23	2.18	121.51	118.08
27	a	414	SQD	O48-C23-O10	-2.18	118.09	123.59
34	c	523	LMG	O8-C28-O10	-2.18	118.09	123.59
26	y	101	BCR	C40-C30-C25	-2.18	106.76	110.30
34	A	422	LMG	C7-O1-C1	-2.18	109.48	113.74
26	b	627	BCR	C29-C30-C25	2.18	113.83	110.48
24	c	508	CLA	CMB-C2B-C3B	2.18	128.75	124.68
24	B	616	CLA	O2A-CGA-CBA	2.18	118.74	111.91
24	B	610	CLA	O2A-CGA-CBA	2.18	118.74	111.91
24	c	505	CLA	C4-C3-C5	2.18	118.93	115.27
24	B	602	CLA	CMC-C2C-C1C	2.18	128.35	125.04
24	b	623	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	b	613	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	b	613	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
24	A	406	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
24	d	402	CLA	CAA-C2A-C3A	-2.18	106.82	112.78
26	H	102	BCR	C10-C11-C12	-2.17	116.43	123.22
24	C	508	CLA	OBD-CAD-C3D	-2.17	123.29	128.52
26	c	527	BCR	C34-C9-C10	-2.17	119.88	122.92
25	a	420[A]	PHO	C4A-C3A-C2A	-2.17	100.77	102.84
26	b	627	BCR	C16-C17-C18	-2.17	124.21	127.31
24	C	503	CLA	C4-C3-C5	2.17	118.92	115.27
24	B	608	CLA	C4-C3-C5	2.17	118.92	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	C4-C3-C5	2.17	118.92	115.27
24	b	622	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
24	b	625	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
26	C	514	BCR	C37-C22-C23	2.17	121.49	118.08
37	H	103	DGD	O6E-C5E-C6E	2.17	111.83	106.44
24	d	401	CLA	CMC-C2C-C1C	2.17	128.34	125.04
24	C	509	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
24	b	624	CLA	CHB-C4A-NA	2.17	127.51	124.51
24	C	506	CLA	O2A-CGA-CBA	2.17	118.70	111.91
24	c	514	CLA	CAC-C3C-C4C	2.16	127.62	124.81
24	C	511	CLA	C1-O2A-CGA	2.16	122.12	116.44
26	D	404	BCR	C16-C17-C18	-2.16	124.22	127.31
26	b	628	BCR	C15-C14-C13	-2.16	124.22	127.31
26	h	101	BCR	C36-C18-C17	-2.16	119.89	122.92
32	d	405[A]	PL9	C25-C24-C26	2.16	118.91	115.27
24	C	502	CLA	CMC-C2C-C1C	2.16	128.33	125.04
26	t	101	BCR	C33-C5-C4	2.16	117.77	113.62
24	C	508	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
24	C	508	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
27	a	414	SQD	O47-C7-O49	-2.16	118.49	123.70
26	a	413	BCR	C37-C22-C21	-2.16	119.90	122.92
26	Y	101	BCR	C21-C20-C19	-2.16	116.49	123.22
24	b	626	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
24	C	513	CLA	C2A-C1A-CHA	-2.16	120.09	123.86
25	A	409[A]	PHO	C4A-C3A-C2A	-2.16	100.79	102.84
24	A	406	CLA	O2A-CGA-CBA	2.15	118.67	111.91
24	B	605	CLA	CHA-C1A-NA	-2.15	121.47	126.40
26	t	101	BCR	C29-C28-C27	-2.15	106.57	111.38
32	d	405[B]	PL9	C51-C49-C50	2.15	119.36	114.60
26	B	619	BCR	C37-C22-C23	2.15	121.47	118.08
39	F	102	HEM	CHA-C4D-ND	2.15	127.04	124.38
24	C	510	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	b	611	CLA	O2A-CGA-CBA	2.15	118.65	111.91
34	B	622	LMG	O8-C28-O10	-2.15	118.17	123.59
25	A	408	PHO	CBA-CAA-C2A	-2.15	107.53	113.81
24	B	617	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
24	C	508	CLA	CHD-C4C-NC	2.15	127.58	124.20
24	C	510	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
24	c	514	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
26	h	101	BCR	C20-C21-C22	-2.14	124.25	127.31
36	C	522	HTG	C1-O5-C5	2.14	116.53	112.58
24	b	625	CLA	C1-O2A-CGA	2.14	122.07	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C11-C10-C8	-2.14	108.99	115.92
24	B	617	CLA	CMB-C2B-C3B	2.14	128.69	124.68
24	B	607	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
25	a	411	PHO	C4A-C3A-C2A	-2.14	100.80	102.84
37	c	521	DGD	C1D-O6D-C5D	2.14	117.88	113.69
38	D	407	LHG	O7-C7-O9	-2.14	118.54	123.70
24	A	406	CLA	CMA-C3A-C2A	-2.14	105.21	113.83
24	a	409	CLA	C7-C6-C5	-2.14	107.56	113.36
24	B	604	CLA	CMB-C2B-C3B	2.14	128.67	124.68
37	C	517	DGD	O1G-C1A-O1A	-2.13	118.21	123.59
34	c	523	LMG	O7-C10-O9	-2.13	118.55	123.70
24	C	513	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
25	A	409[B]	PHO	CMC-C2C-C3C	2.13	128.96	124.94
24	B	612	CLA	CHB-C4A-NA	2.13	127.46	124.51
26	B	618	BCR	C24-C23-C22	-2.13	123.02	126.23
38	L	101	LHG	C5-O7-C7	-2.13	112.56	117.79
26	T	103	BCR	C10-C11-C12	-2.13	116.58	123.22
24	B	611	CLA	C11-C12-C13	-2.13	109.05	115.92
24	a	409	CLA	CHB-C4A-NA	2.12	127.45	124.51
26	c	518	BCR	C36-C18-C17	-2.12	119.95	122.92
24	A	407	CLA	CMA-C3A-C2A	-2.12	105.26	113.83
26	K	101	BCR	C36-C18-C19	2.12	121.42	118.08
24	B	609	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	b	618	CLA	C11-C12-C13	-2.12	109.06	115.92
24	b	621	CLA	CHB-C4A-NA	2.12	127.45	124.51
32	A	420[A]	PL9	C51-C49-C50	2.12	119.29	114.60
24	A	410	CLA	CMB-C2B-C3B	2.12	128.65	124.68
26	K	101	BCR	C29-C30-C25	2.12	113.74	110.48
24	c	508	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
34	j	101	LMG	O8-C28-C29	2.12	118.55	111.91
24	C	506	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
24	B	606	CLA	C1-C2-C3	-2.12	122.38	126.04
24	B	610	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
25	A	409[A]	PHO	CMC-C2C-C3C	2.11	128.93	124.94
27	B	621	SQD	O9-S-C6	2.11	109.45	106.94
24	C	508	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
24	c	514	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
29	M	104	LMT	C1B-O5B-C5B	2.11	117.83	113.69
24	C	509	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	A	416	SQD	O9-S-C6	2.11	109.45	106.94
24	b	611	CLA	CHC-C1C-NC	2.11	127.41	124.20
24	c	510	CLA	O2A-CGA-CBA	2.11	118.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C37-C22-C23	2.11	121.40	118.08
26	b	628	BCR	C39-C30-C25	-2.11	106.88	110.30
37	c	521	DGD	O1G-C1A-O1A	-2.11	118.28	123.59
26	k	101	BCR	C39-C30-C25	-2.10	106.89	110.30
24	a	409	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
32	a	416[A]	PL9	C12-C13-C14	-2.10	122.59	127.66
26	k	101	BCR	C38-C26-C25	-2.10	122.17	124.53
24	C	507	CLA	C4-C3-C5	2.10	118.80	115.27
24	B	616	CLA	C11-C10-C8	-2.10	109.13	115.92
24	C	507	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
25	a	411	PHO	C4-C3-C5	2.10	118.80	115.27
24	d	401	CLA	CED-O2D-CGD	2.10	120.68	115.94
34	b	630	LMG	O7-C10-O9	-2.10	118.64	123.70
38	a	422	LHG	C6-C5-C4	-2.09	106.83	111.79
24	D	403	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	d	401	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
37	H	103	DGD	C2G-O2G-C1B	-2.09	112.64	117.79
24	C	504	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
24	B	603	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	b	613	CLA	CMA-C3A-C2A	-2.09	105.39	113.83
24	d	402	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
24	c	517	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
24	b	613	CLA	C7-C6-C5	-2.09	107.69	113.36
25	a	420[B]	PHO	CMC-C2C-C3C	2.09	128.88	124.94
36	V	207	HTG	O5-C1-C2	-2.09	107.69	110.31
24	b	612	CLA	C1-O2A-CGA	2.09	121.92	116.44
26	a	413	BCR	C8-C7-C6	-2.08	121.35	127.20
29	f	103	LMT	C1B-O5B-C5B	2.08	117.78	113.69
24	b	622	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	B	613	CLA	CMA-C3A-C4A	-2.08	106.18	111.77
24	d	401	CLA	CAC-C3C-C4C	2.08	127.51	124.81
29	M	101	LMT	O6'-C6'-C5'	-2.08	104.15	111.29
36	b	608	HTG	O5-C5-C4	2.08	113.47	109.69
24	C	509	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
24	B	608	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
24	C	511	CLA	C1-C2-C3	-2.08	122.45	126.04
24	b	620	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
29	C	521	LMT	O5'-C5'-C4'	2.07	114.13	109.75
36	B	633	HTG	C1-O5-C5	2.07	116.41	112.58
24	b	616	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
24	B	608	CLA	C1-O2A-CGA	2.07	121.88	116.44
24	C	510	CLA	O1D-CGD-CBD	-2.07	120.25	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	413	BCR	C3-C4-C5	-2.07	110.38	114.08
24	B	617	CLA	O2A-C1-C2	2.07	114.07	108.64
26	B	619	BCR	C30-C25-C26	-2.07	119.70	122.61
24	b	626	CLA	CHC-C1C-NC	2.07	127.34	124.20
24	C	512	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
39	v	205	HEM	O2D-CGD-CBD	2.07	120.67	114.03
24	c	512	CLA	CED-O2D-CGD	2.07	120.61	115.94
34	a	415	LMG	O7-C10-O9	-2.07	118.71	123.70
32	d	405[B]	PL9	C35-C34-C36	2.07	118.75	115.27
39	e	102	HEM	CHD-C1D-C2D	-2.06	121.75	124.98
24	c	512	CLA	C1-O2A-CGA	2.06	121.86	116.44
26	D	404	BCR	C37-C22-C21	-2.06	120.03	122.92
24	c	514	CLA	C4-C3-C2	-2.06	118.39	123.68
27	f	102	SQD	O48-C23-O10	-2.06	118.39	123.59
24	c	510	CLA	CAC-C3C-C4C	2.06	127.48	124.81
27	A	416	SQD	O6-C44-C45	-2.06	105.93	110.90
24	b	611	CLA	C1-O2A-CGA	2.06	121.85	116.44
24	C	511	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
34	D	412	LMG	O8-C28-C29	2.06	118.37	111.91
32	d	405[A]	PL9	C35-C34-C36	2.06	118.73	115.27
26	C	514	BCR	C23-C24-C25	-2.06	121.42	127.20
24	D	403	CLA	CMB-C2B-C3B	2.06	128.53	124.68
36	b	602	HTG	C1-O5-C5	2.06	116.37	112.58
24	B	608	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
26	D	404	BCR	C3-C4-C5	-2.05	110.41	114.08
26	y	101	BCR	C35-C13-C12	2.05	121.31	118.08
24	b	611	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
24	b	612	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
26	c	527	BCR	C36-C18-C17	-2.05	120.05	122.92
24	C	501	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
24	d	401	CLA	C1-C2-C3	-2.05	122.50	126.04
24	b	623	CLA	CMB-C2B-C3B	2.05	128.51	124.68
26	T	103	BCR	C36-C18-C17	-2.05	120.05	122.92
24	C	505	CLA	C4-C3-C5	2.05	118.72	115.27
38	d	407	LHG	O8-C23-O10	-2.05	118.42	123.59
24	C	506	CLA	CED-O2D-CGD	2.05	120.57	115.94
34	A	422	LMG	O7-C10-O9	-2.05	118.75	123.70
24	B	602	CLA	C4-C3-C5	2.05	118.72	115.27
24	a	412	CLA	CMA-C3A-C4A	-2.05	106.27	111.77
29	F	101	LMT	C1B-O5B-C5B	2.05	117.71	113.69
24	D	403	CLA	C1-O2A-CGA	2.05	121.81	116.44
37	c	519	DGD	O1G-C1A-C2A	2.05	118.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	519	LMG	O8-C28-O10	-2.05	118.43	123.59
26	B	620	BCR	C23-C24-C25	-2.04	121.46	127.20
25	a	420[B]	PHO	CMA-C3A-C4A	-2.04	109.90	114.38
24	B	617	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
26	B	619	BCR	C33-C5-C4	2.04	117.54	113.62
32	D	405[A]	PL9	C7-C3-C4	2.04	118.53	116.88
24	b	620	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
36	c	524	HTG	C6-C5-C4	-2.04	108.22	113.00
24	B	603	CLA	CMA-C3A-C2A	-2.04	105.60	113.83
24	A	407	CLA	O2A-CGA-CBA	2.04	118.31	111.91
26	A	411	BCR	C8-C7-C6	-2.04	121.47	127.20
36	B	632	HTG	C6-C5-C4	-2.04	108.23	113.00
24	b	618	CLA	OBD-CAD-C3D	-2.04	123.61	128.52
34	c	523	LMG	O1-C1-C2	2.04	111.48	108.30
24	b	613	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	B	609	CLA	OBD-CAD-C3D	-2.04	123.62	128.52
26	A	411	BCR	C20-C21-C22	-2.04	124.40	127.31
24	d	401	CLA	CAA-CBA-CGA	2.04	119.21	113.25
39	v	205	HEM	CMD-C2D-C1D	2.04	128.14	125.04
26	b	629	BCR	C16-C17-C18	-2.04	124.40	127.31
24	c	513	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
24	c	511	CLA	CMB-C2B-C3B	2.04	128.49	124.68
38	l	101	LHG	O8-C23-O10	-2.04	118.45	123.59
24	b	622	CLA	CMA-C3A-C4A	-2.03	106.30	111.77
26	C	514	BCR	C28-C27-C26	-2.03	110.44	114.08
24	D	402	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
24	a	409	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
24	c	516	CLA	C1-O2A-CGA	2.03	121.78	116.44
24	B	609	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
26	t	101	BCR	C37-C22-C23	2.03	121.28	118.08
36	B	632	HTG	C3-C4-C5	2.03	113.86	110.24
38	E	101	LHG	O8-C23-O10	-2.03	118.47	123.59
27	B	621	SQD	O48-C23-O10	-2.03	118.47	123.59
34	j	101	LMG	O8-C28-O10	-2.03	118.47	123.59
24	C	510	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
27	F	103	SQD	O48-C23-O10	-2.03	118.47	123.59
26	T	103	BCR	C20-C21-C22	-2.03	124.41	127.31
24	b	620	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
26	T	103	BCR	C7-C8-C9	-2.03	123.17	126.23
24	B	608	CLA	CMB-C2B-C3B	2.03	128.47	124.68
24	C	512	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	a	412	CLA	O2A-CGA-O1A	-2.03	118.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	e	101	DGD	O2G-C1B-O1B	-2.03	118.81	123.70
25	A	408	PHO	O2A-CGA-CBA	2.03	118.27	111.91
24	B	609	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
26	k	101	BCR	C3-C4-C5	-2.03	110.46	114.08
36	B	624	HTG	O5-C1-C2	2.02	112.86	110.31
24	b	622	CLA	C11-C10-C8	-2.02	109.38	115.92
24	B	617	CLA	OBD-CAD-C3D	-2.02	123.65	128.52
26	A	411	BCR	C37-C22-C23	2.02	121.26	118.08
26	T	103	BCR	C7-C6-C5	-2.02	116.57	121.46
24	C	508	CLA	CHB-C4A-NA	2.02	127.31	124.51
24	B	607	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	c	509	CLA	CED-O2D-CGD	2.02	120.50	115.94
24	B	603	CLA	C11-C12-C13	-2.02	109.39	115.92
26	b	629	BCR	C3-C4-C5	-2.02	110.47	114.08
32	A	420[B]	PL9	C47-C48-C49	-2.02	120.85	127.75
24	C	507	CLA	CHA-C1A-NA	-2.02	121.78	126.40
24	c	508	CLA	CMA-C3A-C2A	-2.02	105.69	113.83
32	D	405[B]	PL9	C7-C3-C2	-2.02	120.65	123.30
38	l	101	LHG	C6-C5-C4	-2.02	107.02	111.79
32	D	405[A]	PL9	C30-C29-C31	2.02	118.66	115.27
34	c	522	LMG	C30-C29-C28	-2.02	106.29	113.62
26	c	518	BCR	C32-C1-C6	-2.01	107.03	110.30
26	t	101	BCR	C16-C15-C14	2.01	127.60	123.47
32	d	405[B]	PL9	C17-C18-C19	-2.01	122.81	127.66
24	B	610	CLA	CHA-C1A-NA	-2.01	121.79	126.40
26	H	102	BCR	C39-C30-C25	-2.01	107.04	110.30
24	C	502	CLA	C4-C3-C2	-2.01	118.52	123.68
24	c	508	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
25	A	409[B]	PHO	CED-O2D-CGD	2.01	120.48	115.94
26	d	404	BCR	C38-C26-C27	2.01	117.47	113.62
24	B	606	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
24	B	616	CLA	CMB-C2B-C1B	2.01	131.55	128.46
29	m	102	LMT	C1B-O1B-C4'	-2.01	113.00	117.96
32	D	405[A]	PL9	C7-C3-C2	-2.01	120.66	123.30
26	c	518	BCR	C37-C22-C23	2.00	121.24	118.08
24	B	616	CLA	CHA-C1A-NA	-2.00	121.81	126.40
26	b	629	BCR	C15-C14-C13	-2.00	124.45	127.31
24	A	406	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
32	D	405[B]	PL9	C40-C39-C38	-2.00	118.54	123.68
24	C	505	CLA	CHA-C1A-NA	-2.00	121.81	126.40

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	410	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	501	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	402	CLA	ND
24	D	403	CLA	ND
24	a	409	CLA	ND
24	a	412	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	619	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	620	CLA	ND
24	b	622	CLA	ND
24	b	623	CLA	ND
24	b	624	CLA	ND
24	b	625	CLA	ND
24	b	626	CLA	ND
24	c	505	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	c	515	CLA	ND
24	c	516	CLA	ND
24	d	401	CLA	ND
24	d	402	CLA	ND
24	d	403	CLA	ND

All (1308) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	C2-C1-O2A-CGA
24	b	615	CLA	C2-C3-C5-C6
24	b	616	CLA	CHA-CBD-CGD-O1D
24	b	616	CLA	CHA-CBD-CGD-O2D
24	b	624	CLA	CHA-CBD-CGD-O1D
24	b	624	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	b	624	CLA	CAD-CBD-CGD-O1D
24	b	624	CLA	CAD-CBD-CGD-O2D
24	b	624	CLA	C2-C3-C5-C6
24	b	624	CLA	C4-C3-C5-C6
24	c	508	CLA	C2-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
24	c	512	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O2D
26	B	618	BCR	C1-C6-C7-C8
26	D	404	BCR	C1-C6-C7-C8
26	D	404	BCR	C7-C8-C9-C10
26	D	404	BCR	C7-C8-C9-C34
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C37-C22-C23-C24
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C21-C22-C23-C24
26	y	101	BCR	C37-C22-C23-C24
27	A	416	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O9
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
27	F	103	SQD	C5-C6-S-O9
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
28	A	414	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	A	415	GOL	C1-C2-C3-O3
28	B	627	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-C3
28	B	628	GOL	O1-C1-C2-C3
28	B	630	GOL	O1-C1-C2-C3
28	B	630	GOL	C1-C2-C3-O3
28	B	630	GOL	O2-C2-C3-O3
28	C	524	GOL	O1-C1-C2-C3
28	O	301	GOL	O1-C1-C2-C3
28	T	102	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-C3
28	V	201	GOL	O1-C1-C2-C3
28	V	202	GOL	C1-C2-C3-O3
28	V	205	GOL	C1-C2-C3-O3
28	a	402	GOL	O1-C1-C2-C3
28	f	101	GOL	O1-C1-C2-C3
28	v	202	GOL	O1-C1-C2-C3
29	A	417	LMT	C2'-C1'-O1'-C1
29	A	417	LMT	O5'-C1'-O1'-C1
29	B	635	LMT	C2'-C1'-O1'-C1
29	B	635	LMT	O5'-C1'-O1'-C1
29	C	521	LMT	C2'-C1'-O1'-C1
29	C	521	LMT	O5'-C1'-O1'-C1
29	F	101	LMT	C2'-C1'-O1'-C1
29	F	101	LMT	O5'-C1'-O1'-C1
29	M	103	LMT	O5'-C1'-O1'-C1
29	T	104	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
29	a	421	LMT	C2'-C1'-O1'-C1
29	a	421	LMT	O5'-C1'-O1'-C1
29	b	631	LMT	C2'-C1'-O1'-C1
29	b	631	LMT	O5'-C1'-O1'-C1
29	f	103	LMT	C2'-C1'-O1'-C1
29	f	103	LMT	O5'-C1'-O1'-C1
32	a	416[A]	PL9	C12-C11-C9-C10
32	a	416[A]	PL9	C18-C19-C21-C22
32	a	416[A]	PL9	C20-C19-C21-C22
32	a	416[B]	PL9	C12-C11-C9-C10
34	C	520	LMG	O9-C10-O7-C8
34	C	520	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	O9-C10-O7-C8
36	B	624	HTG	C2'-C1'-S1-C1
36	B	625	HTG	O5-C1-S1-C1'
36	c	524	HTG	C2'-C1'-S1-C1
37	D	406	DGD	C2B-C1B-O2G-C2G
37	D	406	DGD	O1B-C1B-O2G-C2G
37	D	406	DGD	C2D-C1D-O3G-C3G
37	D	406	DGD	O6D-C1D-O3G-C3G
37	e	101	DGD	C2B-C1B-O2G-C2G
37	e	101	DGD	O1B-C1B-O2G-C2G
37	e	101	DGD	O6E-C1E-O5D-C6D
38	D	408	LHG	C4-O6-P-O4
38	D	409	LHG	C4-O6-P-O4
38	E	101	LHG	C3-O3-P-O4
38	E	101	LHG	C3-O3-P-O5
38	E	101	LHG	C3-O3-P-O6
38	E	101	LHG	C4-O6-P-O5
38	L	101	LHG	C3-O3-P-O4
38	L	101	LHG	C4-O6-P-O4
38	a	422	LHG	O1-C1-C2-C3
38	a	422	LHG	C3-O3-P-O5
38	a	422	LHG	C3-O3-P-O6
38	d	407	LHG	O2-C2-C3-O3
38	d	407	LHG	C3-O3-P-O4
38	l	101	LHG	C4-O6-P-O4
38	l	101	LHG	C4-O6-P-O5
39	F	102	HEM	C2B-C3B-CAB-CBB
39	v	205	HEM	C2B-C3B-CAB-CBB
38	a	422	LHG	O10-C23-O8-C6
29	C	521	LMT	C3'-C4'-O1B-C1B
29	D	401	LMT	C3'-C4'-O1B-C1B
38	a	422	LHG	C24-C23-O8-C6
24	c	515	CLA	CBD-CGD-O2D-CED
38	E	101	LHG	O10-C23-O8-C6
24	D	403	CLA	C3-C5-C6-C7
24	b	624	CLA	C3-C5-C6-C7
24	c	510	CLA	C3-C5-C6-C7
38	E	101	LHG	C24-C23-O8-C6
27	b	601	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
34	z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	O6-C5-C6-O5
24	b	615	CLA	C4-C3-C5-C6
24	A	410	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
29	M	103	LMT	O5'-C5'-C6'-O6'
24	b	614	CLA	CBD-CGD-O2D-CED
24	B	615	CLA	C3-C5-C6-C7
34	A	422	LMG	C11-C10-O7-C8
24	B	605	CLA	CBD-CGD-O2D-CED
29	f	103	LMT	C4'-C5'-C6'-O6'
37	C	516	DGD	C4A-C5A-C6A-C7A
36	B	625	HTG	O5-C5-C6-O6
24	C	507	CLA	CBD-CGD-O2D-CED
24	c	513	CLA	C3-C5-C6-C7
29	C	521	LMT	O5'-C5'-C6'-O6'
34	C	520	LMG	O6-C5-C6-O5
34	A	422	LMG	O9-C10-O7-C8
34	z	101	LMG	C4-C5-C6-O5
29	M	101	LMT	O5B-C5B-C6B-O6B
32	A	420[A]	PL9	C25-C24-C26-C27
32	A	420[B]	PL9	C25-C24-C26-C27
32	a	416[A]	PL9	C15-C14-C16-C17
32	a	416[A]	PL9	C25-C24-C26-C27
32	a	416[B]	PL9	C15-C14-C16-C17
32	a	416[B]	PL9	C20-C19-C21-C22
32	a	416[B]	PL9	C25-C24-C26-C27
32	A	420[A]	PL9	C23-C24-C26-C27
32	A	420[B]	PL9	C23-C24-C26-C27
32	a	416[A]	PL9	C13-C14-C16-C17
32	a	416[A]	PL9	C23-C24-C26-C27
32	a	416[B]	PL9	C13-C14-C16-C17
32	a	416[B]	PL9	C18-C19-C21-C22
32	a	416[B]	PL9	C23-C24-C26-C27
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	616	CLA	C2A-CAA-CBA-CGA
24	C	509	CLA	O1A-CGA-O2A-C1
29	M	103	LMT	C4'-C5'-C6'-O6'
27	B	621	SQD	O5-C1-O6-C44
34	z	101	LMG	O6-C1-O1-C7
32	d	405[A]	PL9	C39-C41-C42-C43
24	C	509	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	e	101	DGD	C4E-C5E-C6E-O5E
24	c	515	CLA	O1D-CGD-O2D-CED
29	M	101	LMT	C4B-C5B-C6B-O6B
34	a	415	LMG	C17-C18-C19-C20
38	D	408	LHG	O2-C2-C3-O3
38	E	101	LHG	O2-C2-C3-O3
34	Z	101	LMG	C10-C11-C12-C13
29	D	401	LMT	C2'-C1'-O1'-C1
37	e	101	DGD	C2E-C1E-O5D-C6D
29	f	103	LMT	O5'-C5'-C6'-O6'
24	B	602	CLA	C11-C10-C8-C9
24	B	603	CLA	C14-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C9
24	c	510	CLA	C6-C7-C8-C9
24	C	508	CLA	C10-C11-C12-C13
26	Y	101	BCR	C37-C22-C23-C24
36	b	633	HTG	S1-C1'-C2'-C3'
29	m	102	LMT	O5'-C5'-C6'-O6'
34	c	522	LMG	C11-C10-O7-C8
34	C	520	LMG	C28-C29-C30-C31
24	c	507	CLA	CBD-CGD-O2D-CED
24	B	602	CLA	C3-C5-C6-C7
24	C	512	CLA	CBA-CGA-O2A-C1
24	B	602	CLA	C10-C11-C12-C13
24	B	615	CLA	C5-C6-C7-C8
24	B	615	CLA	C10-C11-C12-C13
36	b	633	HTG	O5-C5-C6-O6
24	B	615	CLA	C8-C10-C11-C12
24	C	501	CLA	C15-C16-C17-C18
24	b	625	CLA	C10-C11-C12-C13
28	B	630	GOL	O1-C1-C2-O2
28	b	606	GOL	O1-C1-C2-O2
28	f	101	GOL	O1-C1-C2-O2
28	v	201	GOL	O1-C1-C2-O2
27	A	416	SQD	C23-C24-C25-C26
34	a	415	LMG	C10-C11-C12-C13
24	B	616	CLA	C8-C10-C11-C12
24	b	624	CLA	C5-C6-C7-C8
27	b	601	SQD	C24-C23-O48-C46
36	C	523	HTG	S1-C1'-C2'-C3'
24	B	617	CLA	C2-C1-O2A-CGA
24	b	611	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
34	B	622	LMG	C15-C16-C17-C18
29	A	417	LMT	O5B-C5B-C6B-O6B
24	B	604	CLA	C6-C7-C8-C10
24	B	616	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
24	b	626	CLA	C11-C12-C13-C15
26	T	103	BCR	C13-C14-C15-C16
24	c	512	CLA	C15-C16-C17-C18
36	b	602	HTG	C1'-C2'-C3'-C4'
29	T	104	LMT	O1'-C1-C2-C3
29	D	401	LMT	O5'-C1'-O1'-C1
24	C	506	CLA	C5-C6-C7-C8
32	D	405[B]	PL9	C39-C41-C42-C43
32	a	416[A]	PL9	C9-C11-C12-C13
32	a	416[B]	PL9	C9-C11-C12-C13
32	a	416[B]	PL9	C14-C16-C17-C18
32	d	405[B]	PL9	C39-C41-C42-C43
36	c	524	HTG	S1-C1'-C2'-C3'
34	c	522	LMG	O9-C10-O7-C8
24	B	616	CLA	C5-C6-C7-C8
24	c	517	CLA	C10-C11-C12-C13
34	C	520	LMG	C4-C5-C6-O5
24	A	410	CLA	C13-C15-C16-C17
24	a	412	CLA	C15-C16-C17-C18
37	e	101	DGD	O6D-C5D-C6D-O5D
27	b	601	SQD	O10-C23-O48-C46
24	B	617	CLA	C10-C11-C12-C13
24	C	508	CLA	C5-C6-C7-C8
24	b	616	CLA	C13-C15-C16-C17
24	c	508	CLA	C15-C16-C17-C18
38	L	101	LHG	C4-O6-P-O3
38	d	407	LHG	C3-O3-P-O6
38	l	101	LHG	C4-O6-P-O3
27	F	103	SQD	C26-C27-C28-C29
24	b	611	CLA	C8-C10-C11-C12
24	C	512	CLA	O1A-CGA-O2A-C1
38	E	101	LHG	C1-C2-C3-O3
24	C	506	CLA	C13-C15-C16-C17
24	b	624	CLA	C13-C15-C16-C17
29	D	401	LMT	O5B-C5B-C6B-O6B
34	j	101	LMG	O6-C5-C6-O5
38	a	422	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	C	521	LMT	O5B-C1B-O1B-C4'
38	l	101	LHG	C33-C34-C35-C36
24	B	604	CLA	C5-C6-C7-C8
29	T	104	LMT	C4-C5-C6-C7
37	C	517	DGD	C9A-CAA-CBA-CCA
37	D	406	DGD	C7A-C8A-C9A-CAA
37	c	519	DGD	C9A-CAA-CBA-CCA
37	c	519	DGD	CAB-CBB-CCB-CDB
37	e	101	DGD	CAA-CBA-CCA-CDA
24	C	502	CLA	C16-C17-C18-C20
24	b	621	CLA	C16-C17-C18-C19
36	b	632	HTG	C2'-C3'-C4'-C5'
37	c	521	DGD	C6A-C7A-C8A-C9A
38	L	101	LHG	C14-C15-C16-C17
24	A	410	CLA	C10-C11-C12-C13
37	c	521	DGD	C7B-C8B-C9B-CAB
37	e	101	DGD	C8B-C9B-CAB-CBB
27	A	412	SQD	C9-C10-C11-C12
27	a	414	SQD	C11-C12-C13-C14
29	T	104	LMT	C11-C10-C9-C8
34	A	422	LMG	C30-C31-C32-C33
37	C	516	DGD	C4B-C5B-C6B-C7B
27	b	601	SQD	C12-C13-C14-C15
37	C	517	DGD	C2E-C1E-O5D-C6D
37	c	520	DGD	C2E-C1E-O5D-C6D
37	e	101	DGD	C2D-C1D-O3G-C3G
24	C	511	CLA	CBA-CGA-O2A-C1
29	a	421	LMT	C6-C7-C8-C9
34	A	422	LMG	C11-C12-C13-C14
34	B	622	LMG	C29-C30-C31-C32
24	a	412	CLA	C10-C11-C12-C13
24	C	510	CLA	C4-C3-C5-C6
24	b	619	CLA	C4-C3-C5-C6
25	a	411	PHO	C4-C3-C5-C6
32	D	405[B]	PL9	C15-C14-C16-C17
27	A	412	SQD	C14-C15-C16-C17
34	B	622	LMG	C36-C37-C38-C39
37	C	518	DGD	CAA-CBA-CCA-CDA
37	c	519	DGD	C8B-C9B-CAB-CBB
37	c	521	DGD	CBB-CCB-CDB-CEB
38	d	408	LHG	C29-C30-C31-C32
24	b	619	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	d	405[A]	PL9	C13-C14-C16-C17
24	B	604	CLA	C6-C7-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	C	506	CLA	C6-C7-C8-C9
24	a	410	CLA	C14-C13-C15-C16
24	b	613	CLA	C6-C7-C8-C9
24	b	620	CLA	C11-C12-C13-C14
38	D	407	LHG	C23-C24-C25-C26
29	A	417	LMT	C6-C7-C8-C9
37	C	518	DGD	C8A-C9A-CAA-CBA
37	c	520	DGD	C9A-CAA-CBA-CCA
38	d	406	LHG	C32-C33-C34-C35
28	B	626	GOL	C1-C2-C3-O3
28	B	631	GOL	O1-C1-C2-C3
28	V	203	GOL	O1-C1-C2-C3
28	b	605	GOL	O1-C1-C2-C3
28	b	606	GOL	O1-C1-C2-C3
28	v	201	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
38	D	407	LHG	O1-C1-C2-C3
36	C	523	HTG	O5-C5-C6-O6
34	A	422	LMG	C14-C15-C16-C17
38	a	422	LHG	C24-C25-C26-C27
27	A	416	SQD	C11-C12-C13-C14
27	A	416	SQD	C26-C27-C28-C29
27	a	405	SQD	C31-C32-C33-C34
29	B	635	LMT	C3-C4-C5-C6
34	z	101	LMG	C12-C13-C14-C15
36	B	624	HTG	C2'-C3'-C4'-C5'
37	c	521	DGD	C6B-C7B-C8B-C9B
38	D	407	LHG	C24-C25-C26-C27
34	D	412	LMG	O6-C5-C6-O5
37	C	517	DGD	O6E-C1E-O5D-C6D
37	c	520	DGD	O6E-C1E-O5D-C6D
37	e	101	DGD	O6D-C1D-O3G-C3G
34	C	520	LMG	C13-C14-C15-C16
34	b	630	LMG	C38-C39-C40-C41
36	b	632	HTG	C3'-C4'-C5'-C6'
37	D	406	DGD	C6A-C7A-C8A-C9A
38	d	407	LHG	C34-C35-C36-C37
37	e	101	DGD	C4D-C5D-C6D-O5D
24	C	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	M	103	LMT	C2-C3-C4-C5
29	a	404	LMT	C2-C3-C4-C5
34	A	422	LMG	C32-C33-C34-C35
37	c	520	DGD	C4A-C5A-C6A-C7A
37	c	521	DGD	C7A-C8A-C9A-CAA
34	C	519	LMG	C11-C12-C13-C14
37	H	103	DGD	CBB-CCB-CDB-CEB
38	d	406	LHG	C25-C26-C27-C28
38	l	101	LHG	C27-C28-C29-C30
24	C	509	CLA	C3-C5-C6-C7
24	c	516	CLA	CBA-CGA-O2A-C1
37	c	519	DGD	O6D-C5D-C6D-O5D
34	a	415	LMG	C14-C15-C16-C17
24	D	403	CLA	C8-C10-C11-C12
24	c	514	CLA	C8-C10-C11-C12
26	t	101	BCR	C13-C14-C15-C16
34	j	101	LMG	C19-C20-C21-C22
37	C	516	DGD	C3B-C4B-C5B-C6B
37	D	406	DGD	C2A-C3A-C4A-C5A
37	H	103	DGD	C7A-C8A-C9A-CAA
24	B	616	CLA	C16-C17-C18-C20
24	a	412	CLA	C16-C17-C18-C19
24	a	412	CLA	C16-C17-C18-C20
34	D	412	LMG	C19-C20-C21-C22
34	c	522	LMG	C34-C35-C36-C37
34	c	522	LMG	C7-C8-C9-O8
34	z	101	LMG	O1-C7-C8-C9
29	T	104	LMT	C1-C2-C3-C4
36	b	633	HTG	C1'-C2'-C3'-C4'
38	D	409	LHG	C29-C30-C31-C32
37	C	516	DGD	O6D-C5D-C6D-O5D
32	d	405[B]	PL9	C45-C44-C46-C47
24	C	505	CLA	C2-C3-C5-C6
24	C	510	CLA	C2-C3-C5-C6
32	d	405[A]	PL9	C43-C44-C46-C47
28	A	414	GOL	O2-C2-C3-O3
28	A	415	GOL	O2-C2-C3-O3
28	B	628	GOL	O1-C1-C2-O2
28	O	301	GOL	O1-C1-C2-O2
28	V	203	GOL	O1-C1-C2-O2
28	a	402	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	b	601	SQD	C29-C30-C31-C32
36	b	602	HTG	C3'-C4'-C5'-C6'
29	M	104	LMT	O5'-C5'-C6'-O6'
36	B	632	HTG	C4-C5-C6-O6
24	c	516	CLA	C15-C16-C17-C18
36	B	625	HTG	C4-C5-C6-O6
37	C	516	DGD	C2A-C3A-C4A-C5A
24	C	511	CLA	O1A-CGA-O2A-C1
37	c	521	DGD	C1A-C2A-C3A-C4A
38	d	407	LHG	C1-C2-C3-O3
24	c	513	CLA	C2-C1-O2A-CGA
34	B	622	LMG	C34-C35-C36-C37
34	j	101	LMG	C38-C39-C40-C41
24	a	412	CLA	C8-C10-C11-C12
27	b	601	SQD	C32-C33-C34-C35
37	D	406	DGD	C1B-C2B-C3B-C4B
38	a	422	LHG	C23-C24-C25-C26
26	B	618	BCR	C5-C6-C7-C8
26	D	404	BCR	C5-C6-C7-C8
26	b	627	BCR	C1-C6-C7-C8
26	b	627	BCR	C5-C6-C7-C8
27	A	416	SQD	C30-C31-C32-C33
27	a	414	SQD	C29-C30-C31-C32
36	B	625	HTG	C3'-C4'-C5'-C6'
37	D	406	DGD	C8B-C9B-CAB-CBB
32	D	405[A]	PL9	C15-C14-C16-C17
32	d	405[A]	PL9	C45-C44-C46-C47
24	B	603	CLA	C12-C13-C15-C16
24	B	615	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
24	a	410	CLA	C11-C12-C13-C15
24	a	410	CLA	C12-C13-C15-C16
24	b	611	CLA	C6-C7-C8-C10
24	b	613	CLA	C6-C7-C8-C10
24	c	510	CLA	C6-C7-C8-C10
25	a	411	PHO	C2-C3-C5-C6
32	D	405[A]	PL9	C28-C29-C31-C32
32	d	405[B]	PL9	C13-C14-C16-C17
24	c	516	CLA	O1A-CGA-O2A-C1
37	e	101	DGD	C5A-C6A-C7A-C8A
24	b	612	CLA	C16-C17-C18-C19
27	B	621	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	A	422	LMG	C10-C11-C12-C13
24	a	412	CLA	CBA-CGA-O2A-C1
29	B	635	LMT	C7-C8-C9-C10
38	l	101	LHG	C10-C11-C12-C13
34	a	415	LMG	C29-C30-C31-C32
34	j	101	LMG	C14-C15-C16-C17
34	j	101	LMG	C35-C36-C37-C38
27	b	601	SQD	C7-C8-C9-C10
27	a	405	SQD	C25-C26-C27-C28
27	a	414	SQD	C9-C10-C11-C12
37	C	516	DGD	C5B-C6B-C7B-C8B
34	Z	101	LMG	C19-C20-C21-C22
29	M	103	LMT	O5B-C5B-C6B-O6B
29	T	104	LMT	C7-C8-C9-C10
34	C	520	LMG	C14-C15-C16-C17
37	C	517	DGD	CBB-CCB-CDB-CEB
29	B	635	LMT	C4-C5-C6-C7
36	B	623	HTG	C3'-C4'-C5'-C6'
39	F	102	HEM	C4B-C3B-CAB-CBB
39	v	205	HEM	C4B-C3B-CAB-CBB
34	a	415	LMG	O9-C10-O7-C8
34	b	630	LMG	C32-C33-C34-C35
37	c	519	DGD	O6E-C5E-C6E-O5E
34	B	622	LMG	C31-C32-C33-C34
38	D	409	LHG	C28-C29-C30-C31
34	z	101	LMG	C15-C16-C17-C18
24	C	505	CLA	C4-C3-C5-C6
24	c	514	CLA	C4-C3-C5-C6
32	D	405[A]	PL9	C45-C44-C46-C47
32	d	405[A]	PL9	C15-C14-C16-C17
29	b	631	LMT	C3'-C4'-O1B-C1B
24	c	514	CLA	C2-C3-C5-C6
32	a	416[A]	PL9	C12-C11-C9-C8
32	a	416[B]	PL9	C12-C11-C9-C8
32	A	420[A]	PL9	C4-C3-C7-C8
32	A	420[B]	PL9	C4-C3-C7-C8
32	a	416[A]	PL9	C4-C3-C7-C8
32	a	416[B]	PL9	C4-C3-C7-C8
24	B	615	CLA	C14-C13-C15-C16
24	a	410	CLA	C11-C12-C13-C14
24	b	611	CLA	C11-C10-C8-C9
24	b	624	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	626	CLA	C11-C12-C13-C14
24	c	513	CLA	C11-C10-C8-C9
34	Z	101	LMG	O6-C5-C6-O5
38	d	408	LHG	C31-C32-C33-C34
27	b	601	SQD	C35-C36-C37-C38
34	j	101	LMG	C17-C18-C19-C20
37	c	519	DGD	C7B-C8B-C9B-CAB
24	a	412	CLA	O1A-CGA-O2A-C1
24	C	506	CLA	C1A-C2A-CAA-CBA
34	a	415	LMG	C11-C10-O7-C8
27	B	621	SQD	C11-C10-C9-C8
27	b	601	SQD	C28-C29-C30-C31
37	D	406	DGD	C3B-C4B-C5B-C6B
37	h	102	DGD	CAA-CBA-CCA-CDA
24	C	504	CLA	C15-C16-C17-C18
38	D	408	LHG	C3-O3-P-O6
38	D	408	LHG	C4-O6-P-O3
27	b	601	SQD	C27-C28-C29-C30
34	b	630	LMG	C33-C34-C35-C36
37	C	517	DGD	C8A-C9A-CAA-CBA
37	e	101	DGD	C2A-C3A-C4A-C5A
37	C	518	DGD	C2A-C1A-O1G-C1G
37	e	101	DGD	C2A-C1A-O1G-C1G
34	C	520	LMG	C10-C11-C12-C13
24	c	511	CLA	C5-C6-C7-C8
24	B	616	CLA	C16-C17-C18-C19
24	C	502	CLA	C16-C17-C18-C19
36	b	602	HTG	C2'-C3'-C4'-C5'
34	j	101	LMG	C36-C37-C38-C39
38	L	101	LHG	C13-C14-C15-C16
37	C	516	DGD	C4D-C5D-C6D-O5D
38	d	407	LHG	C24-C23-O8-C6
37	e	101	DGD	O6E-C5E-C6E-O5E
32	d	405[B]	PL9	C43-C44-C46-C47
27	A	412	SQD	C16-C17-C18-C19
27	a	405	SQD	C23-C24-C25-C26
24	d	401	CLA	C2C-C3C-CAC-CBC
37	C	517	DGD	C5A-C6A-C7A-C8A
37	C	516	DGD	O6E-C5E-C6E-O5E
37	c	519	DGD	C4D-C5D-C6D-O5D
27	A	416	SQD	O6-C44-C45-C46
27	B	621	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
27	F	103	SQD	C44-C45-C46-O48
27	a	405	SQD	O6-C44-C45-C46
27	a	414	SQD	O6-C44-C45-C46
34	a	415	LMG	C7-C8-C9-O8
34	b	630	LMG	C40-C41-C42-C43
34	c	522	LMG	O1-C7-C8-C9
34	j	101	LMG	C16-C17-C18-C19
36	b	608	HTG	C4'-C5'-C6'-C7'
37	D	406	DGD	O1G-C1G-C2G-C3G
38	a	422	LHG	C4-C5-C6-O8
34	z	101	LMG	C13-C14-C15-C16
37	C	518	DGD	O1A-C1A-O1G-C1G
34	C	520	LMG	C8-C7-O1-C1
37	C	517	DGD	C5D-C6D-O5D-C1E
37	c	520	DGD	C2G-C3G-O3G-C1D
37	c	520	DGD	C5D-C6D-O5D-C1E
37	e	101	DGD	C4A-C5A-C6A-C7A
38	D	407	LHG	C17-C18-C19-C20
37	e	101	DGD	C9B-CAB-CBB-CCB
34	b	630	LMG	C37-C38-C39-C40
28	C	524	GOL	O1-C1-C2-O2
28	V	201	GOL	O1-C1-C2-O2
28	V	202	GOL	O2-C2-C3-O3
28	v	202	GOL	O1-C1-C2-O2
37	h	102	DGD	C4E-C5E-C6E-O5E
24	c	510	CLA	C15-C16-C17-C18
29	m	102	LMT	C11-C10-C9-C8
38	D	407	LHG	C25-C26-C27-C28
38	E	101	LHG	C24-C25-C26-C27
29	C	521	LMT	O5B-C5B-C6B-O6B
24	c	517	CLA	C2-C1-O2A-CGA
27	a	414	SQD	C15-C16-C17-C18
37	c	521	DGD	C5B-C6B-C7B-C8B
38	d	408	LHG	C28-C29-C30-C31
24	C	509	CLA	C10-C11-C12-C13
34	a	415	LMG	C33-C34-C35-C36
24	c	515	CLA	CBA-CGA-O2A-C1
27	A	416	SQD	C24-C23-O48-C46
24	C	507	CLA	O1D-CGD-O2D-CED
24	b	612	CLA	C16-C17-C18-C20
37	c	520	DGD	C3B-C4B-C5B-C6B
24	B	605	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
38	d	407	LHG	O10-C23-O8-C6
37	c	521	DGD	CBA-CCA-CDA-CEA
27	F	103	SQD	C2-C1-O6-C44
34	Z	101	LMG	C2-C1-O1-C7
27	a	414	SQD	C27-C28-C29-C30
29	B	635	LMT	C11-C10-C9-C8
27	a	414	SQD	O6-C44-C45-O47
27	f	102	SQD	O6-C44-C45-O47
34	A	422	LMG	C13-C14-C15-C16
34	b	630	LMG	C16-C17-C18-C19
37	C	518	DGD	C2A-C3A-C4A-C5A
38	D	409	LHG	C12-C13-C14-C15
24	c	515	CLA	O1A-CGA-O2A-C1
37	e	101	DGD	O1A-C1A-O1G-C1G
24	c	507	CLA	O1D-CGD-O2D-CED
27	F	103	SQD	C32-C33-C34-C35
27	f	102	SQD	C31-C32-C33-C34
37	c	520	DGD	C2B-C3B-C4B-C5B
24	B	616	CLA	C12-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C10
24	C	512	CLA	C11-C10-C8-C7
24	b	624	CLA	C11-C12-C13-C15
24	b	624	CLA	C12-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C10
32	D	405[A]	PL9	C13-C14-C16-C17
32	D	405[B]	PL9	C13-C14-C16-C17
24	B	616	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C9
24	b	611	CLA	C6-C7-C8-C9
24	b	616	CLA	C14-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C9
24	c	513	CLA	C14-C13-C15-C16
29	D	401	LMT	O1'-C1-C2-C3
34	a	415	LMG	C21-C22-C23-C24
24	C	503	CLA	C8-C10-C11-C12
29	a	404	LMT	C6-C7-C8-C9
27	a	414	SQD	C19-C20-C21-C22
38	l	101	LHG	C11-C12-C13-C14
26	Y	101	BCR	C21-C22-C23-C24
38	d	408	LHG	C33-C34-C35-C36
37	h	102	DGD	C5B-C6B-C7B-C8B
24	b	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
38	D	409	LHG	C24-C23-O8-C6
29	C	521	LMT	O1'-C1-C2-C3
37	C	517	DGD	C4A-C5A-C6A-C7A
37	c	520	DGD	C1A-C2A-C3A-C4A
38	d	406	LHG	C7-C8-C9-C10
24	B	614	CLA	C13-C15-C16-C17
34	c	523	LMG	C32-C33-C34-C35
29	M	104	LMT	O5'-C1'-O1'-C1
38	D	408	LHG	C32-C33-C34-C35
24	C	509	CLA	C8-C10-C11-C12
24	b	626	CLA	C10-C11-C12-C13
34	b	630	LMG	C39-C40-C41-C42
24	B	602	CLA	CBA-CGA-O2A-C1
27	f	102	SQD	C24-C25-C26-C27
34	a	415	LMG	C12-C13-C14-C15
29	M	103	LMT	C2-C1-O1'-C1'
34	a	415	LMG	C35-C36-C37-C38
24	b	613	CLA	C5-C6-C7-C8
37	c	521	DGD	C4A-C5A-C6A-C7A
34	c	523	LMG	O6-C5-C6-O5
24	C	510	CLA	CBA-CGA-O2A-C1
27	b	601	SQD	C44-C45-C46-O48
34	A	422	LMG	C7-C8-C9-O8
34	C	520	LMG	C7-C8-C9-O8
34	Z	101	LMG	C7-C8-C9-O8
37	e	101	DGD	O1G-C1G-C2G-C3G
38	E	101	LHG	C4-C5-C6-O8
38	D	407	LHG	C34-C35-C36-C37
24	A	410	CLA	C8-C10-C11-C12
24	c	506	CLA	C16-C17-C18-C19
24	b	614	CLA	O1D-CGD-O2D-CED
38	L	101	LHG	C33-C34-C35-C36
34	c	522	LMG	C10-C11-C12-C13
37	C	517	DGD	C1A-C2A-C3A-C4A
28	V	205	GOL	O2-C2-C3-O3
38	D	407	LHG	O1-C1-C2-O2
27	F	103	SQD	C31-C32-C33-C34
27	a	405	SQD	C19-C20-C21-C22
24	A	405	CLA	C13-C15-C16-C17
24	c	513	CLA	C10-C11-C12-C13
27	a	414	SQD	C35-C36-C37-C38
24	b	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	C	517	DGD	CAB-CBB-CCB-CDB
24	B	614	CLA	C15-C16-C17-C18
38	D	409	LHG	O10-C23-O8-C6
27	b	601	SQD	C31-C32-C33-C34
27	F	103	SQD	O47-C45-C46-O48
34	Z	101	LMG	O1-C7-C8-O7
34	Z	101	LMG	O7-C8-C9-O8
34	z	101	LMG	O1-C7-C8-O7
32	D	405[A]	PL9	C9-C11-C12-C13
32	D	405[A]	PL9	C39-C41-C42-C43
38	d	406	LHG	C11-C10-C9-C8
24	C	513	CLA	C2-C1-O2A-CGA
24	b	624	CLA	C2-C1-O2A-CGA
24	c	515	CLA	C2-C1-O2A-CGA
24	c	516	CLA	C2-C1-O2A-CGA
37	e	101	DGD	C2B-C3B-C4B-C5B
24	A	410	CLA	C6-C7-C8-C9
24	b	624	CLA	C11-C10-C8-C9
27	b	601	SQD	C11-C12-C13-C14
29	F	101	LMT	O1'-C1-C2-C3
34	A	422	LMG	C12-C13-C14-C15
37	H	103	DGD	CCA-CDA-CEA-CFA
24	b	611	CLA	C13-C15-C16-C17
24	C	510	CLA	O1A-CGA-O2A-C1
34	C	519	LMG	C30-C31-C32-C33
38	D	408	LHG	C33-C34-C35-C36
24	B	611	CLA	C16-C17-C18-C19
26	C	514	BCR	C1-C6-C7-C8
26	C	514	BCR	C5-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C26
26	c	518	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C30
24	B	602	CLA	C8-C10-C11-C12
24	c	513	CLA	C15-C16-C17-C18
37	D	406	DGD	C2B-C3B-C4B-C5B
36	V	207	HTG	S1-C1'-C2'-C3'
27	A	416	SQD	O10-C23-O48-C46
24	b	611	CLA	C10-C11-C12-C13
37	h	102	DGD	C6A-C7A-C8A-C9A
24	B	607	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	611	CLA	C16-C17-C18-C20
24	C	509	CLA	C16-C17-C18-C19
24	b	621	CLA	C16-C17-C18-C20
24	A	406	CLA	C2C-C3C-CAC-CBC
34	C	519	LMG	C14-C15-C16-C17
34	C	519	LMG	C29-C30-C31-C32
34	D	412	LMG	C13-C14-C15-C16
37	H	103	DGD	CDB-CEB-CFB-CGB
27	A	412	SQD	C15-C16-C17-C18
27	b	601	SQD	C30-C31-C32-C33
29	B	635	LMT	C2-C3-C4-C5
38	l	101	LHG	O6-C4-C5-C6
24	A	410	CLA	C6-C7-C8-C10
24	c	510	CLA	C11-C10-C8-C7
24	c	513	CLA	C12-C13-C15-C16
24	c	516	CLA	C11-C10-C8-C7
24	b	611	CLA	O1A-CGA-O2A-C1
37	H	103	DGD	CDA-CEA-CFA-CGA
24	A	405	CLA	C16-C17-C18-C19
37	e	101	DGD	C6A-C7A-C8A-C9A
27	B	621	SQD	C31-C32-C33-C34
36	V	207	HTG	O5-C1-S1-C1'
36	b	633	HTG	C2'-C1'-S1-C1
37	C	517	DGD	C4B-C5B-C6B-C7B
37	H	103	DGD	C9B-CAB-CBB-CCB
37	c	519	DGD	CBA-CCA-CDA-CEA
37	C	516	DGD	C6A-C7A-C8A-C9A
38	a	422	LHG	C13-C14-C15-C16
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	D	403	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	626	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
39	V	206	HEM	C2B-C3B-CAB-CBB
39	e	102	HEM	C2B-C3B-CAB-CBB
34	c	522	LMG	C39-C40-C41-C42
38	D	407	LHG	C11-C10-C9-C8
27	F	103	SQD	O5-C1-O6-C44
29	M	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
24	b	621	CLA	C8-C10-C11-C12
29	f	103	LMT	C4-C5-C6-C7
34	C	520	LMG	C39-C40-C41-C42
37	c	519	DGD	C2A-C3A-C4A-C5A
34	A	422	LMG	O1-C7-C8-C9
38	D	409	LHG	C2-C3-O3-P
38	d	408	LHG	C2-C3-O3-P
36	b	633	HTG	C4-C5-C6-O6
38	a	422	LHG	O6-C4-C5-O7
24	b	622	CLA	C8-C10-C11-C12
24	b	620	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	611	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
29	a	404	LMT	C4B-C5B-C6B-O6B
24	B	602	CLA	O1A-CGA-O2A-C1
34	C	519	LMG	C31-C32-C33-C34
34	C	519	LMG	C12-C13-C14-C15
37	c	520	DGD	C9B-CAB-CBB-CCB
27	B	621	SQD	O47-C45-C46-O48
27	b	601	SQD	O47-C45-C46-O48
34	a	415	LMG	O7-C8-C9-O8
37	D	406	DGD	O1G-C1G-C2G-O2G
37	e	101	DGD	O1G-C1G-C2G-O2G
29	M	104	LMT	C1-C2-C3-C4
24	b	618	CLA	C13-C15-C16-C17
27	a	414	SQD	C17-C18-C19-C20
28	c	502	GOL	O1-C1-C2-O2
28	f	101	GOL	O2-C2-C3-O3
38	a	422	LHG	O1-C1-C2-O2
32	A	420[A]	PL9	C15-C14-C16-C17
27	B	621	SQD	C19-C20-C21-C22
27	a	405	SQD	C35-C36-C37-C38
25	A	408	PHO	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	d	405[A]	PL9	C28-C29-C31-C32
24	c	513	CLA	C11-C12-C13-C14
27	a	405	SQD	C27-C28-C29-C30
24	b	620	CLA	C15-C16-C17-C18
27	F	103	SQD	C5-C6-S-O8
24	c	506	CLA	C16-C17-C18-C20
29	D	401	LMT	O5B-C1B-O1B-C4'
24	C	509	CLA	O1D-CGD-O2D-CED
38	d	406	LHG	C30-C31-C32-C33
28	b	607	GOL	O1-C1-C2-C3
28	b	607	GOL	C1-C2-C3-O3
24	b	624	CLA	C15-C16-C17-C18
24	c	512	CLA	C1A-C2A-CAA-CBA
38	l	101	LHG	C7-C8-C9-C10
38	E	101	LHG	C4-O6-P-O3
36	B	632	HTG	O5-C5-C6-O6
24	b	626	CLA	C4-C3-C5-C6
32	d	405[B]	PL9	C15-C14-C16-C17
37	c	520	DGD	C6A-C7A-C8A-C9A
38	D	408	LHG	C4-O6-P-O5
38	L	101	LHG	C4-O6-P-O5
27	F	103	SQD	C7-C8-C9-C10
34	A	422	LMG	C18-C19-C20-C21
37	c	521	DGD	C2A-C1A-O1G-C1G
27	F	103	SQD	C34-C35-C36-C37
37	h	102	DGD	CBB-CCB-CDB-CEB
24	b	624	CLA	C16-C17-C18-C19
27	B	621	SQD	C33-C34-C35-C36
36	B	623	HTG	C4'-C5'-C6'-C7'
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	608	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	b	615	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
38	D	408	LHG	C26-C27-C28-C29
38	E	101	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	B	621	SQD	C24-C23-O48-C46
38	D	408	LHG	C1-C2-C3-O3
24	d	401	CLA	C4C-C3C-CAC-CBC
27	f	102	SQD	C25-C26-C27-C28
38	E	101	LHG	C15-C16-C17-C18
24	b	625	CLA	C16-C17-C18-C19
25	A	408	PHO	C4-C3-C5-C6
24	B	602	CLA	C11-C10-C8-C7
24	B	604	CLA	C11-C10-C8-C7
24	C	504	CLA	C12-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C15
36	V	207	HTG	C2-C1-S1-C1'
38	l	101	LHG	O6-C4-C5-O7
37	h	102	DGD	O2G-C1B-C2B-C3B
27	a	405	SQD	C24-C25-C26-C27
29	f	103	LMT	C5-C6-C7-C8
38	D	408	LHG	C13-C14-C15-C16
34	Z	101	LMG	O1-C7-C8-C9
38	l	101	LHG	C28-C29-C30-C31
34	A	422	LMG	O1-C7-C8-O7
34	c	522	LMG	O1-C7-C8-O7
34	c	522	LMG	O7-C8-C9-O8
38	E	101	LHG	O7-C5-C6-O8
27	a	414	SQD	C30-C31-C32-C33
34	a	415	LMG	C34-C35-C36-C37
38	a	422	LHG	C14-C15-C16-C17
37	C	517	DGD	C2G-C3G-O3G-C1D
24	C	501	CLA	C13-C15-C16-C17
37	c	520	DGD	C2A-C3A-C4A-C5A
32	A	420[B]	PL9	C15-C14-C16-C17
37	H	103	DGD	O2G-C1B-C2B-C3B
27	F	103	SQD	C30-C31-C32-C33
24	C	502	CLA	C11-C12-C13-C14
24	b	616	CLA	C11-C10-C8-C9
24	c	510	CLA	C11-C10-C8-C9
24	C	513	CLA	O1A-CGA-O2A-C1
37	C	518	DGD	C9A-CAA-CBA-CCA
32	D	405[B]	PL9	C9-C11-C12-C13
32	a	416[A]	PL9	C14-C16-C17-C18
27	B	621	SQD	C35-C36-C37-C38
34	C	519	LMG	O10-C28-O8-C9
28	b	607	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
29	C	521	LMT	C5'-C4'-O1B-C1B
34	z	101	LMG	C16-C17-C18-C19
24	C	512	CLA	C3-C5-C6-C7
24	C	513	CLA	C3-C5-C6-C7
37	C	518	DGD	CDA-CEA-CFA-CGA
24	b	624	CLA	C16-C17-C18-C20
24	B	605	CLA	C4-C3-C5-C6
27	b	601	SQD	C11-C10-C9-C8
34	j	101	LMG	C15-C16-C17-C18
37	H	103	DGD	C5B-C6B-C7B-C8B
37	c	519	DGD	CBB-CCB-CDB-CEB
38	D	408	LHG	C31-C32-C33-C34
24	b	626	CLA	C2-C3-C5-C6
32	D	405[B]	PL9	C43-C44-C46-C47
34	C	519	LMG	C28-C29-C30-C31
37	c	520	DGD	C3A-C4A-C5A-C6A
38	d	408	LHG	C11-C10-C9-C8
37	h	102	DGD	O6E-C5E-C6E-O5E
37	D	406	DGD	C4A-C5A-C6A-C7A
24	C	502	CLA	C3-C5-C6-C7
37	C	517	DGD	C6B-C7B-C8B-C9B
27	B	621	SQD	C46-C45-O47-C7
27	b	601	SQD	C46-C45-O47-C7
24	D	402	CLA	C2-C1-O2A-CGA
24	b	623	CLA	C2-C1-O2A-CGA
27	B	621	SQD	O10-C23-O48-C46
37	c	521	DGD	O1A-C1A-O1G-C1G
37	C	518	DGD	CBA-CCA-CDA-CEA
24	C	506	CLA	C4-C3-C5-C6
26	D	404	BCR	C23-C24-C25-C30
26	c	518	BCR	C1-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C26
38	E	101	LHG	C16-C17-C18-C19
24	C	513	CLA	CBA-CGA-O2A-C1
38	L	101	LHG	C16-C17-C18-C19
36	c	524	HTG	C1'-C2'-C3'-C4'
37	C	516	DGD	O6E-C1E-O5D-C6D
29	M	101	LMT	C2'-C1'-O1'-C1
29	M	104	LMT	C2'-C1'-O1'-C1
38	a	422	LHG	O7-C5-C6-O8
27	a	405	SQD	C18-C19-C20-C21
27	a	414	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
34	A	422	LMG	C17-C18-C19-C20
38	L	101	LHG	C3-O3-P-O6
38	a	422	LHG	C4-O6-P-O3
34	B	622	LMG	C16-C17-C18-C19
34	C	519	LMG	C35-C36-C37-C38
24	b	626	CLA	C16-C17-C18-C19
34	a	415	LMG	C30-C31-C32-C33
37	h	102	DGD	CDB-CEB-CFB-CGB
24	A	405	CLA	C15-C16-C17-C18
27	a	405	SQD	C28-C29-C30-C31
29	M	103	LMT	C2B-C1B-O1B-C4'
27	f	102	SQD	O6-C44-C45-C46
24	a	412	CLA	C4-C3-C5-C6
32	D	405[B]	PL9	C35-C34-C36-C37
32	D	405[B]	PL9	C45-C44-C46-C47
32	a	416[A]	PL9	C45-C44-C46-C47
27	A	416	SQD	C24-C25-C26-C27
24	C	502	CLA	C11-C12-C13-C15
24	b	611	CLA	C11-C10-C8-C7
24	A	405	CLA	C2C-C3C-CAC-CBC
27	F	103	SQD	C33-C34-C35-C36
38	d	406	LHG	C33-C34-C35-C36
24	B	604	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C12-C13-C14
38	L	101	LHG	C10-C11-C12-C13
27	f	102	SQD	C26-C27-C28-C29
29	C	521	LMT	C4'-C5'-C6'-O6'
37	c	519	DGD	CDA-CEA-CFA-CGA
24	c	513	CLA	C13-C15-C16-C17
24	b	625	CLA	C16-C17-C18-C20
34	C	519	LMG	C29-C28-O8-C9
29	M	104	LMT	C5-C6-C7-C8
29	f	103	LMT	C2B-C1B-O1B-C4'
28	V	204	GOL	O2-C2-C3-O3
38	d	406	LHG	C26-C27-C28-C29
29	D	401	LMT	C2B-C1B-O1B-C4'
27	B	621	SQD	C14-C15-C16-C17
27	B	621	SQD	C17-C18-C19-C20
27	b	601	SQD	C33-C34-C35-C36
37	c	520	DGD	C8B-C9B-CAB-CBB
38	E	101	LHG	C14-C15-C16-C17
24	c	514	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	c	514	CLA	CBA-CGA-O2A-C1
37	H	103	DGD	C4E-C5E-C6E-O5E
37	c	519	DGD	O6E-C1E-O5D-C6D
38	a	422	LHG	O6-C4-C5-C6
24	b	614	CLA	C3-C5-C6-C7
37	C	518	DGD	C8B-C9B-CAB-CBB
38	d	406	LHG	C29-C30-C31-C32
37	D	406	DGD	CBA-CCA-CDA-CEA
27	A	416	SQD	C12-C13-C14-C15
39	V	206	HEM	C4B-C3B-CAB-CBB
34	D	412	LMG	C20-C21-C22-C23
38	D	408	LHG	C34-C35-C36-C37
34	a	415	LMG	C31-C32-C33-C34
32	A	420[A]	PL9	C13-C14-C16-C17
24	B	602	CLA	C2-C1-O2A-CGA
24	b	620	CLA	C16-C17-C18-C19
27	B	621	SQD	C12-C13-C14-C15
27	A	416	SQD	C2-C1-O6-C44
34	c	522	LMG	C2-C1-O1-C7
37	C	516	DGD	C2E-C1E-O5D-C6D
27	A	412	SQD	C18-C19-C20-C21
29	a	404	LMT	C3-C4-C5-C6
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	612	CLA	C2A-CAA-CBA-CGA
24	c	505	CLA	C2A-CAA-CBA-CGA
34	c	523	LMG	O7-C8-C9-O8
24	B	602	CLA	CAA-CBA-CGA-O2A
37	C	516	DGD	C1B-C2B-C3B-C4B
34	C	519	LMG	C21-C22-C23-C24
38	d	408	LHG	C35-C36-C37-C38
24	B	608	CLA	C3A-C2A-CAA-CBA
27	a	414	SQD	C33-C34-C35-C36
27	b	601	SQD	C14-C15-C16-C17
37	H	103	DGD	C4B-C5B-C6B-C7B
24	B	616	CLA	C4-C3-C5-C6
32	d	405[A]	PL9	C30-C29-C31-C32
32	a	416[A]	PL9	C43-C44-C46-C47
34	A	422	LMG	C36-C37-C38-C39
24	C	504	CLA	C14-C13-C15-C16
24	D	403	CLA	C6-C7-C8-C9
24	c	514	CLA	C11-C12-C13-C14
24	d	402	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C16-C17-C18-C19
24	b	620	CLA	C16-C17-C18-C20
27	a	405	SQD	C34-C35-C36-C37
39	V	206	HEM	CAD-CBD-CGD-O2D
37	H	103	DGD	C5A-C6A-C7A-C8A
37	h	102	DGD	O1G-C1G-C2G-C3G
29	M	104	LMT	C11-C10-C9-C8
36	B	632	HTG	C4'-C5'-C6'-C7'
37	C	516	DGD	CAA-CBA-CCA-CDA
34	b	630	LMG	C29-C28-O8-C9
27	A	416	SQD	O5-C1-O6-C44
34	A	422	LMG	O6-C1-O1-C7
34	c	522	LMG	O6-C1-O1-C7
38	D	409	LHG	C10-C11-C12-C13
24	B	609	CLA	C13-C15-C16-C17
32	a	416[B]	PL9	C45-C44-C46-C47
27	a	414	SQD	C10-C11-C12-C13
34	j	101	LMG	C13-C14-C15-C16
24	A	407	CLA	C11-C10-C8-C7
24	c	514	CLA	C12-C13-C15-C16
38	d	408	LHG	C9-C10-C11-C12
36	C	523	HTG	C1'-C2'-C3'-C4'
29	C	521	LMT	C3-C4-C5-C6
34	B	622	LMG	C22-C23-C24-C25
39	F	102	HEM	CAD-CBD-CGD-O1D
24	B	605	CLA	C13-C15-C16-C17
24	b	614	CLA	C13-C15-C16-C17
24	B	610	CLA	C16-C17-C18-C19
38	E	101	LHG	C17-C18-C19-C20
24	a	409	CLA	C2A-CAA-CBA-CGA
24	C	513	CLA	C5-C6-C7-C8
29	f	103	LMT	C9-C10-C11-C12
38	L	101	LHG	C12-C13-C14-C15
37	c	521	DGD	C3A-C4A-C5A-C6A
24	B	608	CLA	C16-C17-C18-C19
24	d	403	CLA	C15-C16-C17-C18
34	D	412	LMG	C16-C17-C18-C19
24	c	517	CLA	C4-C3-C5-C6
34	C	520	LMG	C11-C12-C13-C14
34	c	522	LMG	C36-C37-C38-C39
24	B	616	CLA	C2-C3-C5-C6
39	e	102	HEM	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
39	V	206	HEM	CAD-CBD-CGD-O1D
37	D	406	DGD	C4B-C5B-C6B-C7B
24	A	405	CLA	C16-C17-C18-C20
37	D	406	DGD	O2G-C2G-C3G-O3G
29	C	521	LMT	C1-C2-C3-C4
37	H	103	DGD	C3B-C4B-C5B-C6B
27	b	601	SQD	C10-C11-C12-C13
24	B	613	CLA	C8-C10-C11-C12
24	A	410	CLA	C15-C16-C17-C18
32	A	420[A]	PL9	C19-C21-C22-C23
32	a	416[A]	PL9	C39-C41-C42-C43
37	C	517	DGD	C1B-C2B-C3B-C4B
29	A	417	LMT	O1'-C1-C2-C3
24	C	511	CLA	C2-C1-O2A-CGA
24	c	510	CLA	C2-C1-O2A-CGA
32	A	420[A]	PL9	C43-C44-C46-C47
32	A	420[B]	PL9	C43-C44-C46-C47
32	a	416[B]	PL9	C43-C44-C46-C47
24	a	410	CLA	C10-C11-C12-C13
39	e	102	HEM	CAD-CBD-CGD-O1D
34	B	622	LMG	O8-C28-C29-C30
24	B	615	CLA	C6-C7-C8-C9
24	C	505	CLA	C11-C12-C13-C14
34	a	415	LMG	C15-C16-C17-C18
39	F	102	HEM	CAD-CBD-CGD-O2D
29	m	102	LMT	C4-C5-C6-C7
37	C	516	DGD	C8B-C9B-CAB-CBB
38	D	407	LHG	C33-C34-C35-C36
38	E	101	LHG	C12-C13-C14-C15
24	A	406	CLA	C15-C16-C17-C18
27	a	405	SQD	O10-C23-O48-C46
34	b	630	LMG	O10-C28-O8-C9
26	b	628	BCR	C23-C24-C25-C30
24	d	401	CLA	C15-C16-C17-C18
28	A	413	GOL	C1-C2-C3-O3
28	B	629	GOL	O1-C1-C2-C3
38	d	408	LHG	O1-C1-C2-C3
26	H	102	BCR	C9-C10-C11-C12
27	a	405	SQD	C24-C23-O48-C46
24	b	616	CLA	C8-C10-C11-C12
24	a	412	CLA	C2-C3-C5-C6
32	A	420[B]	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
34	A	422	LMG	O8-C28-C29-C30
24	b	611	CLA	C3-C5-C6-C7
38	d	407	LHG	C14-C15-C16-C17
34	Z	101	LMG	C8-C7-O1-C1
24	C	509	CLA	C13-C15-C16-C17
24	c	510	CLA	C13-C15-C16-C17
25	a	420[B]	PHO	C8-C10-C11-C12
29	m	102	LMT	C7-C8-C9-C10
24	C	510	CLA	C8-C10-C11-C12
37	c	520	DGD	C7A-C8A-C9A-CAA
34	D	412	LMG	C30-C31-C32-C33
38	d	408	LHG	C10-C11-C12-C13
32	A	420[A]	PL9	C30-C29-C31-C32
32	A	420[B]	PL9	C30-C29-C31-C32
24	B	610	CLA	C2-C3-C5-C6
24	C	505	CLA	C11-C12-C13-C15
24	b	616	CLA	C11-C10-C8-C7
24	A	406	CLA	C4C-C3C-CAC-CBC
26	h	101	BCR	C9-C10-C11-C12
26	k	101	BCR	C9-C10-C11-C12
37	c	519	DGD	C2E-C1E-O5D-C6D
39	v	205	HEM	CAD-CBD-CGD-O2D
38	d	407	LHG	O7-C5-C6-O8
36	B	623	HTG	C4-C5-C6-O6
27	a	405	SQD	C29-C30-C31-C32
24	c	507	CLA	C8-C10-C11-C12
36	B	623	HTG	C2'-C1'-S1-C1
24	C	512	CLA	CAA-CBA-CGA-O2A
34	Z	101	LMG	O7-C10-C11-C12
34	z	101	LMG	O7-C10-C11-C12
38	a	422	LHG	O8-C23-C24-C25
34	A	422	LMG	C33-C34-C35-C36
24	b	611	CLA	C4-C3-C5-C6
32	A	420[B]	PL9	C45-C44-C46-C47
32	D	405[A]	PL9	C35-C34-C36-C37
24	B	605	CLA	C2-C3-C5-C6
29	m	102	LMT	C4'-C5'-C6'-O6'
24	C	507	CLA	C11-C10-C8-C9
24	c	516	CLA	C11-C10-C8-C9
29	M	103	LMT	O1'-C1-C2-C3
34	C	519	LMG	C16-C17-C18-C19
24	C	513	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	b	619	CLA	C3A-C2A-CAA-CBA
37	C	518	DGD	O1G-C1A-C2A-C3A
37	h	102	DGD	CDA-CEA-CFA-CGA
39	e	102	HEM	CAA-CBA-CGA-O1A
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	b	613	CLA	CAD-CBD-CGD-O2D
24	b	620	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D
24	c	516	CLA	CAD-CBD-CGD-O2D
34	A	422	LMG	C16-C17-C18-C19
37	c	519	DGD	C5A-C6A-C7A-C8A
24	b	618	CLA	C2-C1-O2A-CGA
24	d	402	CLA	C2-C1-O2A-CGA
39	F	102	HEM	CAA-CBA-CGA-O2A
27	f	102	SQD	O47-C7-C8-C9
29	b	631	LMT	C6-C7-C8-C9
24	c	511	CLA	C4-C3-C5-C6
32	A	420[A]	PL9	C20-C19-C21-C22
32	A	420[A]	PL9	C45-C44-C46-C47
39	e	102	HEM	CAD-CBD-CGD-O2D
24	c	517	CLA	C2-C3-C5-C6
37	c	521	DGD	O1G-C1A-C2A-C3A
37	e	101	DGD	O2G-C1B-C2B-C3B
38	E	101	LHG	C25-C26-C27-C28
26	K	101	BCR	C7-C8-C9-C10
34	c	522	LMG	C17-C18-C19-C20
38	l	101	LHG	C17-C18-C19-C20
25	a	411	PHO	C2C-C3C-CAC-CBC
25	a	420[A]	PHO	C2C-C3C-CAC-CBC
37	H	103	DGD	C1G-C2G-C3G-O3G
39	F	102	HEM	CAA-CBA-CGA-O1A
29	m	102	LMT	C5-C6-C7-C8
37	D	406	DGD	O1G-C1A-C2A-C3A
29	D	401	LMT	C5-C6-C7-C8
24	A	406	CLA	C13-C15-C16-C17
24	D	403	CLA	O2A-C1-C2-C3
24	d	403	CLA	O2A-C1-C2-C3
25	A	408	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	a	411	PHO	O2A-C1-C2-C3
39	e	102	HEM	C4B-C3B-CAB-CBB
24	b	624	CLA	C2A-CAA-CBA-CGA
27	A	416	SQD	C15-C16-C17-C18
27	f	102	SQD	C33-C34-C35-C36
24	b	611	CLA	CAA-CBA-CGA-O1A
39	v	205	HEM	CAD-CBD-CGD-O1D
29	a	421	LMT	C5-C6-C7-C8
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	b	615	CLA	CHA-CBD-CGD-O1D
24	c	510	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O2D
37	c	521	DGD	O6E-C5E-C6E-O5E
24	A	405	CLA	C4C-C3C-CAC-CBC
37	e	101	DGD	C7B-C8B-C9B-CAB
38	L	101	LHG	C30-C31-C32-C33
24	c	516	CLA	CAA-CBA-CGA-O2A
38	L	101	LHG	O7-C7-C8-C9
38	d	406	LHG	O8-C23-C24-C25
27	A	412	SQD	O6-C44-C45-O47
24	c	510	CLA	O1A-CGA-O2A-C1
38	D	407	LHG	C7-C8-C9-C10
24	C	510	CLA	CAA-CBA-CGA-O2A
25	A	409[B]	PHO	CHA-CBD-CGD-O2D
25	a	420[B]	PHO	CHA-CBD-CGD-O1D
25	a	420[B]	PHO	CHA-CBD-CGD-O2D
28	T	101	GOL	O1-C1-C2-O2
24	b	624	CLA	C10-C11-C12-C13
38	D	407	LHG	C26-C27-C28-C29
38	l	101	LHG	O7-C7-C8-C9
38	D	407	LHG	C28-C29-C30-C31
38	a	422	LHG	O10-C23-C24-C25
34	j	101	LMG	C29-C30-C31-C32
37	c	520	DGD	C8A-C9A-CAA-CBA
24	a	410	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
27	A	412	SQD	O49-C7-O47-C45
39	e	102	HEM	CAA-CBA-CGA-O2A
24	A	407	CLA	C11-C10-C8-C9
24	D	403	CLA	C11-C10-C8-C9
24	b	626	CLA	C14-C13-C15-C16
34	C	519	LMG	C40-C41-C42-C43
24	C	512	CLA	CAA-CBA-CGA-O1A
27	A	412	SQD	C8-C7-O47-C45
32	a	416[B]	PL9	C11-C12-C13-C14
34	Z	101	LMG	O9-C10-C11-C12
24	c	514	CLA	CAA-CBA-CGA-O2A
37	C	516	DGD	O2G-C1B-C2B-C3B
27	A	416	SQD	C18-C19-C20-C21
38	D	409	LHG	C33-C34-C35-C36
34	z	101	LMG	O9-C10-C11-C12
24	c	510	CLA	C16-C17-C18-C19
24	d	403	CLA	C4-C3-C5-C6
38	L	101	LHG	C26-C27-C28-C29
28	T	101	GOL	O1-C1-C2-C3
24	C	506	CLA	C2-C3-C5-C6
37	e	101	DGD	C3A-C4A-C5A-C6A
38	D	409	LHG	C9-C10-C11-C12
38	l	101	LHG	C9-C10-C11-C12
24	c	505	CLA	C1A-C2A-CAA-CBA
37	e	101	DGD	O1B-C1B-C2B-C3B
24	c	508	CLA	C2-C1-O2A-CGA
24	c	510	CLA	CBA-CGA-O2A-C1
29	f	103	LMT	O5B-C1B-O1B-C4'
37	C	518	DGD	O1A-C1A-C2A-C3A
29	f	103	LMT	C1-C2-C3-C4
29	a	404	LMT	C7-C8-C9-C10
37	D	406	DGD	C1G-C2G-C3G-O3G
29	m	102	LMT	C9-C10-C11-C12
34	c	522	LMG	C40-C41-C42-C43
24	a	409	CLA	C13-C15-C16-C17
24	B	603	CLA	C2A-CAA-CBA-CGA
24	b	613	CLA	C2A-CAA-CBA-CGA
24	C	509	CLA	C16-C17-C18-C20
36	d	411	HTG	C1'-C2'-C3'-C4'
37	C	517	DGD	C3A-C4A-C5A-C6A
24	c	510	CLA	C4-C3-C5-C6
24	B	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	c	520	DGD	O2G-C1B-C2B-C3B
29	M	103	LMT	O5B-C1B-O1B-C4'
37	D	406	DGD	O1A-C1A-C2A-C3A
37	c	521	DGD	O1A-C1A-C2A-C3A
38	d	406	LHG	O10-C23-C24-C25
38	D	409	LHG	C4-O6-P-O5
38	L	101	LHG	C3-O3-P-O5
38	a	422	LHG	C4-O6-P-O5
24	c	514	CLA	CAA-CBA-CGA-O1A
24	c	516	CLA	CAA-CBA-CGA-O1A
27	f	102	SQD	O49-C7-C8-C9
24	b	623	CLA	CAA-CBA-CGA-O2A
24	B	606	CLA	O1A-CGA-O2A-C1
26	T	103	BCR	C1-C6-C7-C8
26	T	103	BCR	C5-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
32	A	420[B]	PL9	C19-C21-C22-C23
24	B	608	CLA	C16-C17-C18-C20
24	d	401	CLA	C16-C17-C18-C20
24	A	405	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C2A-CAA-CBA-CGA
24	B	613	CLA	C13-C15-C16-C17
38	D	407	LHG	C27-C28-C29-C30
36	b	632	HTG	S1-C1'-C2'-C3'
27	a	405	SQD	C32-C33-C34-C35
24	b	619	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CAD-CBD-CGD-O1D
24	c	515	CLA	CAD-CBD-CGD-O1D
34	B	622	LMG	C9-C8-O7-C10
24	a	409	CLA	C2C-C3C-CAC-CBC
38	L	101	LHG	C9-C10-C11-C12
38	d	407	LHG	C32-C33-C34-C35
24	C	507	CLA	C11-C12-C13-C14
38	l	101	LHG	O9-C7-C8-C9
24	c	509	CLA	CAA-CBA-CGA-O2A
37	C	517	DGD	O2G-C1B-C2B-C3B
38	E	101	LHG	O8-C23-C24-C25
38	D	409	LHG	C30-C31-C32-C33
27	A	416	SQD	C29-C30-C31-C32
24	C	501	CLA	CAA-CBA-CGA-O2A
34	c	522	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	d	408	LHG	O8-C23-C24-C25
24	b	625	CLA	C13-C15-C16-C17
32	A	420[B]	PL9	C20-C19-C21-C22
32	D	405[A]	PL9	C30-C29-C31-C32
29	a	404	LMT	C9-C10-C11-C12
34	z	101	LMG	C11-C12-C13-C14
24	C	507	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
24	b	614	CLA	C6-C7-C8-C10
24	b	626	CLA	C12-C13-C15-C16
24	c	506	CLA	C11-C12-C13-C15
32	d	405[A]	PL9	C18-C19-C21-C22
39	F	102	HEM	C2A-CAA-CBA-CGA
38	L	101	LHG	O9-C7-C8-C9
24	C	505	CLA	CAA-CBA-CGA-O2A
24	a	409	CLA	C4C-C3C-CAC-CBC
26	k	101	BCR	C19-C20-C21-C22
29	M	104	LMT	C9-C10-C11-C12
37	D	406	DGD	C9B-CAB-CBB-CCB
37	e	101	DGD	CAB-CBB-CCB-CDB
24	B	613	CLA	CAA-CBA-CGA-O2A
34	b	630	LMG	O8-C28-C29-C30
37	C	517	DGD	O1B-C1B-C2B-C3B
29	a	404	LMT	O5B-C5B-C6B-O6B
34	A	422	LMG	O7-C10-C11-C12
24	C	510	CLA	CAA-CBA-CGA-O1A
24	C	508	CLA	C13-C15-C16-C17
37	c	520	DGD	O1B-C1B-C2B-C3B
34	D	412	LMG	O7-C10-C11-C12

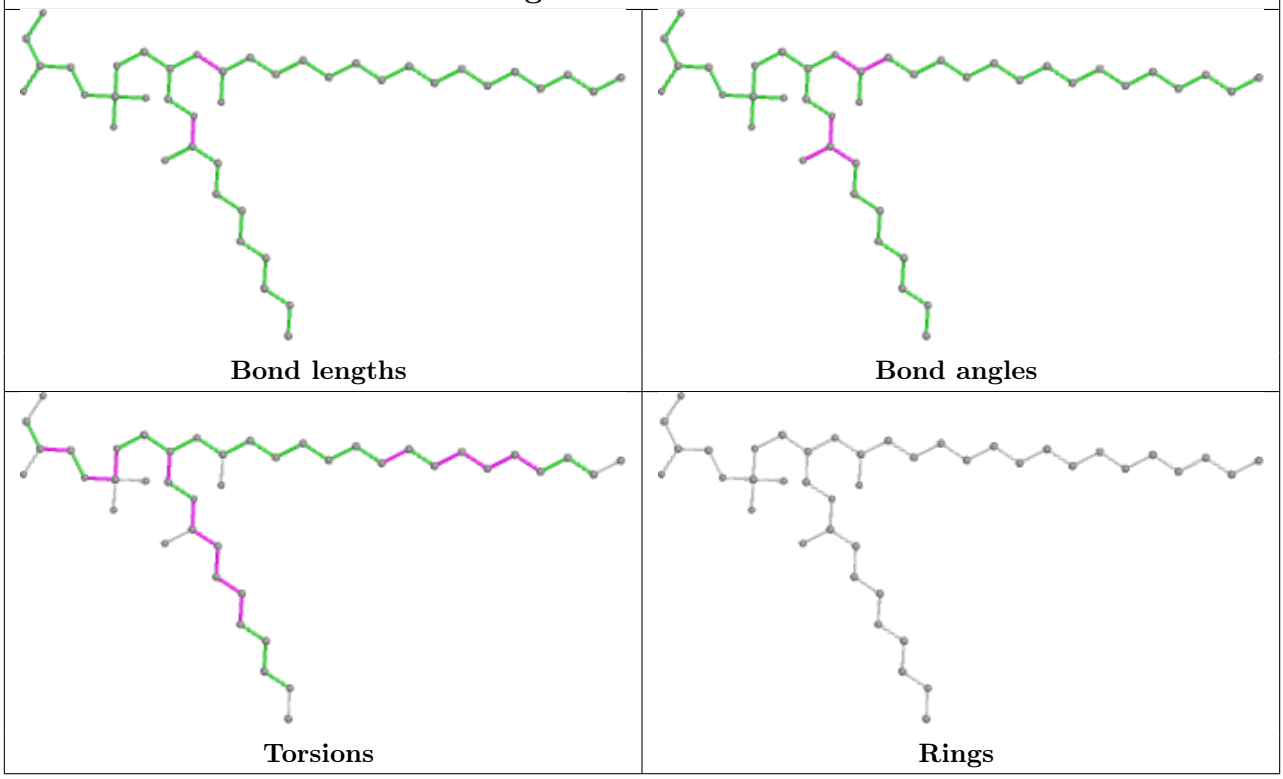
There are no ring outliers.

No monomer is involved in short contacts.

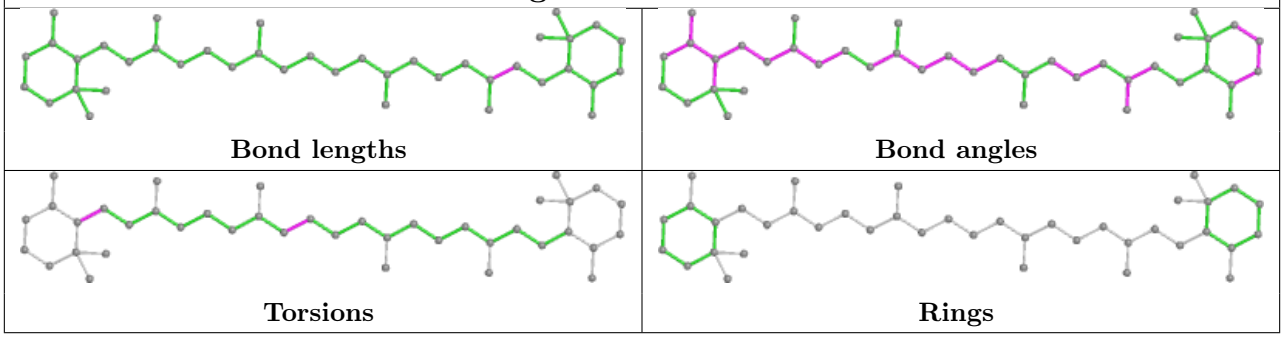
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

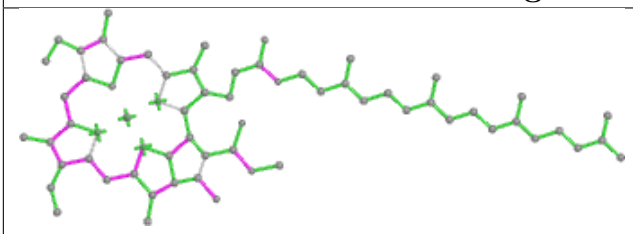
Ligand LHG E 101



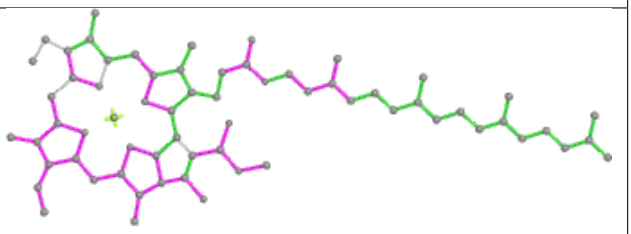
Ligand BCR t 101



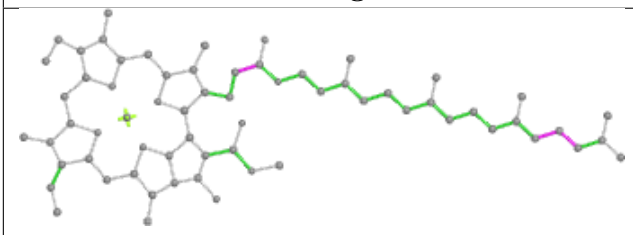
Ligand CLA B 614



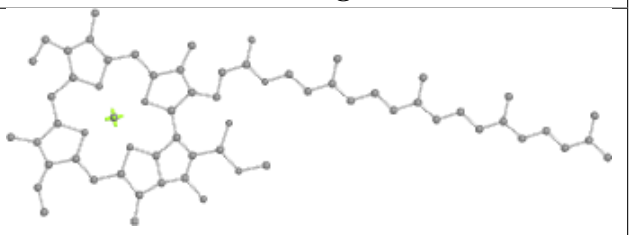
Bond lengths



Bond angles

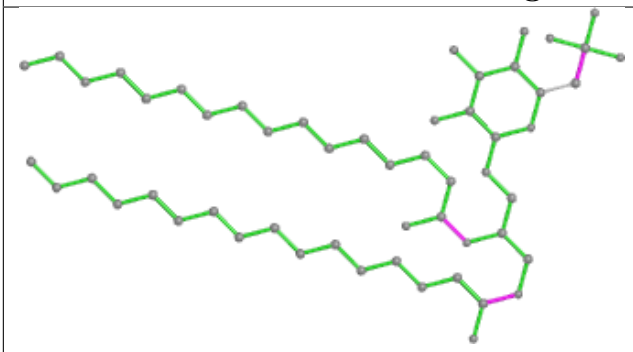


Torsions

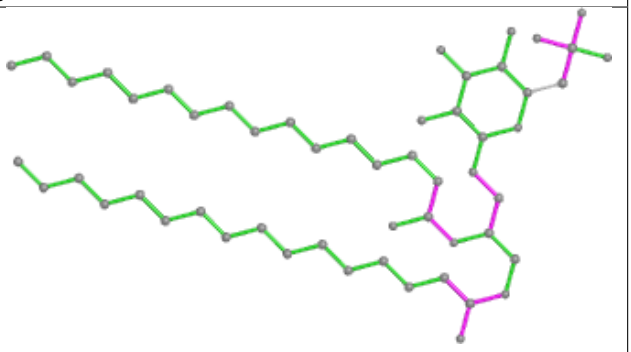


Rings

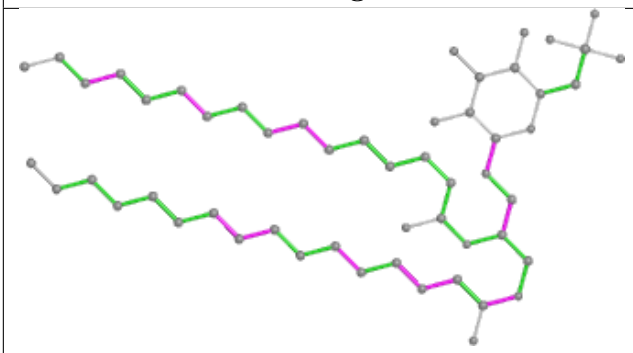
Ligand SQD A 416



Bond lengths



Bond angles



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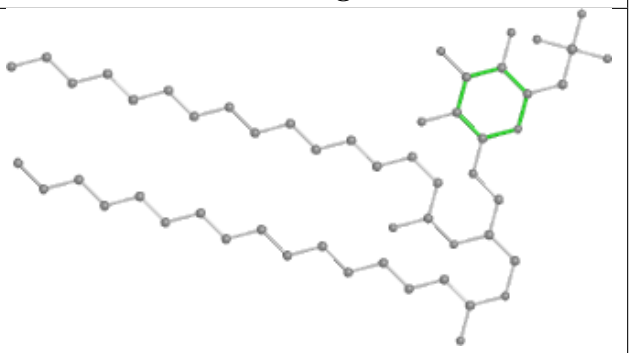
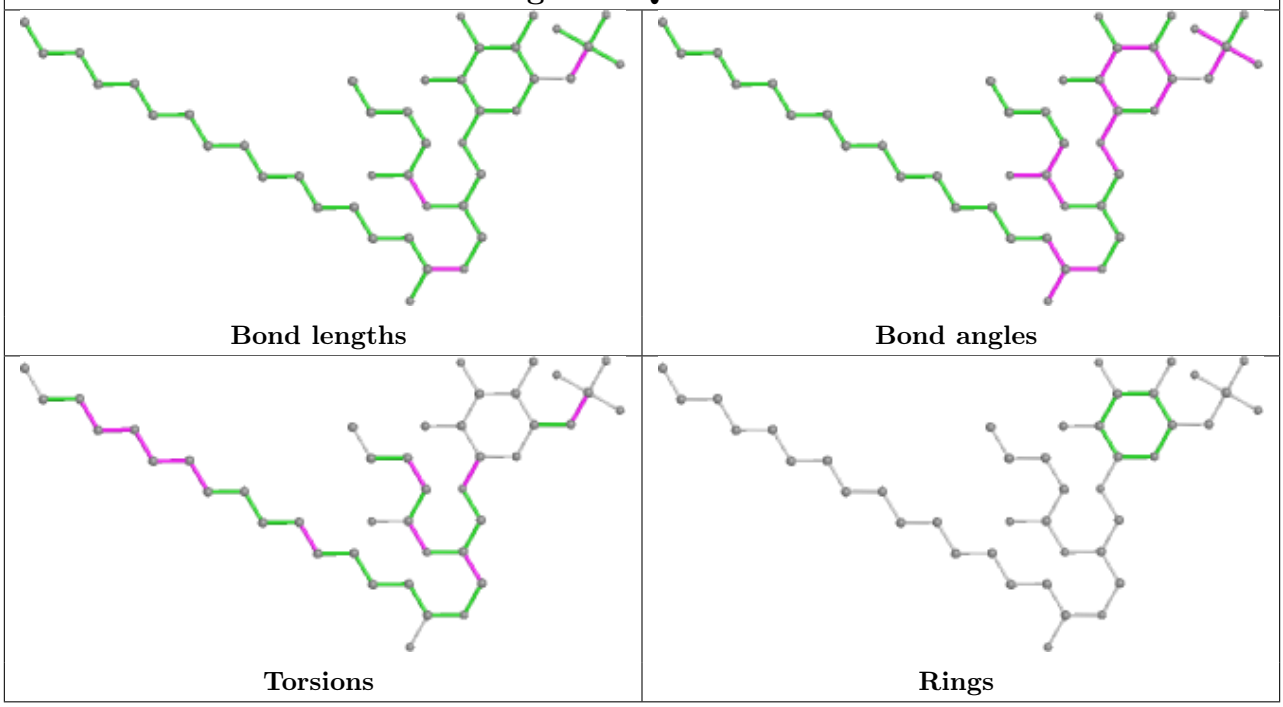
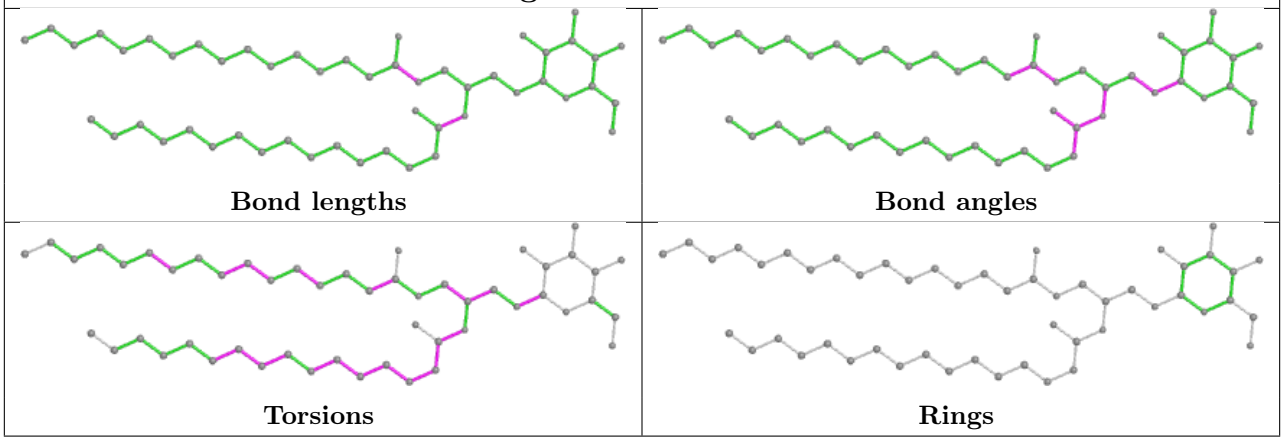


Rings

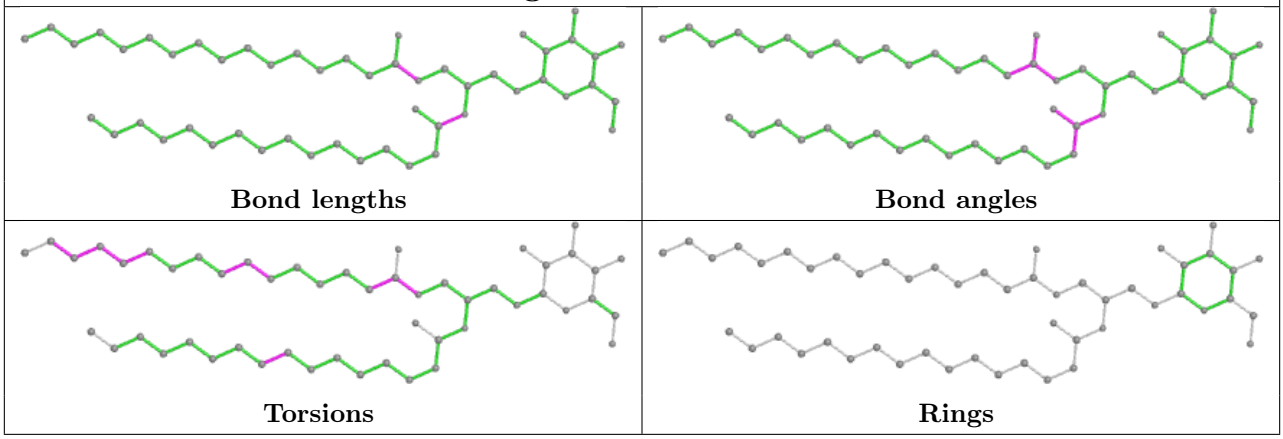
Ligand SQD F 103



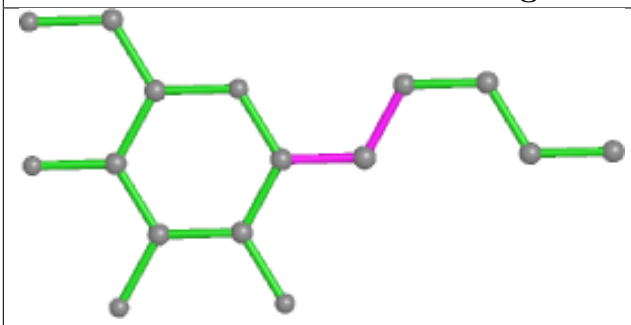
Ligand LMG A 422



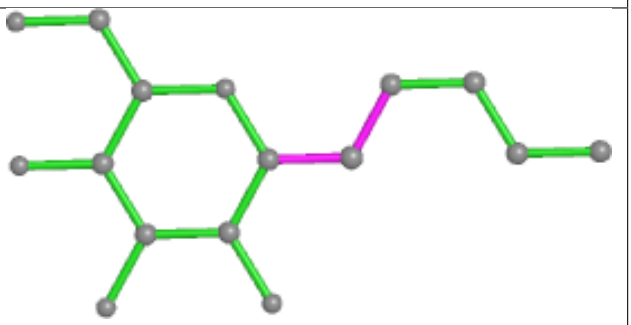
Ligand LMG b 630



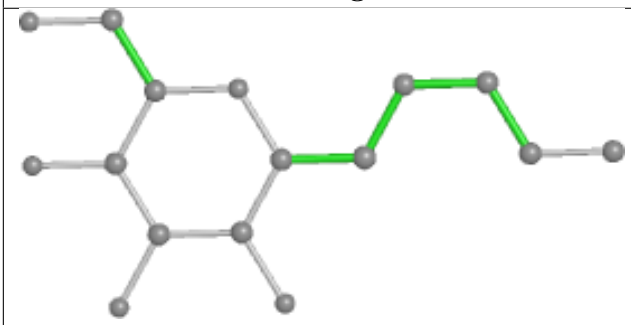
Ligand HTG H 101



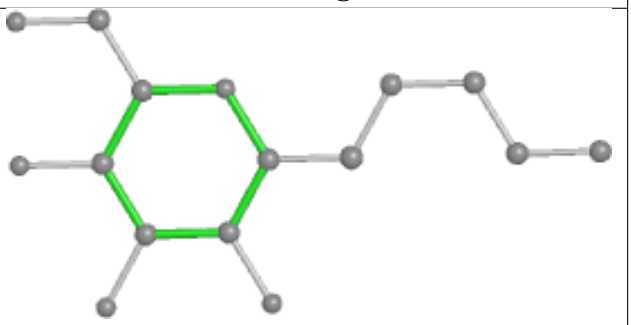
Bond lengths



Bond angles

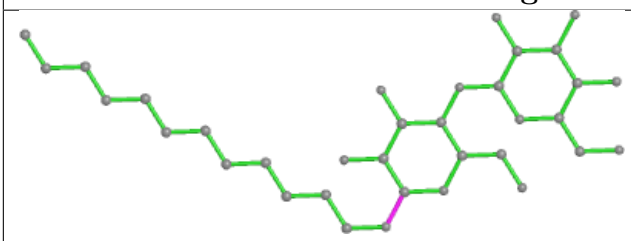


Torsions



Rings

Ligand LMT A 417



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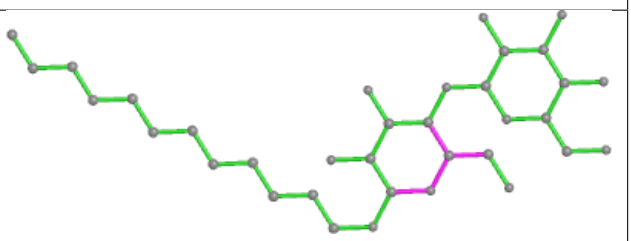
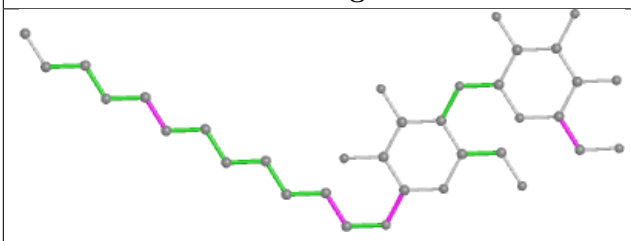
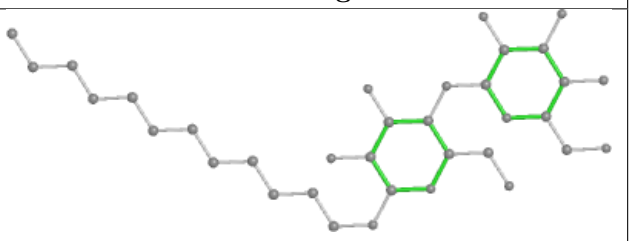


Bond angles

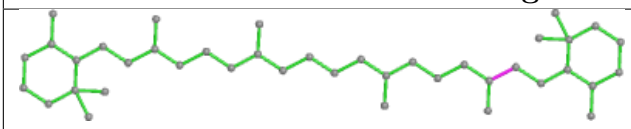


Torsions

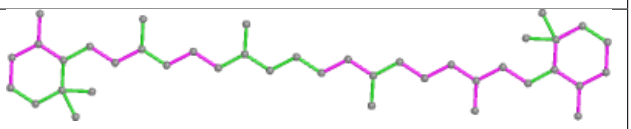


Rings

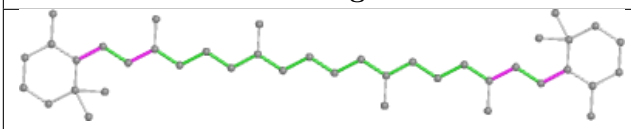
Ligand BCR D 404



Bond lengths



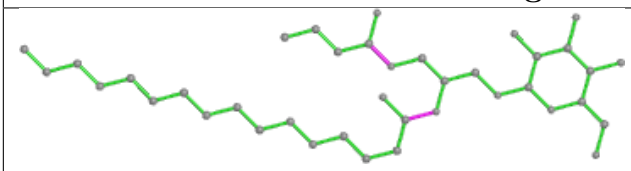
Bond angles



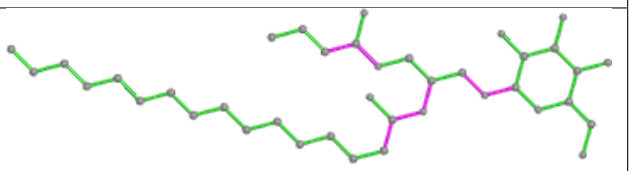
Torsions

Rings

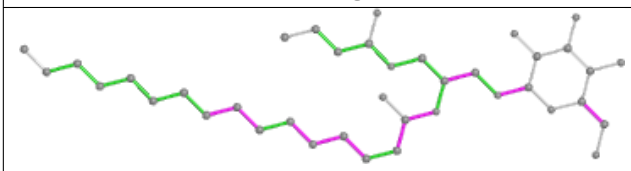
Ligand LMG z 101



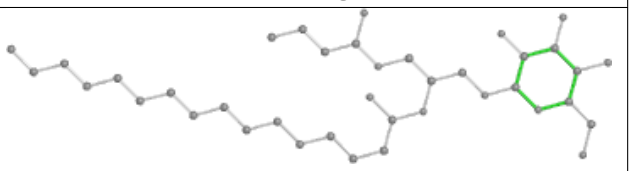
Bond lengths



Bond angles

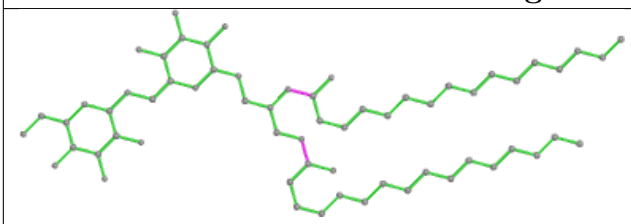


Torsions

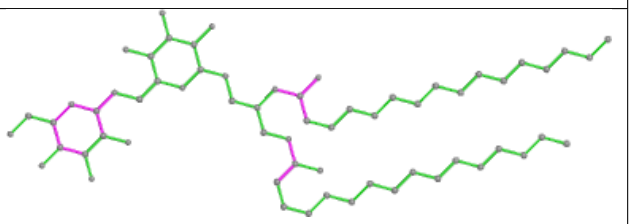


Rings

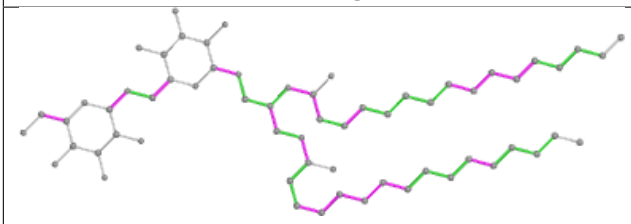
Ligand DGD e 101



Bond lengths



Bond angles



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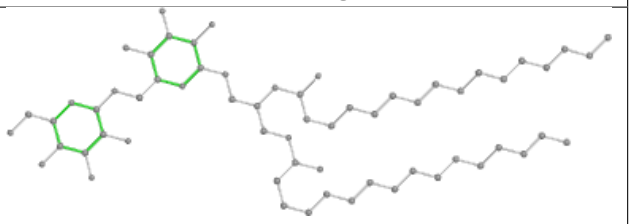
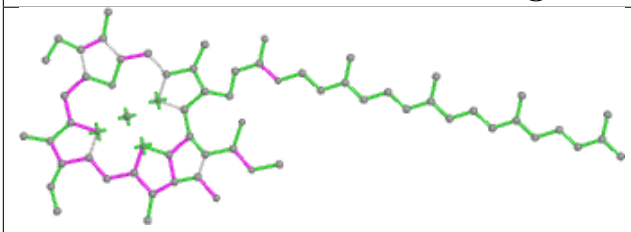
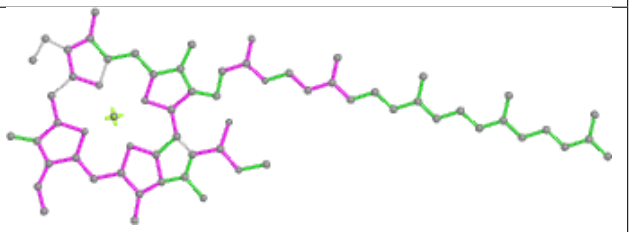


Rings

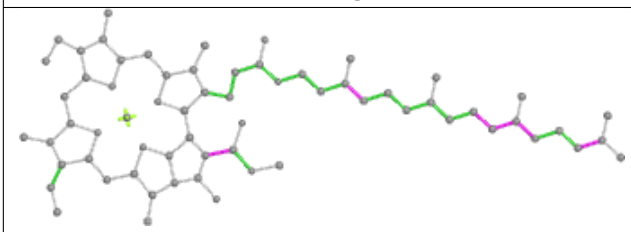
Ligand CLA b 626



Bond lengths



Bond angles



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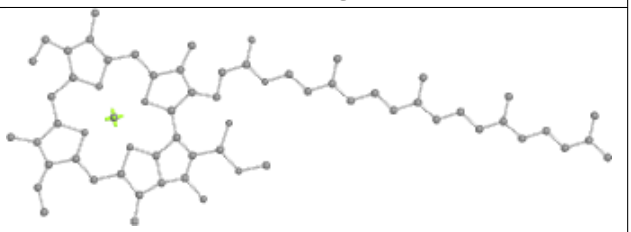
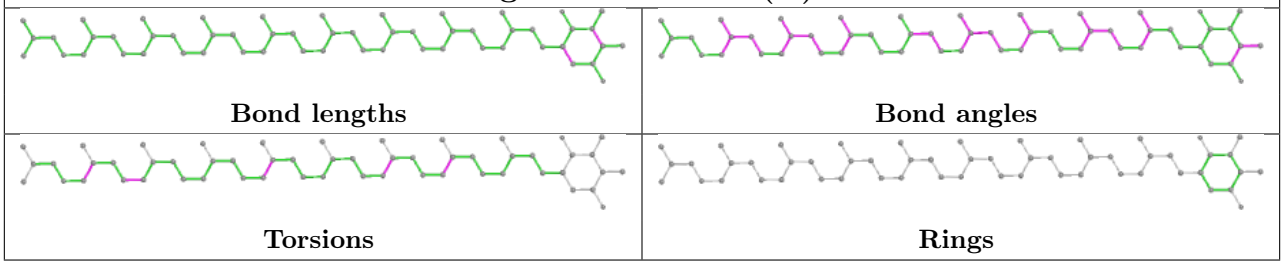
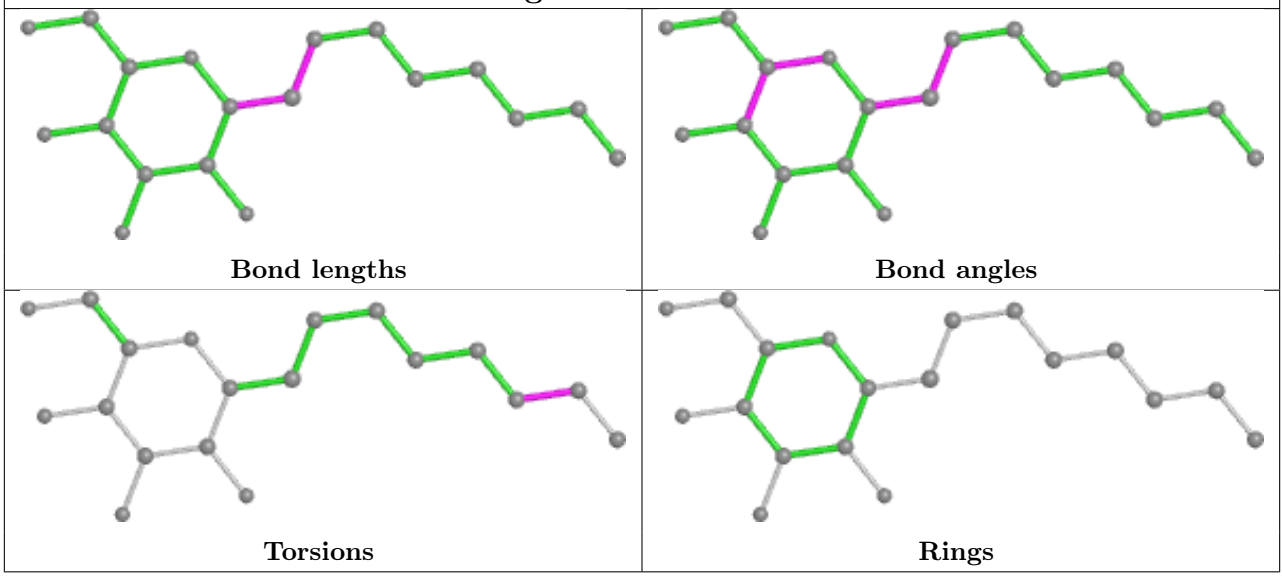


Rings

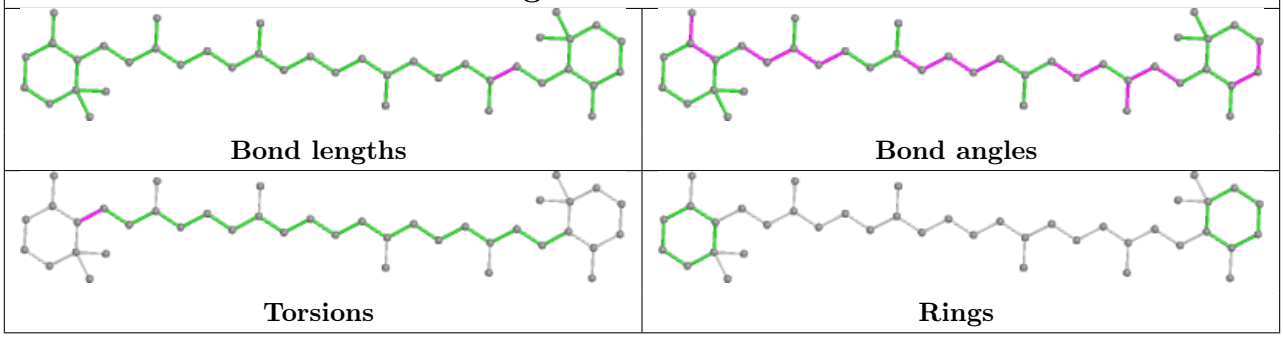
Ligand PL9 d 405 (A)



Ligand HTG b 608



Ligand BCR C 515



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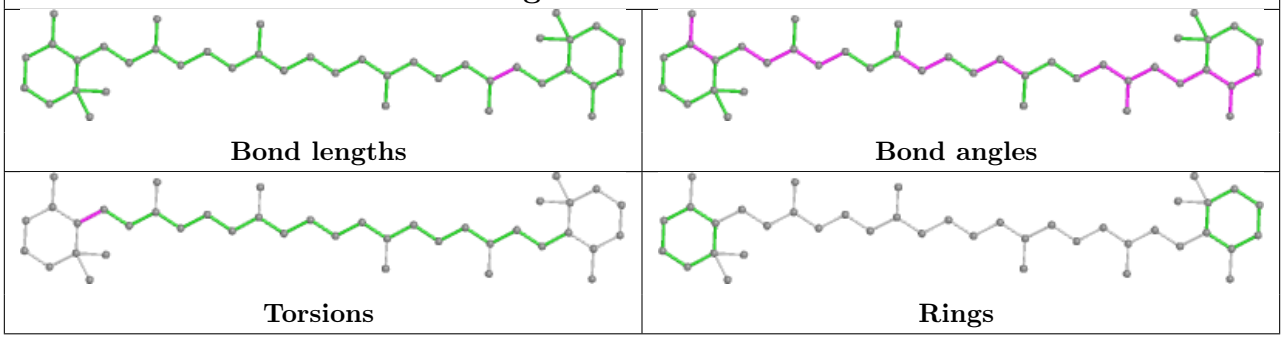
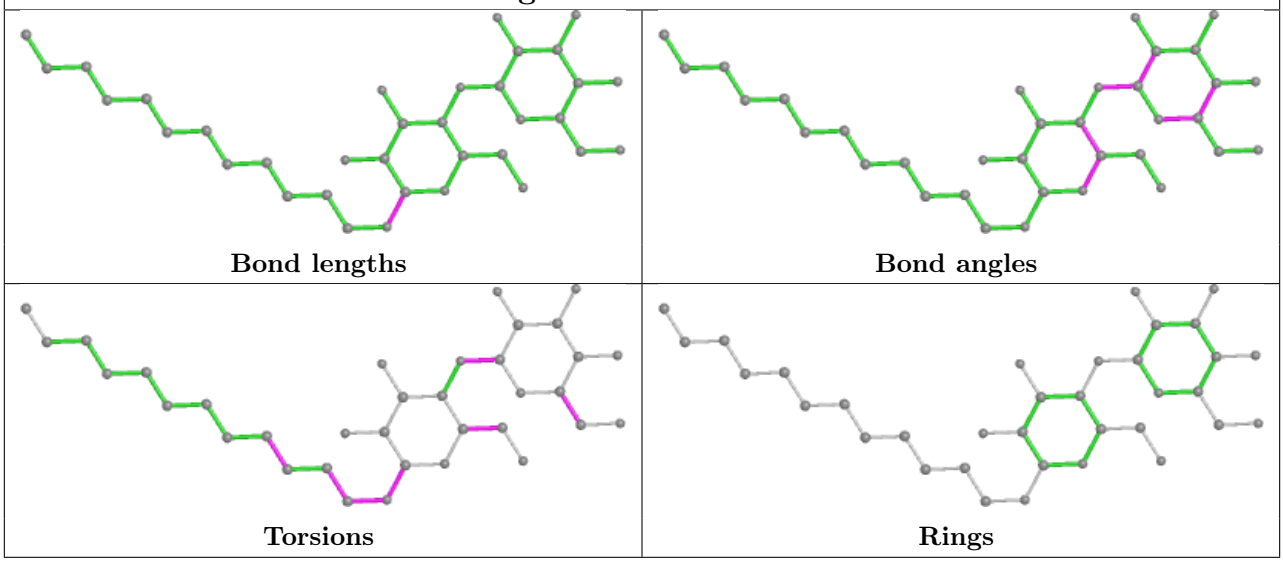
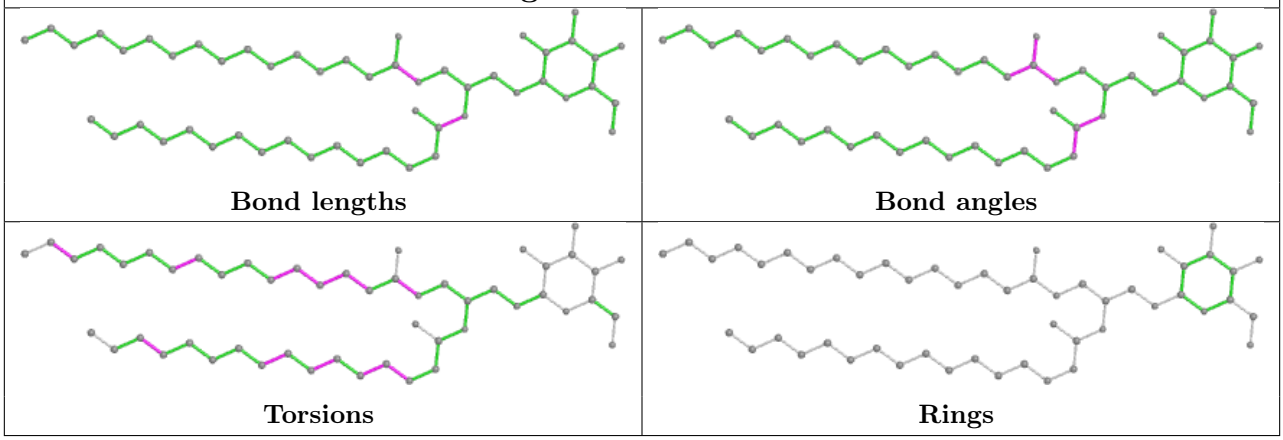


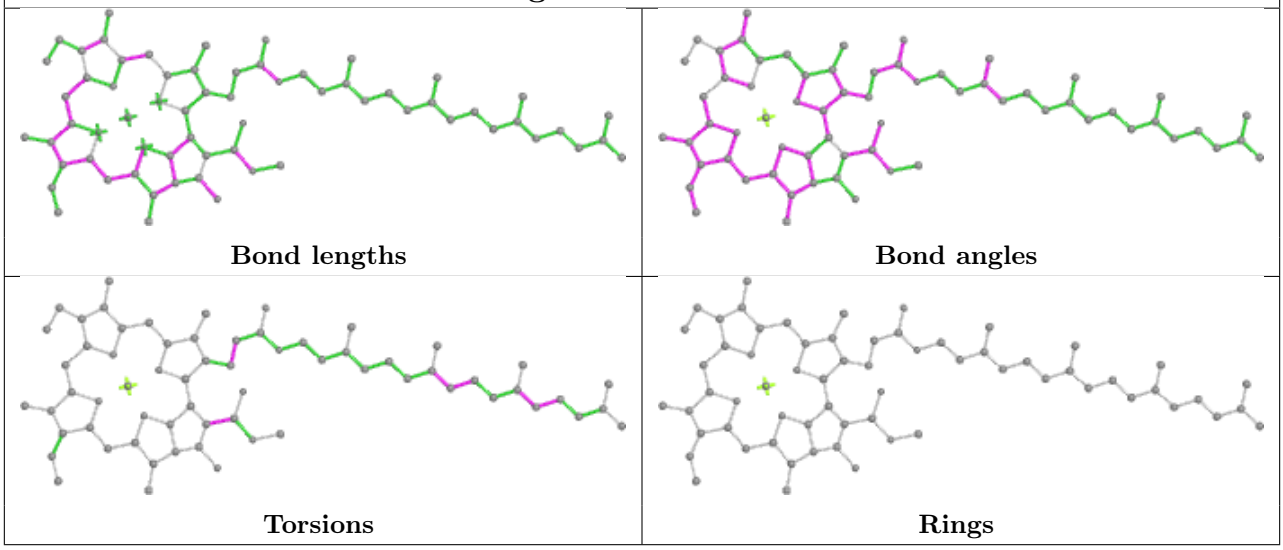
Ligand LMT M 103

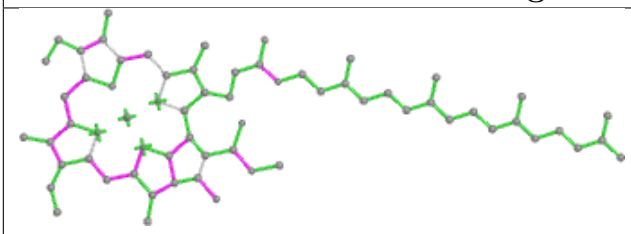
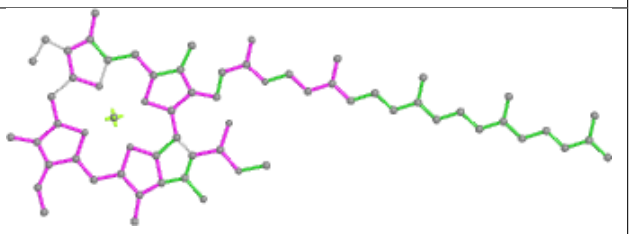
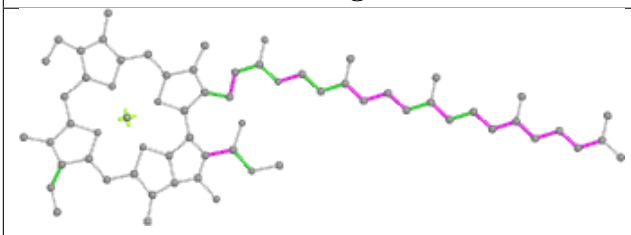
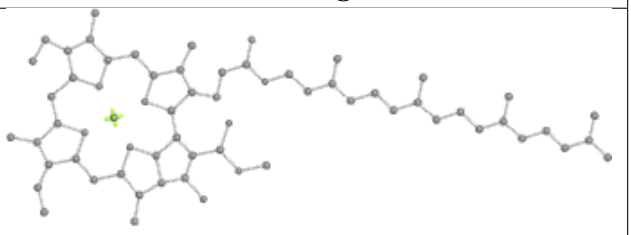


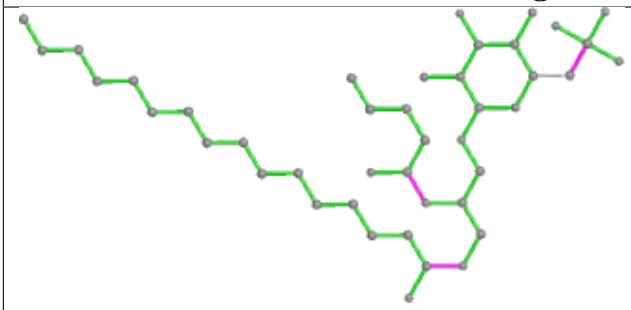
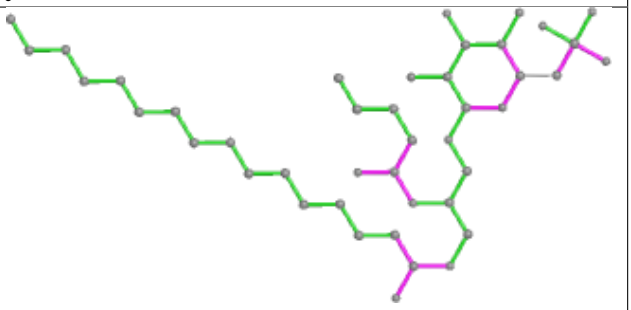
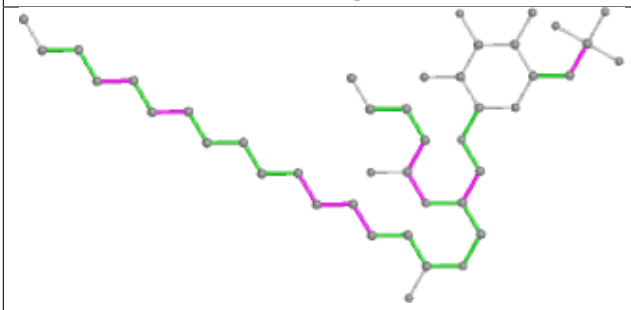
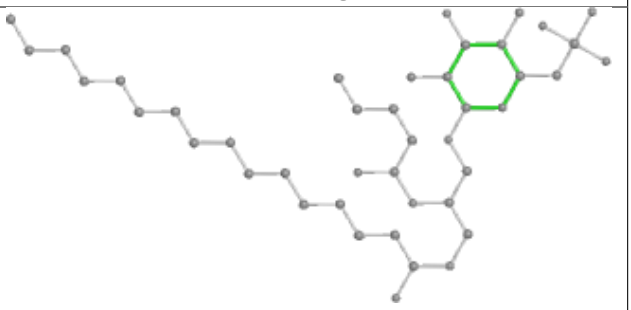
Ligand LMG C 519



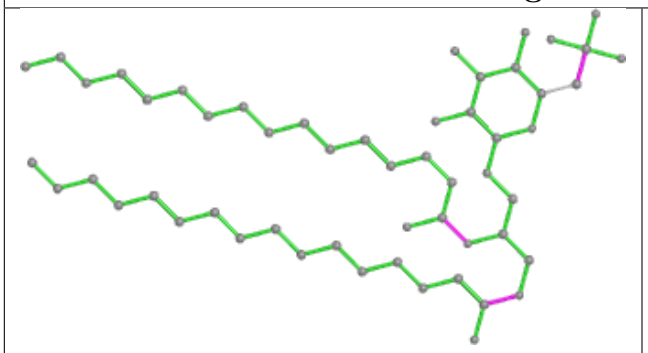
Ligand CLA b 616



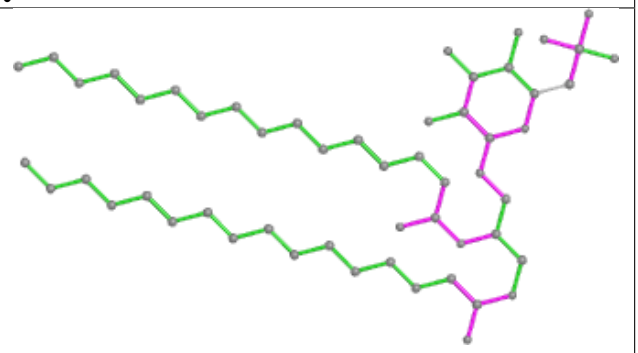
Ligand CLA b 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD f 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

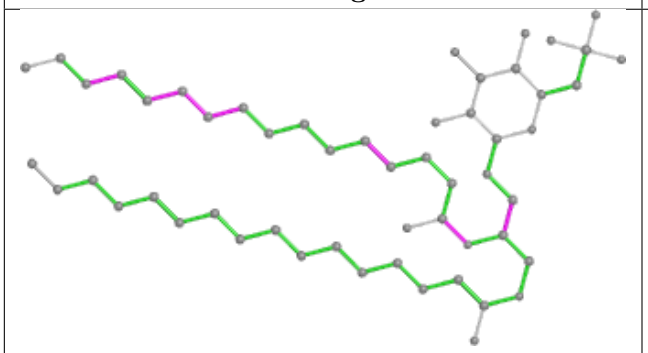
Ligand SQD A 412



Bond lengths



Bond angles



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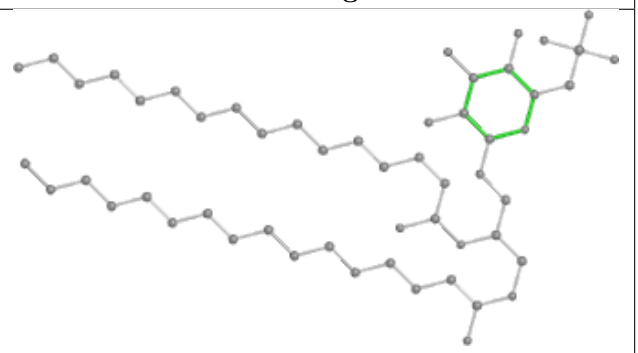
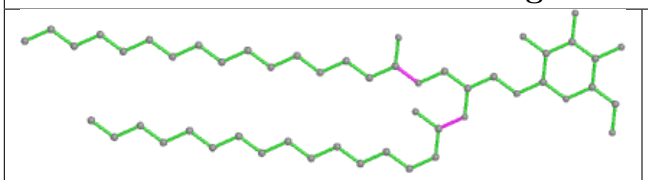
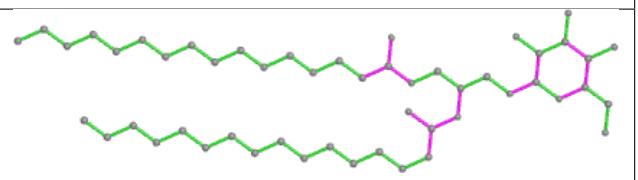


Rings

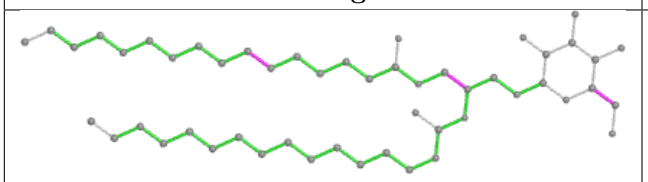
Ligand LMG c 523



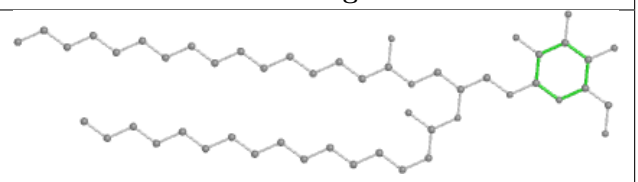
Bond lengths



Bond angles

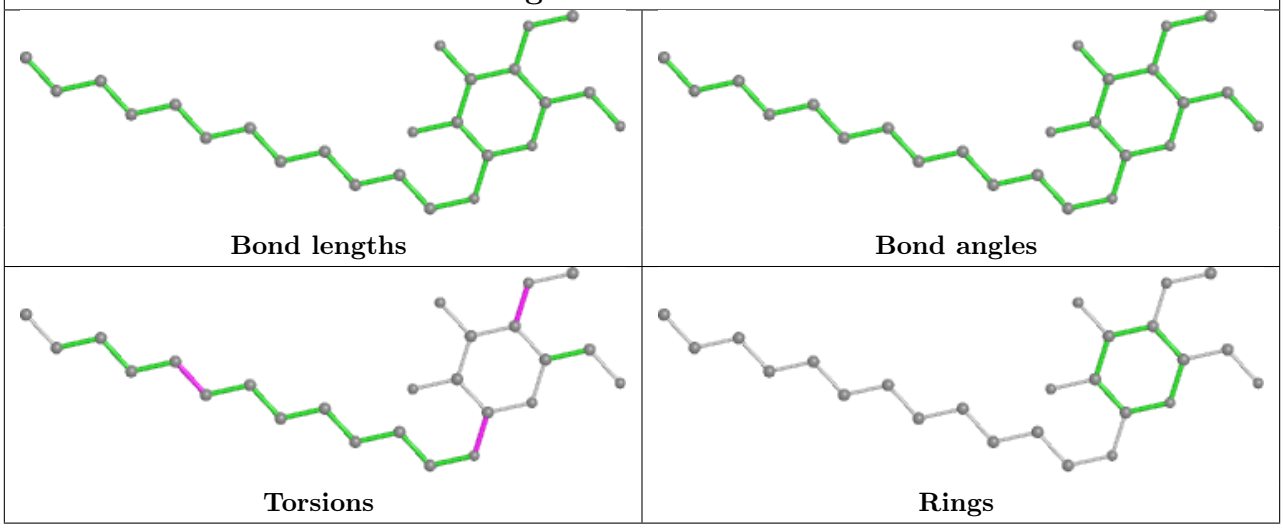


Torsions

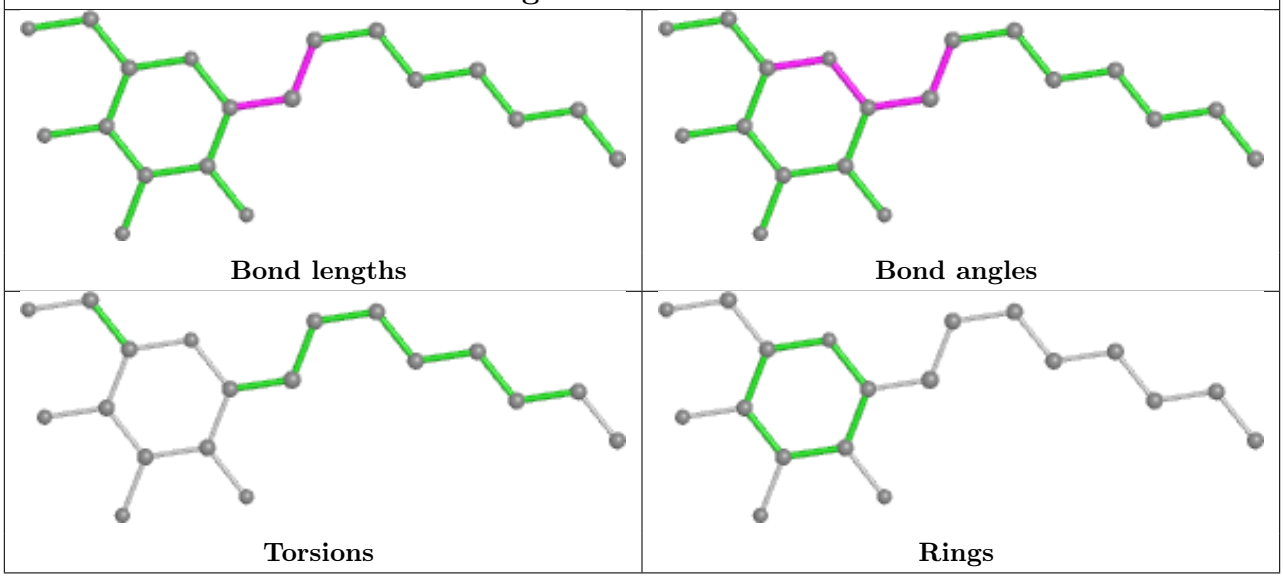


Rings

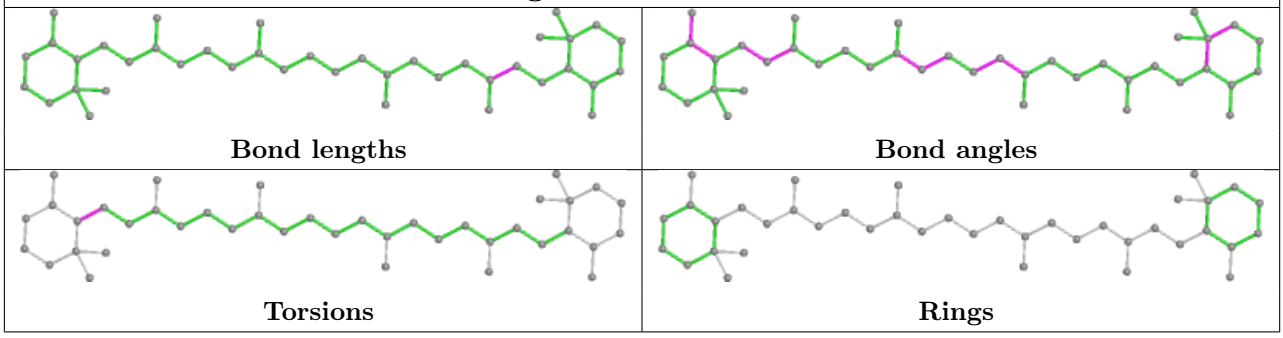
Ligand LMT b 631



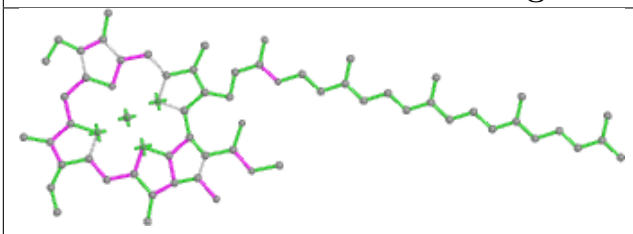
Ligand HTG B 633



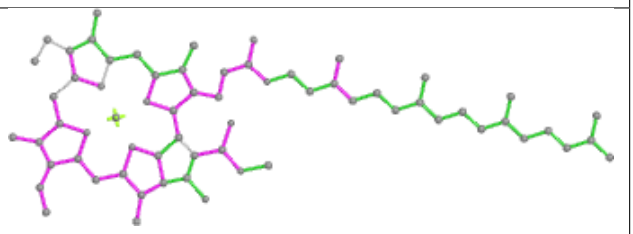
Ligand BCR b 627



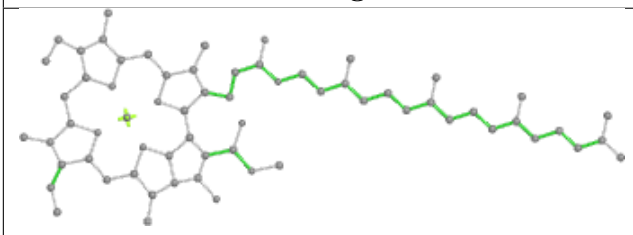
Ligand CLA b 617



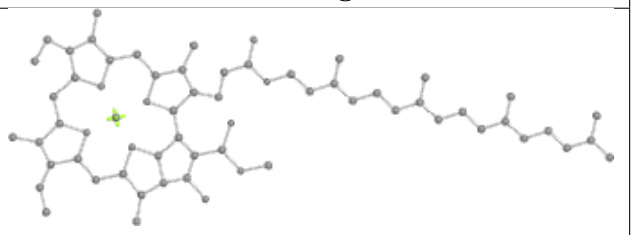
Bond lengths



Bond angles

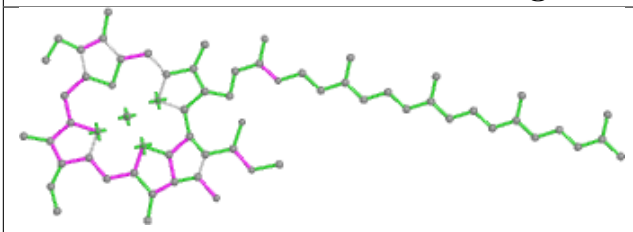


Torsions



Rings

Ligand CLA c 506



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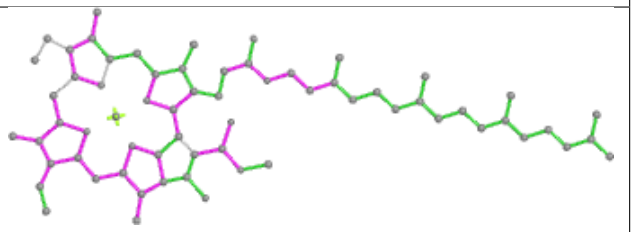
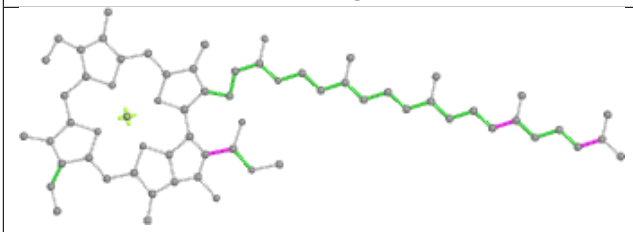
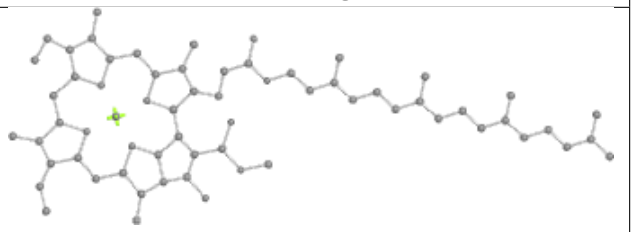


Bond angles

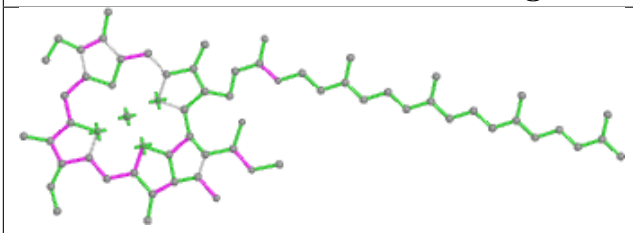


Torsions

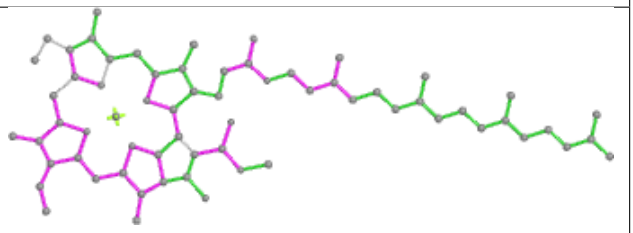


Rings

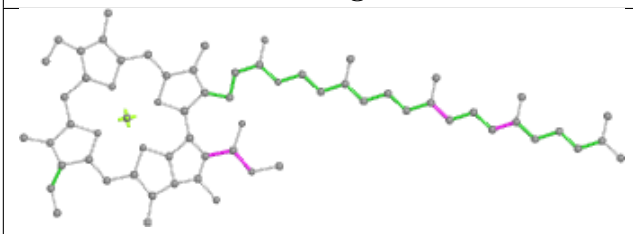
Ligand CLA C 507



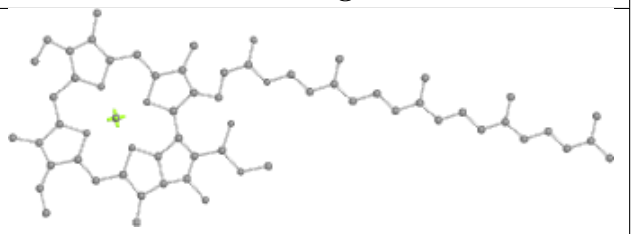
Bond lengths



Bond angles

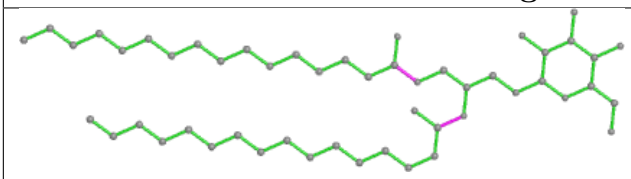


Torsions

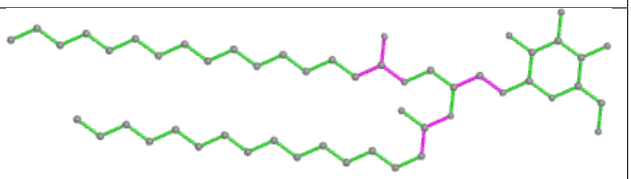


Rings

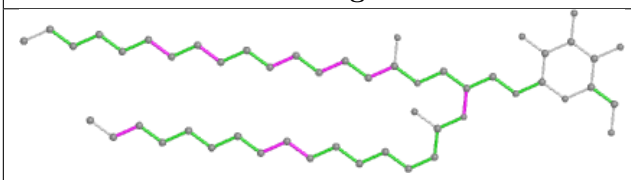
Ligand LMG B 622



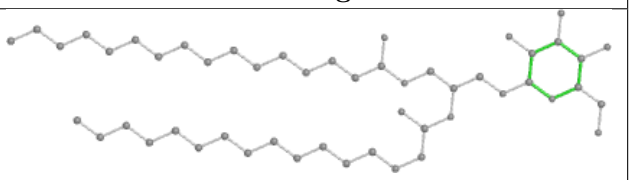
Bond lengths



Bond angles

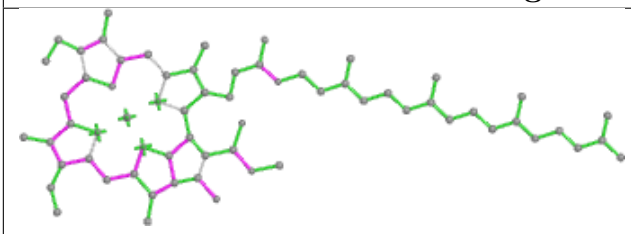


Torsions

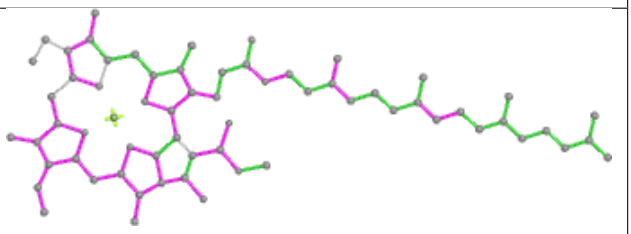


Rings

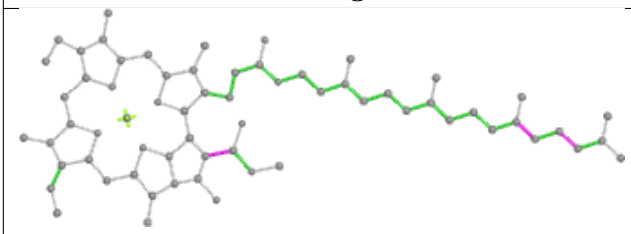
Ligand CLA C 504



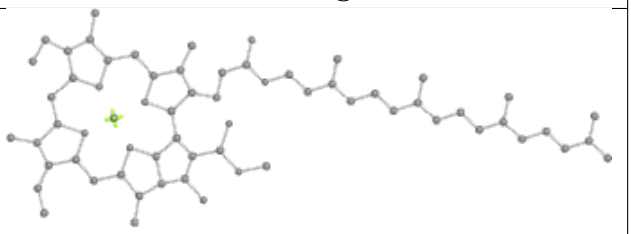
Bond lengths



Bond angles

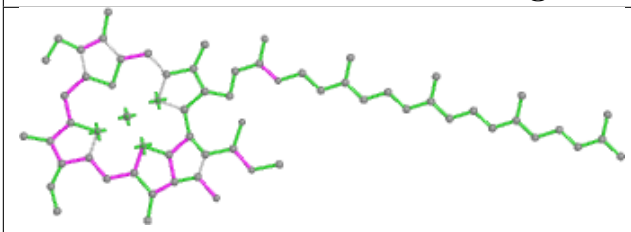


Torsions



Rings

Ligand CLA c 515



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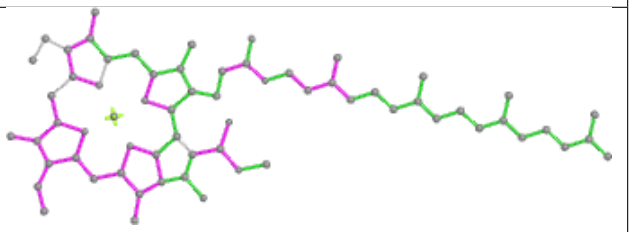

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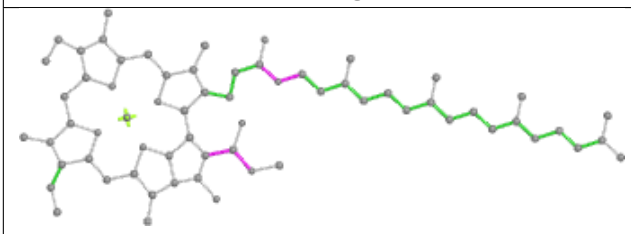

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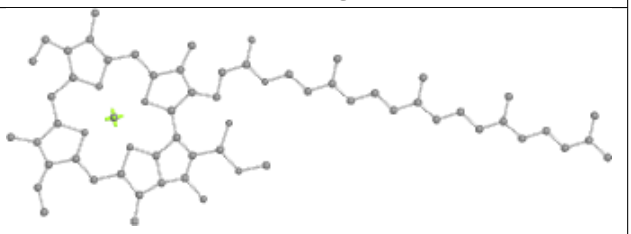
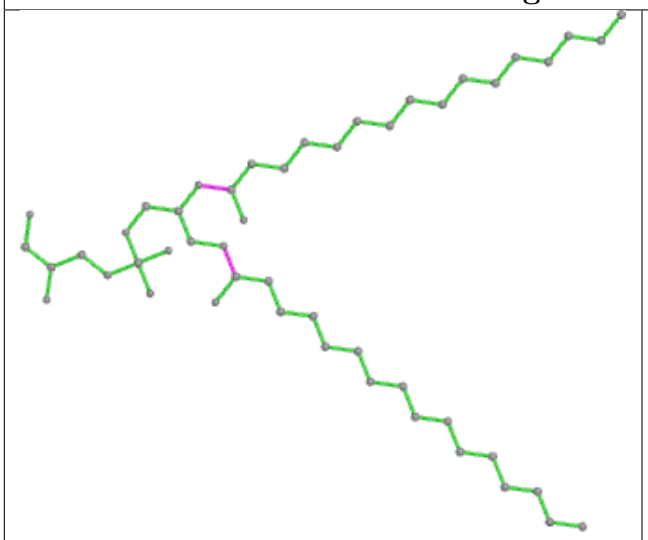


Rings

Ligand LHG D 407



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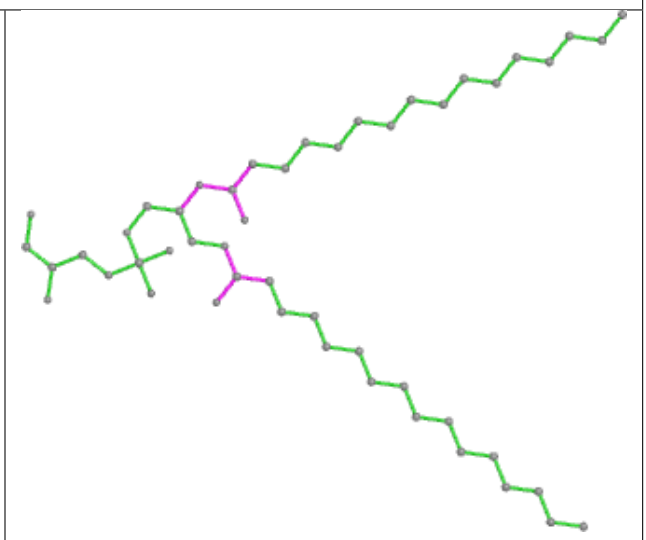
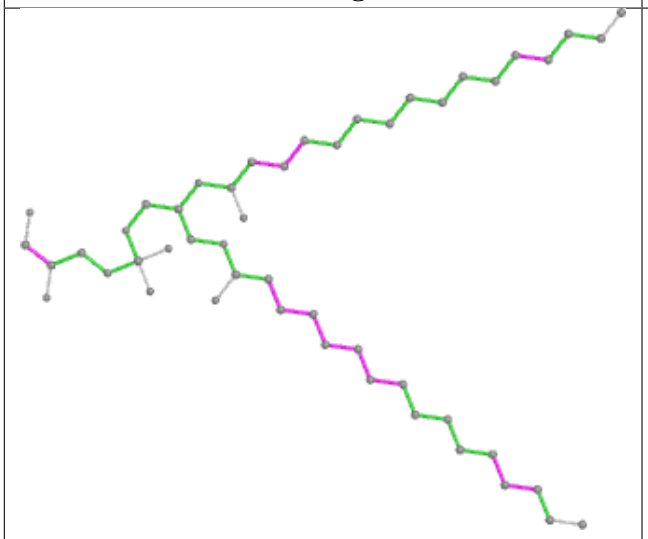
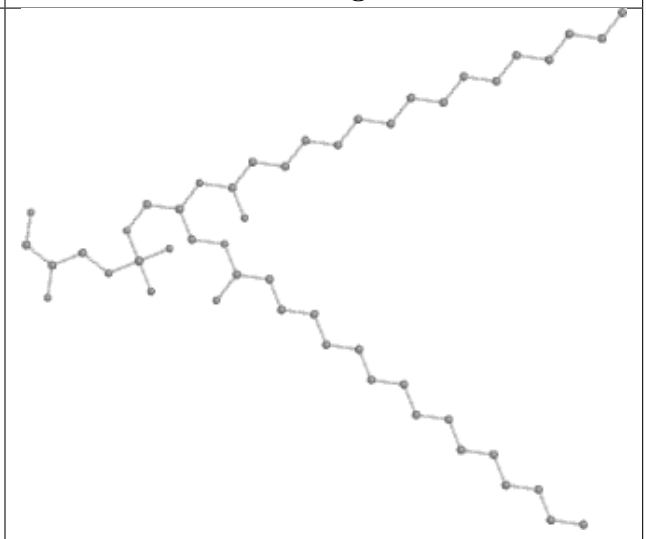


Bond angles

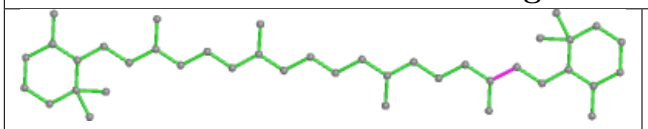


Torsions



Rings

Ligand BCR B 619



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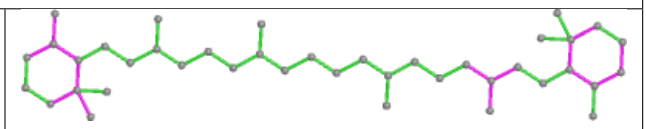
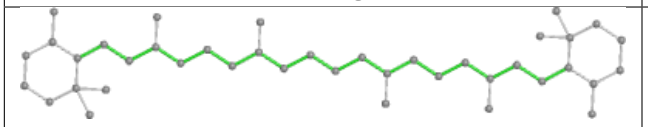
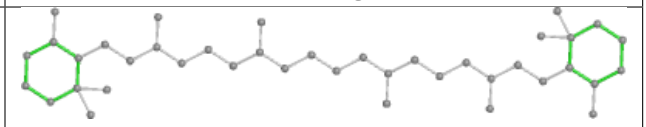


Bond angles

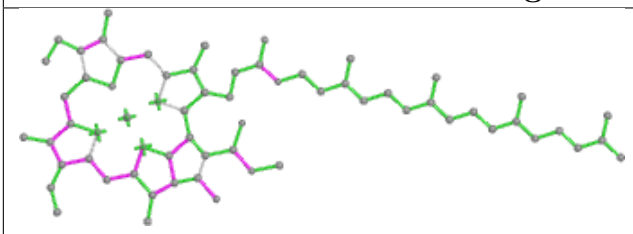


Torsions



Rings

Ligand CLA C 511



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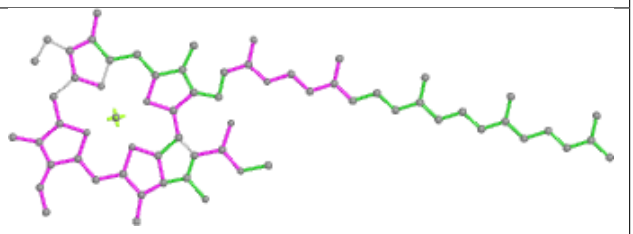
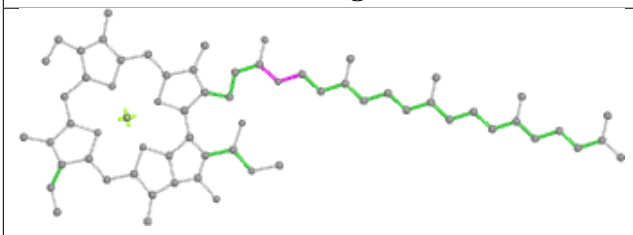


Bond angles



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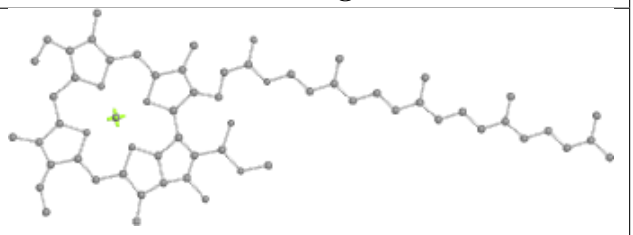
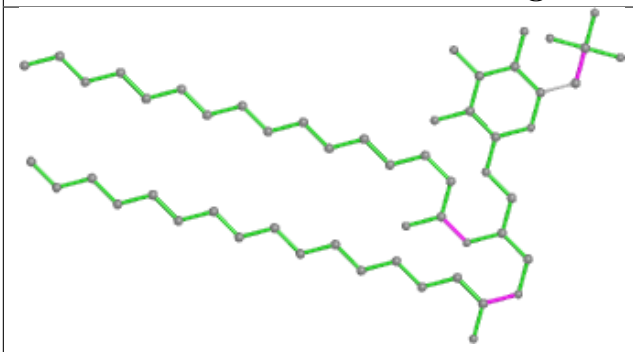


Rings

Ligand SQD b 601



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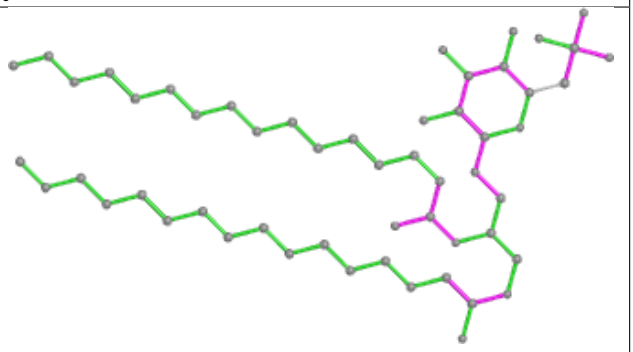
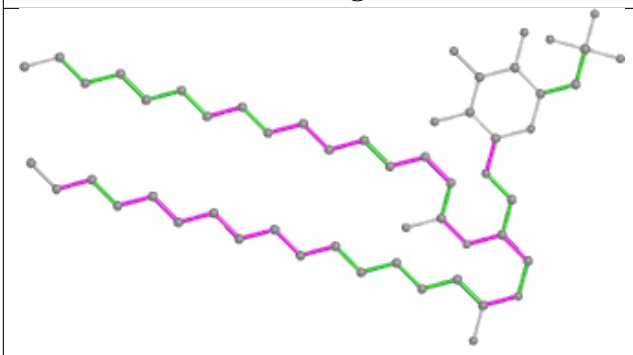
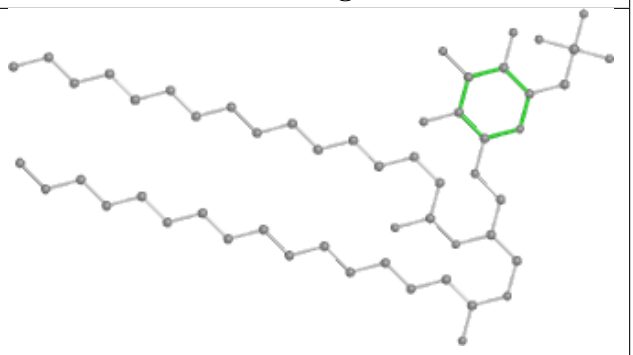


Bond angles

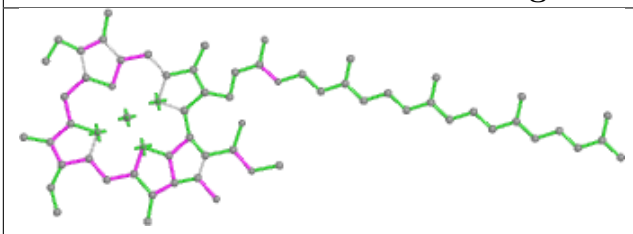


Torsions



Rings

Ligand CLA c 508



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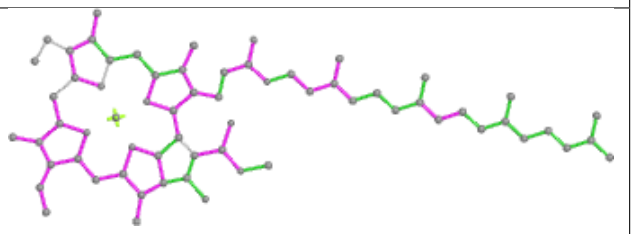
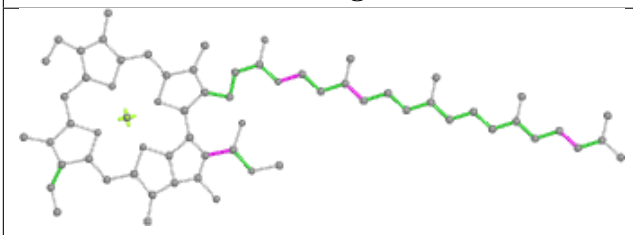


Bond angles



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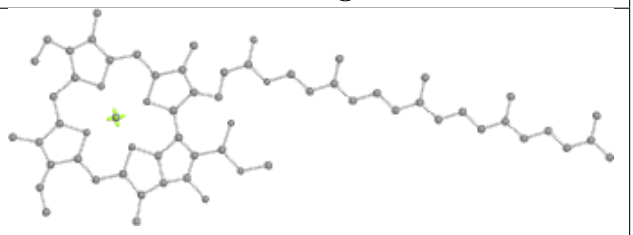
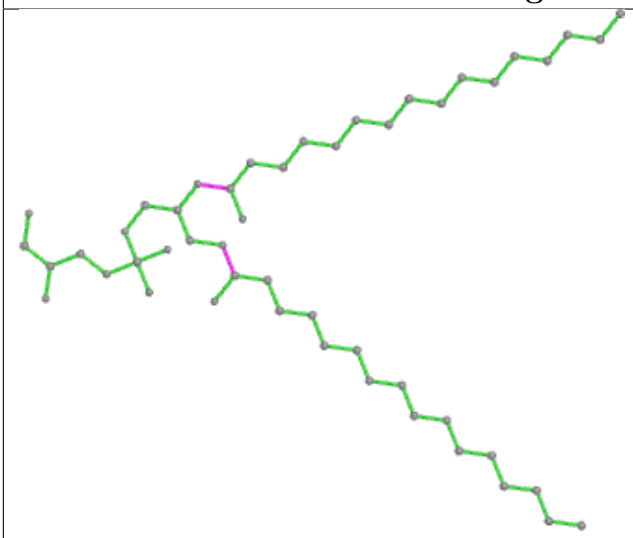


Rings

Ligand LHG d 408



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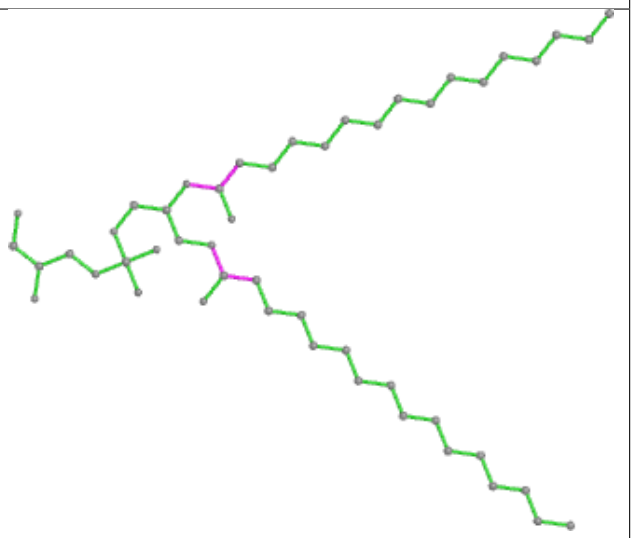
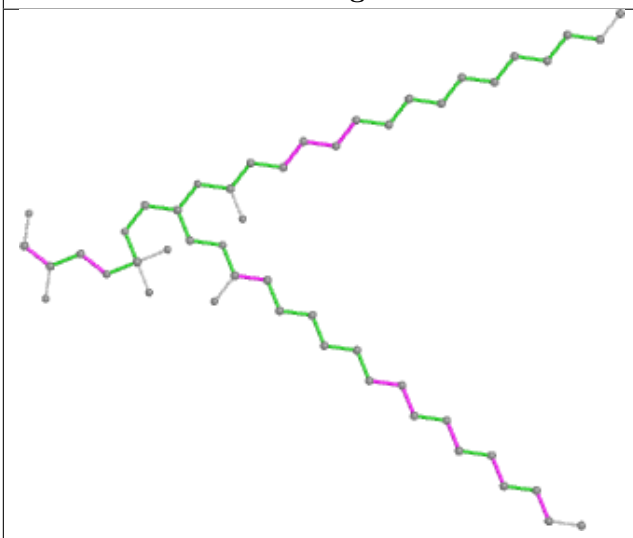


Bond angles



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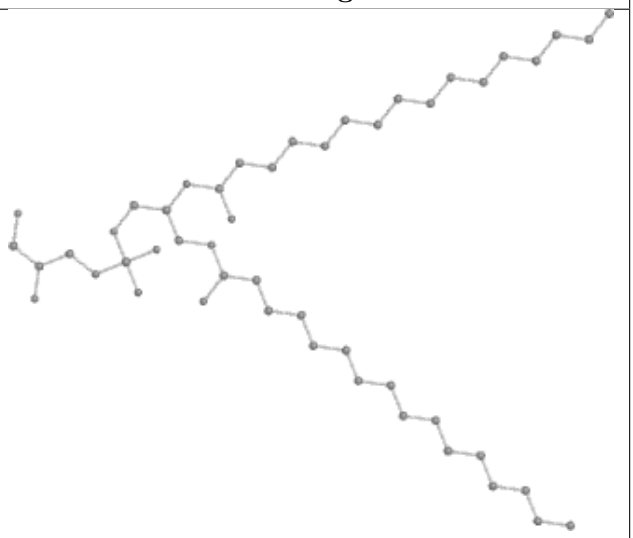
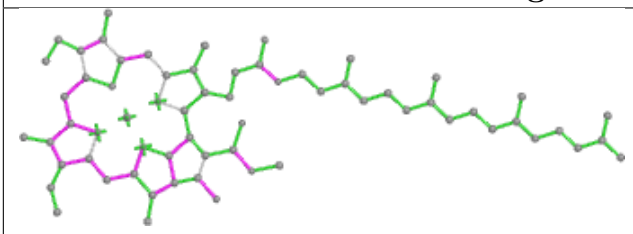
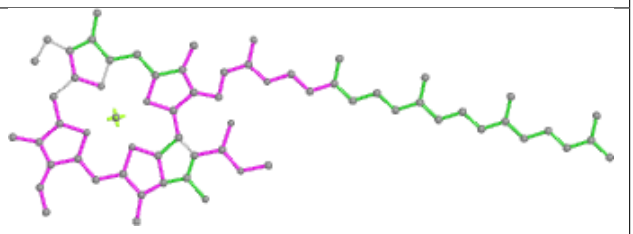


Rings

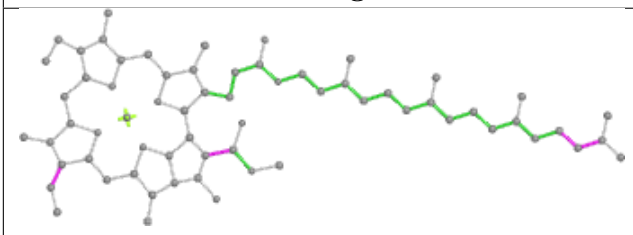
Ligand CLA d 401



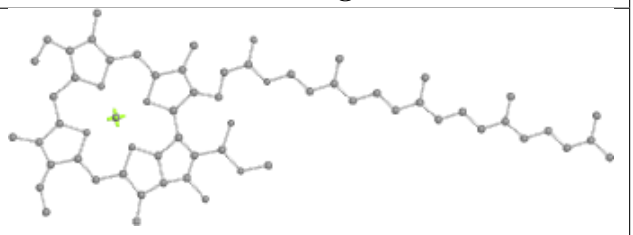
Bond lengths



Bond angles

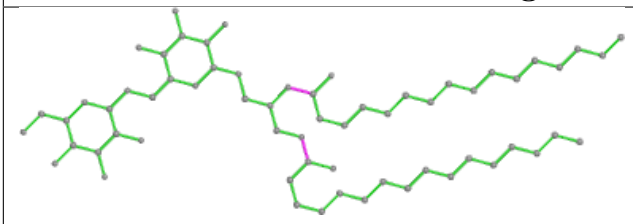


Torsions



Rings

Ligand DGD C 516



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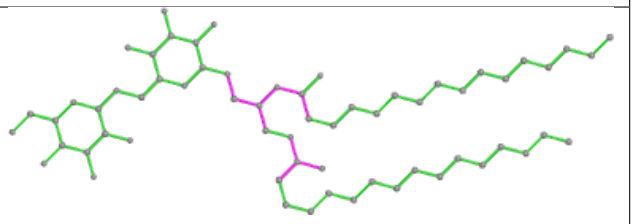
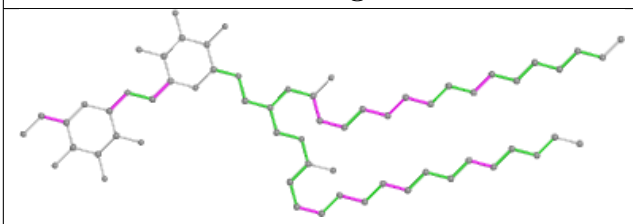


Bond angles



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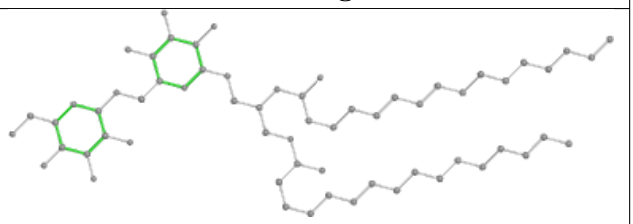
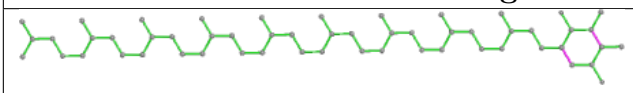


Rings

Ligand PL9 d 405 (B)



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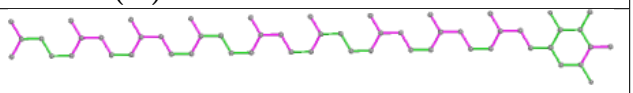
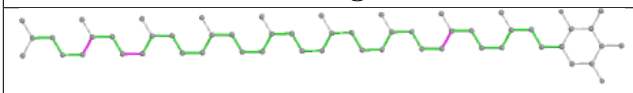


Bond angles



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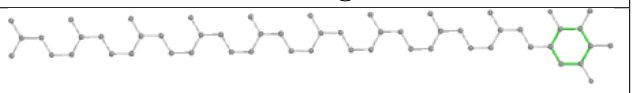
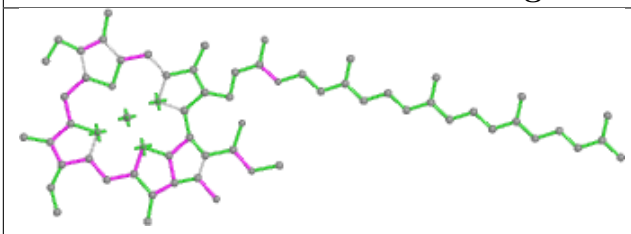
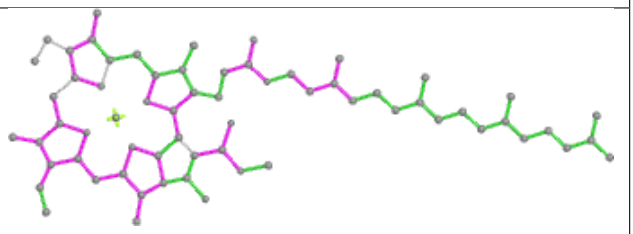


Rings

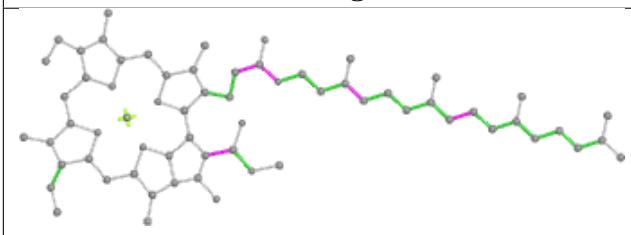
Ligand CLA C 510



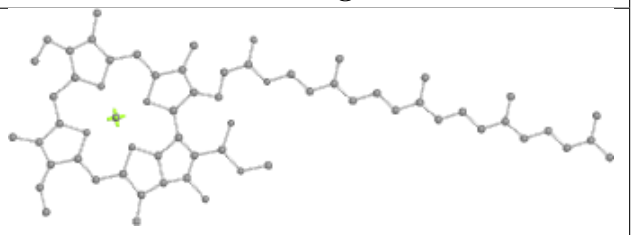
Bond lengths



Bond angles

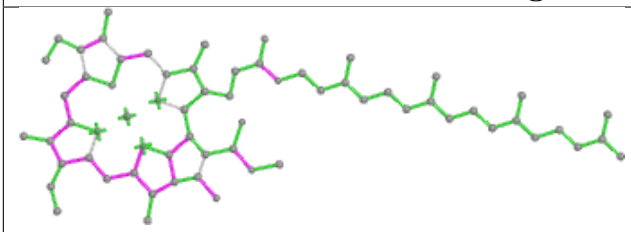


Torsions

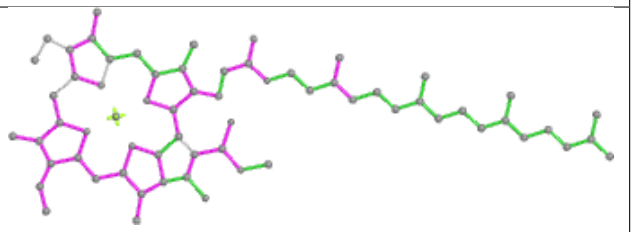


Rings

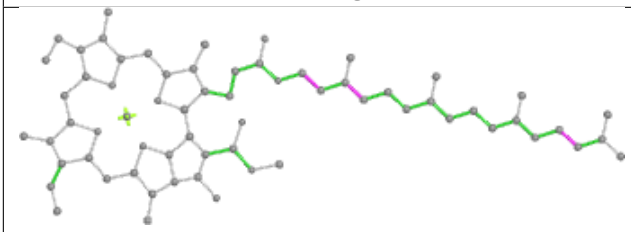
Ligand CLA d 403



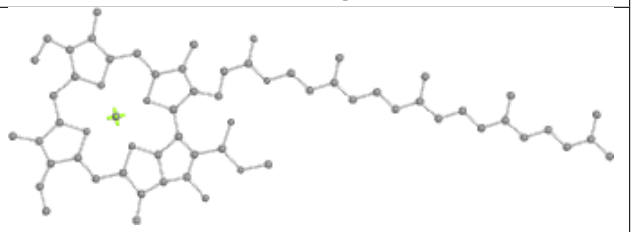
Bond lengths



Bond angles

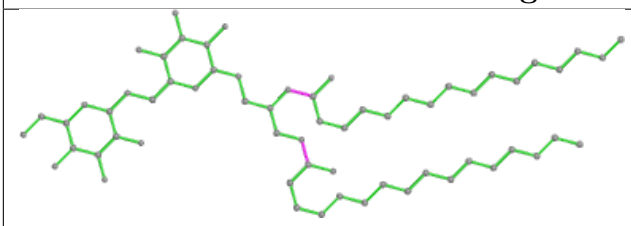


Torsions

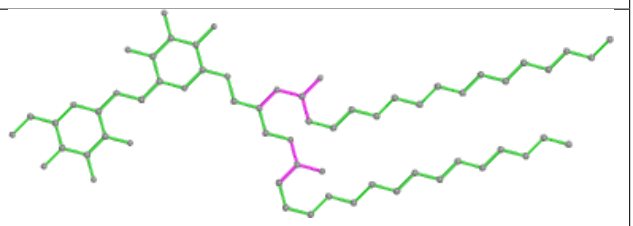


Rings

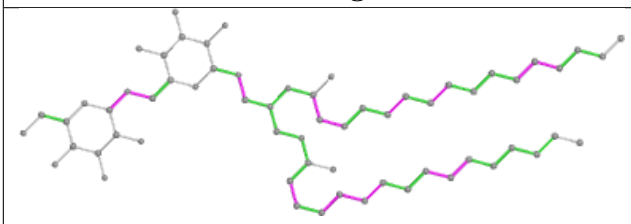
Ligand DGD C 517



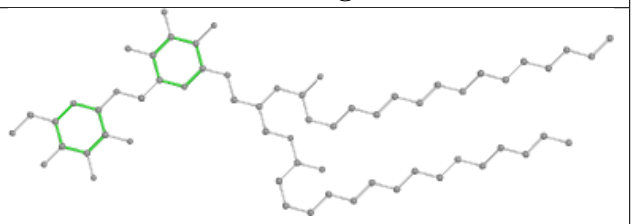
Bond lengths



Bond angles

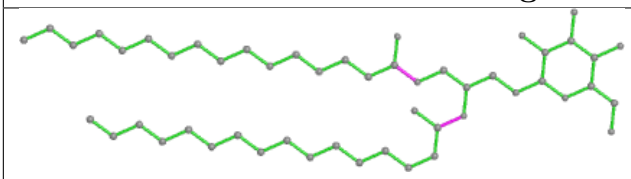


Torsions



Rings

Ligand LMG C 520



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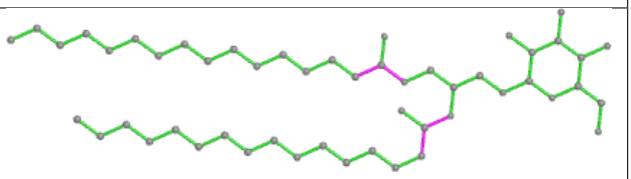

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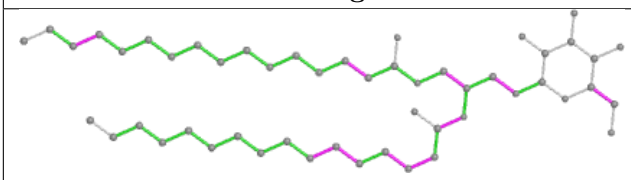

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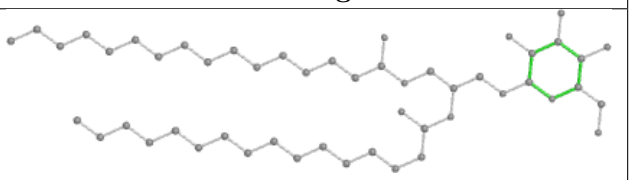
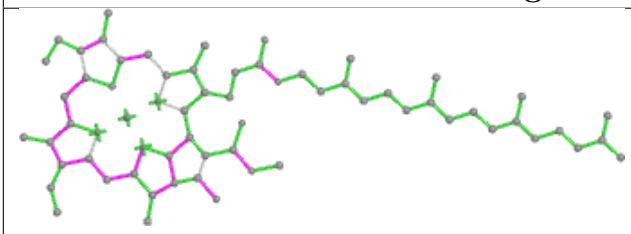
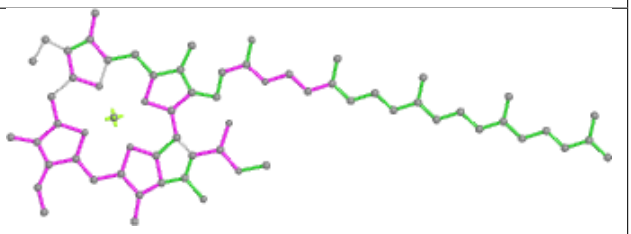


Rings

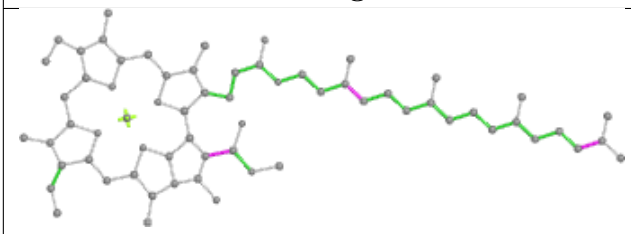
Ligand CLA B 610



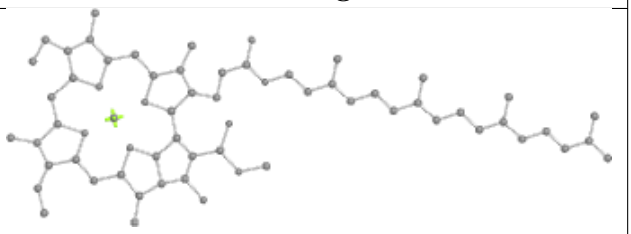
Bond lengths



Bond angles

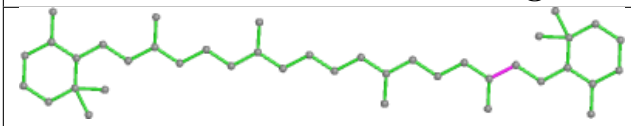


Torsions



Rings

Ligand BCR y 101



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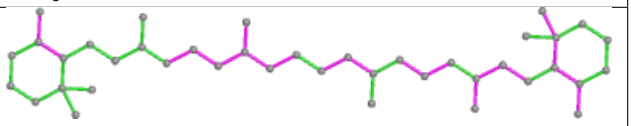
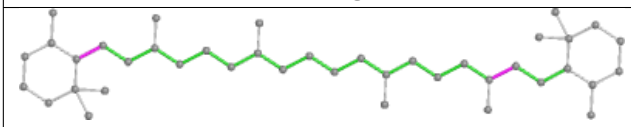


Bond angles



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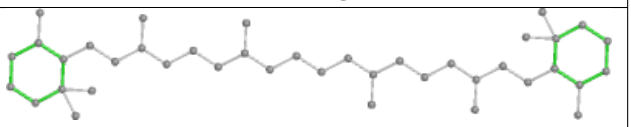
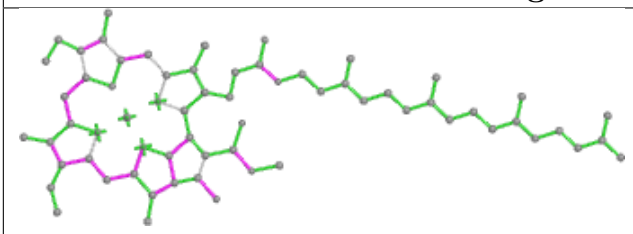


Rings

Ligand CLA b 621



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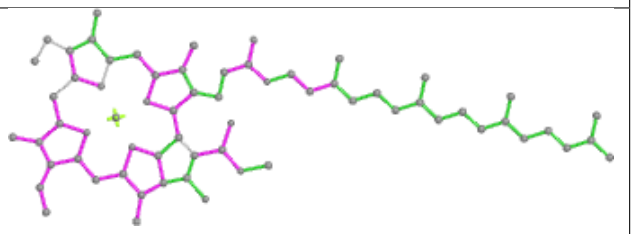
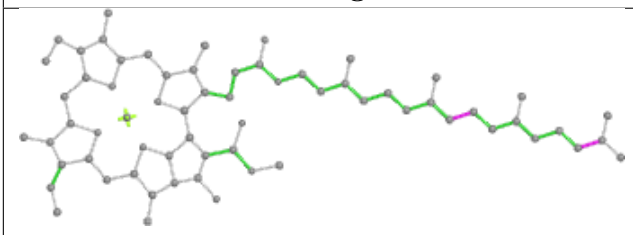


Bond angles



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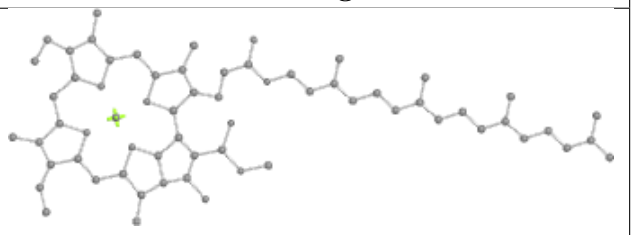
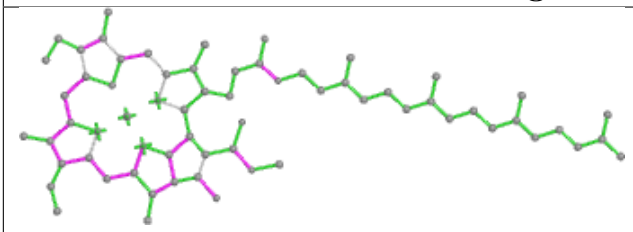


Rings

Ligand CLA b 618



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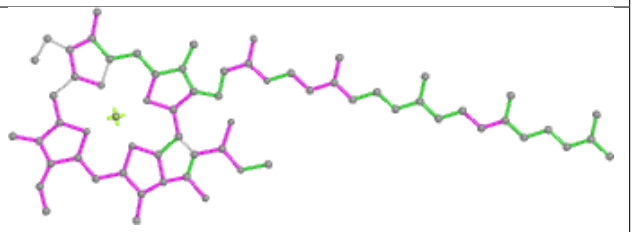
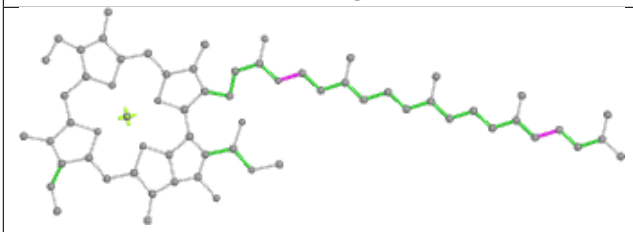
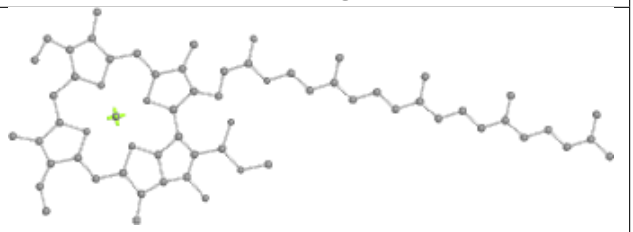


Bond angles

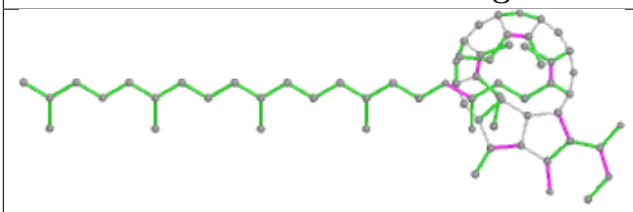


Torsions



Rings

Ligand PHO a 420 (A)



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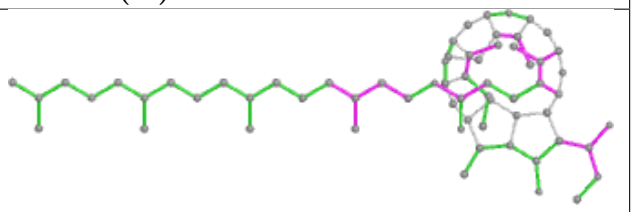
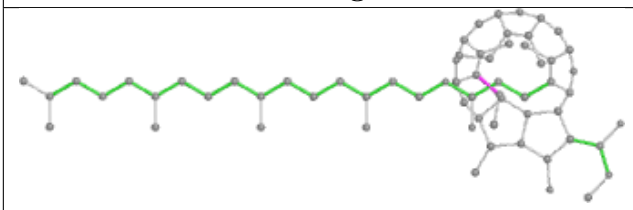


Bond angles



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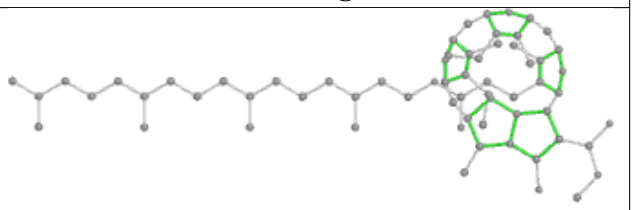
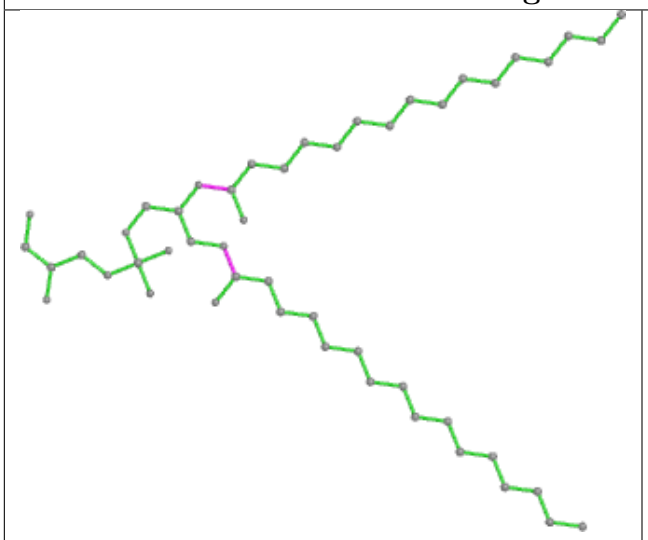


Rings

Ligand LHG D 408



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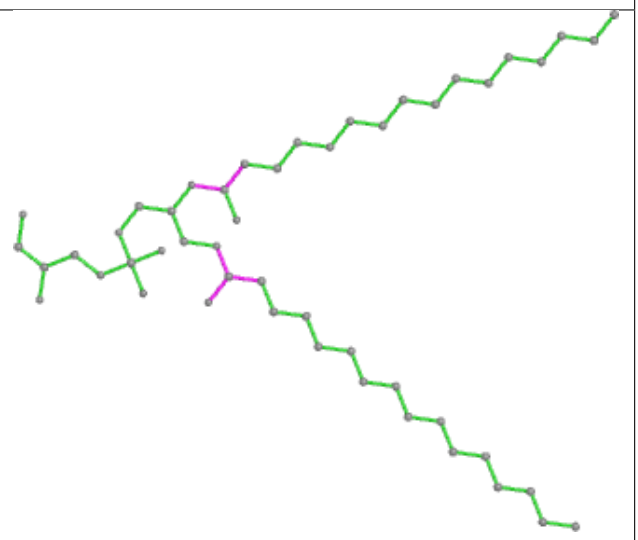
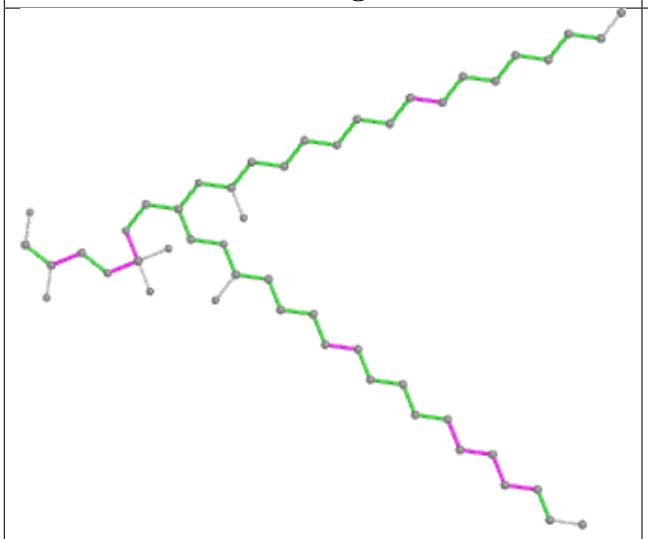


Bond angles



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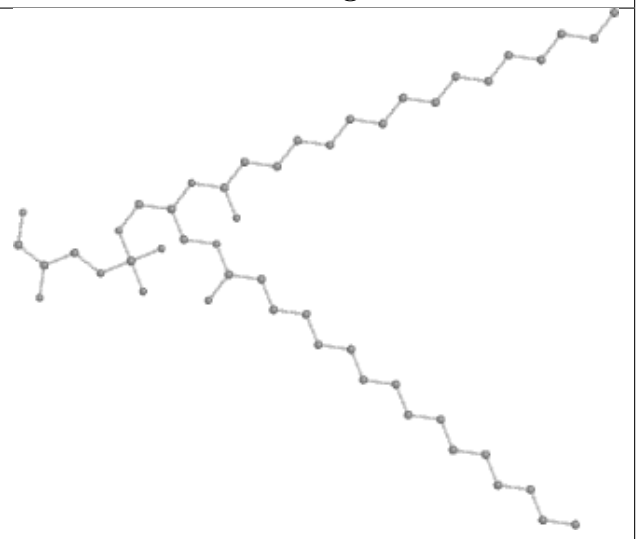
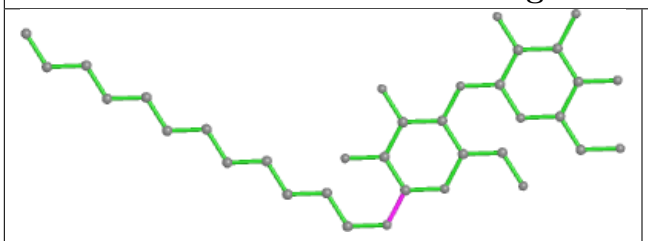


Rings

Ligand LMT a 404



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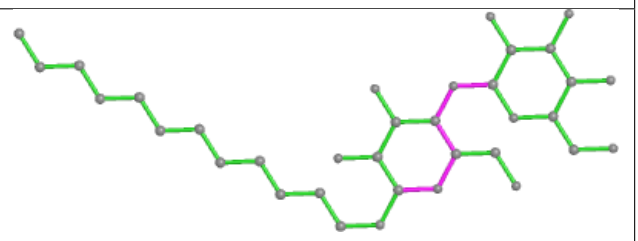
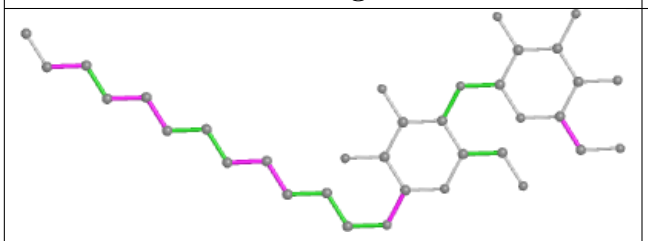


Bond angles



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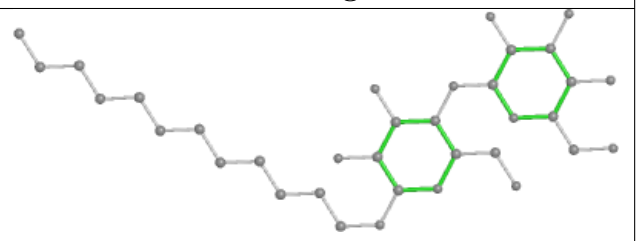
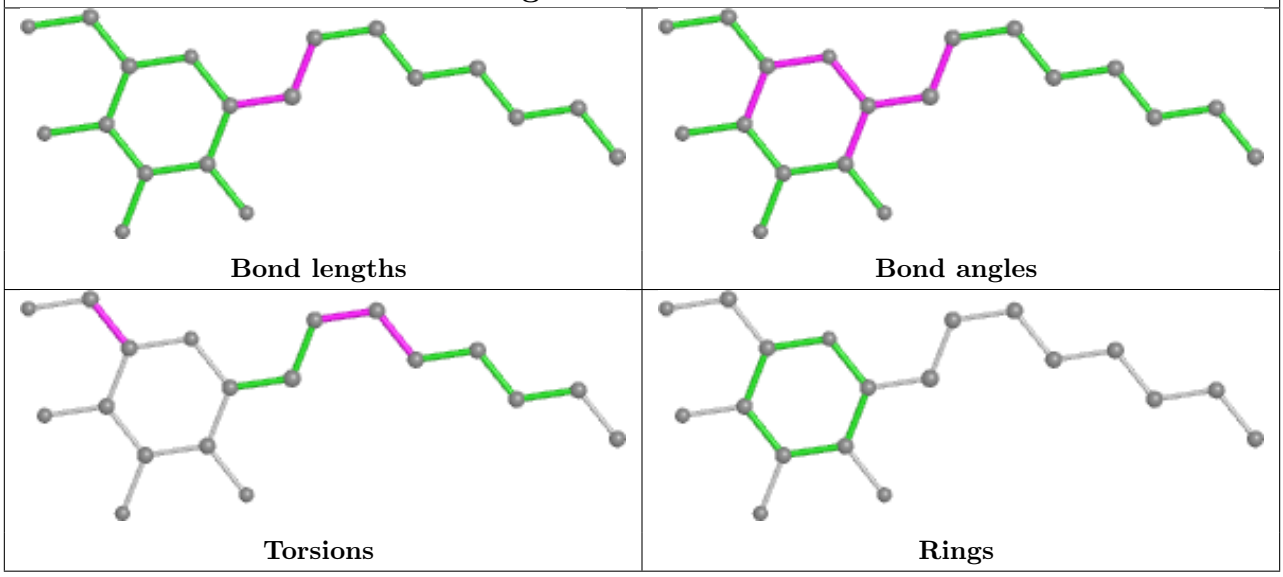
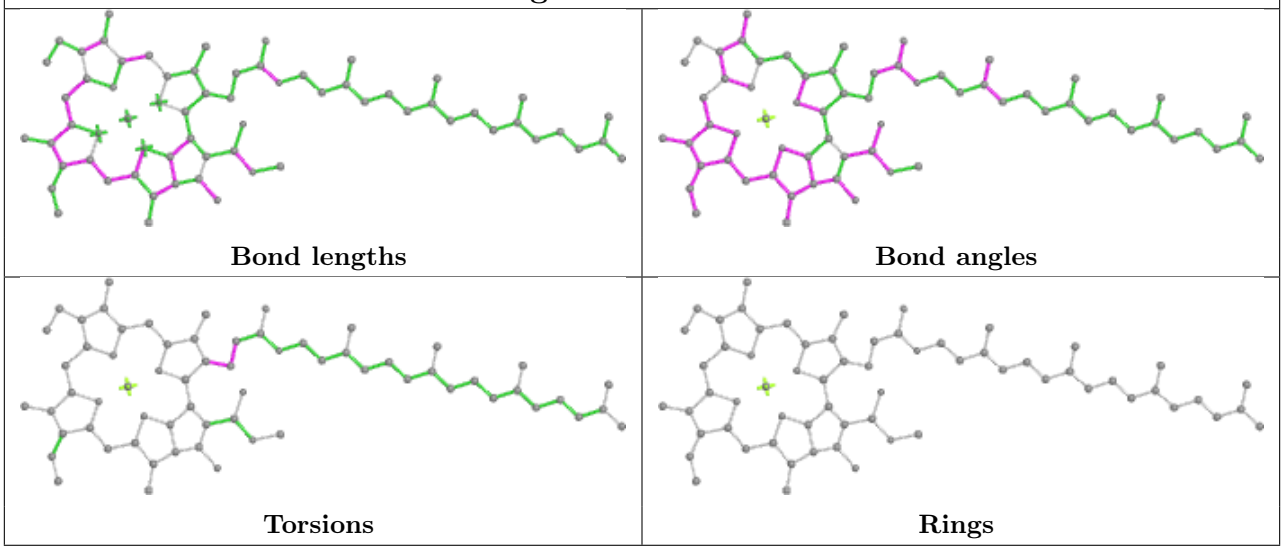


Rings

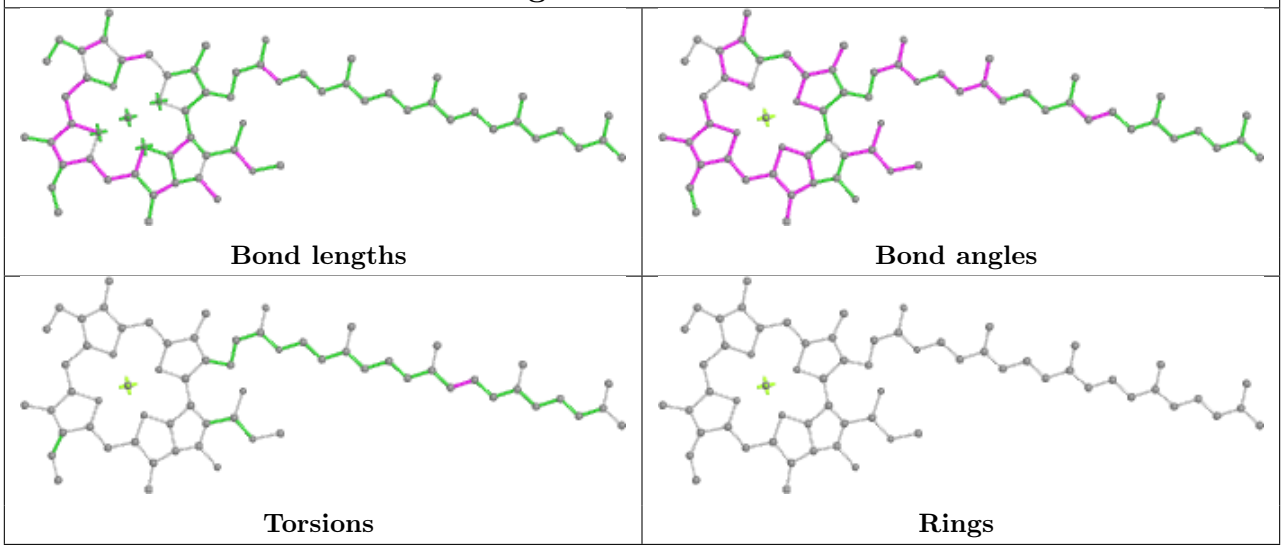
Ligand HTG C 523



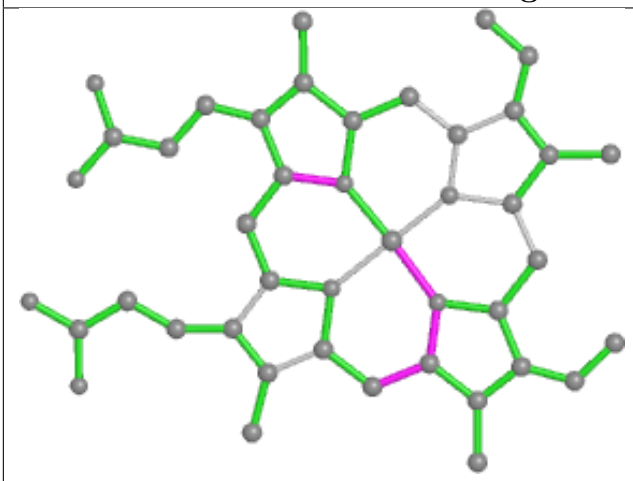
Ligand CLA c 505



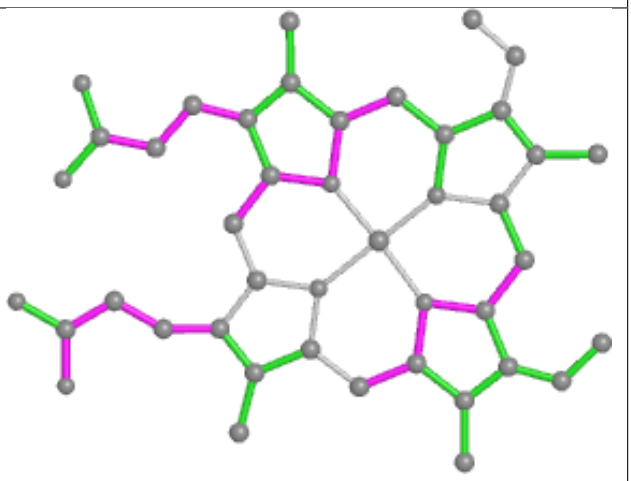
Ligand CLA b 622



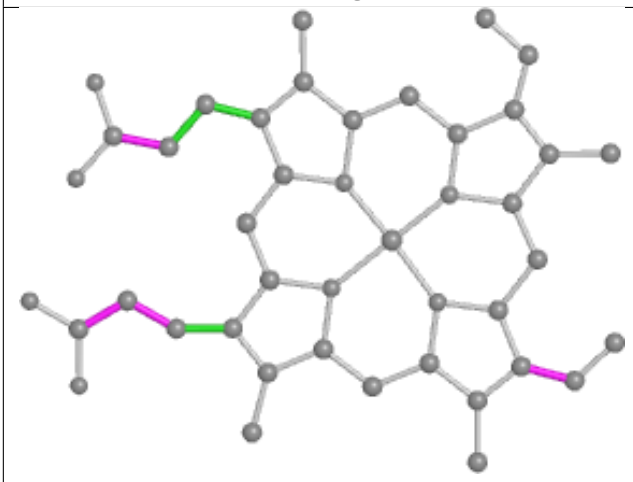
Ligand HEM F 102



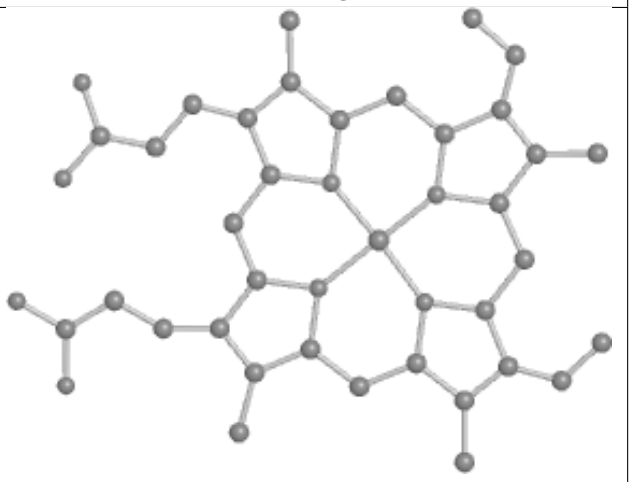
Bond lengths



Bond angles

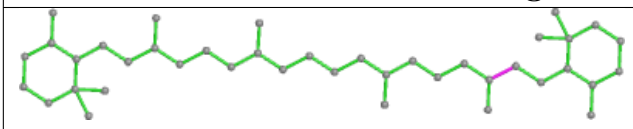


Torsions



Rings

Ligand BCR b 629



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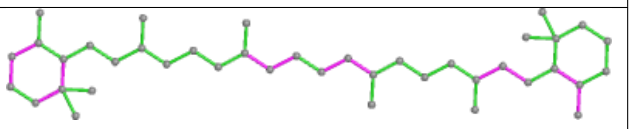
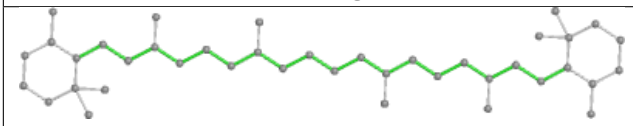


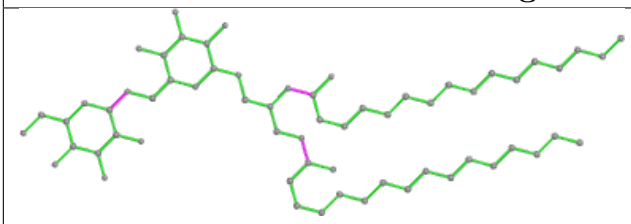
Bond angles



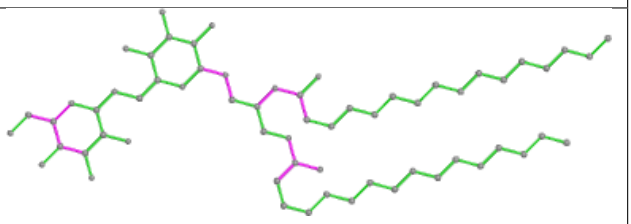
Torsions

Rings

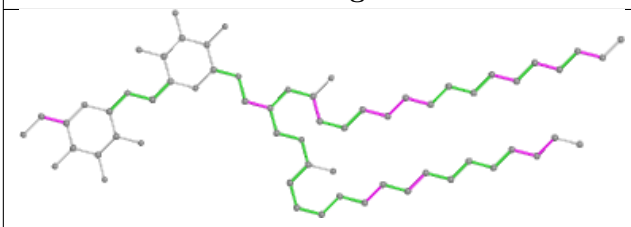
Ligand DGD H 103



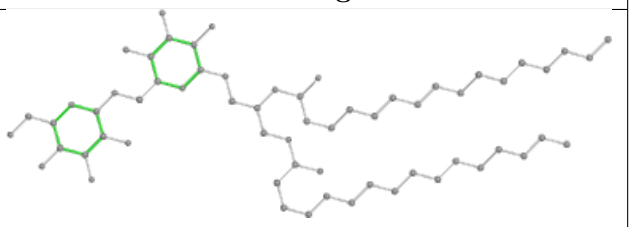
Bond lengths



Bond angles

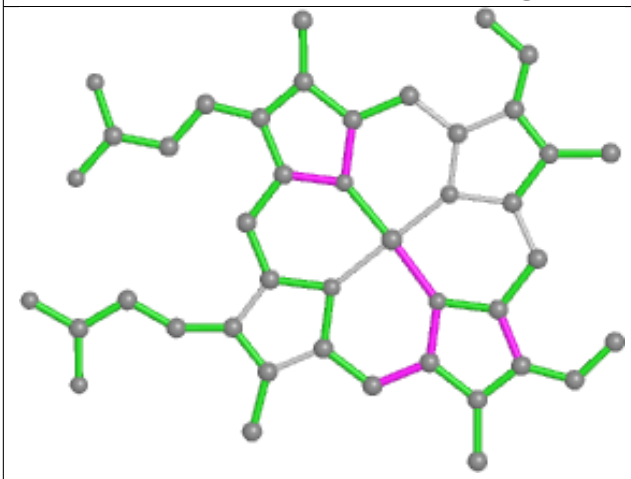


Torsions



Rings

Ligand HEM V 206



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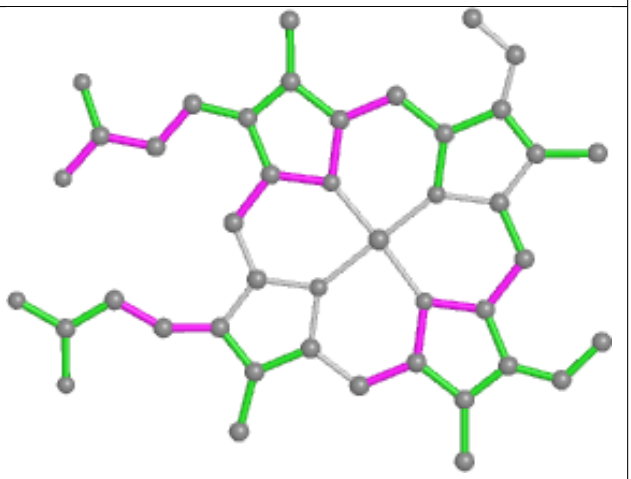
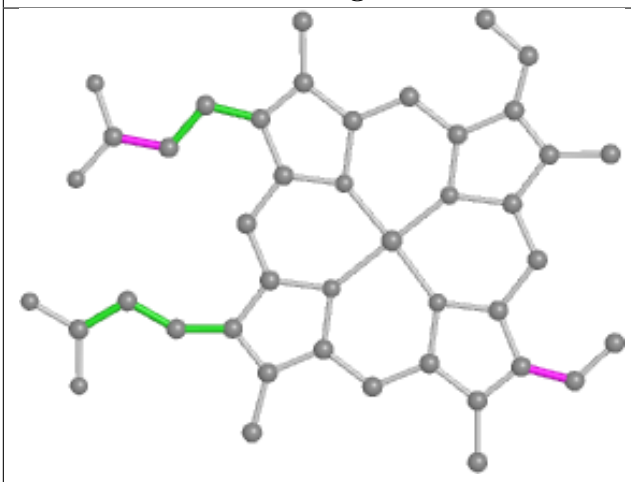
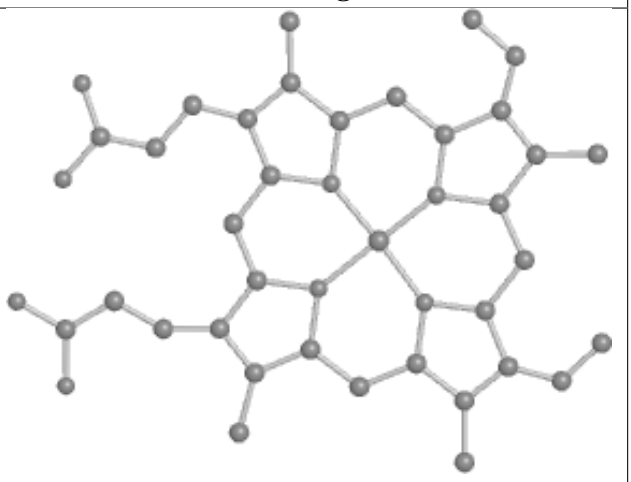


Bond angles

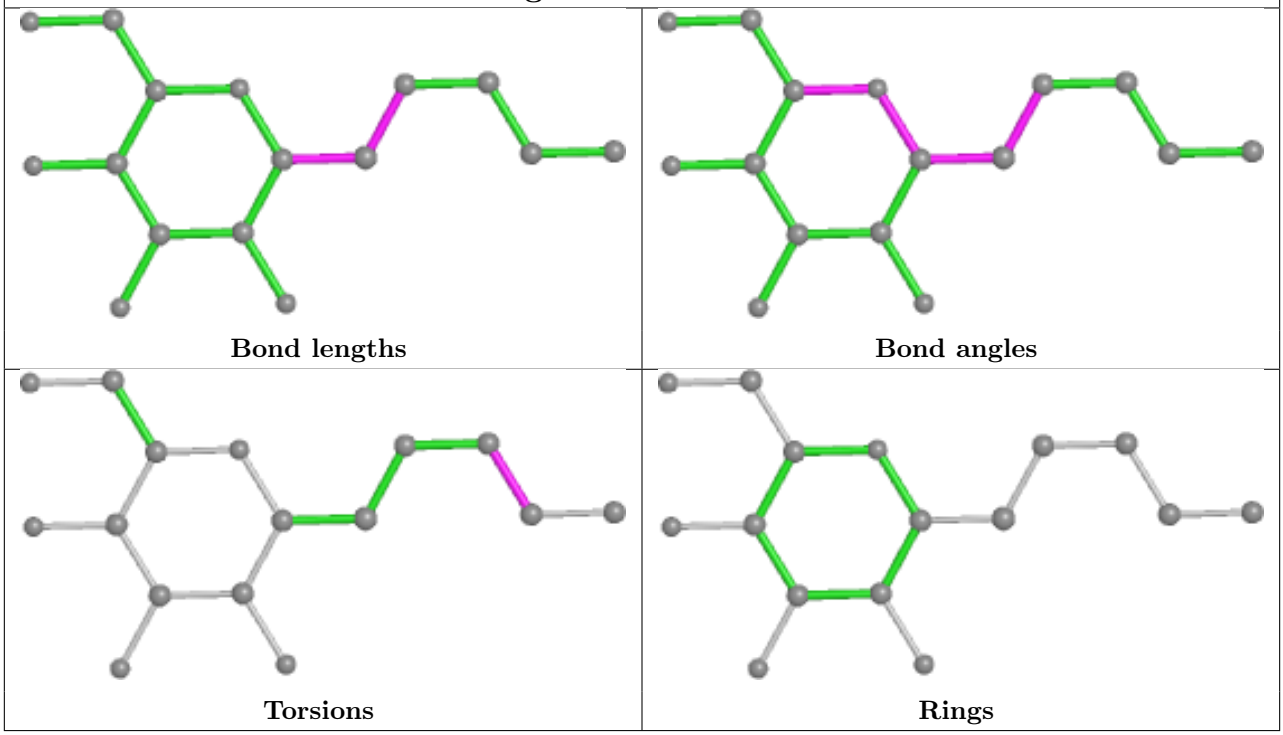


Torsions

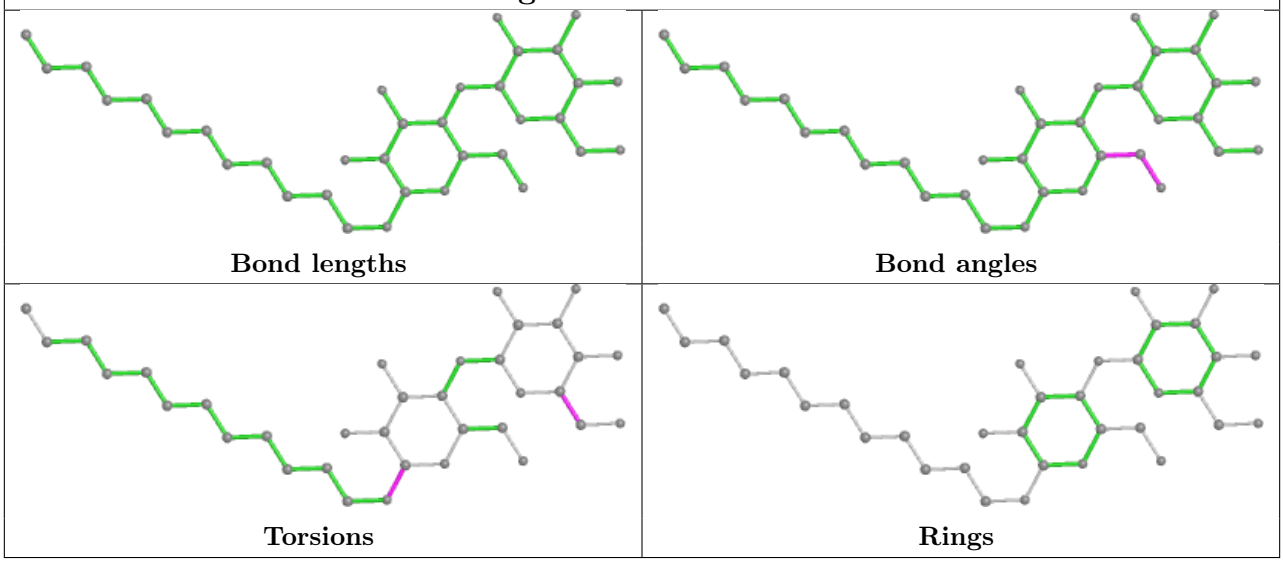


Rings

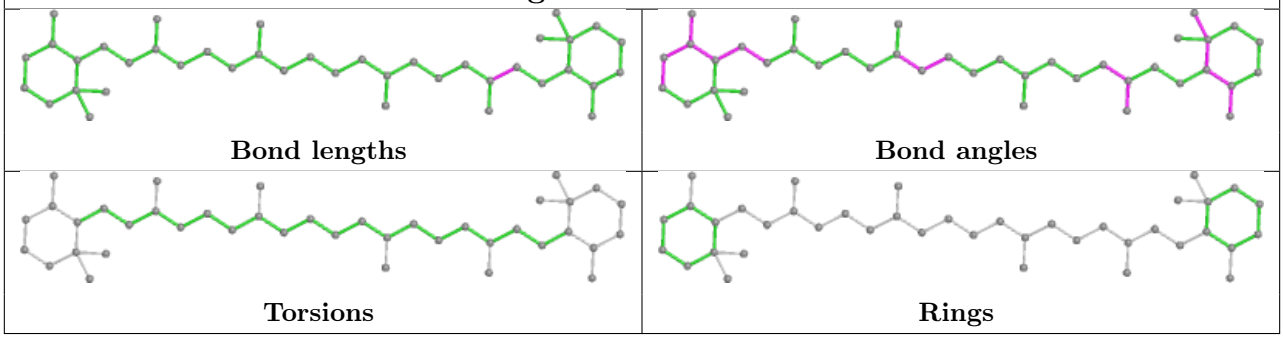
Ligand HTG d 411



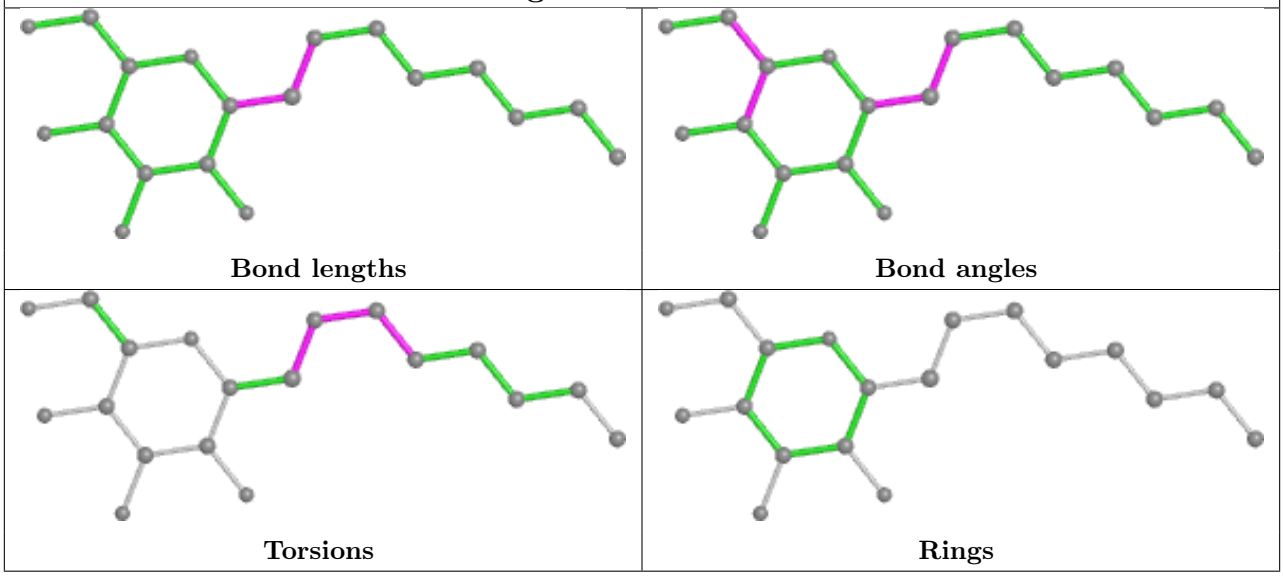
Ligand LMT M 101



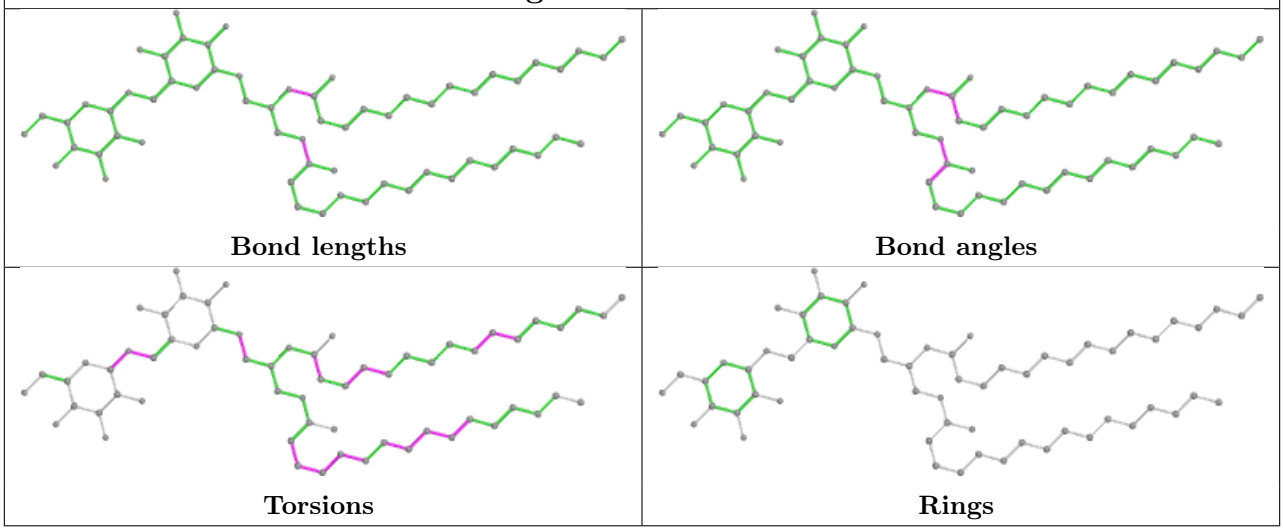
Ligand BCR a 413



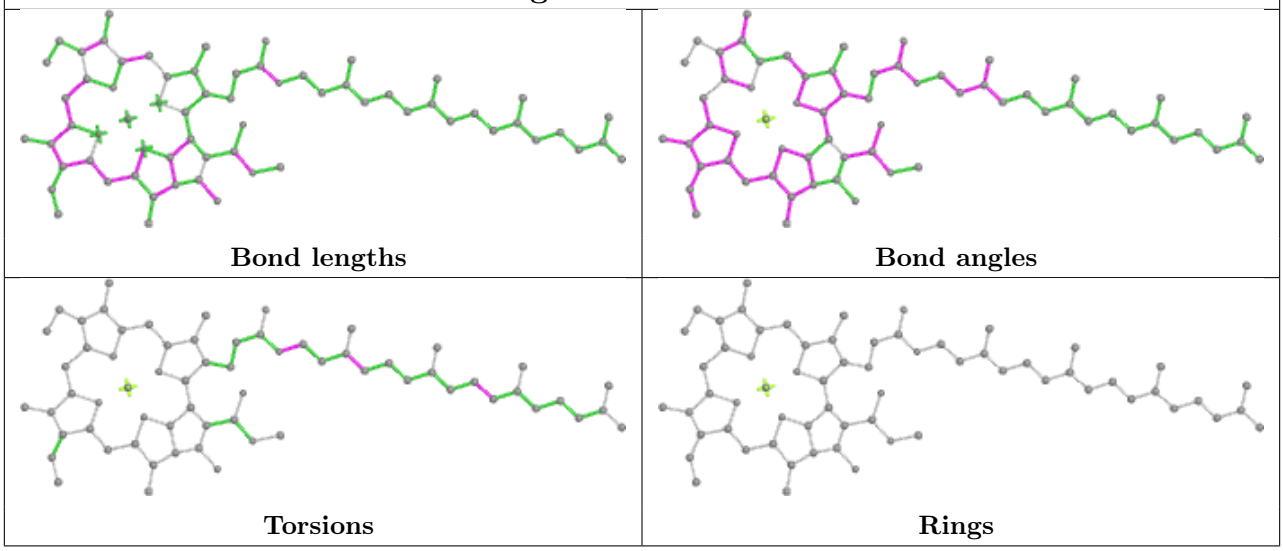
Ligand HTG c 524



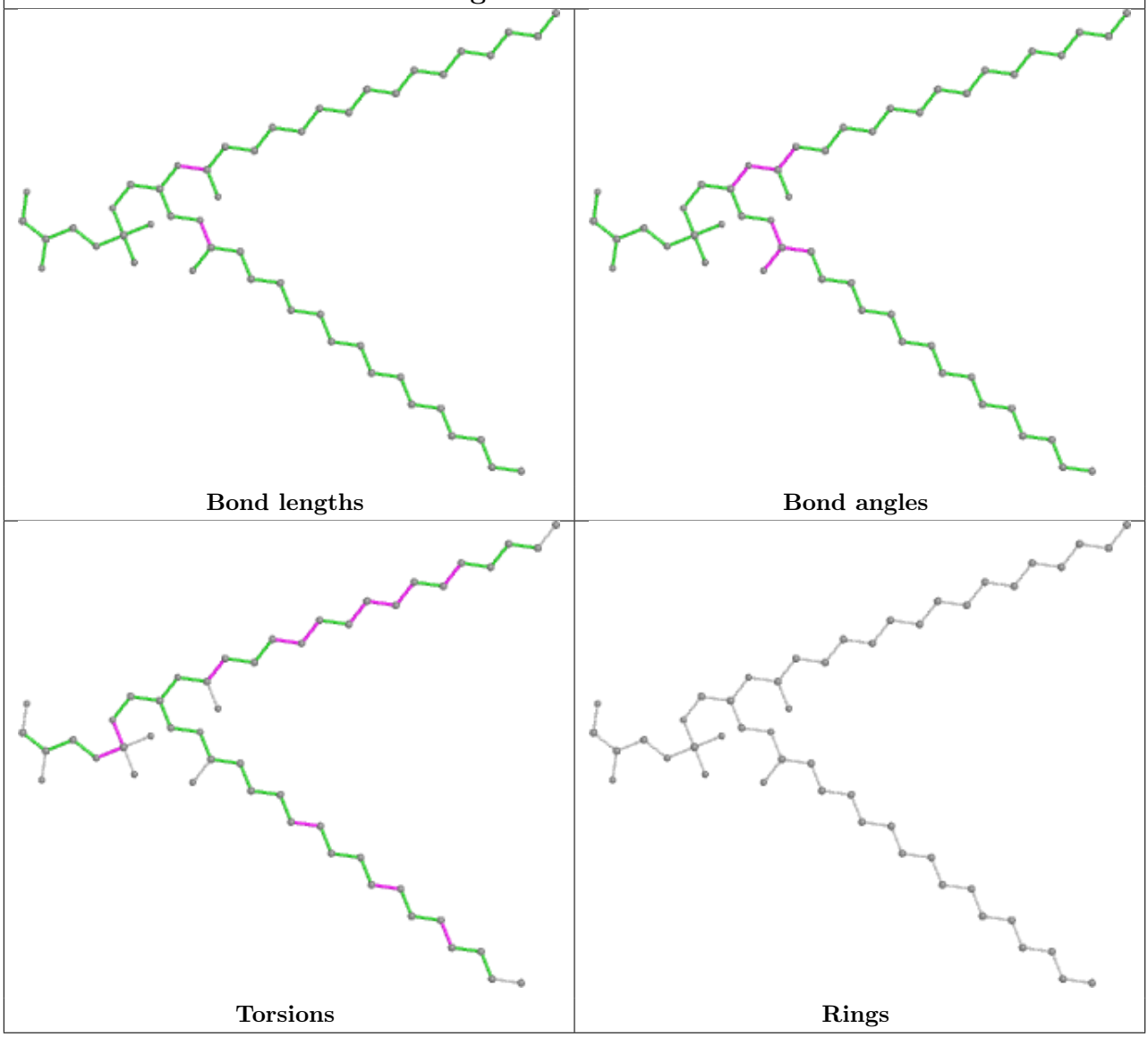
Ligand DGD c 520



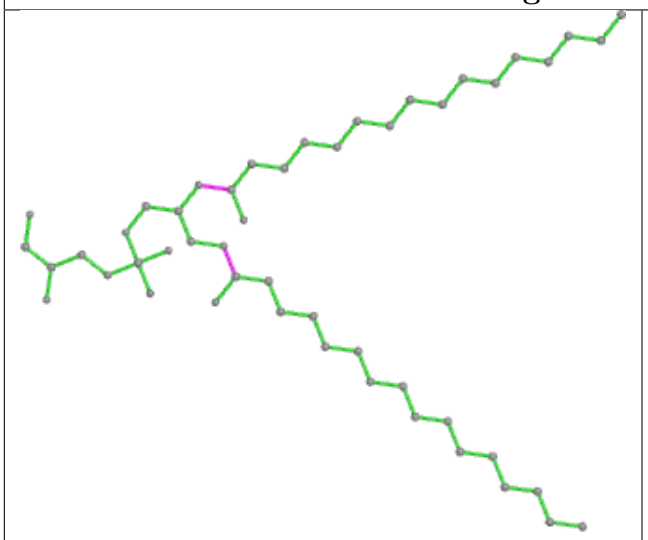
Ligand CLA c 517



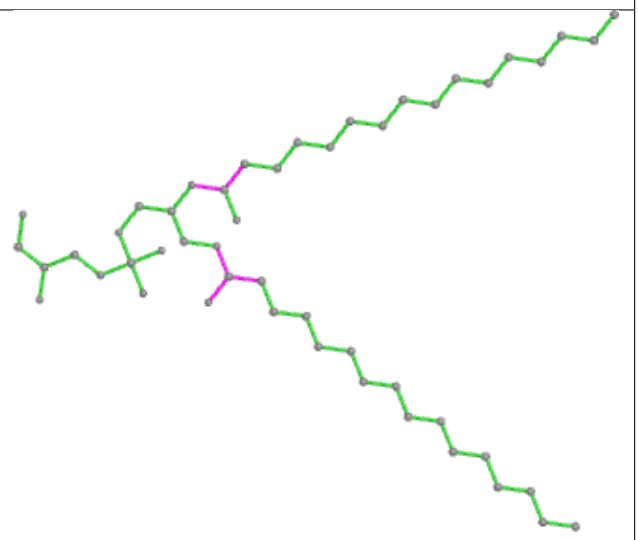
Ligand LHG L 101



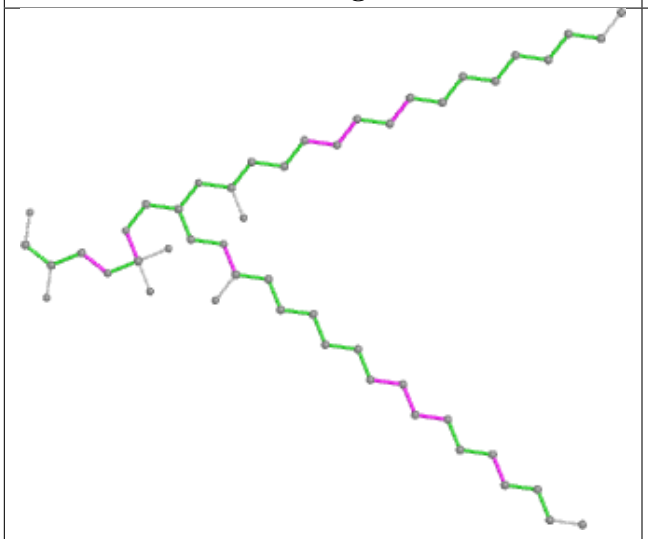
Ligand LHG D 409



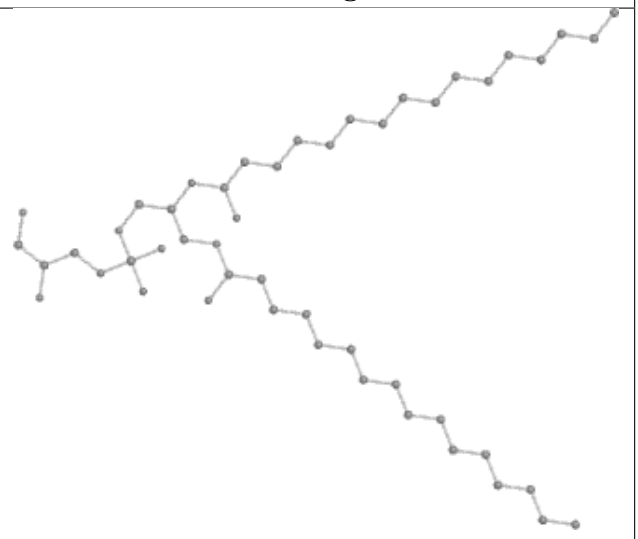
Bond lengths



Bond angles

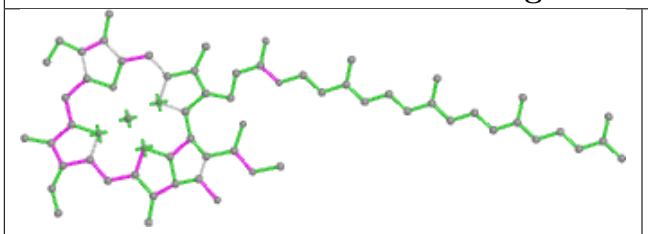


Torsions

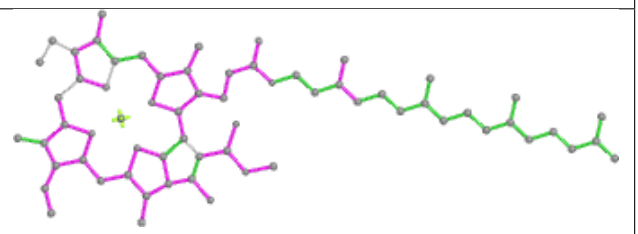


Rings

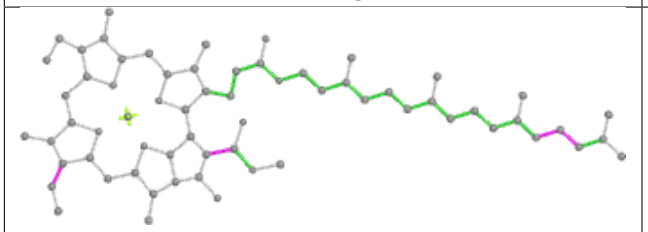
Ligand CLA A 406



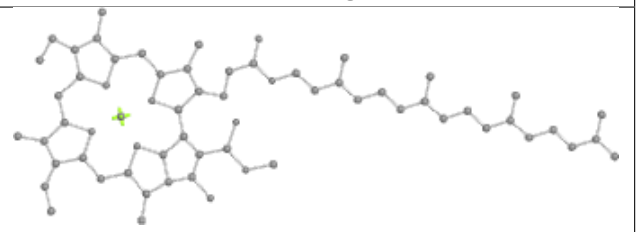
Bond lengths



Bond angles

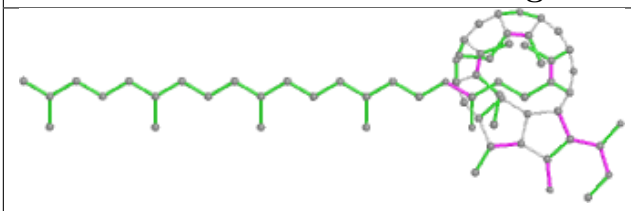


Torsions

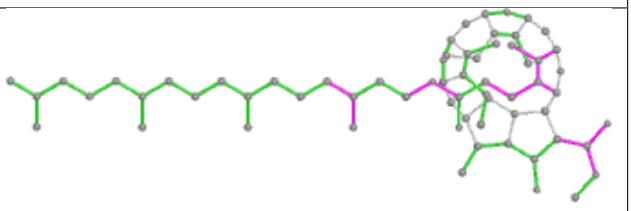


Rings

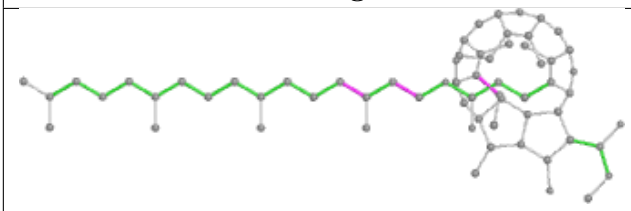
Ligand PHO a 411



Bond lengths



Bond angles



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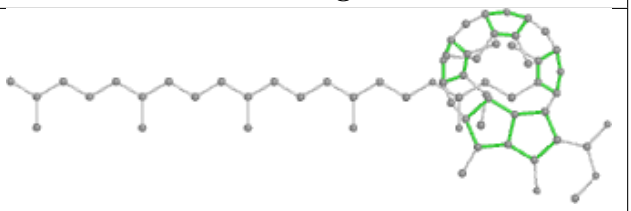
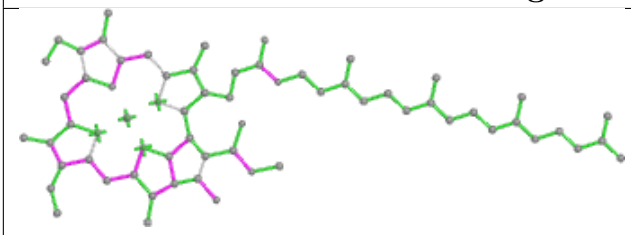
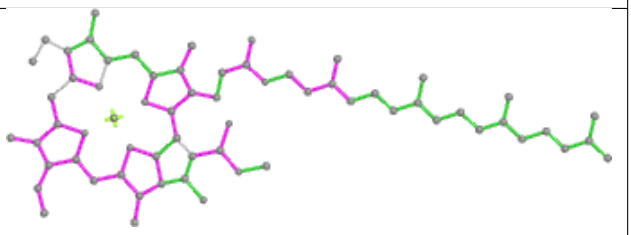


Rings

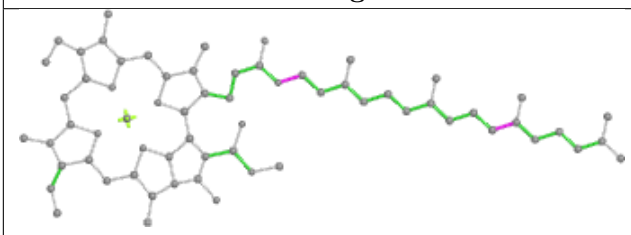
Ligand CLA d 402



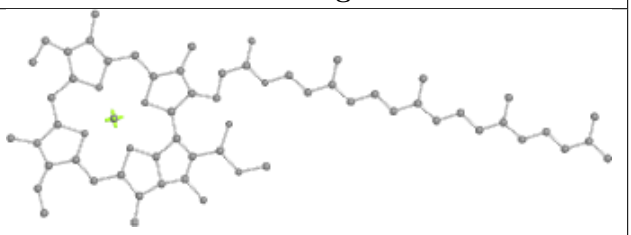
Bond lengths



Bond angles

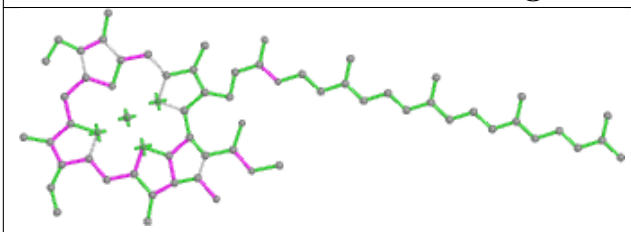


Torsions

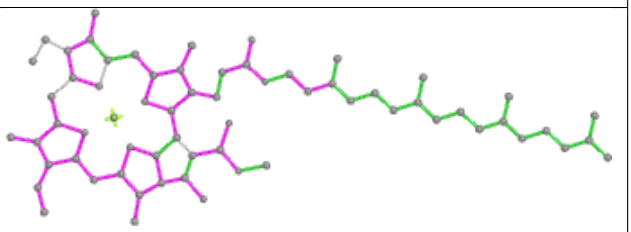


Rings

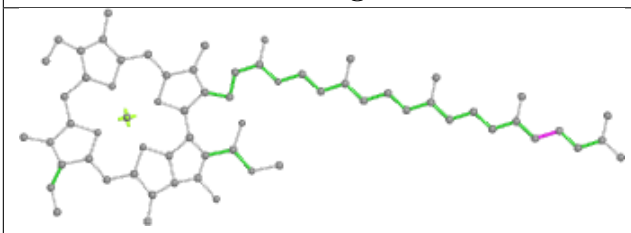
Ligand CLA B 609



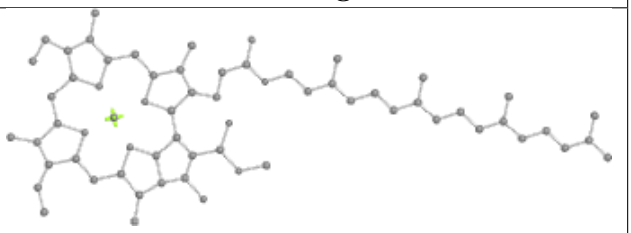
Bond lengths



Bond angles

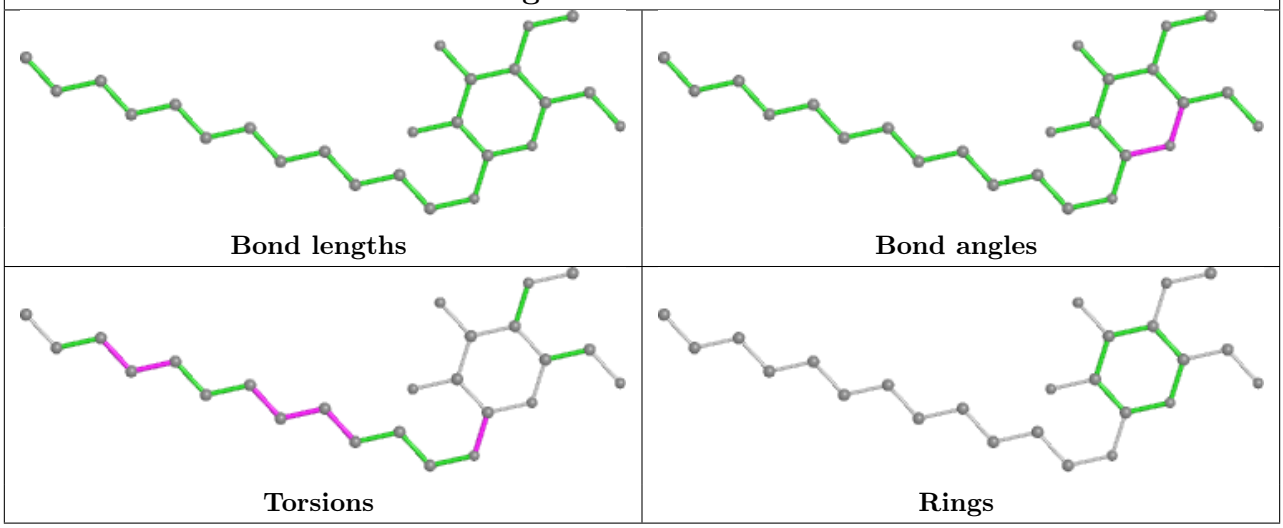


Torsions

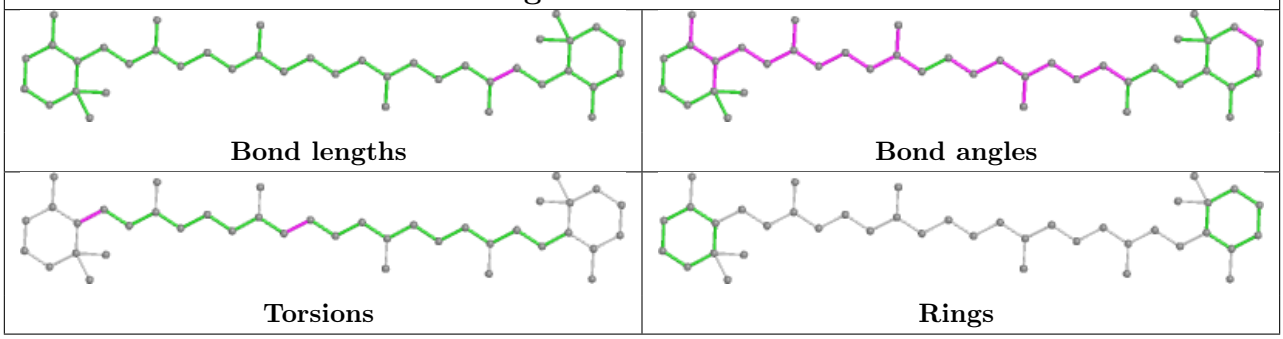


Rings

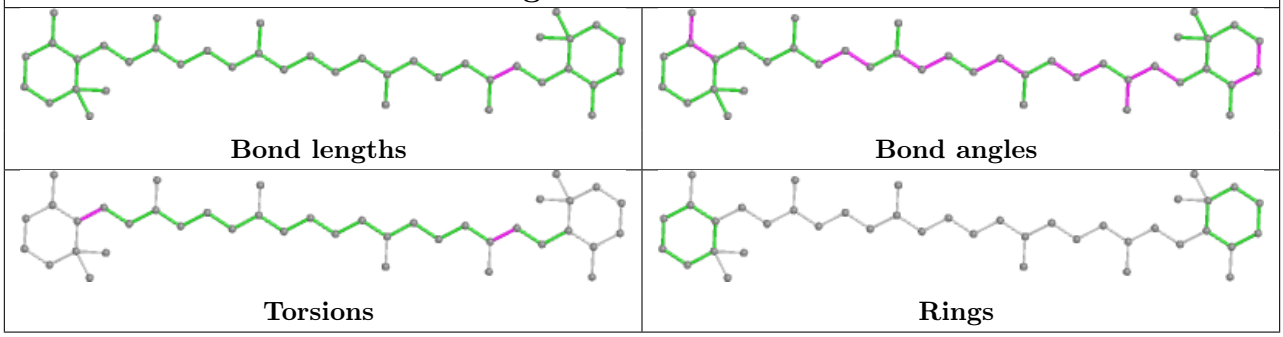
Ligand LMT B 635



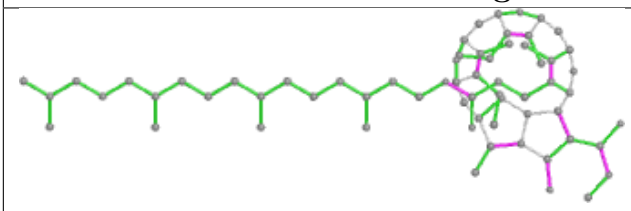
Ligand BCR T 103



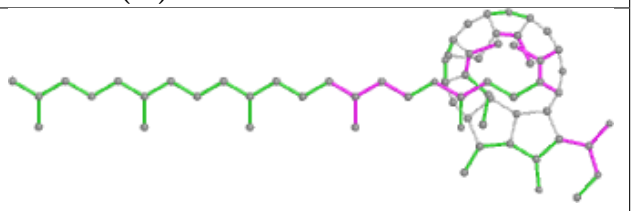
Ligand BCR Y 101



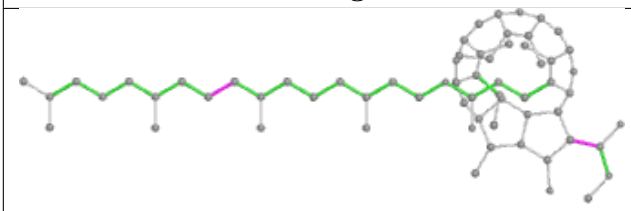
Ligand PHO a 420 (B)



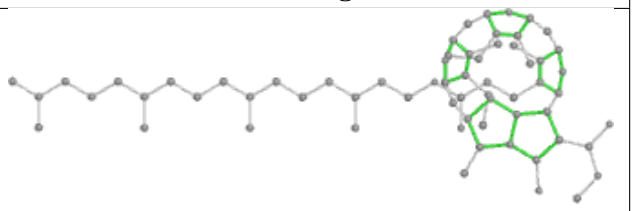
Bond lengths



Bond angles

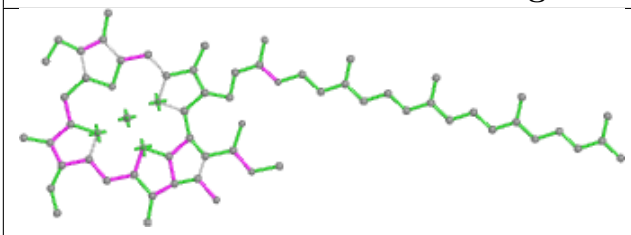


Torsions

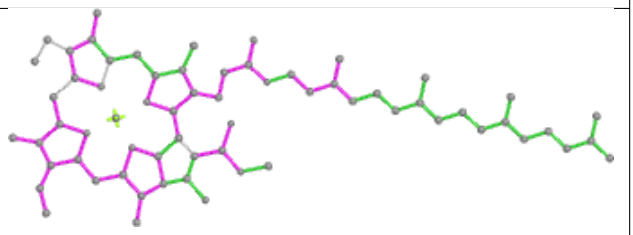


Rings

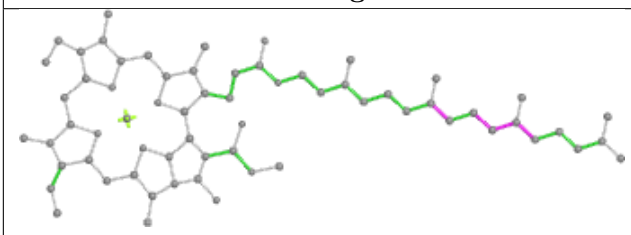
Ligand CLA a 410



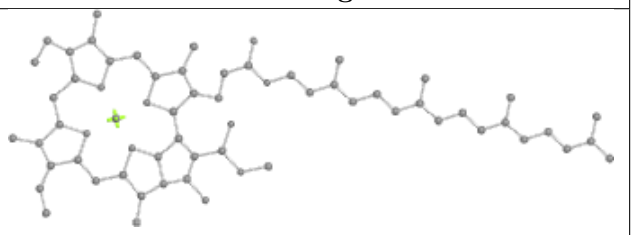
Bond lengths



Bond angles

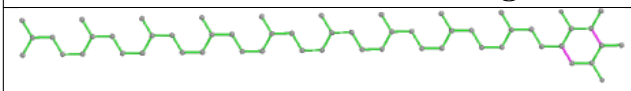


Torsions

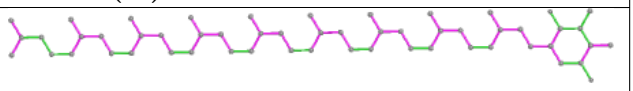


Rings

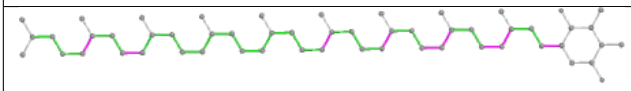
Ligand PL9 a 416 (A)



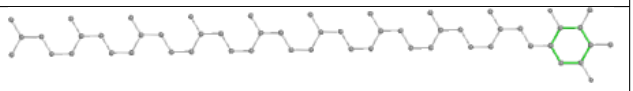
Bond lengths



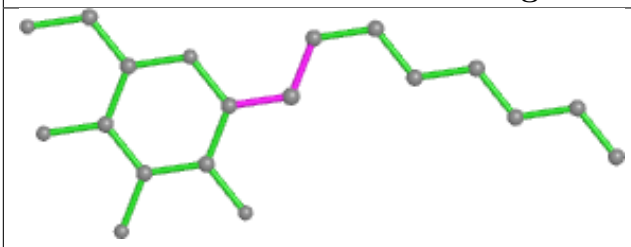
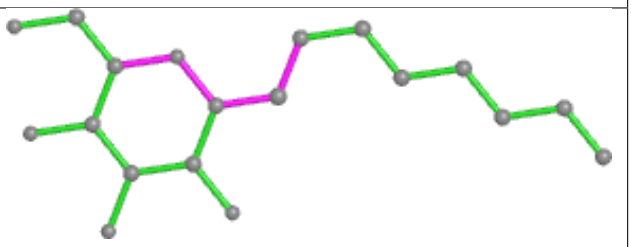
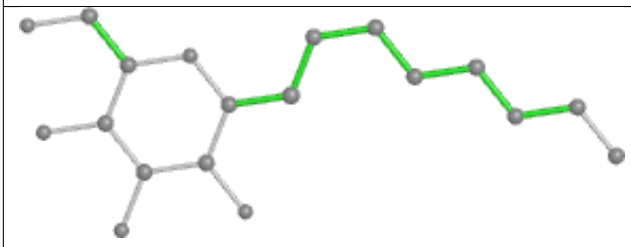
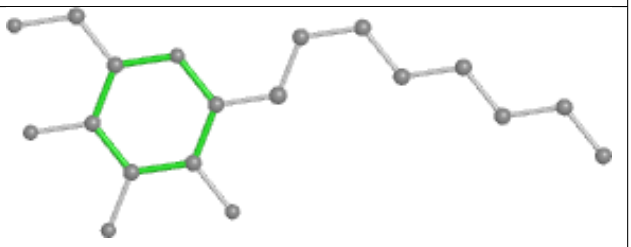
Bond angles

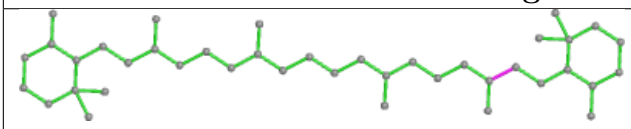
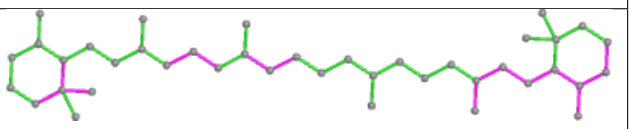
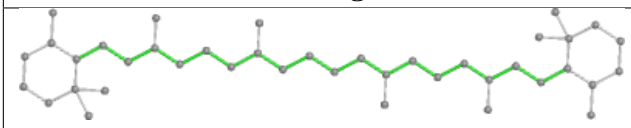
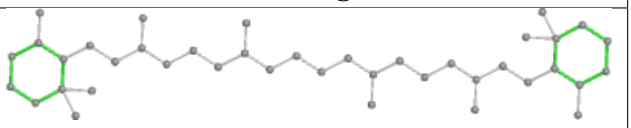


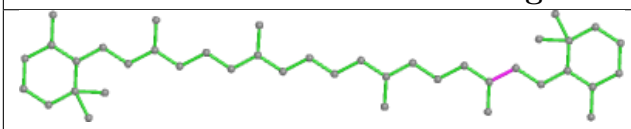
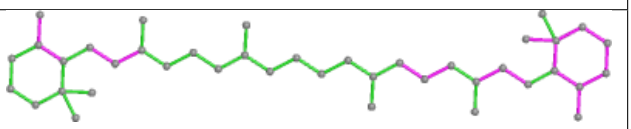
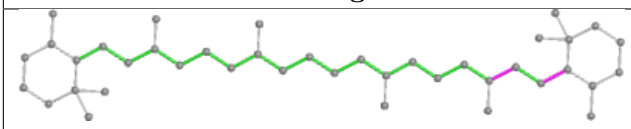
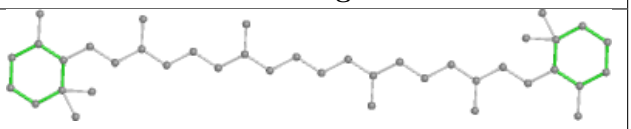
Torsions



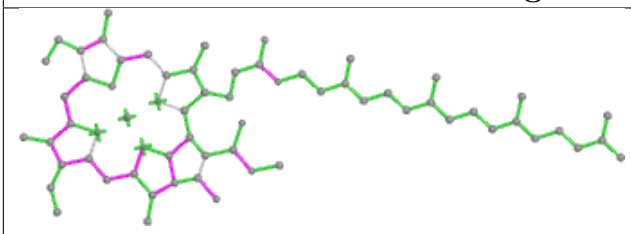
Rings

Ligand HTG C 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

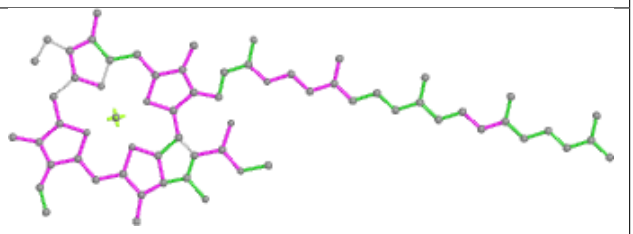
Ligand BCR B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

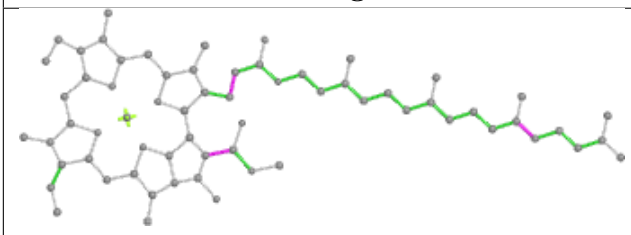
Ligand CLA B 603



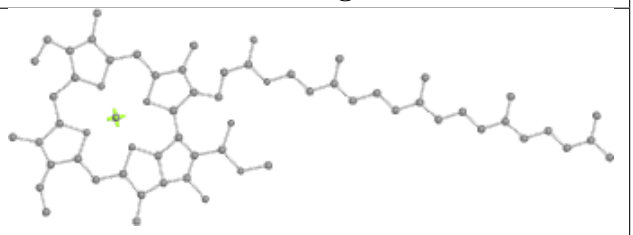
Bond lengths



Bond angles

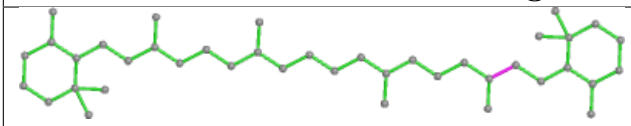


Torsions



Rings

Ligand BCR k 101



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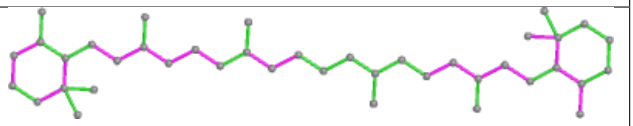
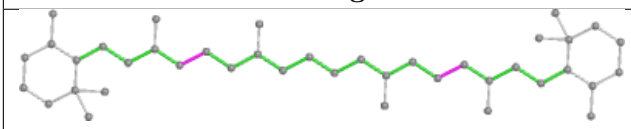


Bond angles



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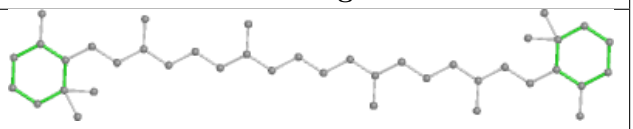
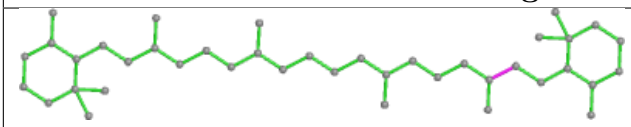


Rings

Ligand BCR K 101



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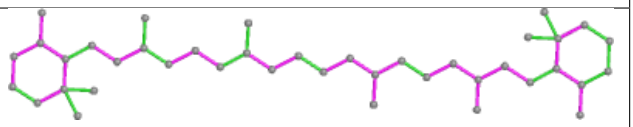
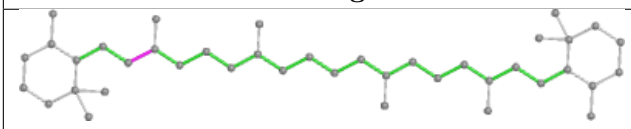


Bond angles



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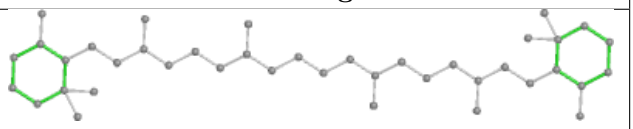
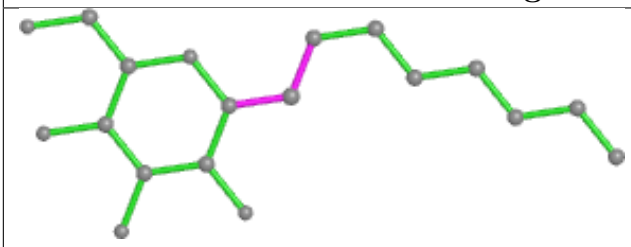


Rings

Ligand HTG b 609



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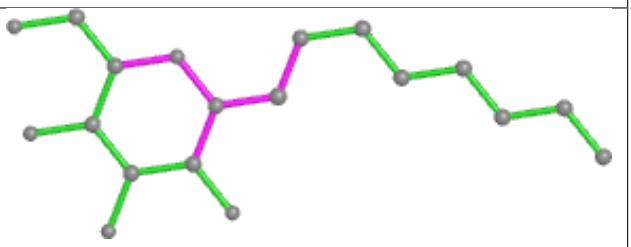
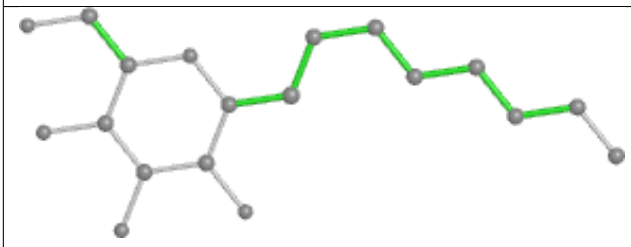


Bond angles



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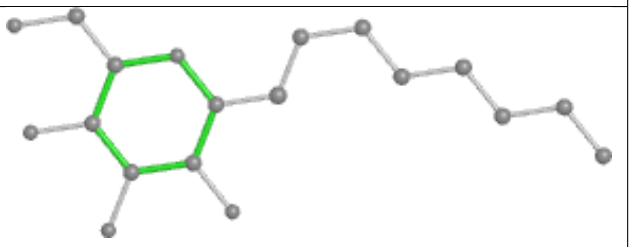
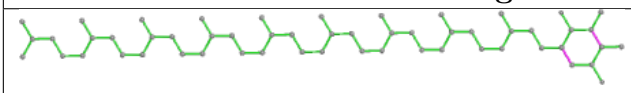


Rings

Ligand PL9 D 405 (A)



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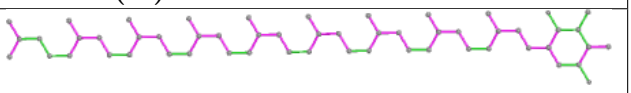

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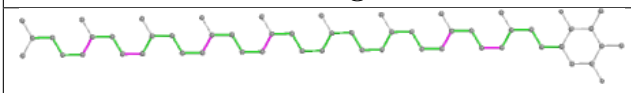

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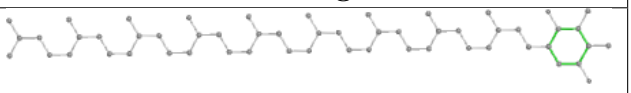
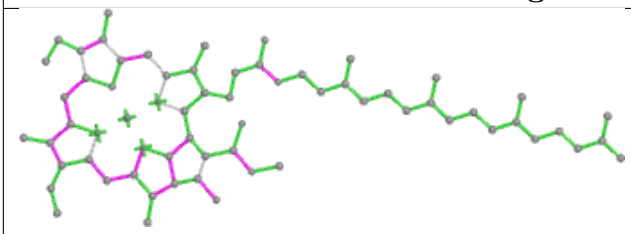


Rings

Ligand CLA b 611



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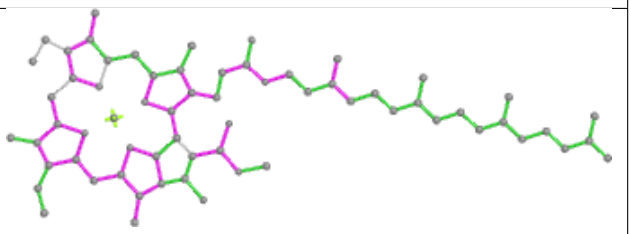
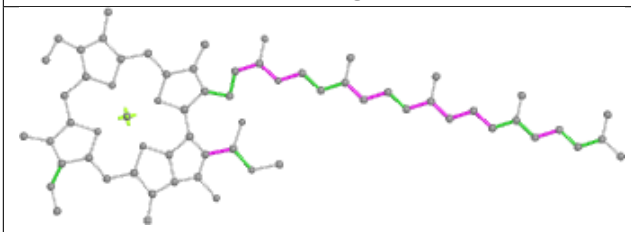


Bond angles



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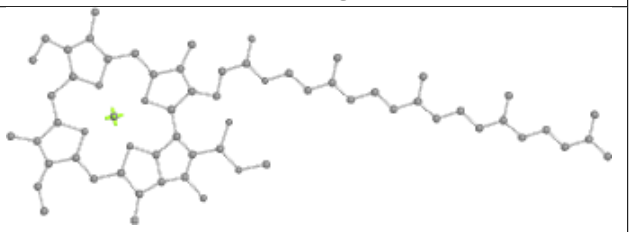
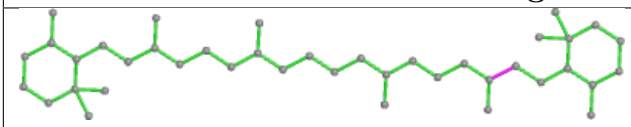


Rings

Ligand BCR c 527



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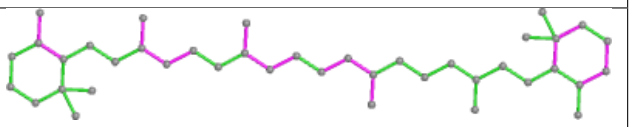
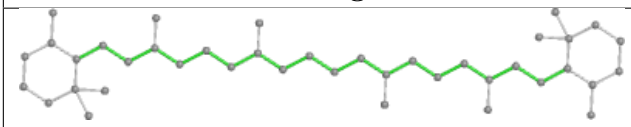


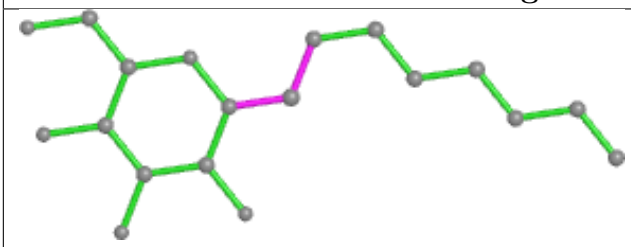
Bond angles



Torsions

Rings

Ligand HTG B 625



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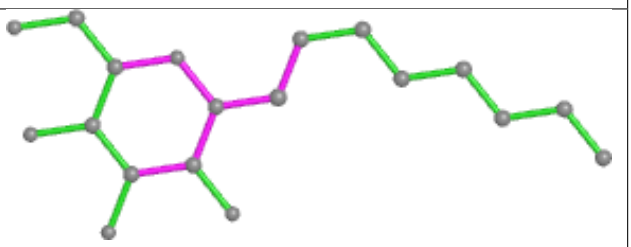
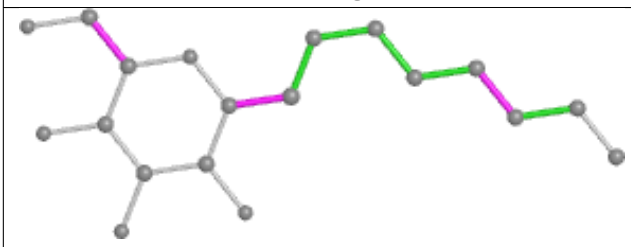
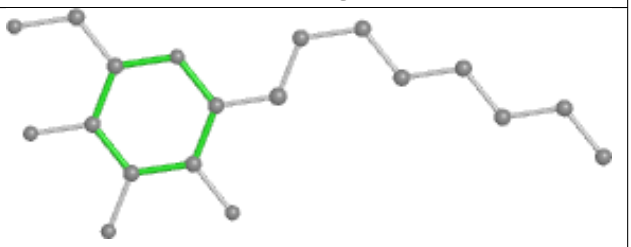


Bond angles

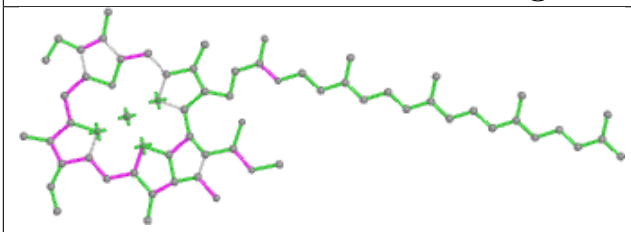


Torsions



Rings

Ligand CLA c 509



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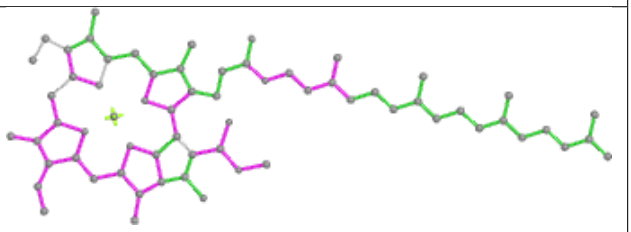
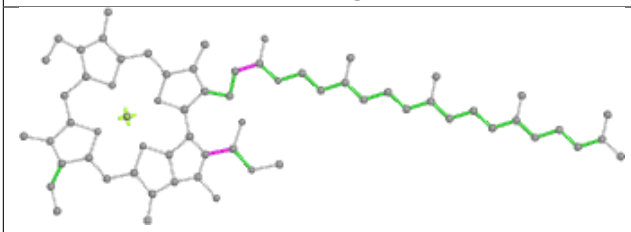
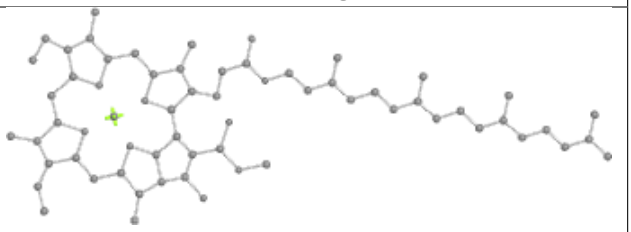


Bond angles

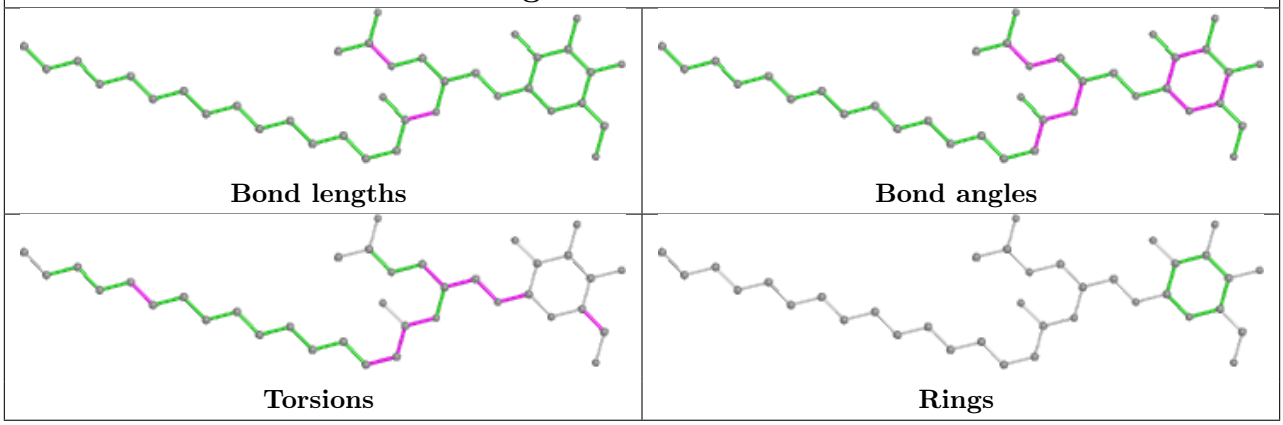


Torsions



Rings

Ligand LMG Z 101



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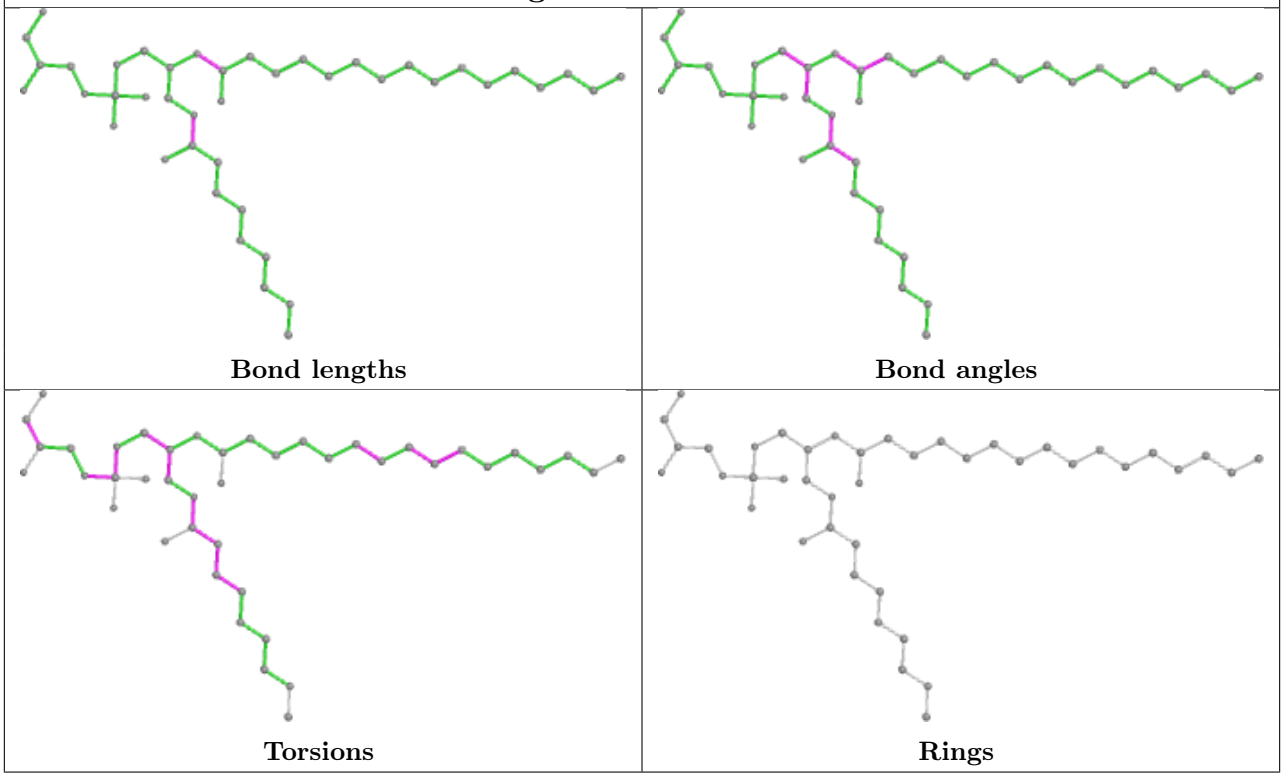

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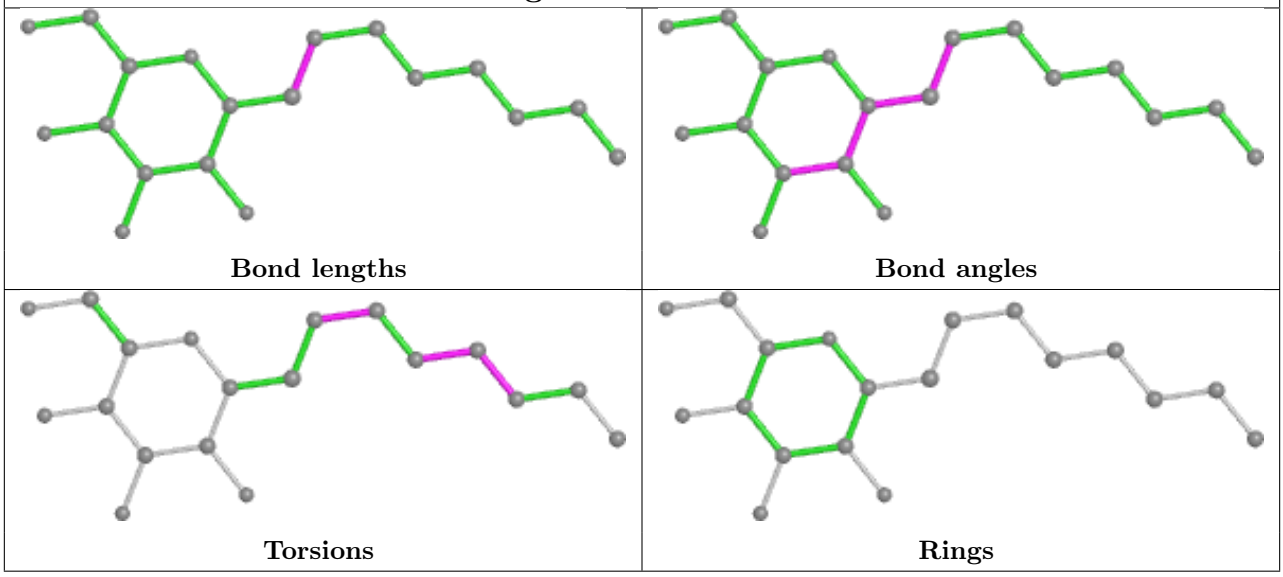

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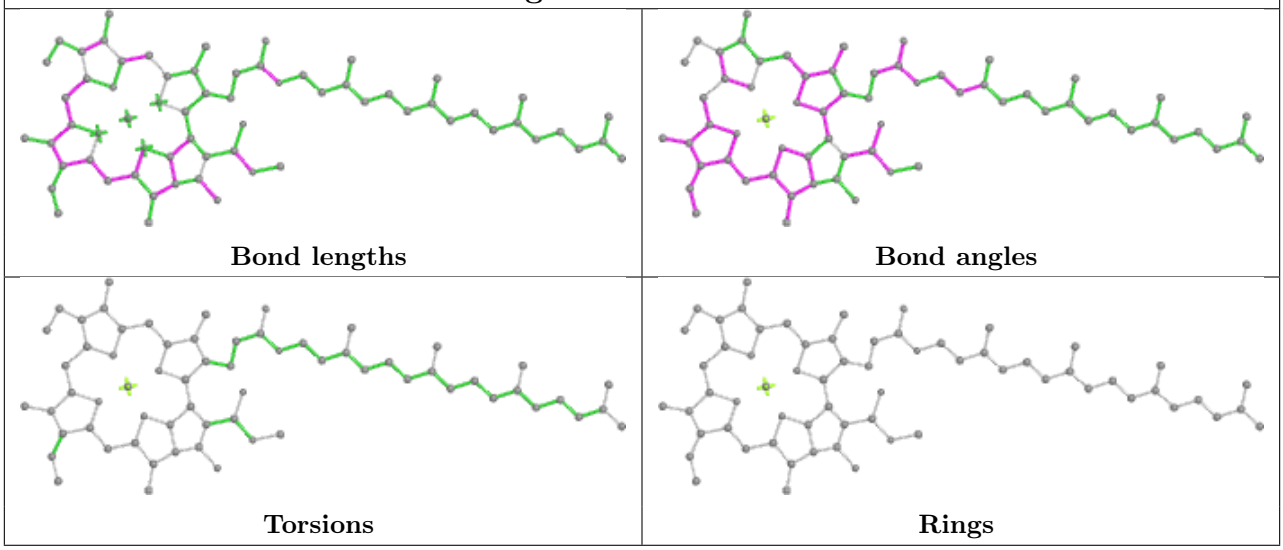

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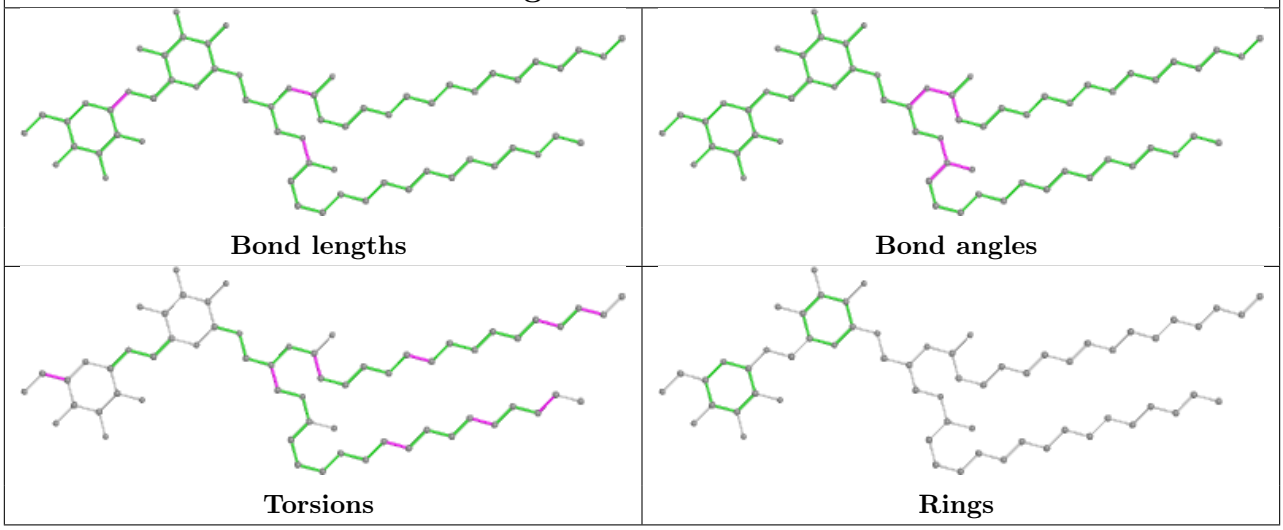

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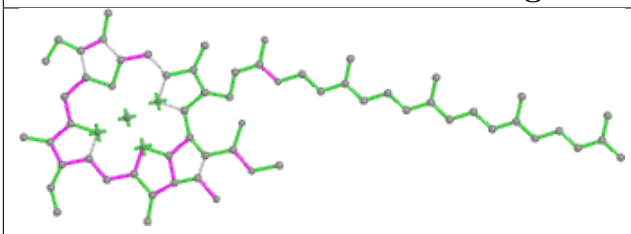

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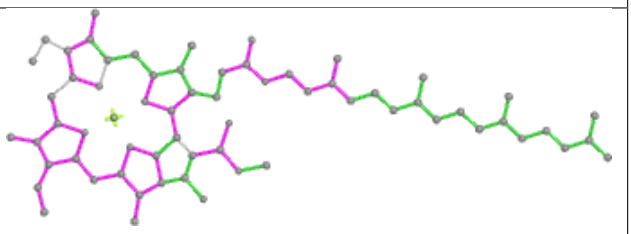
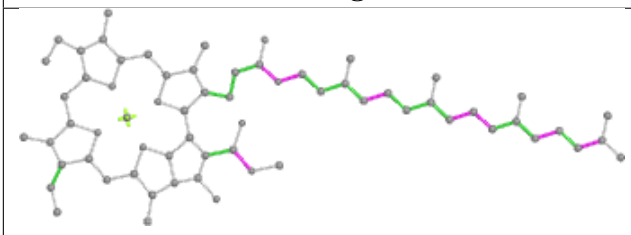
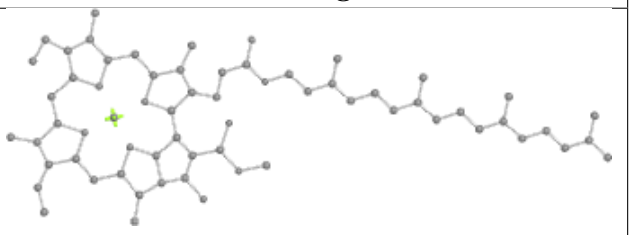


Bond angles

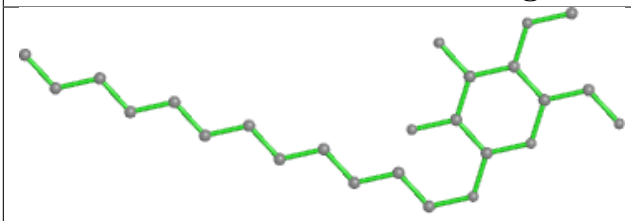


Torsions



Rings

Ligand LMT T 104



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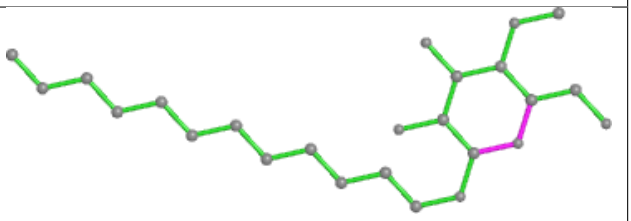

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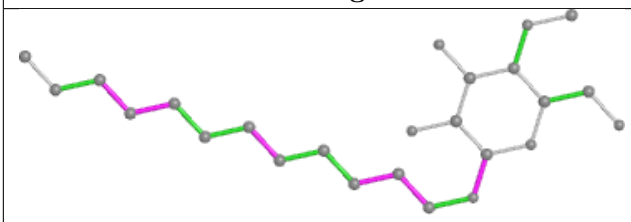

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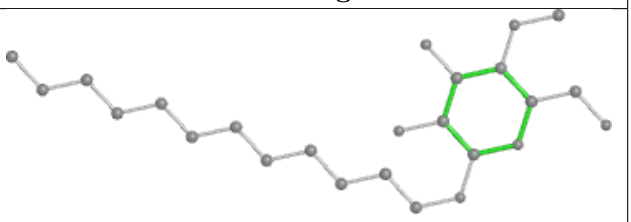
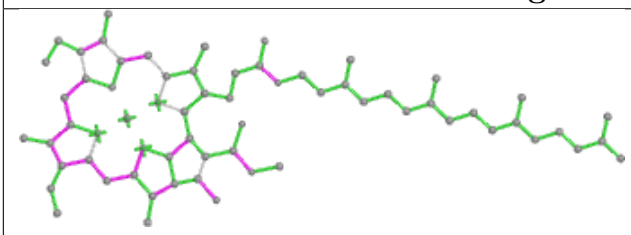
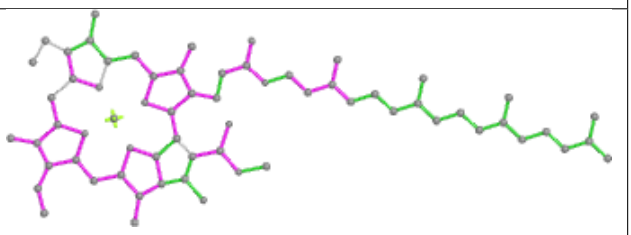


Rings

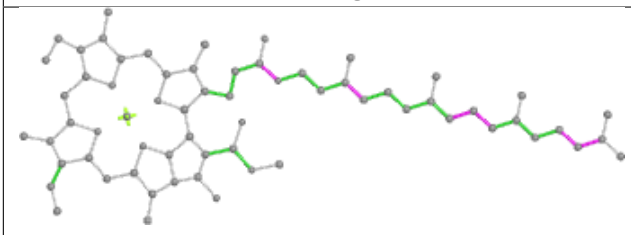
Ligand CLA a 412



Bond lengths



Bond angles



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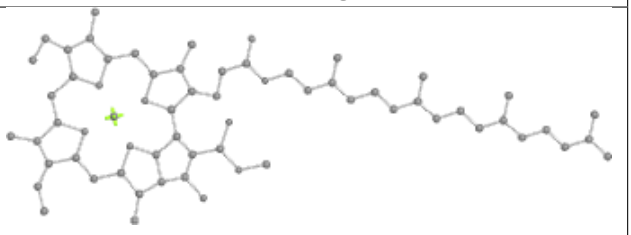
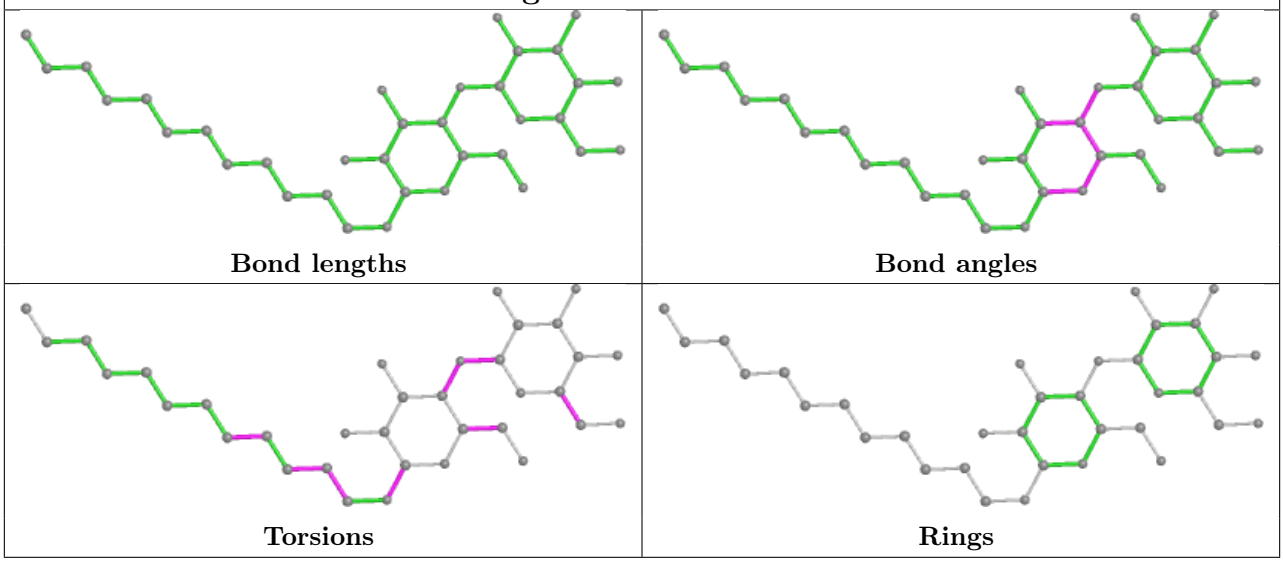
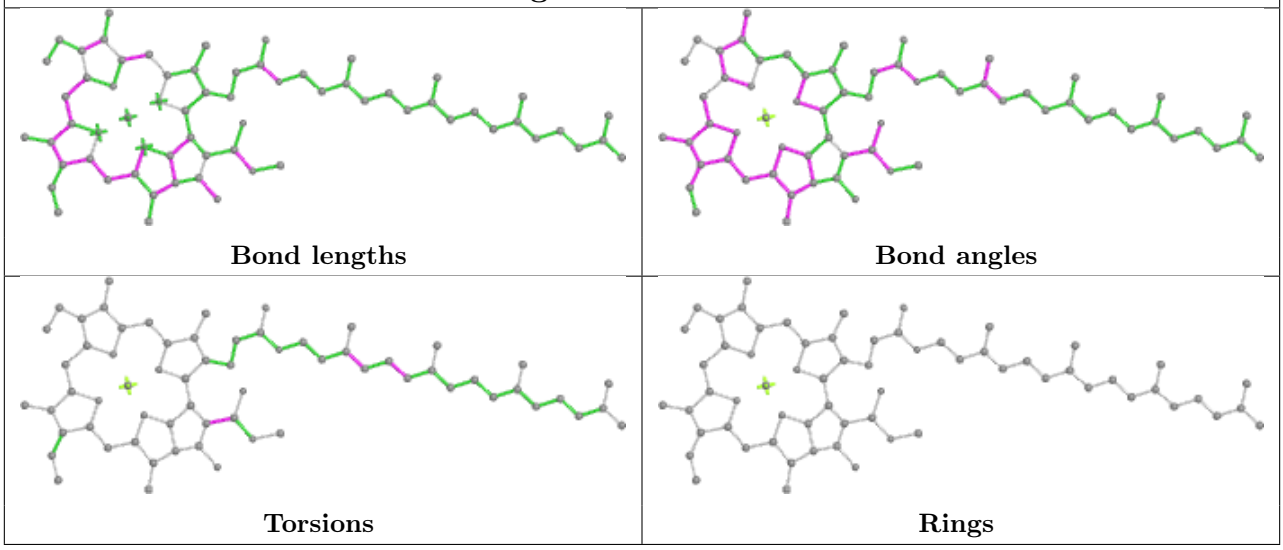


Rings

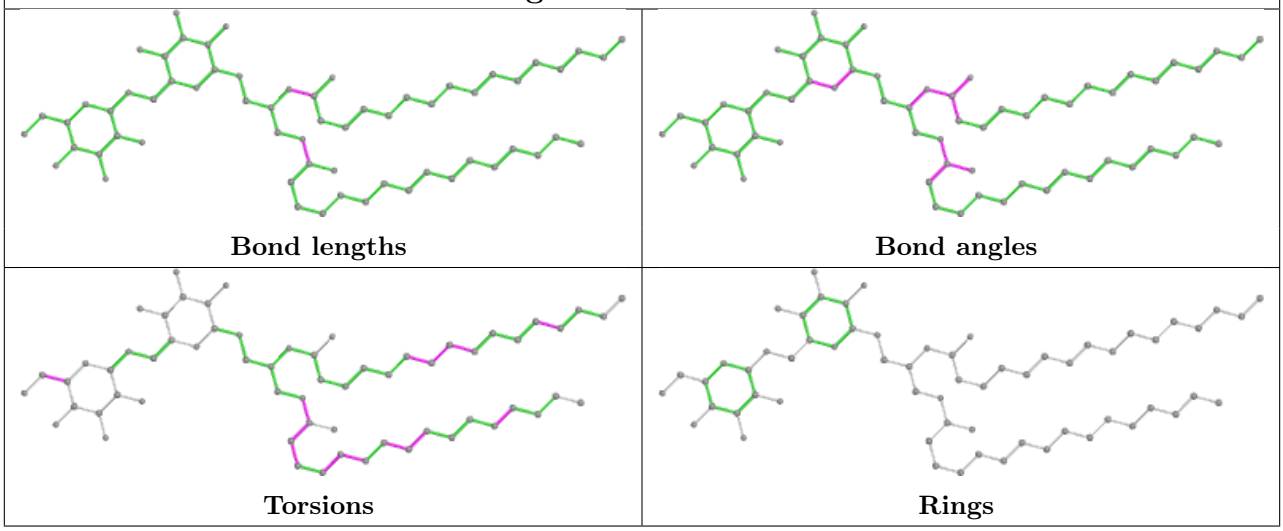
Ligand LMT C 521

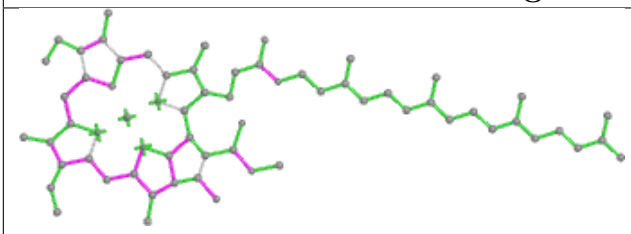
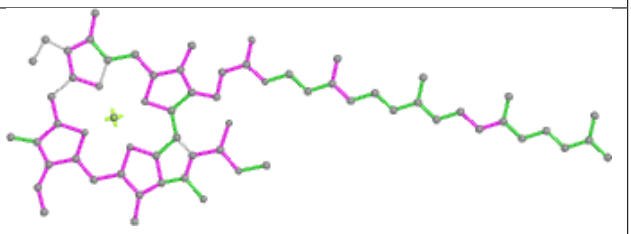
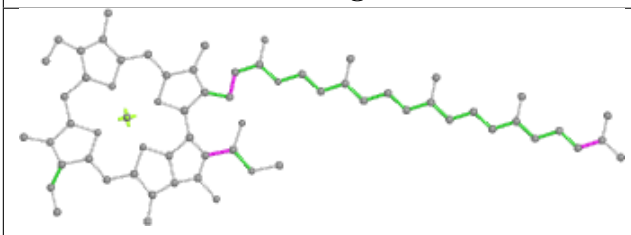
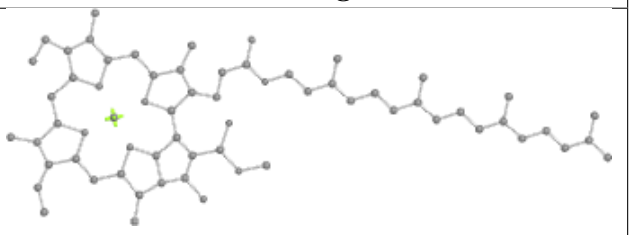


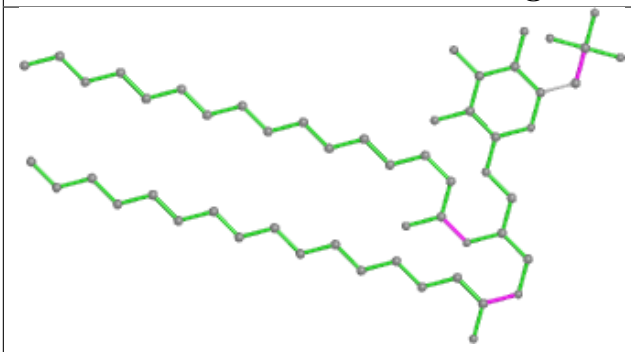
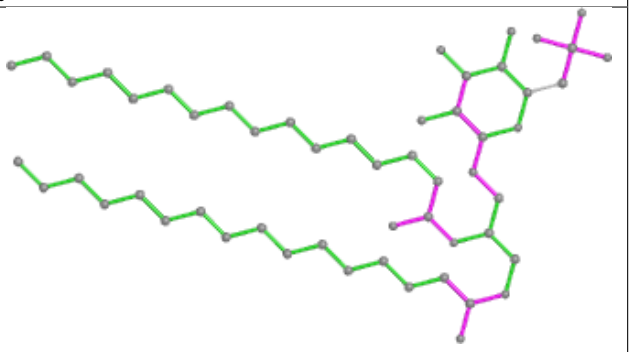
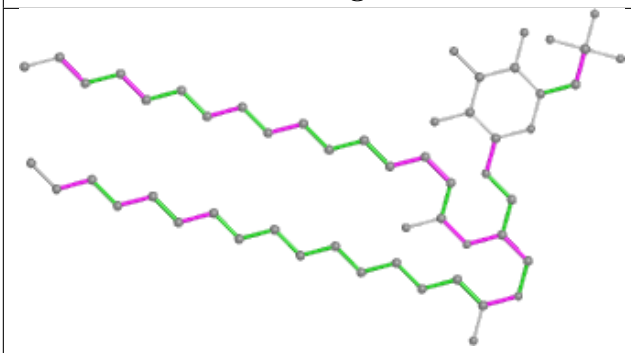
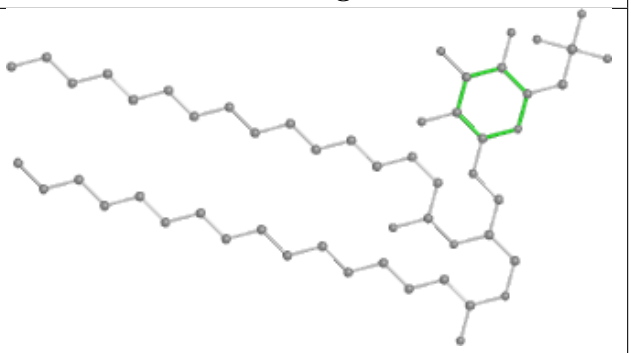
Ligand CLA c 511



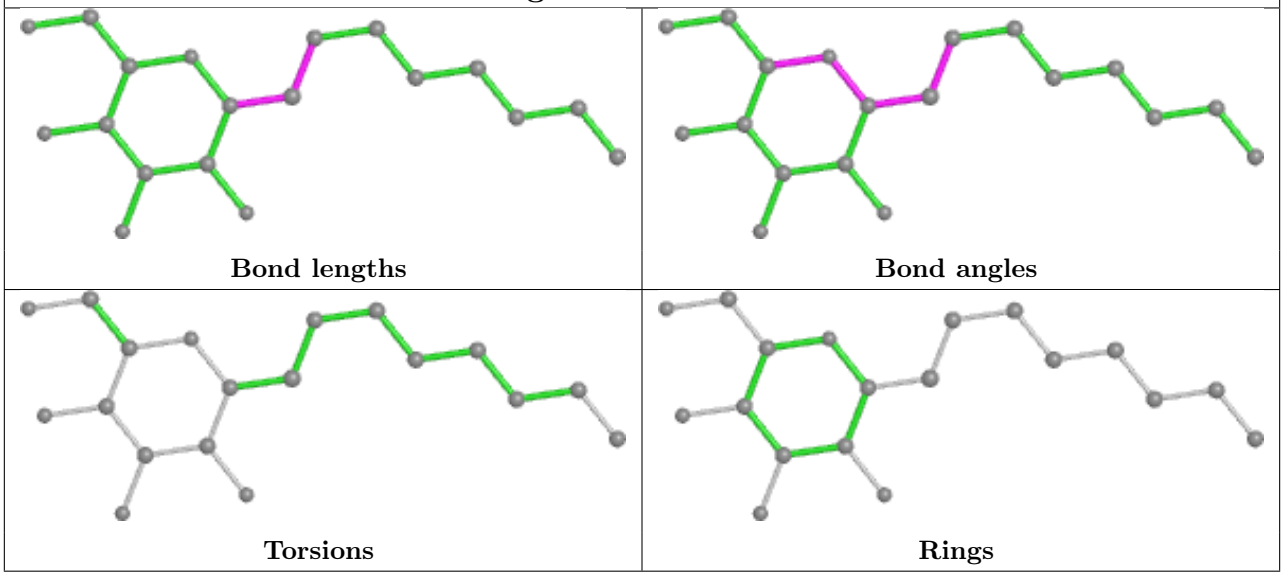
Ligand DGD c 521



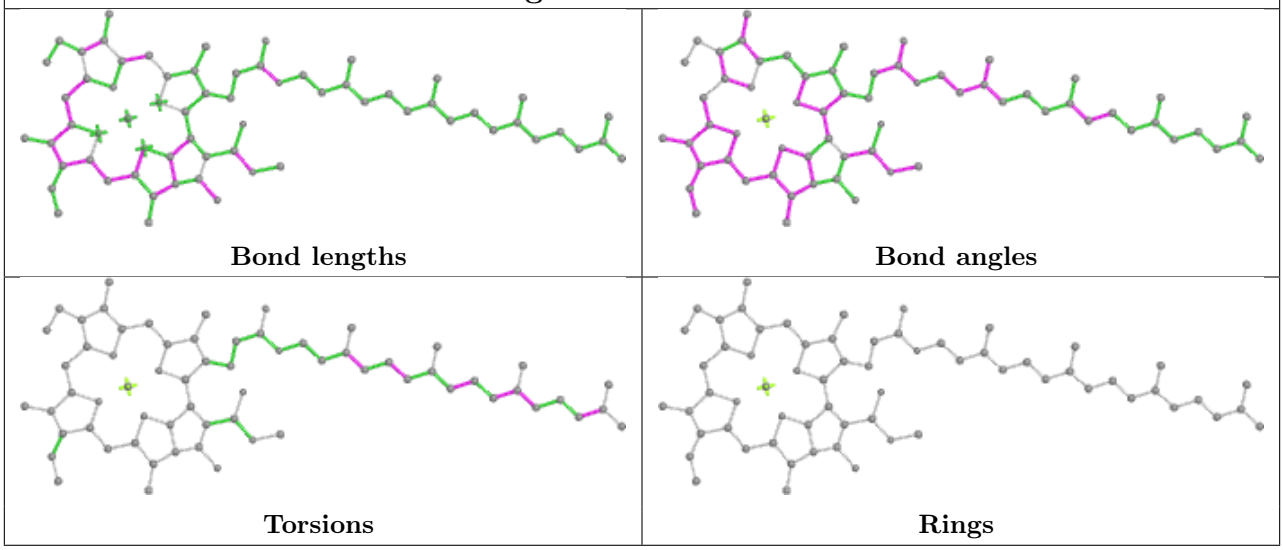
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

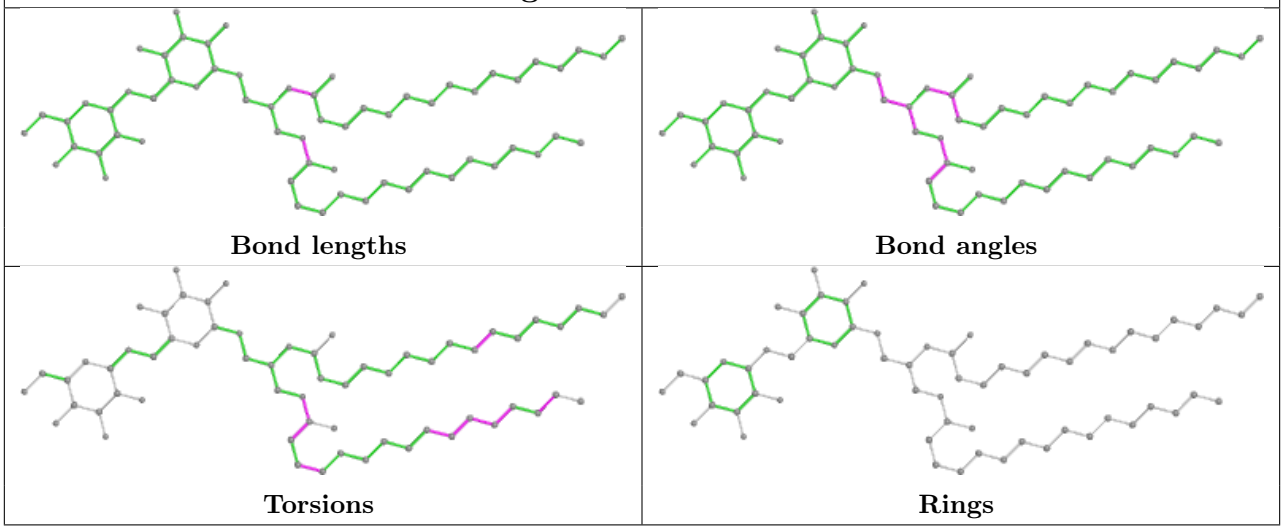
Ligand HTG c 525



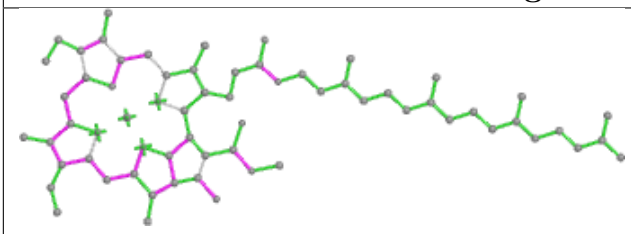
Ligand CLA B 616



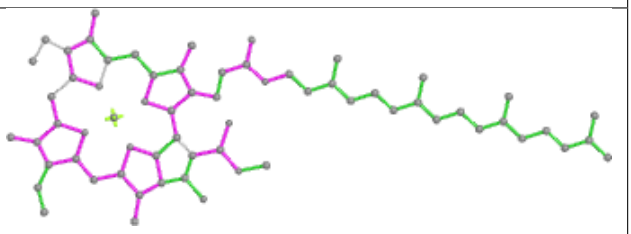
Ligand DGD C 518



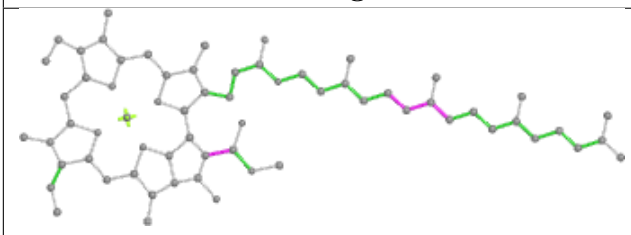
Ligand CLA B 604



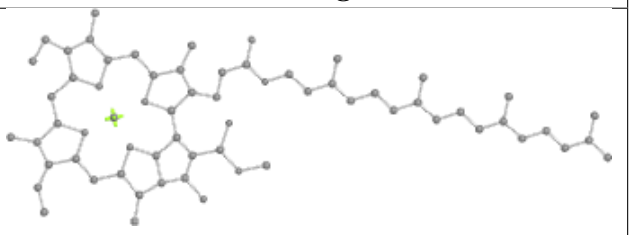
Bond lengths



Bond angles

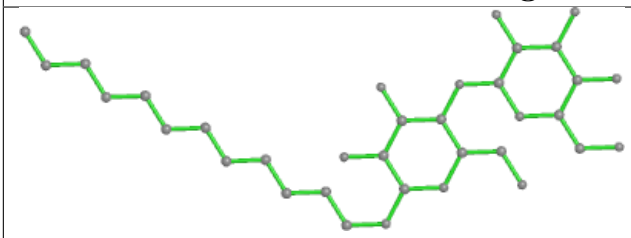


Torsions

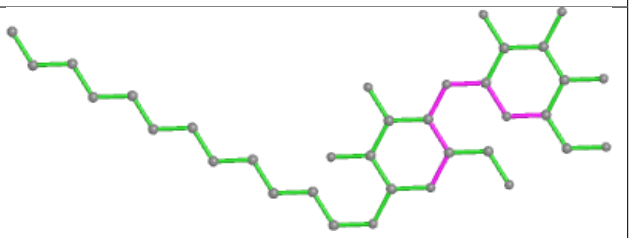


Rings

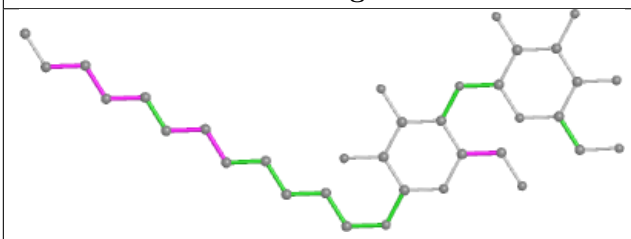
Ligand LMT m 102



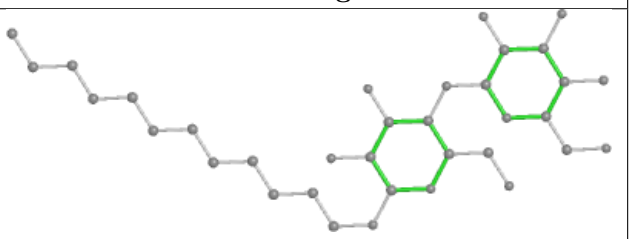
Bond lengths



Bond angles

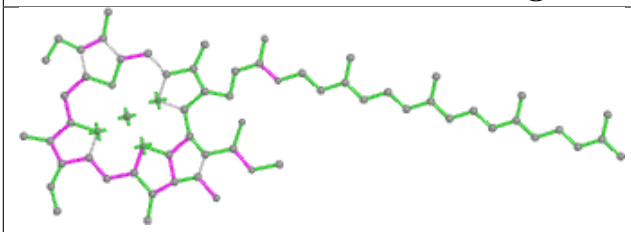


Torsions



Rings

Ligand CLA b 620



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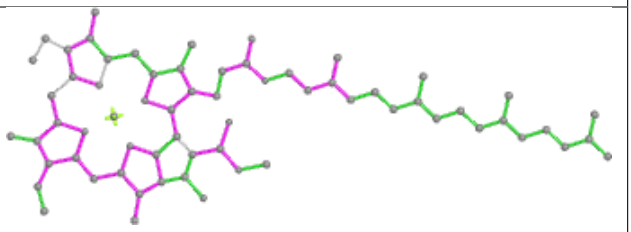
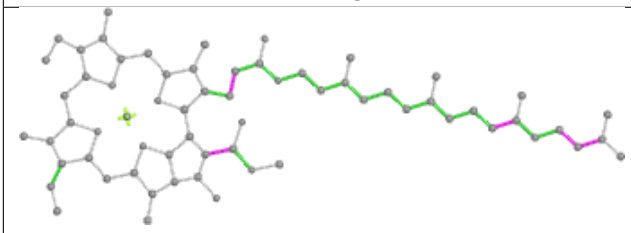
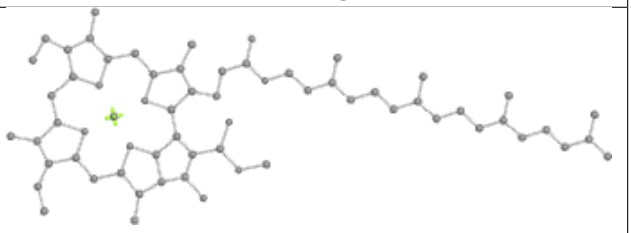


Bond angles

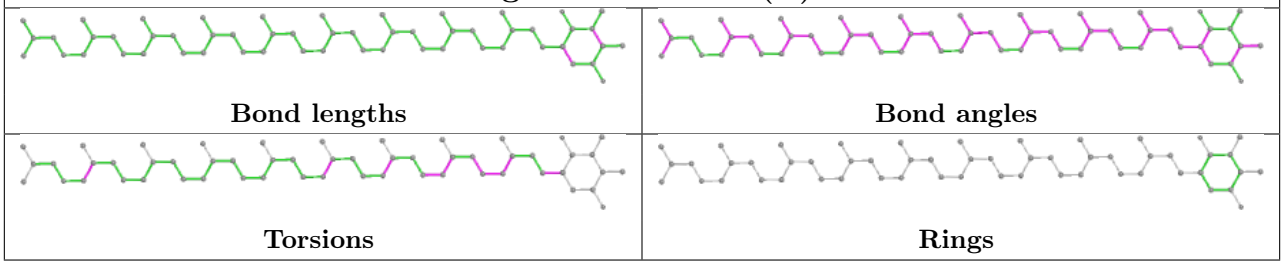


Torsions

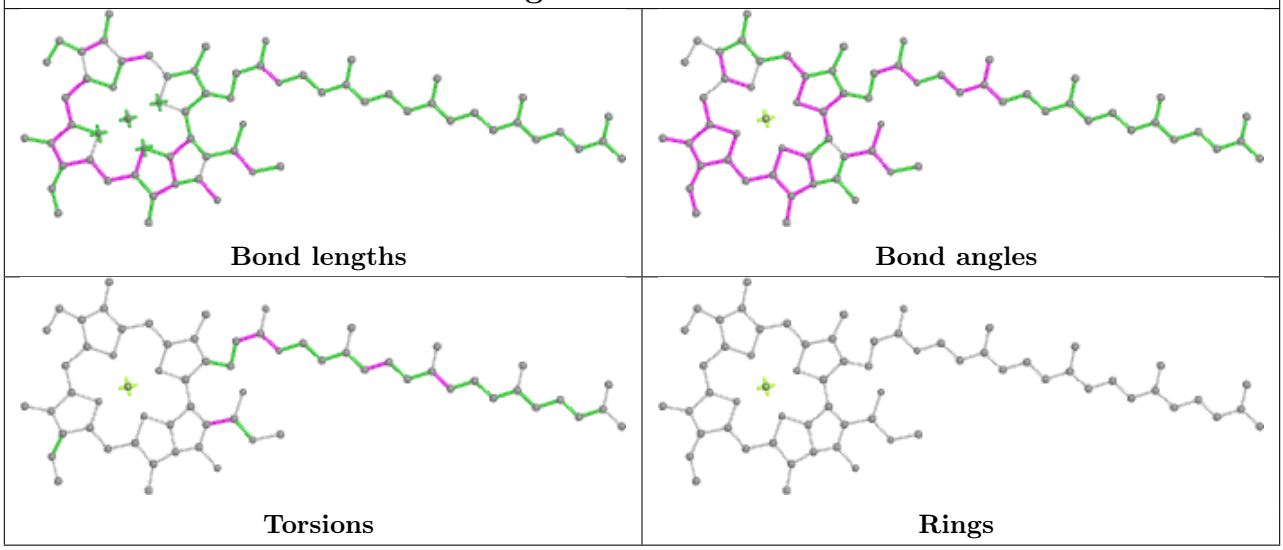


Rings

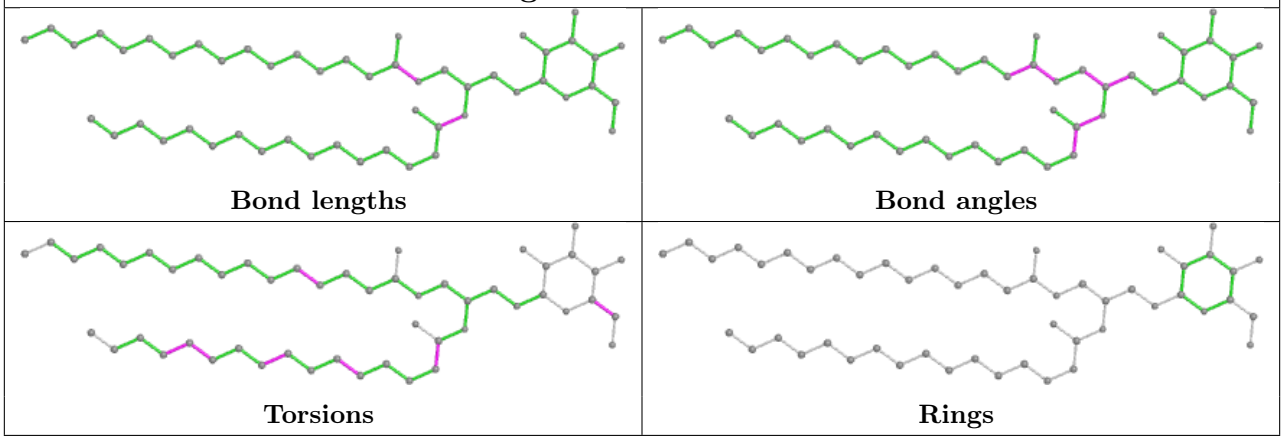
Ligand PL9 a 416 (B)



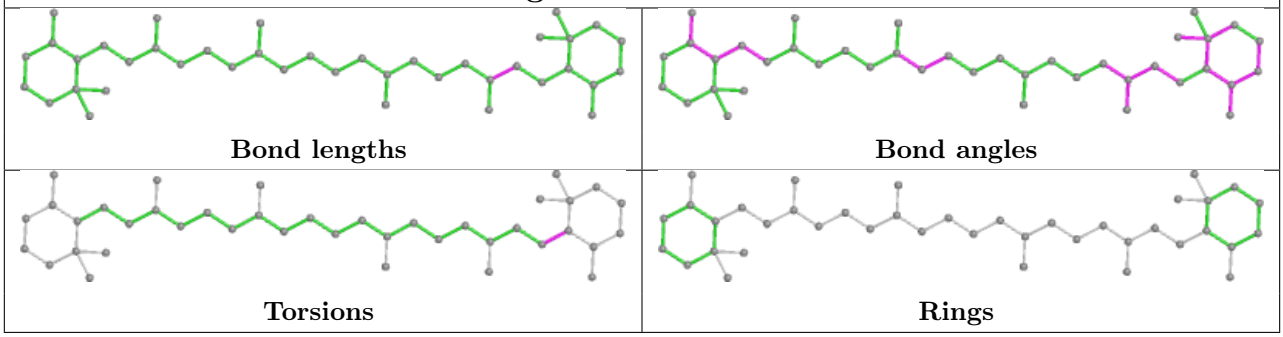
Ligand CLA C 512



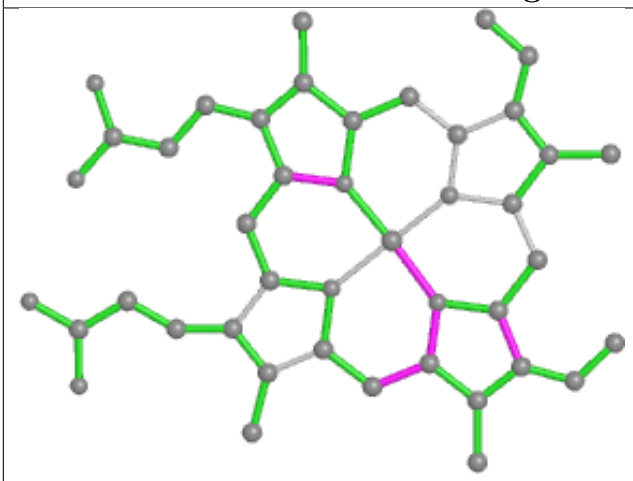
Ligand LMG D 412



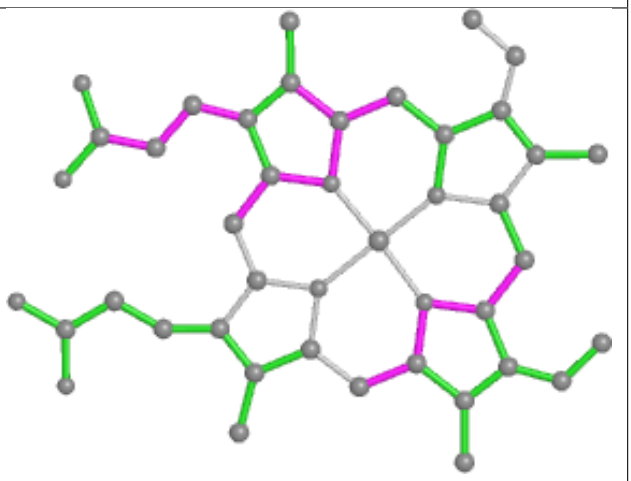
Ligand BCR b 628



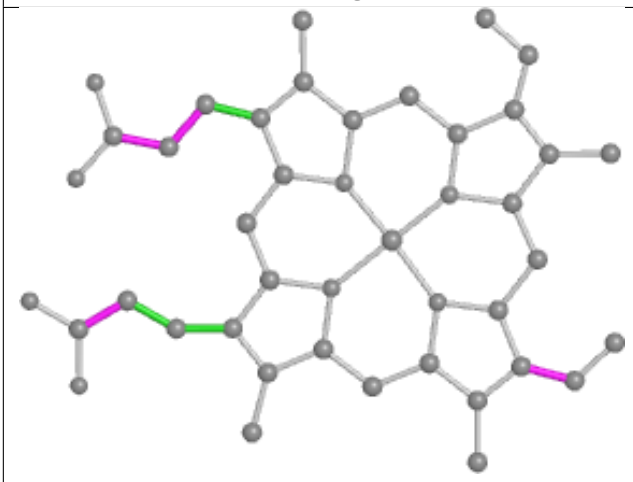
Ligand HEM e 102



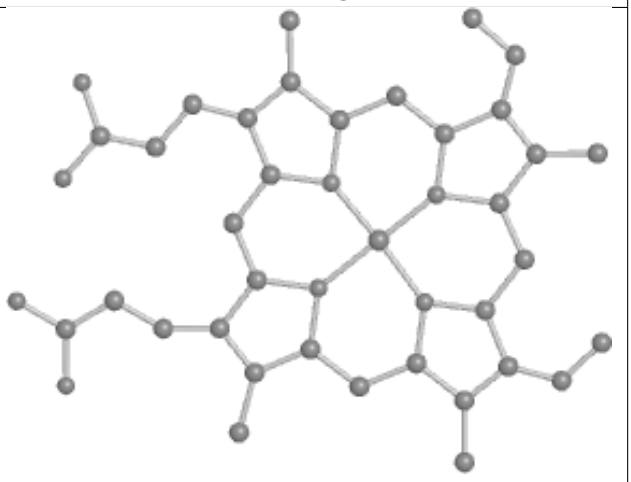
Bond lengths



Bond angles

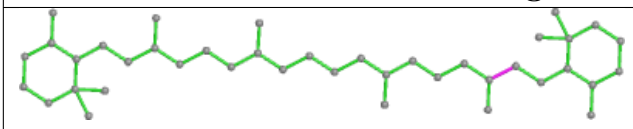


Torsions



Rings

Ligand BCR h 101



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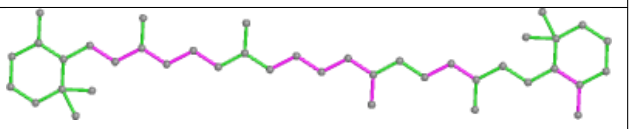
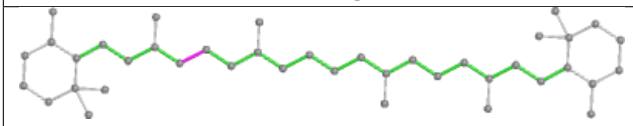


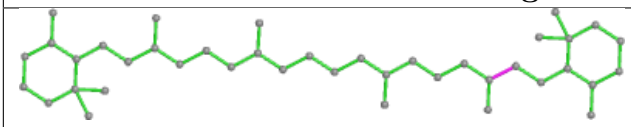
Bond angles



Torsions

Rings

Ligand BCR H 102



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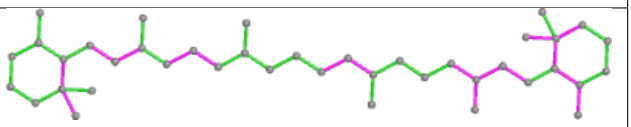
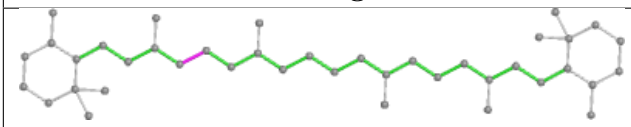


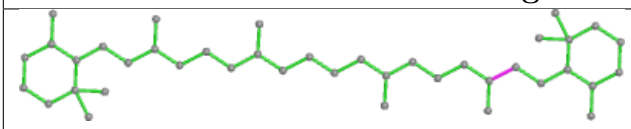
Bond angles



Torsions

Rings

Ligand BCR A 411



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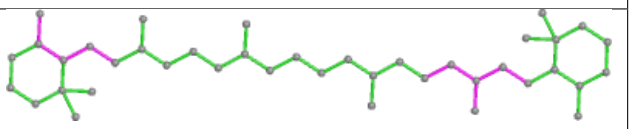
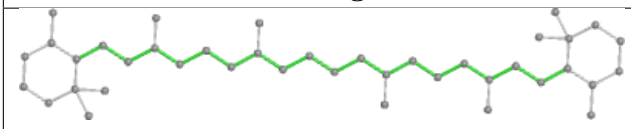
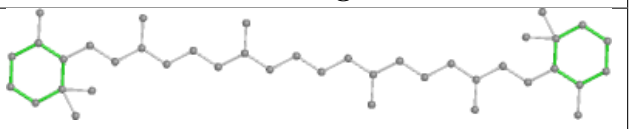


Bond angles

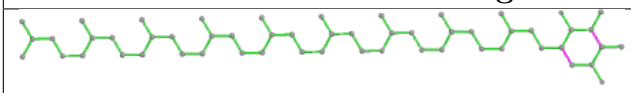


Torsions

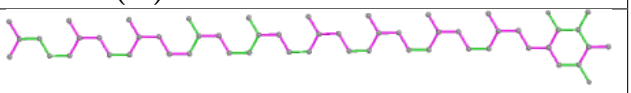


Rings

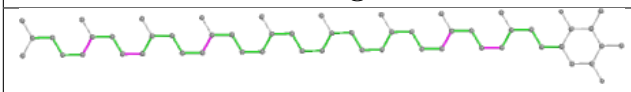
Ligand PL9 D 405 (B)



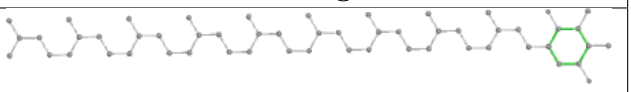
Bond lengths



Bond angles

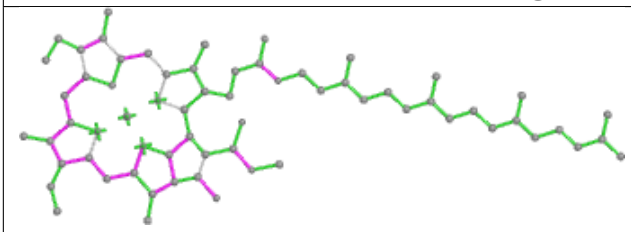


Torsions



Rings

Ligand CLA c 514



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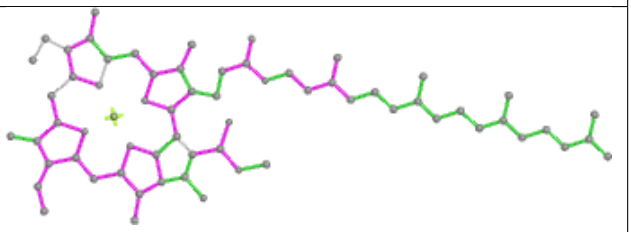
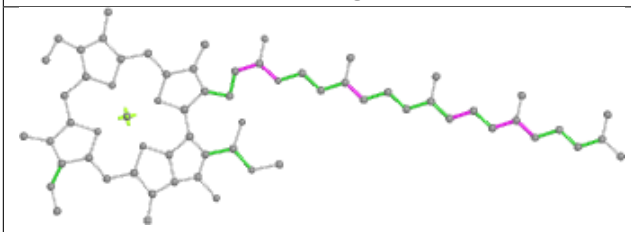
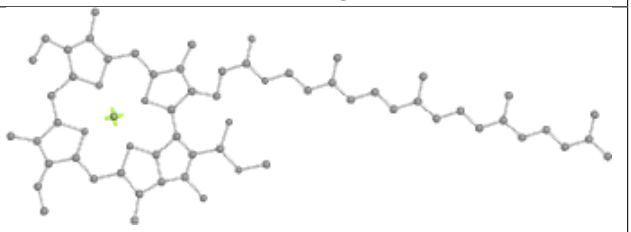


Bond angles

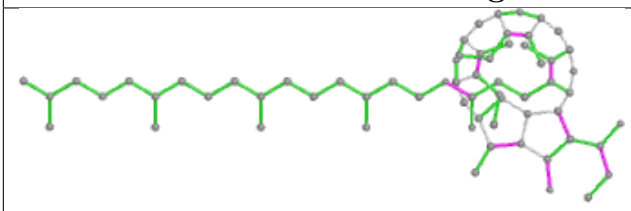


Torsions

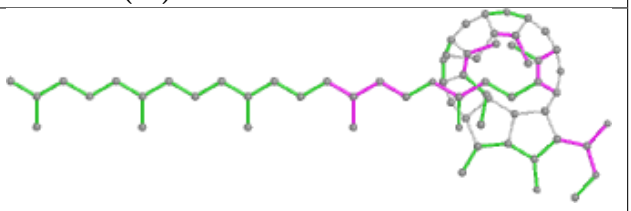


Rings

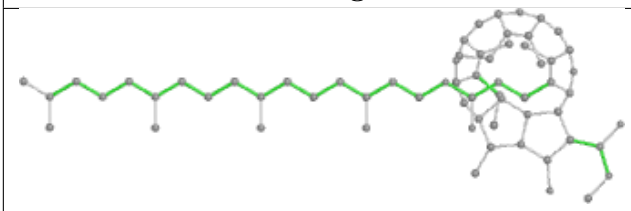
Ligand PHO A 409 (A)



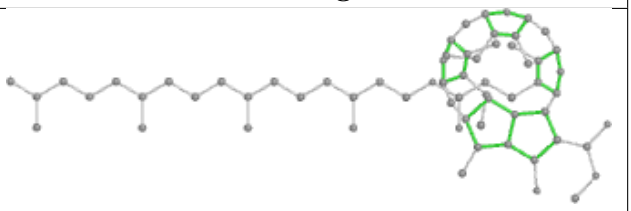
Bond lengths



Bond angles

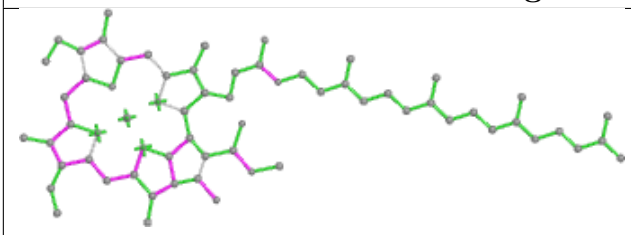


Torsions

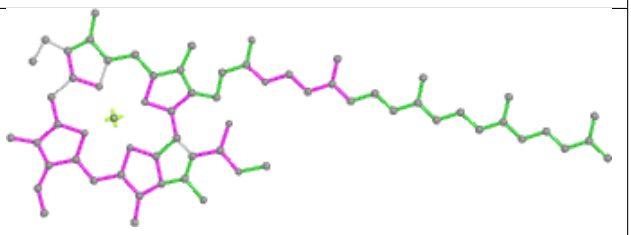


Rings

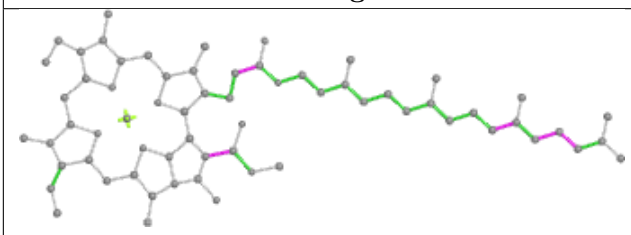
Ligand CLA C 501



Bond lengths



Bond angles



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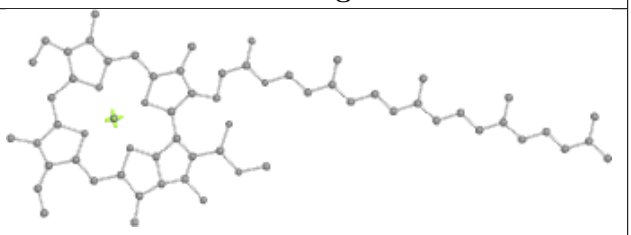
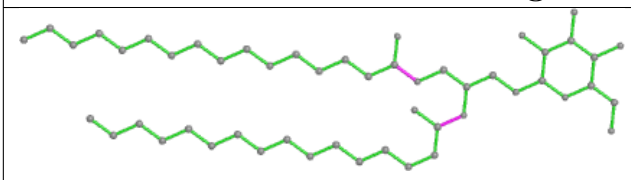


Rings

Ligand LMG j 101



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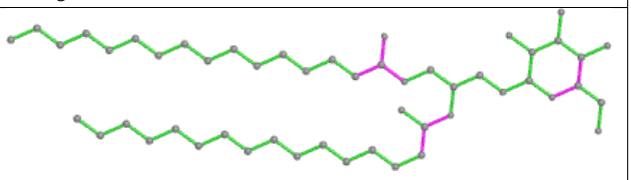
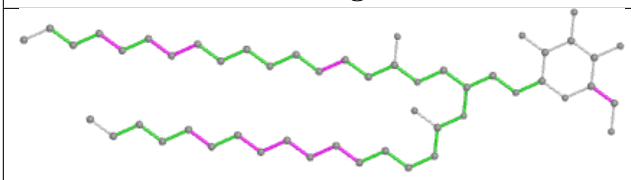


Bond angles



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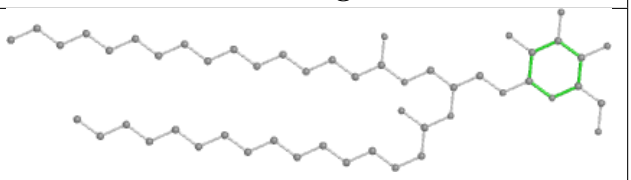
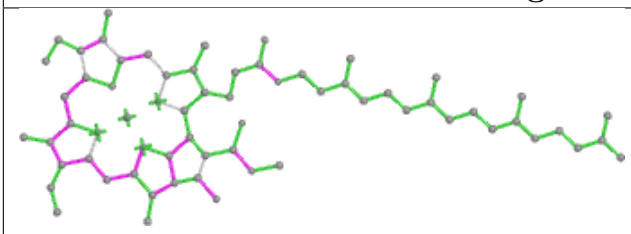
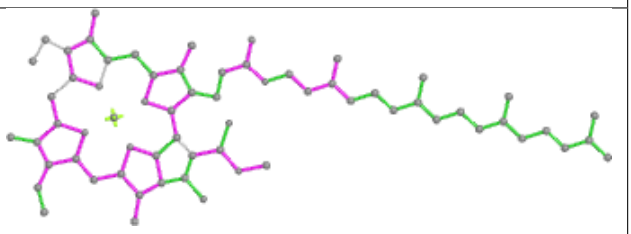
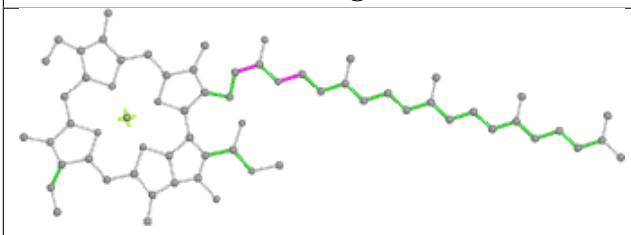
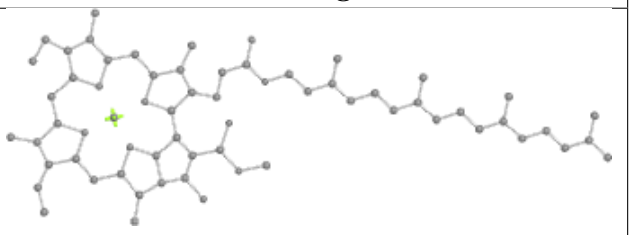
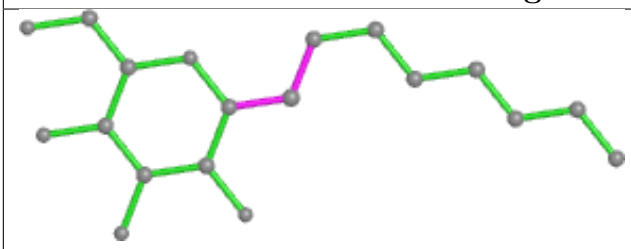
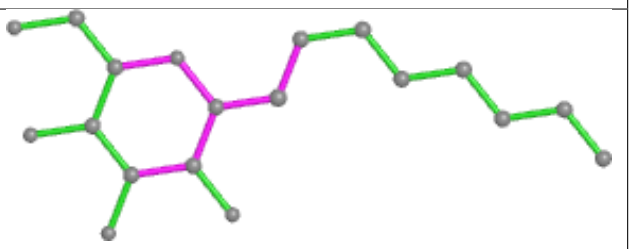
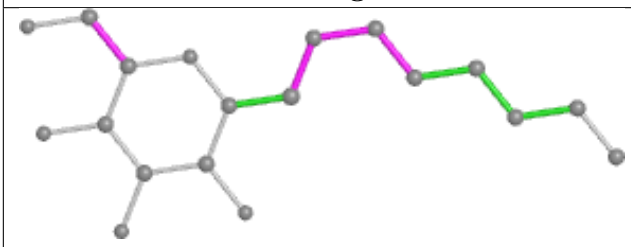
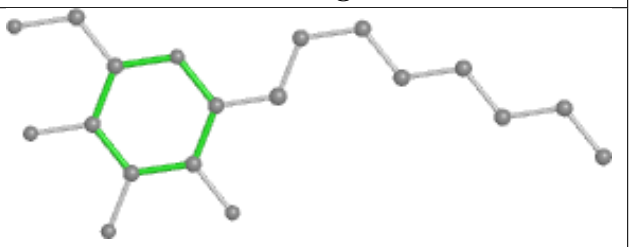


Rings

Ligand CLA b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG b 633	
 Bond lengths	 Bond angles
 Torsions	 Rings

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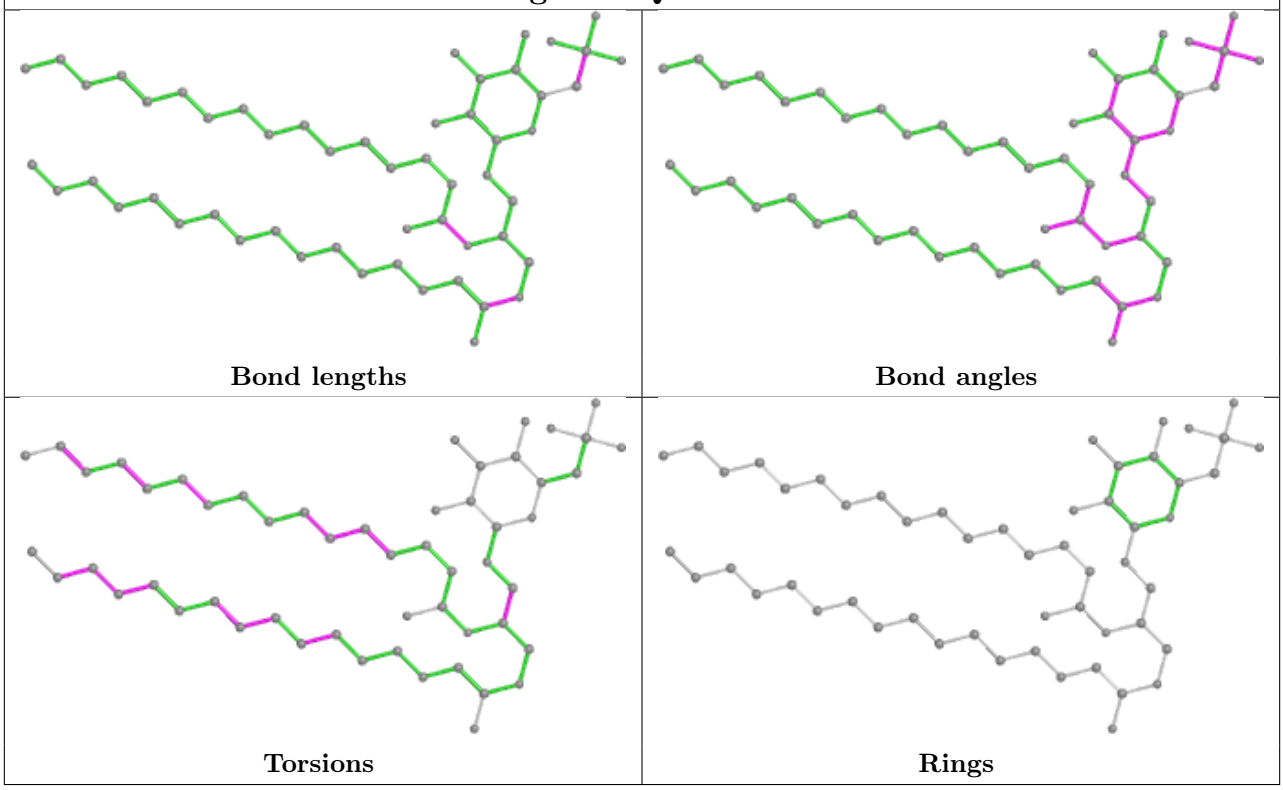

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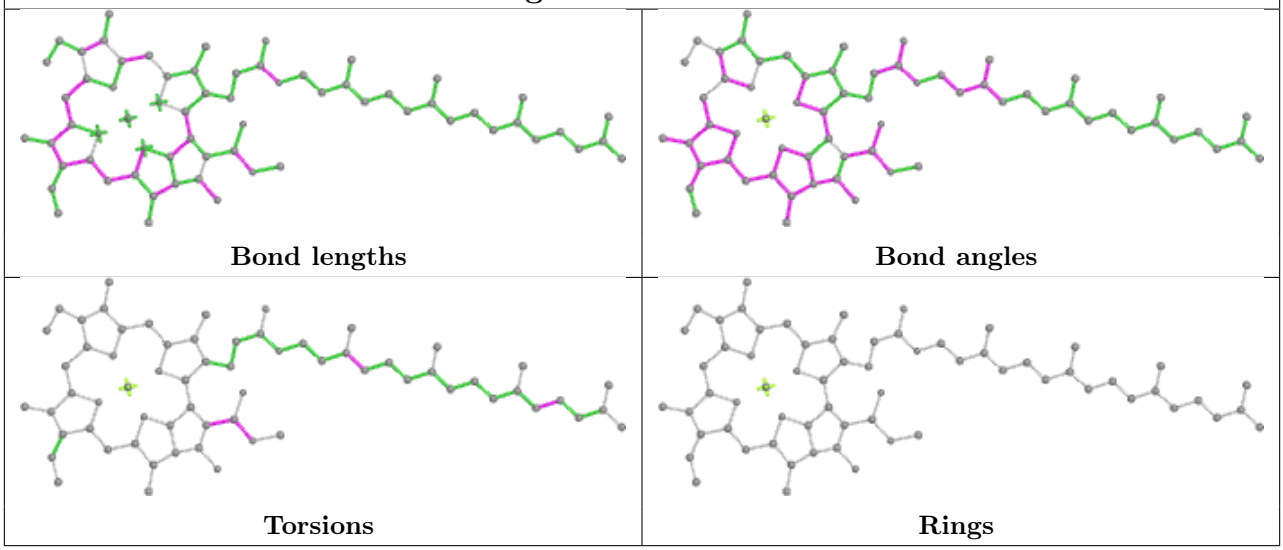

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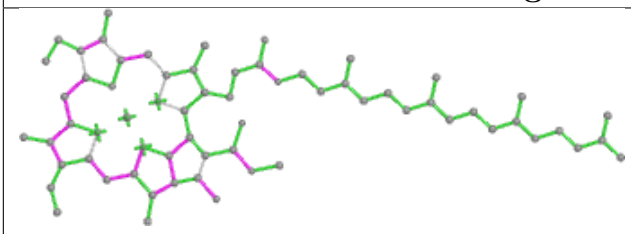
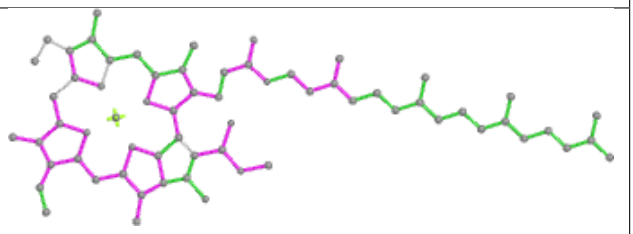
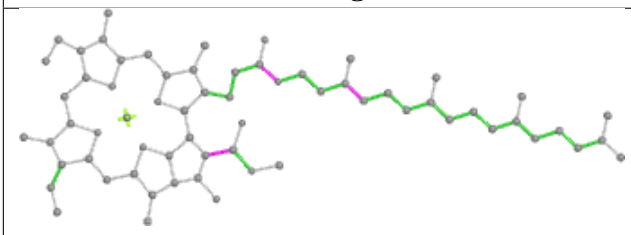


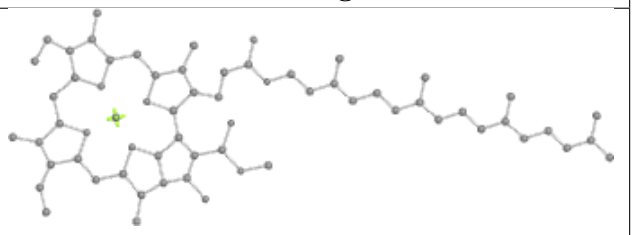
Bond lengths



Bond angles

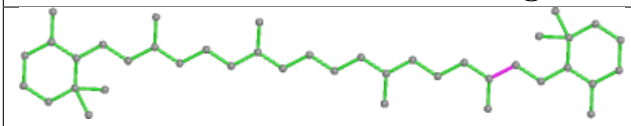


Torsions

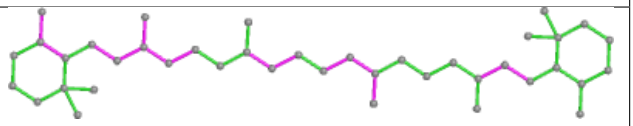


Rings

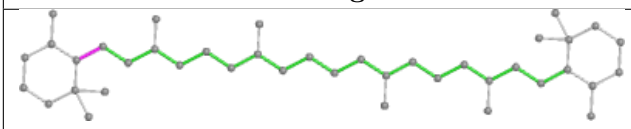
Ligand BCR B 618



Bond lengths



Bond angles



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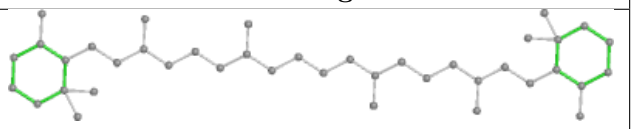
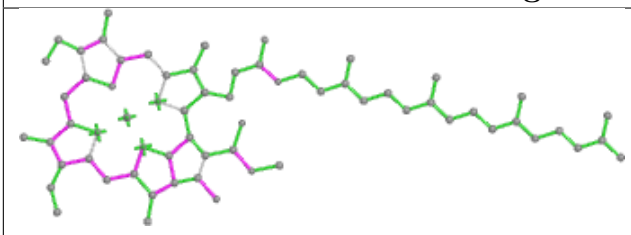


Rings

Ligand CLA D 402



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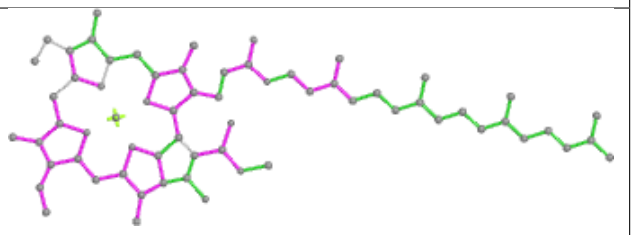
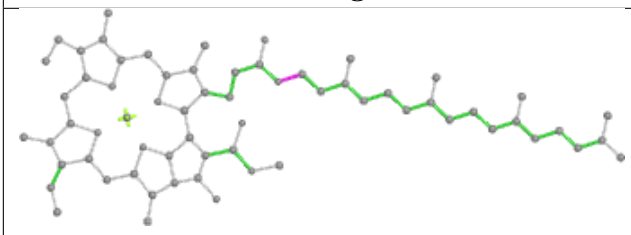


Bond angles



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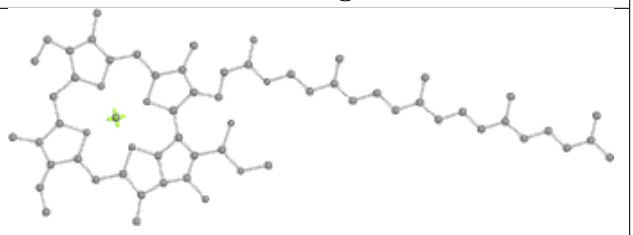
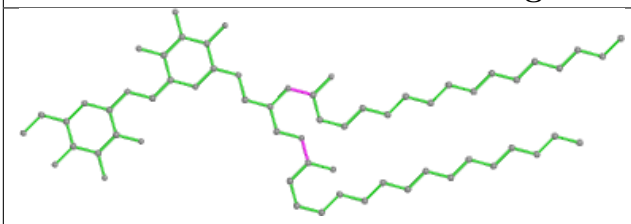


Rings

Ligand DGD c 519



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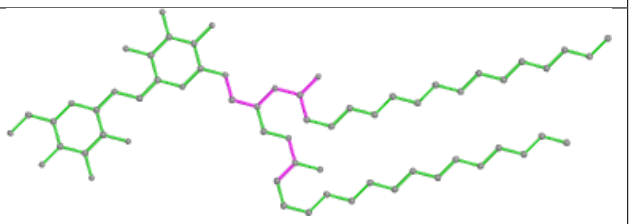

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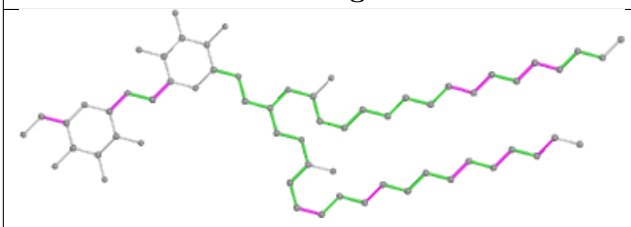

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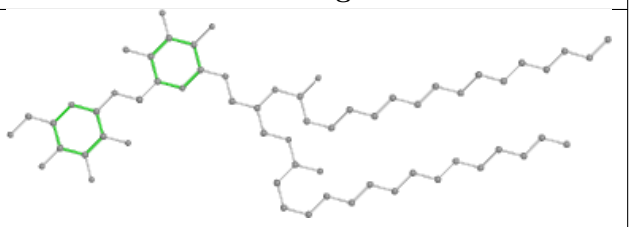
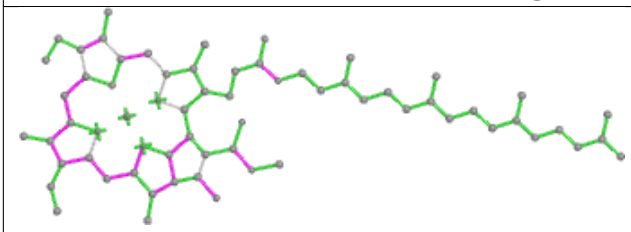


Rings

Ligand CLA a 409



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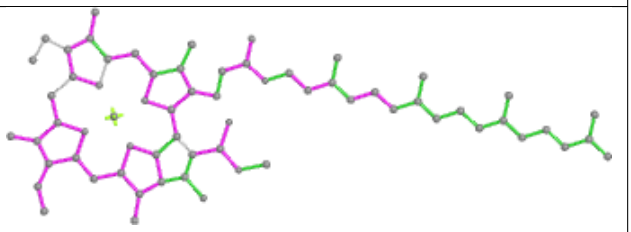
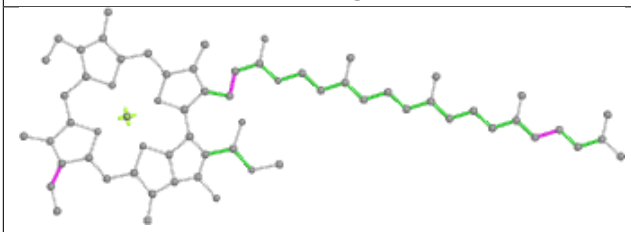


Bond angles



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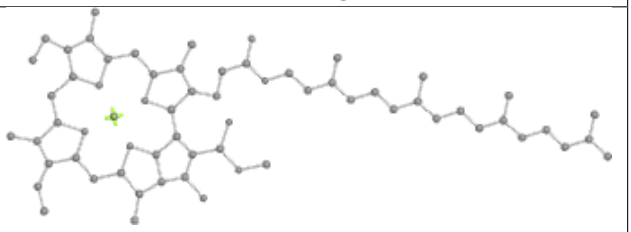
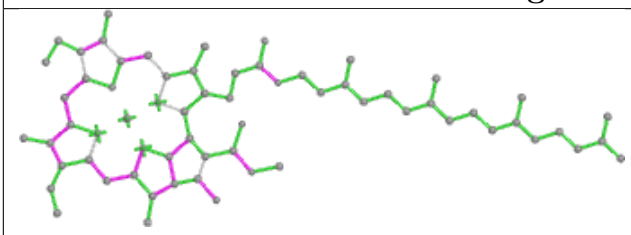


Rings

Ligand CLA b 615



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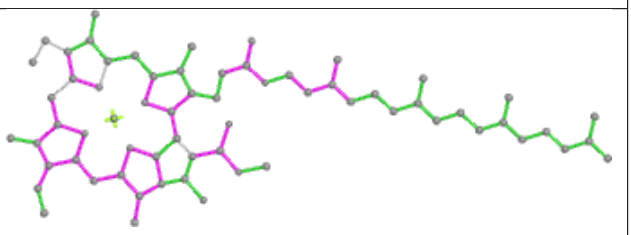
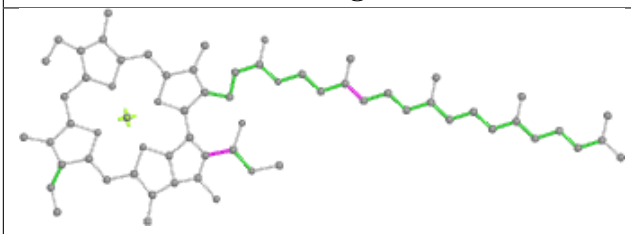
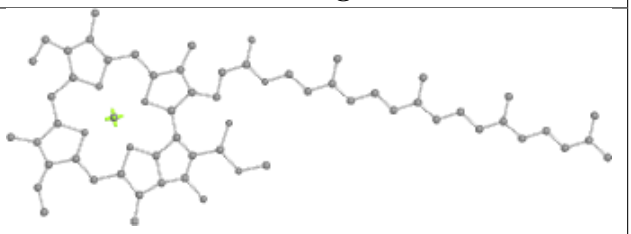


Bond angles

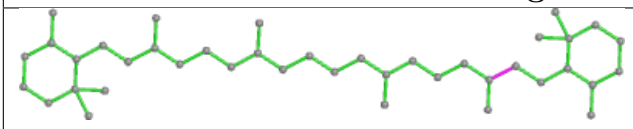


Torsions



Rings

Ligand BCR c 518



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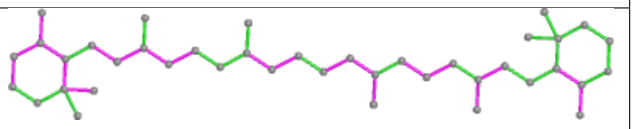
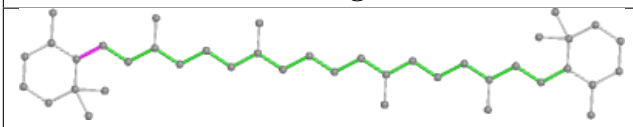


Bond angles



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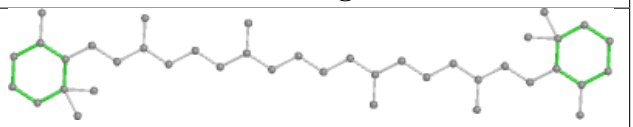
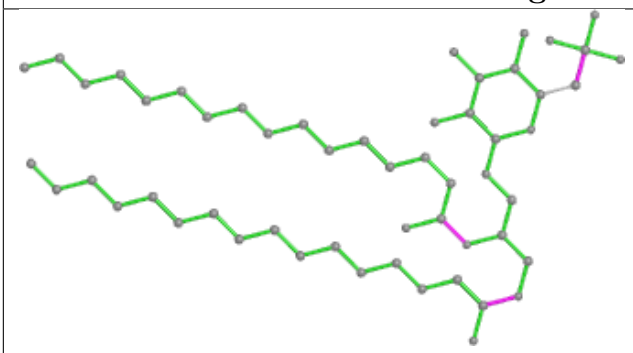


Rings

Ligand SQD a 405



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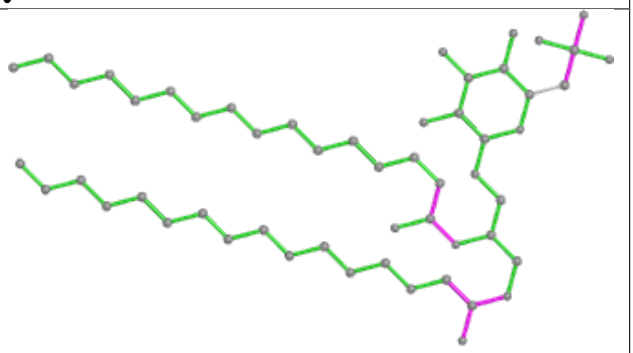
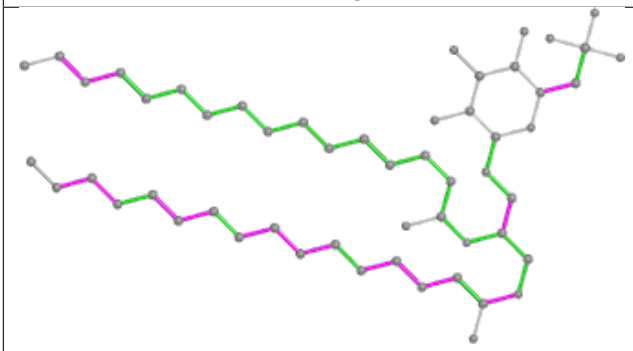
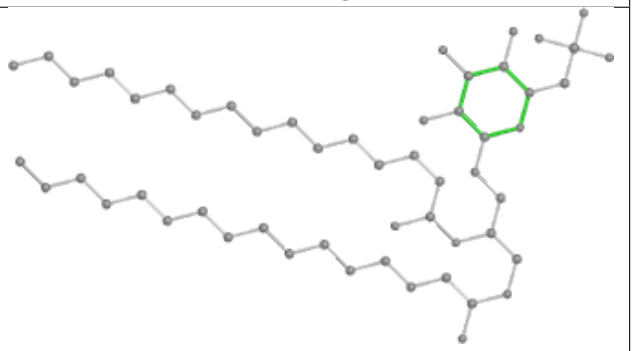


Bond angles

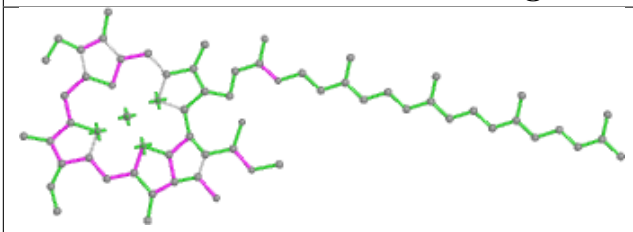


Torsions

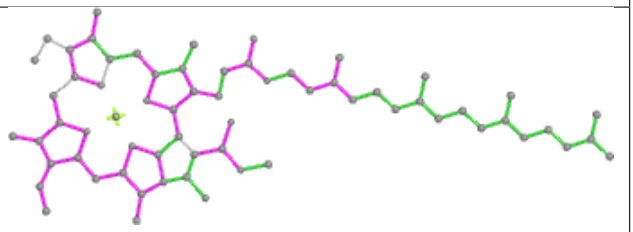


Rings

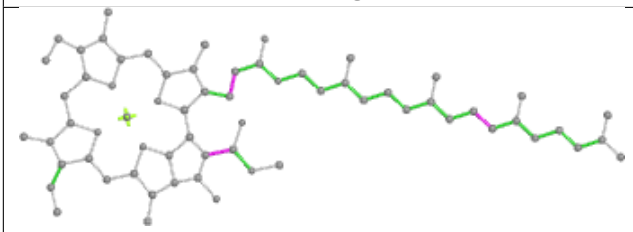
Ligand CLA B 607



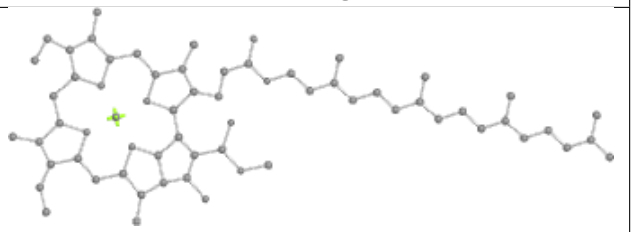
Bond lengths



Bond angles

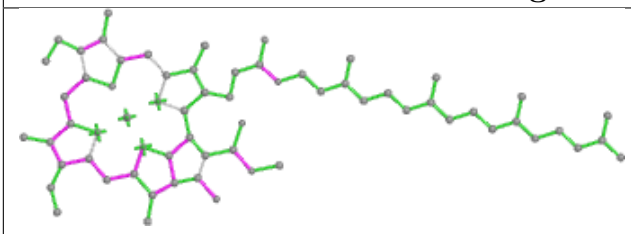


Torsions

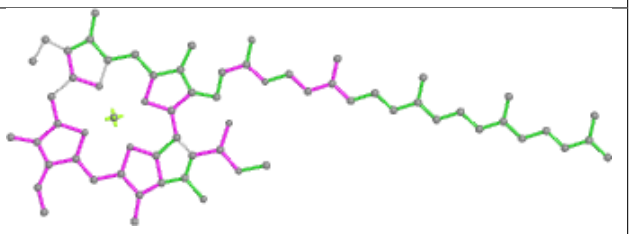


Rings

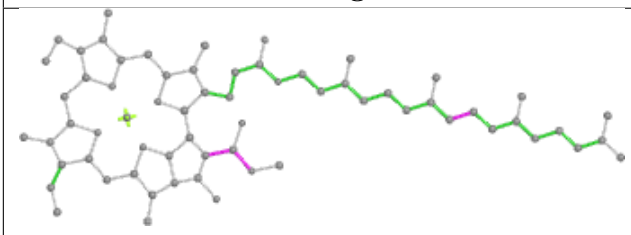
Ligand CLA c 507



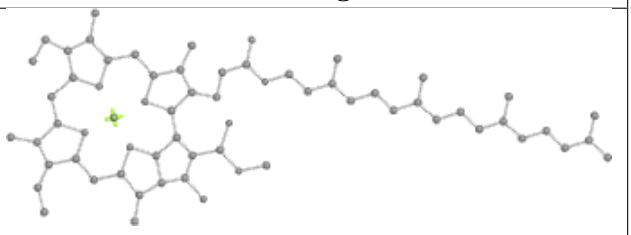
Bond lengths



Bond angles

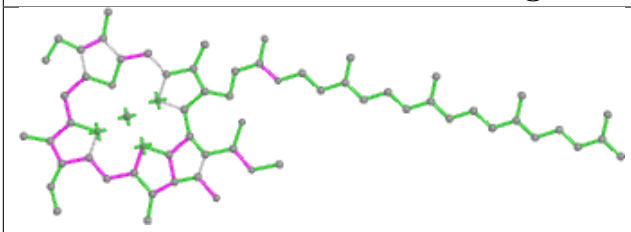


Torsions

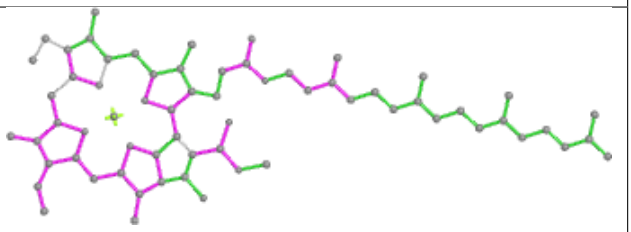


Rings

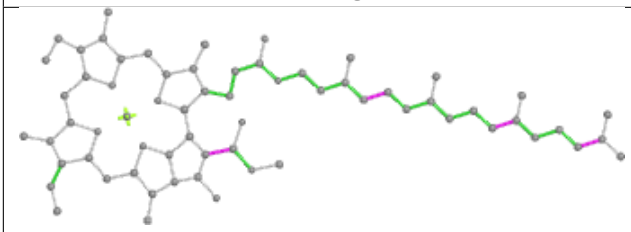
Ligand CLA C 502



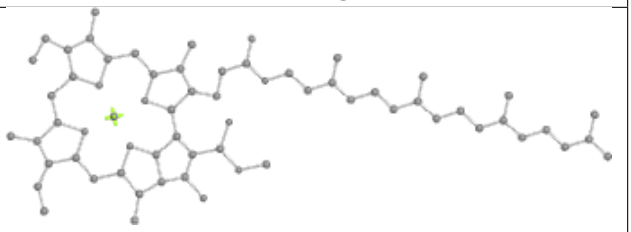
Bond lengths



Bond angles

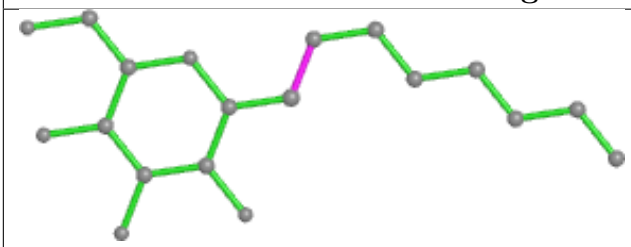


Torsions

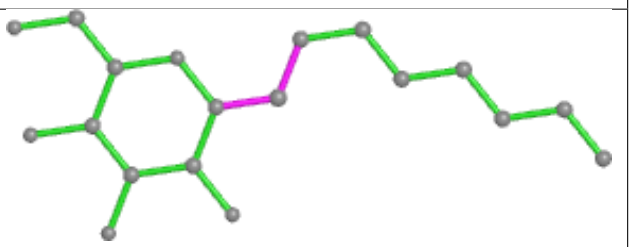


Rings

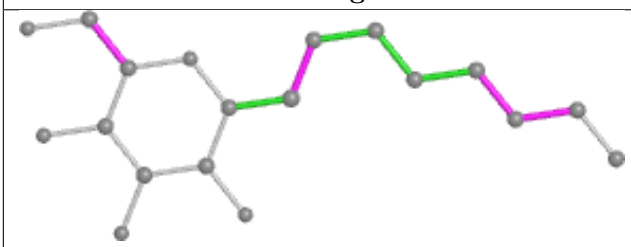
Ligand HTG B 623



Bond lengths



Bond angles



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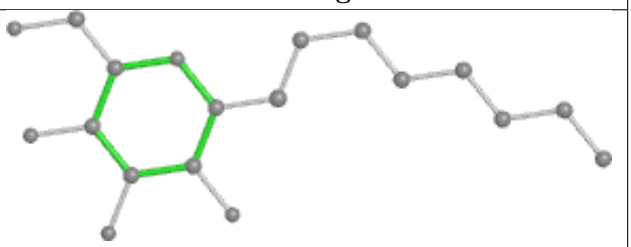
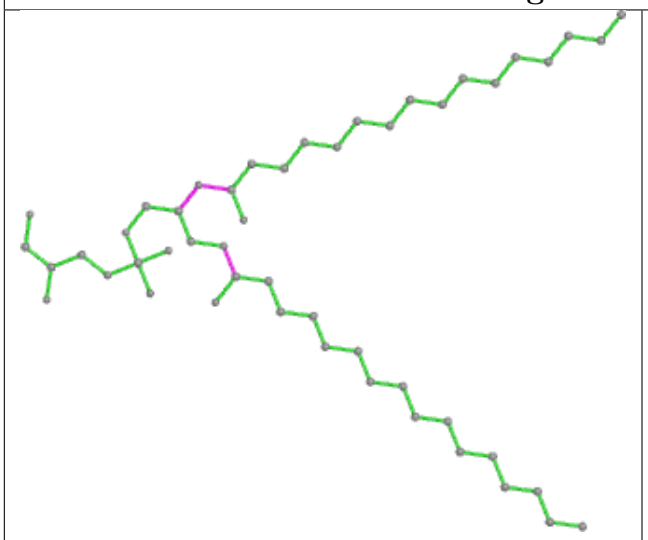
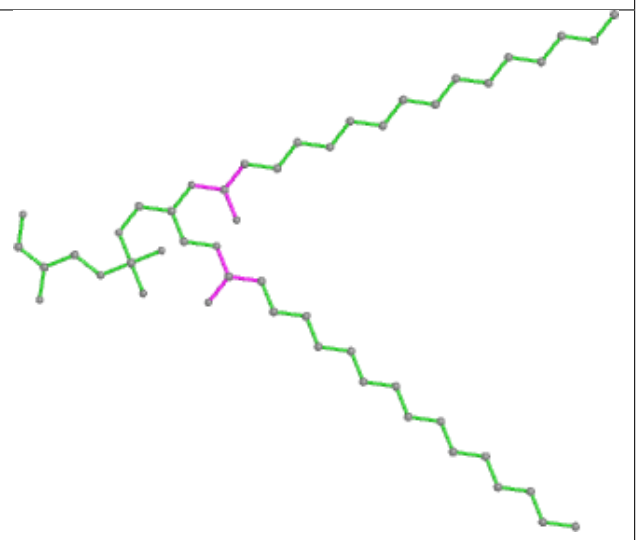


Rings

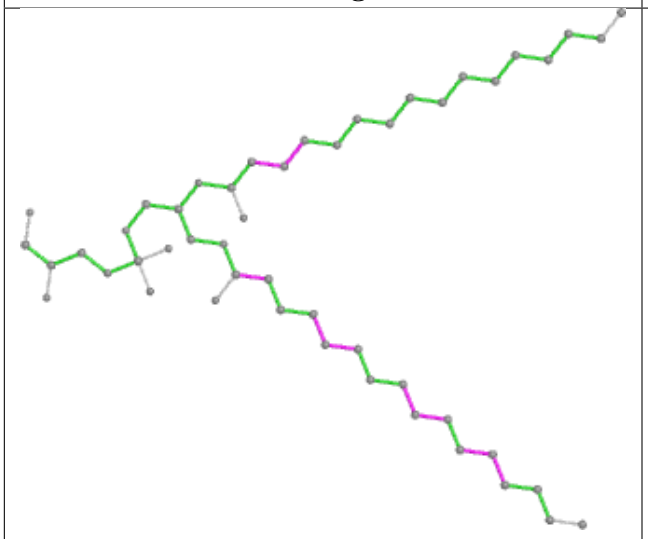
Ligand LHG d 406



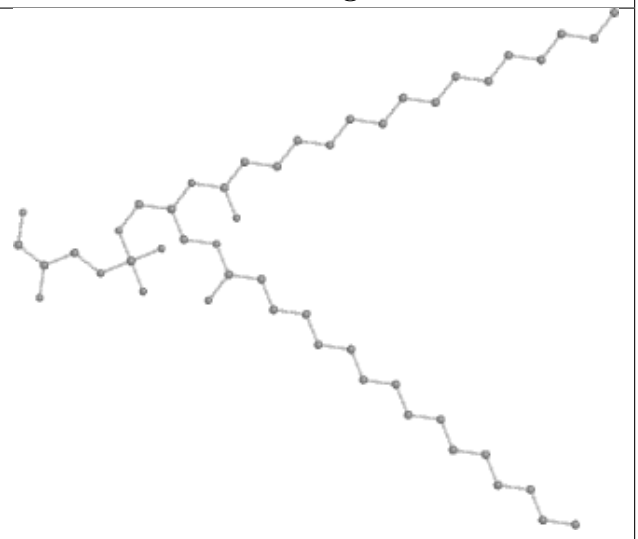
Bond lengths



Bond angles

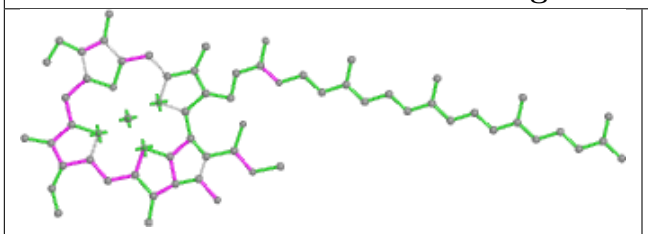


Torsions

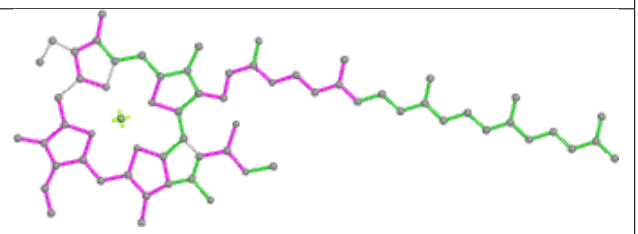


Rings

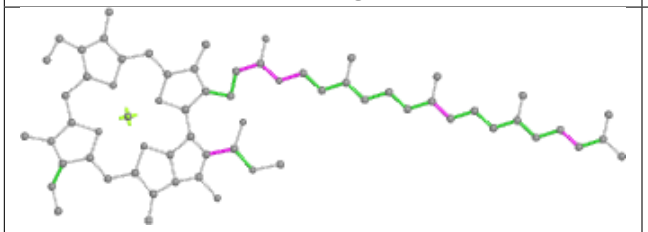
Ligand CLA c 516



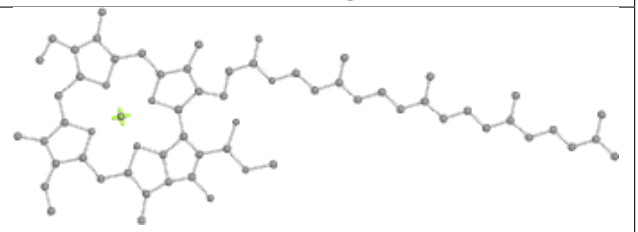
Bond lengths



Bond angles

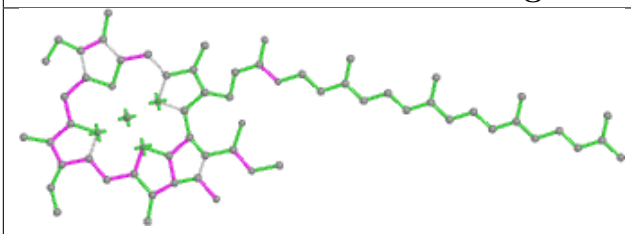


Torsions



Rings

Ligand CLA B 617



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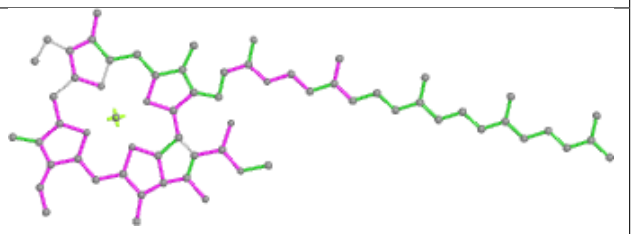
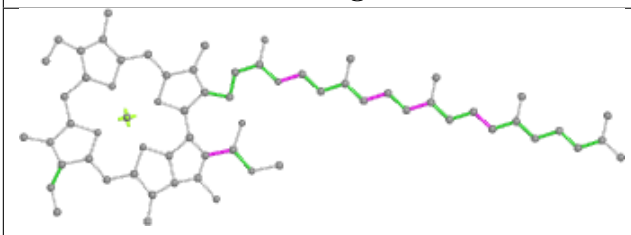


Bond angles



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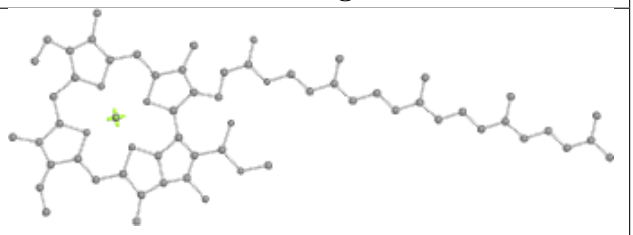
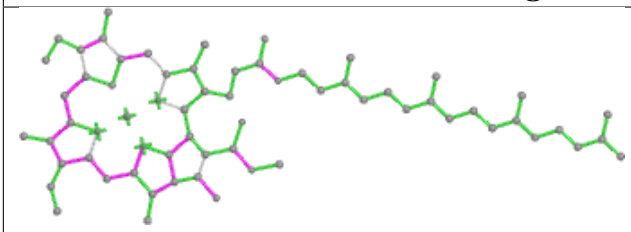


Rings

Ligand CLA C 506



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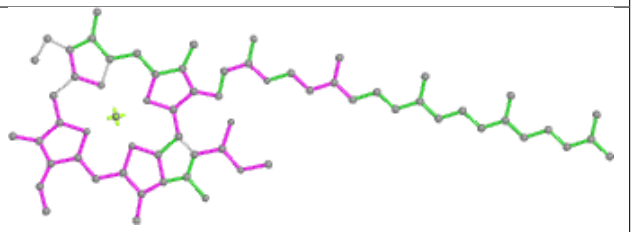
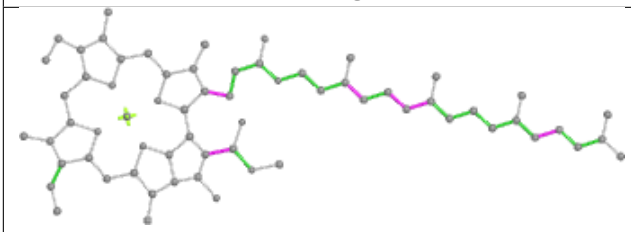
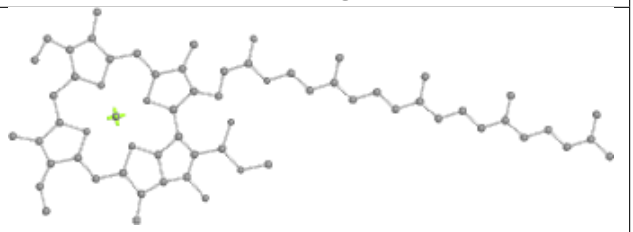


Bond angles

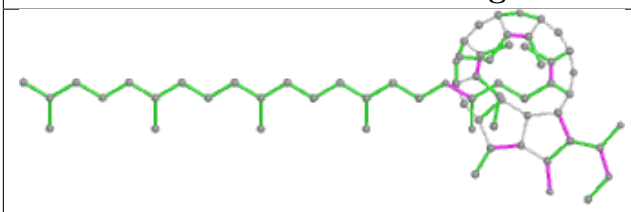


Torsions

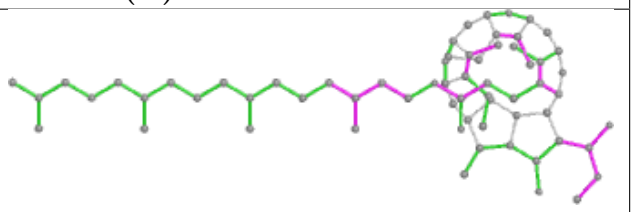


Rings

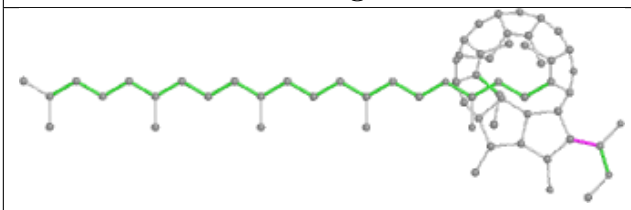
Ligand PHO A 409 (B)



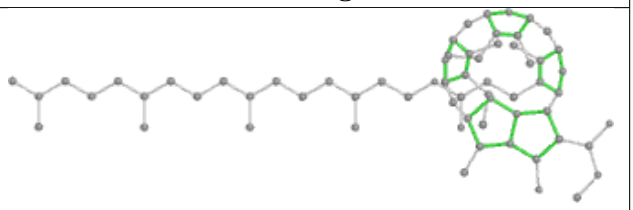
Bond lengths



Bond angles

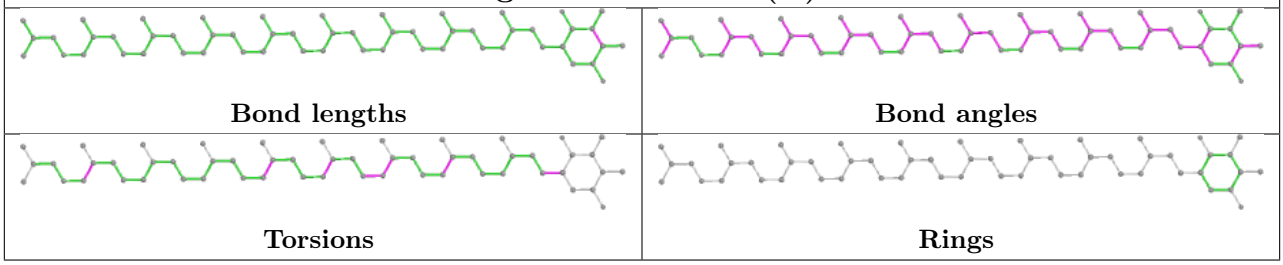


Torsions

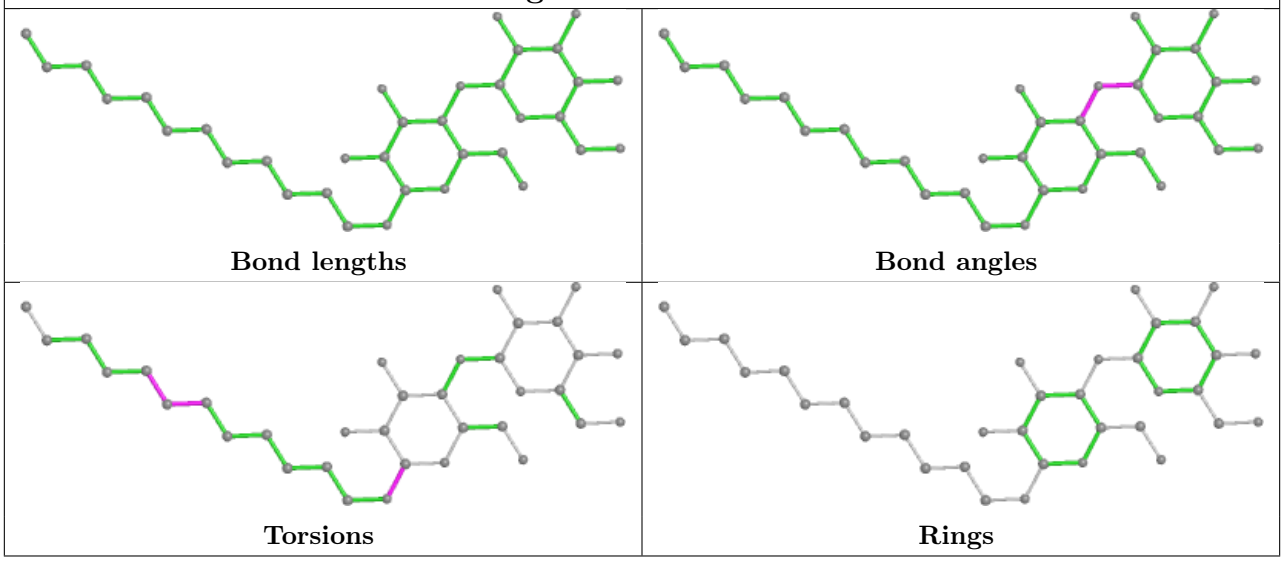


Rings

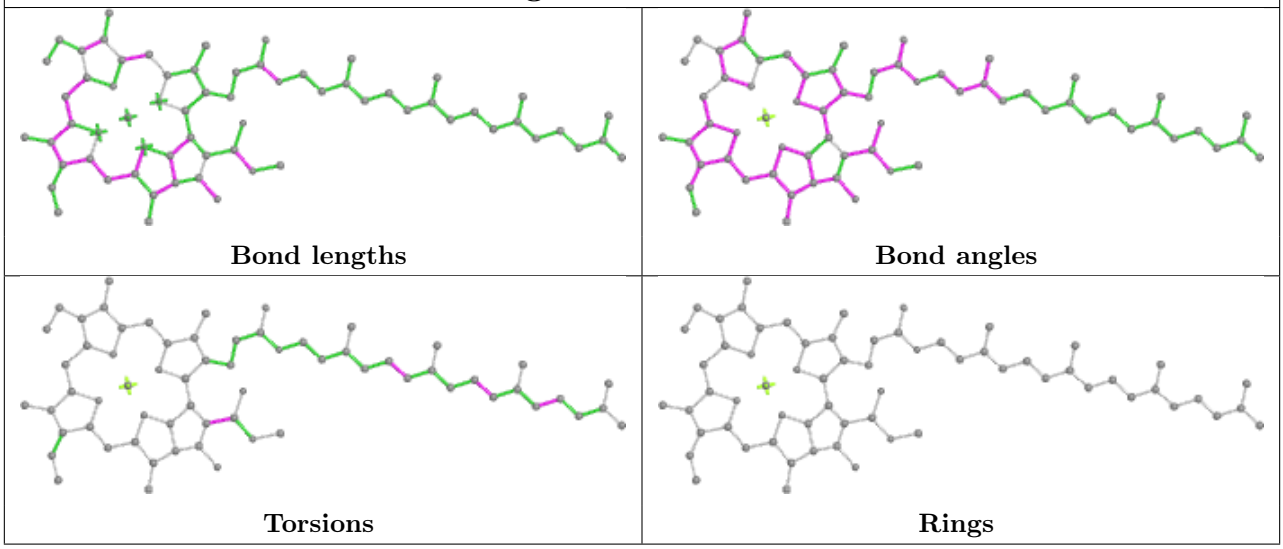
Ligand PL9 A 420 (A)



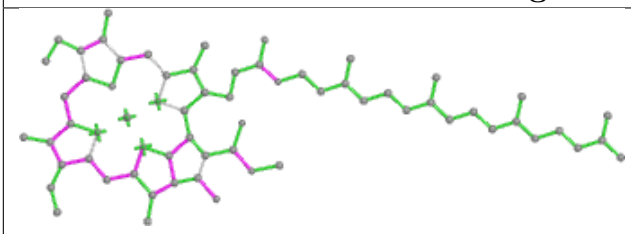
Ligand LMT a 421



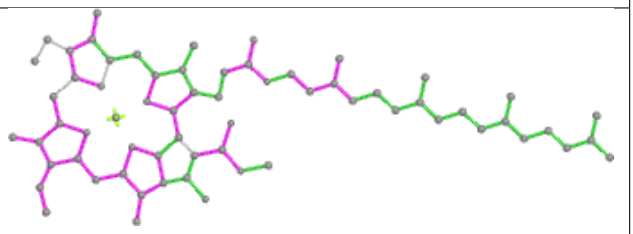
Ligand CLA C 508



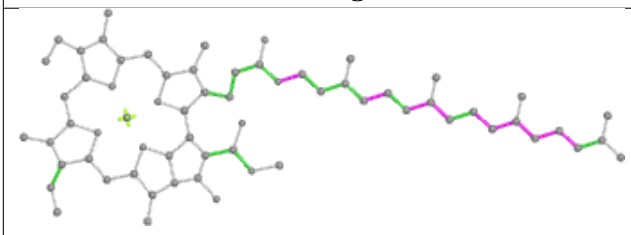
Ligand CLA c 513



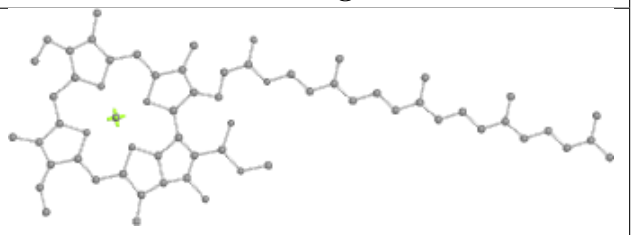
Bond lengths



Bond angles

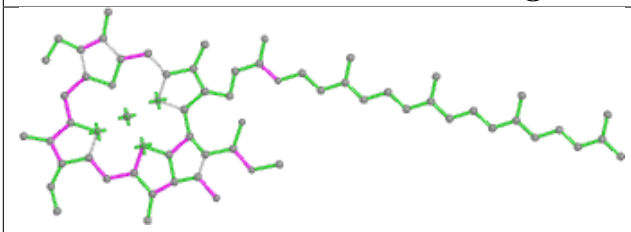


Torsions

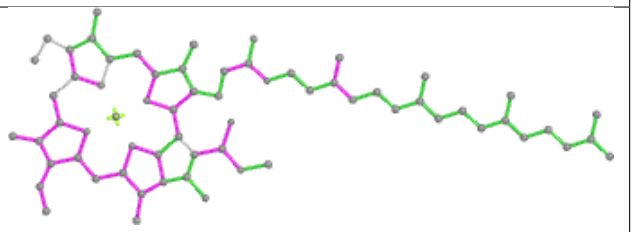


Rings

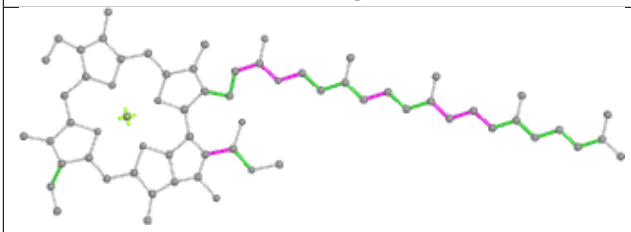
Ligand CLA B 602



Bond lengths



Bond angles



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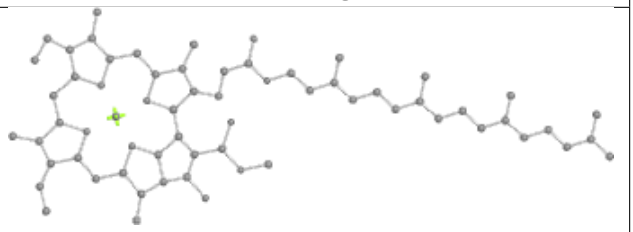
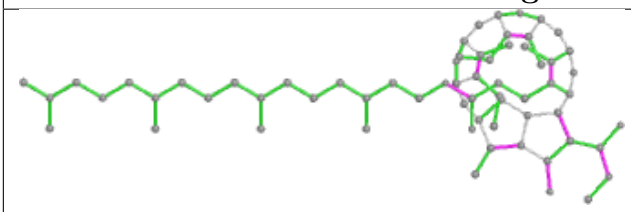
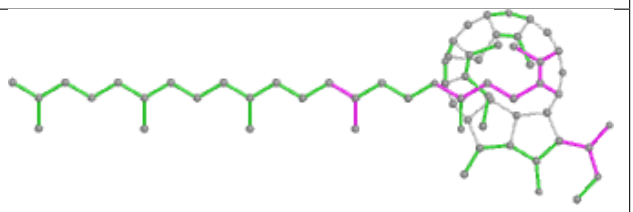


Rings

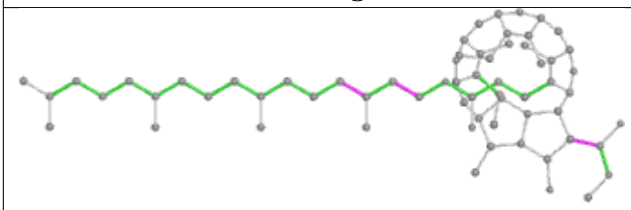
Ligand PHO A 408



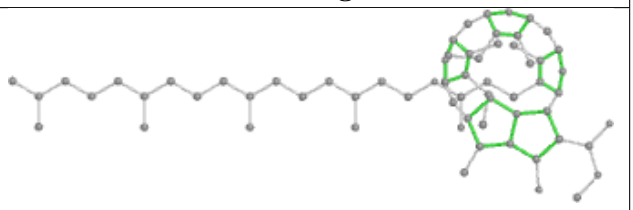
Bond lengths



Bond angles

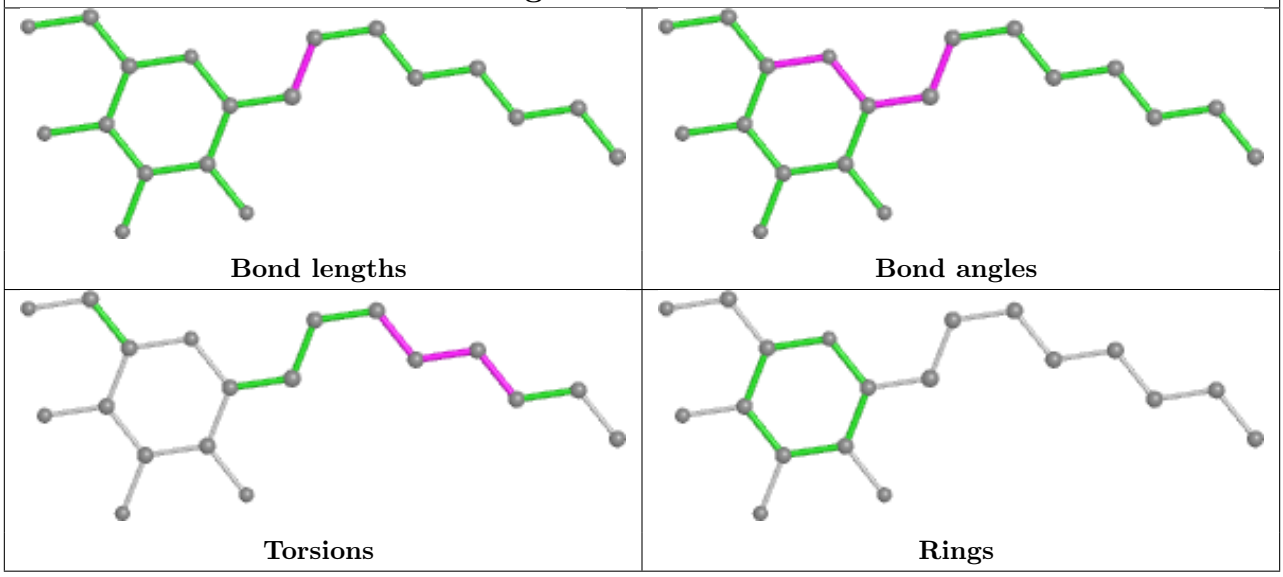


Torsions

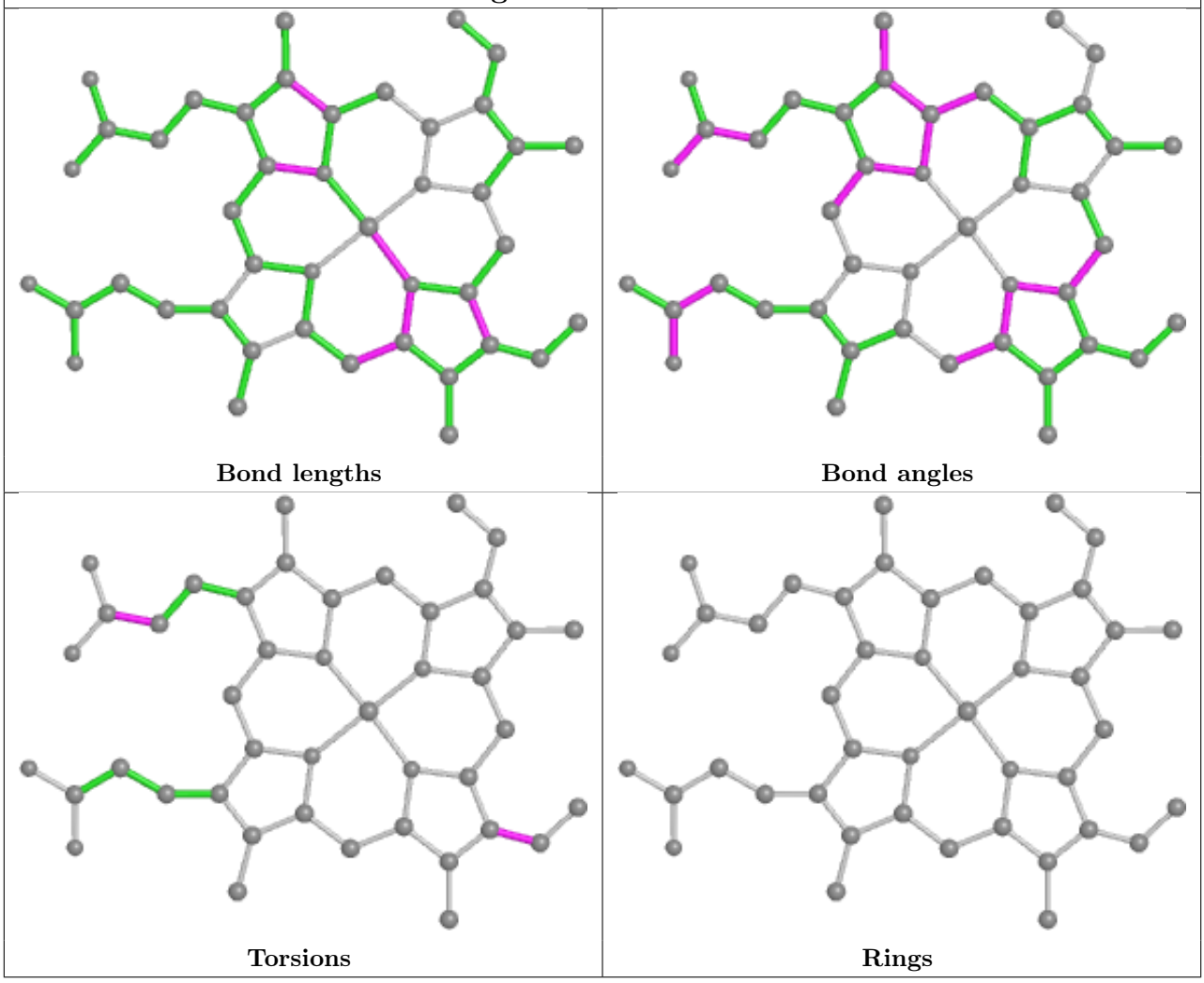


Rings

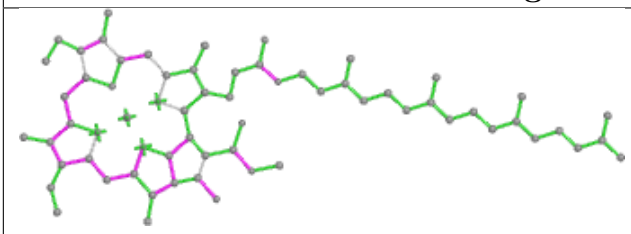
Ligand HTG b 602



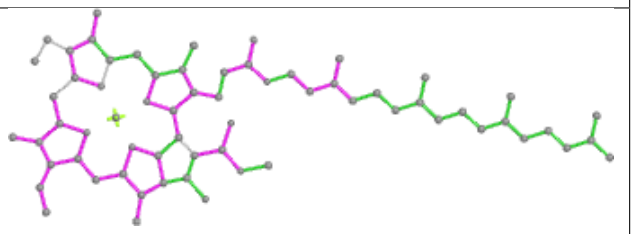
Ligand HEM v 205



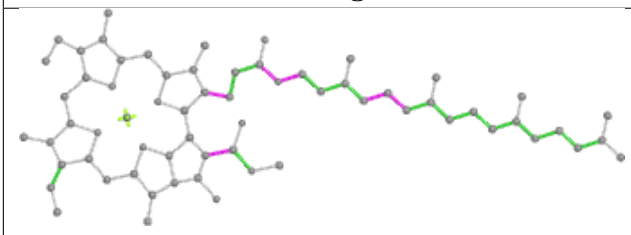
Ligand CLA C 513



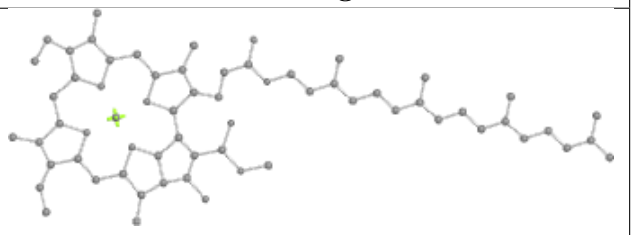
Bond lengths



Bond angles

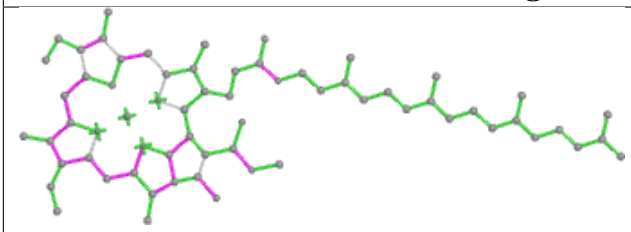


Torsions



Rings

Ligand CLA C 503



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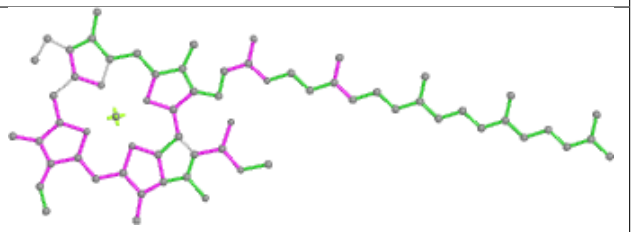

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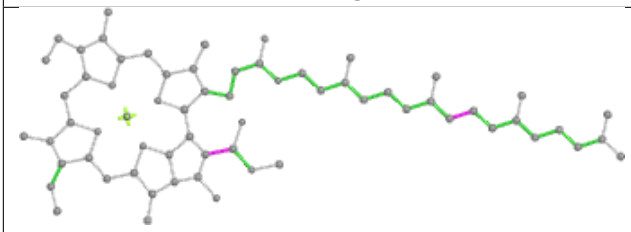

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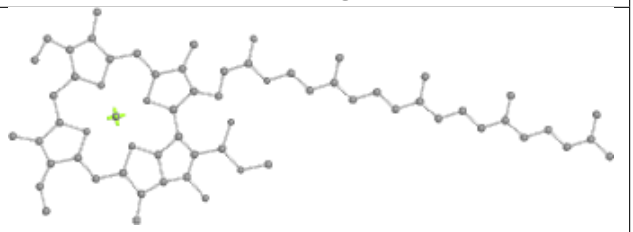
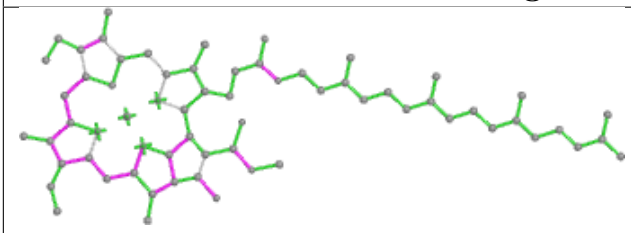


Rings

Ligand CLA A 405



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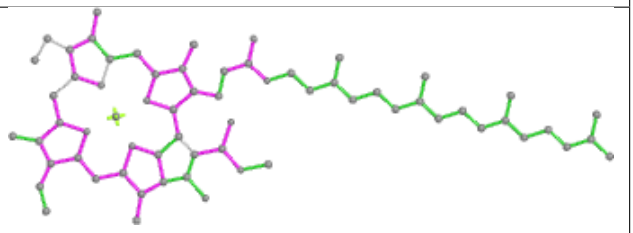
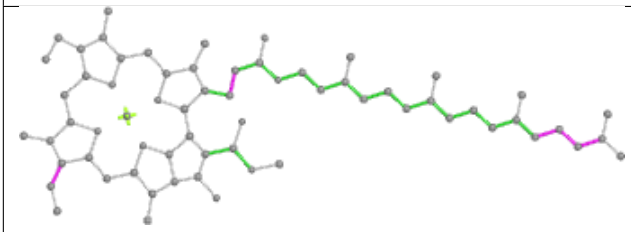


Bond angles



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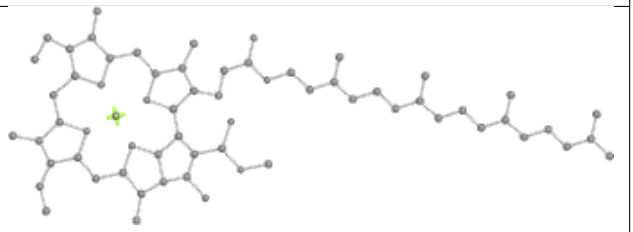
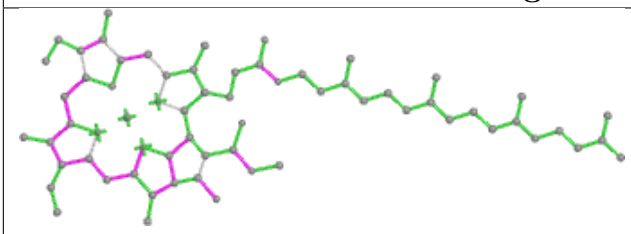


Rings

Ligand CLA A 410



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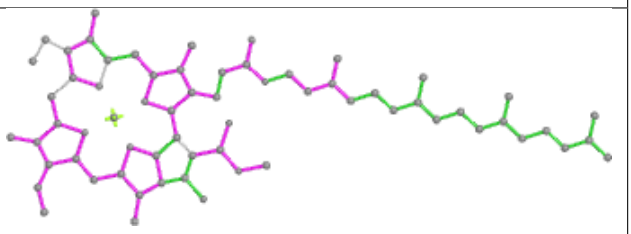
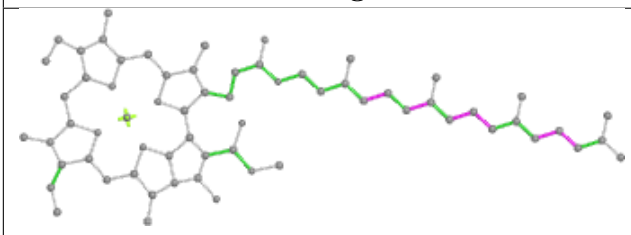
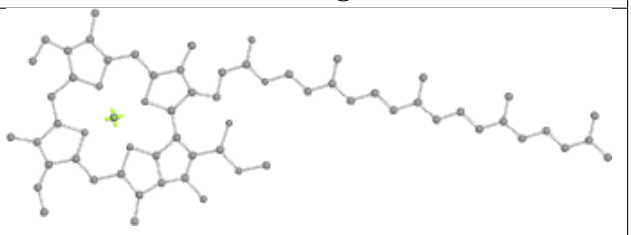


Bond angles

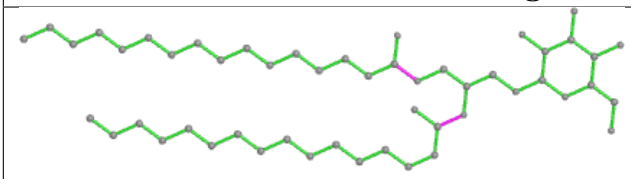


Torsions



Rings

Ligand LMG a 415



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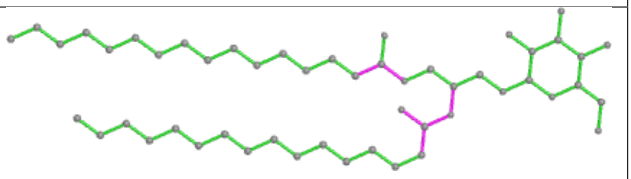
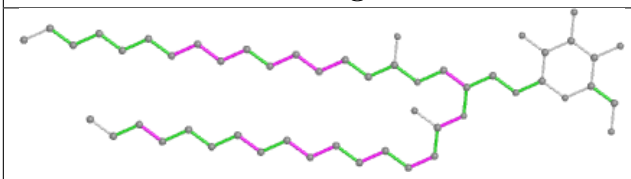


Bond angles



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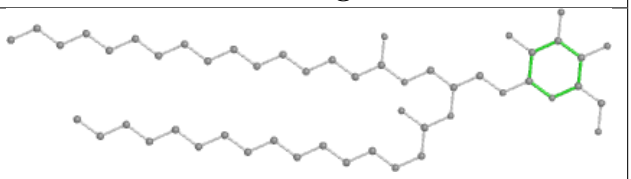
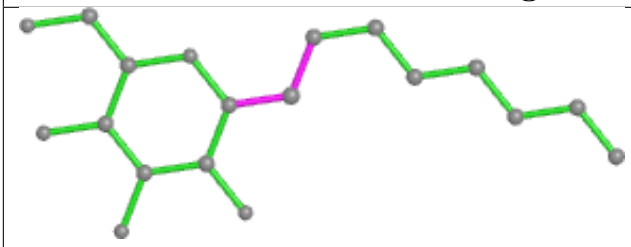


Rings

Ligand HTG V 207



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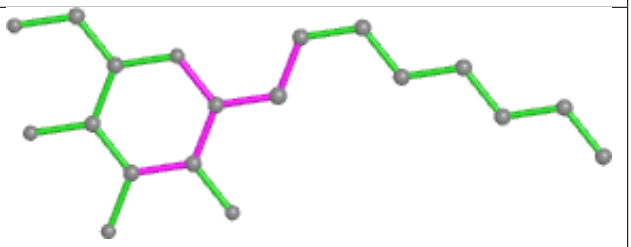
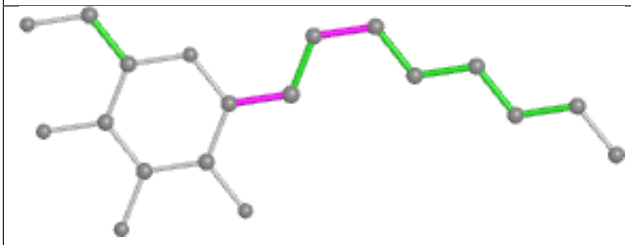


Bond angles



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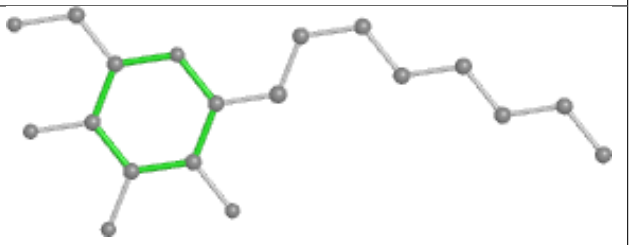
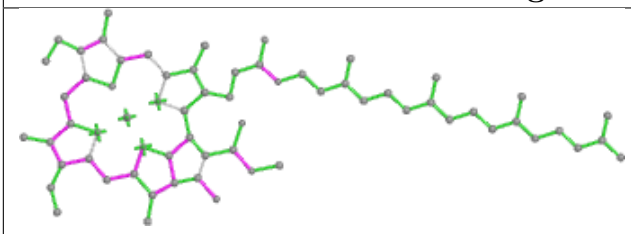


Rings

Ligand CLA b 613



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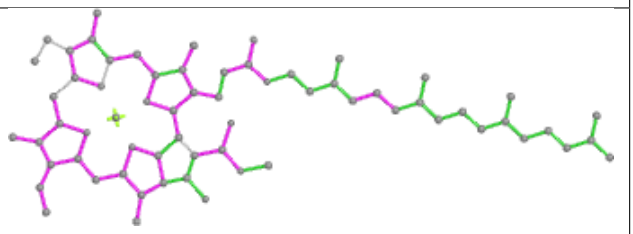
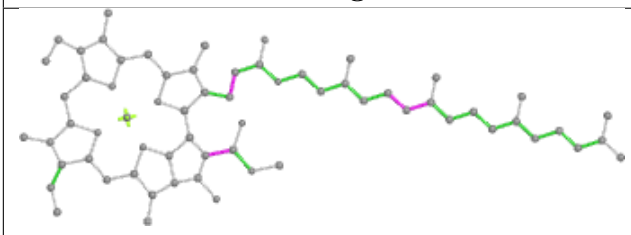


Bond angles



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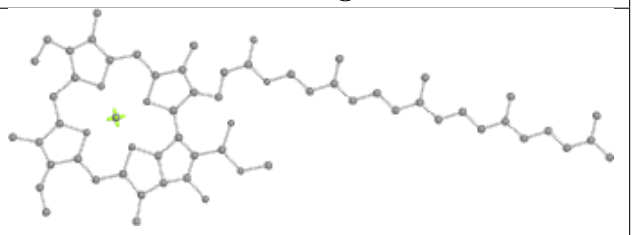

Rings

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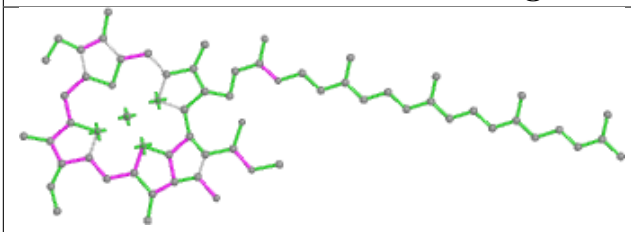

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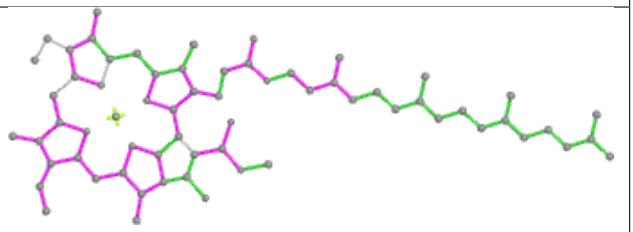
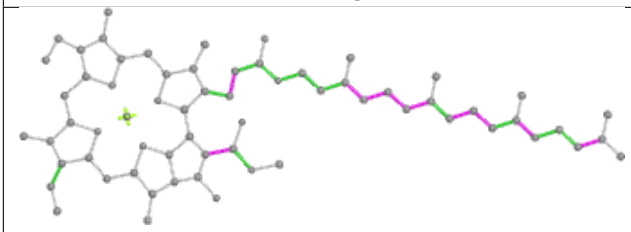


Bond angles



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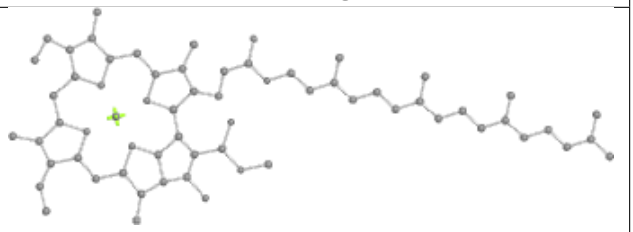
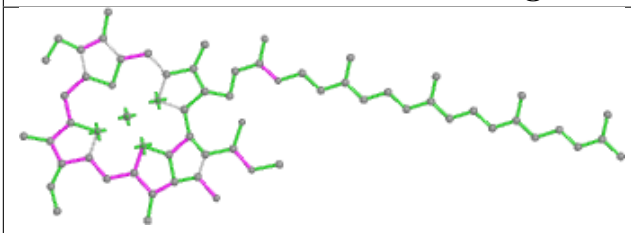


Rings

Ligand CLA B 608



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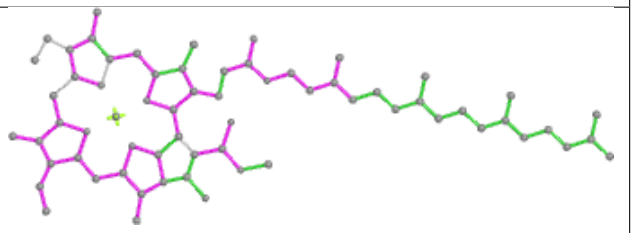
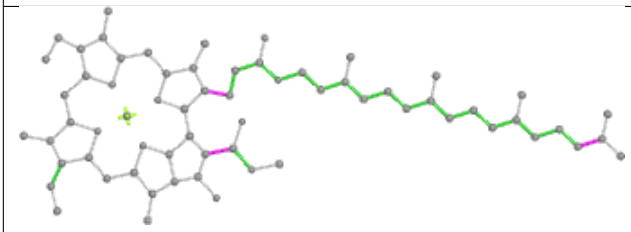


Bond angles



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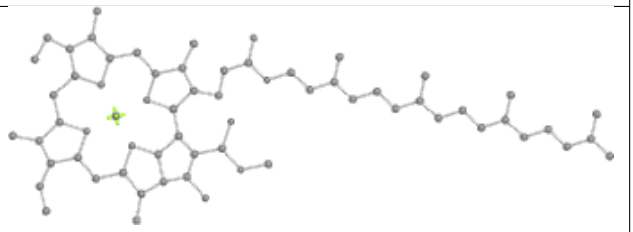
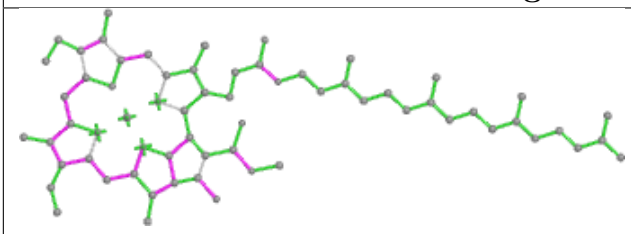


Rings

Ligand CLA A 407



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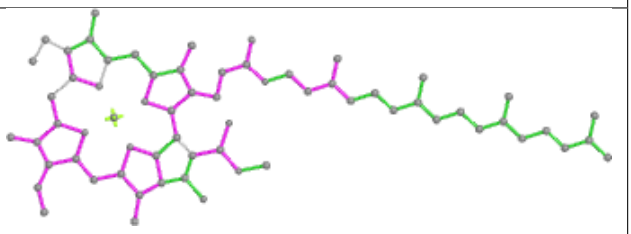
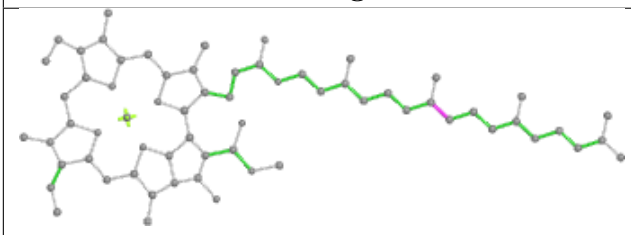


Bond angles



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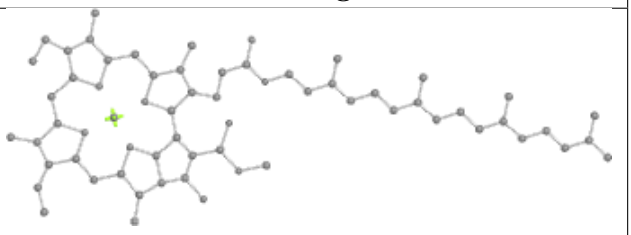
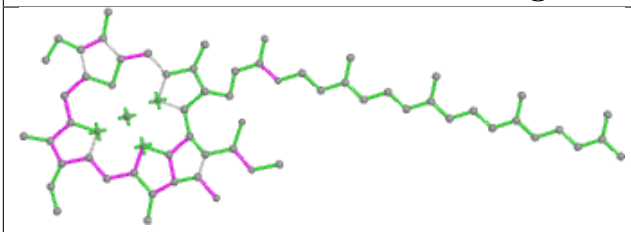


Rings

Ligand CLA c 512



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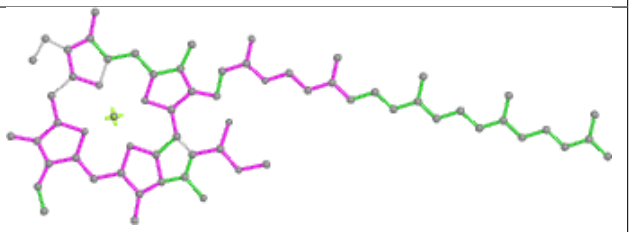
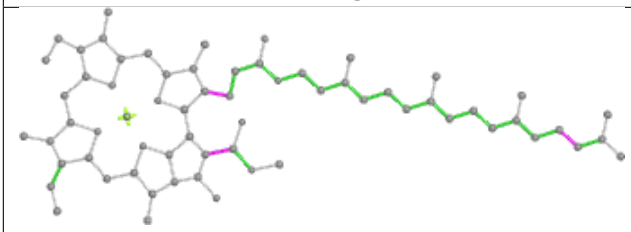


Bond angles



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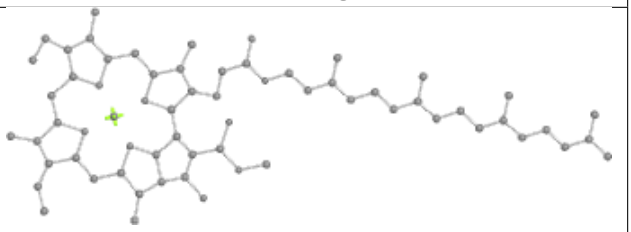
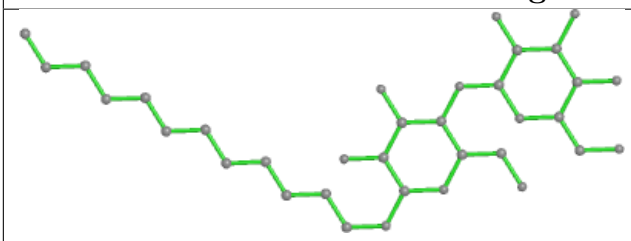


Rings

Ligand LMT f 103



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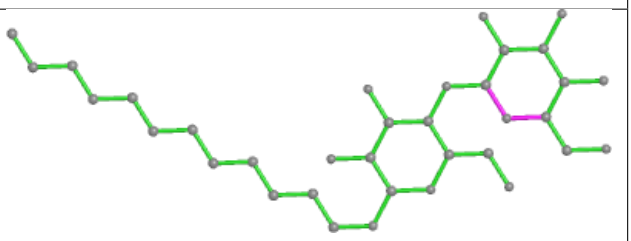
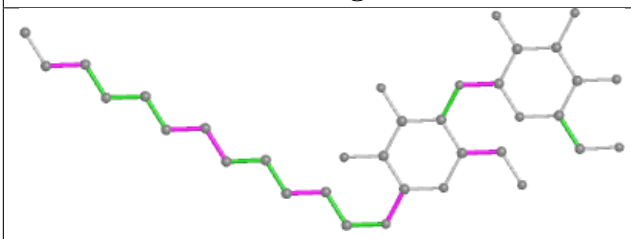


Bond angles



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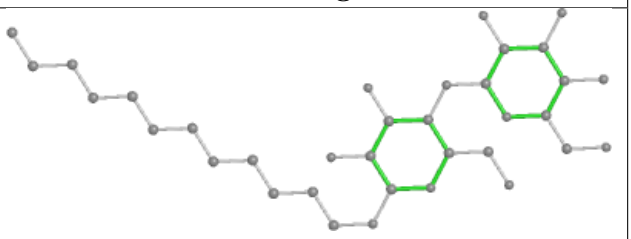
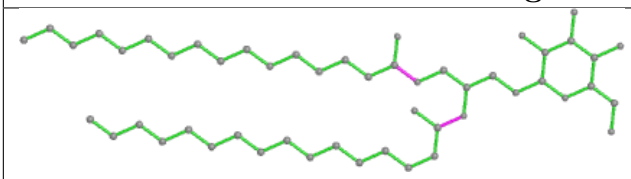


Rings

Ligand LMG c 522



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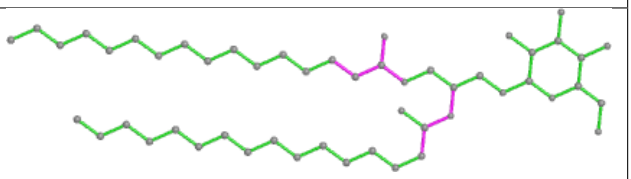
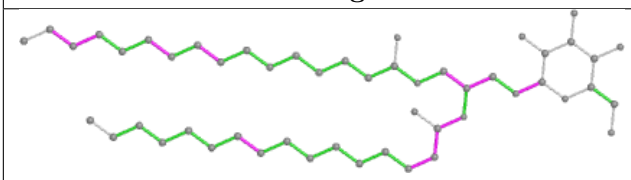


Bond angles



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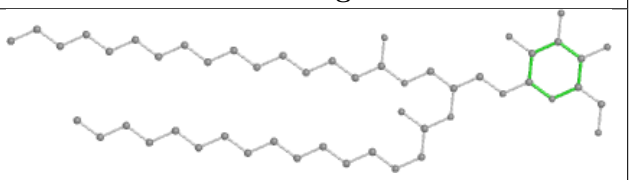
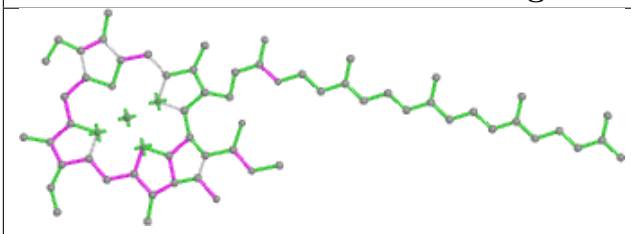


Rings

Ligand CLA b 612



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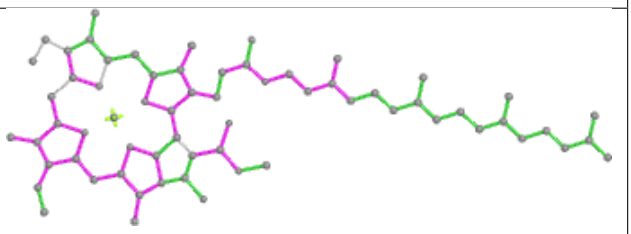
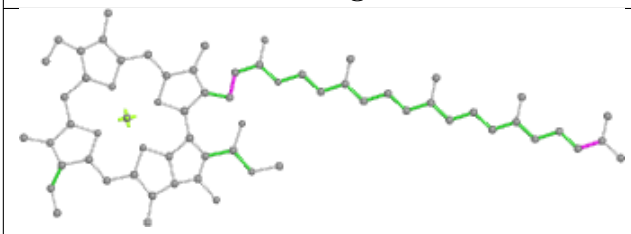
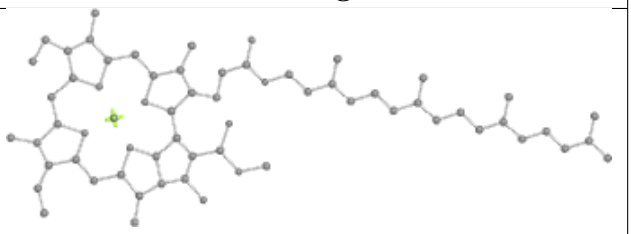


Bond angles

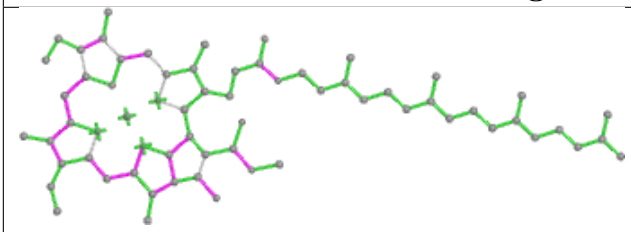


Torsions

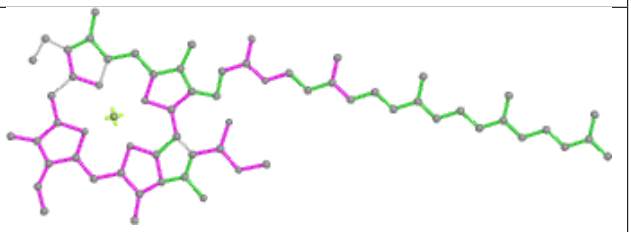


Rings

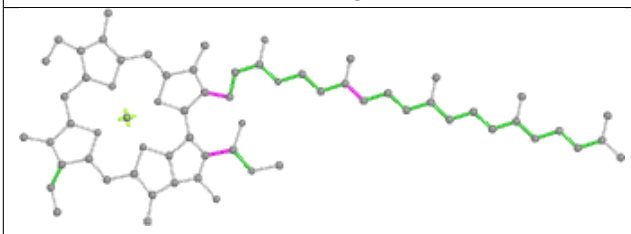
Ligand CLA b 619



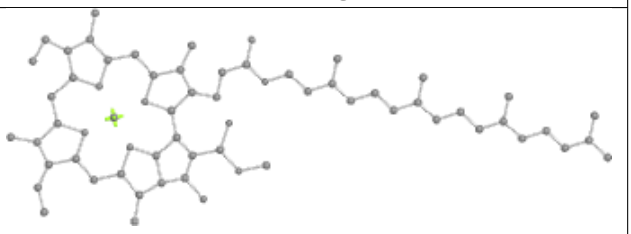
Bond lengths



Bond angles

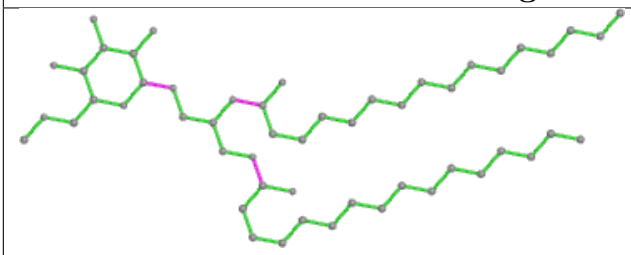


Torsions

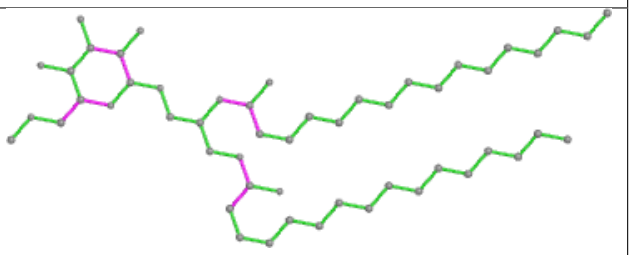


Rings

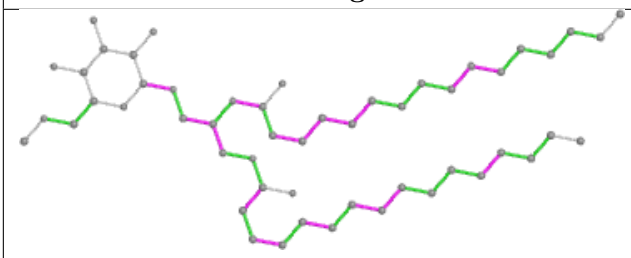
Ligand DGD D 406



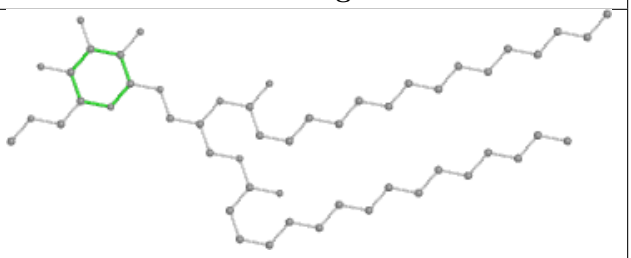
Bond lengths



Bond angles

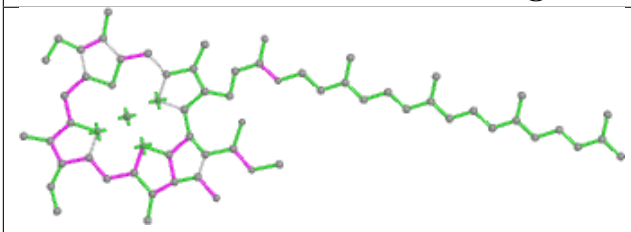


Torsions

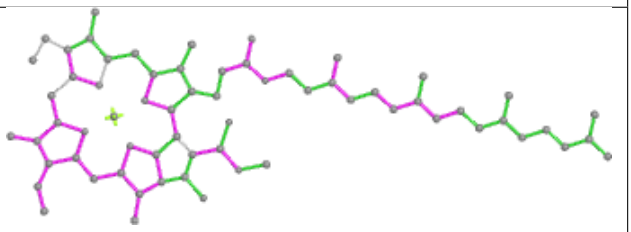


Rings

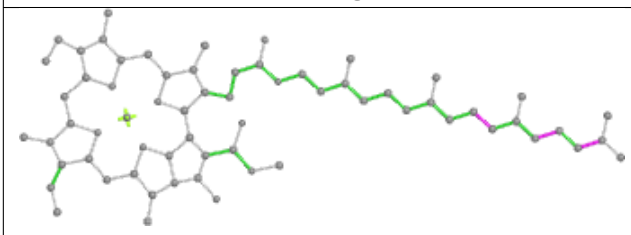
Ligand CLA b 625



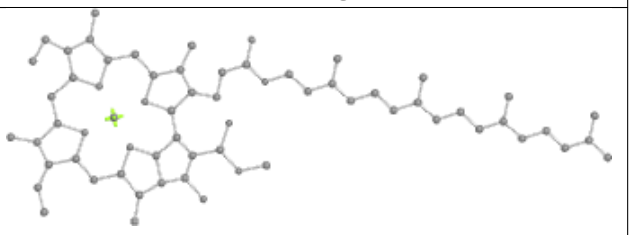
Bond lengths



Bond angles

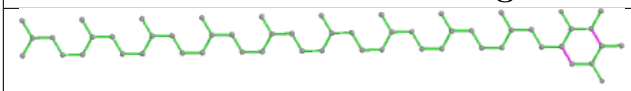


Torsions

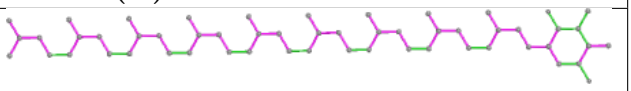


Rings

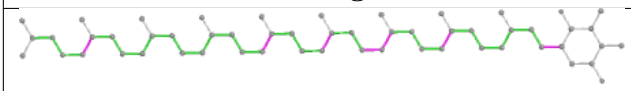
Ligand PL9 A 420 (B)



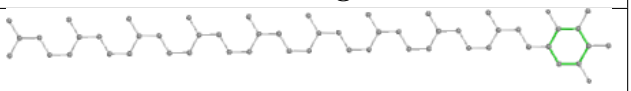
Bond lengths



Bond angles

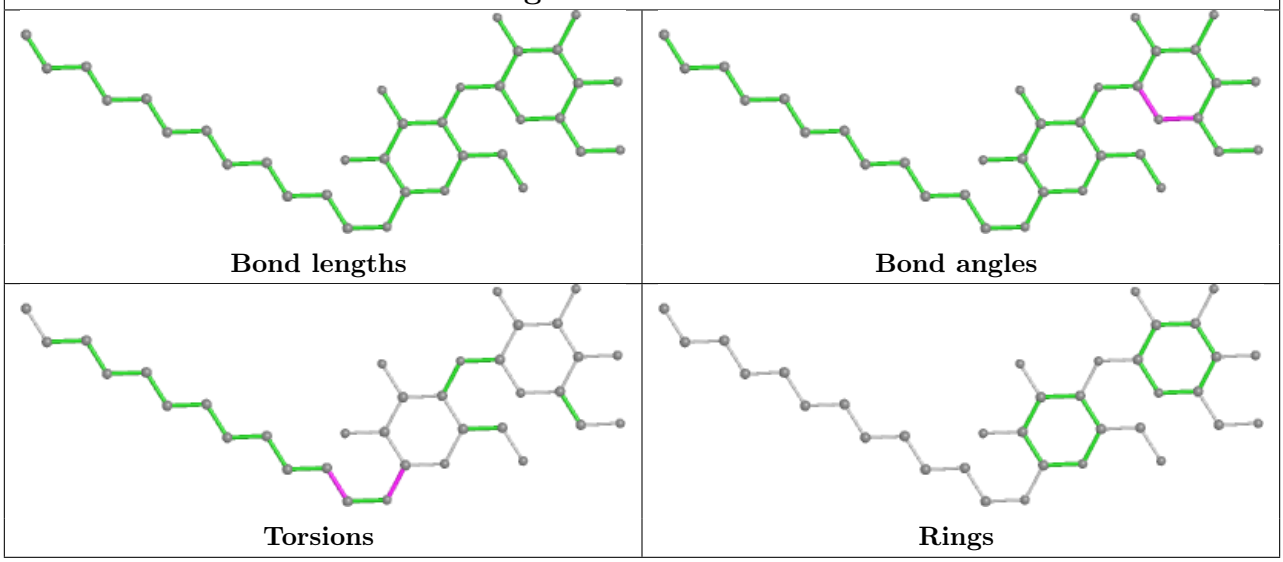


Torsions

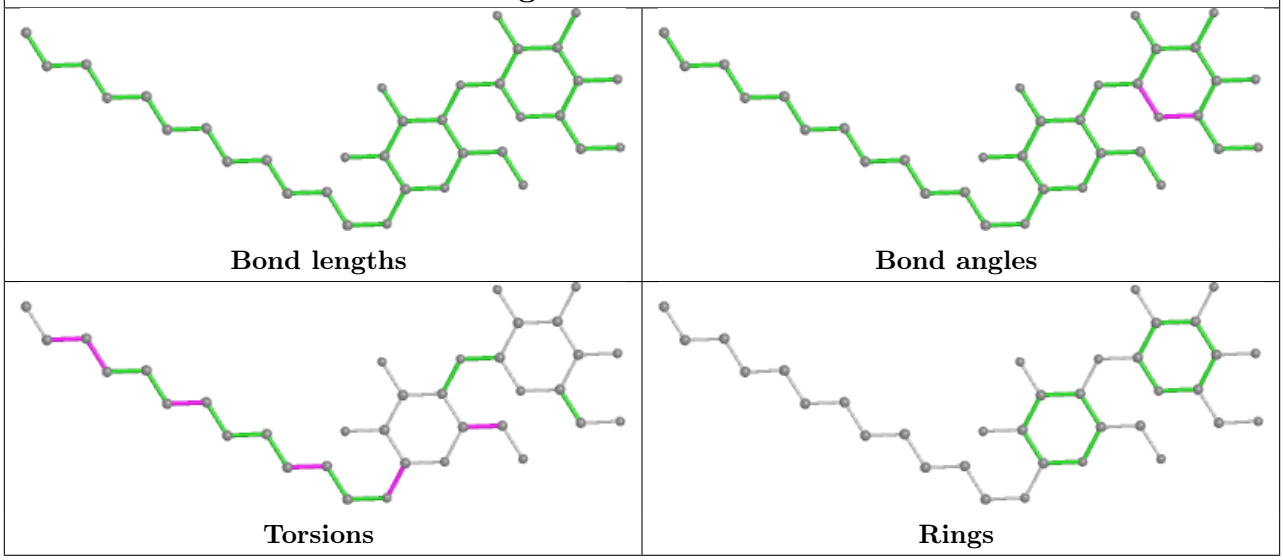


Rings

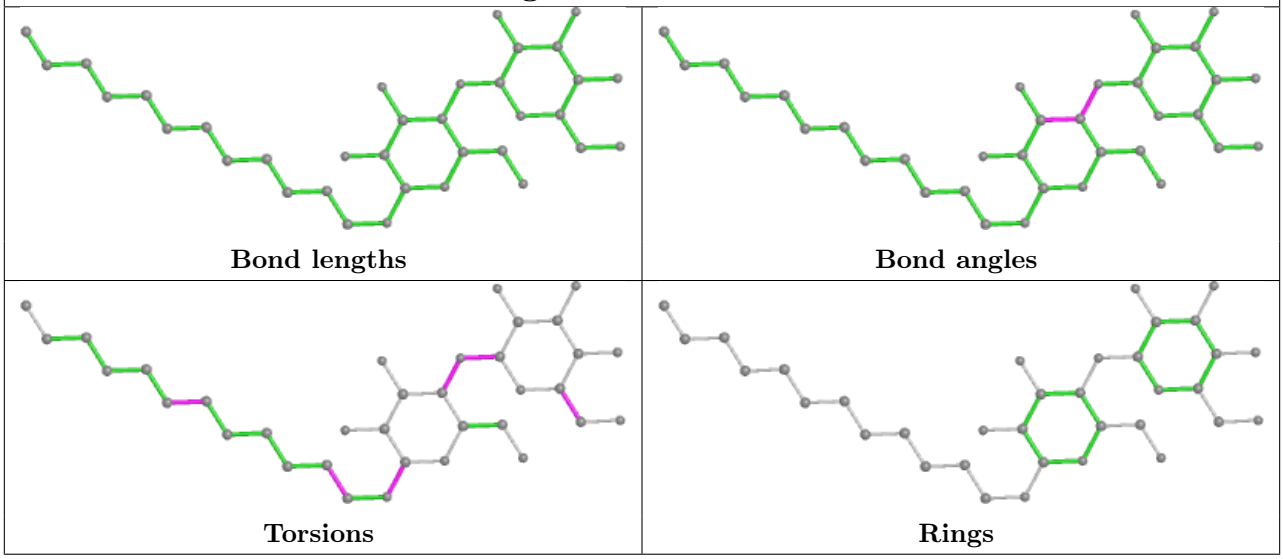
Ligand LMT F 101



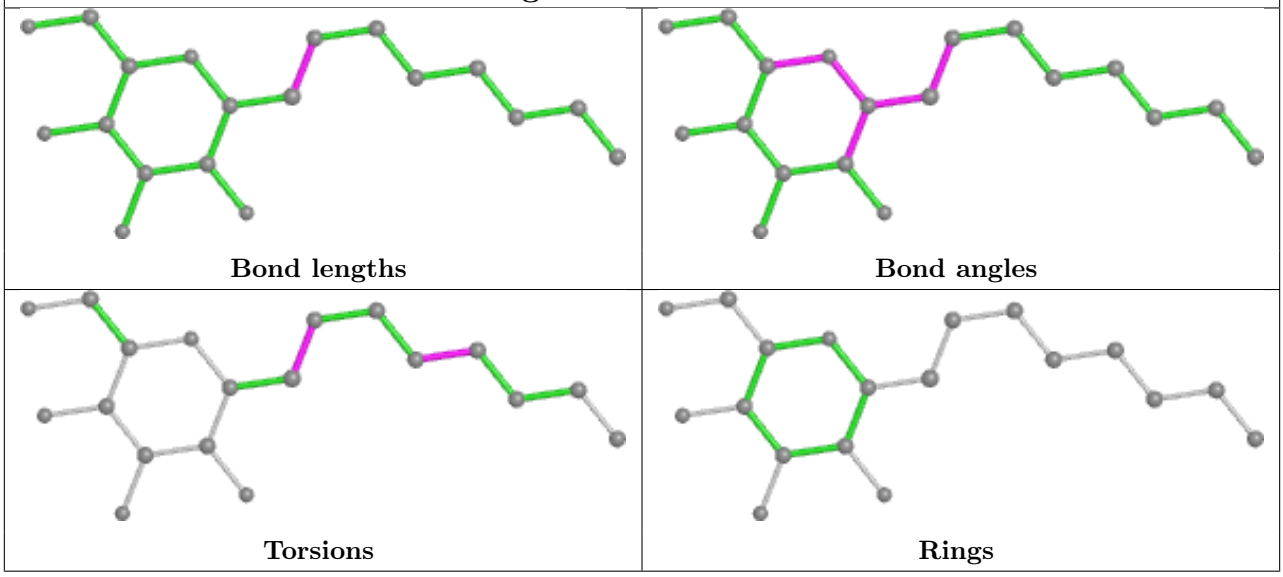
Ligand LMT M 104



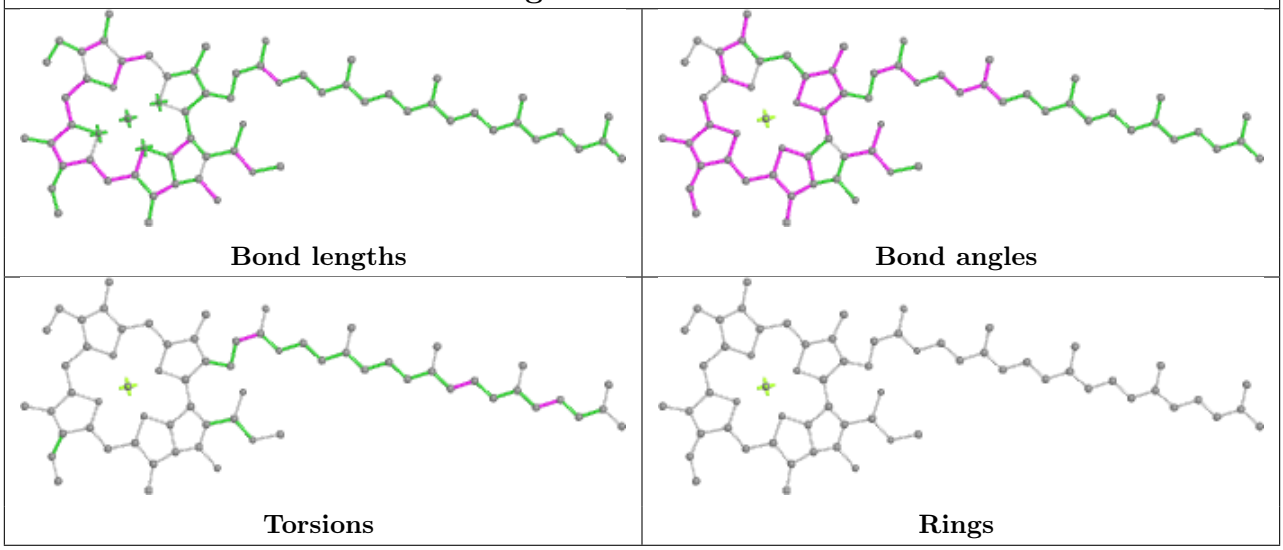
Ligand LMT D 401



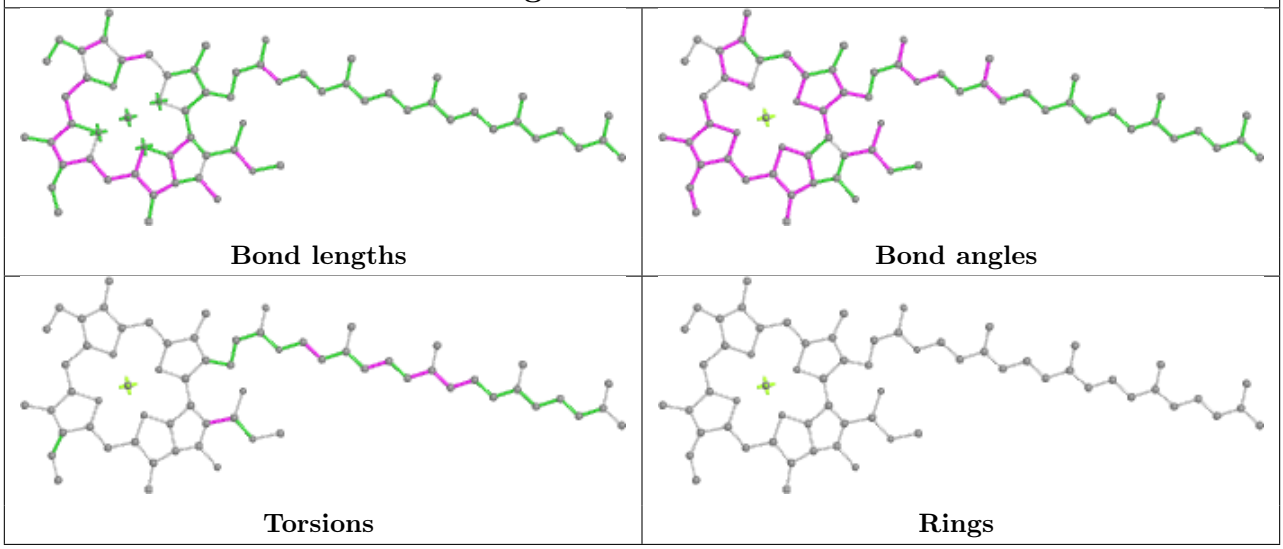
Ligand HTG B 624



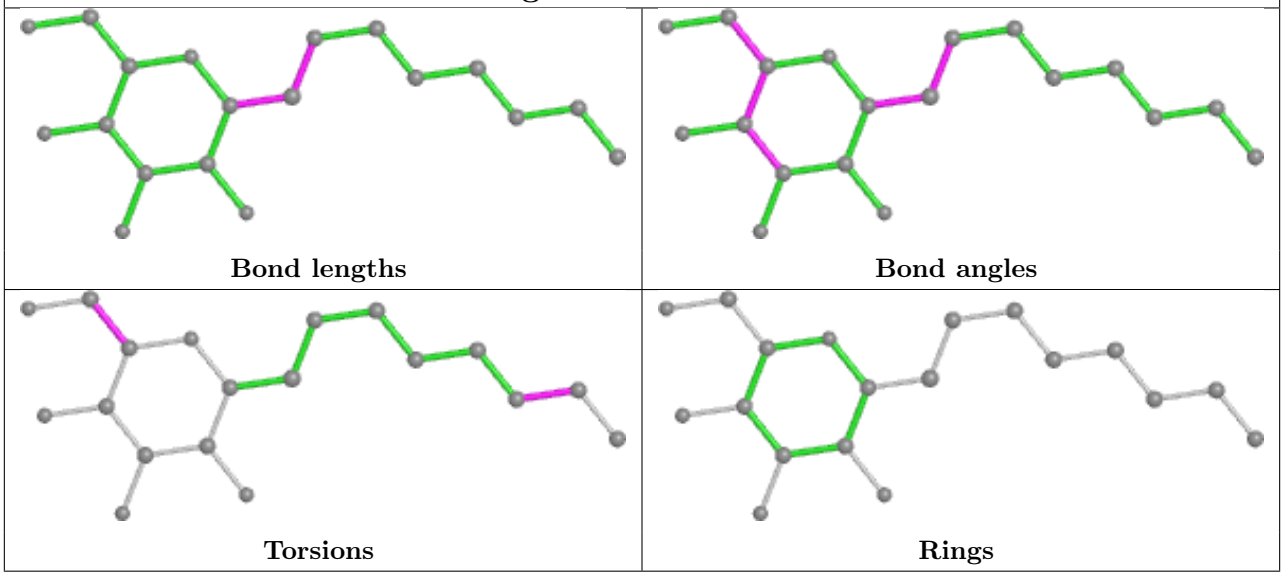
Ligand CLA B 613



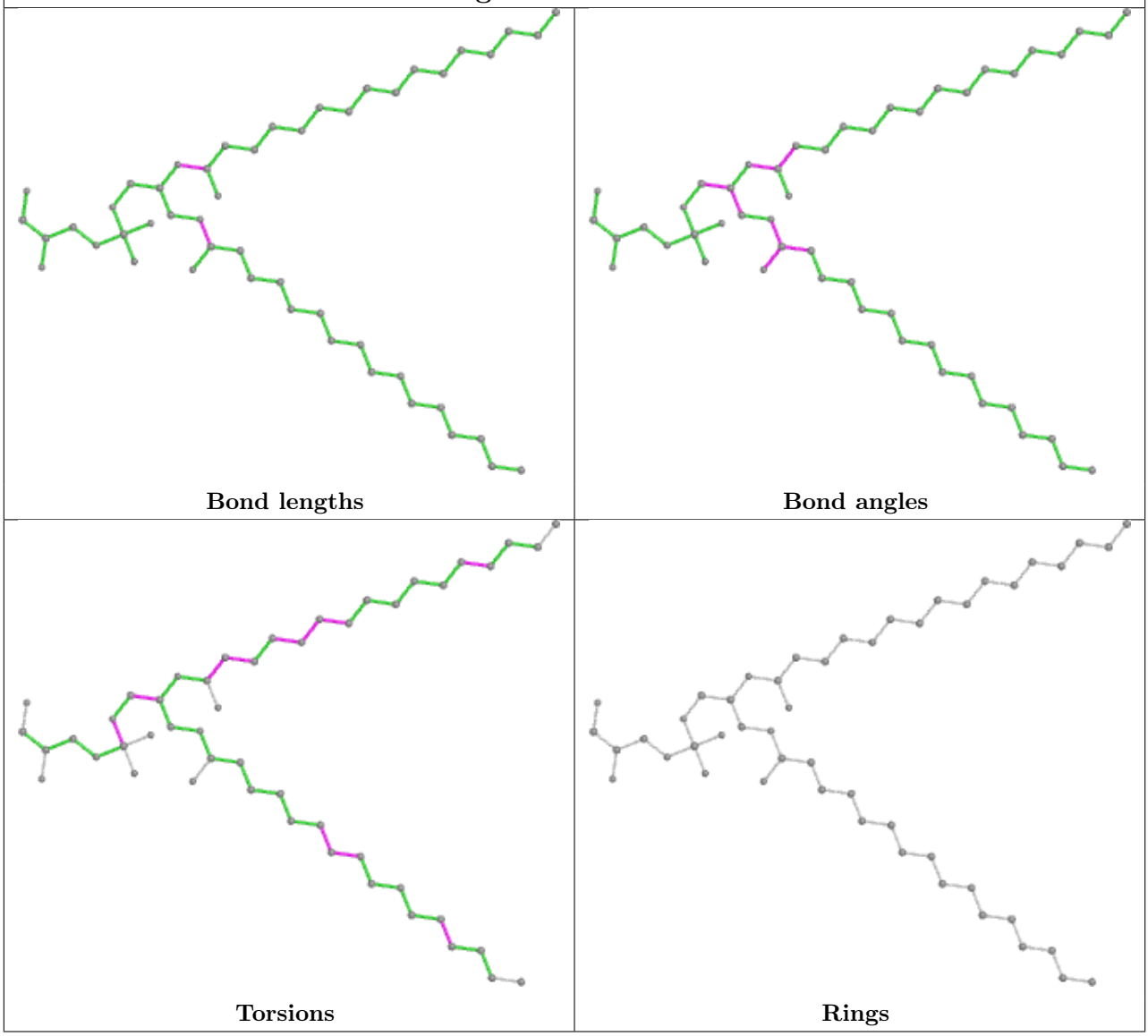
Ligand CLA D 403



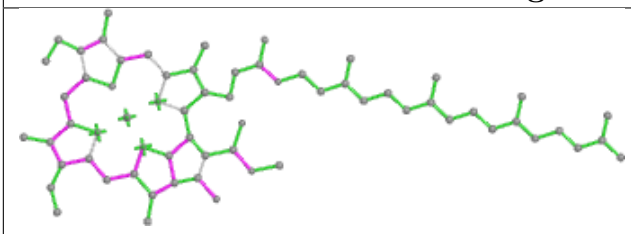
Ligand HTG B 632



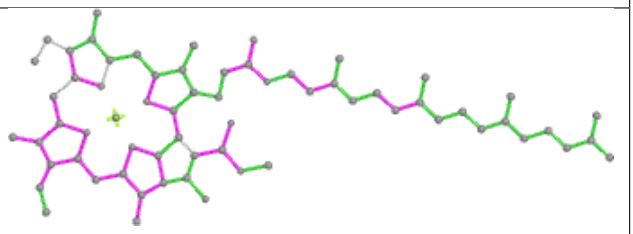
Ligand LHG l 101



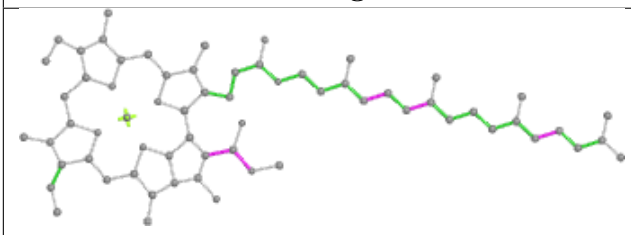
Ligand CLA b 614



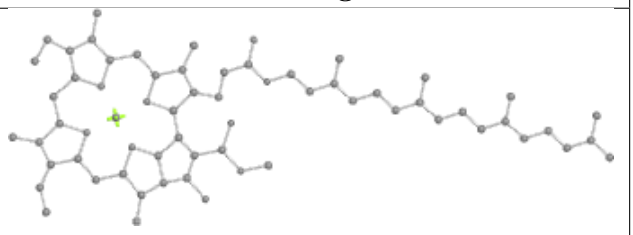
Bond lengths



Bond angles

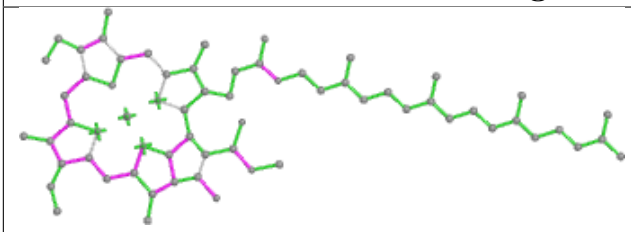


Torsions

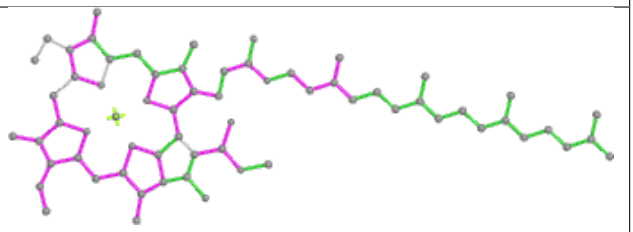


Rings

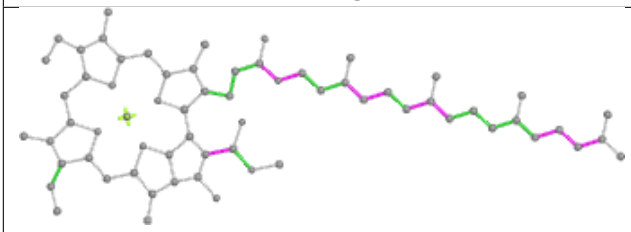
Ligand CLA c 510



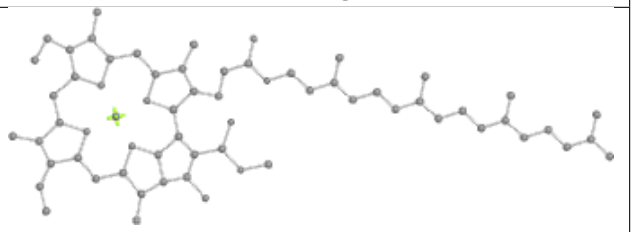
Bond lengths



Bond angles

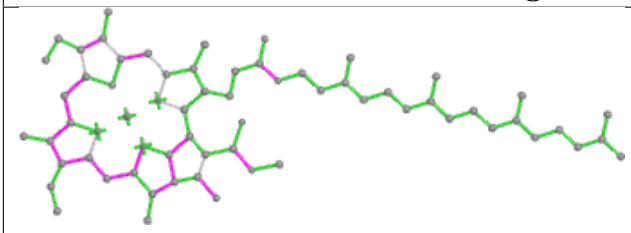


Torsions

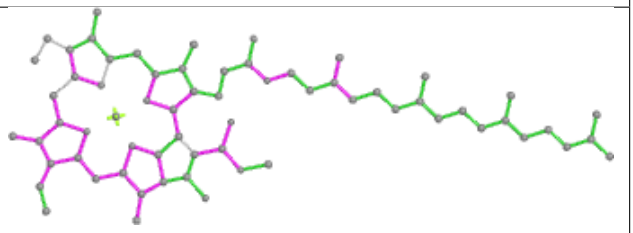


Rings

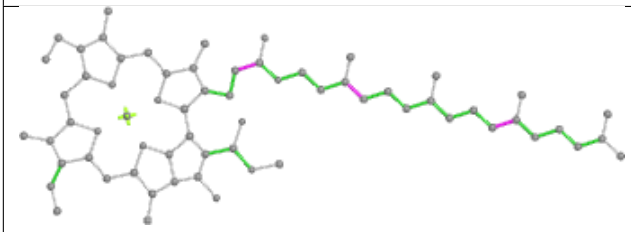
Ligand CLA C 505



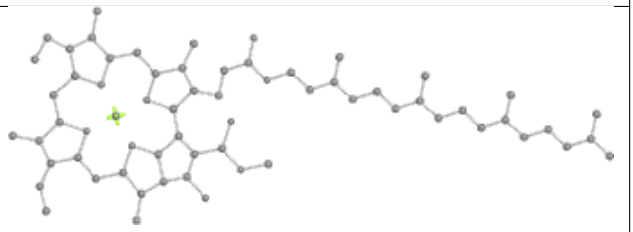
Bond lengths



Bond angles

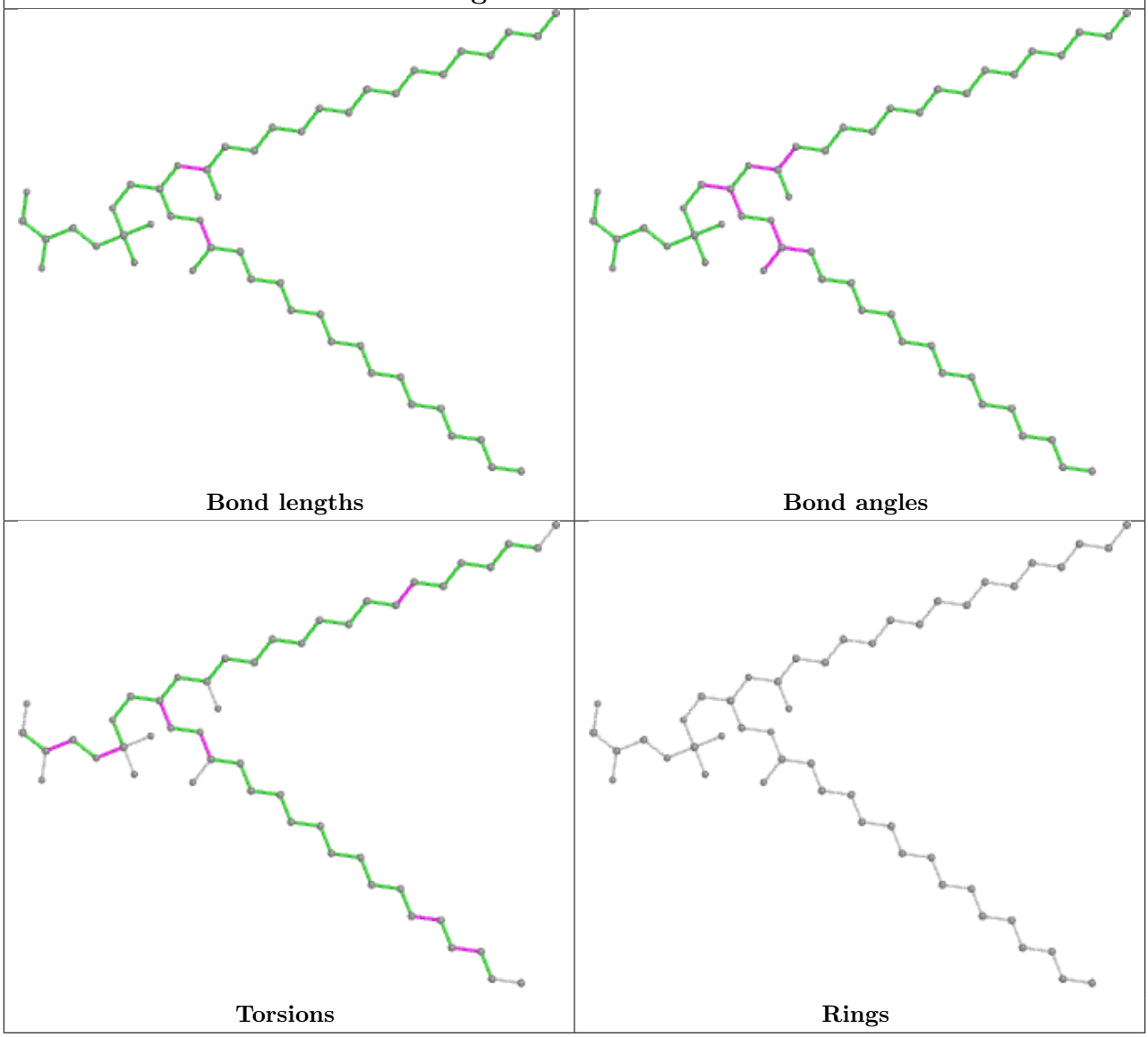


Torsions



Rings

Ligand LHG d 407



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	0.06	2 (0%) 89 91	28, 37, 66, 107	0
1	a	334/344 (97%)	0.17	10 (2%) 50 59	29, 38, 73, 150	0
2	B	504/505 (99%)	0.08	7 (1%) 75 80	29, 42, 76, 120	0
2	b	503/505 (99%)	0.21	24 (4%) 30 39	30, 43, 83, 162	0
3	C	451/455 (99%)	0.02	3 (0%) 87 91	32, 49, 69, 110	0
3	c	455/455 (100%)	0.07	4 (0%) 84 88	36, 53, 70, 121	0
4	D	341/342 (99%)	0.02	1 (0%) 94 95	27, 38, 62, 134	0
4	d	341/342 (99%)	0.02	2 (0%) 89 91	28, 41, 65, 112	0
5	E	81/84 (96%)	0.62	8 (9%) 7 11	44, 62, 92, 139	0
5	e	81/84 (96%)	0.90	10 (12%) 4 5	47, 65, 110, 167	0
6	F	34/44 (77%)	0.31	3 (8%) 10 14	45, 54, 92, 96	0
6	f	32/44 (72%)	0.29	2 (6%) 20 27	45, 54, 112, 130	0
7	H	65/65 (100%)	0.19	3 (4%) 32 42	39, 52, 68, 144	0
7	h	65/65 (100%)	0.09	2 (3%) 49 58	40, 54, 74, 162	0
8	I	37/38 (97%)	0.21	3 (8%) 12 16	44, 52, 104, 148	0
8	i	37/38 (97%)	0.18	2 (5%) 25 34	41, 50, 97, 126	0
9	J	38/39 (97%)	0.48	3 (7%) 12 17	42, 58, 135, 165	0
9	j	39/39 (100%)	0.74	4 (10%) 6 9	46, 59, 130, 162	0
10	K	37/37 (100%)	-0.03	0 100 100	50, 58, 72, 91	0
10	k	37/37 (100%)	0.23	0 100 100	50, 63, 79, 98	0
11	L	37/37 (100%)	0.14	1 (2%) 54 63	28, 34, 94, 106	0
11	l	37/37 (100%)	0.18	1 (2%) 54 63	30, 36, 90, 121	0
12	M	33/36 (91%)	0.27	2 (6%) 21 28	28, 36, 61, 112	0
12	m	33/36 (91%)	0.27	0 100 100	30, 37, 66, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.02	3 (1%) 79 83	29, 47, 91, 130	0
13	o	243/244 (99%)	0.10	4 (1%) 72 77	31, 49, 103, 167	0
14	T	29/32 (90%)	0.16	1 (3%) 45 53	30, 36, 62, 135	0
14	t	29/32 (90%)	0.11	0 100 100	31, 37, 64, 128	0
15	U	97/104 (93%)	-0.08	0 100 100	35, 46, 75, 109	0
15	u	97/104 (93%)	-0.03	0 100 100	37, 49, 68, 117	0
16	V	137/137 (100%)	-0.06	0 100 100	31, 45, 65, 84	0
16	v	137/137 (100%)	0.08	1 (0%) 87 91	39, 56, 82, 129	0
17	Y	29/30 (96%)	1.78	7 (24%) 0 0	60, 71, 151, 153	0
17	y	29/30 (96%)	0.80	2 (6%) 16 23	68, 80, 106, 124	0
18	X	39/40 (97%)	0.48	4 (10%) 6 9	47, 60, 112, 132	0
18	x	38/40 (95%)	0.53	4 (10%) 6 9	52, 61, 113, 134	0
19	Z	62/62 (100%)	0.54	7 (11%) 5 7	56, 72, 108, 126	0
19	z	62/62 (100%)	1.11	10 (16%) 1 2	70, 83, 128, 175	0
20	R	18/34 (52%)	7.53	18 (100%) 0 0	111, 142, 168, 174	0
All	All	5275/5384 (97%)	0.17	158 (2%) 50 59	27, 47, 89, 175	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	16.6
20	R	18	TRP	14.5
20	R	15	ALA	13.8
5	e	5	THR	13.8
2	b	496	TYR	10.6
20	R	16	ALA	9.7
9	j	1	MET	9.7
20	R	6	LEU	9.6
20	R	5	VAL	9.5
20	R	12	VAL	9.3
20	R	9	LEU	9.1
19	z	3	ILE	8.5
20	R	3	TRP	8.3
2	b	494	GLY	8.2
17	Y	19	ILE	8.1
2	b	495	PHE	7.7
17	Y	20	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
20	R	14	LEU	7.2
20	R	17	GLY	7.0
2	b	499	VAL	6.8
7	h	65	LEU	6.7
20	R	11	PRO	6.7
2	b	489	GLU	6.4
20	R	13	LEU	6.1
20	R	8	VAL	6.1
2	b	486	LEU	5.9
19	Z	62	VAL	5.8
5	e	4	THR	5.5
13	o	58	ASN	5.4
3	C	23	ALA	5.4
1	a	264[A]	SER	5.4
5	e	6	GLY	5.3
9	J	5	GLY	5.3
2	b	493	TRP	5.2
5	E	6	GLY	5.1
20	R	19	ALA	4.9
18	x	2	THR	4.9
18	X	37	VAL	4.8
2	B	479	PHE	4.8
13	O	56	PRO	4.8
19	Z	31	GLN	4.8
18	x	37	VAL	4.8
1	a	262	TYR	4.6
17	Y	21	GLN	4.5
2	b	488	PRO	4.5
19	z	62	VAL	4.4
17	y	20	ALA	4.3
5	E	5	THR	4.3
13	O	60	ARG	4.2
7	h	66	GLY	4.2
2	B	495	PHE	4.1
9	j	3	GLU	4.0
18	x	38	GLN	3.9
13	o	59	LYS	3.9
20	R	2	ASP	3.9
1	a	263	ALA	3.8
2	b	487	SER	3.8
17	Y	22	LEU	3.8
2	b	502	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	b	497	GLN	3.8
2	B	496	TYR	3.7
19	z	32	ASP	3.7
5	E	4	THR	3.7
9	j	4	GLY	3.7
5	e	7	GLU	3.6
19	z	61	VAL	3.6
2	B	494	GLY	3.6
20	R	10	LEU	3.6
19	z	5	PHE	3.5
19	z	35	ARG	3.5
19	Z	33	TRP	3.5
8	I	37	LEU	3.5
2	b	500	GLY	3.5
5	E	84	LYS	3.5
6	F	16	PHE	3.5
2	b	498	LYS	3.4
9	J	2	SER	3.4
19	z	33	TRP	3.4
2	b	86[A]	ILE	3.3
20	R	4	ARG	3.3
8	I	34	ARG	3.2
2	b	504	THR	3.2
2	b	501	ASP	3.2
19	z	41	PHE	3.2
2	b	485	GLU	3.1
2	b	484	PRO	3.1
13	o	56	PRO	3.1
5	E	79	PHE	3.1
1	a	261	GLN	3.1
19	z	2	THR	3.1
20	R	7	VAL	3.1
7	H	65	LEU	3.0
4	D	12	ARG	3.0
2	b	491	VAL	3.0
2	b	490	GLN	3.0
5	E	83	LEU	2.9
2	b	503	THR	2.9
19	Z	61	VAL	2.9
6	f	14	PRO	2.9
2	B	504	THR	2.9
9	J	3	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
16	v	106	ASN	2.9
3	C	145[A]	SER	2.9
9	j	2	SER	2.9
2	b	85	GLY	2.8
5	e	10	PHE	2.8
2	B	501	ASP	2.8
1	a	248[A]	ILE	2.8
13	O	62	GLU	2.7
4	d	236[A]	ASN	2.7
1	a	260	PHE	2.7
1	a	265[A]	PHE	2.7
18	X	40	SER	2.6
5	E	19	TYR	2.6
2	B	483	ASP	2.6
2	b	492	GLU	2.6
1	A	12	ASN	2.6
5	e	61	ARG	2.5
6	F	14	PRO	2.5
1	a	229	GLU	2.5
5	E	15	THR	2.5
5	e	72	ALA	2.5
11	l	3	PRO	2.4
3	c	143	TYR	2.4
12	M	33	GLN	2.4
7	H	64	ALA	2.4
1	a	11	ALA	2.4
7	H	66	GLY	2.3
19	Z	32	ASP	2.3
1	A	13	LEU	2.3
14	T	30	THR	2.3
6	F	15	ILE	2.3
17	Y	26	ALA	2.2
18	X	2	THR	2.2
19	Z	29	SER	2.2
2	b	478	VAL	2.2
3	c	207	ARG	2.2
12	M	34	LYS	2.2
11	L	1	MET	2.2
1	a	307[A]	ILE	2.1
3	c	21	ILE	2.1
6	f	16	PHE	2.1
18	x	35	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	240[A]	ALA	2.1
17	y	25	ILE	2.1
8	i	34	ARG	2.1
5	e	14	ILE	2.1
19	z	28	ALA	2.1
8	i	36	ASP	2.1
18	X	39	ARG	2.1
3	c	140	LEU	2.1
5	e	59	GLU	2.1
3	C	25	ASN	2.0
17	Y	25	ILE	2.0
13	o	246	ALA	2.0
8	I	36	ASP	2.0
19	Z	3	ILE	2.0
5	e	74	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.94	0.11	37,40,54,78	0
12	FME	M	1	10/11	0.97	0.13	26,45,71,76	0
8	FME	i	1	10/11	0.97	0.13	39,48,57,57	0
12	FME	m	1	10/11	0.97	0.16	34,45,87,98	0
8	FME	I	1	10/11	0.98	0.11	36,46,51,55	0
14	FME	t	1	10/11	0.98	0.12	28,35,39,84	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	DGD	e	101	62/66	0.44	0.39	66,114,163,166	0
29	LMT	F	101	35/35	0.54	0.33	97,128,145,146	0
29	LMT	C	521	35/35	0.57	0.32	94,119,146,148	0
29	LMT	b	631	25/35	0.58	0.32	72,95,139,144	0
33	UNL	C	527	34/-	0.59	0.22	76,103,111,117	0
38	LHG	a	422	42/49	0.59	0.30	78,125,159,162	0
33	UNL	a	403	30/-	0.62	0.24	77,91,116,118	0
37	DGD	D	406	52/66	0.63	0.28	67,101,132,138	0
29	LMT	a	421	35/35	0.64	0.37	94,110,132,135	0
33	UNL	A	421	28/-	0.66	0.22	68,84,98,99	0
33	UNL	c	526	32/-	0.66	0.23	77,98,122,128	0
33	UNL	j	102	10/-	0.66	0.21	70,80,90,91	0
29	LMT	M	103	35/35	0.67	0.25	45,92,128,137	0
36	HTG	c	525	19/19	0.67	0.34	68,104,113,143	0
36	HTG	d	411	16/19	0.67	0.19	70,111,121,126	0
29	LMT	D	401	35/35	0.68	0.28	75,118,137,137	0
29	LMT	f	103	35/35	0.70	0.29	72,117,137,137	0
36	HTG	H	101	16/19	0.71	0.27	70,131,138,139	0
33	UNL	B	634	33/-	0.72	0.24	54,88,123,126	0
27	SQD	f	102	43/54	0.72	0.27	97,116,146,147	0
33	UNL	J	101	10/-	0.72	0.22	46,70,80,85	0
29	LMT	a	404	35/35	0.73	0.24	47,86,111,123	0
34	LMG	Z	101	37/55	0.73	0.27	57,108,124,127	0
35	CA	b	610	1/1	0.73	0.17	130,130,130,130	0
36	HTG	b	609	19/19	0.74	0.21	62,113,140,141	0
33	UNL	m	101	10/-	0.74	0.22	50,57,79,81	0
29	LMT	m	102	35/35	0.75	0.23	47,95,121,125	0
36	HTG	B	633	19/19	0.76	0.21	53,110,132,175	0
32	PL9	a	416[A]	55/55	0.76	0.25	83,102,111,114	55
32	PL9	a	416[B]	55/55	0.76	0.25	84,102,111,114	55
36	HTG	B	625	19/19	0.76	0.26	64,120,133,158	0
29	LMT	A	417	35/35	0.77	0.21	41,79,99,112	0
38	LHG	E	101	42/49	0.77	0.22	69,98,119,122	0
29	LMT	M	104	35/35	0.77	0.22	46,79,89,95	0
33	UNL	b	634	33/-	0.78	0.25	48,98,141,142	0
27	SQD	b	601	54/54	0.78	0.18	52,72,120,129	0
28	GOL	V	202	6/6	0.79	0.38	62,77,81,82	0
33	UNL	d	410	36/-	0.80	0.20	53,77,122,126	0
27	SQD	A	416	54/54	0.80	0.19	47,73,104,112	0
33	UNL	I	101	40/-	0.80	0.25	43,83,129,135	0
32	PL9	A	420[A]	55/55	0.81	0.23	70,87,101,101	55
33	UNL	i	101	40/-	0.81	0.23	50,74,125,128	0
32	PL9	A	420[B]	55/55	0.81	0.23	71,87,101,101	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMT	T	104	25/35	0.81	0.23	38,71,116,121	0
28	GOL	v	201	6/6	0.81	0.34	78,85,89,90	0
36	HTG	b	633	19/19	0.81	0.22	70,120,135,135	0
27	SQD	B	621	54/54	0.82	0.19	48,81,143,146	0
34	LMG	C	519	51/55	0.82	0.19	50,78,102,103	0
29	LMT	B	635	25/35	0.82	0.24	38,73,124,127	0
34	LMG	z	101	39/55	0.83	0.24	69,112,127,136	0
29	LMT	M	101	35/35	0.83	0.20	39,82,98,103	0
28	GOL	T	102	6/6	0.83	0.28	103,114,116,120	0
34	LMG	C	520	51/55	0.83	0.20	53,105,116,119	0
36	HTG	C	523	19/19	0.83	0.22	75,95,121,124	0
27	SQD	a	405	54/54	0.83	0.16	45,76,111,114	0
34	LMG	c	523	51/55	0.83	0.23	49,106,118,120	0
33	UNL	M	102	10/-	0.84	0.19	50,64,69,73	0
34	LMG	a	415	51/55	0.85	0.18	58,75,96,97	0
33	UNL	D	411	40/-	0.85	0.18	57,79,113,123	0
34	LMG	A	422	51/55	0.86	0.17	56,79,99,104	0
37	DGD	C	517	62/66	0.86	0.15	37,52,86,94	0
34	LMG	b	630	51/55	0.86	0.17	39,48,68,82	0
27	SQD	F	103	43/54	0.87	0.21	74,97,116,118	0
34	LMG	c	522	51/55	0.87	0.18	52,86,107,110	0
28	GOL	b	607	6/6	0.87	0.16	64,77,80,80	0
33	UNL	X	101	18/-	0.87	0.16	58,70,93,100	0
28	GOL	c	502	6/6	0.87	0.43	70,79,91,98	0
28	GOL	t	102	6/6	0.87	0.42	49,76,86,89	0
36	HTG	B	624	19/19	0.88	0.17	54,64,74,81	0
33	UNL	d	412	18/-	0.88	0.20	61,68,102,107	0
37	DGD	h	102	62/66	0.88	0.15	35,48,63,73	0
28	GOL	A	415	6/6	0.88	0.17	54,73,76,79	0
36	HTG	b	632	19/19	0.88	0.24	51,67,77,78	0
28	GOL	a	402	6/6	0.89	0.22	76,90,92,92	0
37	DGD	c	520	62/66	0.89	0.16	38,51,100,112	0
28	GOL	O	301	6/6	0.89	0.10	68,76,77,77	0
24	CLA	C	513	65/65	0.89	0.17	50,64,93,98	0
28	GOL	C	524	6/6	0.89	0.28	63,65,79,82	0
34	LMG	B	622	51/55	0.89	0.16	32,49,69,85	0
28	GOL	A	413	6/6	0.90	0.12	43,44,56,59	0
37	DGD	H	103	62/66	0.90	0.16	32,47,70,74	0
28	GOL	A	414	6/6	0.90	0.25	52,54,57,60	0
36	HTG	c	524	19/19	0.90	0.14	81,89,96,118	0
27	SQD	A	412	54/54	0.90	0.17	43,76,91,94	0
36	HTG	b	608	19/19	0.90	0.13	48,68,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	B	636	6/6	0.90	0.12	48,51,55,55	0
24	CLA	c	517	65/65	0.91	0.15	61,77,92,94	0
24	CLA	c	511	65/65	0.91	0.14	43,54,62,67	0
36	HTG	V	207	19/19	0.91	0.24	63,87,104,205	0
28	GOL	T	101	6/6	0.91	0.34	55,69,88,96	0
28	GOL	B	630	6/6	0.91	0.24	50,66,68,71	0
37	DGD	c	521	62/66	0.91	0.15	39,51,82,89	0
27	SQD	a	414	54/54	0.91	0.15	54,77,98,101	0
36	HTG	B	632	19/19	0.91	0.13	41,75,91,92	0
38	LHG	D	407	49/49	0.91	0.17	35,47,59,64	0
28	GOL	v	202	6/6	0.91	0.19	72,79,89,99	0
36	HTG	C	522	19/19	0.91	0.15	72,80,91,95	0
34	LMG	j	101	51/55	0.92	0.15	46,56,92,106	0
28	GOL	b	606	6/6	0.92	0.19	75,79,94,95	0
24	CLA	c	515	65/65	0.92	0.15	43,55,73,80	0
35	CA	f	104	1/1	0.92	0.09	97,97,97,97	0
24	CLA	b	619	65/65	0.92	0.15	35,49,56,65	0
28	GOL	f	101	6/6	0.92	0.20	74,84,86,89	0
38	LHG	D	409	49/49	0.92	0.19	37,54,105,113	0
37	DGD	C	518	62/66	0.92	0.14	37,47,75,87	0
24	CLA	C	506	65/65	0.92	0.14	44,60,101,105	0
24	CLA	C	511	65/65	0.93	0.12	42,56,67,78	0
36	HTG	b	602	19/19	0.93	0.12	35,49,65,66	0
24	CLA	B	602	65/65	0.93	0.16	44,61,94,111	0
34	LMG	D	412	51/55	0.93	0.16	35,55,100,106	0
24	CLA	b	611	65/65	0.93	0.15	46,69,101,116	0
24	CLA	b	612	65/65	0.93	0.15	33,44,51,57	0
28	GOL	V	203	6/6	0.93	0.15	39,50,64,67	0
28	GOL	a	401	6/6	0.93	0.27	50,61,66,76	0
24	CLA	b	616	65/65	0.93	0.14	30,43,84,96	0
24	CLA	b	617	65/65	0.93	0.14	26,34,42,50	0
24	CLA	B	614	65/65	0.93	0.14	25,35,63,75	0
24	CLA	b	626	65/65	0.93	0.13	35,50,97,100	0
33	UNL	d	409	17/-	0.93	0.18	46,63,91,92	0
36	HTG	B	623	19/19	0.93	0.14	37,51,65,70	0
24	CLA	c	507	65/65	0.93	0.13	41,51,60,77	0
24	CLA	C	501	65/65	0.93	0.14	38,47,69,78	0
28	GOL	B	628	6/6	0.93	0.16	52,70,78,85	0
24	CLA	C	504	65/65	0.93	0.15	35,46,77,83	0
28	GOL	v	203	6/6	0.93	0.17	46,50,57,61	0
22	CL	v	204	1/1	0.93	0.11	88,88,88,88	0
24	CLA	C	507	65/65	0.93	0.14	40,52,67,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	b	621	65/65	0.94	0.13	26,38,48,55	0
24	CLA	C	508	65/65	0.94	0.13	35,48,107,117	0
28	GOL	V	205	6/6	0.94	0.20	71,75,81,91	0
24	CLA	c	505	65/65	0.94	0.13	40,54,62,66	0
24	CLA	C	509	65/65	0.94	0.14	41,52,73,76	0
24	CLA	c	508	65/65	0.94	0.12	38,50,71,75	0
24	CLA	c	509	65/65	0.94	0.12	34,45,64,72	0
24	CLA	c	510	65/65	0.94	0.12	44,62,87,95	0
24	CLA	B	607	65/65	0.94	0.14	31,43,85,91	0
28	GOL	o	301	6/6	0.94	0.17	64,70,80,88	0
24	CLA	c	512	65/65	0.94	0.13	36,46,109,121	0
24	CLA	c	514	65/65	0.94	0.12	38,50,60,68	0
24	CLA	C	512	65/65	0.94	0.12	46,64,76,80	0
33	UNL	D	410	17/-	0.94	0.16	39,67,83,87	0
28	GOL	B	626	6/6	0.94	0.14	39,52,57,71	0
24	CLA	c	516	65/65	0.94	0.13	51,62,77,83	0
24	CLA	B	603	65/65	0.94	0.13	33,42,47,53	0
37	DGD	c	519	62/66	0.94	0.13	37,46,91,95	0
35	CA	B	601	1/1	0.94	0.07	118,118,118,118	0
35	CA	F	104	1/1	0.94	0.07	82,82,82,82	0
26	BCR	b	628	40/40	0.94	0.14	31,43,54,61	0
26	BCR	c	527	40/40	0.94	0.12	56,72,78,81	0
26	BCR	h	101	40/40	0.94	0.12	39,54,64,66	0
26	BCR	k	101	40/40	0.94	0.14	44,60,70,74	0
26	BCR	y	101	40/40	0.94	0.14	43,60,68,76	0
28	GOL	V	201	6/6	0.94	0.21	68,75,76,79	0
38	LHG	d	406	49/49	0.94	0.16	41,49,58,63	0
38	LHG	d	407	49/49	0.94	0.16	30,39,57,75	0
38	LHG	l	101	49/49	0.94	0.16	33,44,53,59	0
32	PL9	D	405[B]	55/55	0.95	0.15	27,35,43,47	55
26	BCR	D	404	40/40	0.95	0.14	36,49,79,88	0
26	BCR	H	102	40/40	0.95	0.13	36,52,65,68	0
26	BCR	K	101	40/40	0.95	0.14	43,55,62,63	0
26	BCR	T	103	40/40	0.95	0.12	28,45,55,58	0
26	BCR	Y	101	40/40	0.95	0.11	48,59,67,72	0
24	CLA	C	510	65/65	0.95	0.12	39,51,60,69	0
26	BCR	c	518	40/40	0.95	0.14	39,55,64,64	0
28	GOL	b	603	6/6	0.95	0.20	53,57,64,80	0
24	CLA	b	622	65/65	0.95	0.13	29,39,47,49	0
26	BCR	d	404	40/40	0.95	0.14	38,50,73,79	0
24	CLA	b	624	65/65	0.95	0.14	27,39,83,97	0
24	CLA	b	625	65/65	0.95	0.12	34,44,62,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	B	608	65/65	0.95	0.13	24,33,44,53	0
24	CLA	C	503	65/65	0.95	0.13	39,50,59,65	0
24	CLA	B	610	65/65	0.95	0.13	35,46,55,71	0
24	CLA	D	403	65/65	0.95	0.13	39,49,99,104	0
24	CLA	a	409	65/65	0.95	0.14	27,32,48,57	0
24	CLA	C	505	65/65	0.95	0.13	32,47,66,74	0
37	DGD	C	516	62/66	0.95	0.14	33,44,85,86	0
24	CLA	B	604	65/65	0.95	0.13	33,43,50,53	0
24	CLA	b	613	65/65	0.95	0.13	34,43,52,58	0
24	CLA	c	513	65/65	0.95	0.13	43,54,67,82	0
24	CLA	B	615	65/65	0.95	0.14	27,38,82,86	0
24	CLA	B	616	65/65	0.95	0.13	33,44,60,68	0
24	CLA	b	618	65/65	0.95	0.12	32,42,51,56	0
24	CLA	B	617	65/65	0.95	0.15	31,50,107,110	0
28	GOL	B	627	6/6	0.95	0.22	56,65,80,92	0
24	CLA	d	401	65/65	0.95	0.13	26,32,41,51	0
24	CLA	d	403	65/65	0.95	0.13	39,49,98,106	0
38	LHG	D	408	49/49	0.95	0.16	30,41,62,74	0
28	GOL	B	631	6/6	0.95	0.32	48,62,69,70	0
25	PHO	a	420[A]	64/64	0.95	0.14	31,41,46,49	64
38	LHG	L	101	49/49	0.95	0.15	31,43,54,61	0
25	PHO	a	420[B]	64/64	0.95	0.14	31,40,46,50	64
26	BCR	B	620	40/40	0.95	0.14	31,43,57,59	0
26	BCR	C	514	40/40	0.95	0.13	49,65,73,78	0
38	LHG	d	408	49/49	0.95	0.17	34,52,103,105	0
32	PL9	D	405[A]	55/55	0.95	0.15	28,35,45,49	55
25	PHO	A	409[B]	64/64	0.96	0.14	30,39,44,49	64
24	CLA	B	609	65/65	0.96	0.14	32,42,52,54	0
23	BCT	a	419[A]	4/4	0.96	0.13	53,54,57,63	4
26	BCR	A	411	40/40	0.96	0.15	29,37,44,45	0
26	BCR	B	619	40/40	0.96	0.14	26,36,55,58	0
24	CLA	a	410	65/65	0.96	0.14	29,40,99,105	0
24	CLA	a	412	65/65	0.96	0.15	32,45,111,115	0
26	BCR	C	515	40/40	0.96	0.15	39,53,60,63	0
24	CLA	c	506	65/65	0.96	0.13	38,50,63,69	0
28	GOL	B	629	6/6	0.96	0.13	43,47,50,52	0
24	CLA	B	611	65/65	0.96	0.13	35,44,50,57	0
24	CLA	B	612	65/65	0.96	0.14	26,35,47,53	0
23	BCT	a	419[B]	4/4	0.96	0.13	53,53,57,64	4
24	CLA	b	614	65/65	0.96	0.13	26,39,70,74	0
28	GOL	C	525	6/6	0.96	0.12	39,48,50,51	0
24	CLA	b	615	65/65	0.96	0.13	28,38,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	A	405	65/65	0.96	0.14	25,32,41,57	0
24	CLA	B	605	65/65	0.96	0.13	25,35,67,69	0
24	CLA	B	606	65/65	0.96	0.13	28,37,50,52	0
24	CLA	A	406	65/65	0.96	0.14	24,32,38,45	0
24	CLA	b	620	65/65	0.96	0.13	33,44,51,57	0
28	GOL	V	204	6/6	0.96	0.12	55,61,65,65	0
26	BCR	t	101	40/40	0.96	0.13	30,43,60,68	0
24	CLA	A	410	65/65	0.96	0.13	29,47,108,113	0
24	CLA	D	402	65/65	0.96	0.14	24,33,52,57	0
24	CLA	d	402	65/65	0.96	0.13	26,35,54,64	0
32	PL9	d	405[A]	55/55	0.96	0.16	25,35,44,49	55
32	PL9	d	405[B]	55/55	0.96	0.16	25,35,43,49	55
28	GOL	b	604	6/6	0.96	0.16	41,56,70,75	0
28	GOL	b	605	6/6	0.96	0.21	53,64,74,84	0
24	CLA	b	623	65/65	0.96	0.14	28,39,55,57	0
25	PHO	A	408	64/64	0.96	0.13	26,32,38,43	0
25	PHO	A	409[A]	64/64	0.96	0.14	29,40,44,47	64
39	HEM	e	102	43/43	0.96	0.17	53,76,114,130	0
40	MG	j	103	1/1	0.96	0.17	55,55,55,55	0
25	PHO	a	411	64/64	0.97	0.14	26,34,40,45	0
24	CLA	B	613	65/65	0.97	0.12	27,36,45,47	0
24	CLA	A	407	65/65	0.97	0.12	27,37,90,96	0
24	CLA	C	502	65/65	0.97	0.12	36,44,55,70	0
26	BCR	a	413	40/40	0.97	0.12	28,38,46,47	0
26	BCR	b	627	40/40	0.97	0.14	30,39,47,47	0
26	BCR	B	618	40/40	0.97	0.14	28,37,45,45	0
40	MG	J	102	1/1	0.97	0.09	50,50,50,50	0
26	BCR	b	629	40/40	0.97	0.14	37,48,60,64	0
23	BCT	A	404[A]	4/4	0.98	0.12	51,52,57,63	4
23	BCT	A	404[B]	4/4	0.98	0.12	51,52,57,63	4
28	GOL	c	501	6/6	0.98	0.14	43,46,52,53	0
35	CA	C	526	1/1	0.98	0.07	67,67,67,67	0
22	CL	A	403[B]	1/1	0.98	0.12	33,33,33,33	1
22	CL	U	201	1/1	0.98	0.17	93,93,93,93	0
35	CA	c	503	1/1	0.98	0.08	63,63,63,63	0
39	HEM	F	102	43/43	0.98	0.13	46,64,75,83	0
39	HEM	V	206	43/43	0.98	0.12	34,39,47,50	0
35	CA	c	504	1/1	0.98	0.06	73,73,73,73	0
39	HEM	v	205	43/43	0.98	0.11	41,49,55,57	0
22	CL	A	403[A]	1/1	0.98	0.12	33,33,33,33	1
35	CA	o	302	1/1	0.98	0.06	86,86,86,86	0
30	OEX	a	417[A]	10/10	0.99	0.12	31,37,39,45	10

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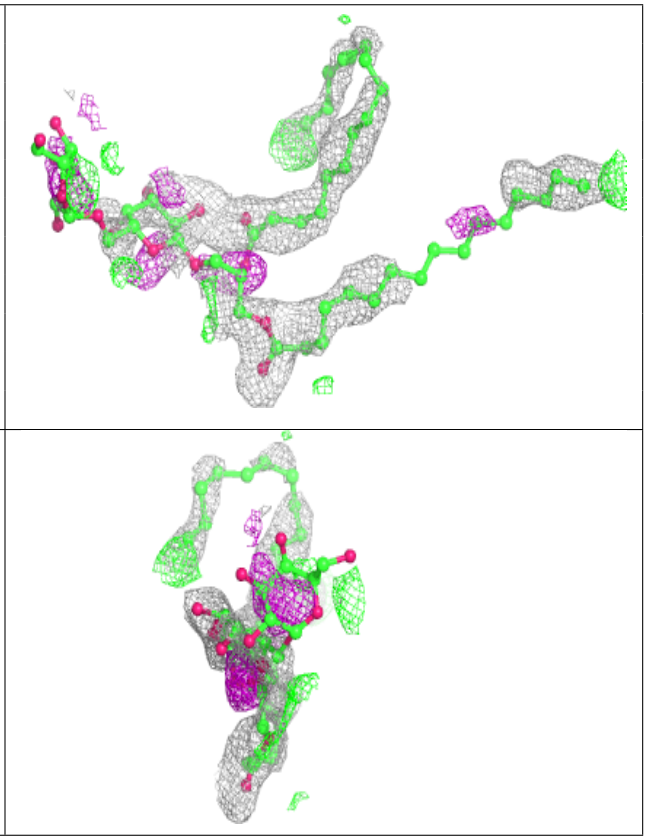
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	OEY	A	419[B]	11/11	0.99	0.14	31,36,42,47	11
31	OEY	a	418[B]	11/11	0.99	0.13	32,37,44,57	11
22	CL	a	408[B]	1/1	0.99	0.10	38,38,38,38	1
21	FE2	a	406[B]	1/1	0.99	0.13	46,46,46,46	0
22	CL	A	402[A]	1/1	0.99	0.12	30,30,30,30	1
22	CL	A	402[B]	1/1	0.99	0.12	31,31,31,31	1
22	CL	a	407[A]	1/1	0.99	0.09	34,34,34,34	1
22	CL	a	407[B]	1/1	0.99	0.09	33,33,33,33	1
22	CL	a	408[A]	1/1	0.99	0.10	40,40,40,40	1
30	OEX	A	418[A]	10/10	0.99	0.13	31,35,38,46	10
35	CA	O	302	1/1	0.99	0.05	80,80,80,80	0
21	FE2	A	401[A]	1/1	1.00	0.11	45,45,45,45	1
21	FE2	A	401[B]	1/1	1.00	0.11	47,47,47,47	1

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

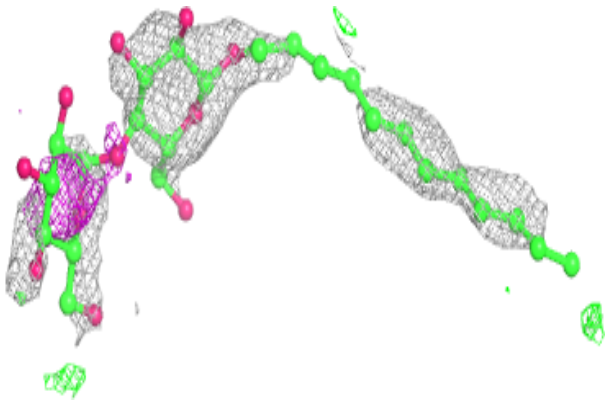
Electron density around DGD e 101:

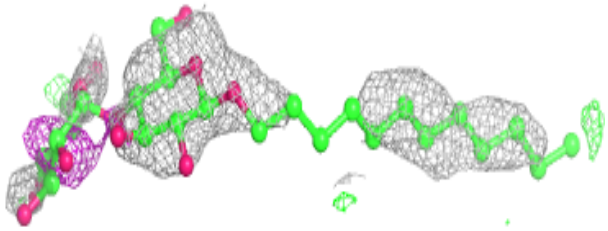
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

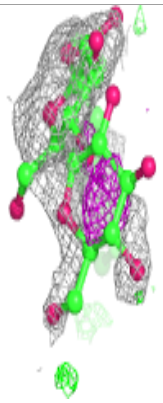


Electron density around LMT F 101:

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

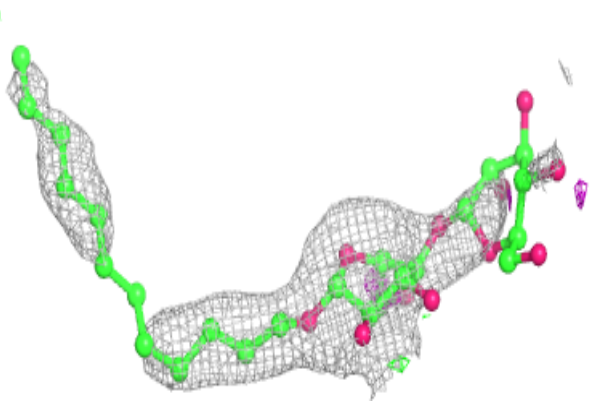


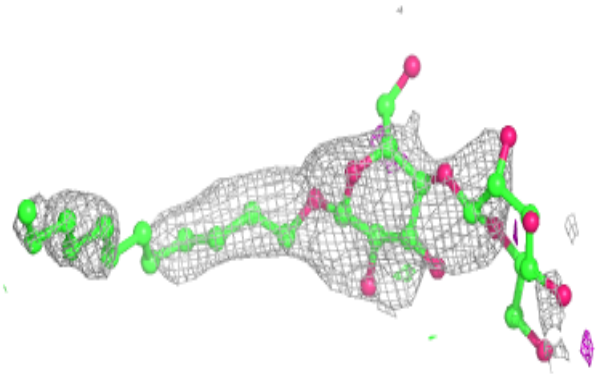


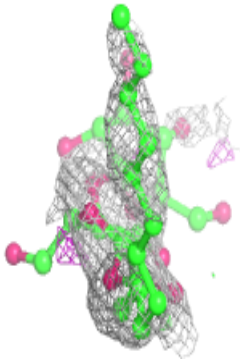


Electron density around LMT C 521:

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

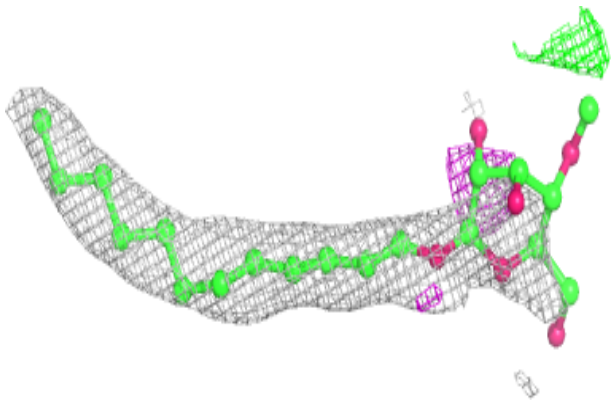


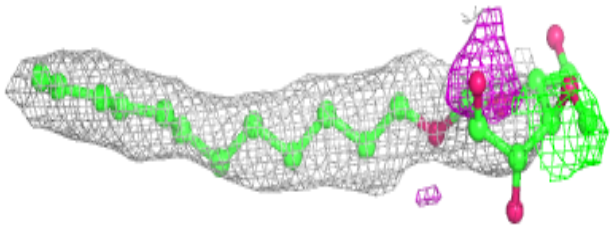


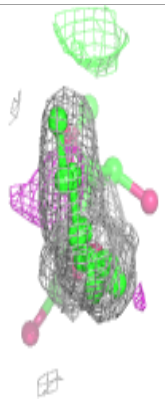


Electron density around LMT b 631:

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

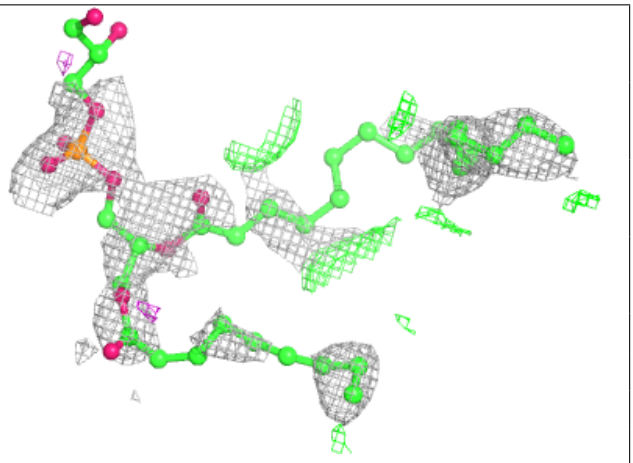


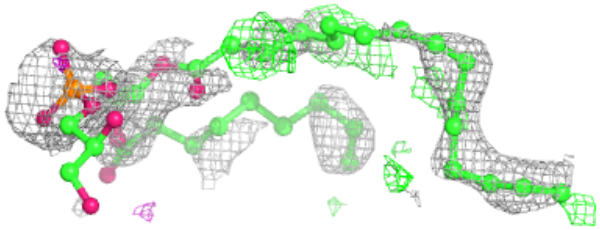


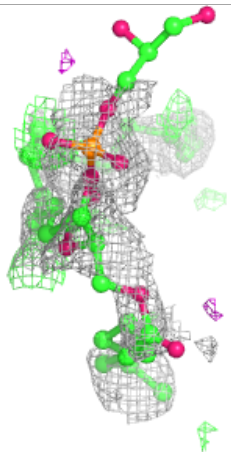


Electron density around LHG a 422:

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

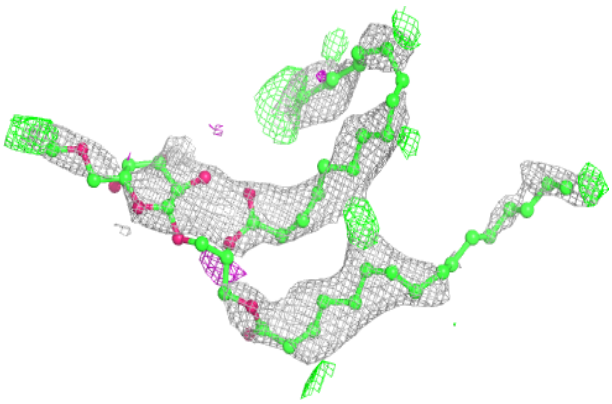


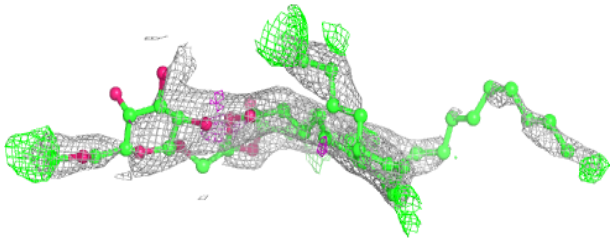


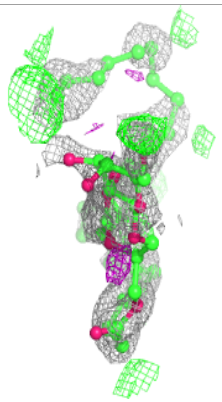


Electron density around DGD D 406:

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

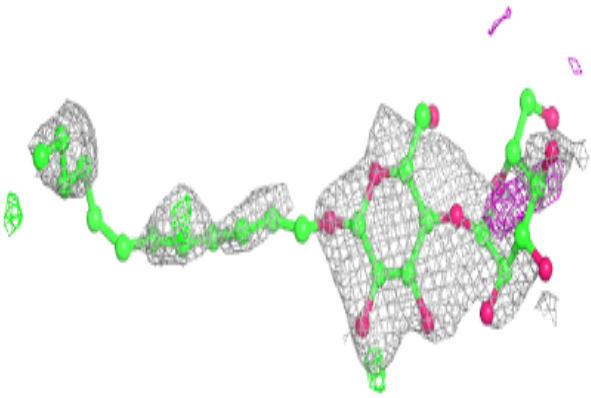


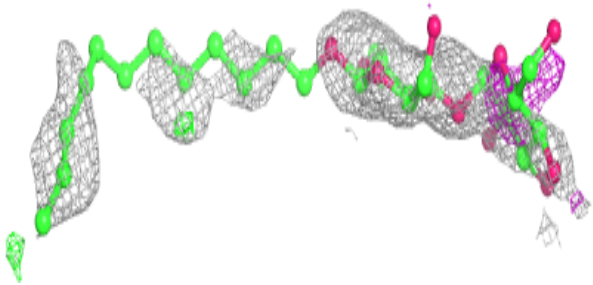


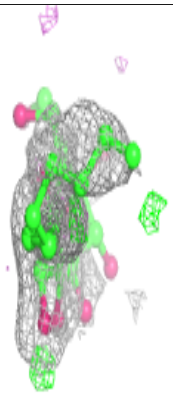


Electron density around LMT a 421:

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

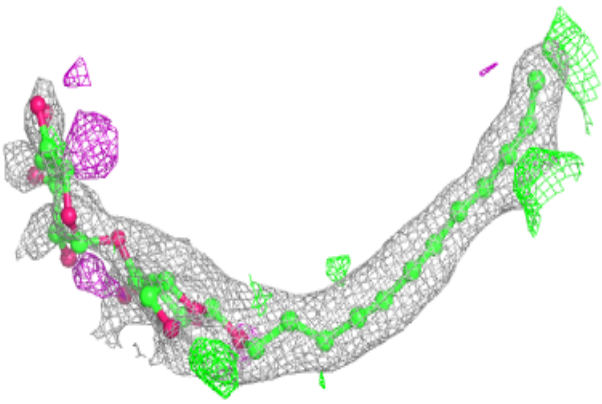


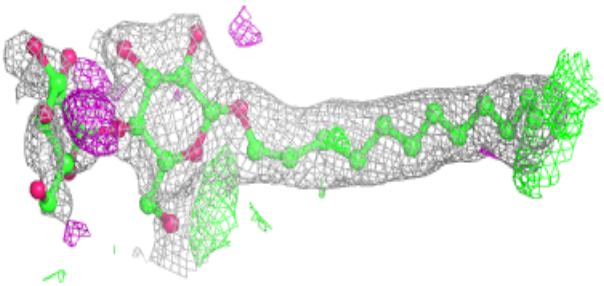


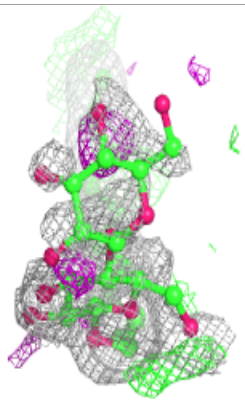


Electron density around LMT M 103:

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

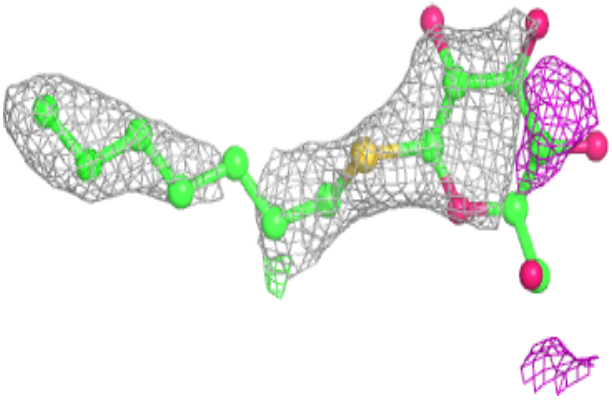


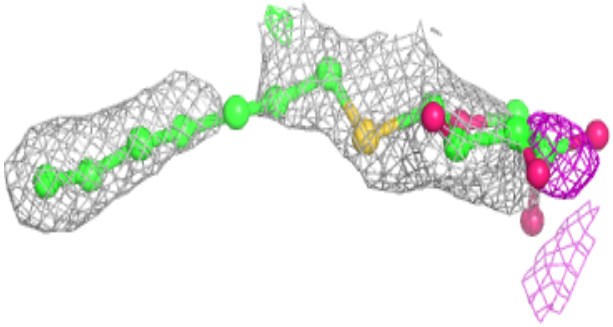


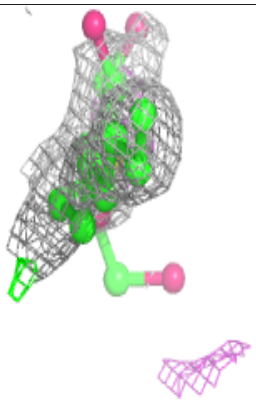


Electron density around HTG c 525:

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

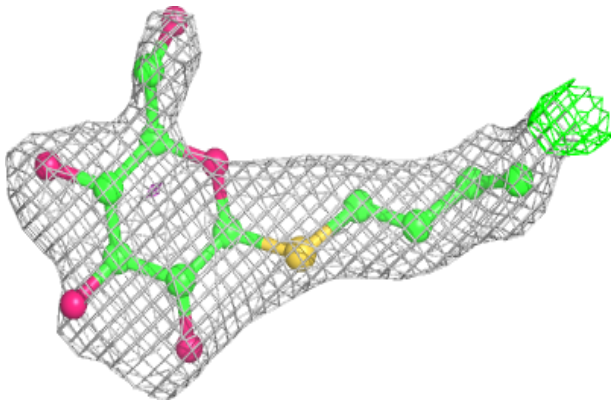


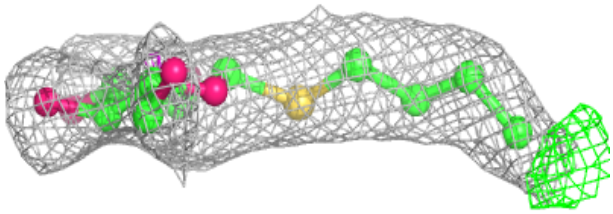


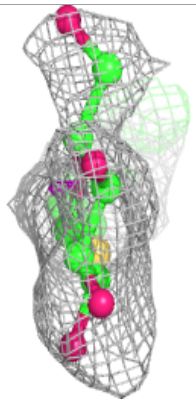


Electron density around HTG d 411:

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

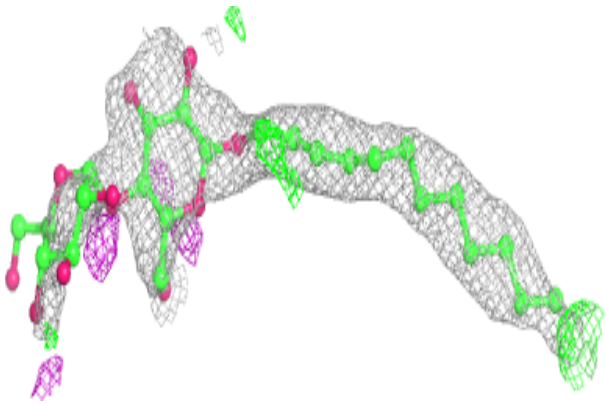


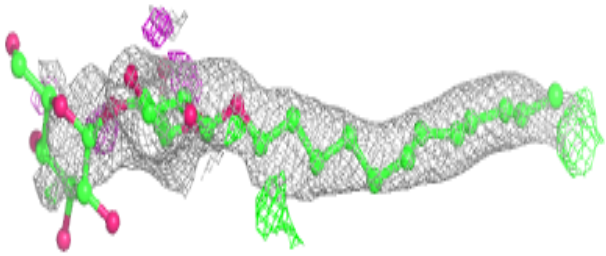


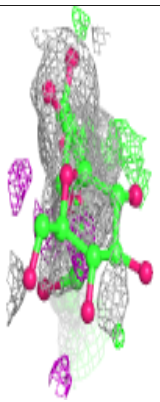


Electron density around LMT D 401:

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

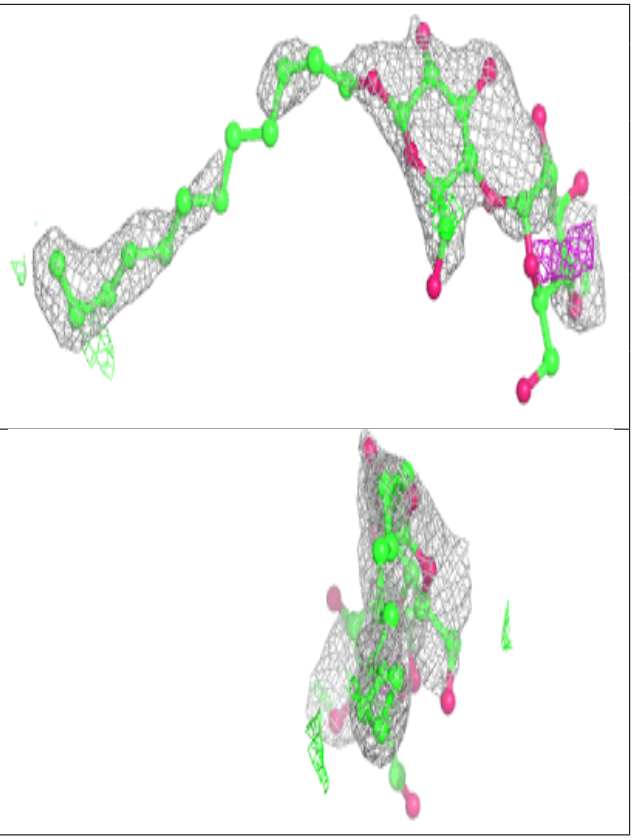


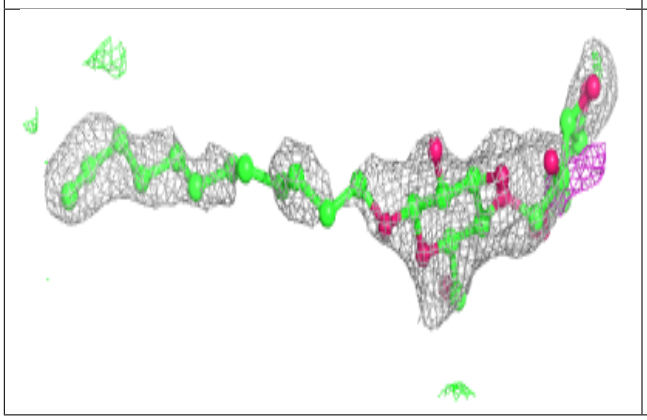




Electron density around LMT f 103:

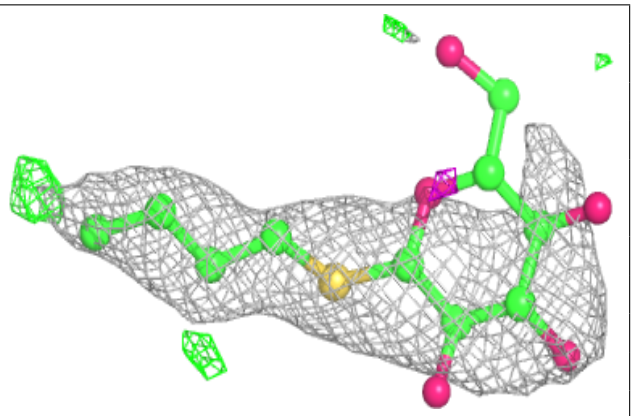
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

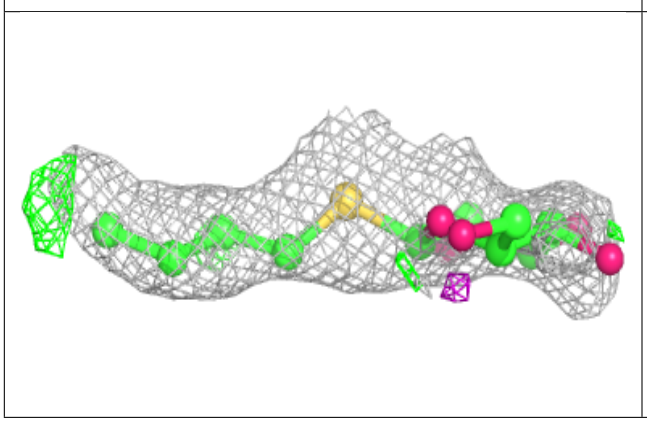


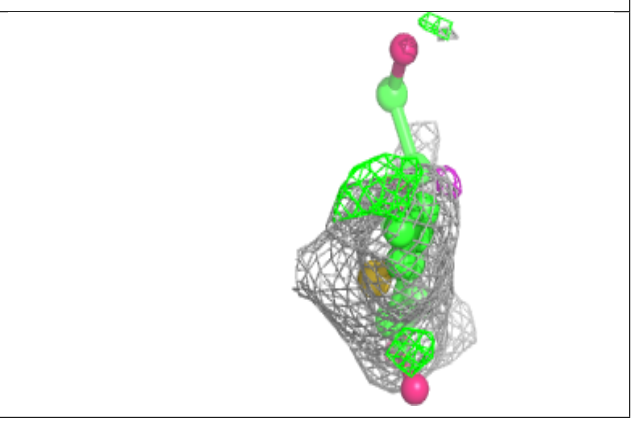


Electron density around HTG H 101:

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

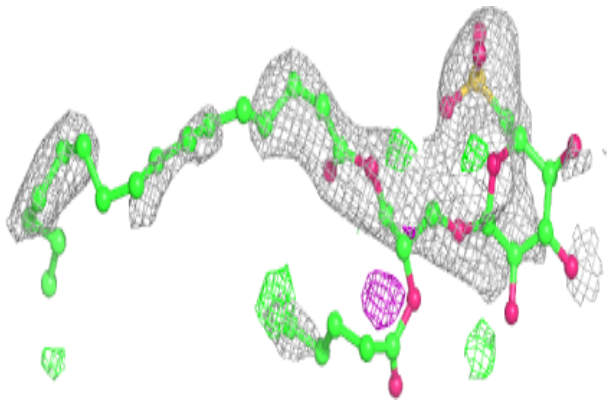


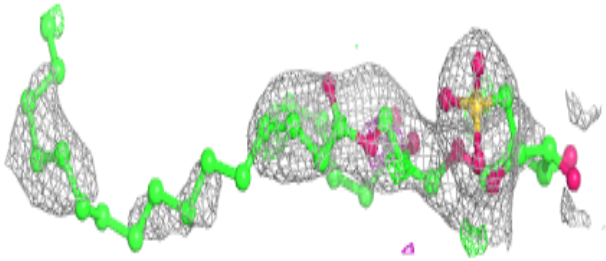


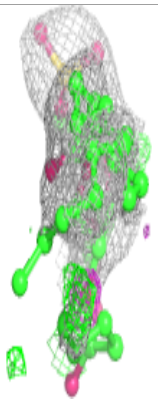


Electron density around SQD f 102:

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

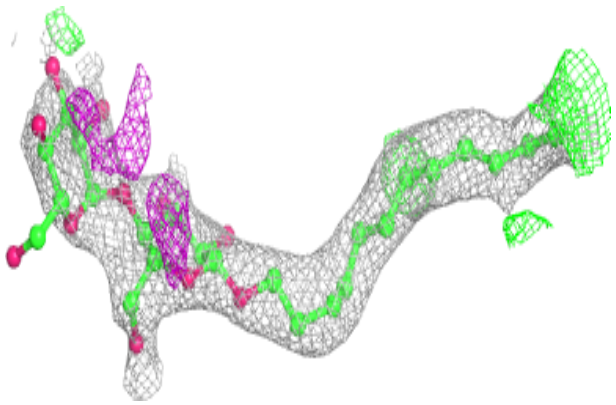


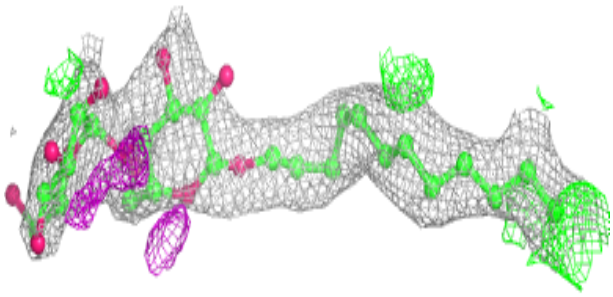


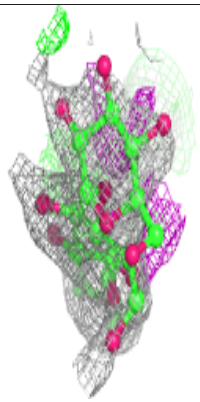


Electron density around LMT a 404:

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

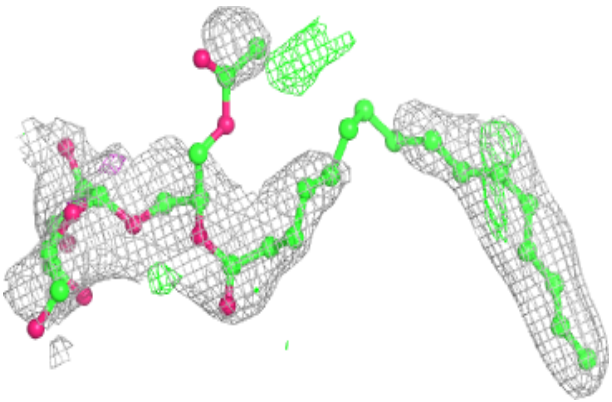


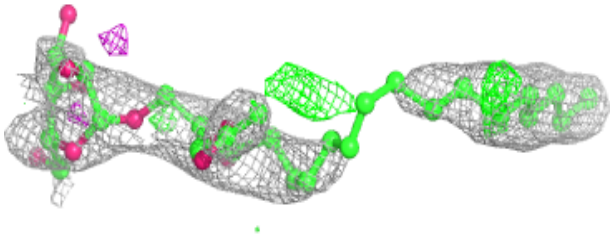


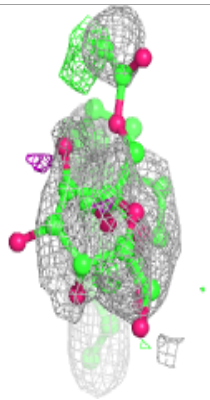


Electron density around LMG Z 101:

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

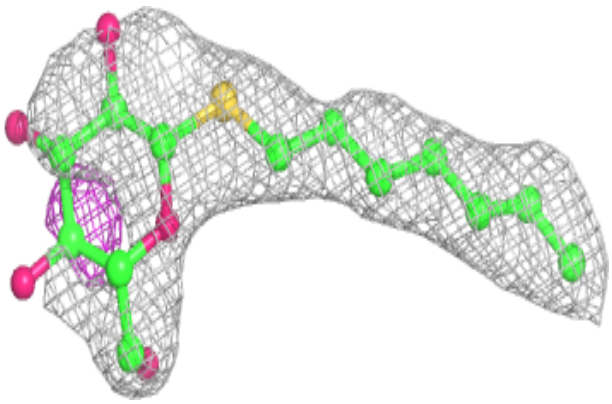


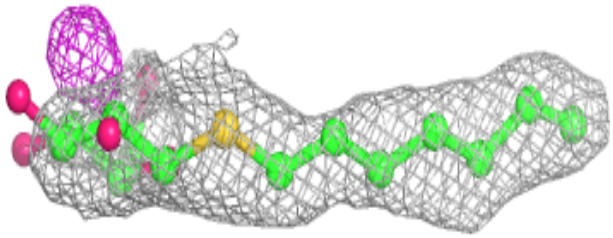


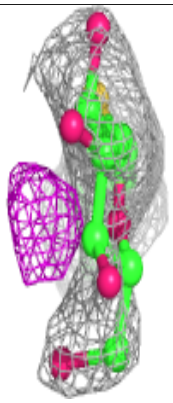


Electron density around HTG b 609:

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

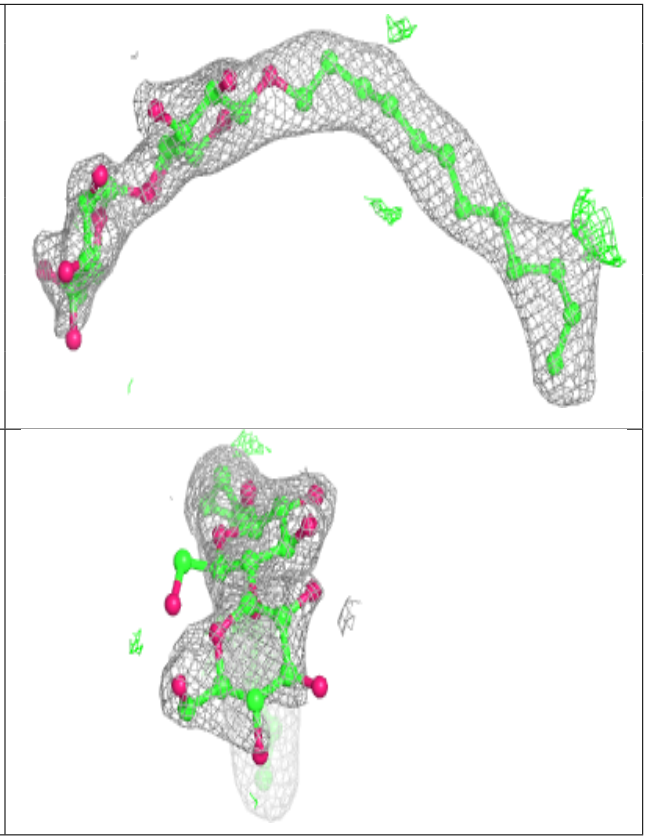






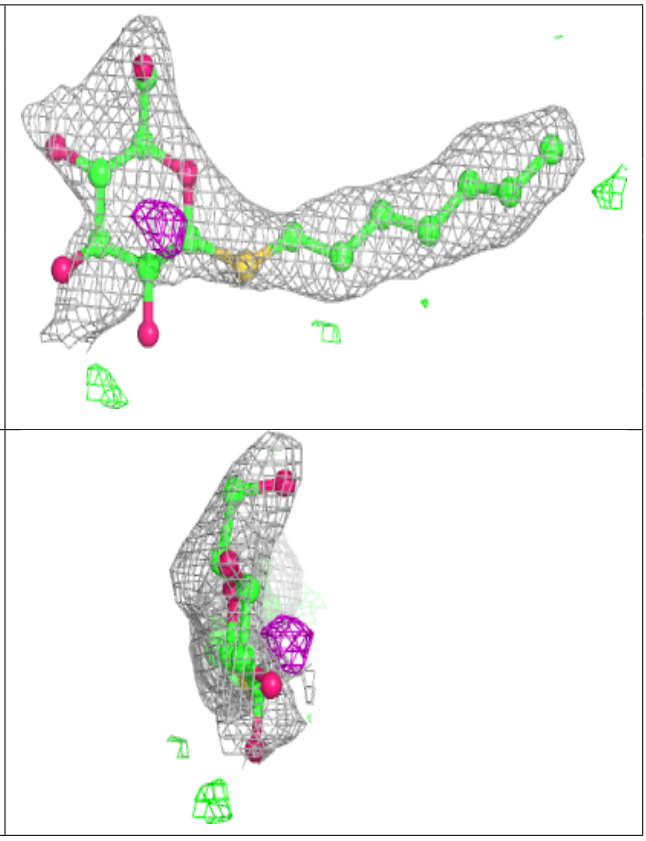
Electron density around LMT m 102:

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



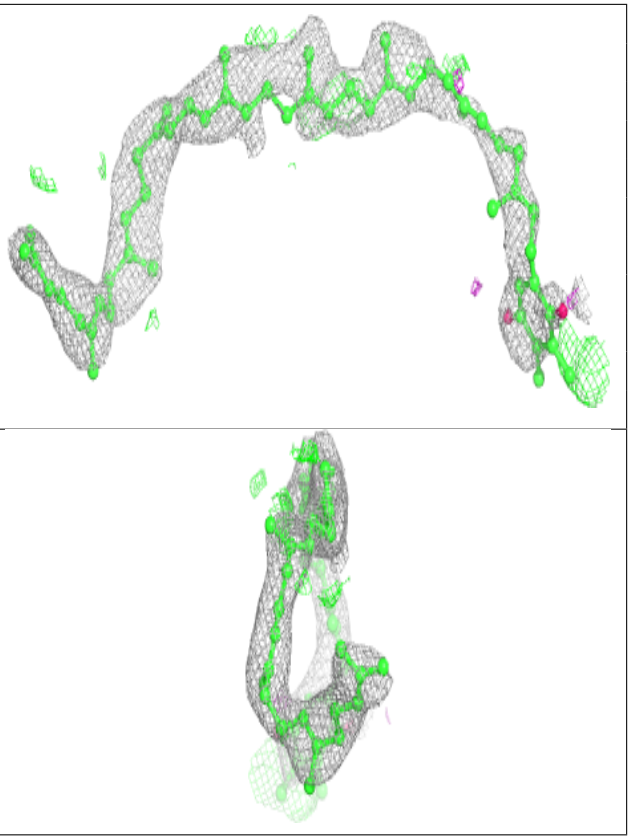
Electron density around HTG B 633:

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



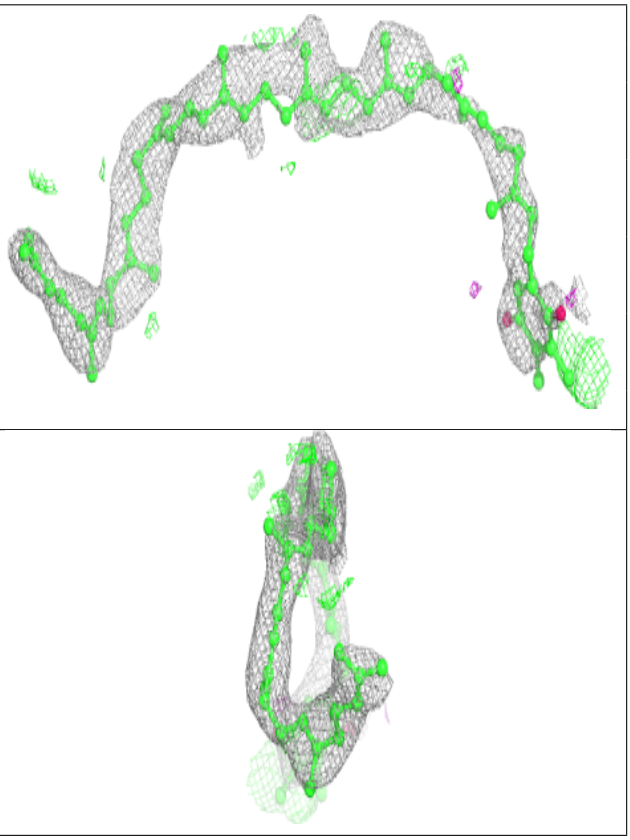
Electron density around PL9 a 416 (A):

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



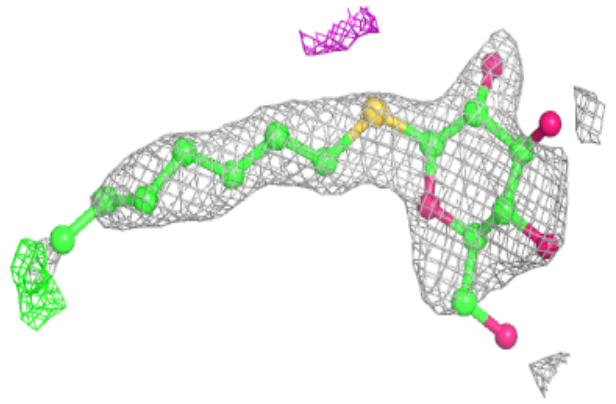
Electron density around PL9 a 416 (B):

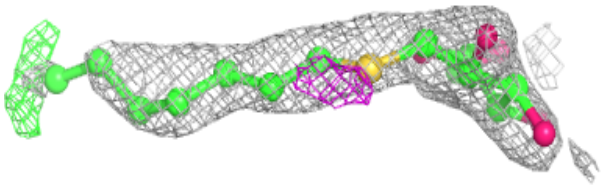
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

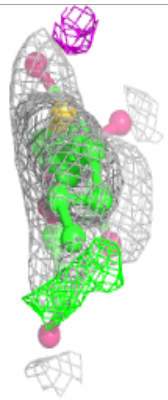


Electron density around HTG B 625:

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

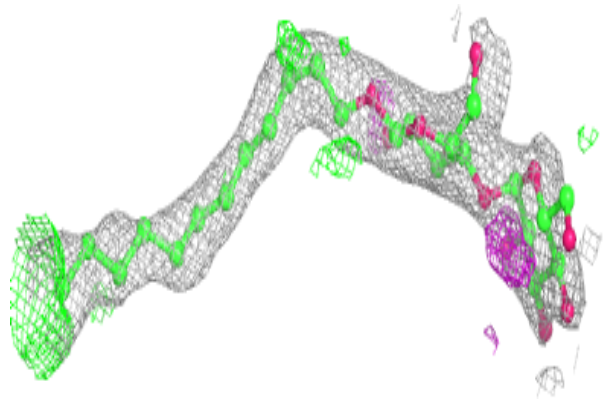


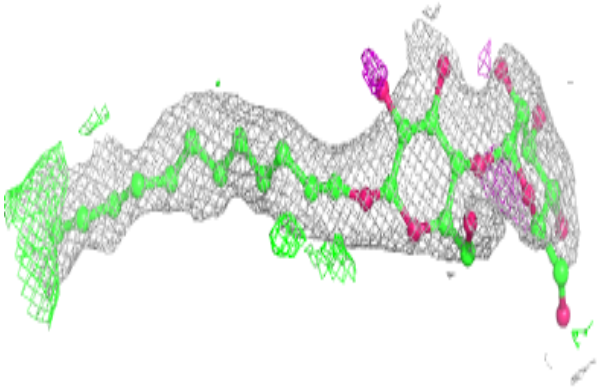


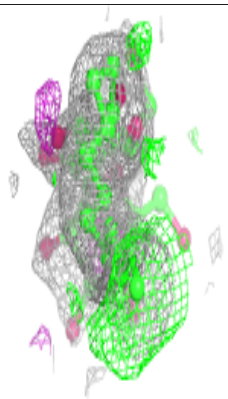


Electron density around LMT A 417:

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

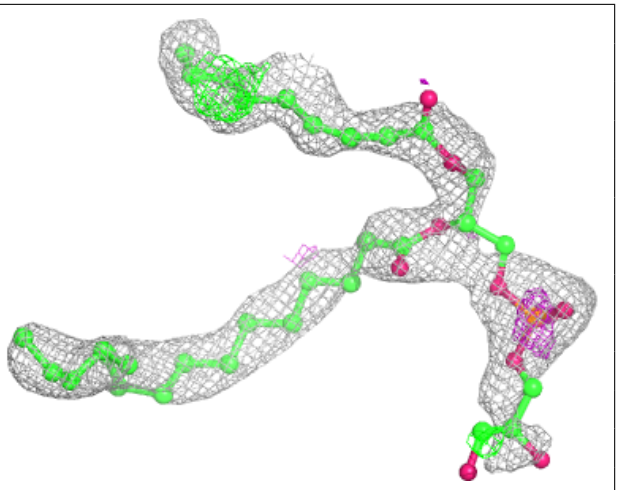


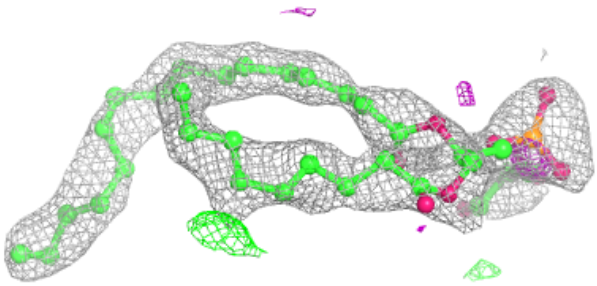


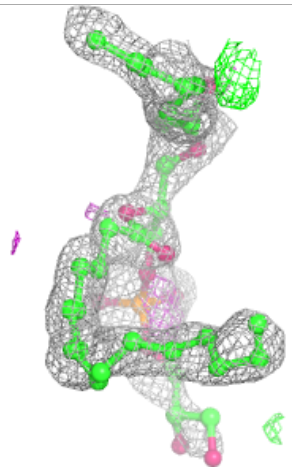


Electron density around LHG E 101:

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

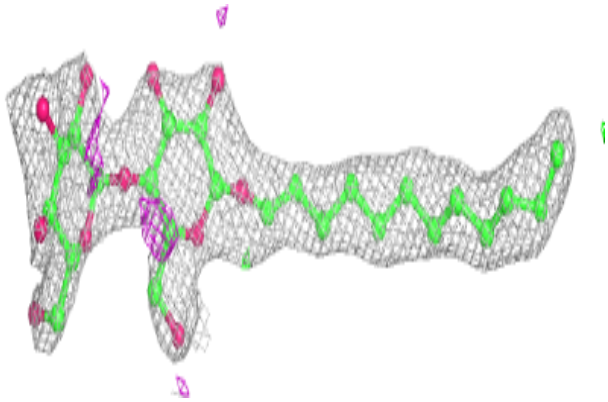


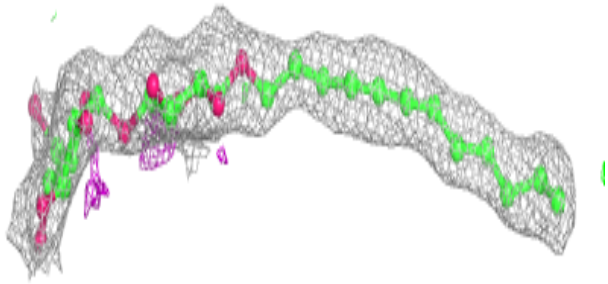


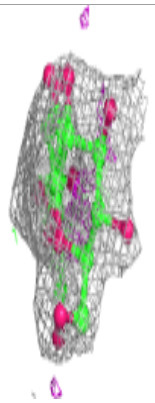


Electron density around LMT M 104:

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

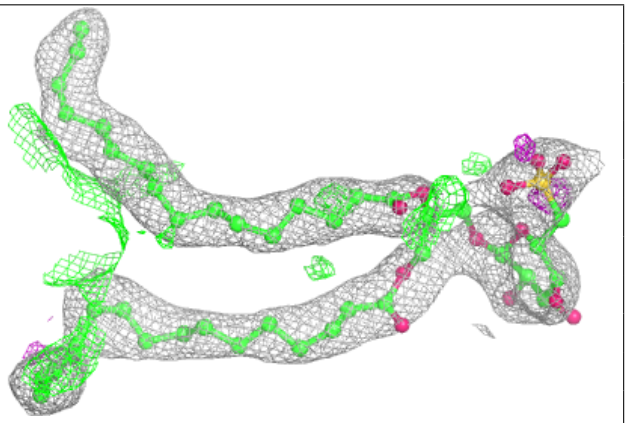


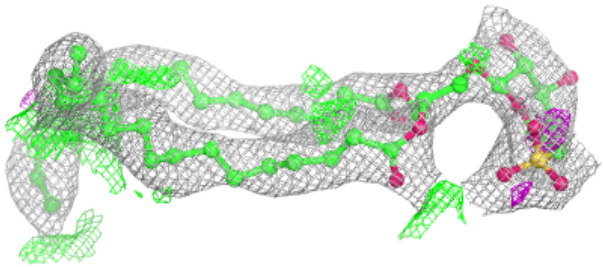


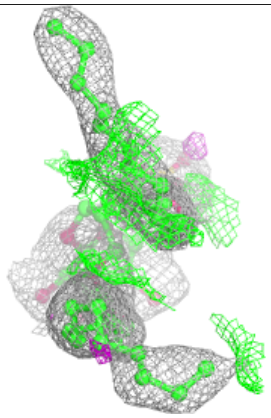


Electron density around SQD b 601:

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

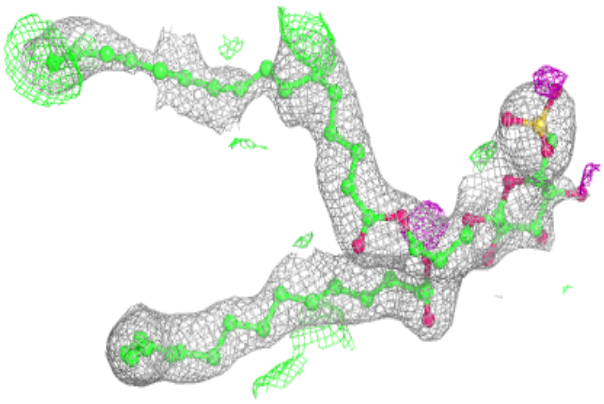


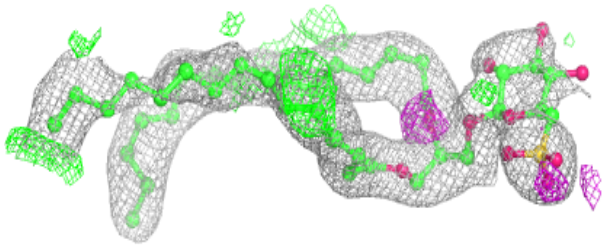


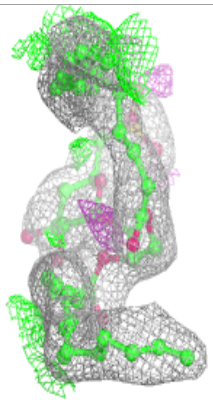


Electron density around SQD A 416:

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

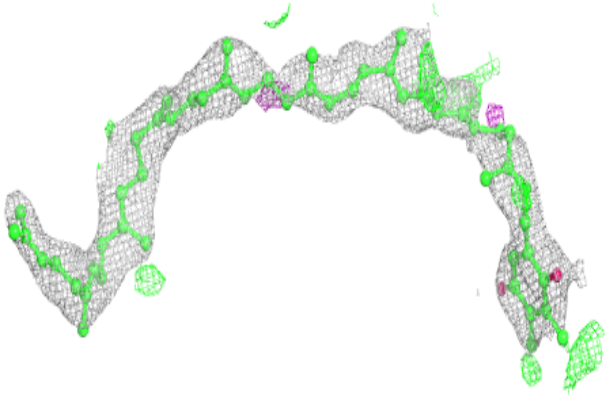


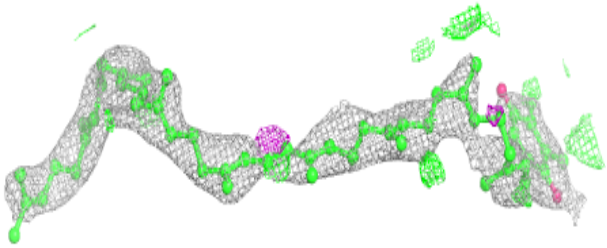


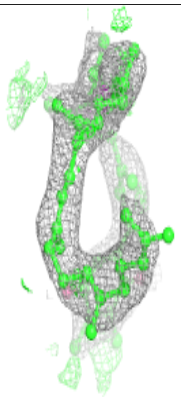


Electron density around PL9 A 420 (A):

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

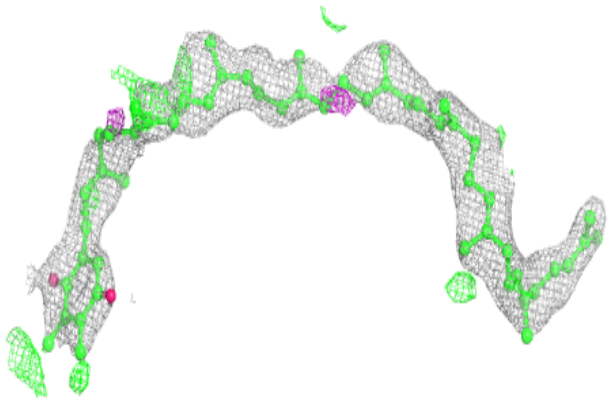


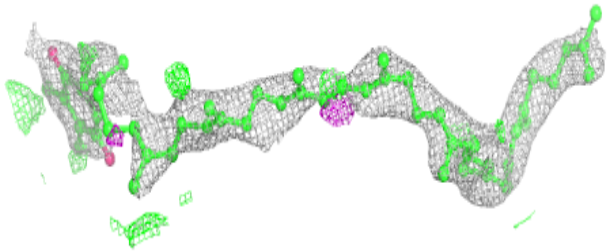


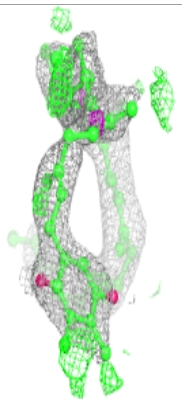


Electron density around PL9 A 420 (B):

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

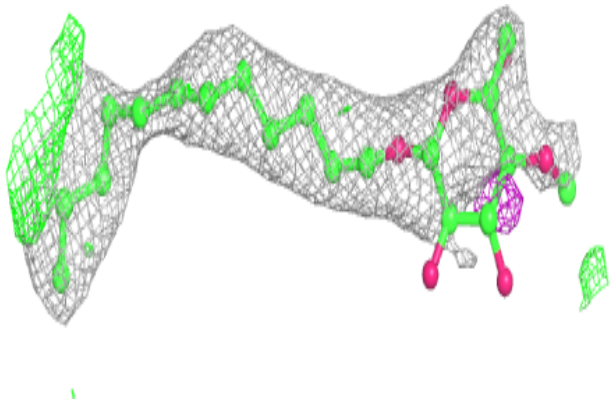


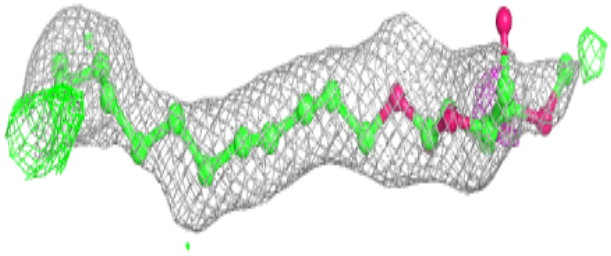


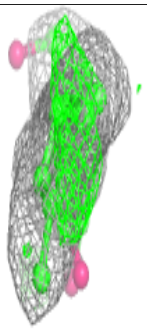


Electron density around LMT T 104:

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

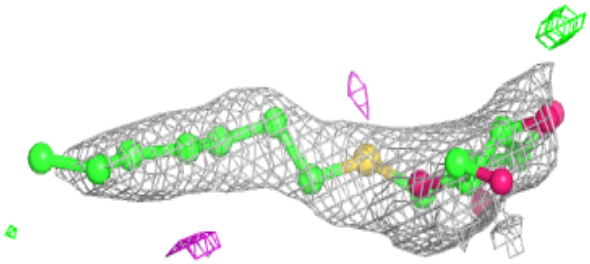


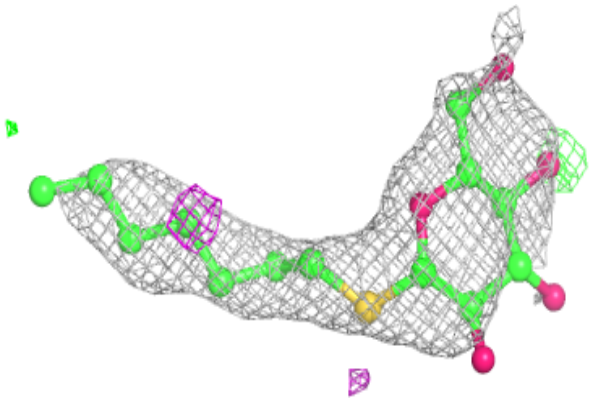


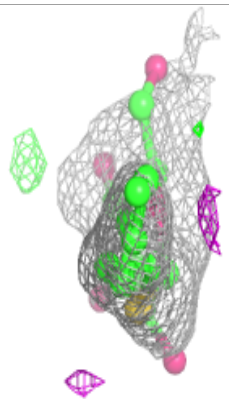


Electron density around HTG b 633:

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

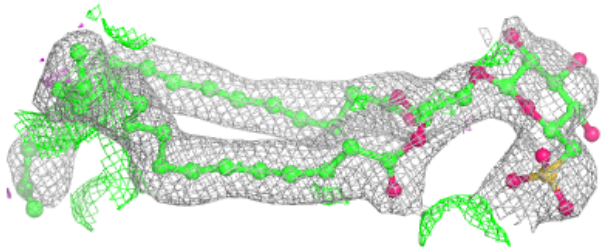


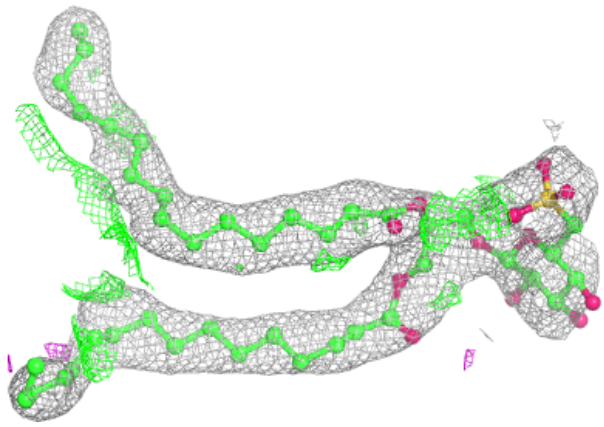


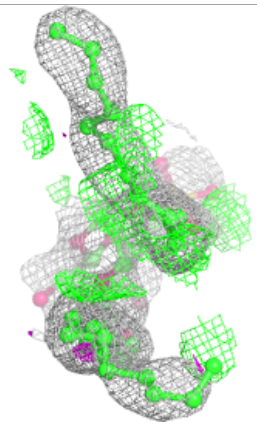


Electron density around SQD B 621:

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

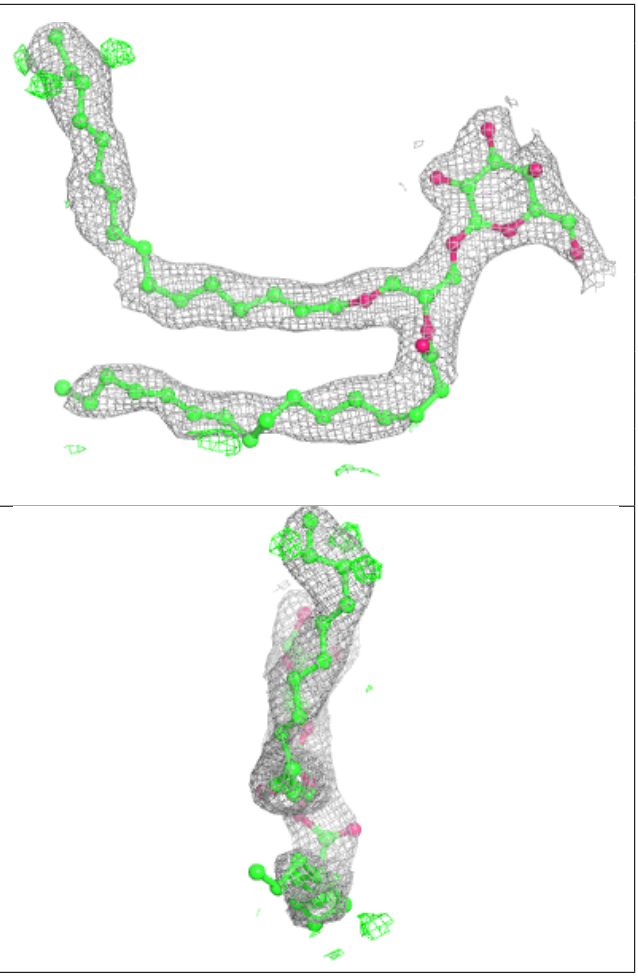






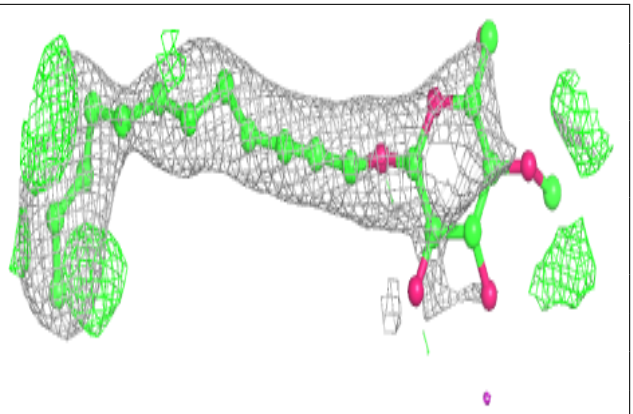
Electron density around LMG C 519:

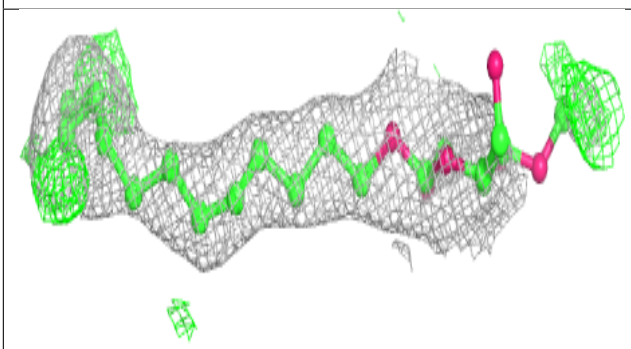
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

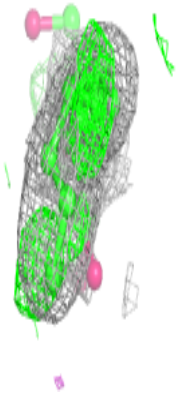


Electron density around LMT B 635:

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

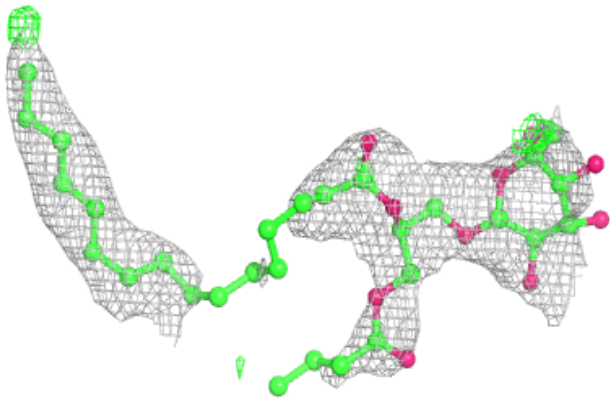


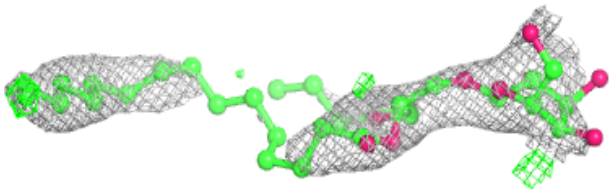


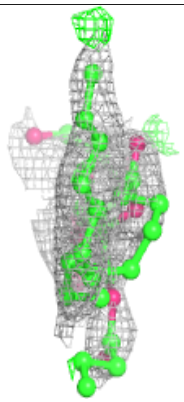


Electron density around LMG z 101:

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

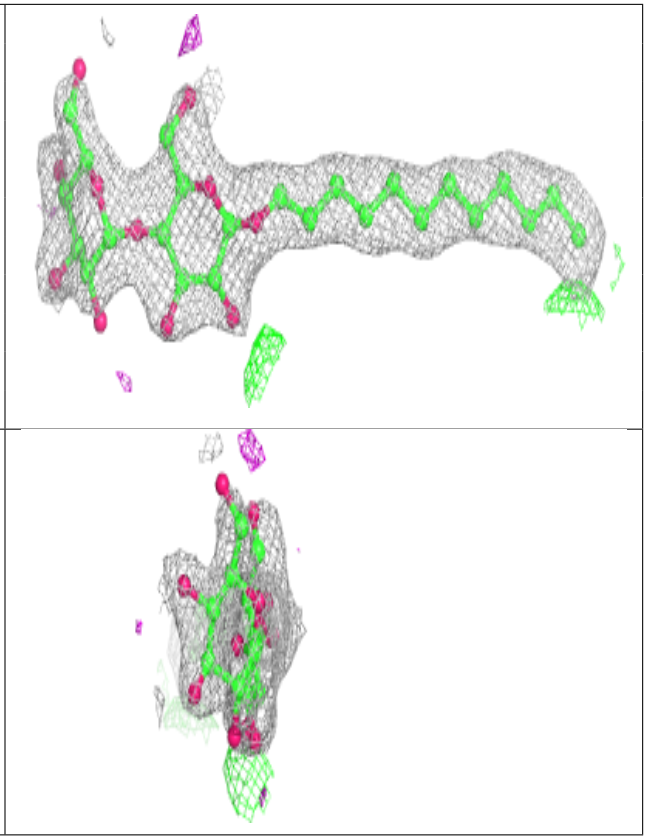


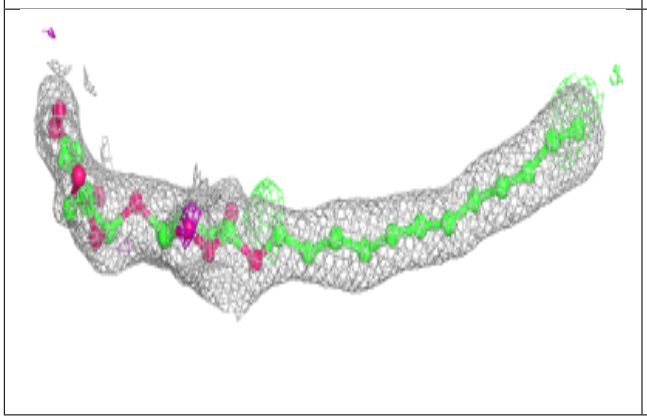




Electron density around LMT M 101:

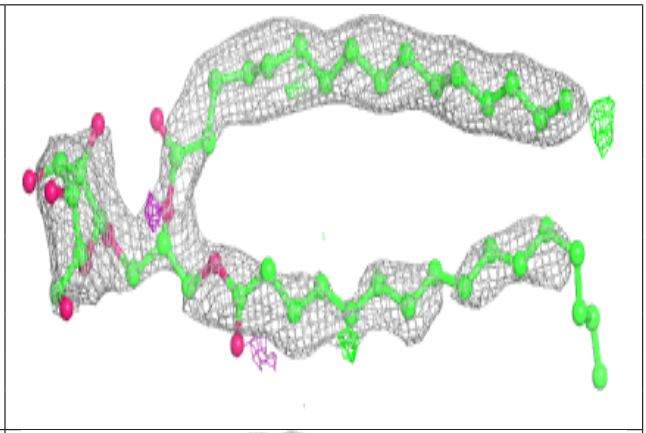
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

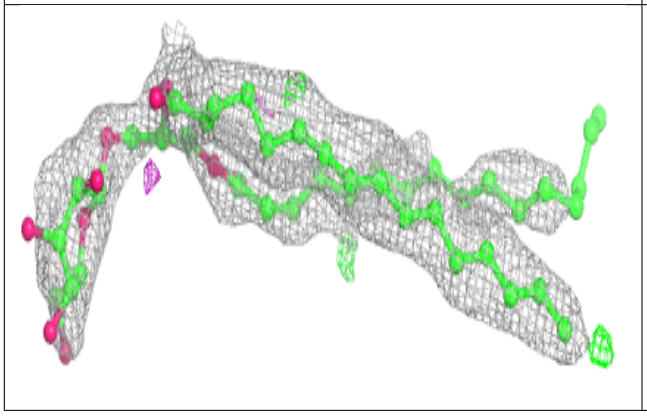


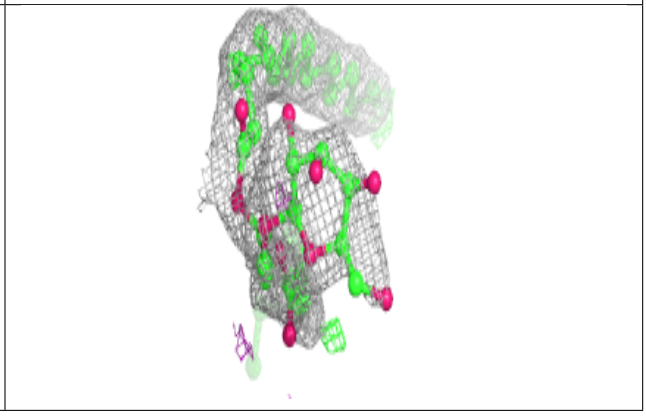


Electron density around LMG C 520:

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

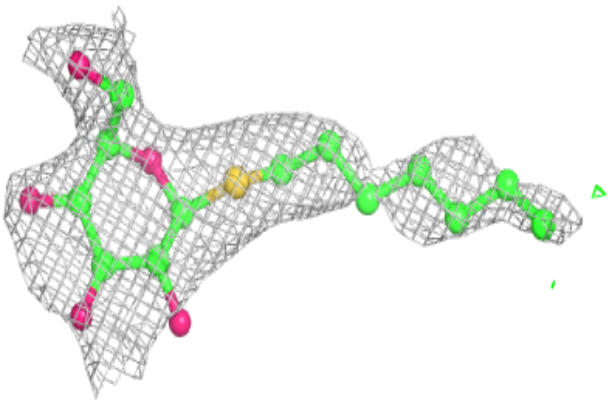


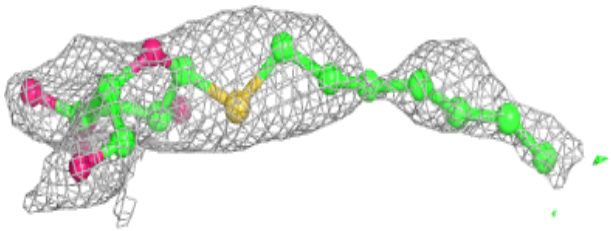


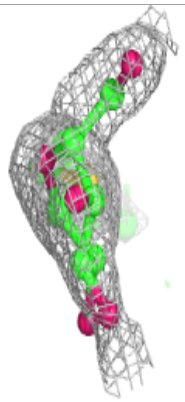


Electron density around HTG C 523:

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

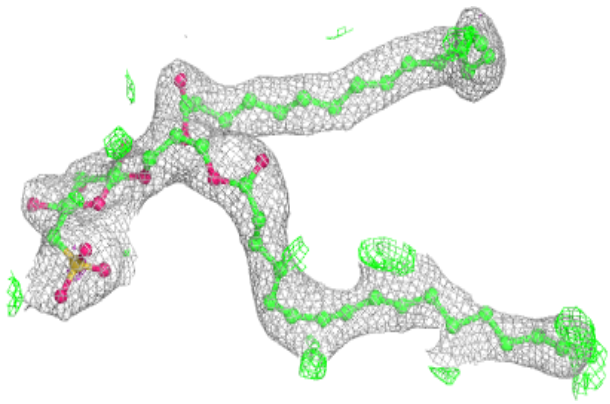


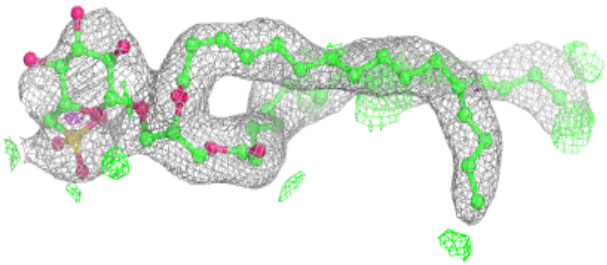


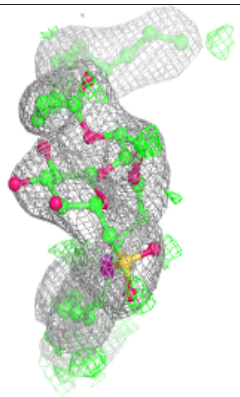


Electron density around SQD a 405:

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

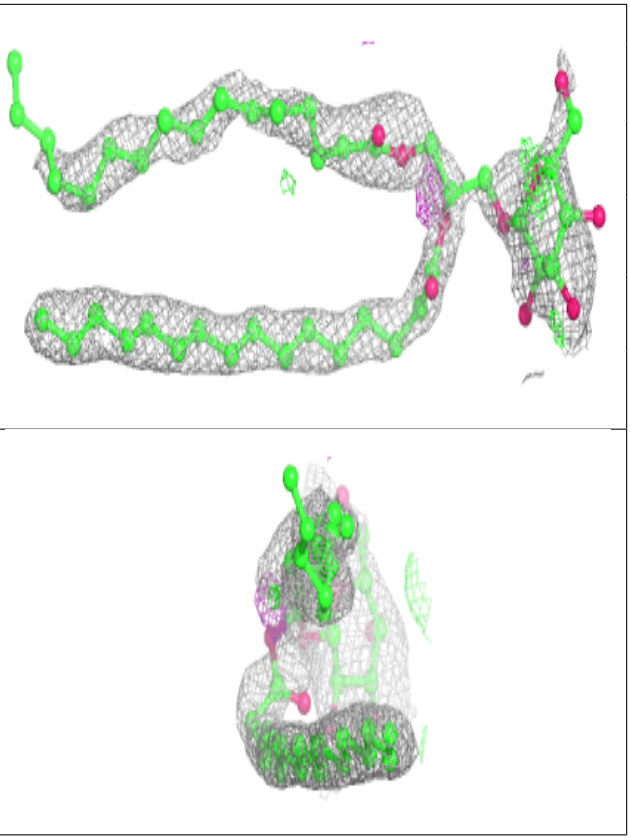






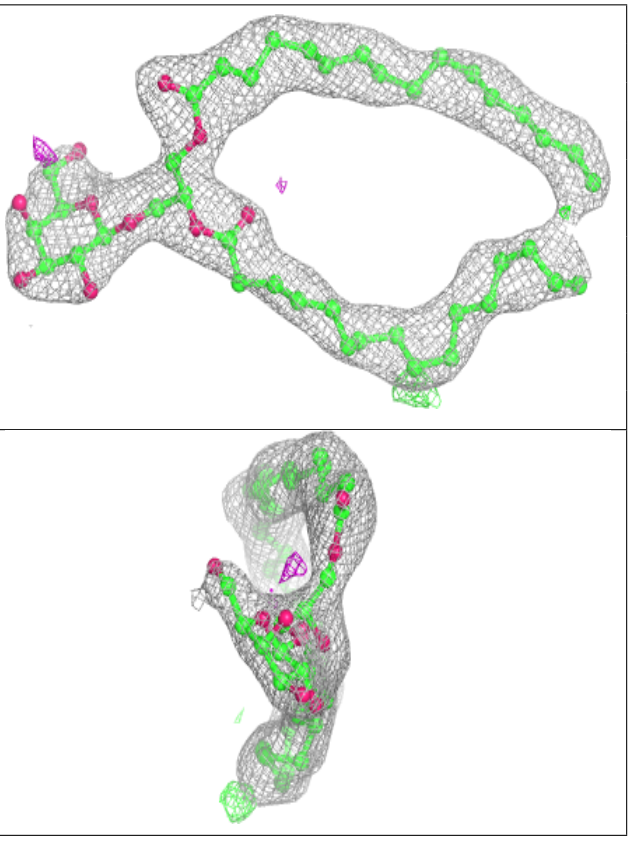
Electron density around LMG c 523:

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



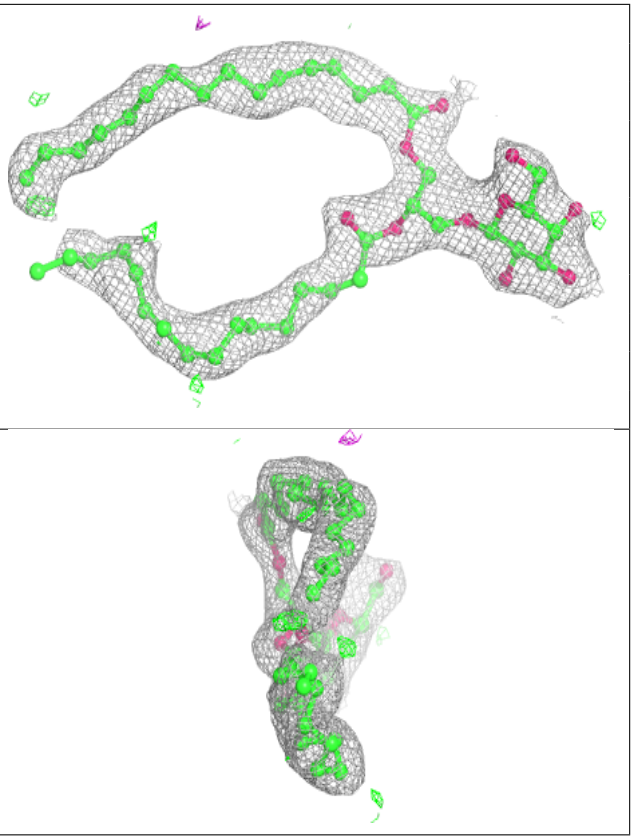
Electron density around LMG a 415:

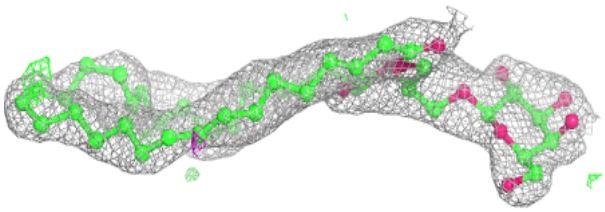
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMG A 422:

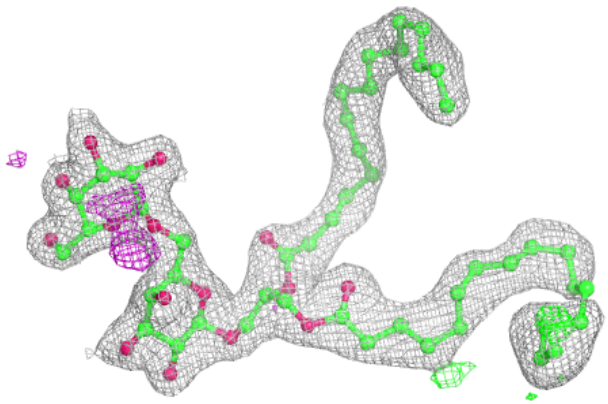
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

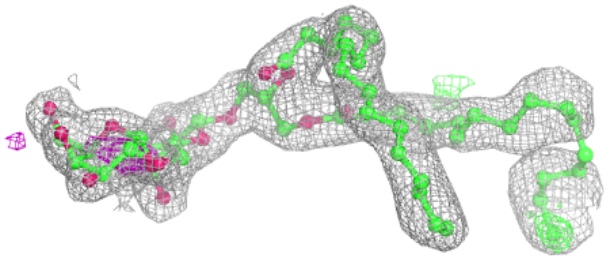


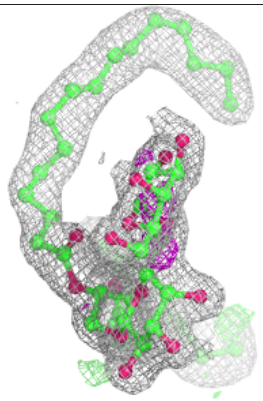


Electron density around DGD C 517:

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

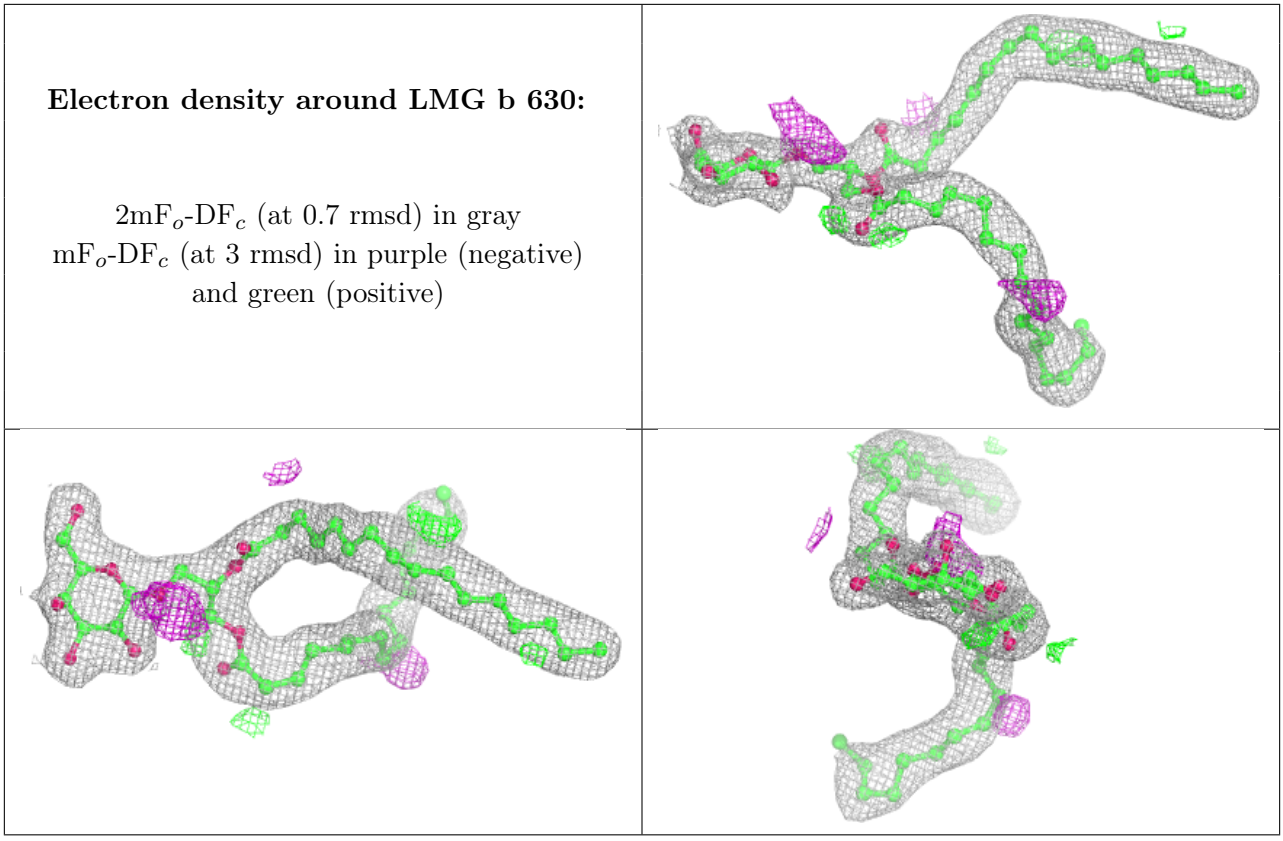






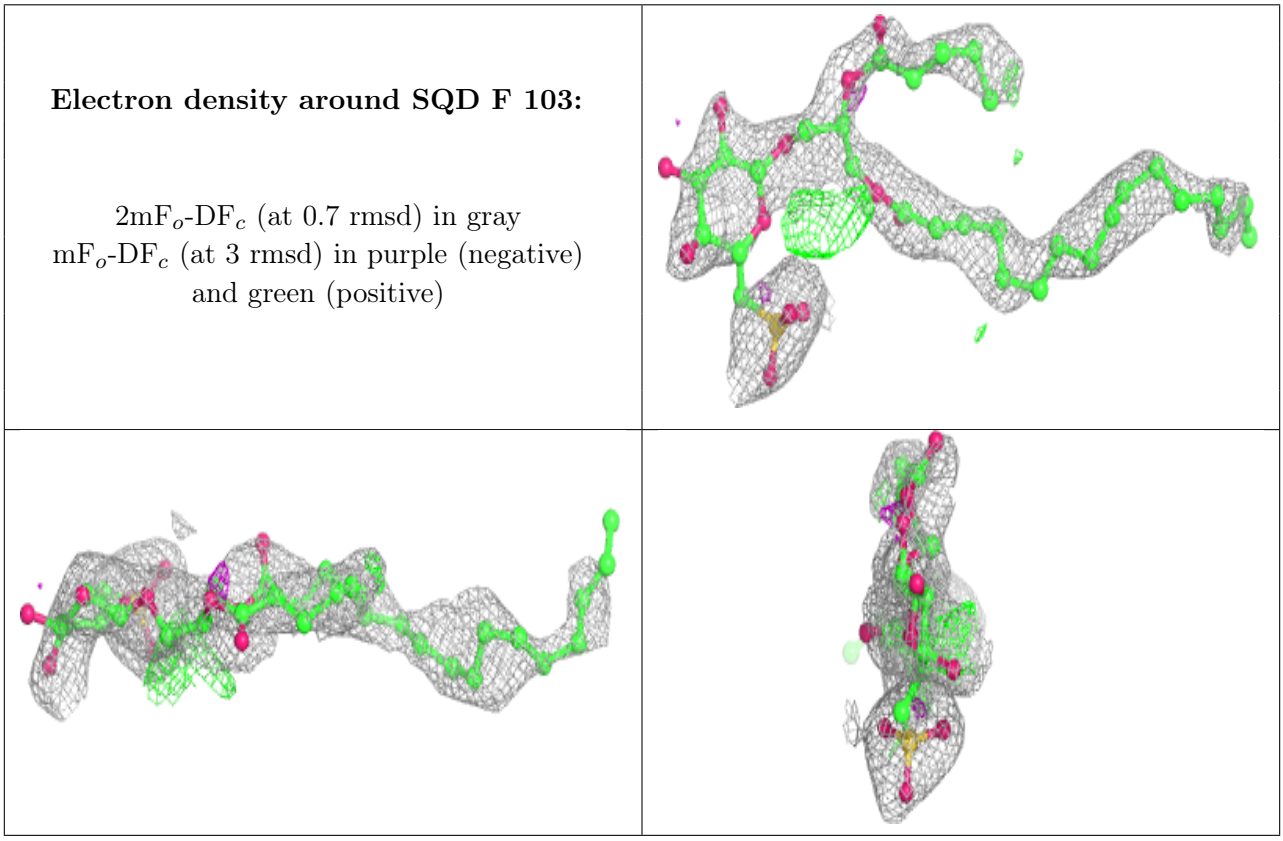
Electron density around LMG b 630:

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



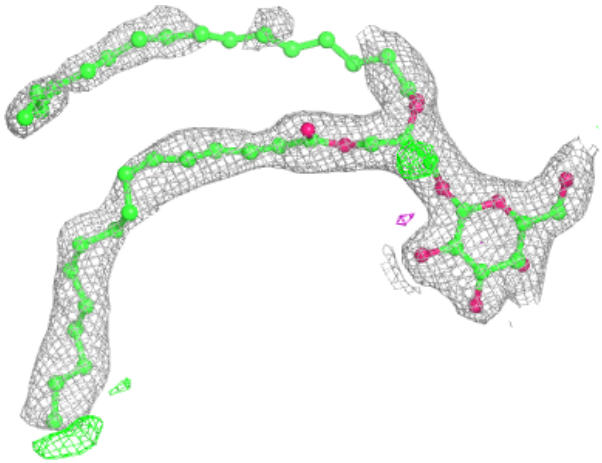
Electron density around SQD F 103:

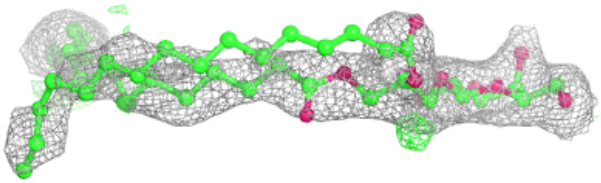
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

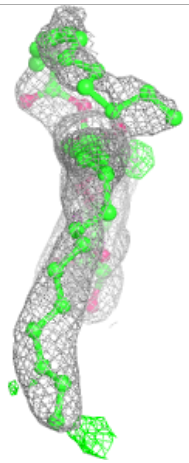


Electron density around LMG c 522:

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

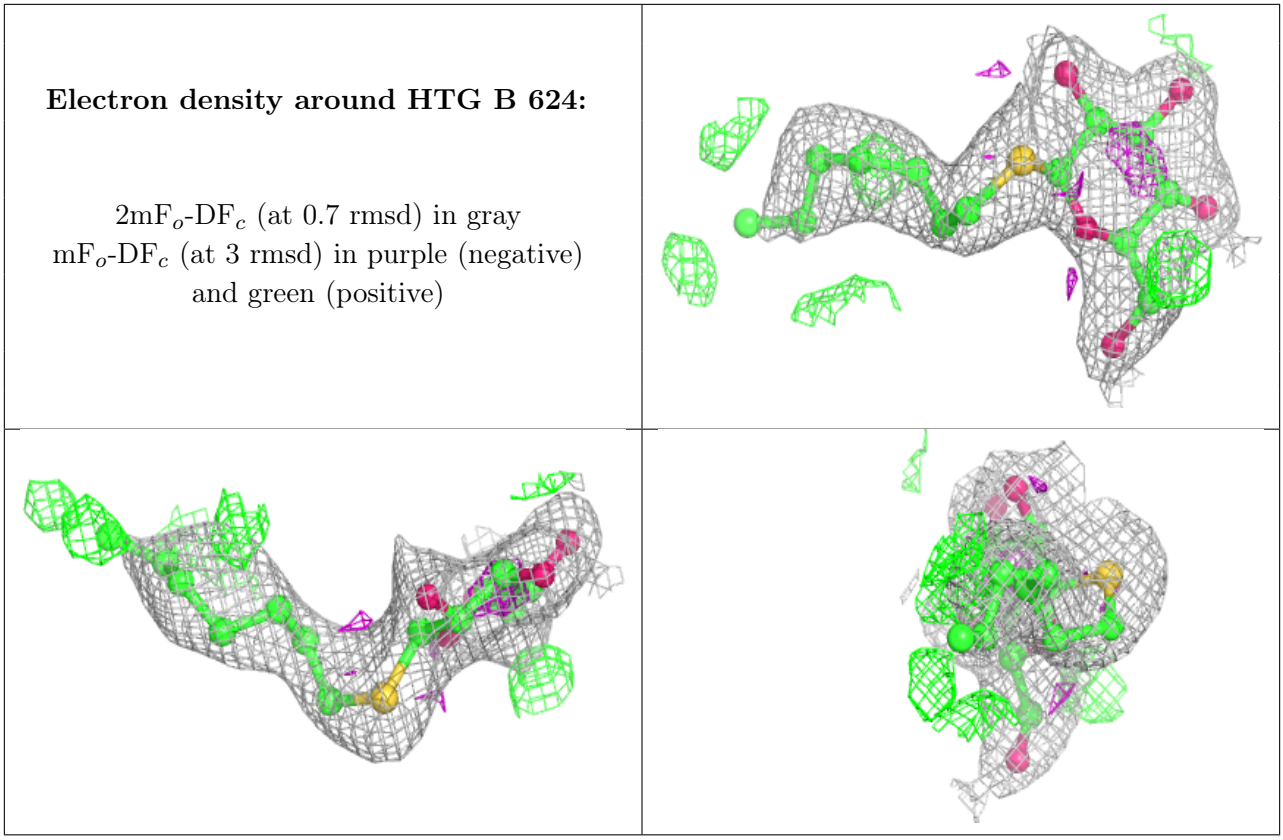






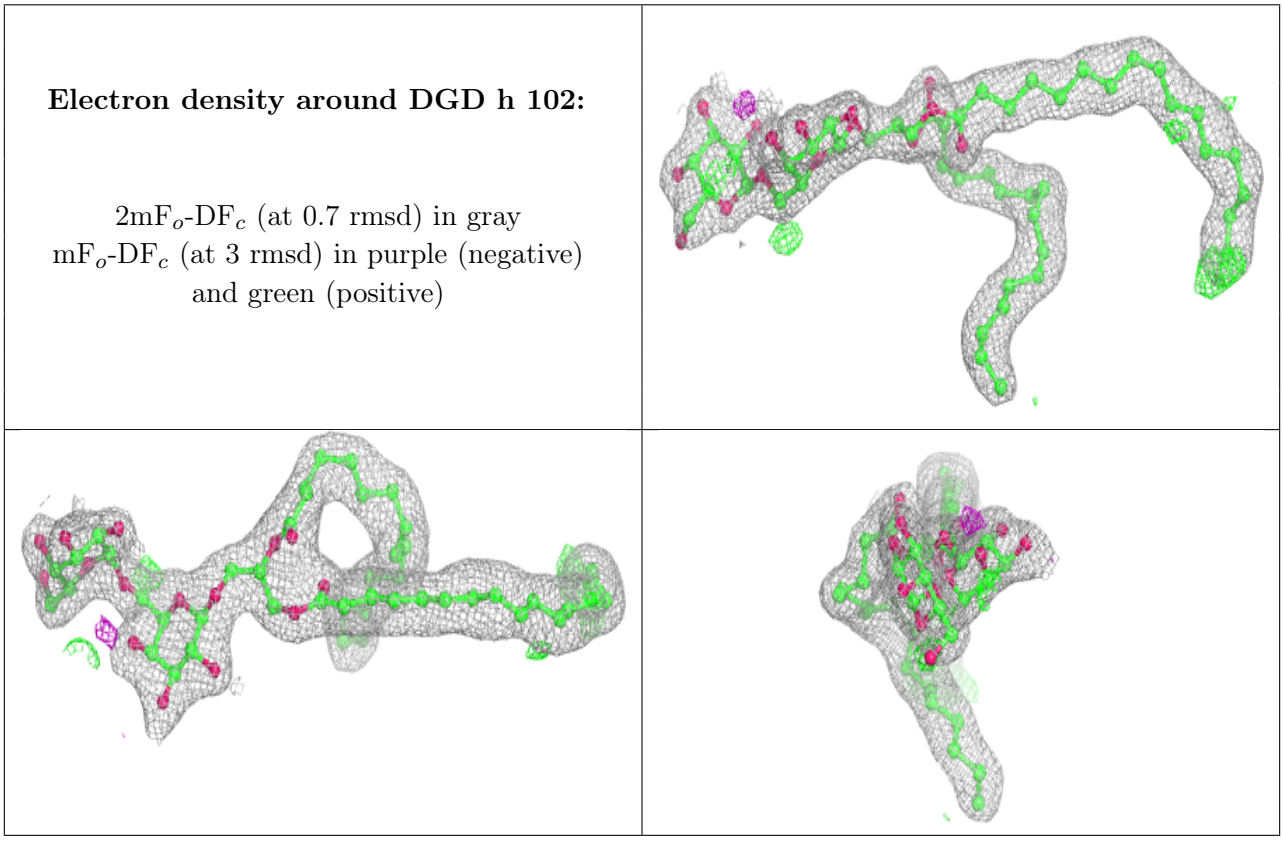
Electron density around HTG B 624:

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



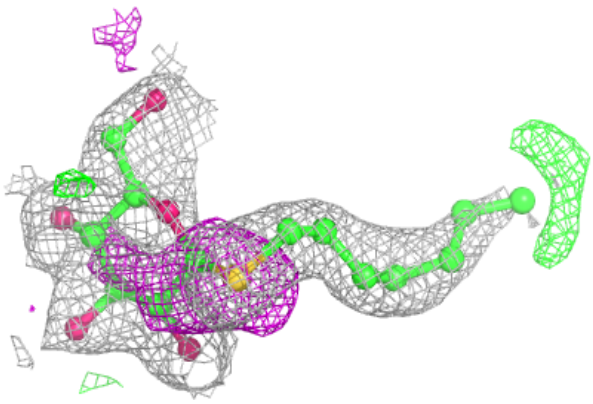
Electron density around DGD h 102:

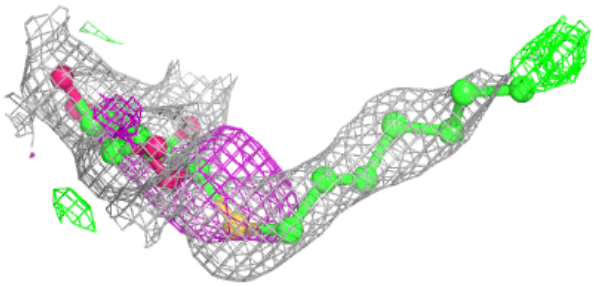
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

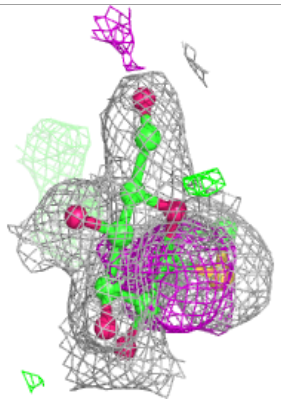


Electron density around HTG b 632:

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

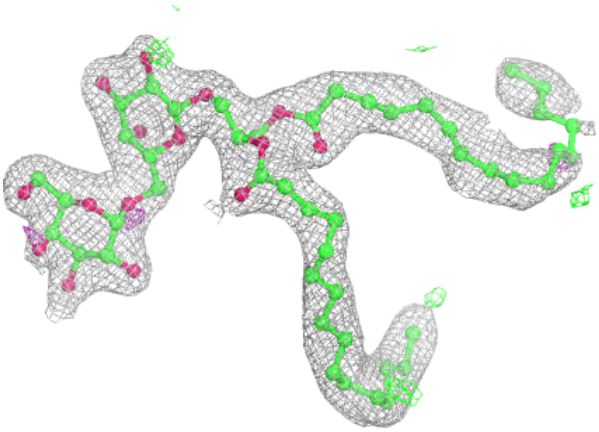


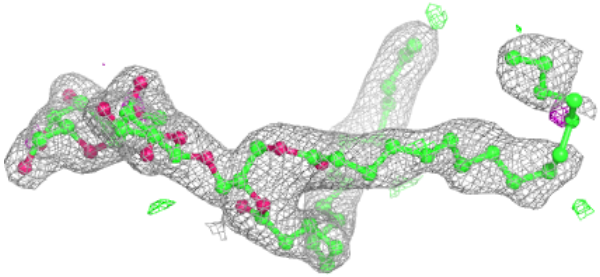


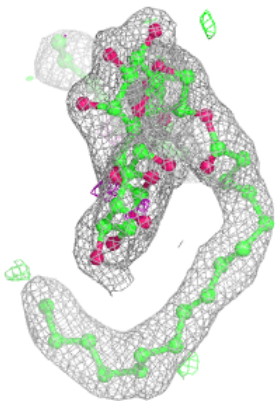


Electron density around DGD c 520:

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

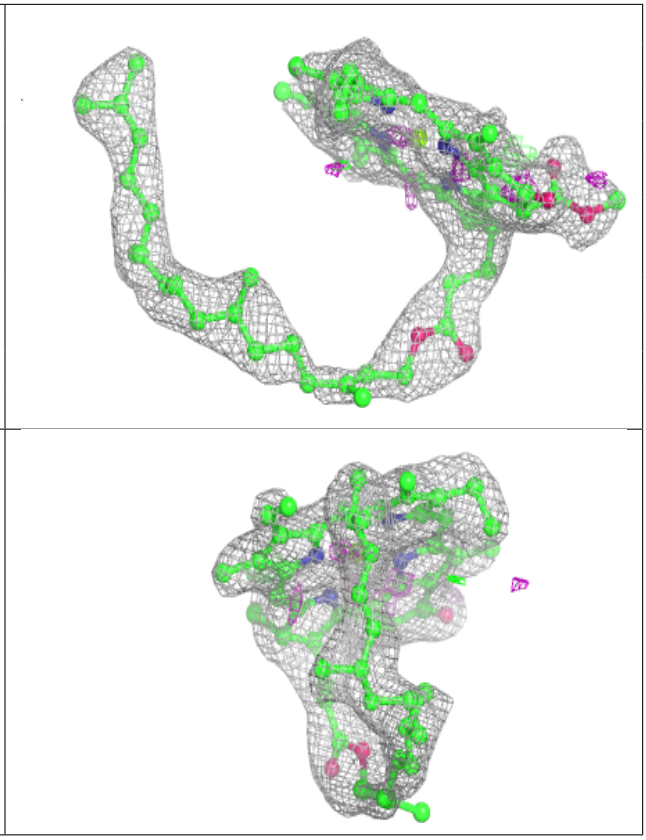






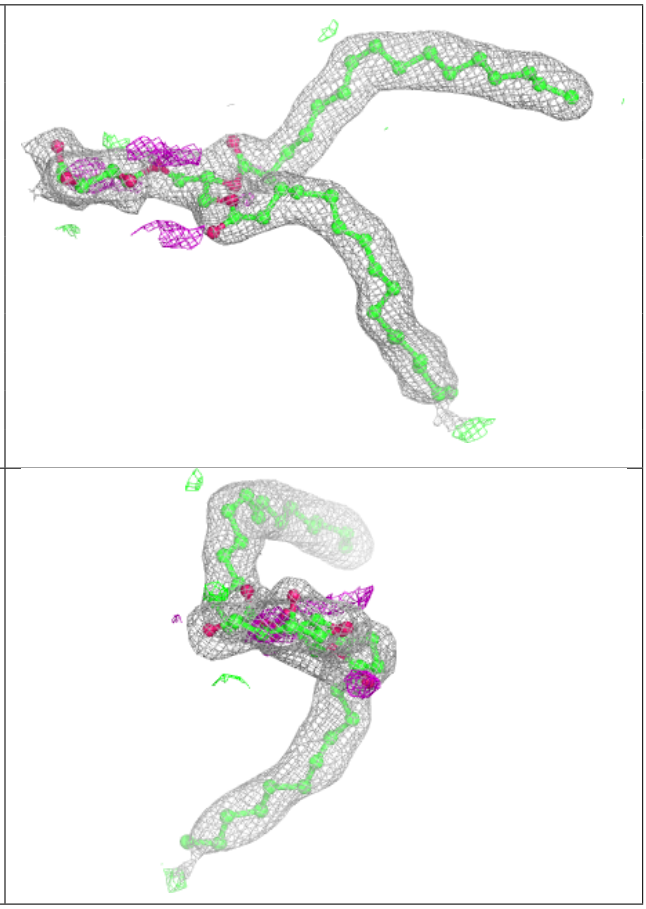
Electron density around CLA C 513:

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



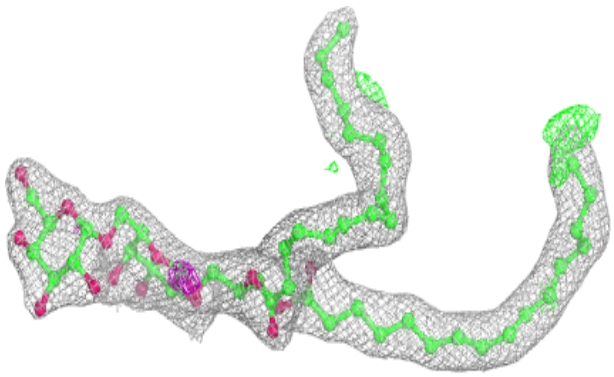
Electron density around LMG B 622:

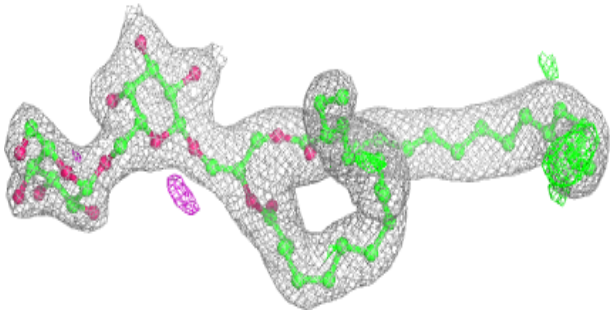
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

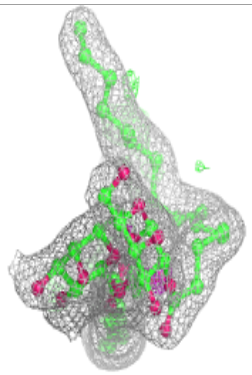


Electron density around DGD H 103:

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

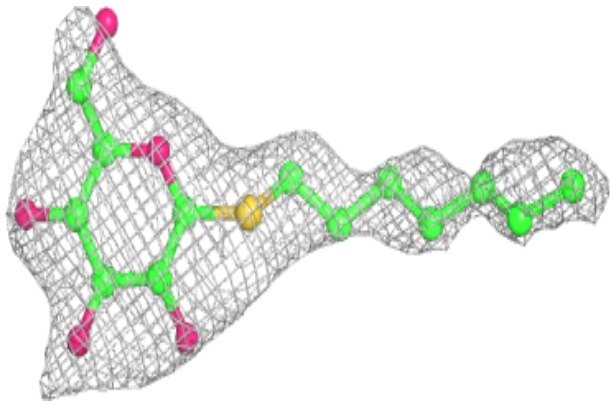


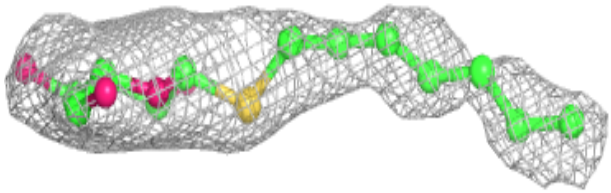


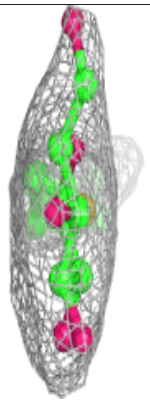


Electron density around HTG c 524:

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

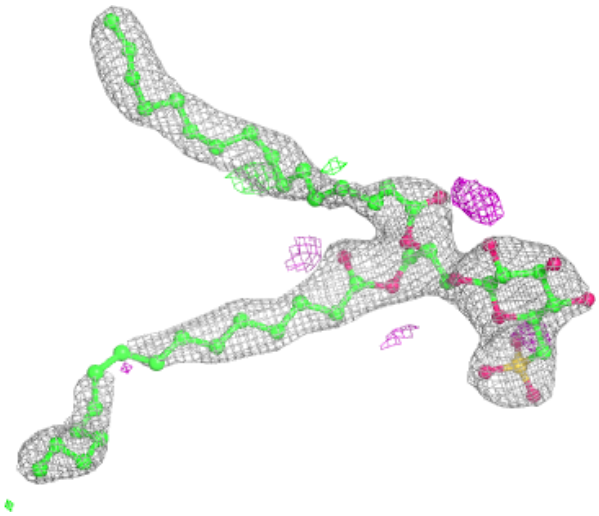


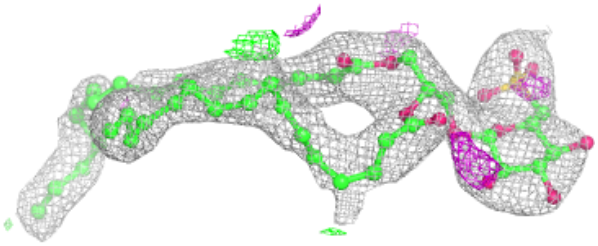


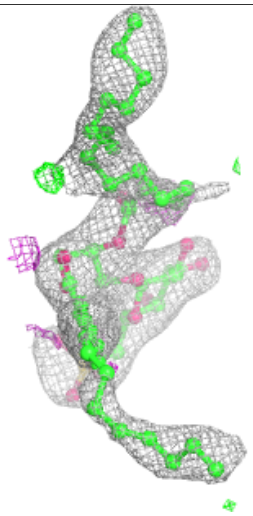


Electron density around SQD A 412:

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

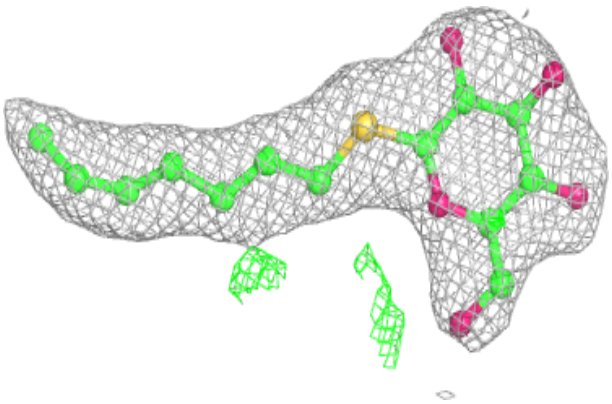


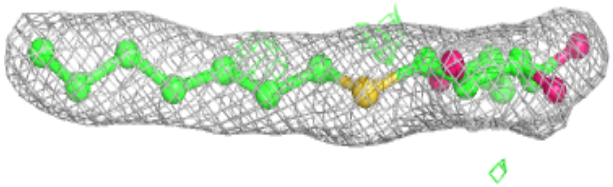


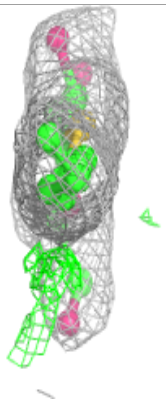


Electron density around HTG b 608:

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

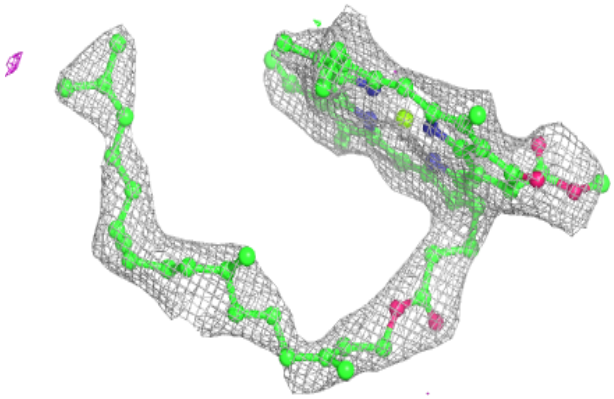


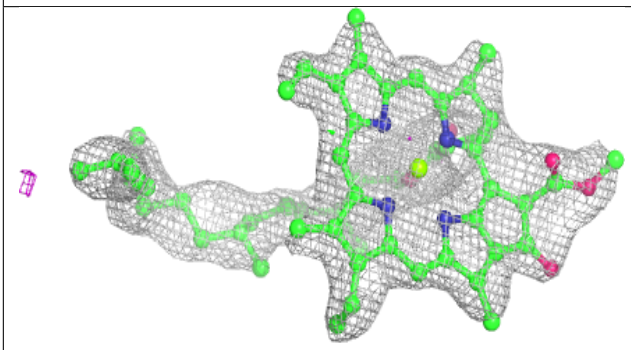


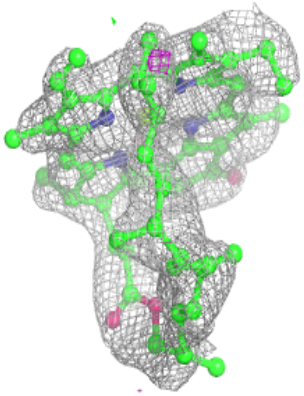


Electron density around CLA c 517:

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

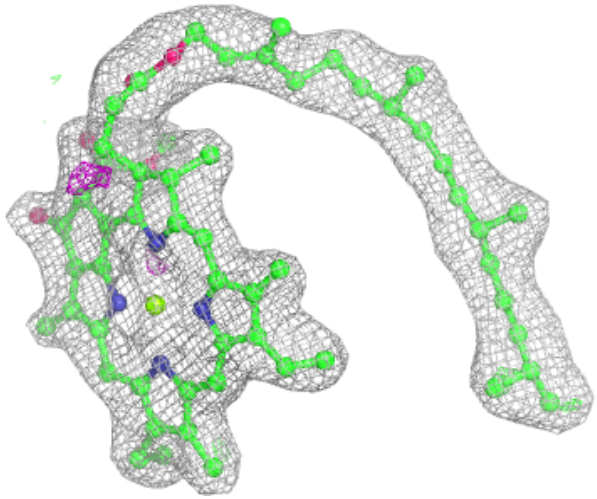


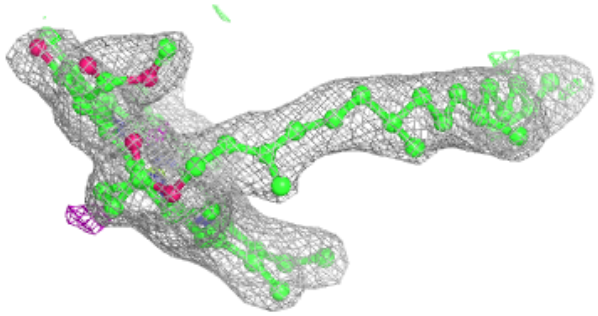


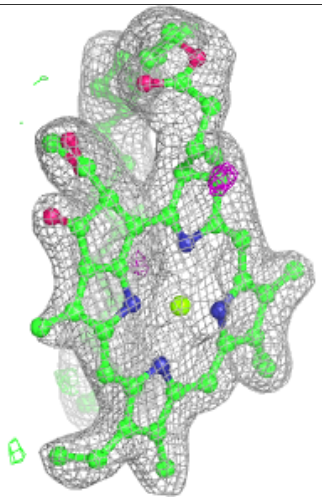


Electron density around CLA c 511:

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

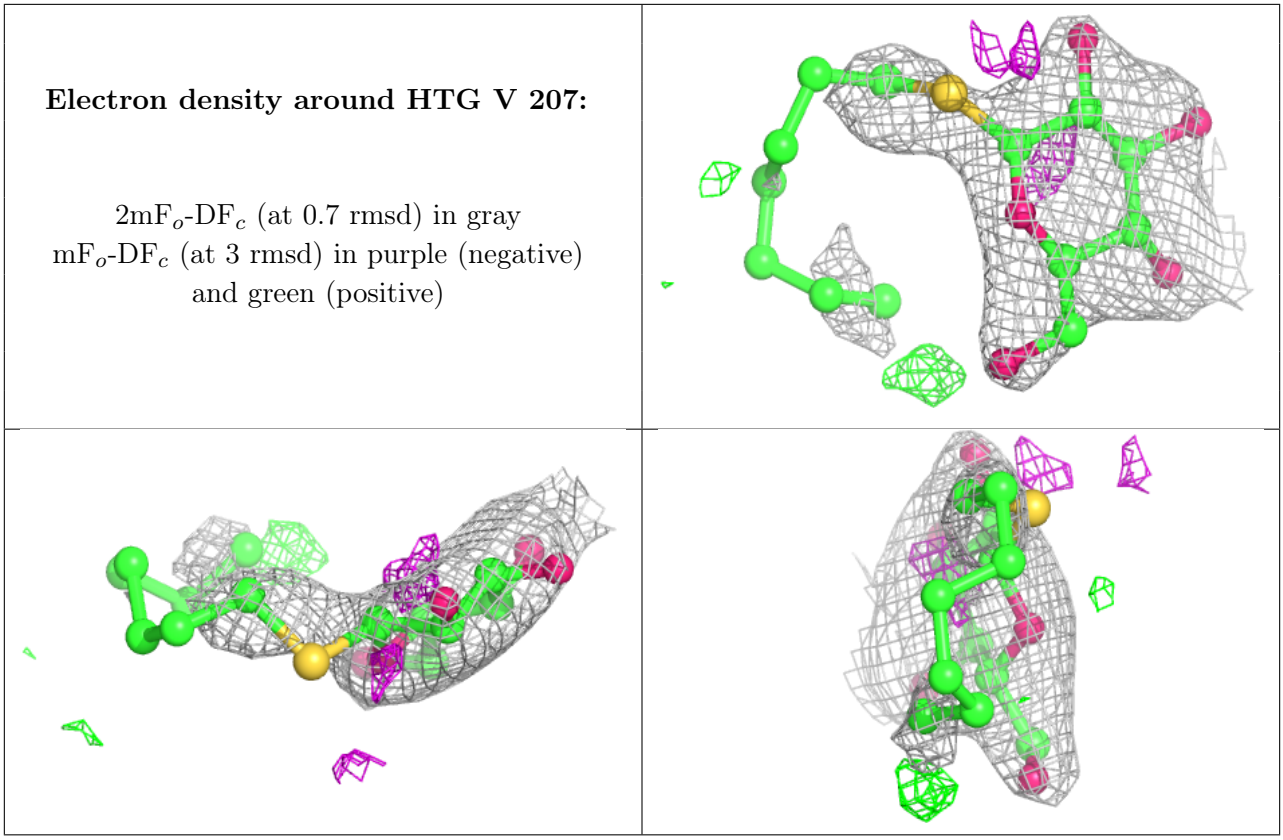






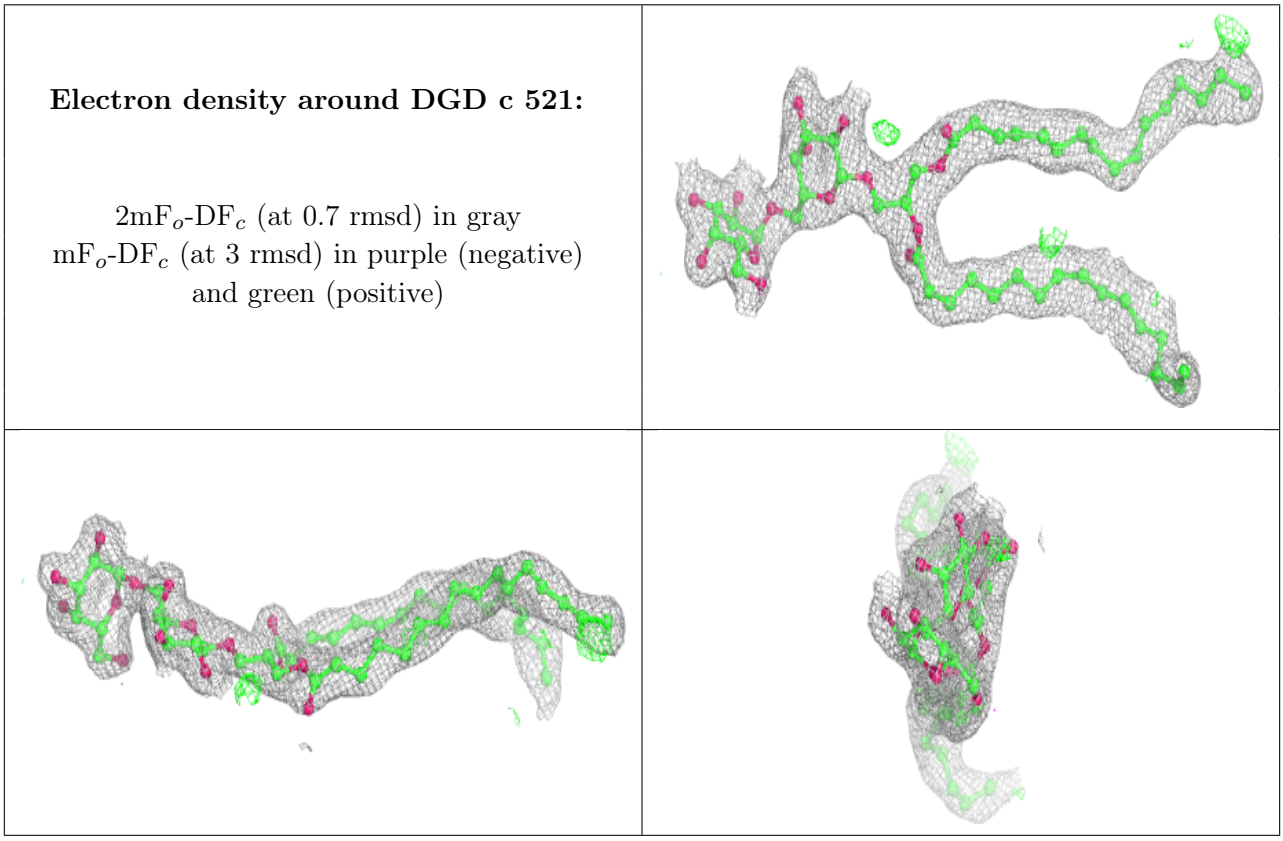
Electron density around HTG V 207:

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



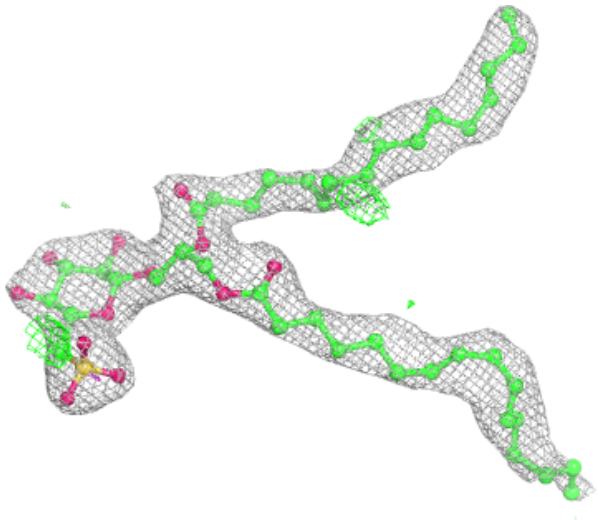
Electron density around DGD c 521:

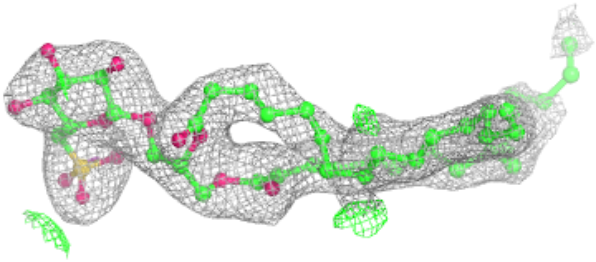
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

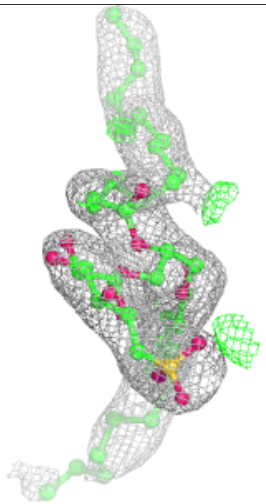


Electron density around SQD a 414:

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

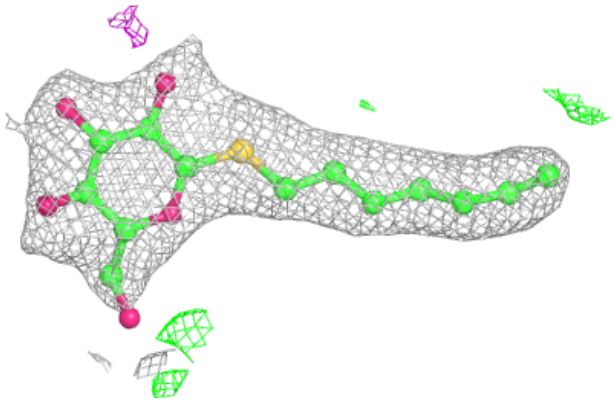


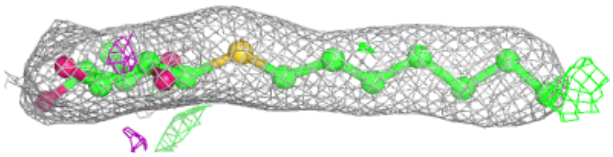


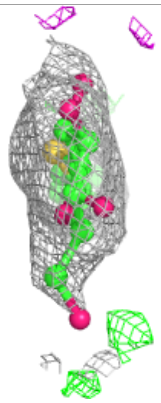


Electron density around HTG B 632:

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

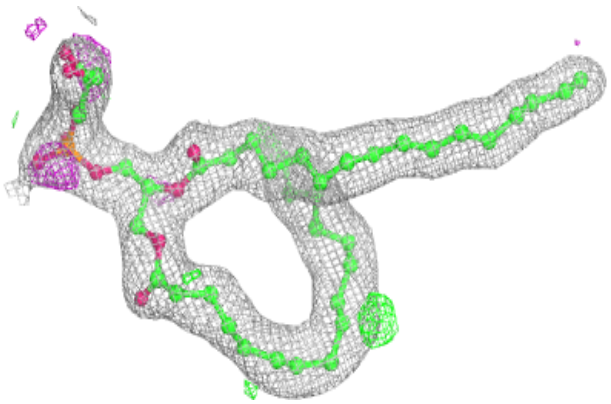


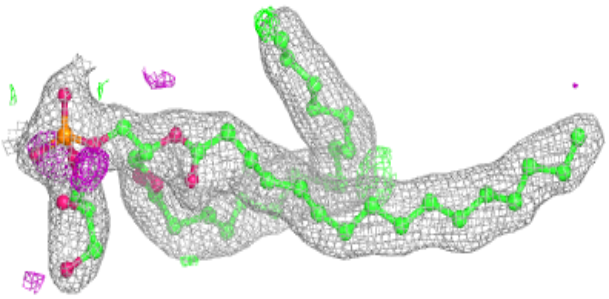




Electron density around LHG D 407:

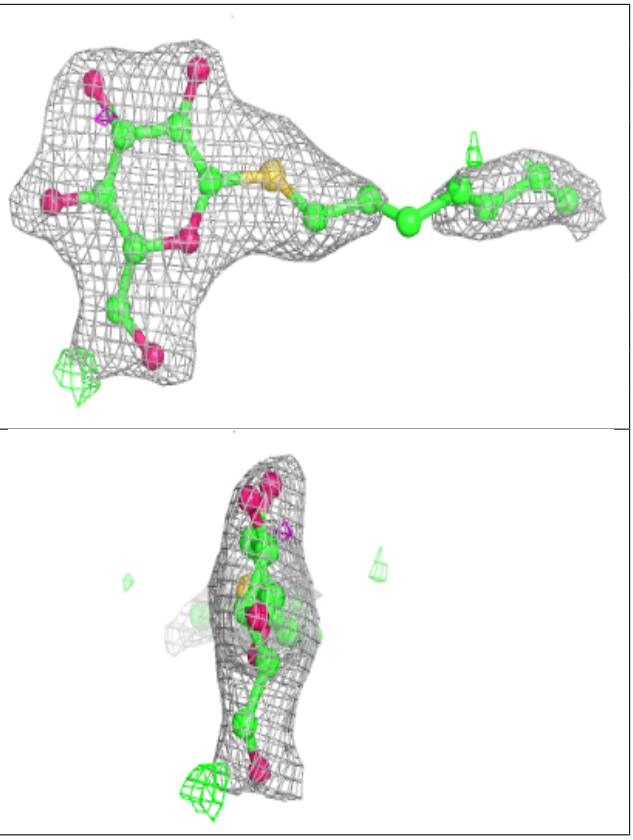
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





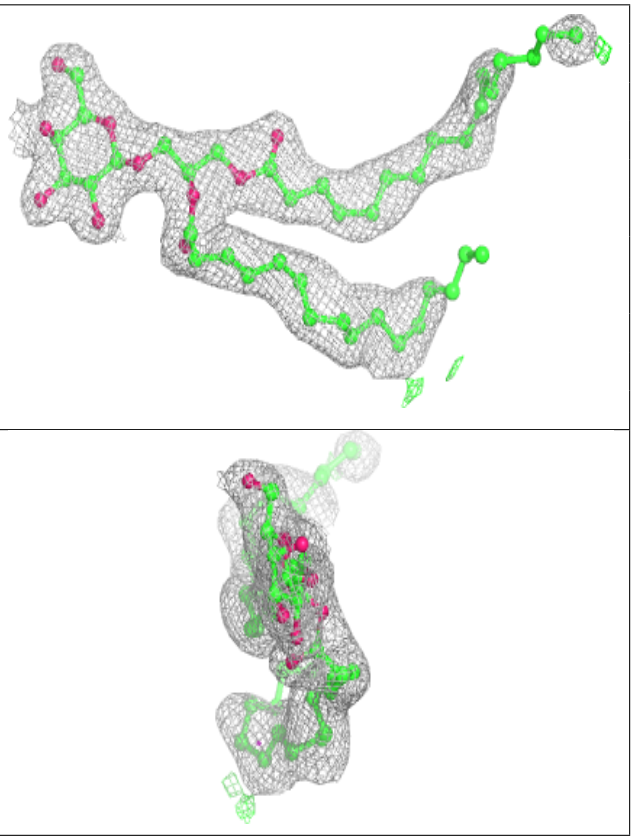
Electron density around HTG C 522:

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



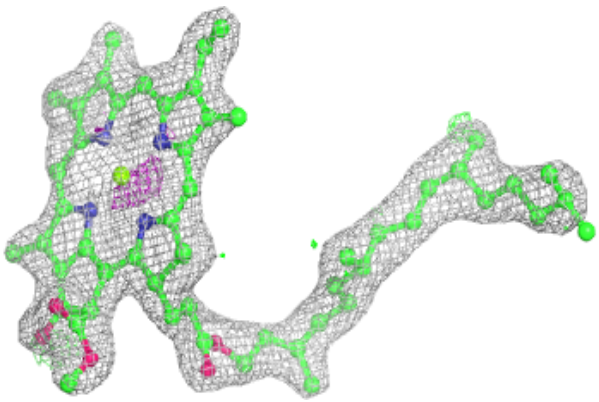
Electron density around LMG j 101:

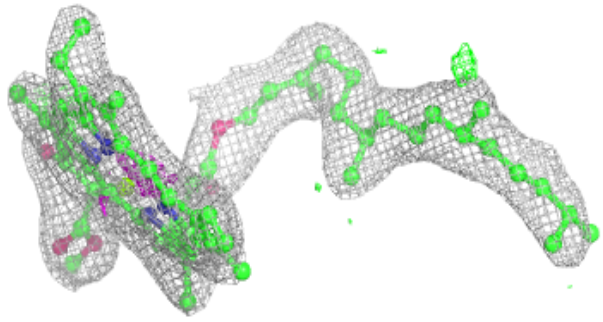
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

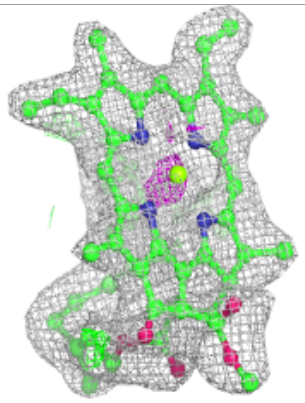


Electron density around CLA c 515:

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

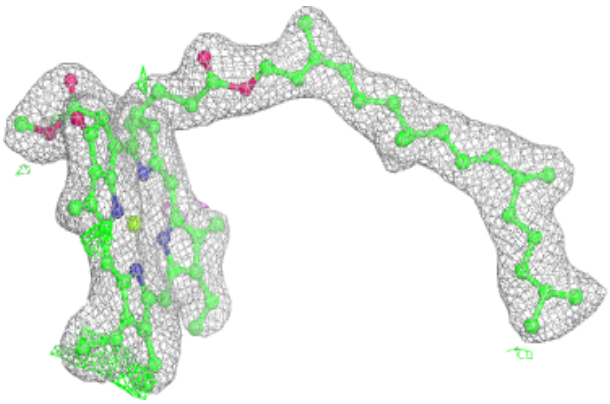


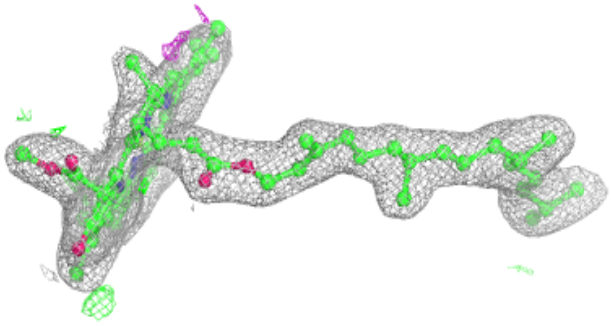


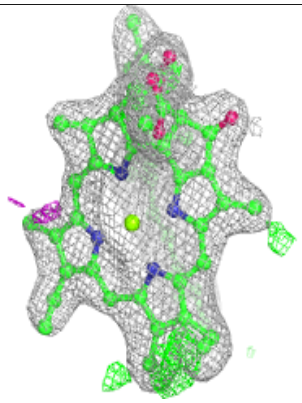


Electron density around CLA b 619:

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

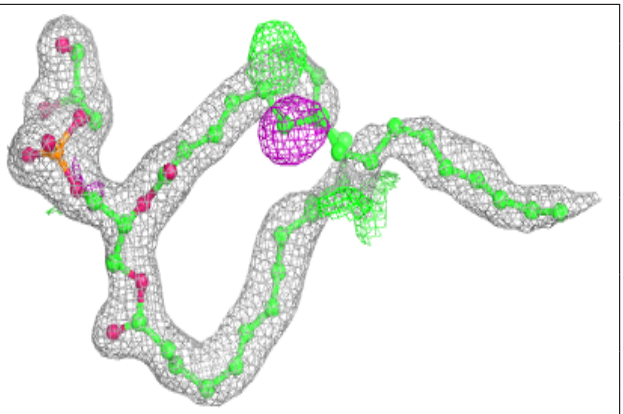


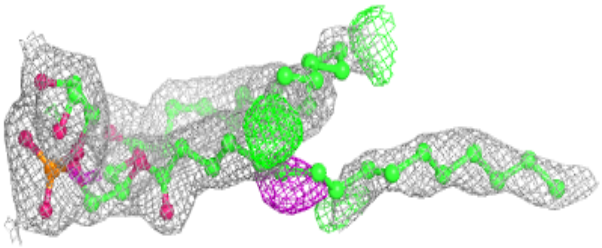


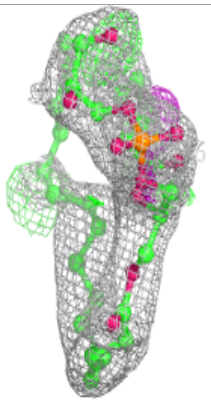


Electron density around LHG D 409:

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

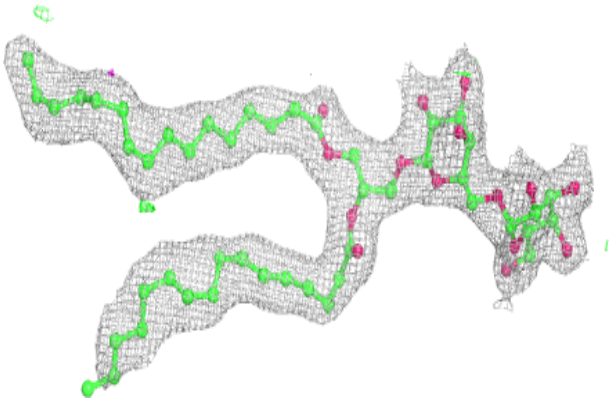


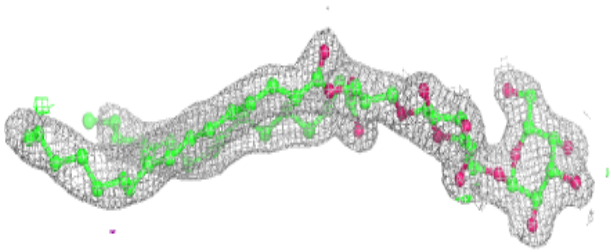


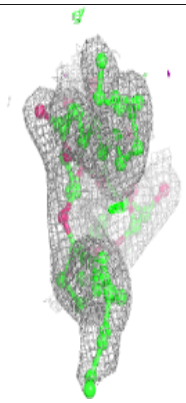


Electron density around DGD C 518:

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

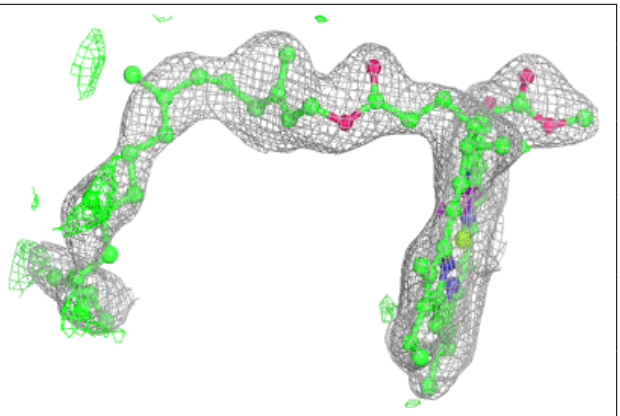


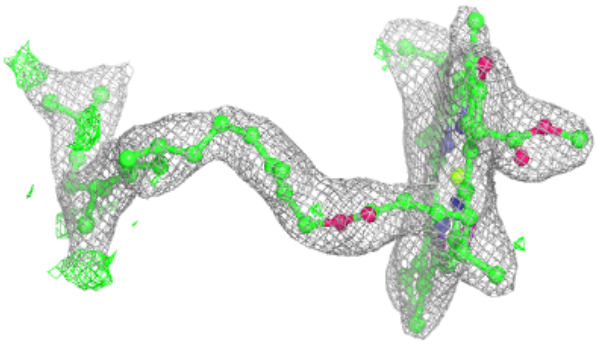


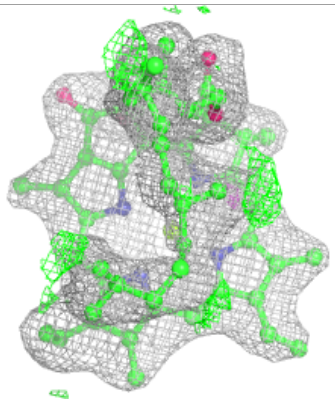


Electron density around CLA C 506:

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

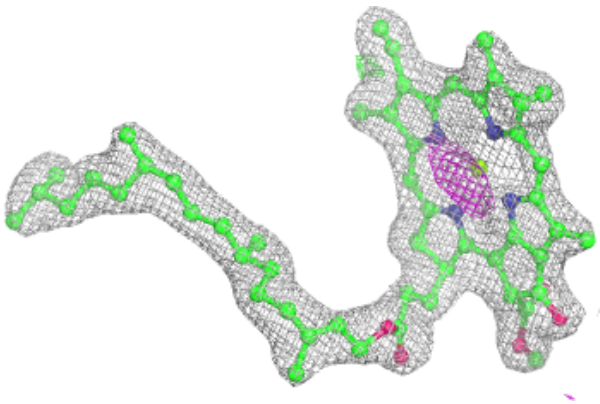


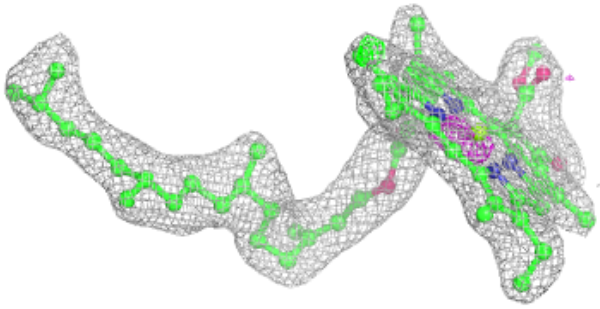


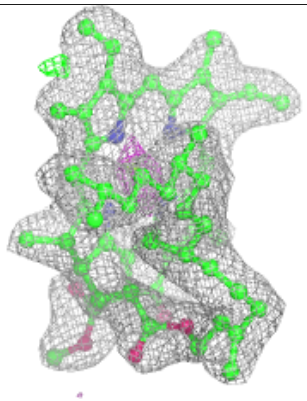


Electron density around CLA C 511:

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

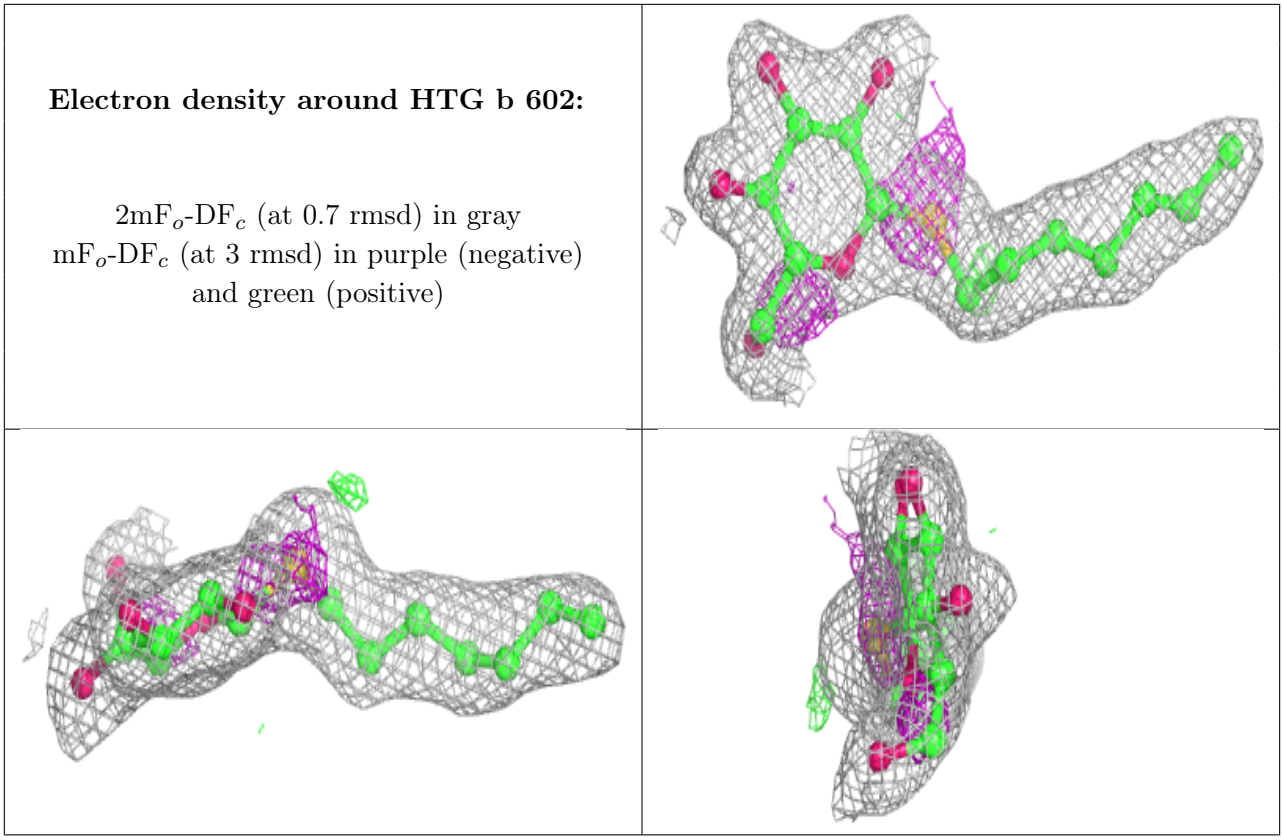






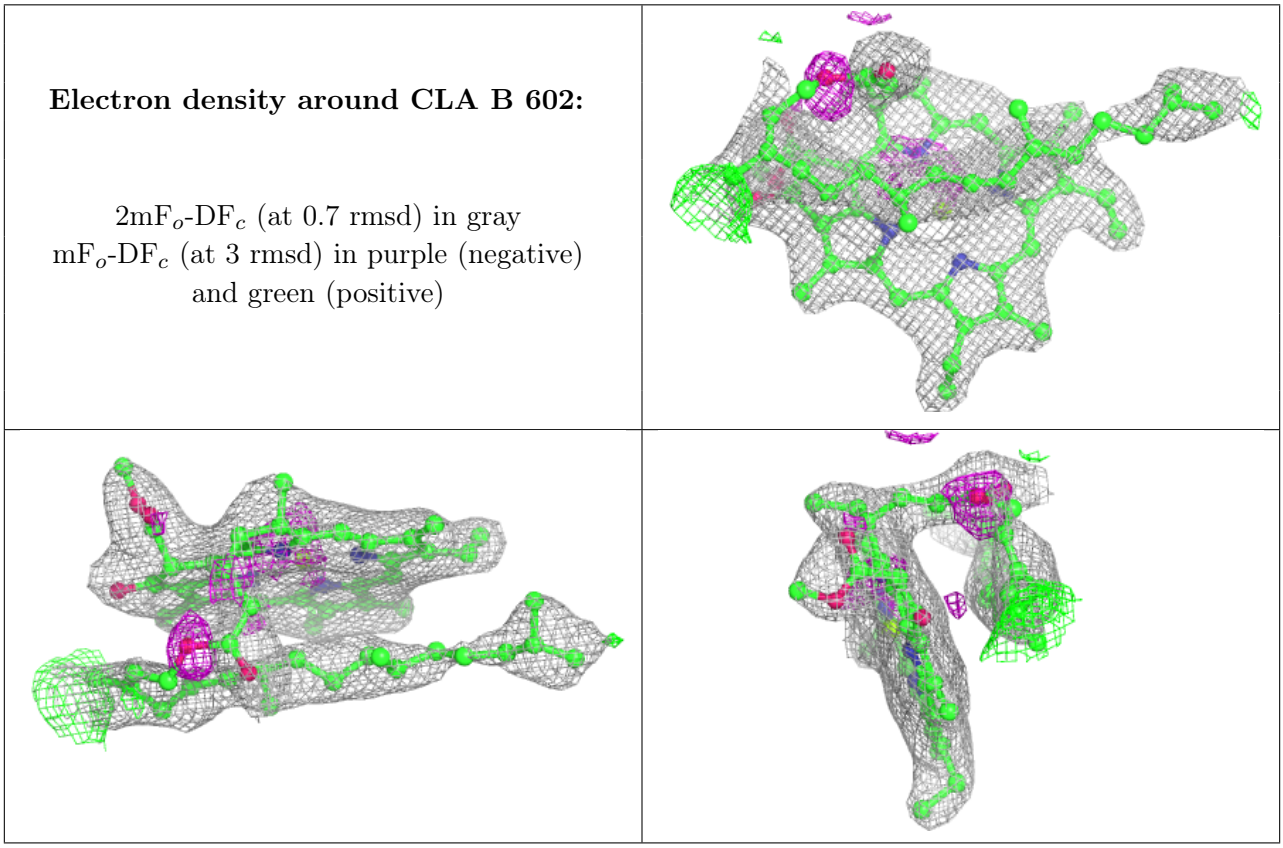
Electron density around HTG b 602:

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



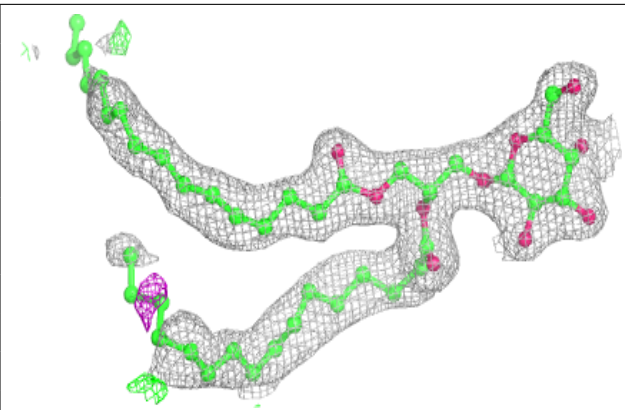
Electron density around CLA B 602:

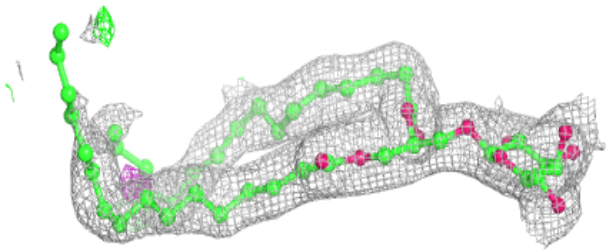
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

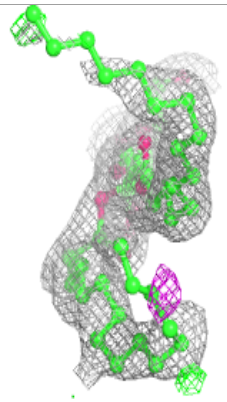


Electron density around LMG D 412:

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

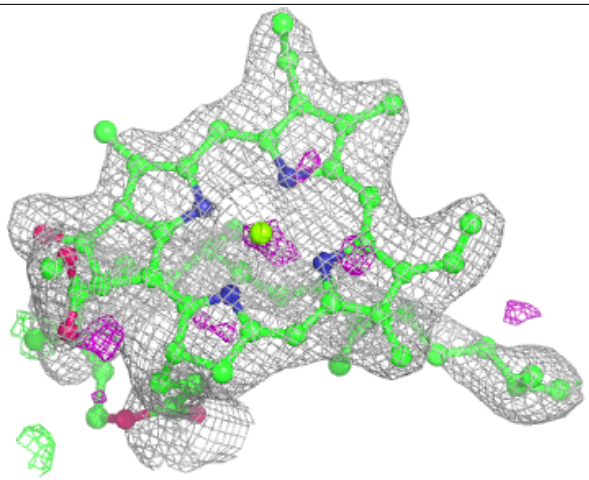


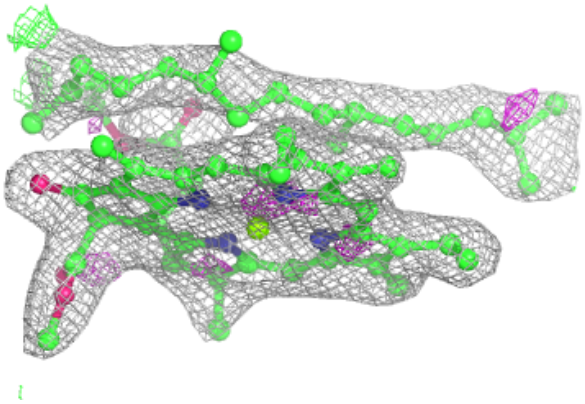


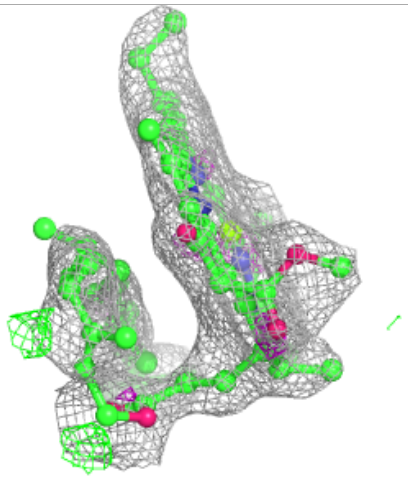


Electron density around CLA b 611:

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

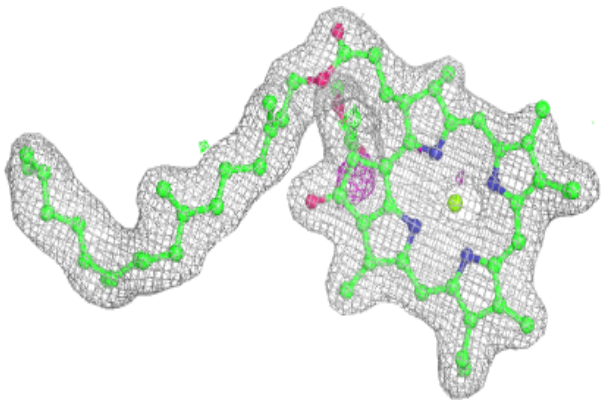


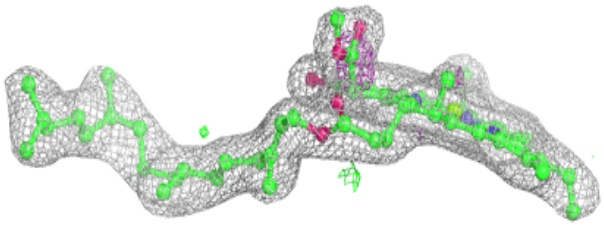




Electron density around CLA b 612:

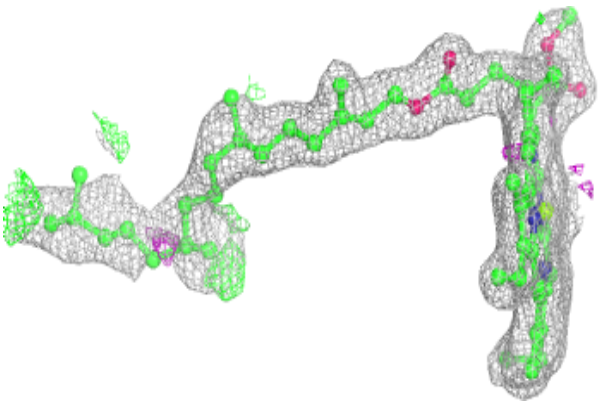
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

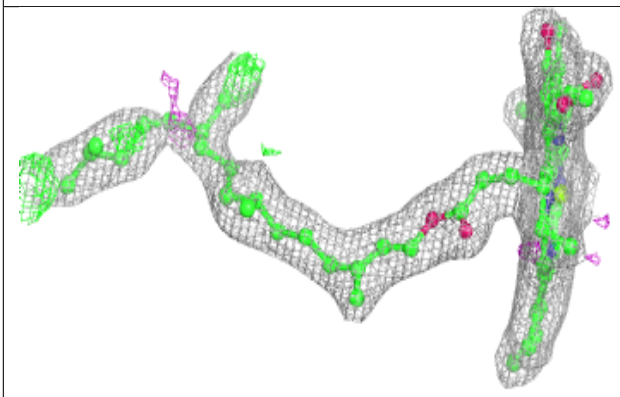


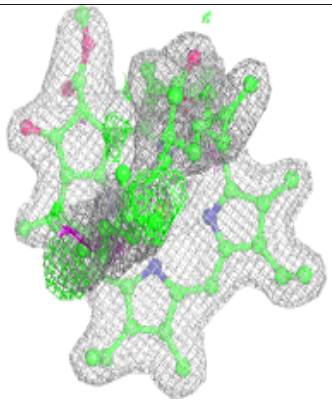


Electron density around CLA b 616:

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

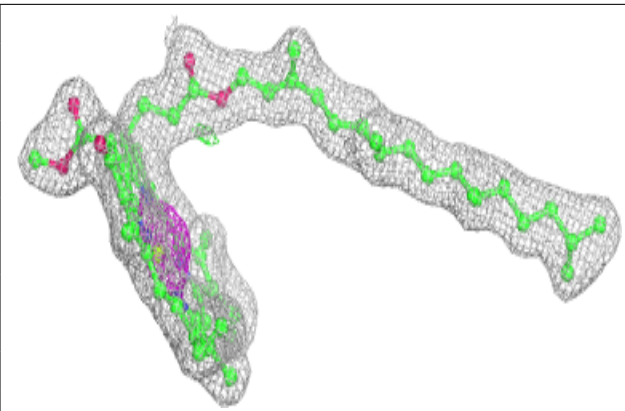


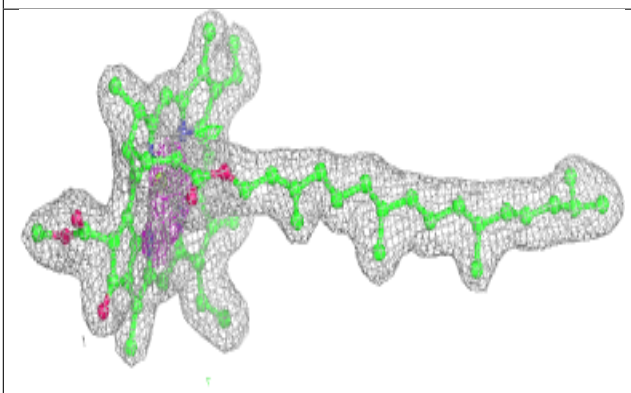


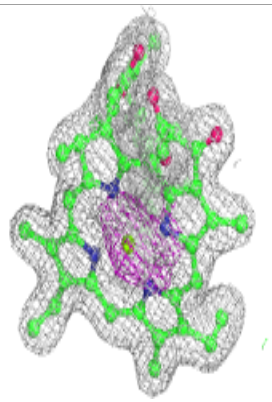


Electron density around CLA b 617:

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

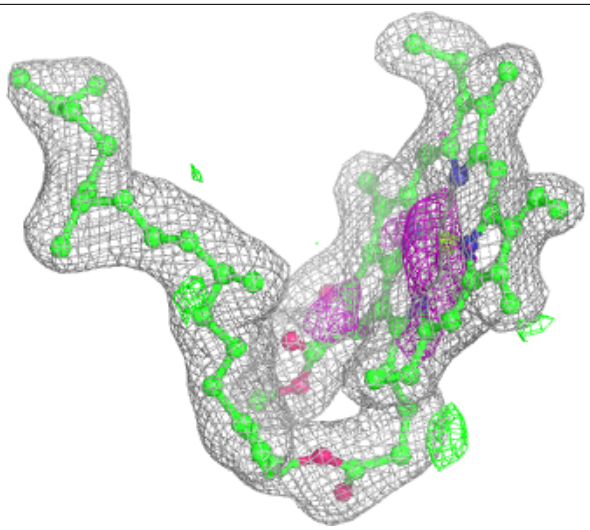


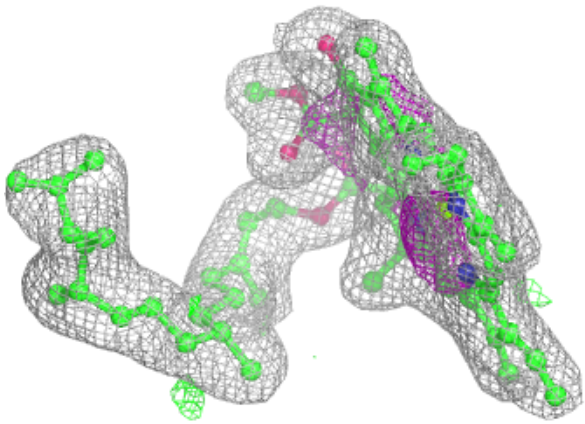


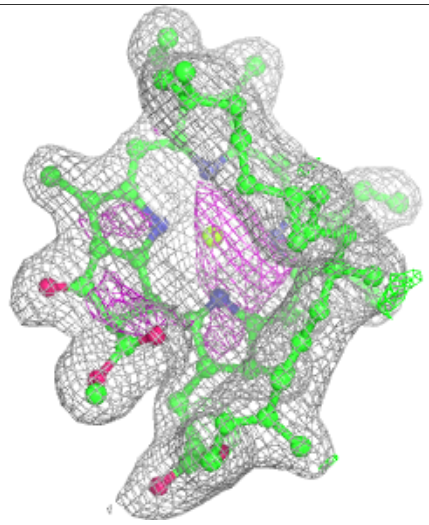


Electron density around CLA B 614:

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

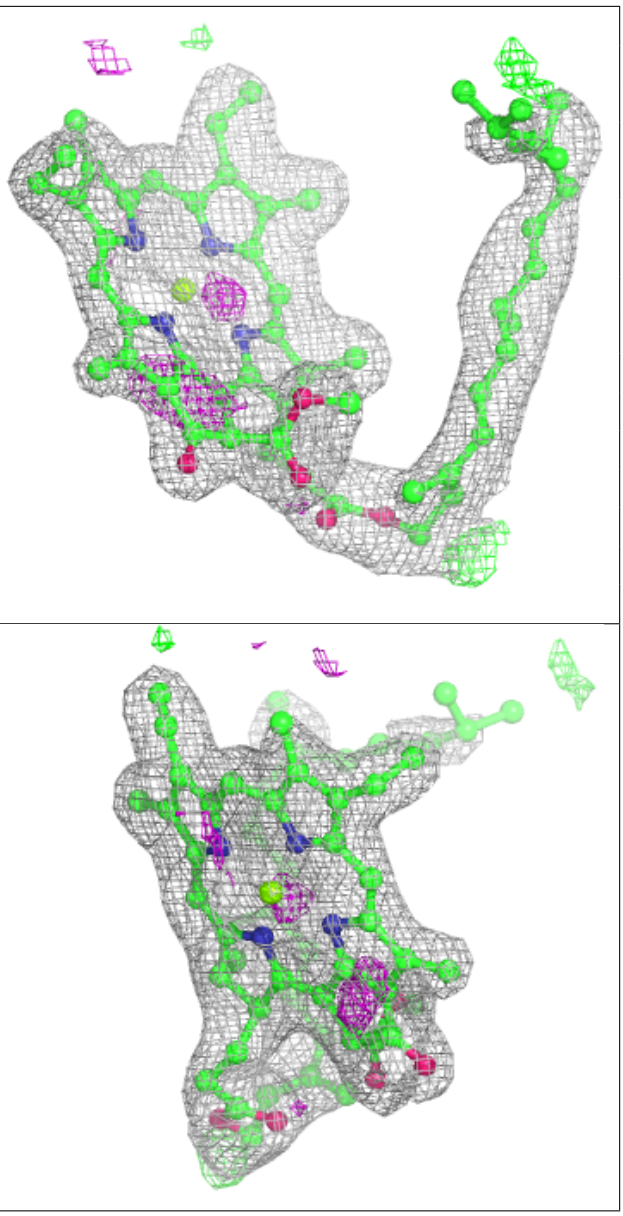






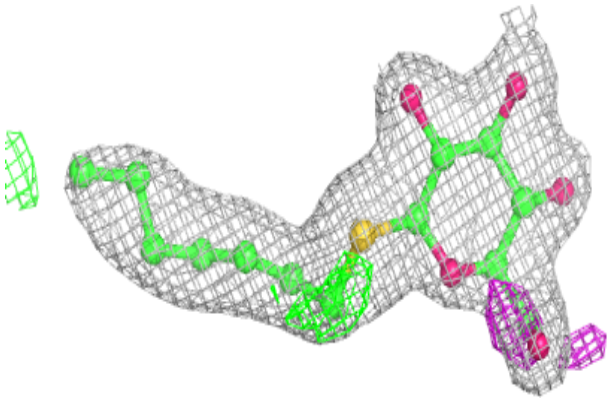
Electron density around CLA b 626:

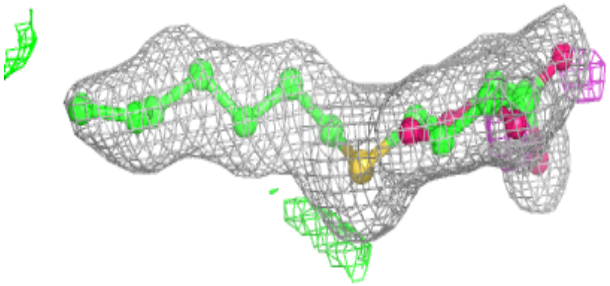
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

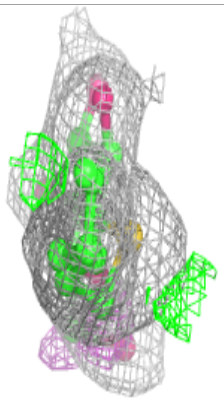


Electron density around HTG B 623:

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

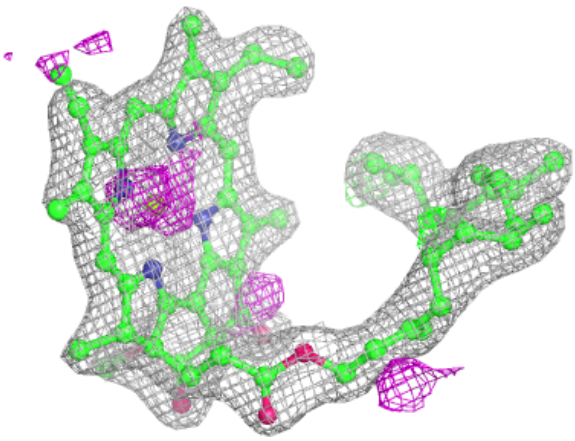


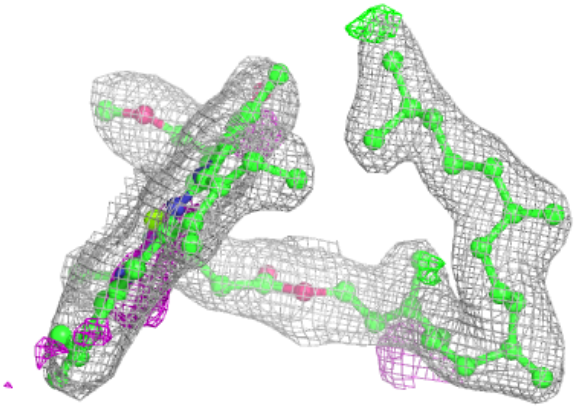


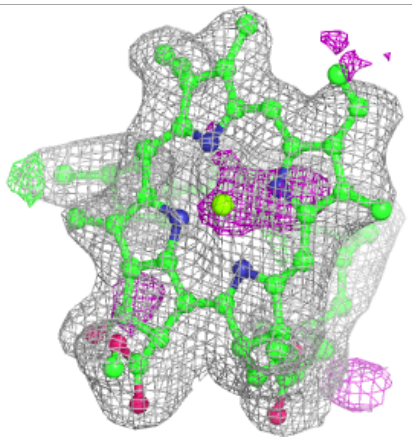


Electron density around CLA c 507:

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

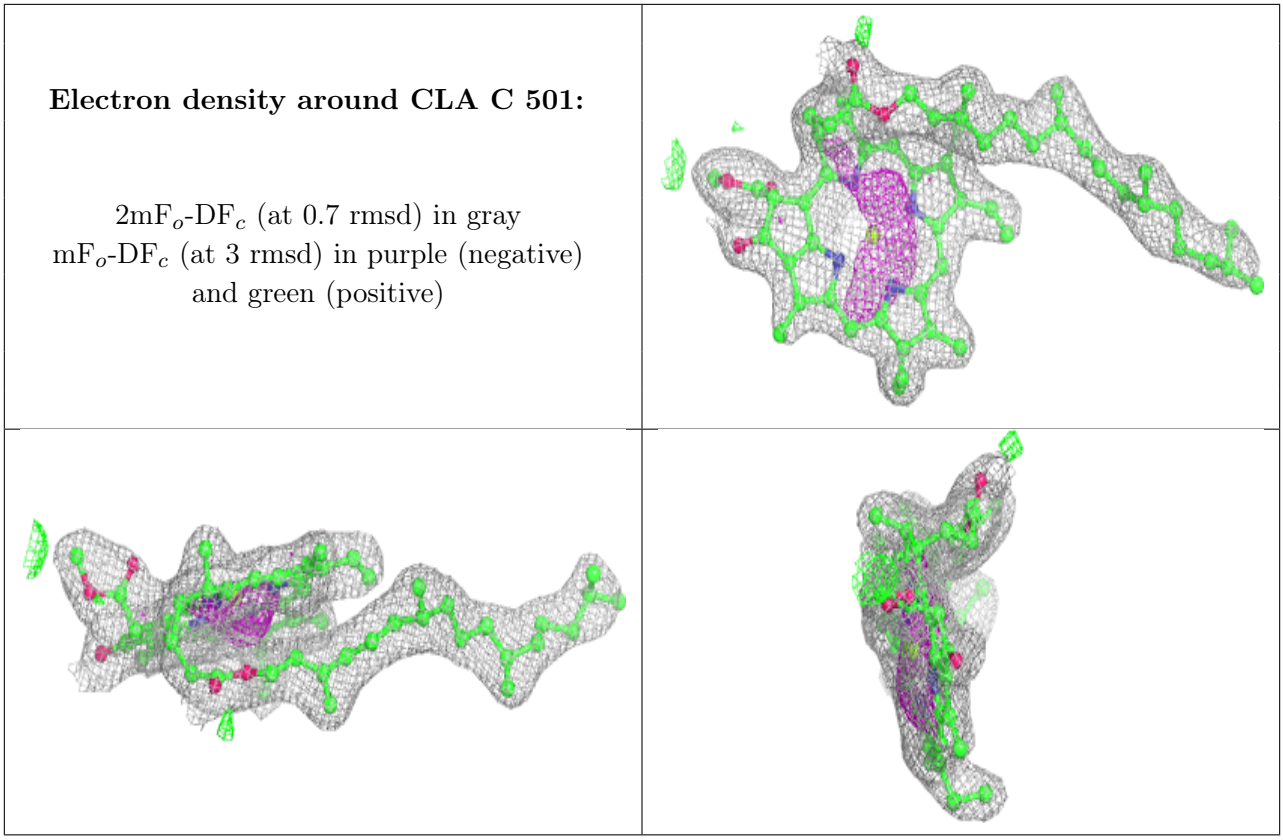






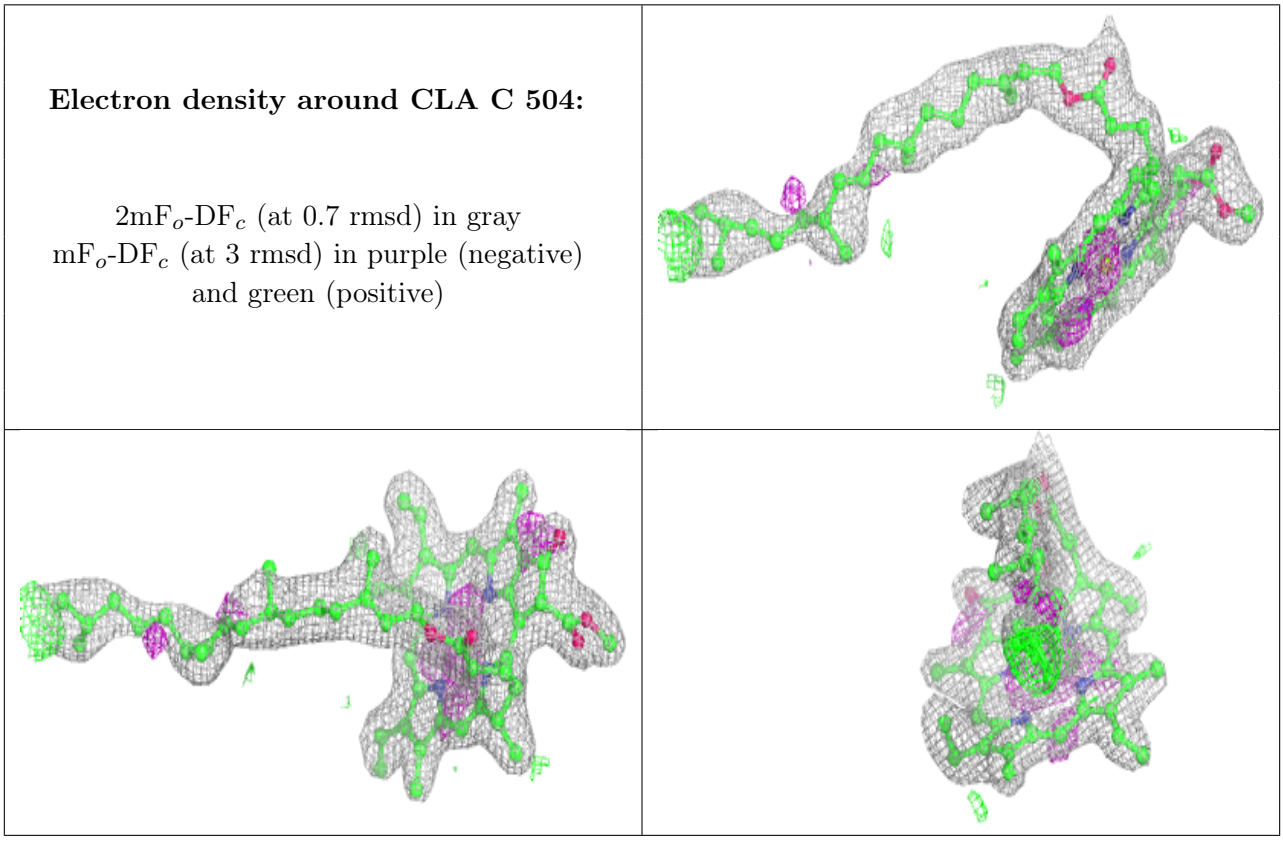
Electron density around CLA C 501:

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



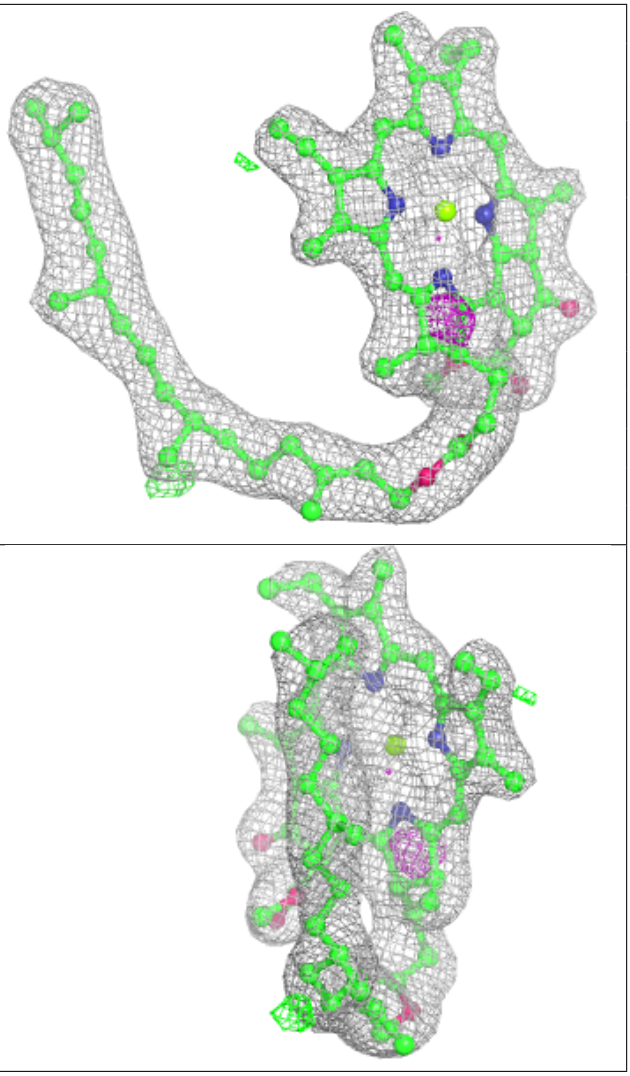
Electron density around CLA C 504:

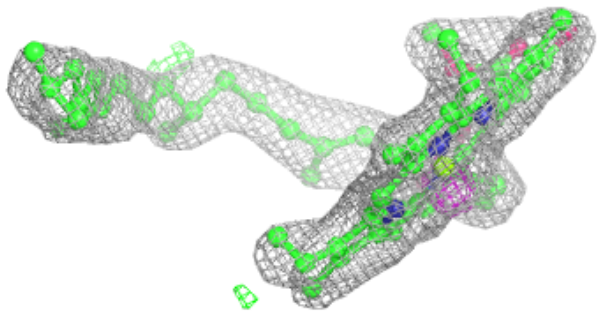
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA C 507:

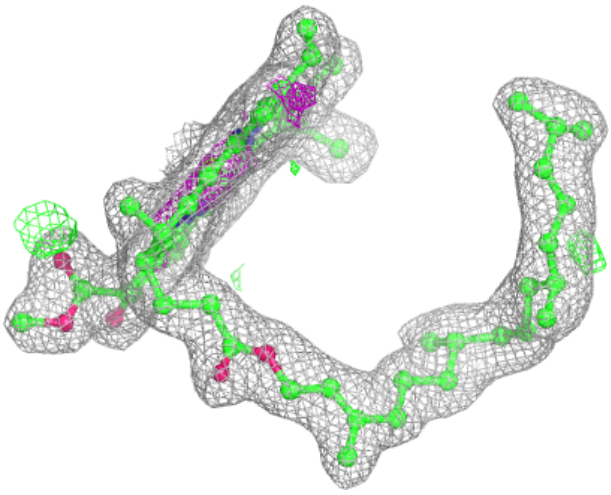
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

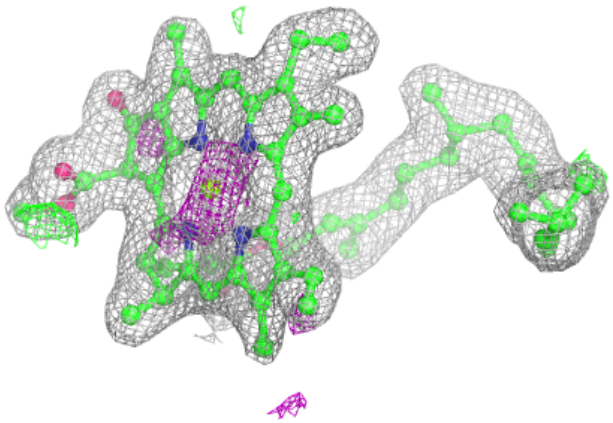


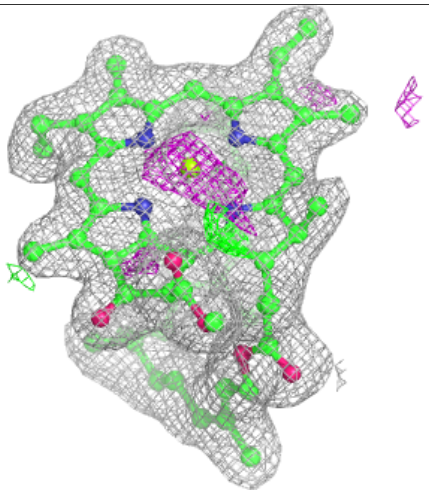


Electron density around CLA b 621:

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

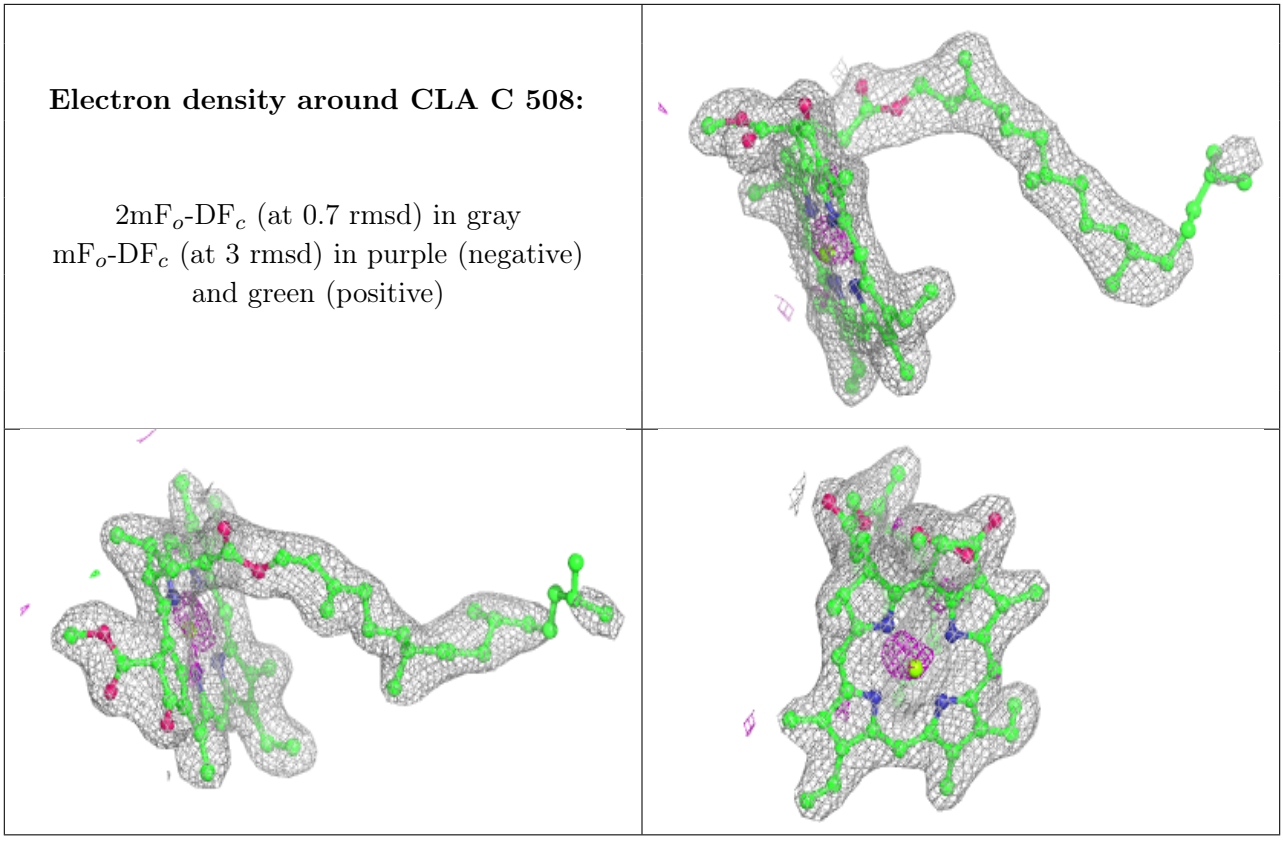






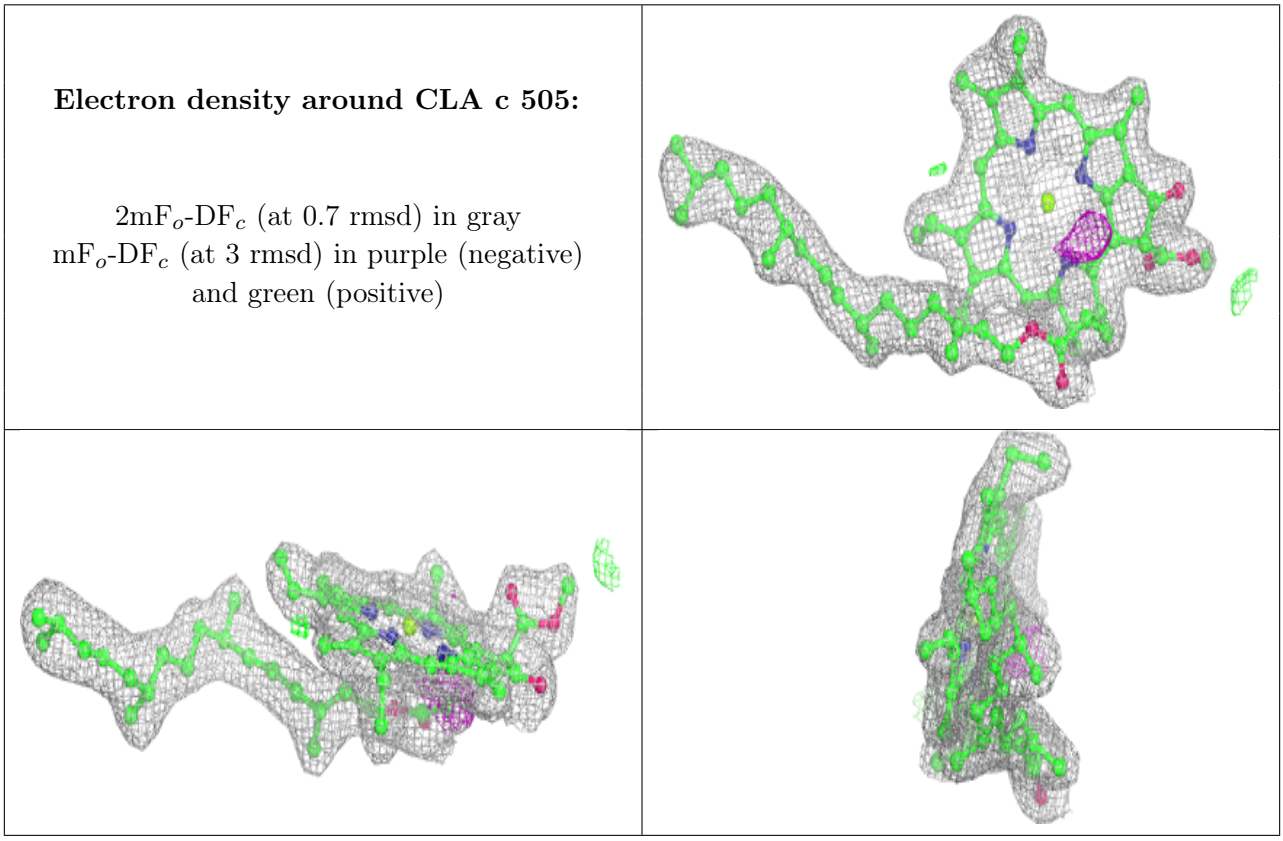
Electron density around CLA C 508:

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



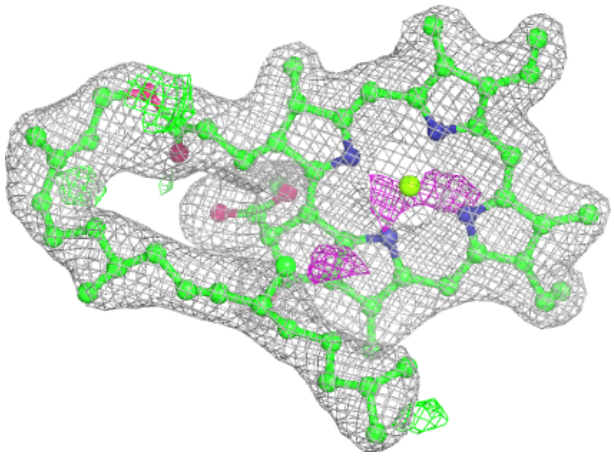
Electron density around CLA c 505:

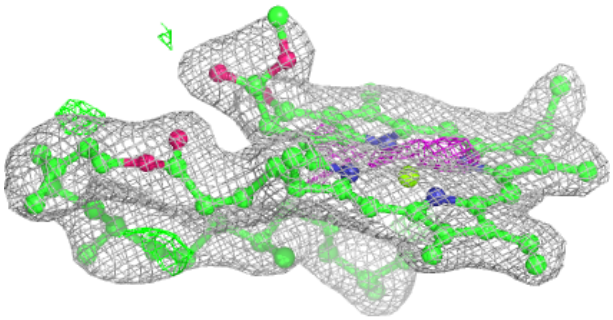
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

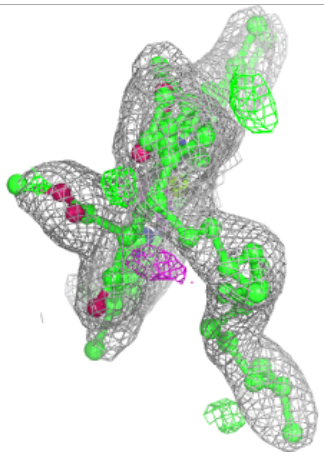


Electron density around CLA C 509:

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

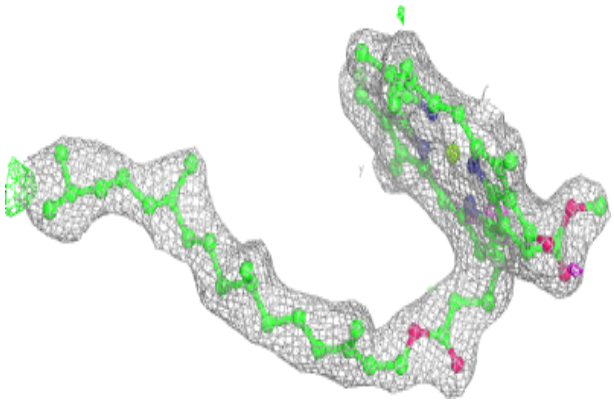


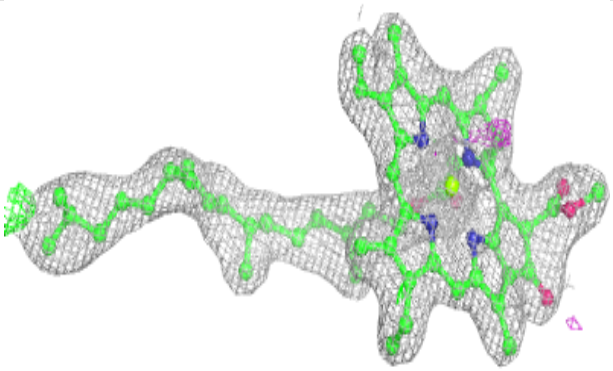


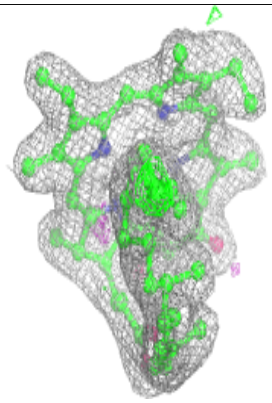


Electron density around CLA c 508:

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

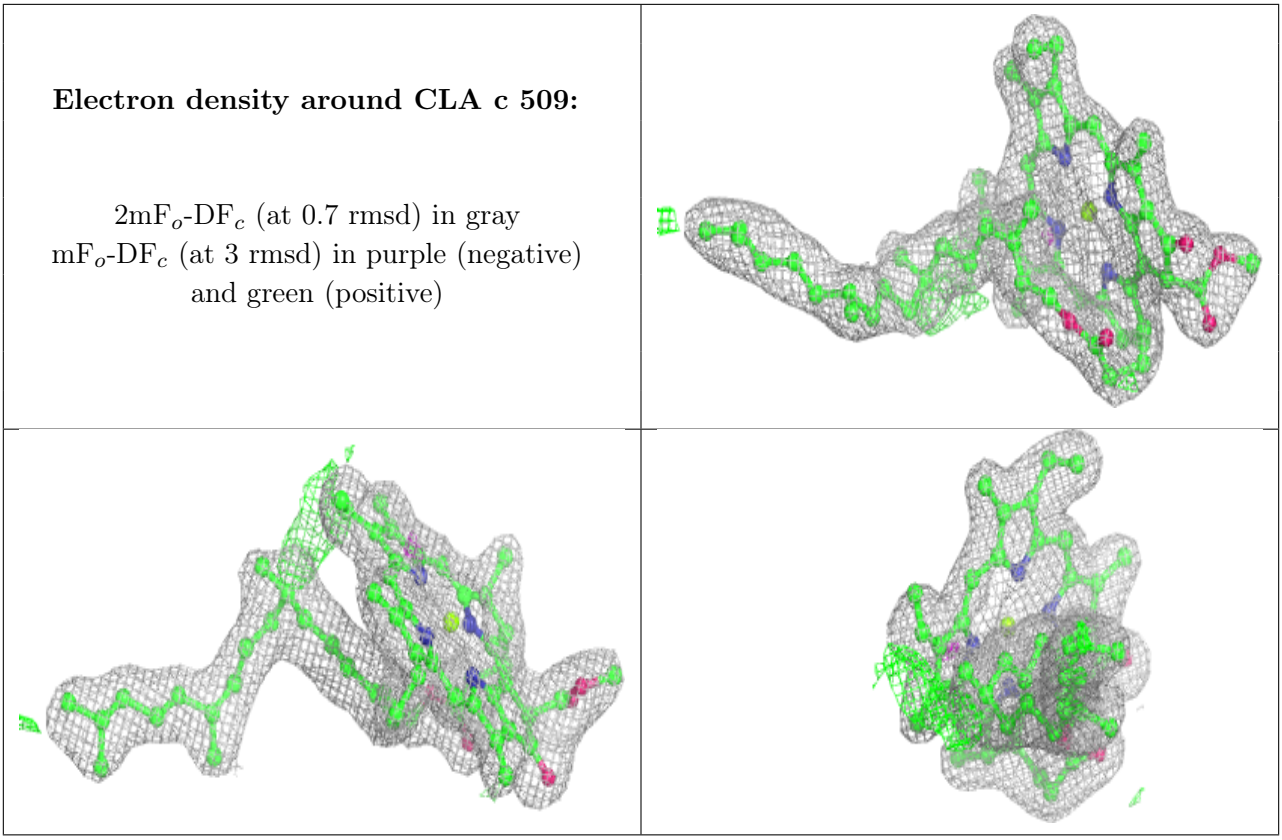






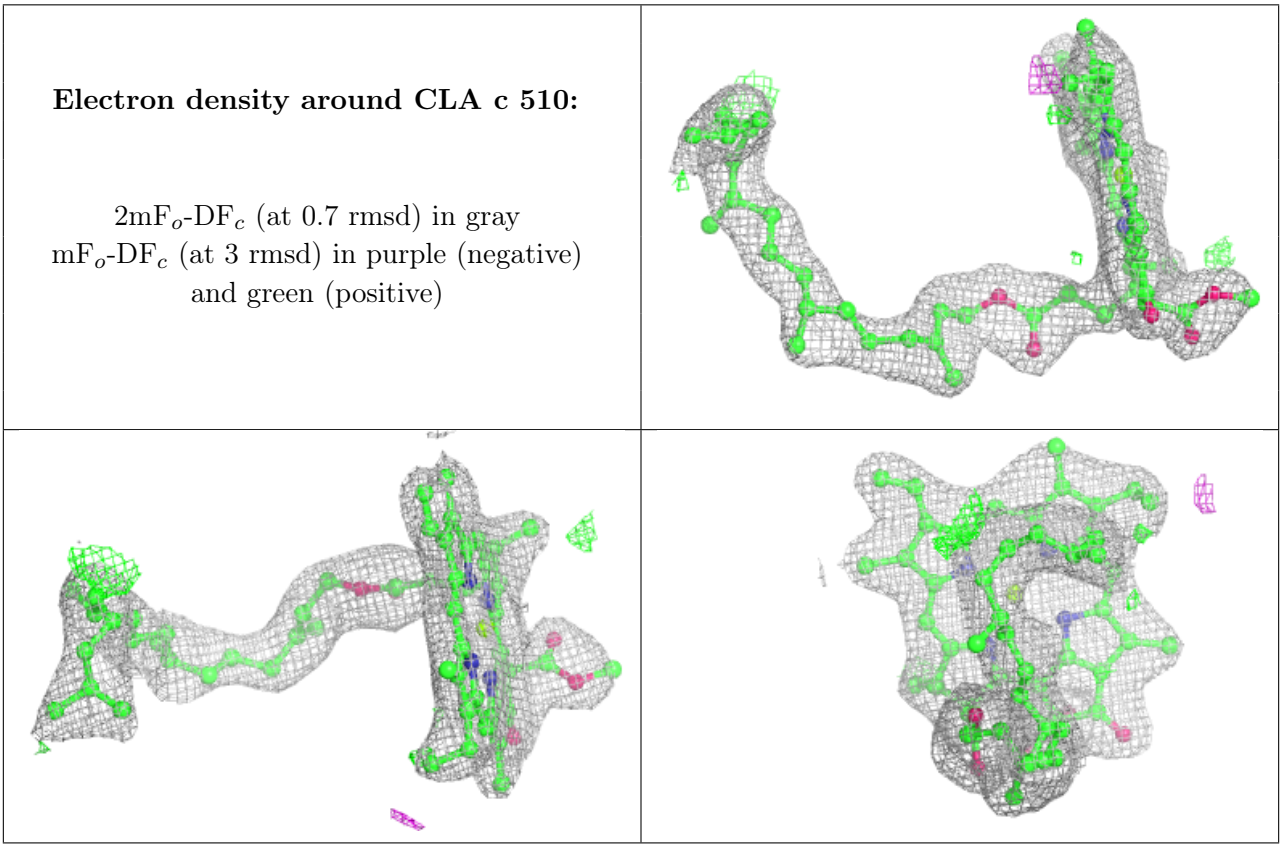
Electron density around CLA c 509:

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



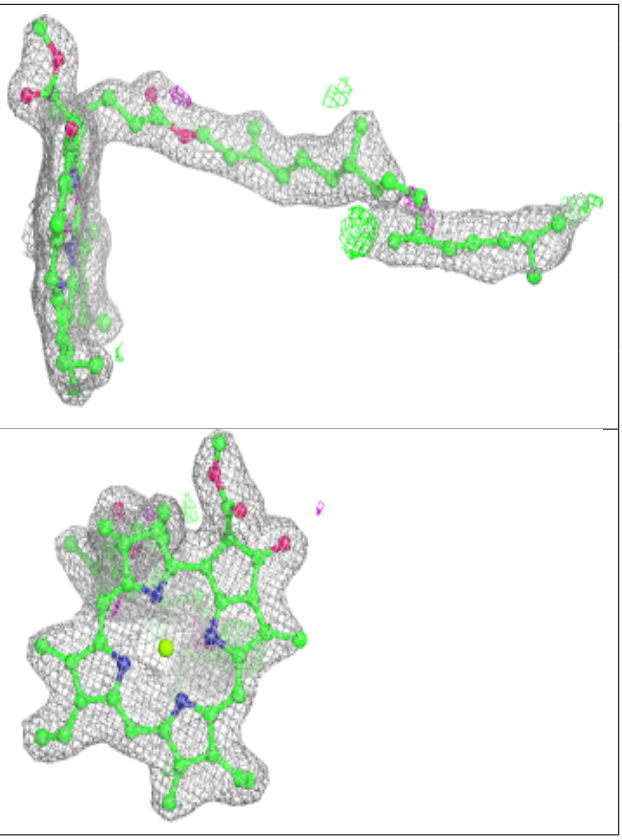
Electron density around CLA c 510:

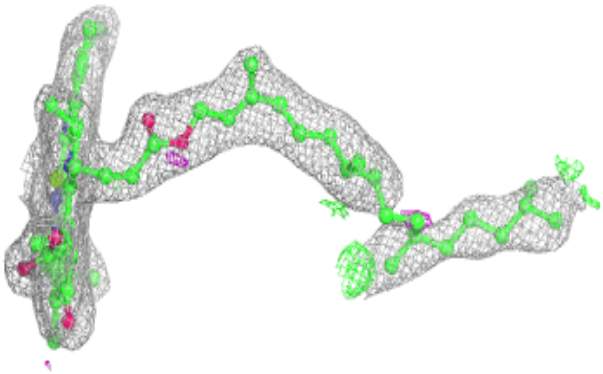
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 607:

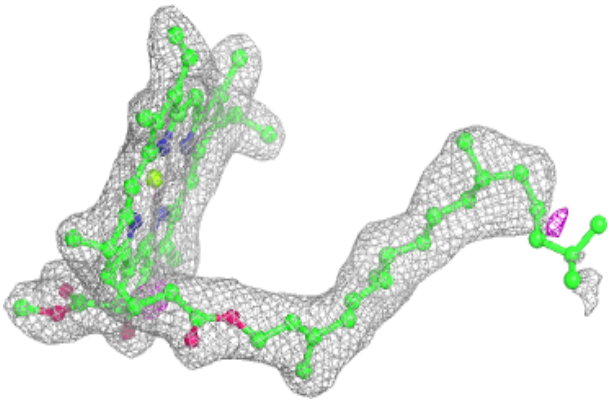
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

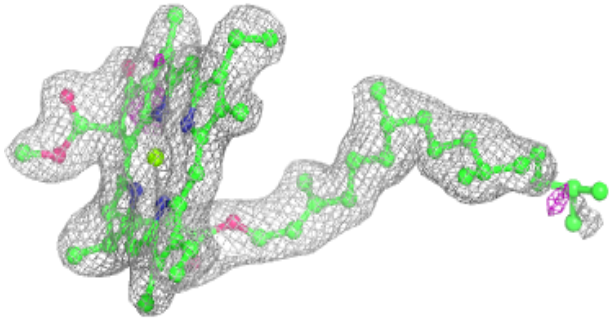


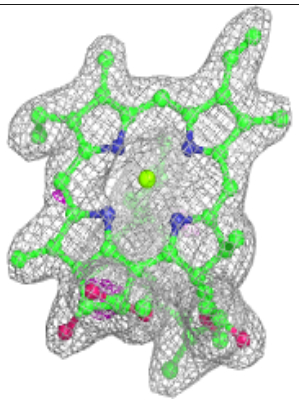


Electron density around CLA c 512:

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

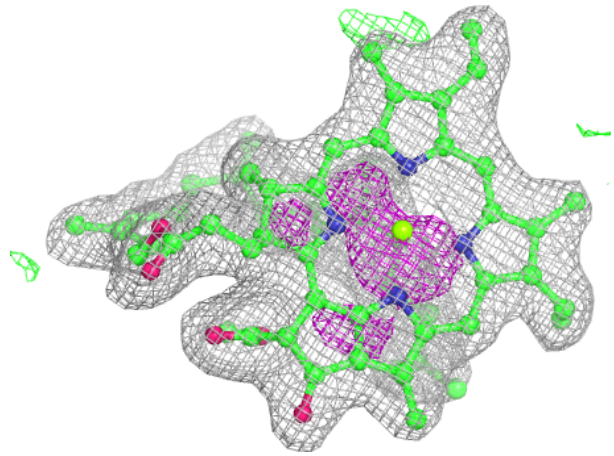


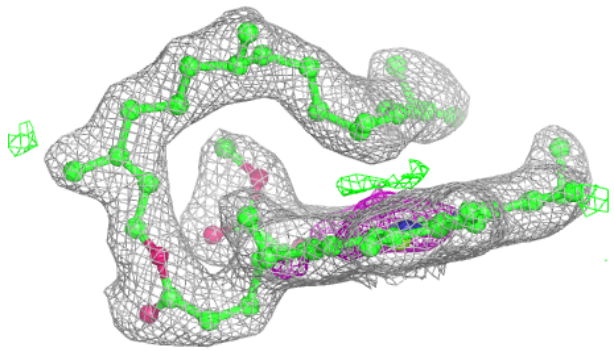


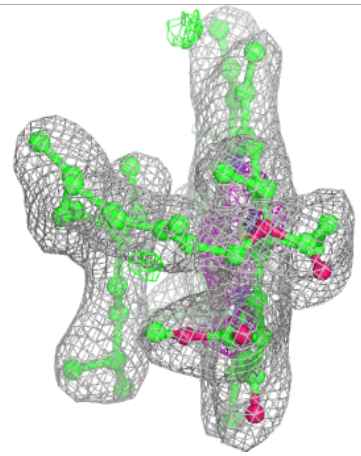


Electron density around CLA c 514:

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

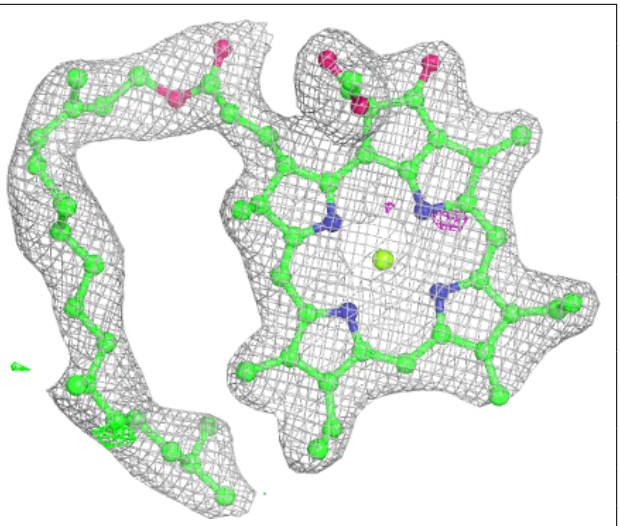


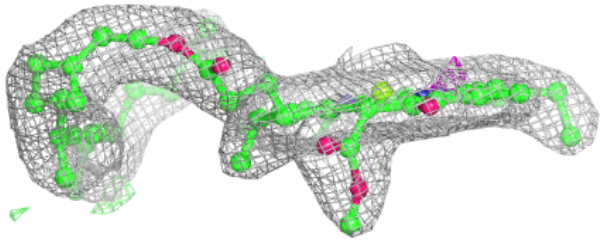


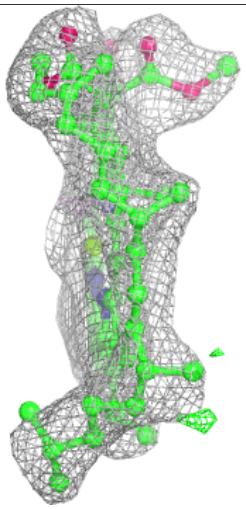


Electron density around CLA C 512:

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

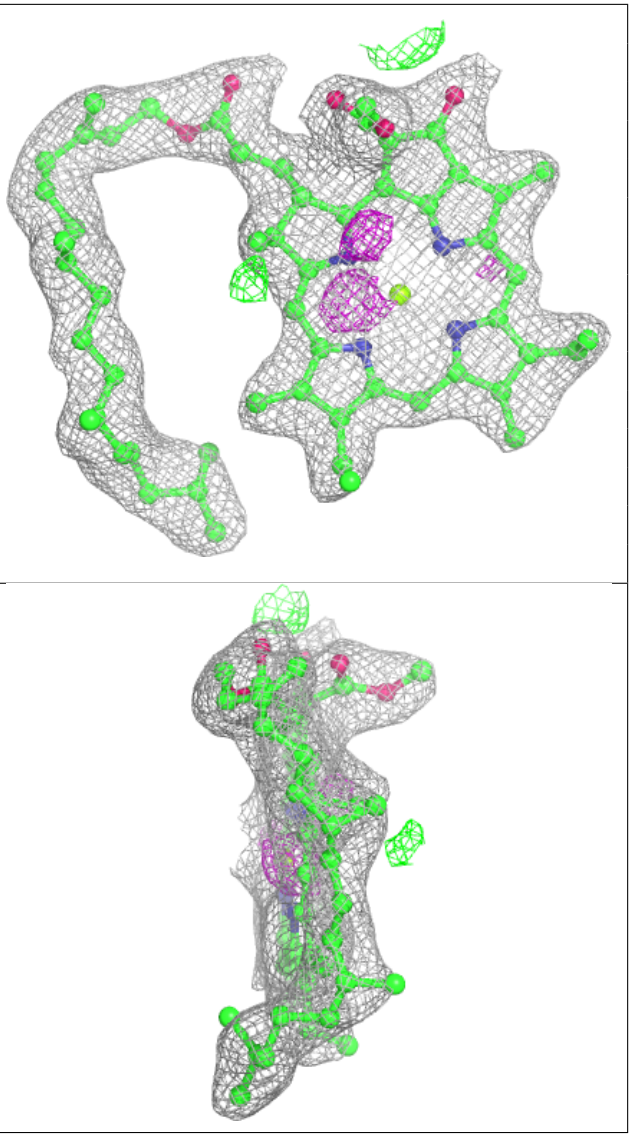






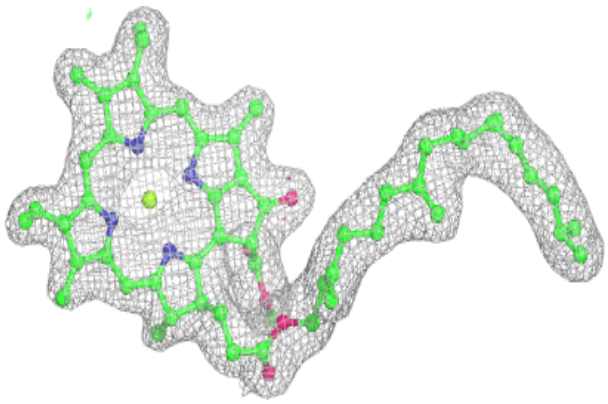
Electron density around CLA c 516:

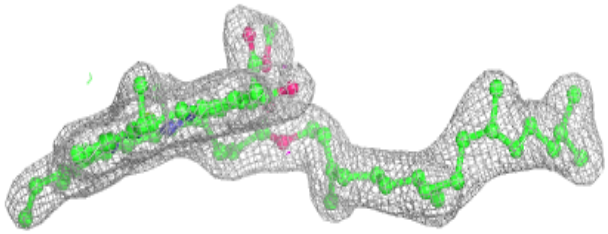
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

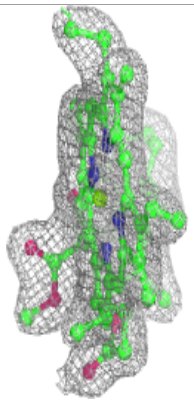


Electron density around CLA B 603:

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

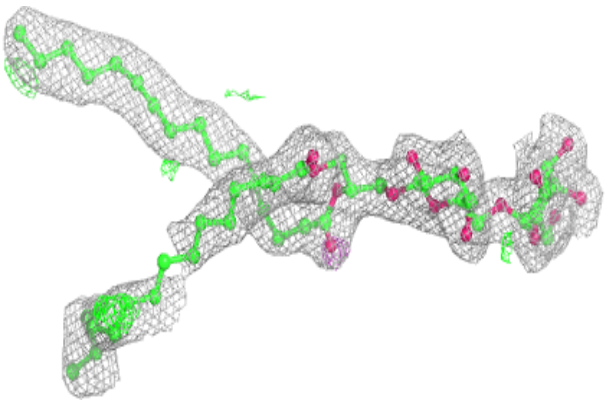


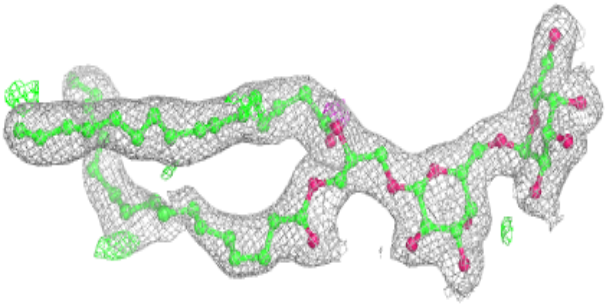


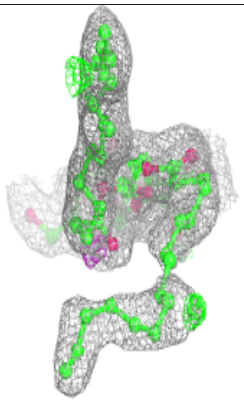


Electron density around DGD c 519:

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

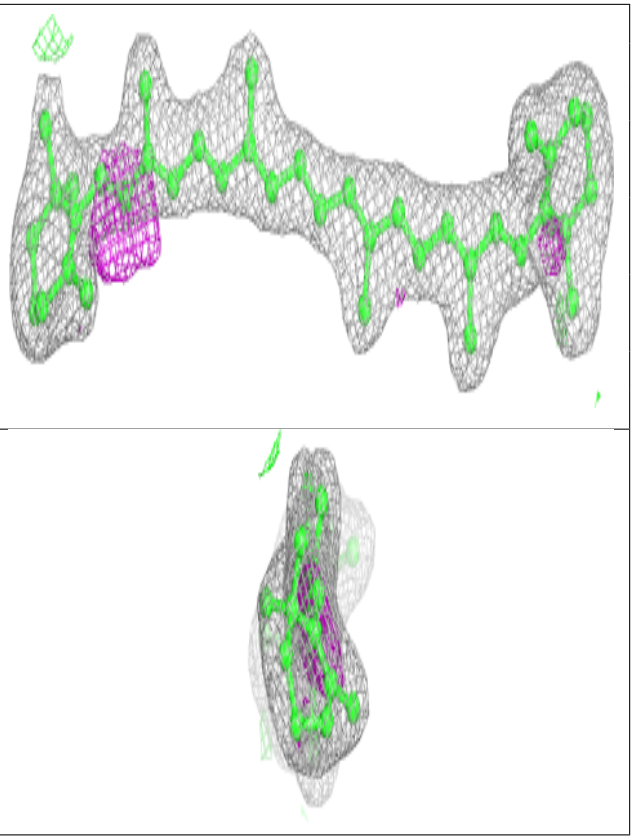






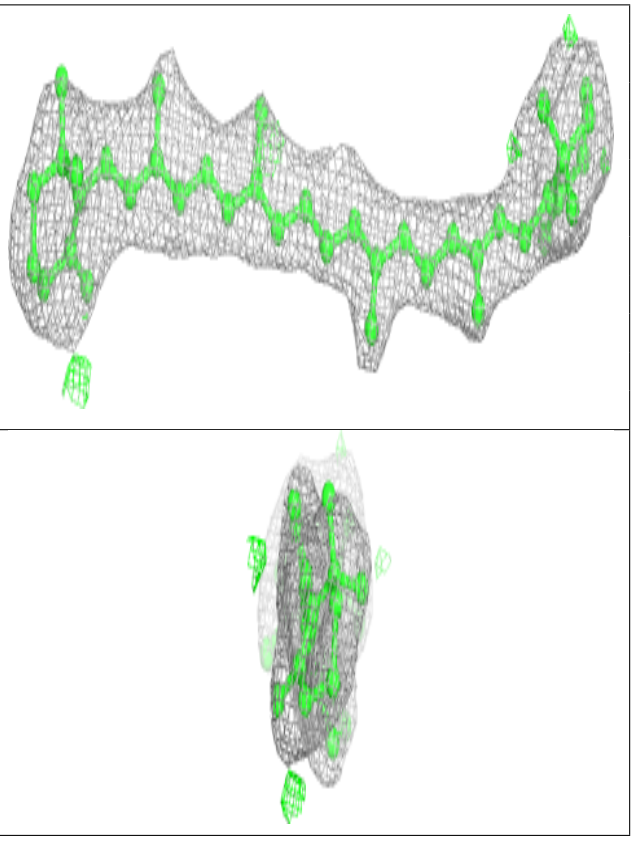
Electron density around BCR b 628:

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



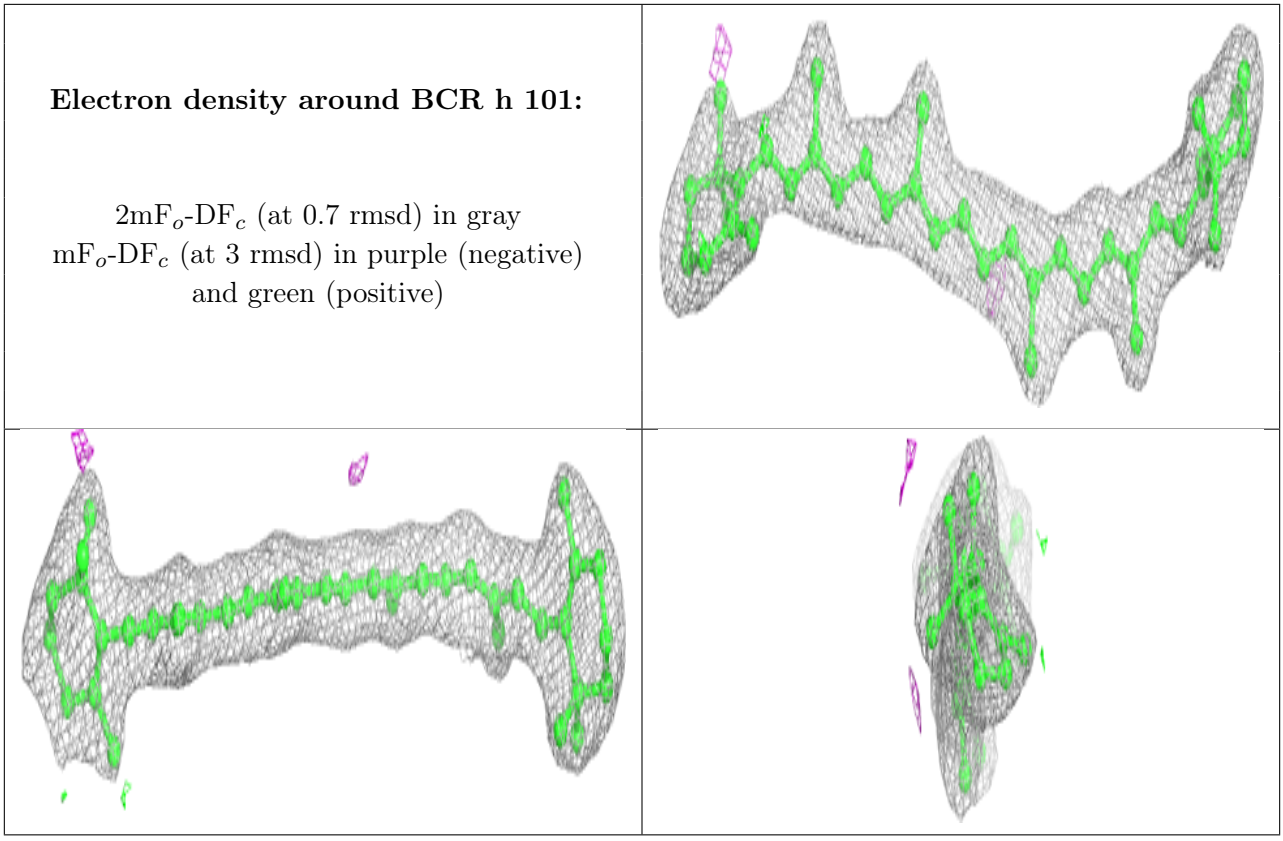
Electron density around BCR c 527:

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



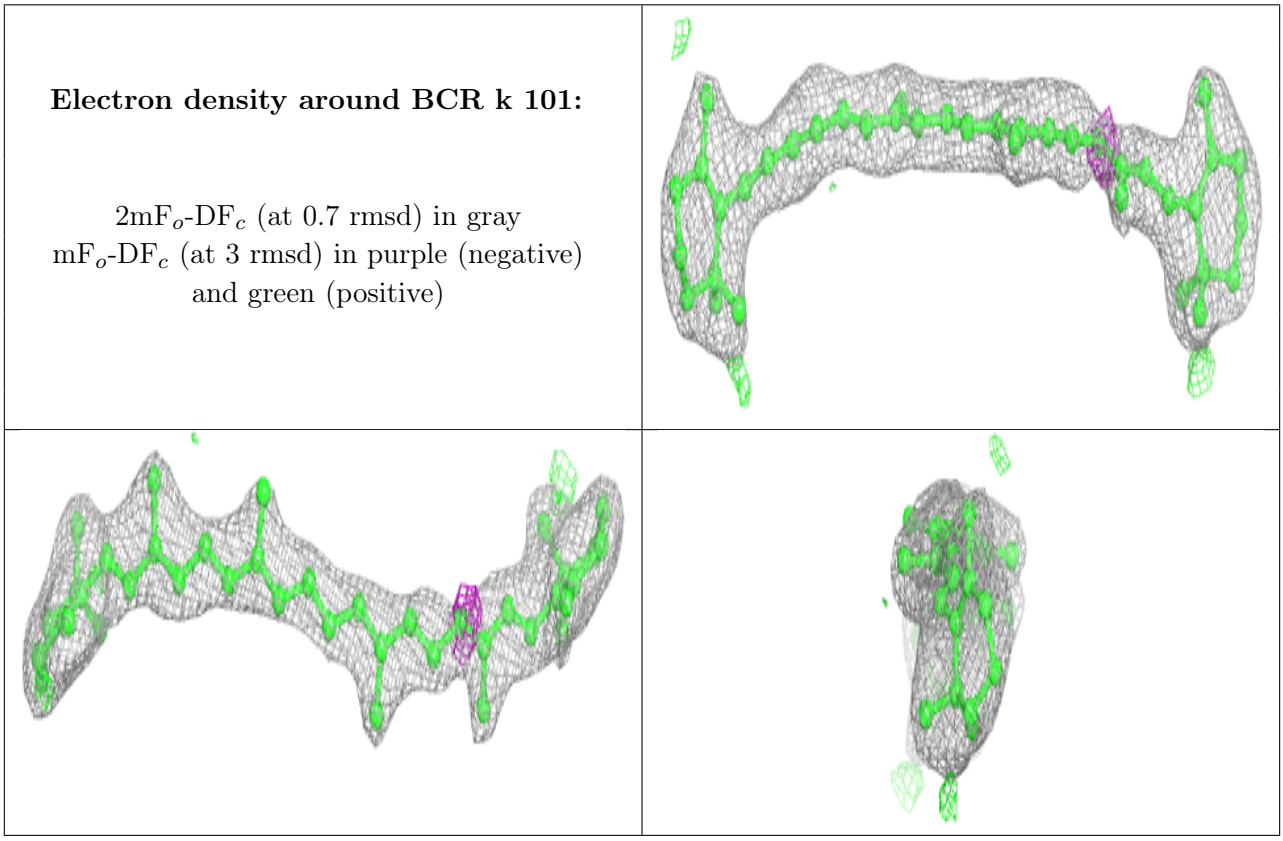
Electron density around BCR h 101:

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



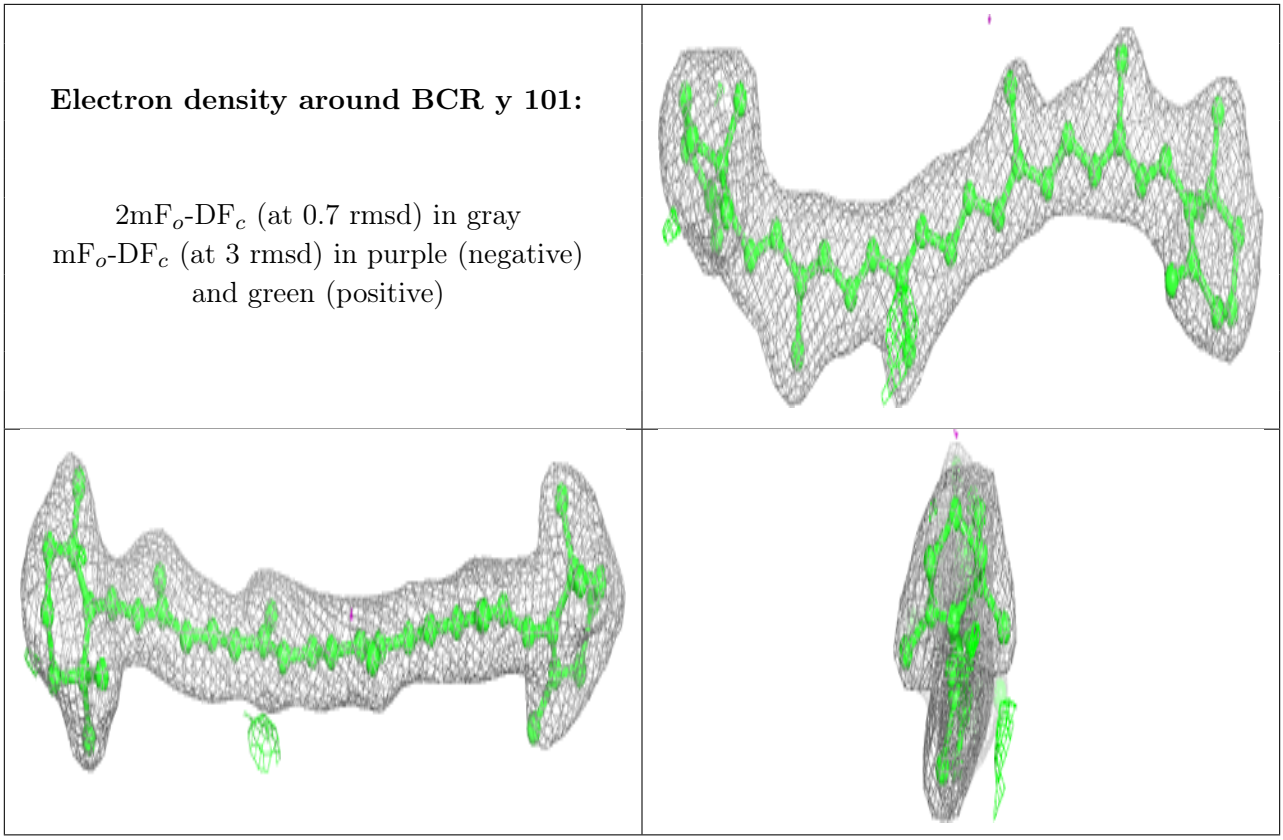
Electron density around BCR k 101:

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



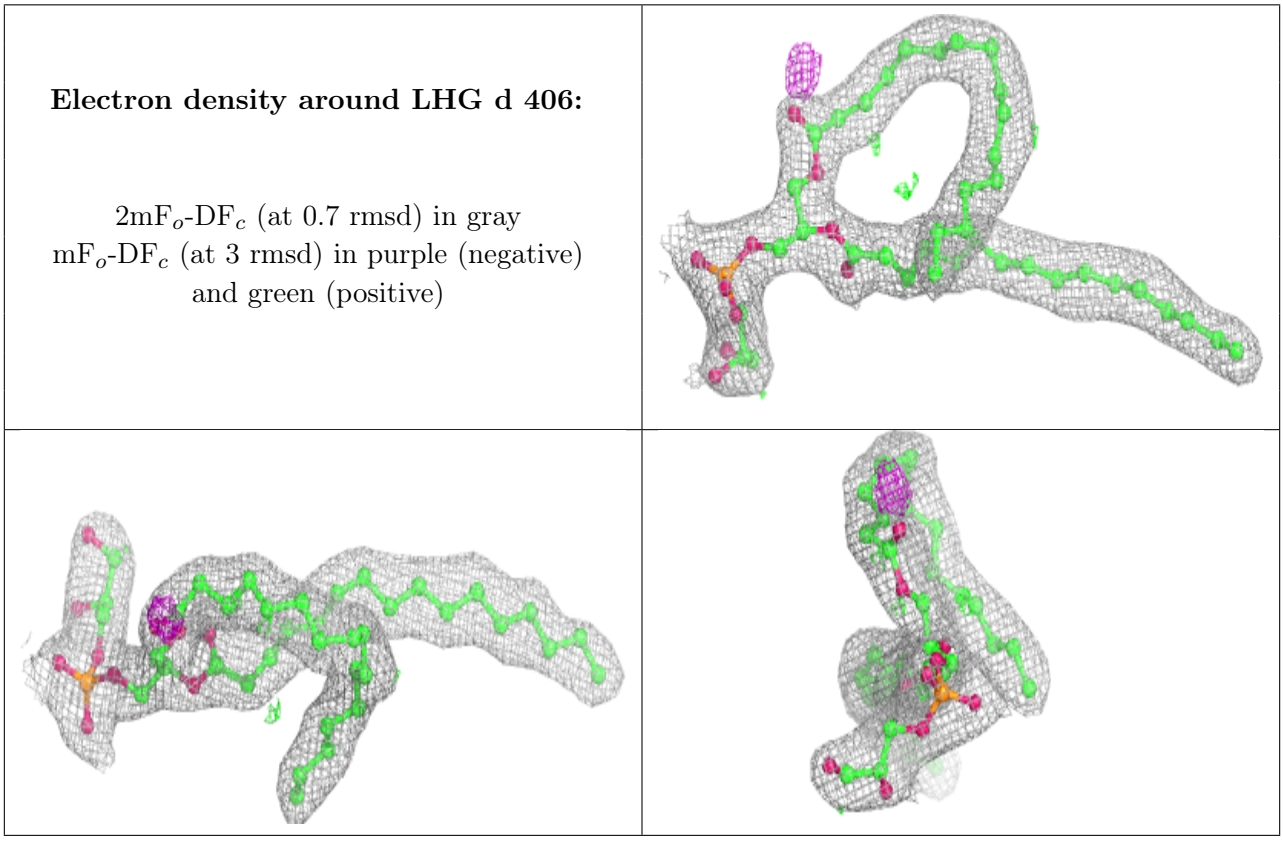
Electron density around BCR y 101:

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



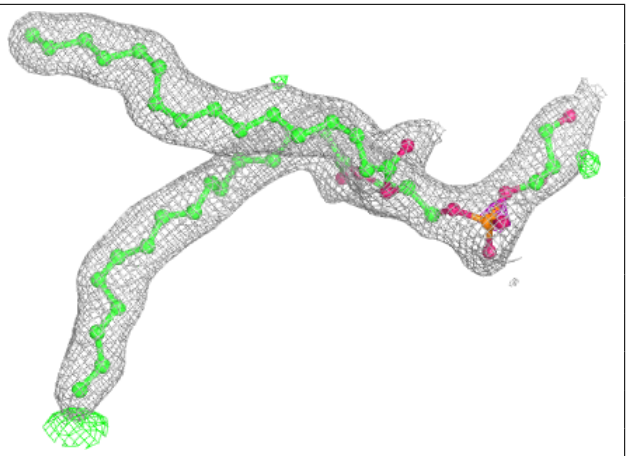
Electron density around LHG d 406:

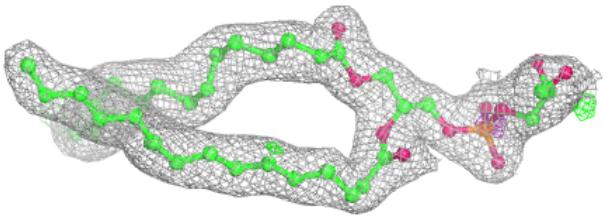
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

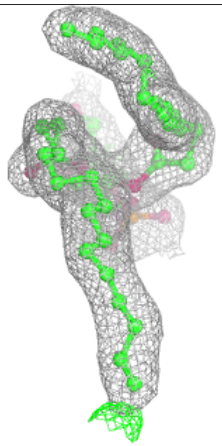


Electron density around LHG d 407:

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

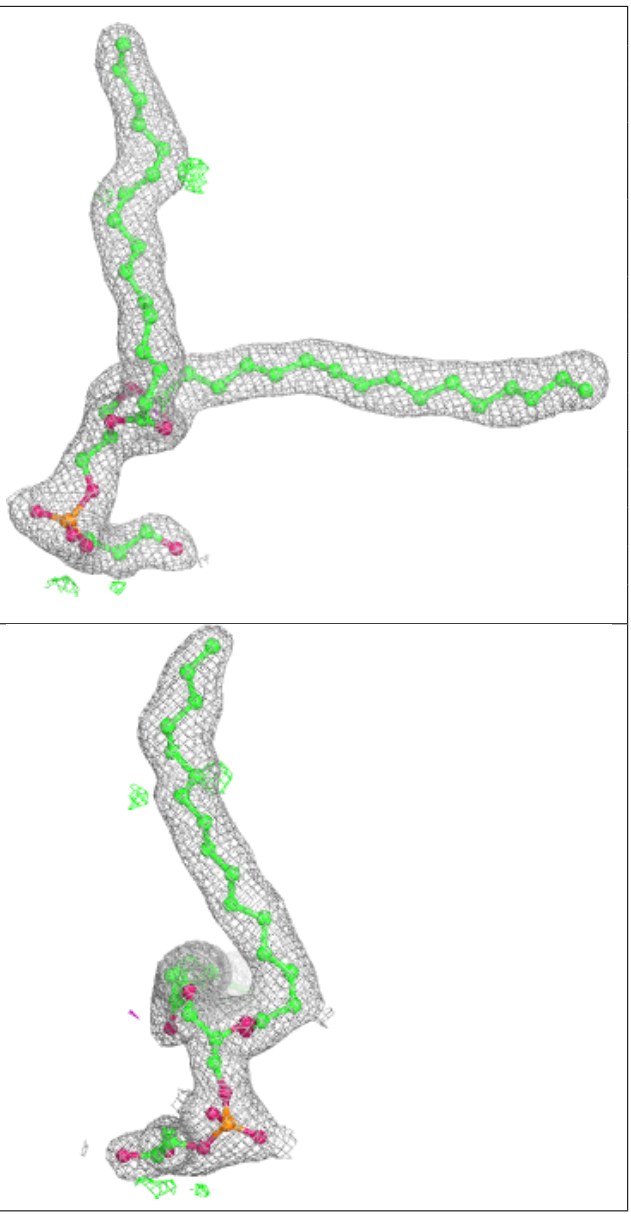






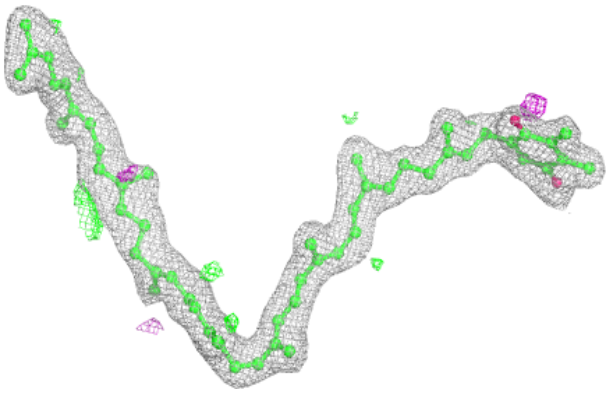
Electron density around LHG l 101:

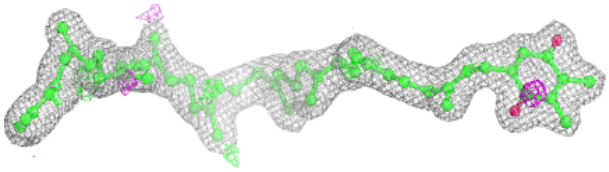
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

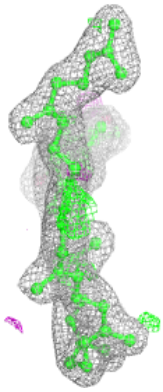


Electron density around PL9 D 405 (B):

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

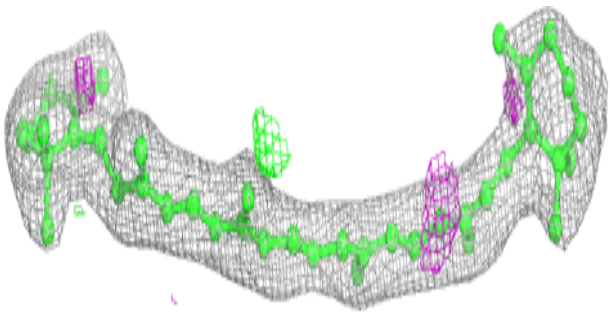


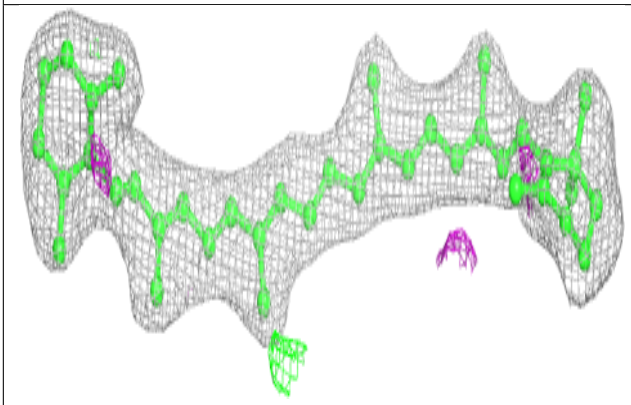


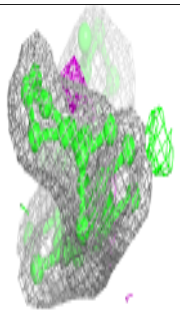


Electron density around BCR D 404:

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

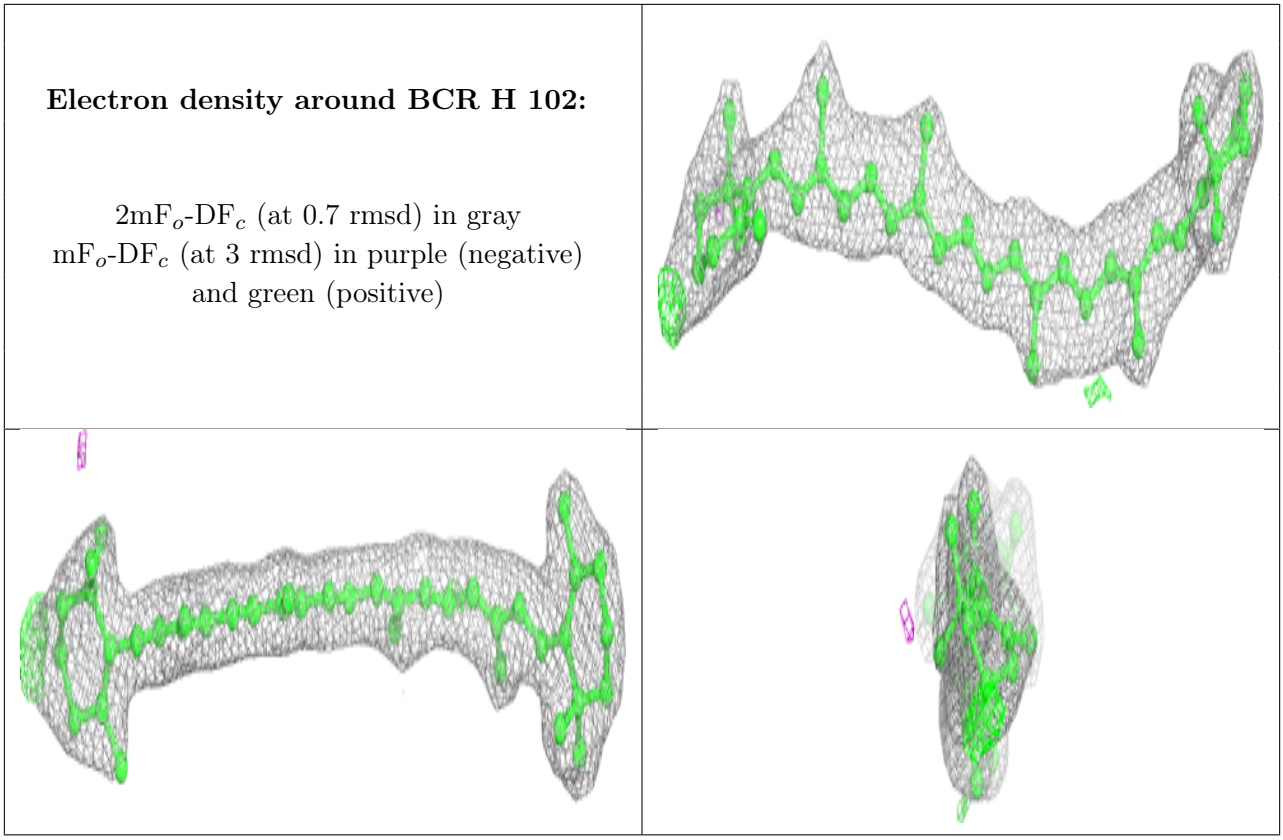






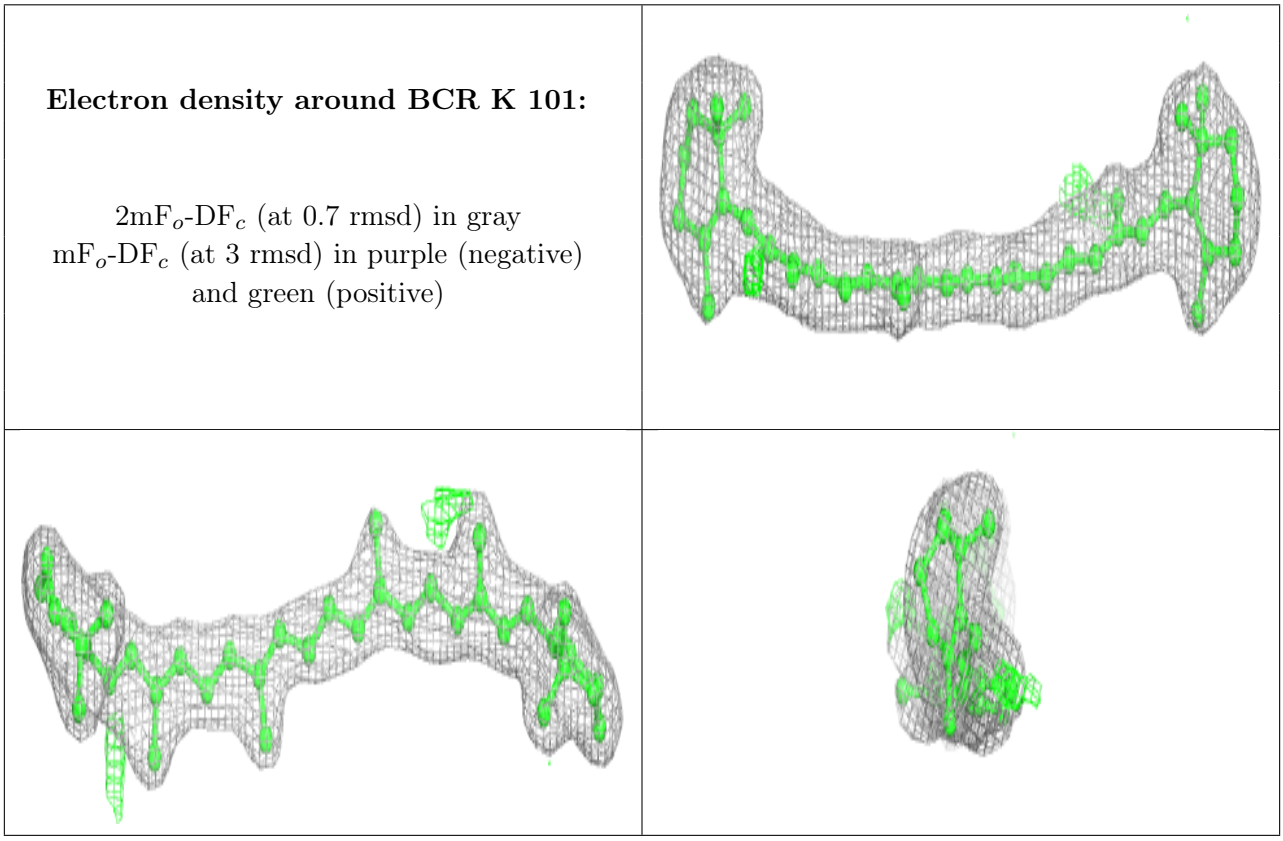
Electron density around BCR H 102:

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



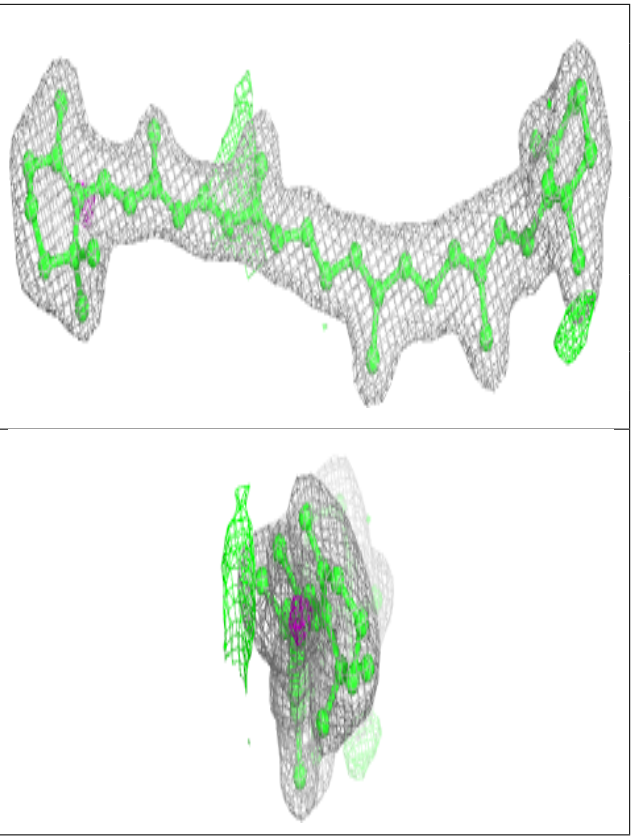
Electron density around BCR K 101:

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



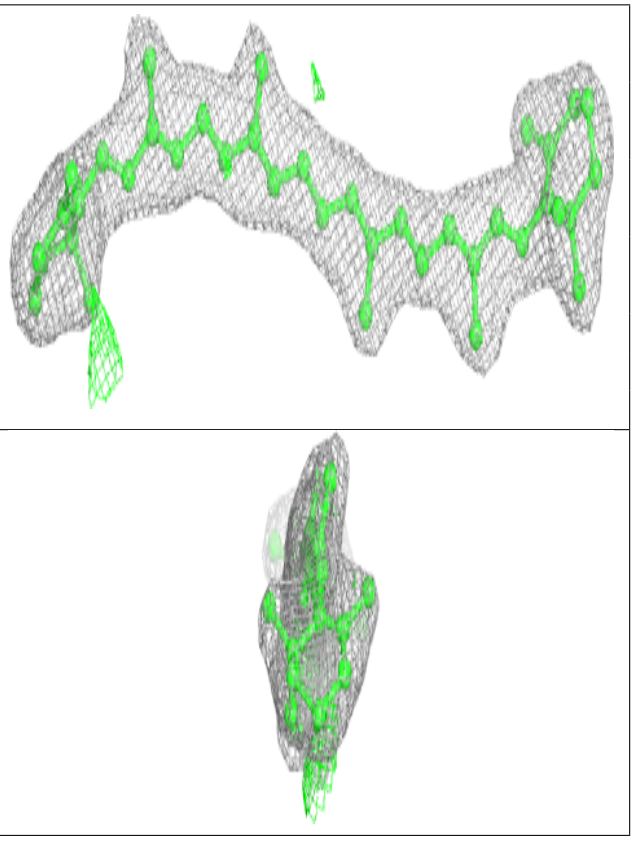
Electron density around BCR T 103:

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



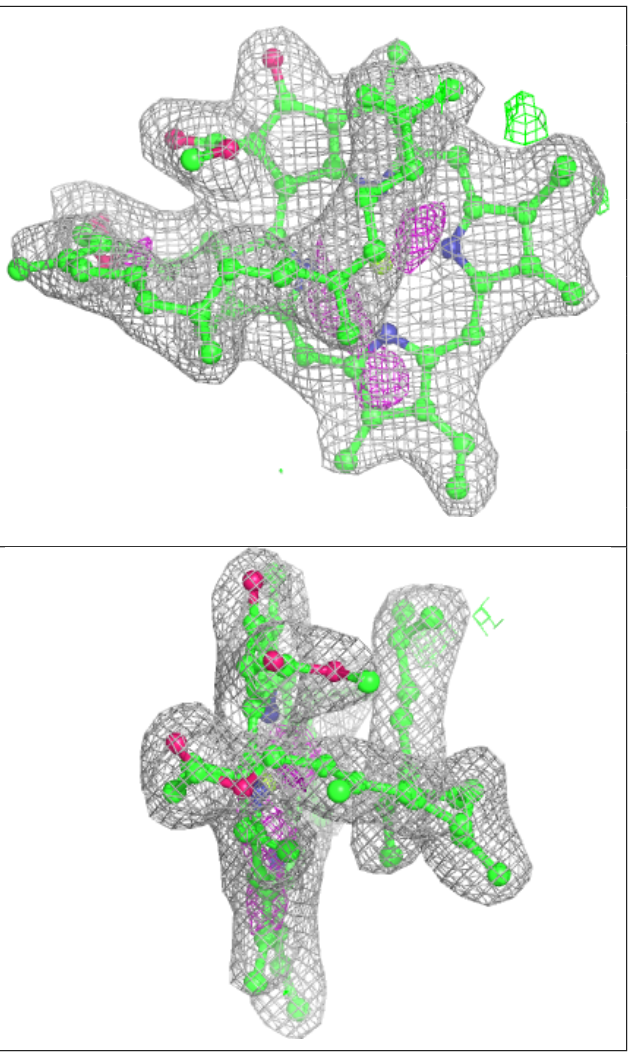
Electron density around BCR Y 101:

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



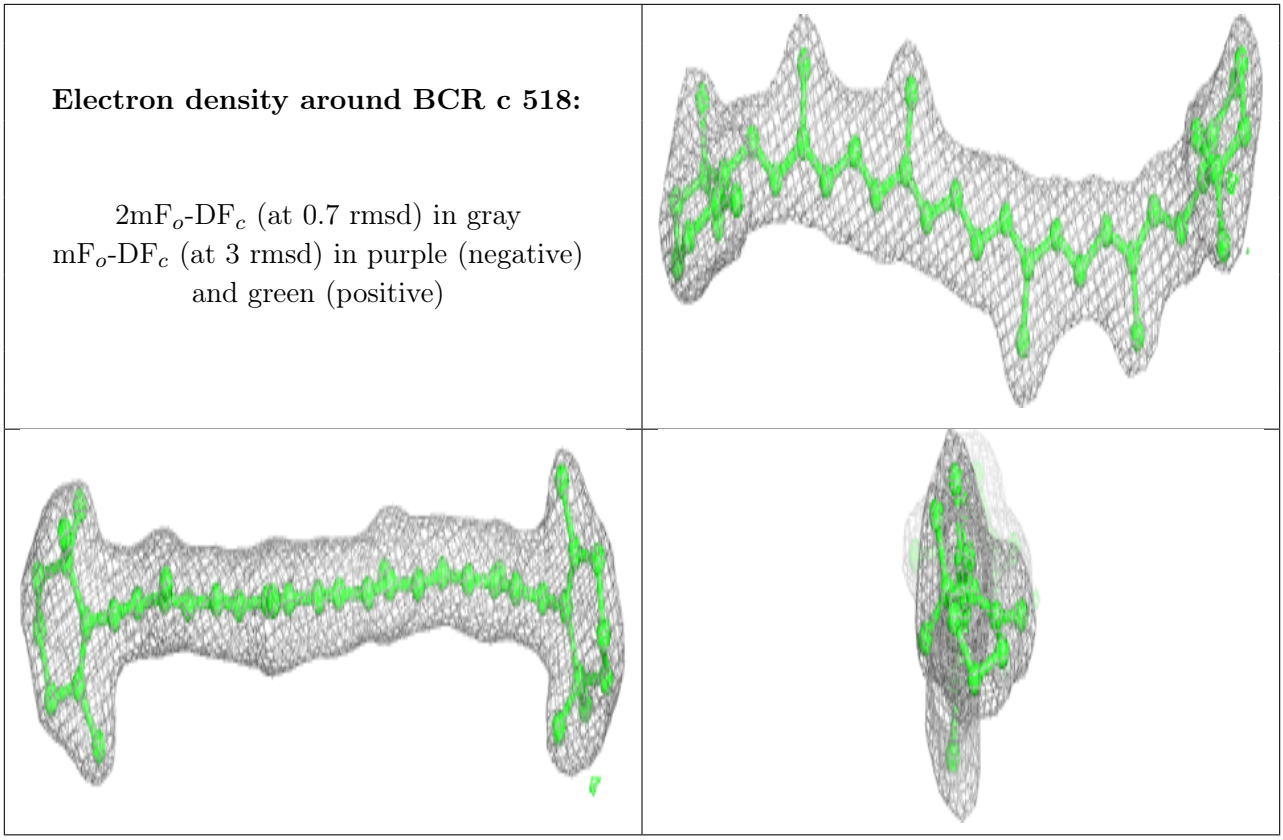
Electron density around CLA C 510:

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



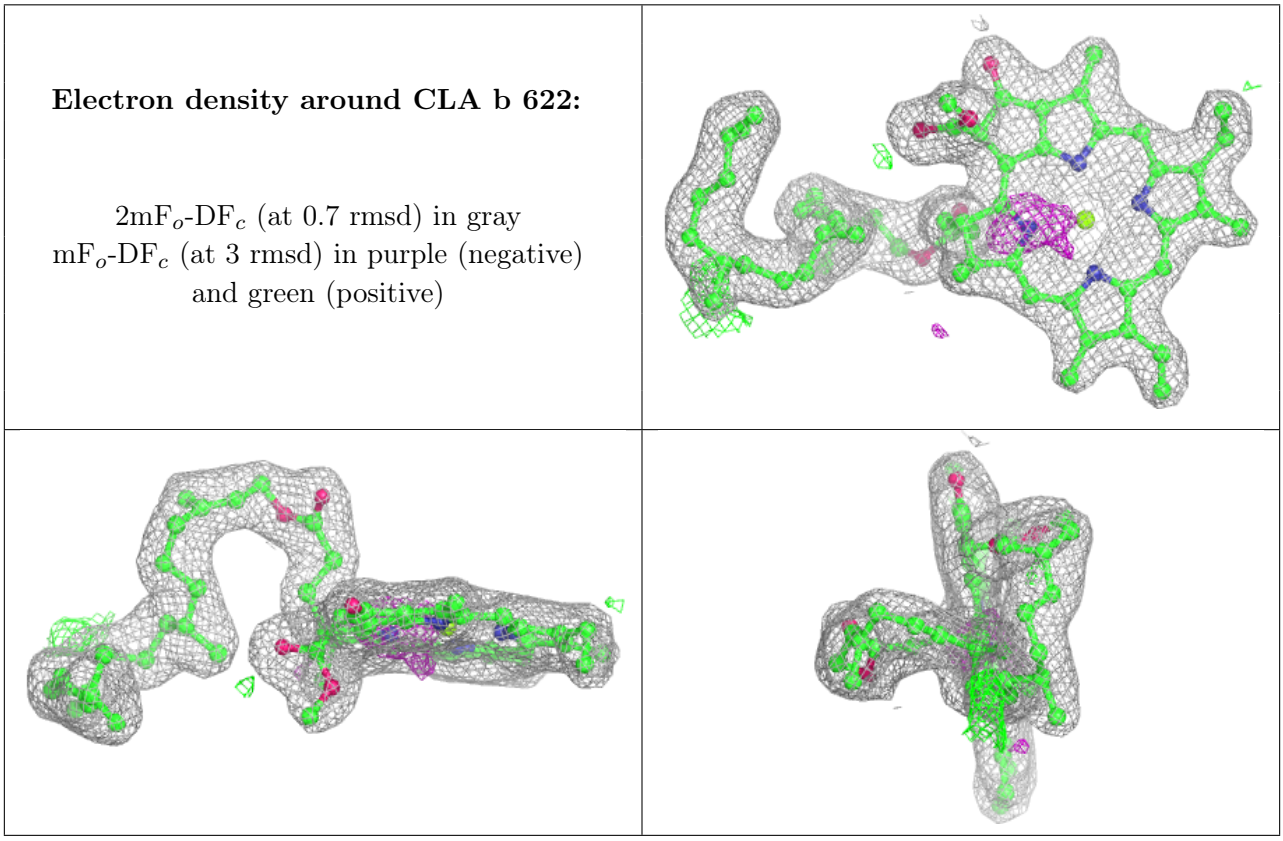
Electron density around BCR c 518:

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



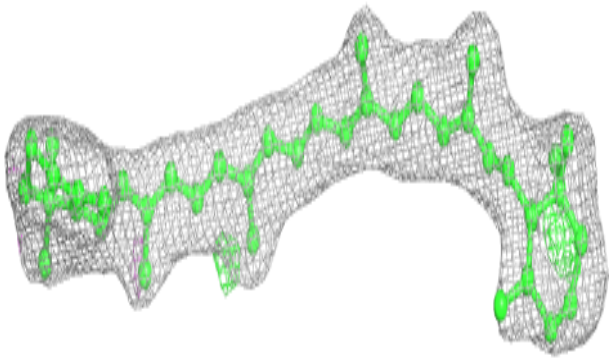
Electron density around CLA b 622:

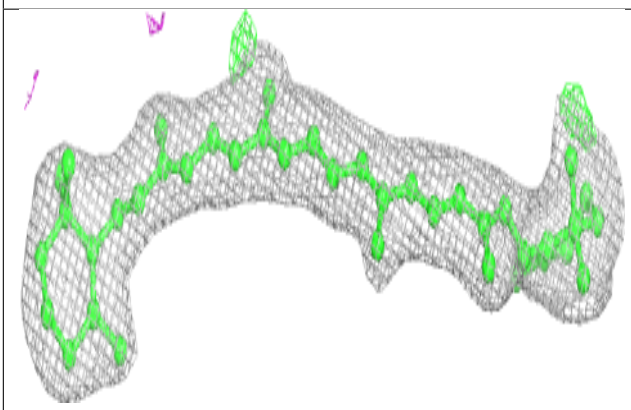
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

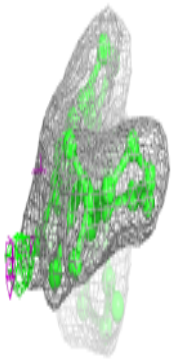


Electron density around BCR d 404:

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

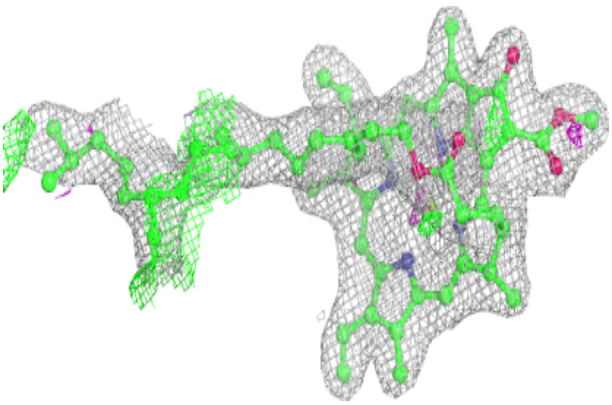


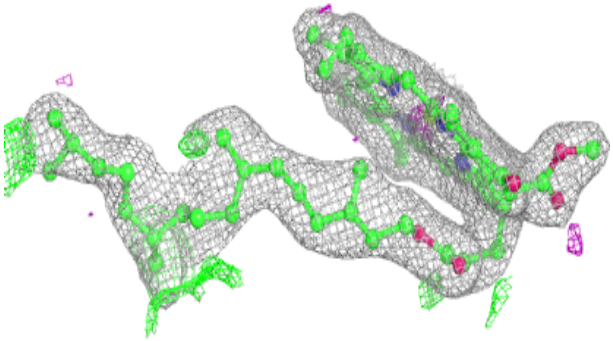


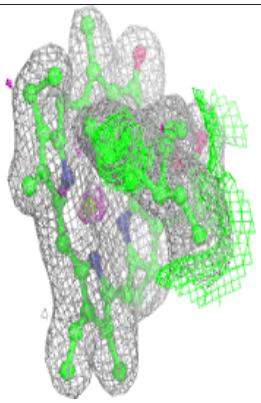


Electron density around CLA b 624:

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

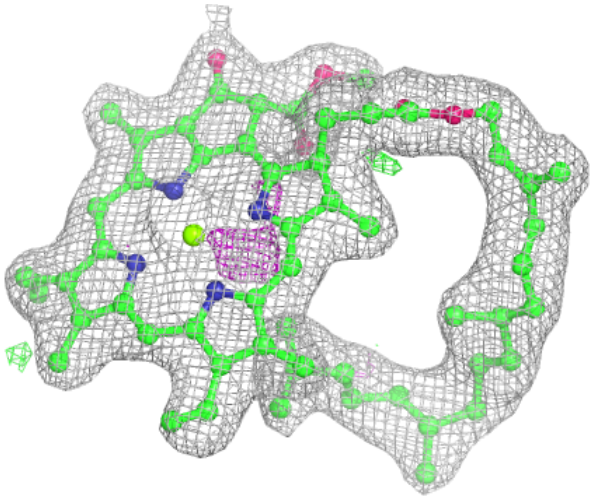


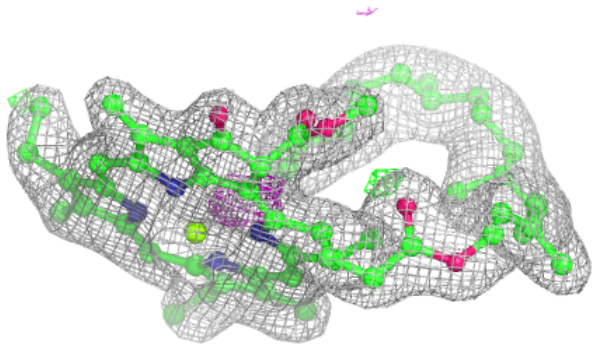


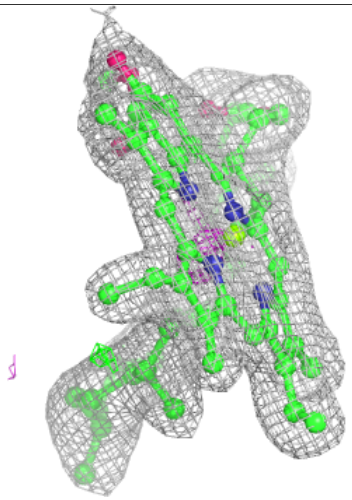


Electron density around CLA b 625:

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

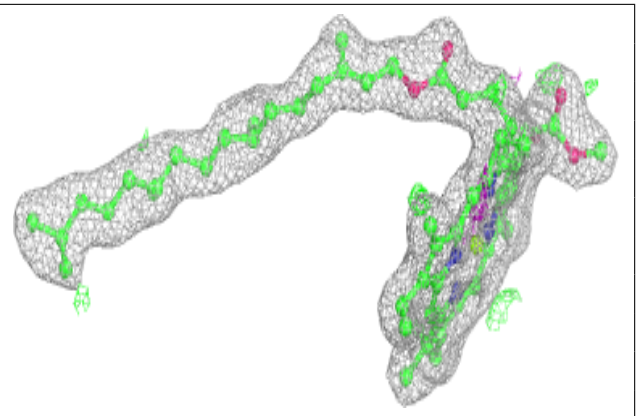


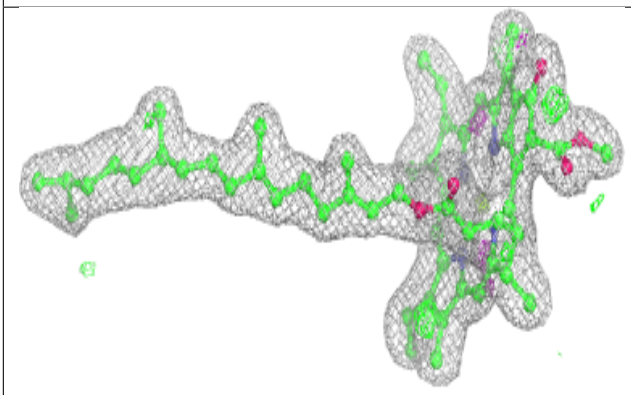


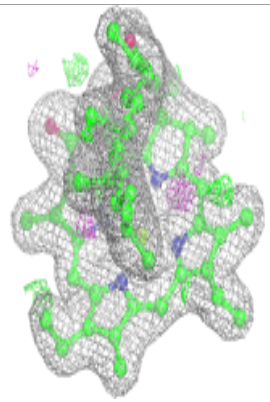


Electron density around CLA B 608:

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

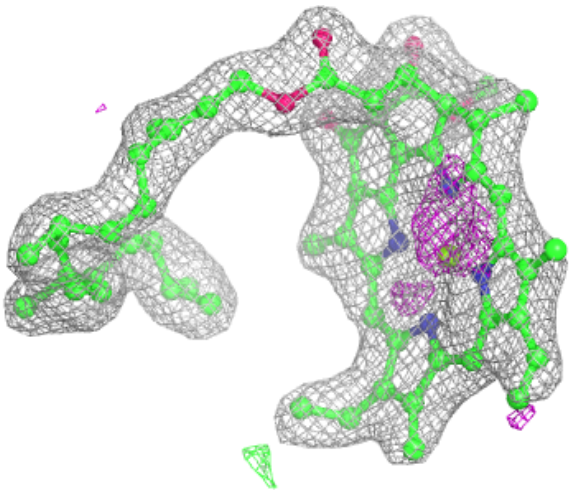


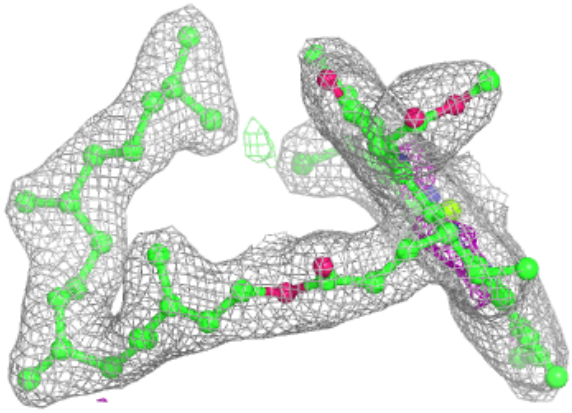


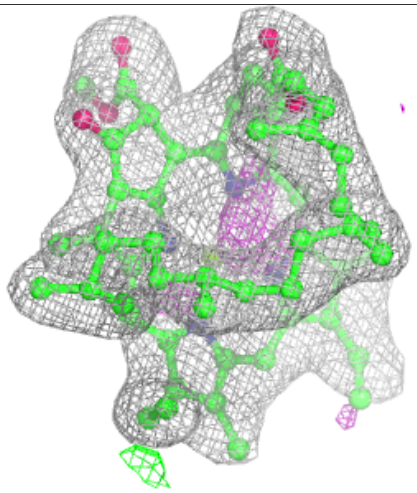


Electron density around CLA C 503:

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

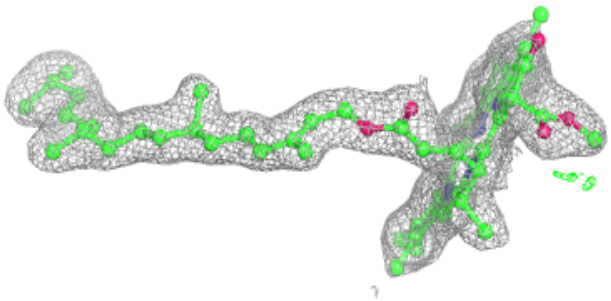






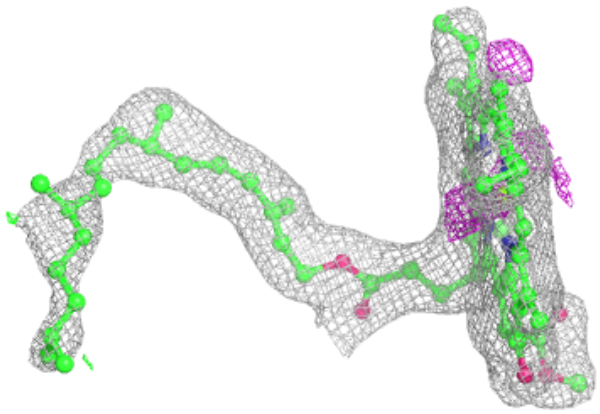
Electron density around CLA B 610:

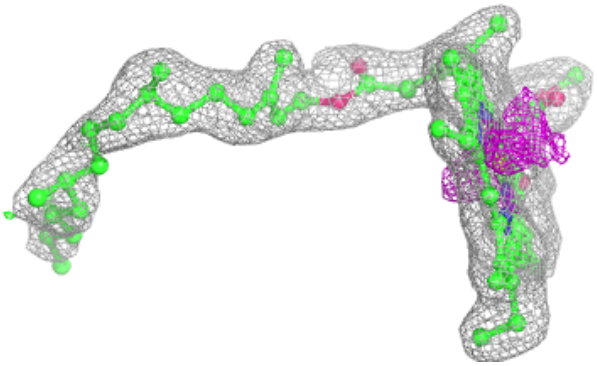
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

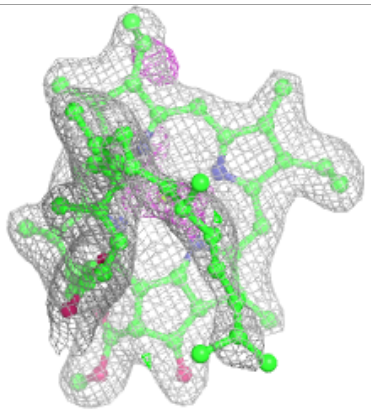


Electron density around CLA D 403:

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

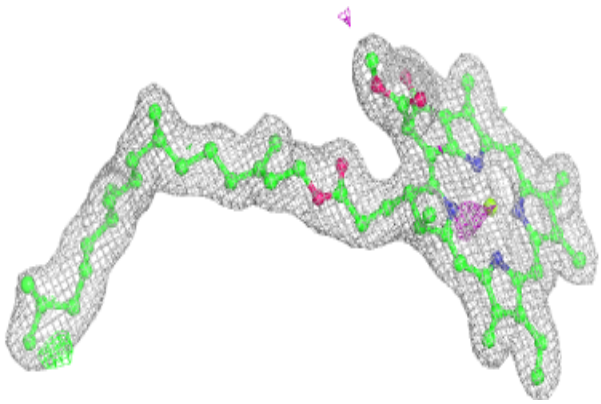


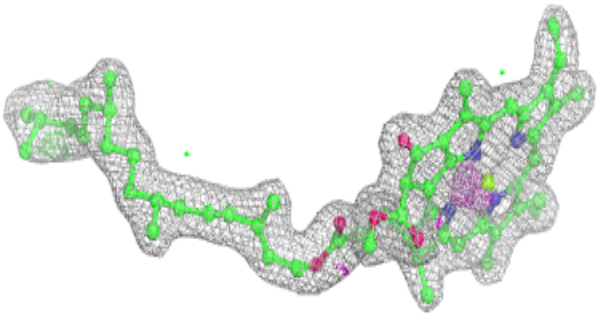


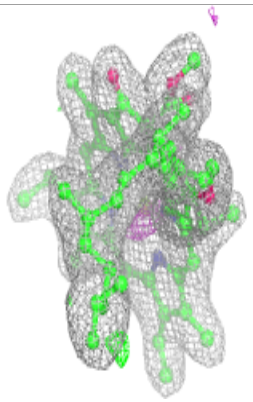


Electron density around CLA a 409:

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

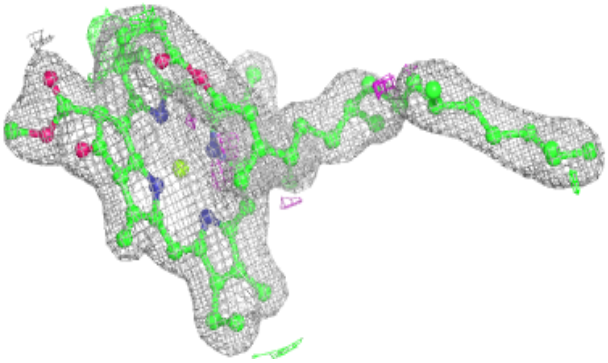


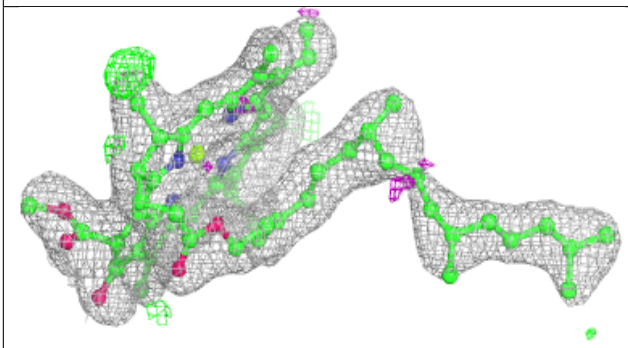


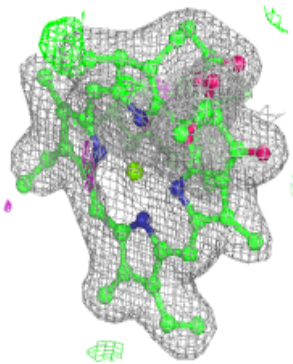


Electron density around CLA C 505:

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

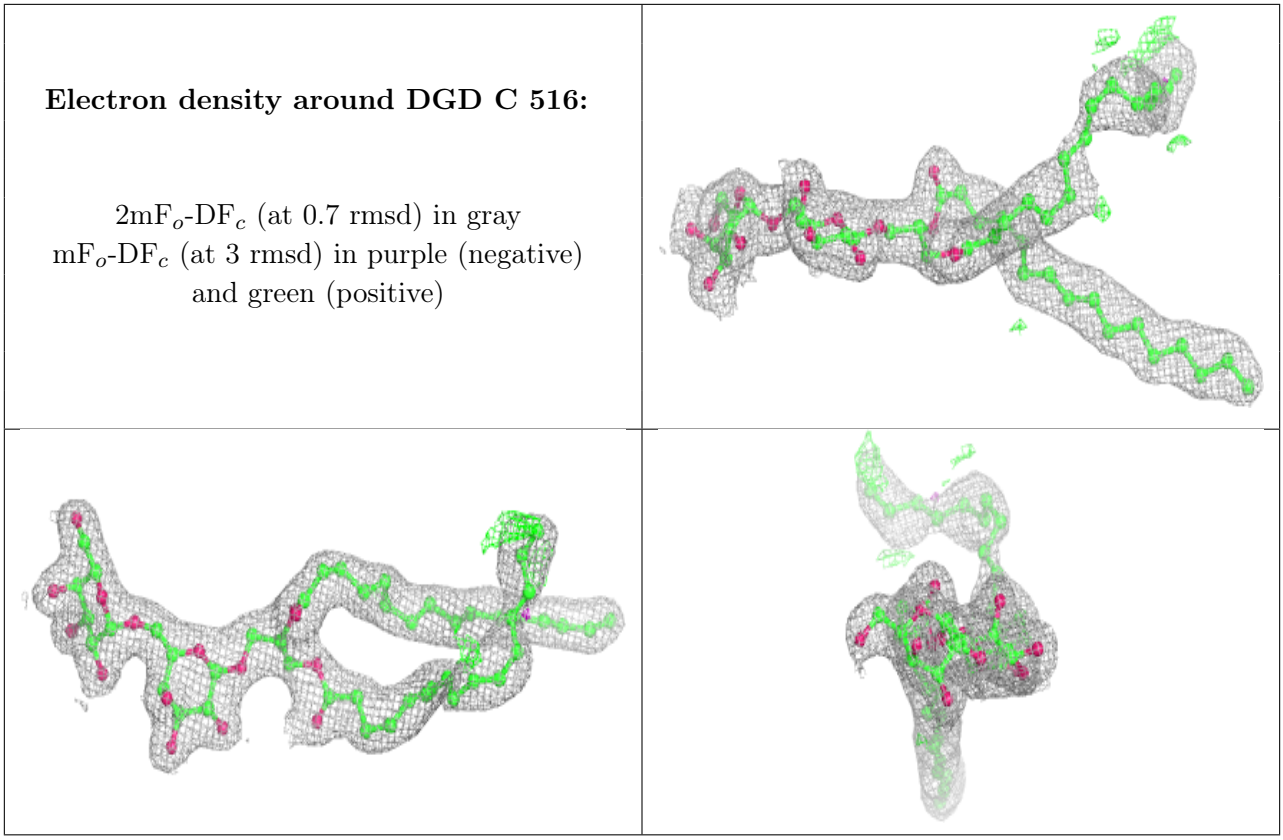






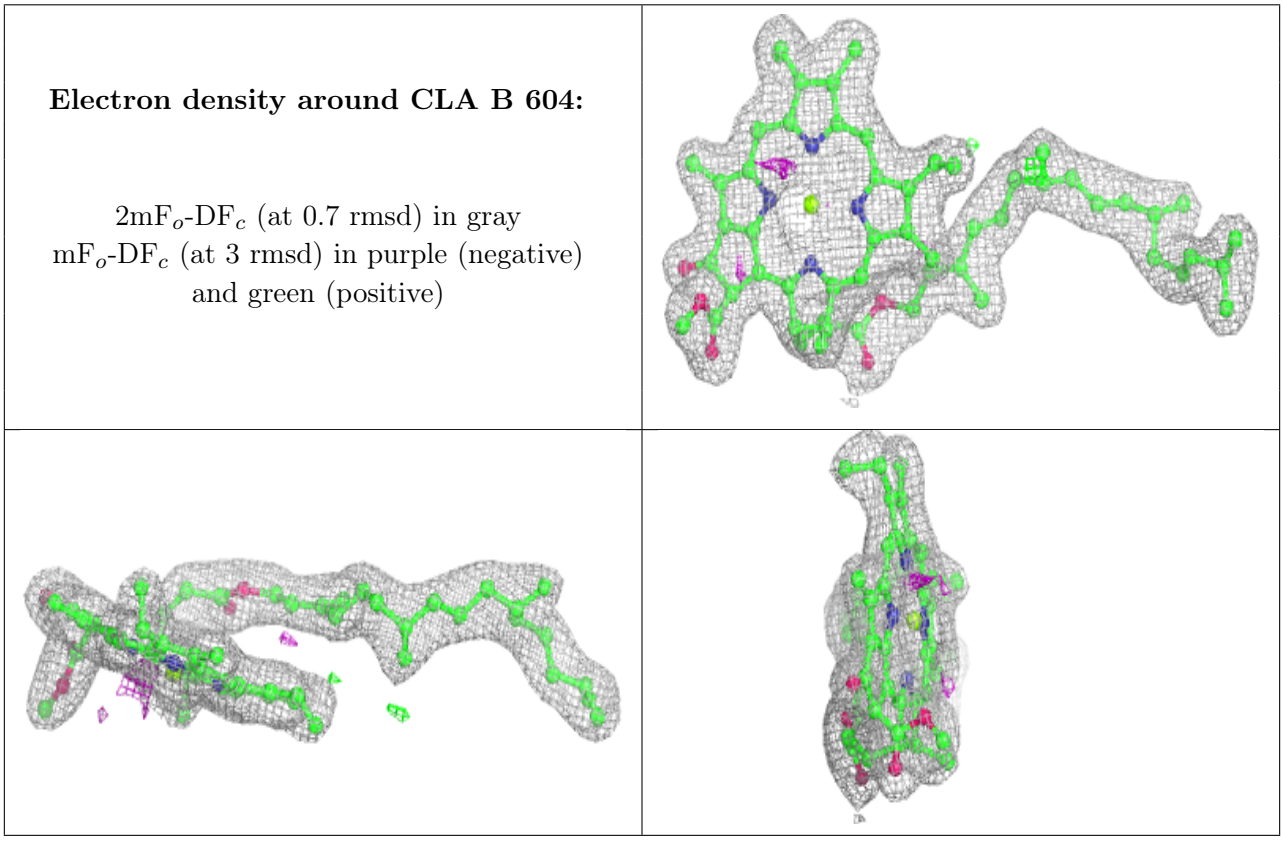
Electron density around DGD C 516:

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



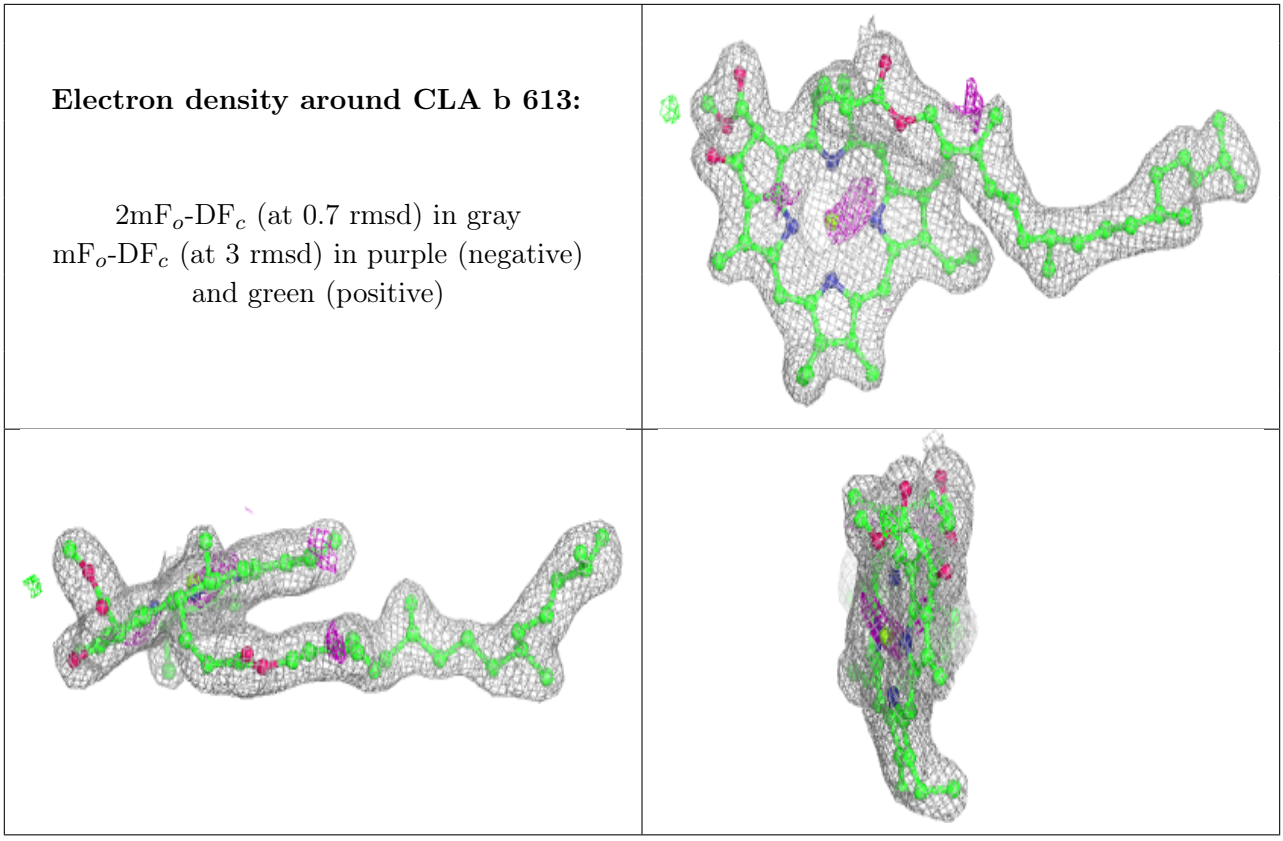
Electron density around CLA B 604:

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



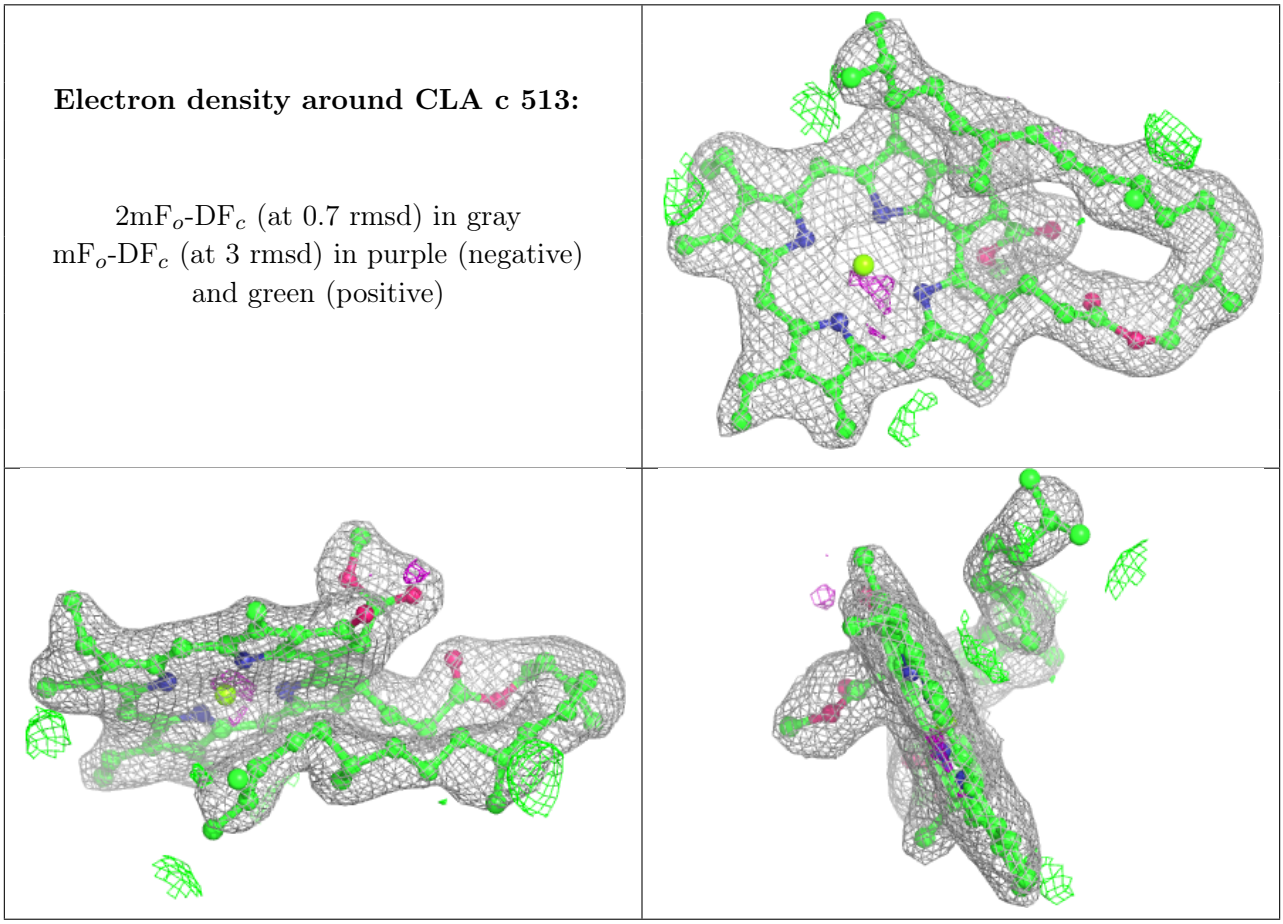
Electron density around CLA b 613:

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



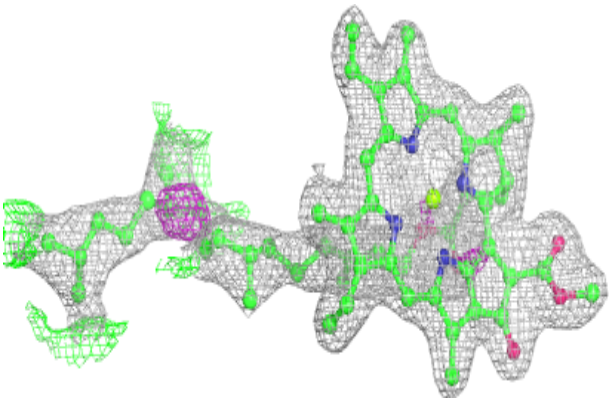
Electron density around CLA c 513:

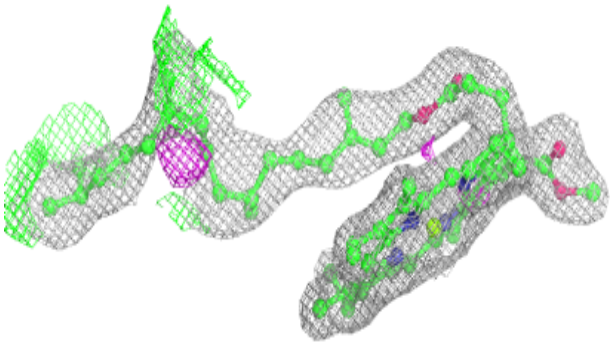
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

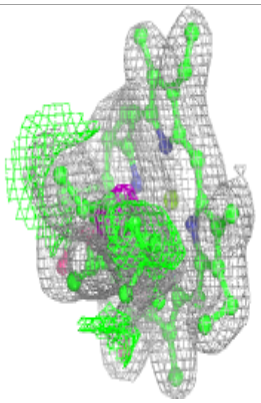


Electron density around CLA B 615:

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

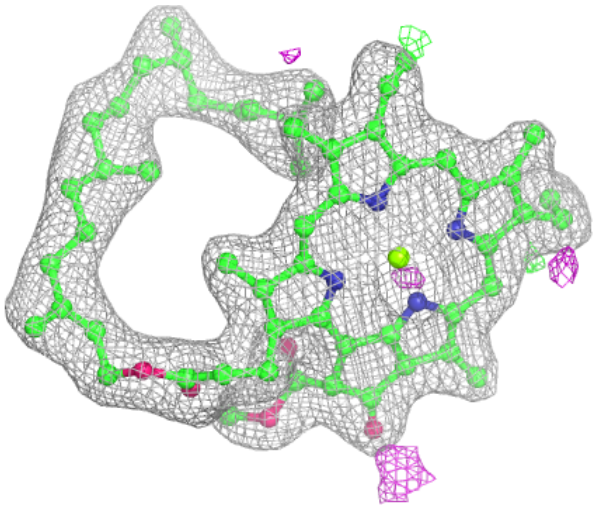


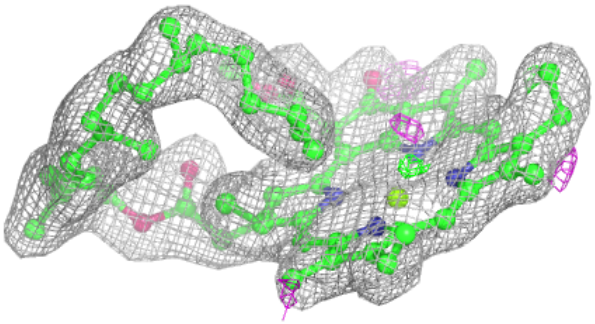


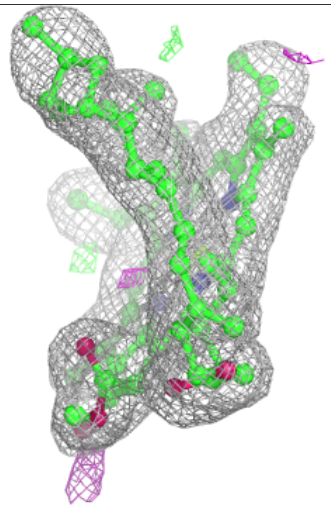


Electron density around CLA B 616:

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

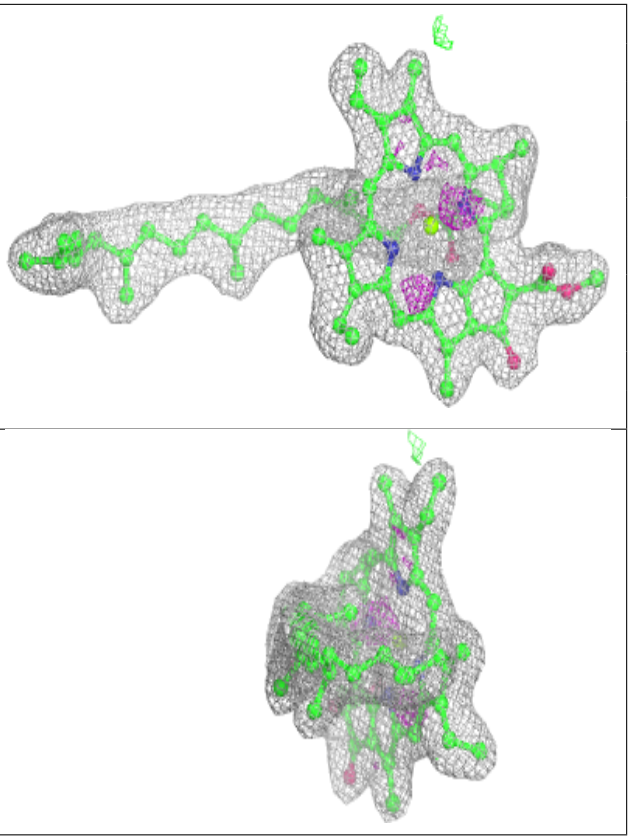


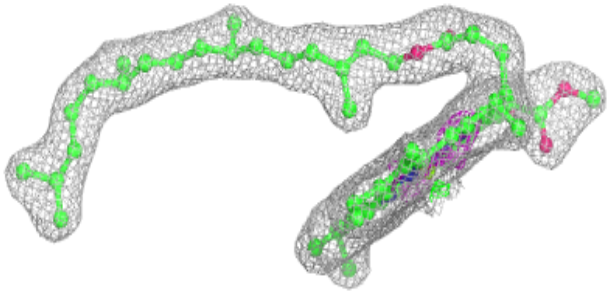




Electron density around CLA b 618:

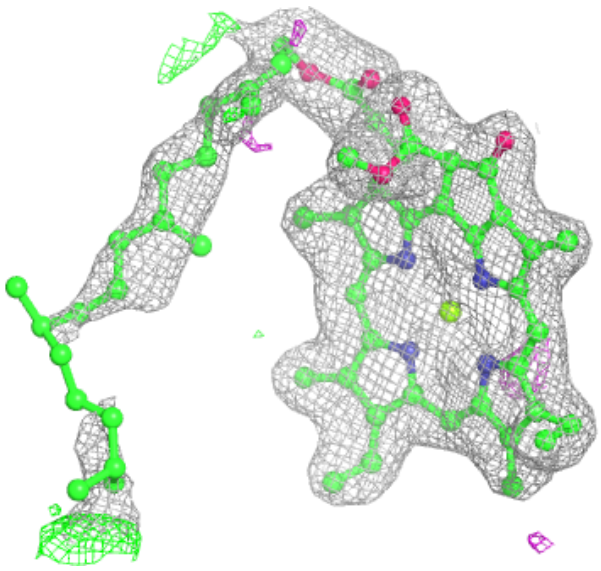
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

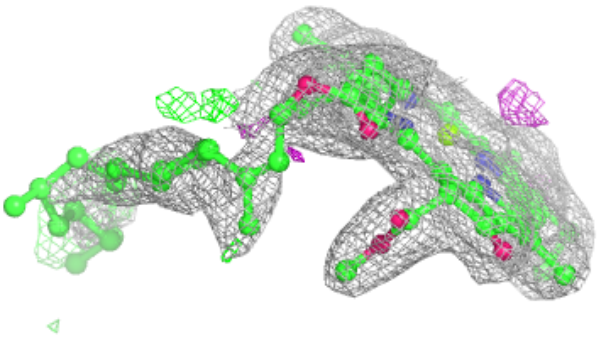


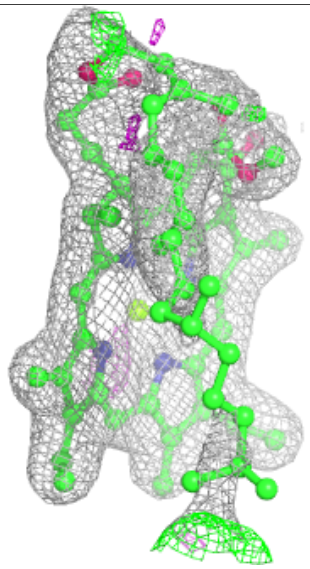


Electron density around CLA B 617:

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

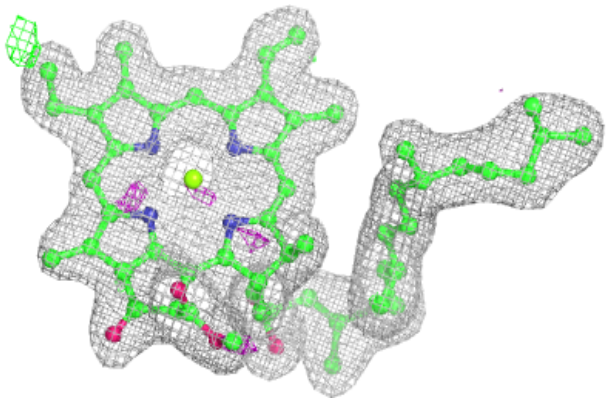


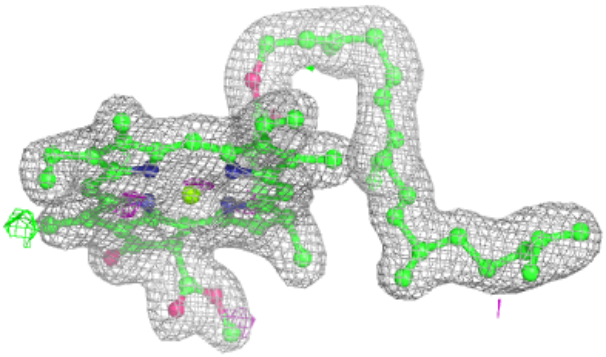


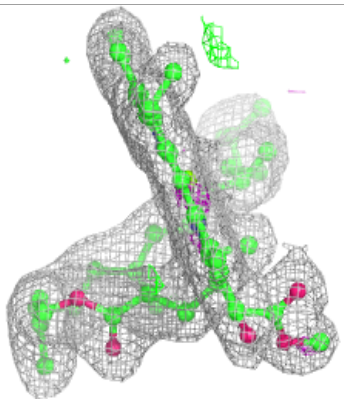


Electron density around CLA d 401:

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

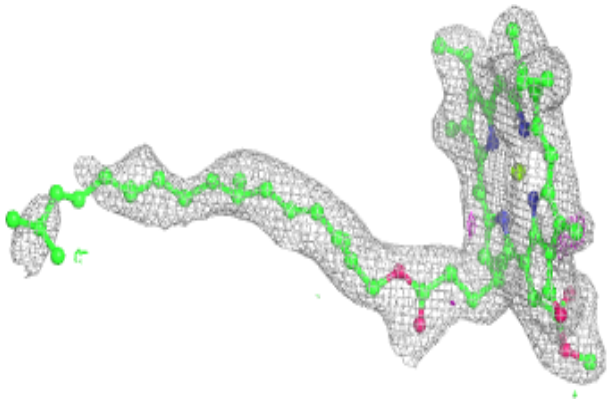


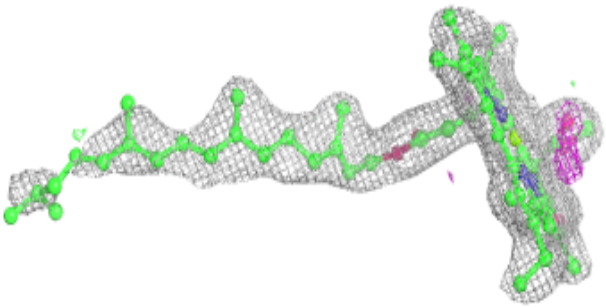


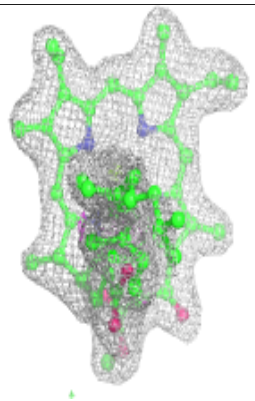


Electron density around CLA d 403:

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

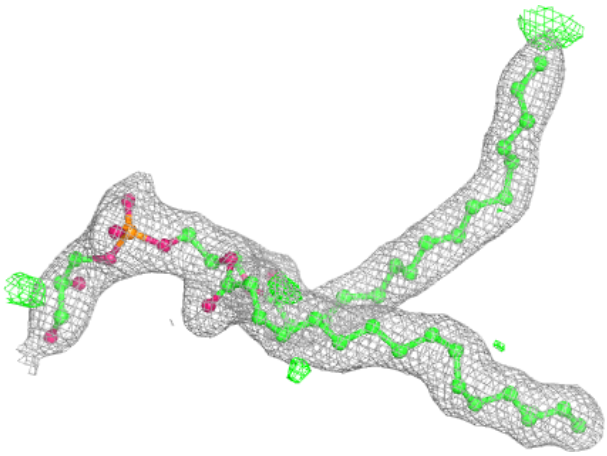


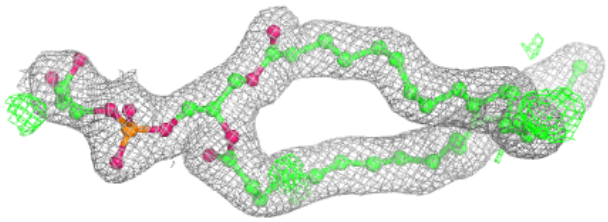


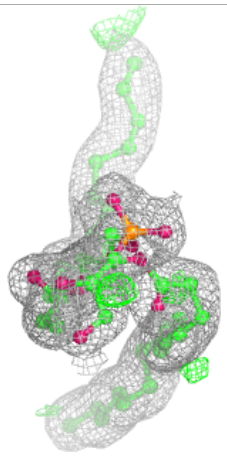


Electron density around LHG D 408:

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

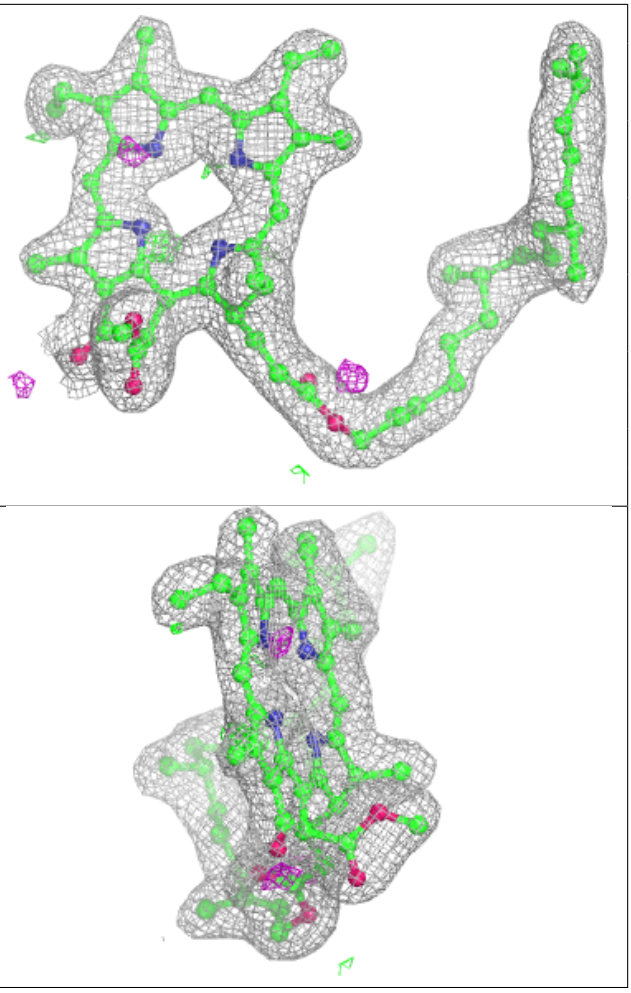






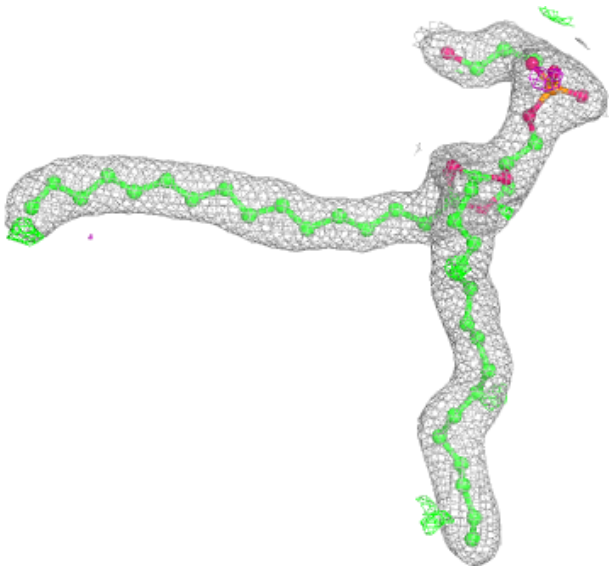
Electron density around PHO a 420 (A):

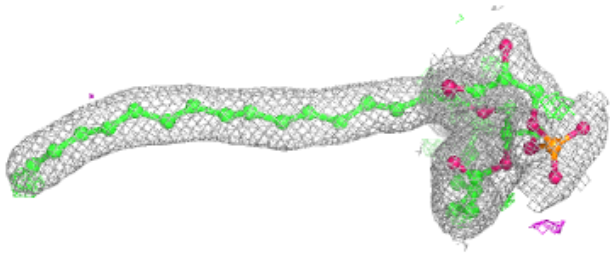
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

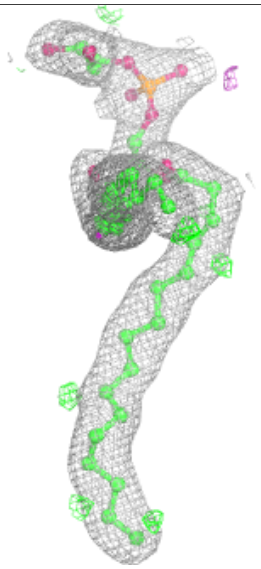


Electron density around LHG L 101:

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

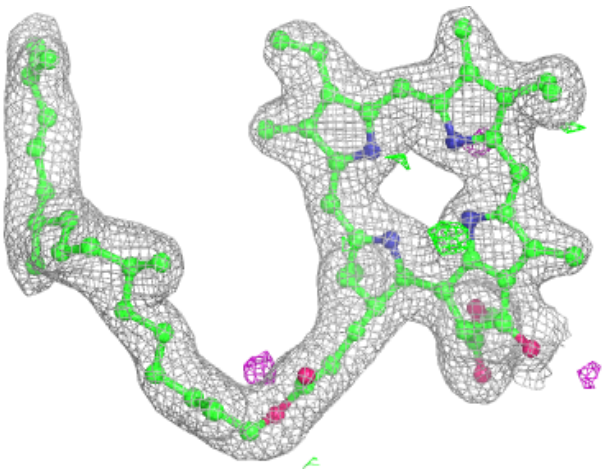


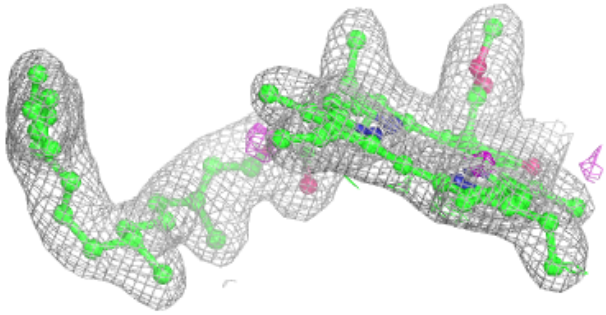


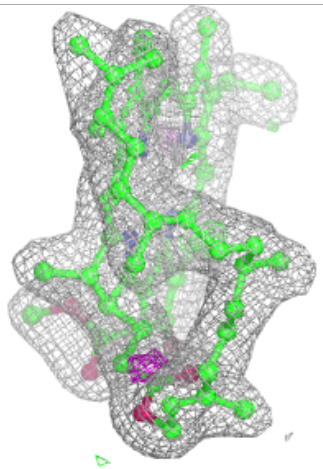


Electron density around PHO a 420 (B):

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

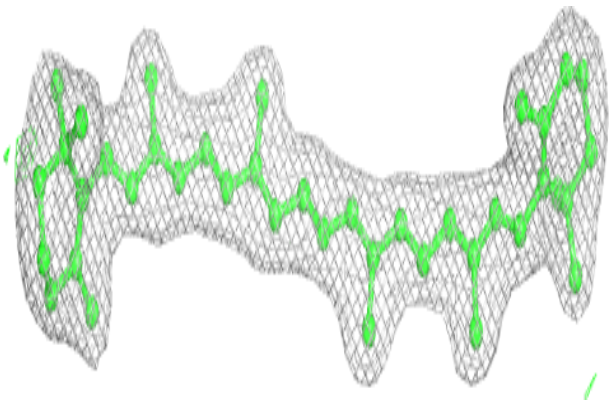


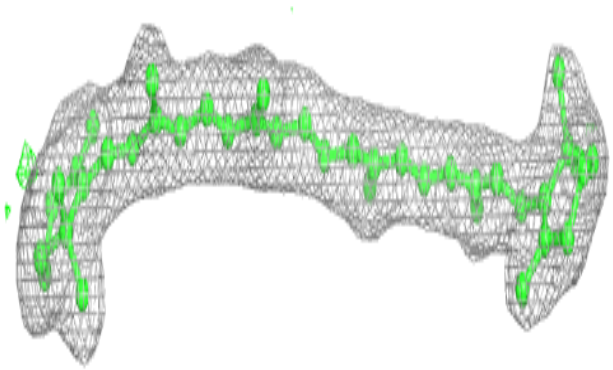


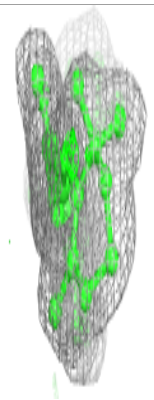


Electron density around BCR B 620:

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

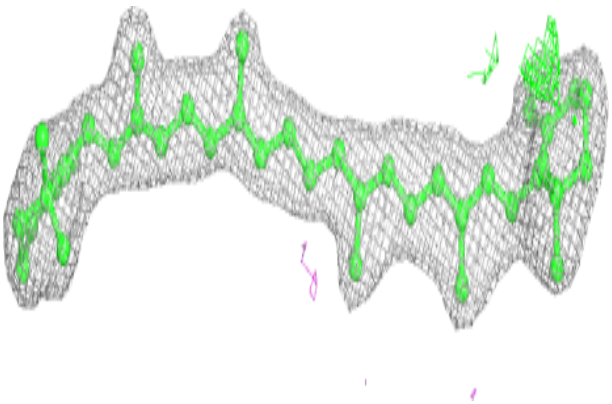


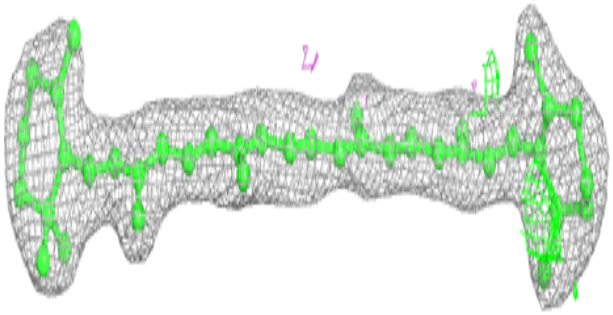


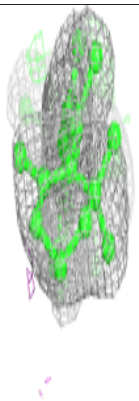


Electron density around BCR C 514:

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

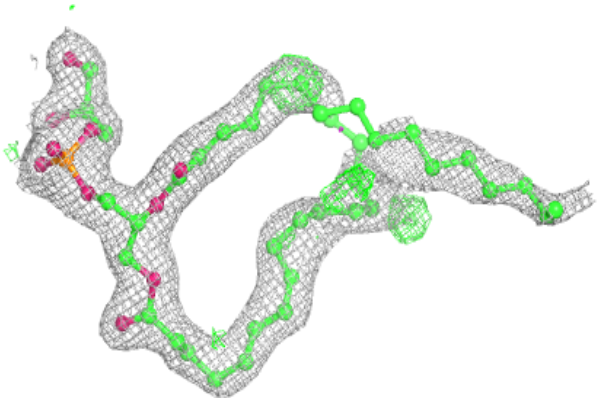


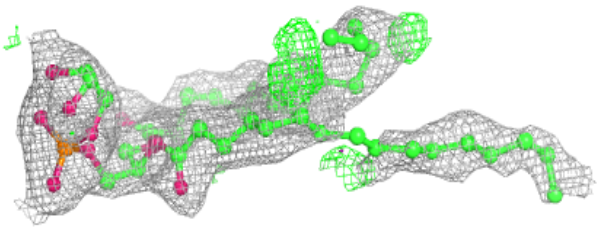


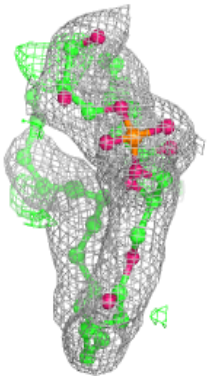


Electron density around LHG d 408:

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

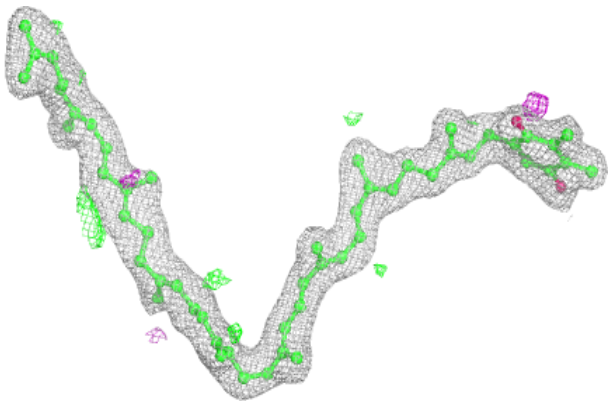


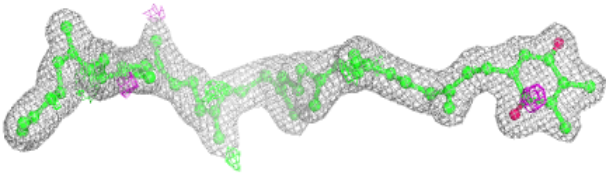


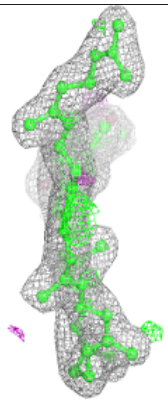


Electron density around PL9 D 405 (A):

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

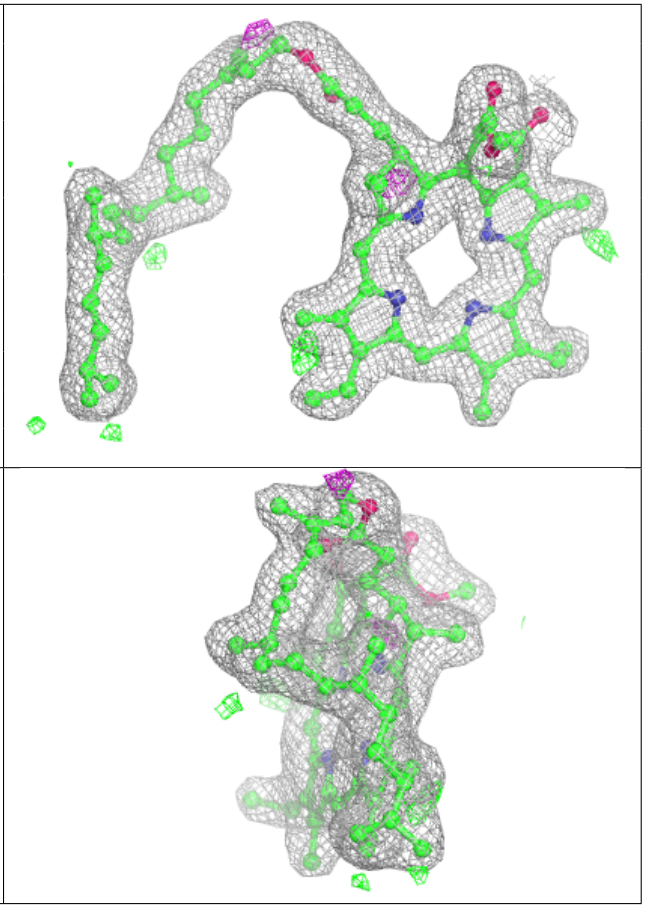






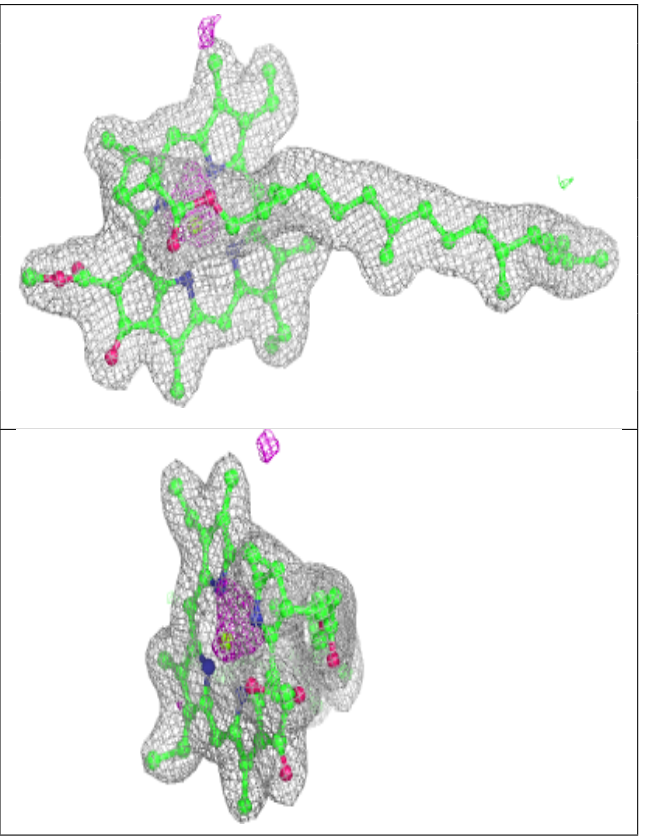
Electron density around PHO A 409 (B):

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



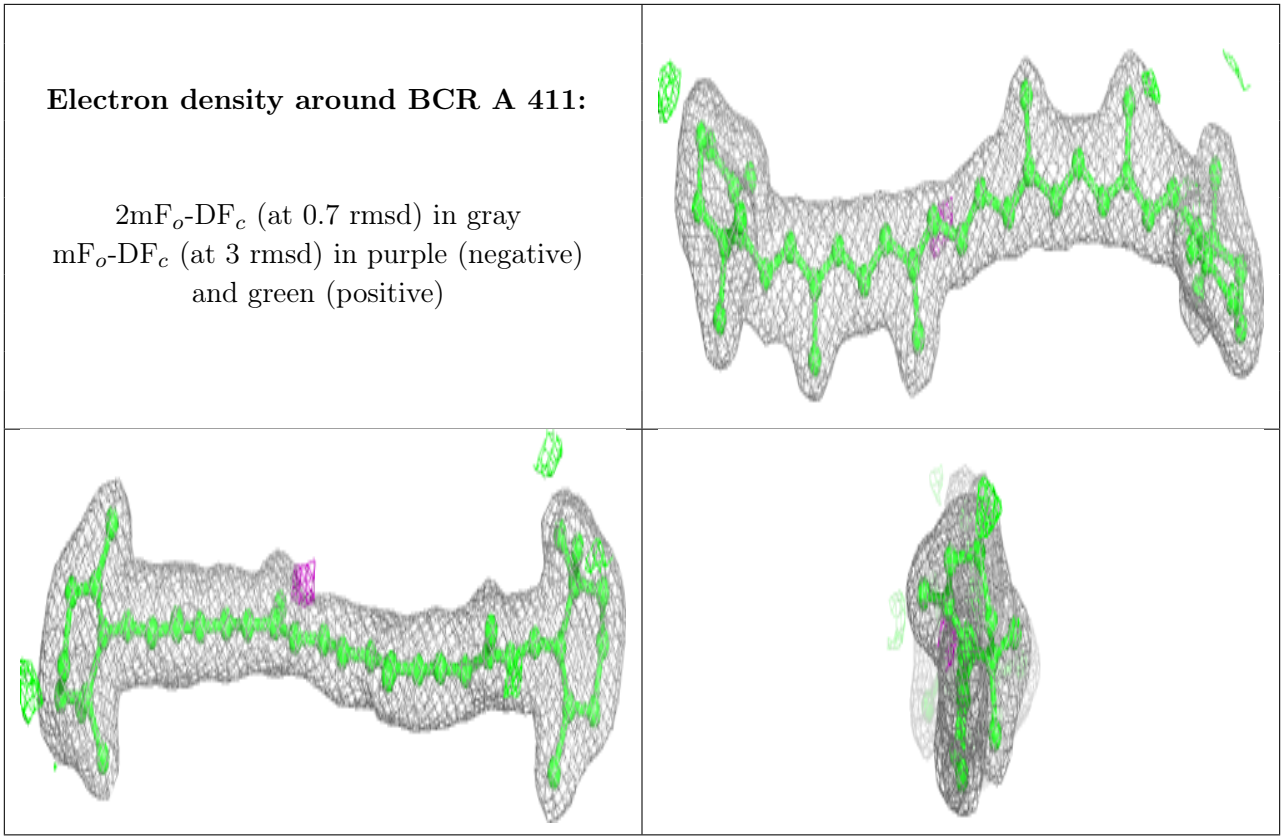
Electron density around CLA B 609:

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



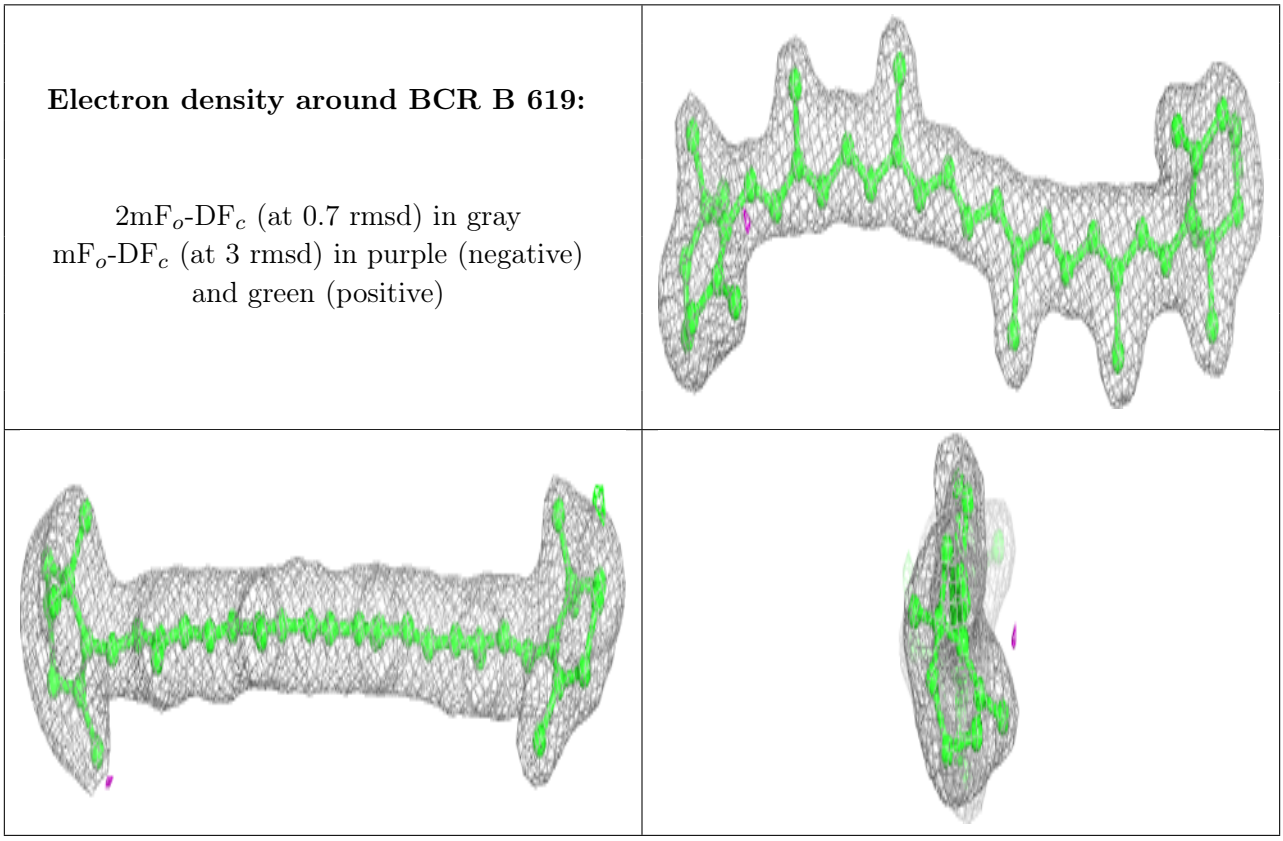
Electron density around BCR A 411:

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



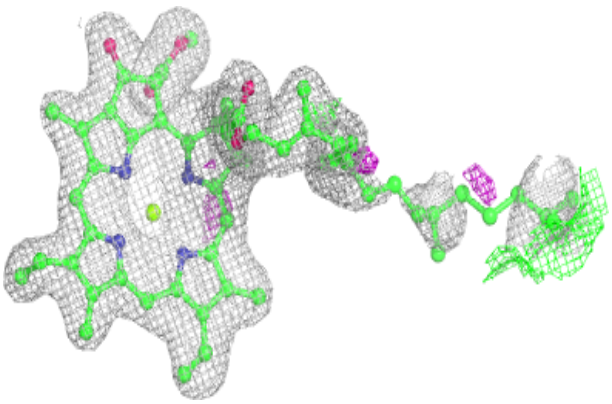
Electron density around BCR B 619:

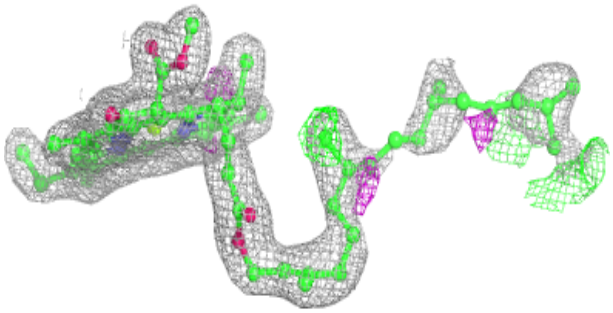
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

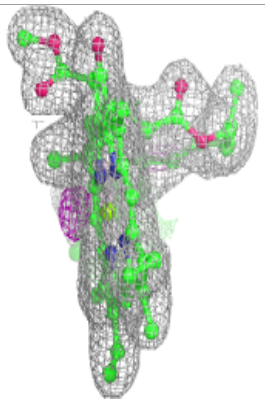


Electron density around CLA a 410:

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

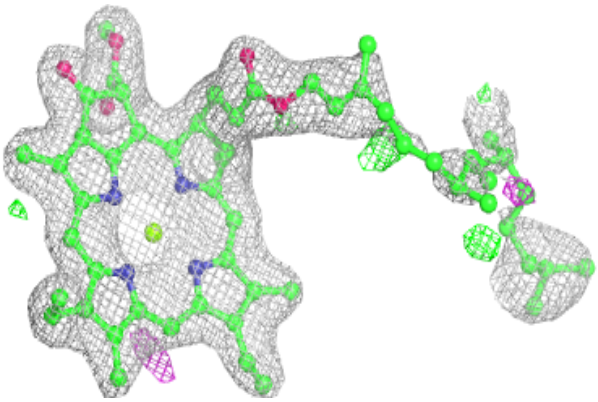


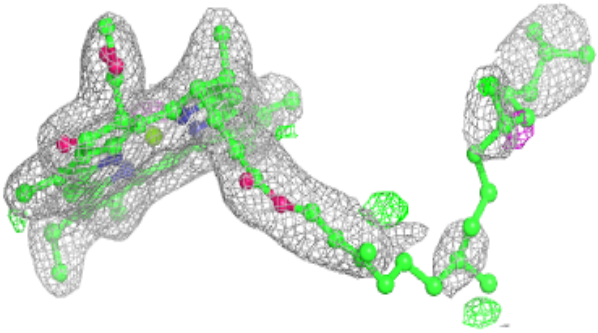


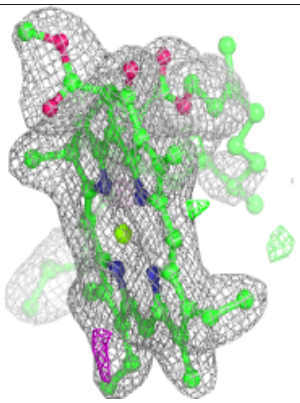


Electron density around CLA a 412:

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

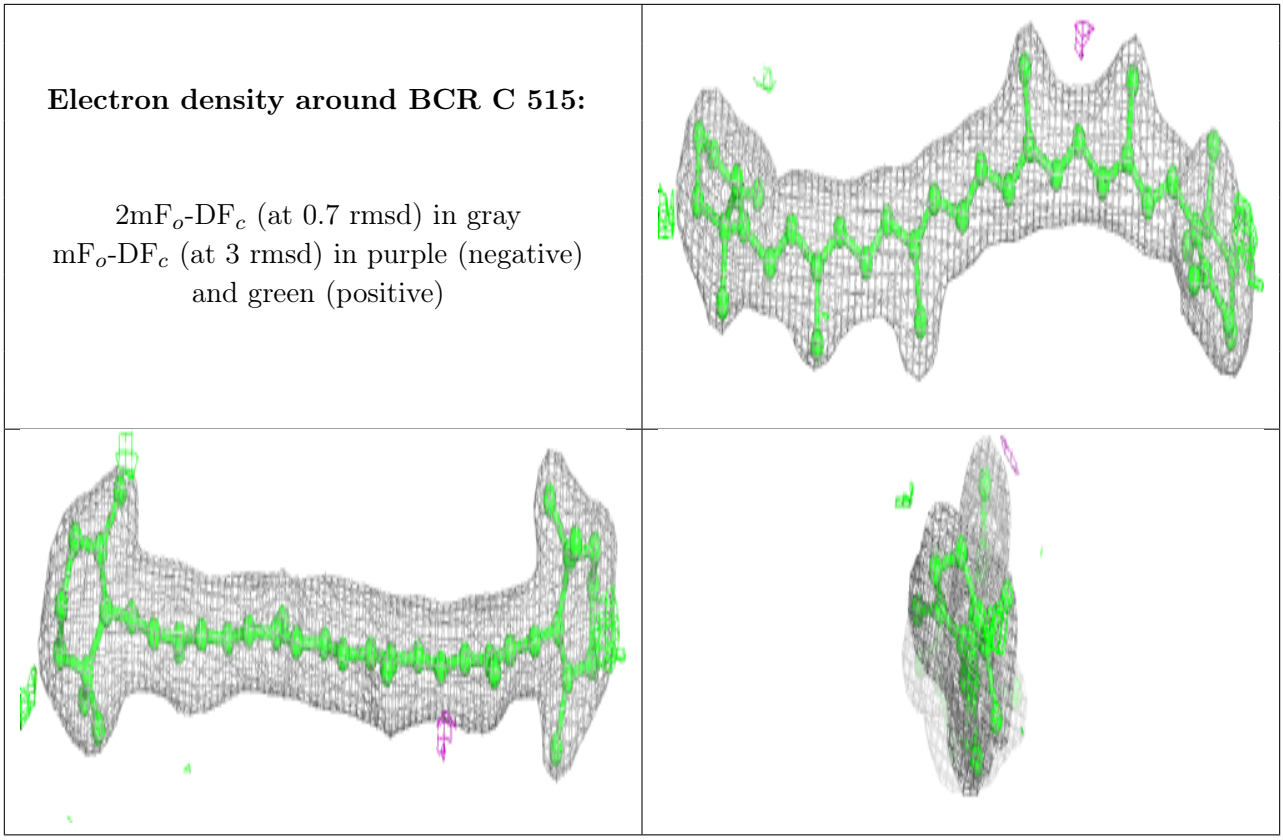






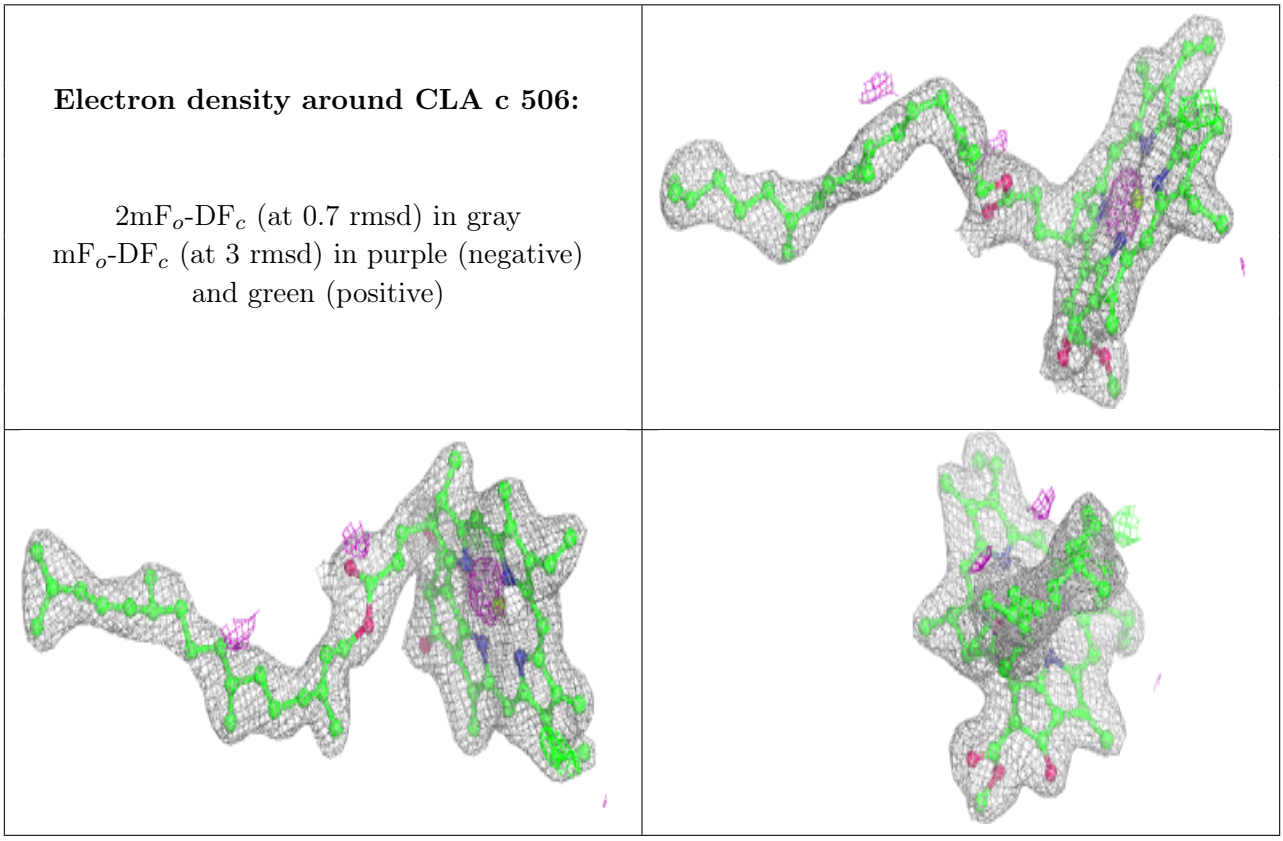
Electron density around BCR C 515:

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



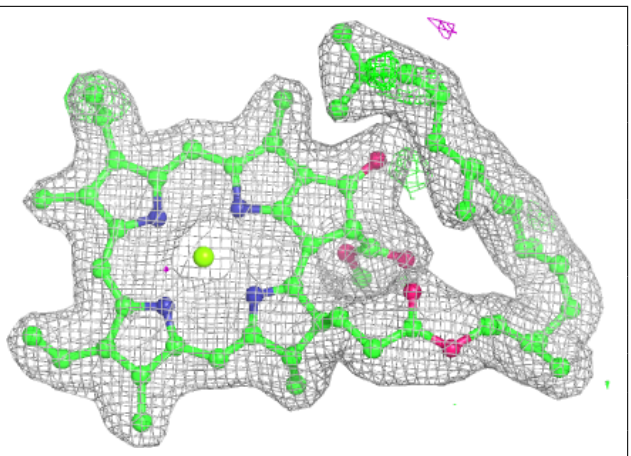
Electron density around CLA c 506:

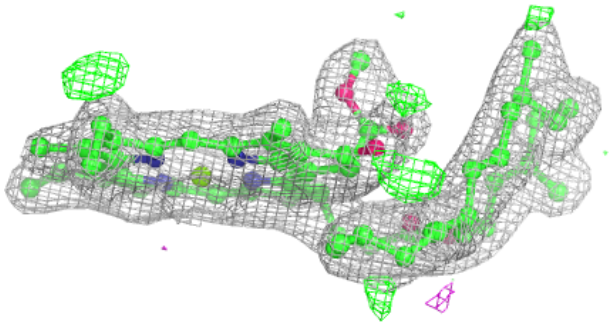
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

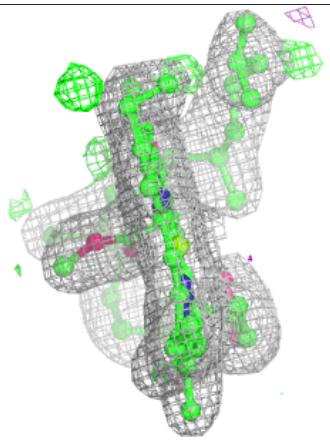


Electron density around CLA B 611:

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

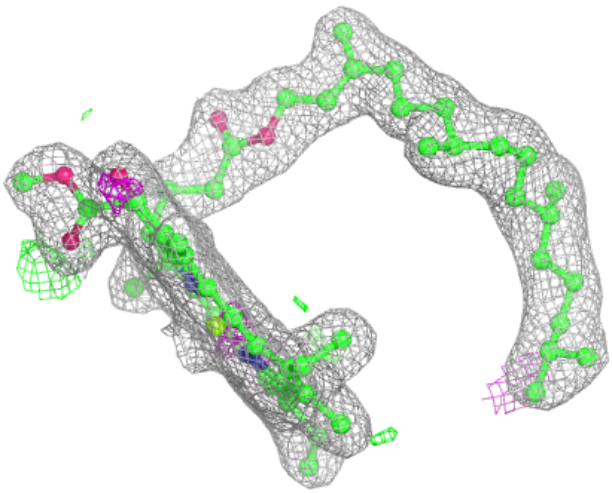


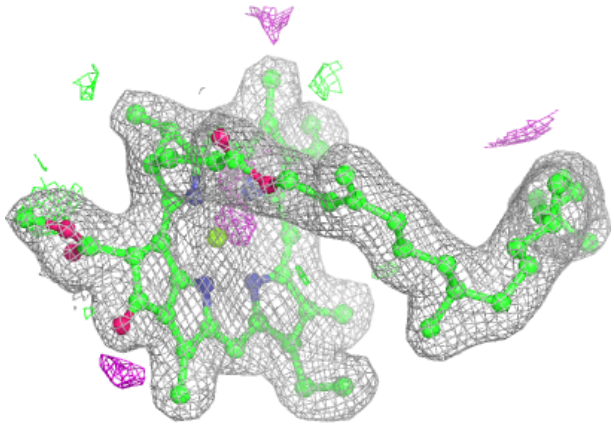


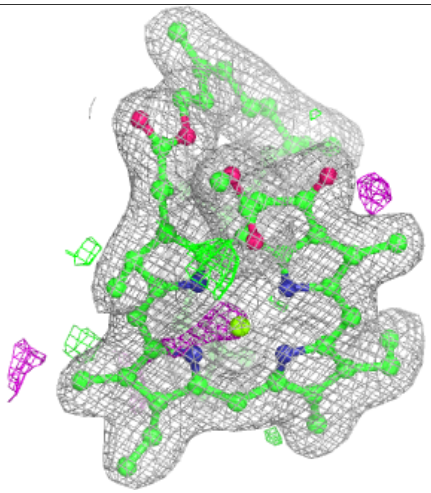


Electron density around CLA B 612:

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

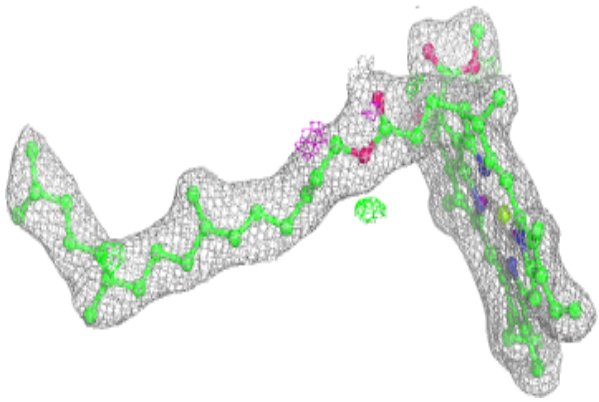


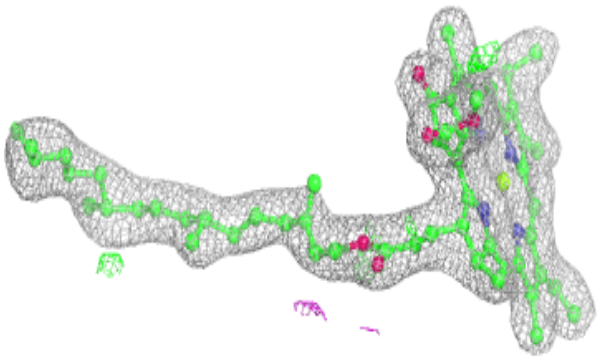


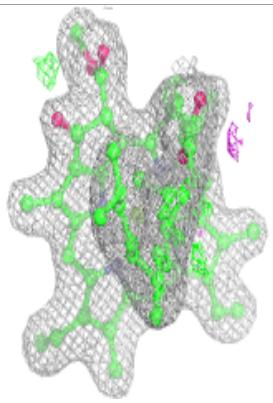


Electron density around CLA b 614:

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

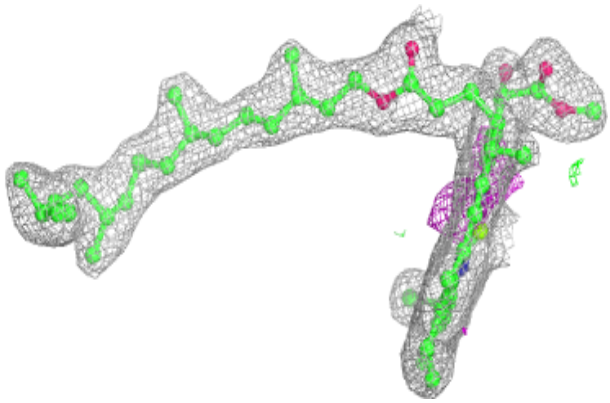


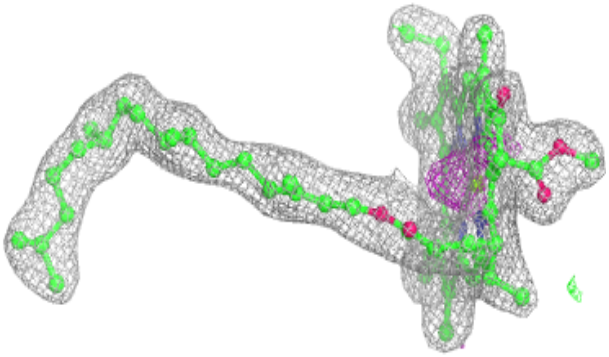


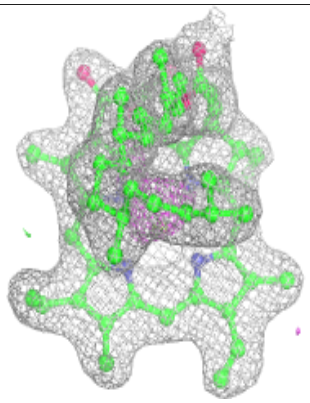


Electron density around CLA b 615:

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

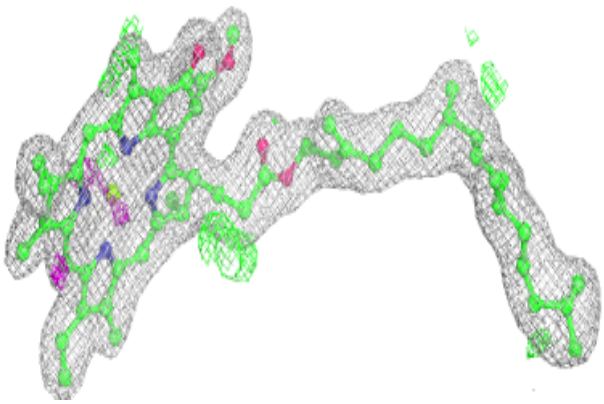


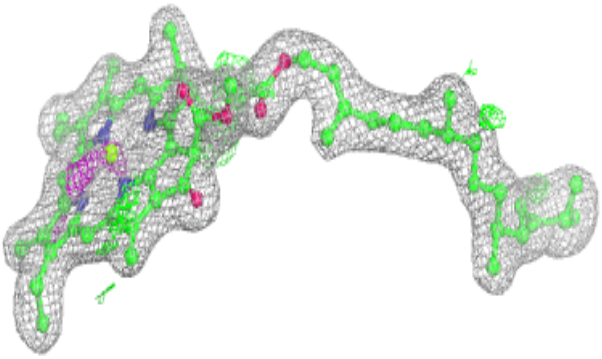


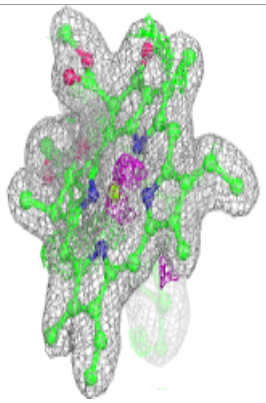


Electron density around CLA A 405:

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

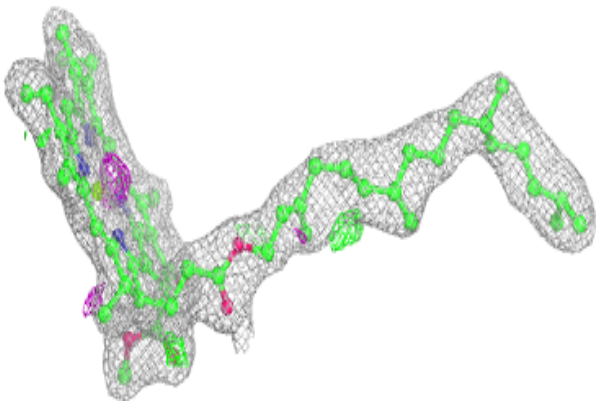


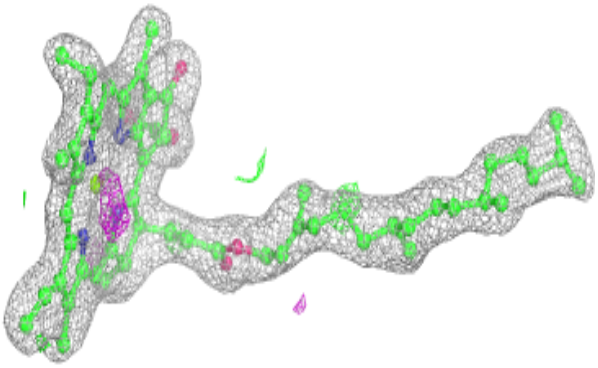


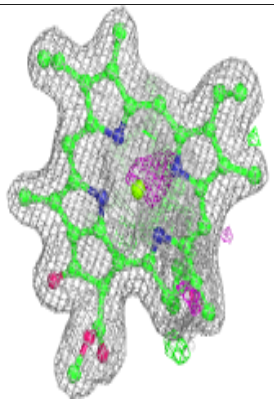


Electron density around CLA B 605:

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

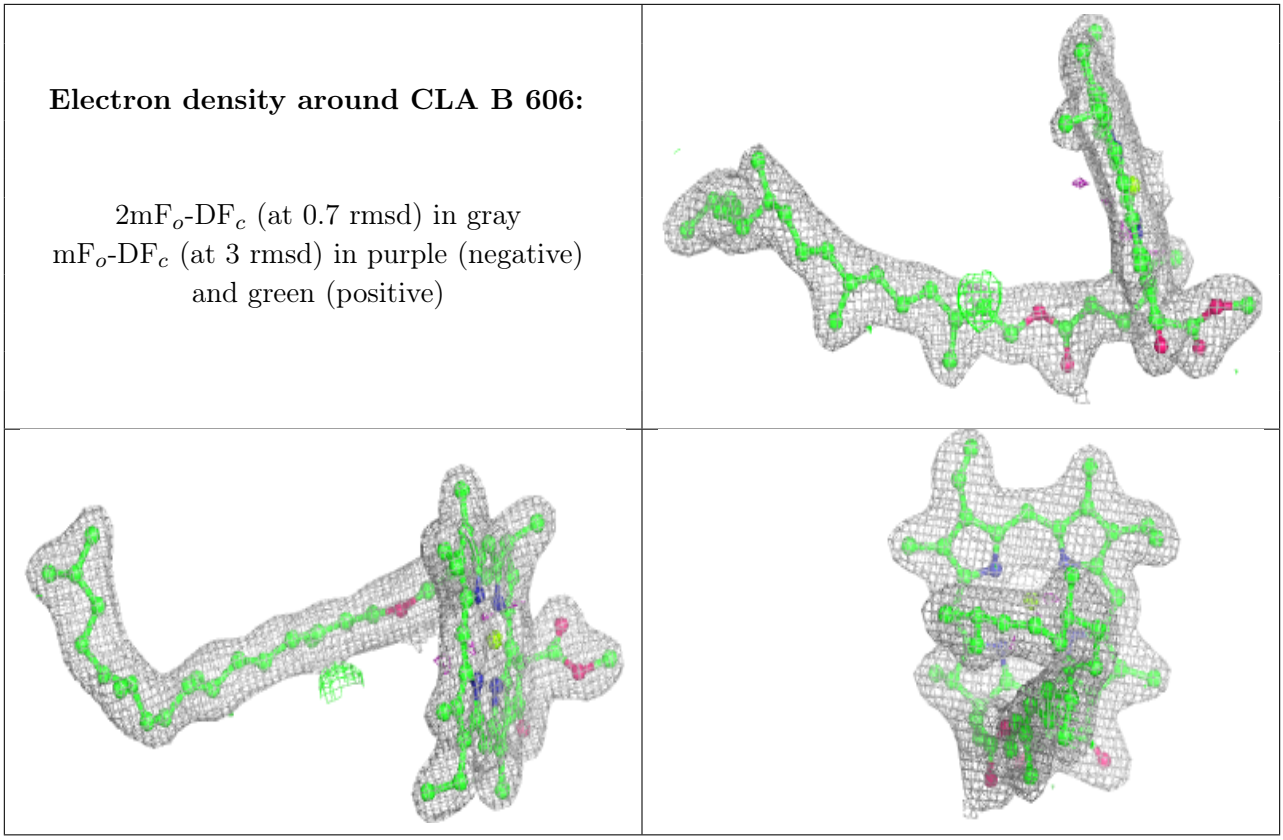






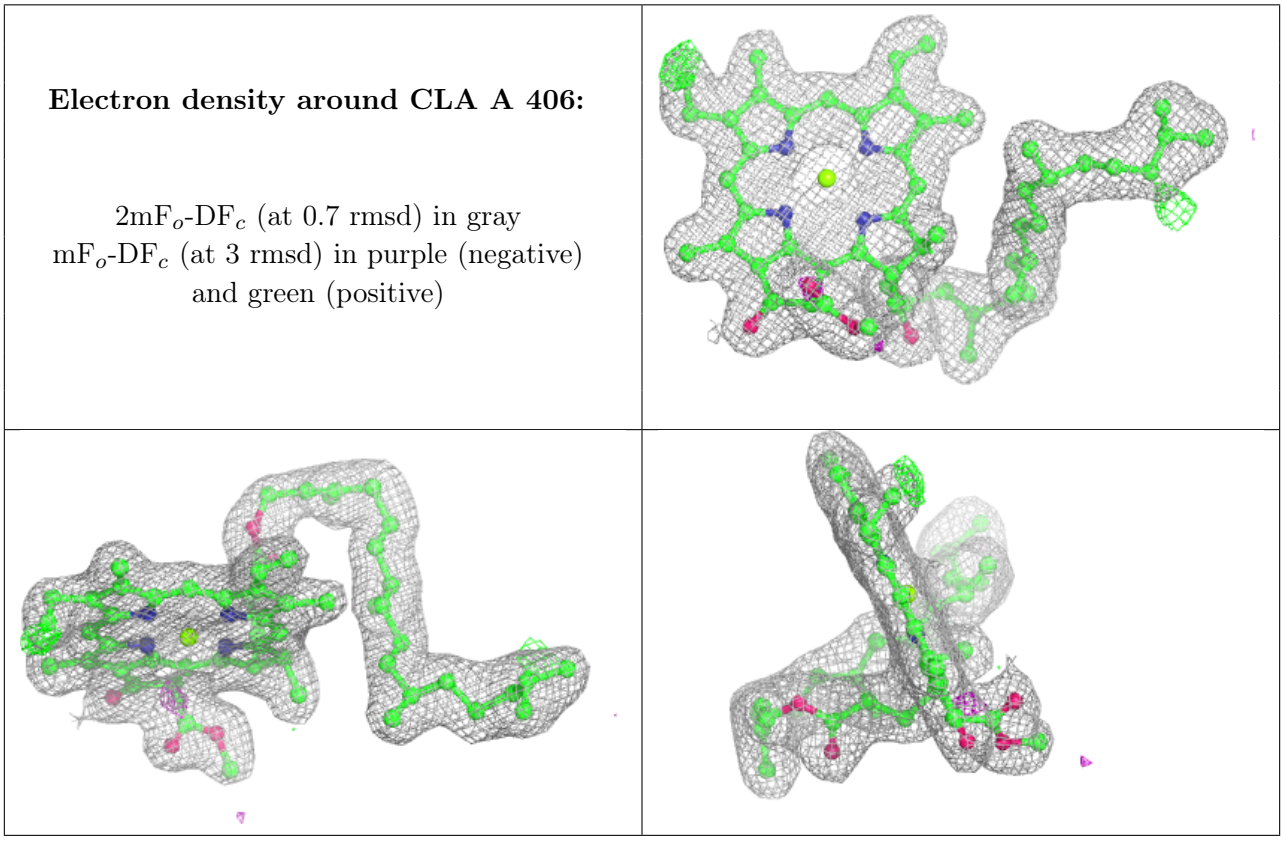
Electron density around CLA B 606:

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



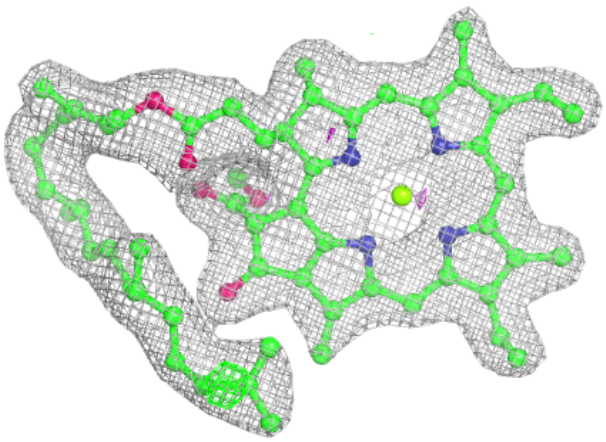
Electron density around CLA A 406:

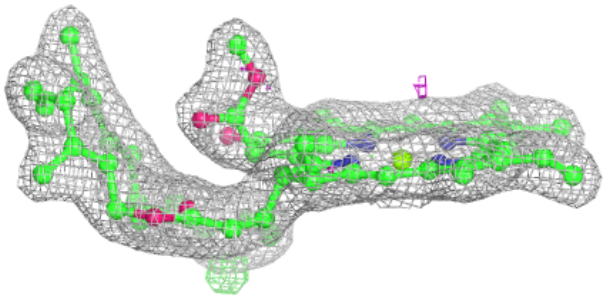
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

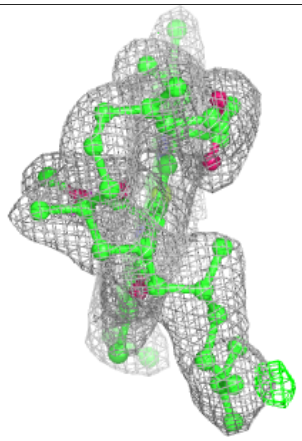


Electron density around CLA b 620:

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

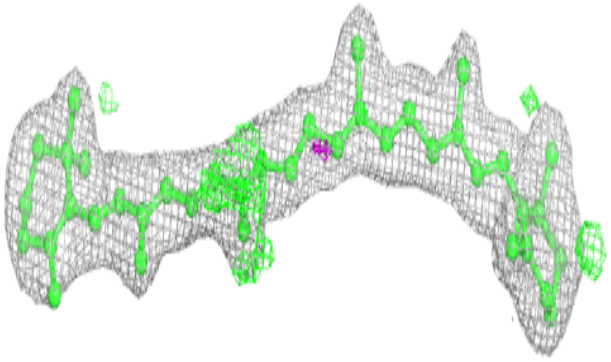


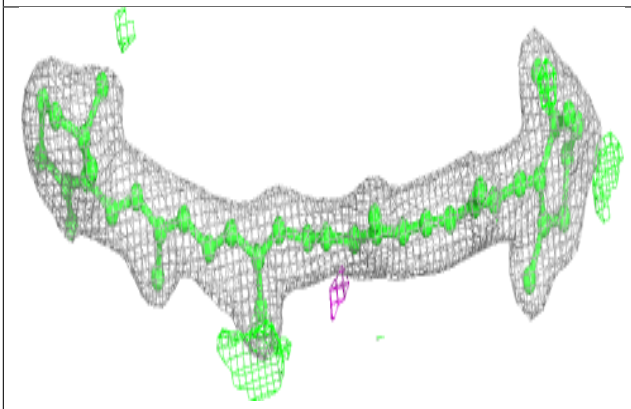


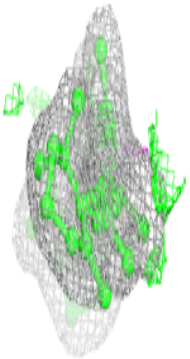


Electron density around BCR t 101:

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

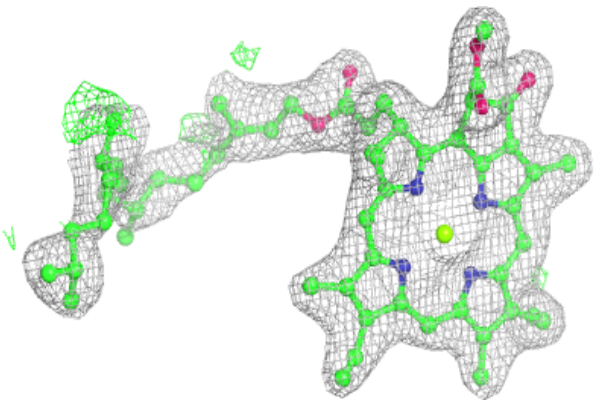


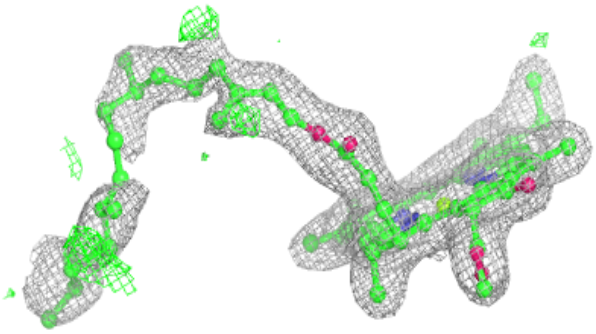


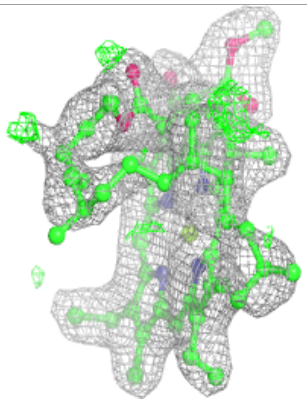


Electron density around CLA A 410:

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

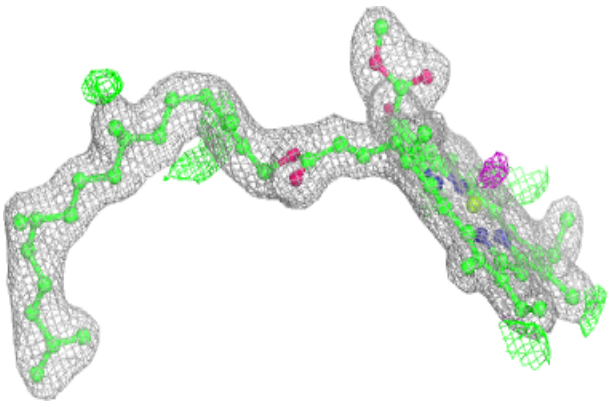


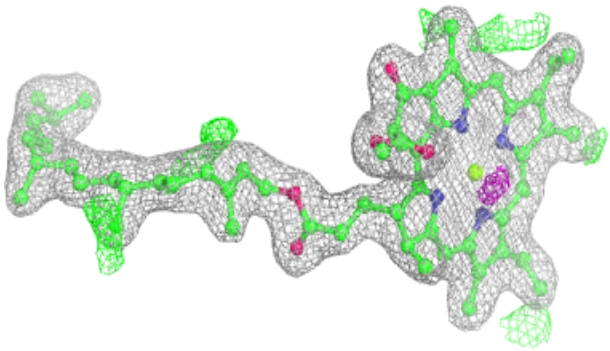




Electron density around CLA D 402:

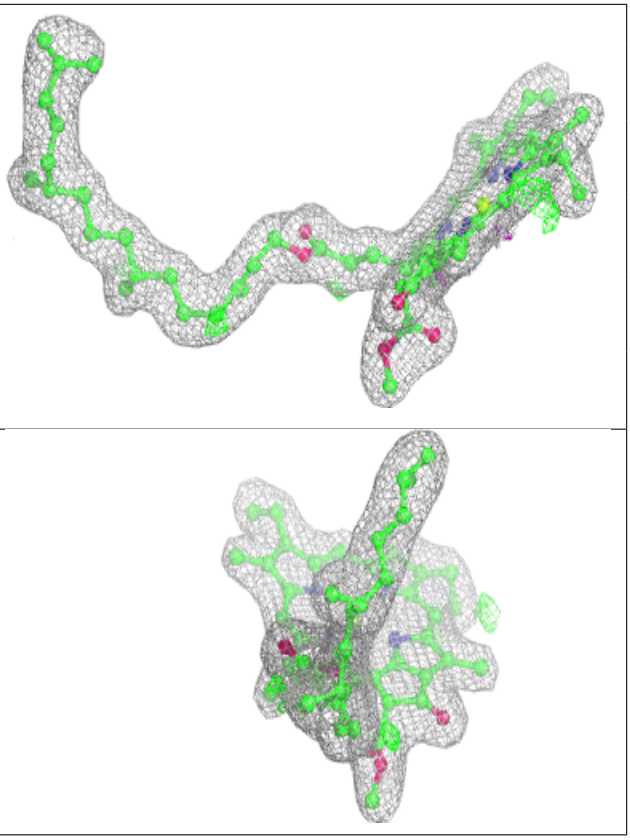
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

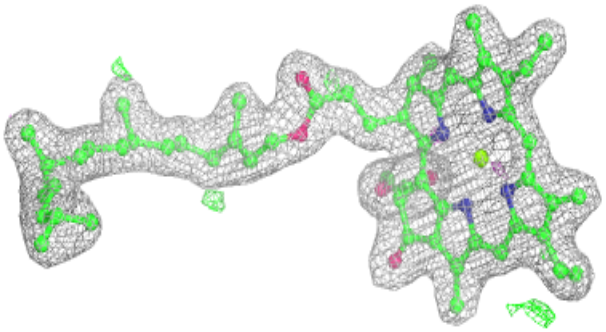




Electron density around CLA d 402:

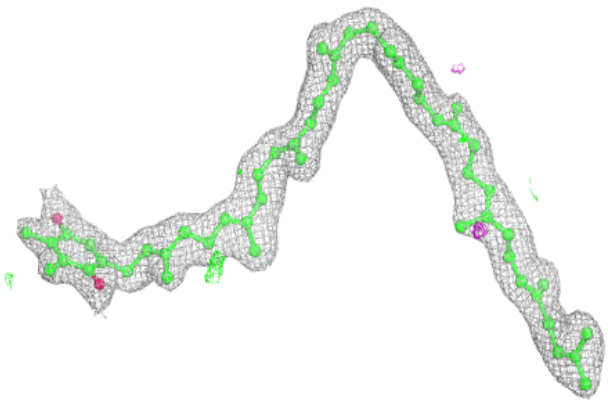
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

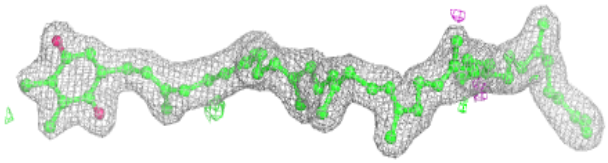


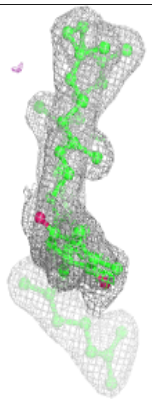


Electron density around PL9 d 405 (A):

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

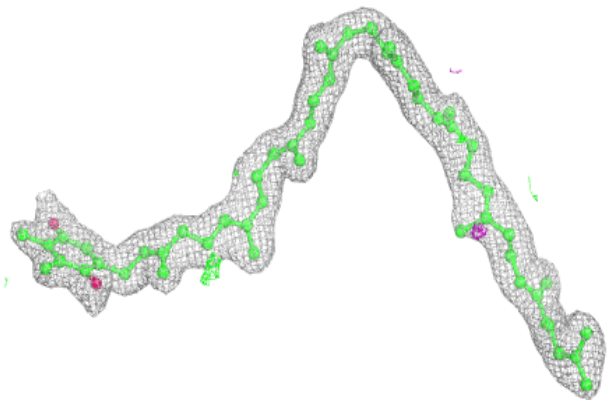


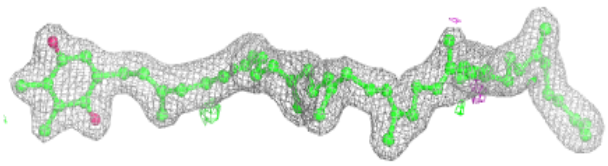




Electron density around PL9 d 405 (B):

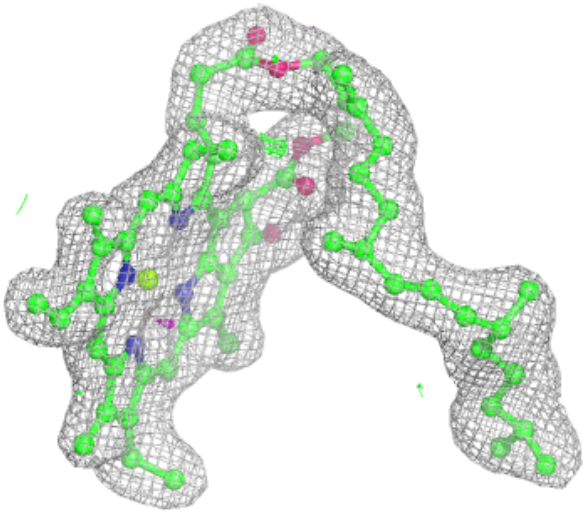
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

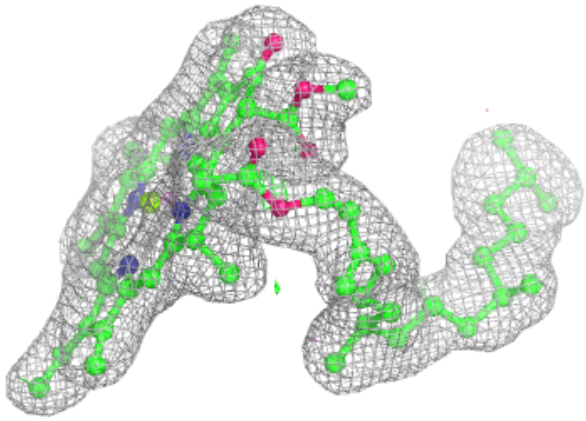


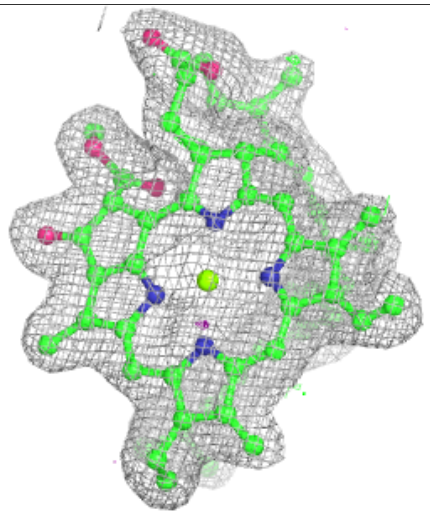


Electron density around CLA b 623:

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

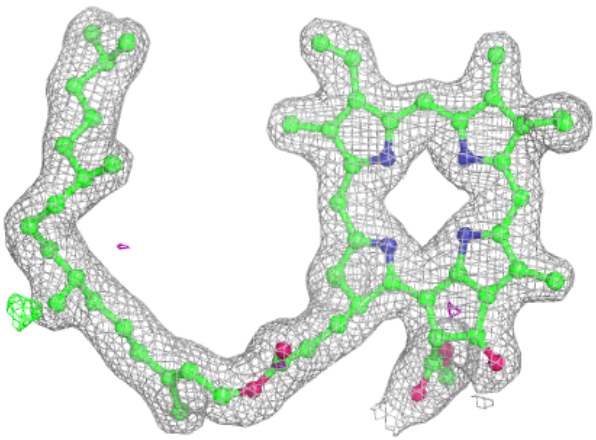


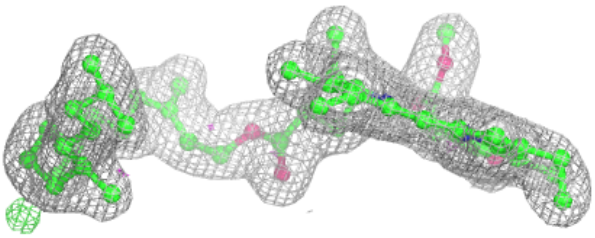


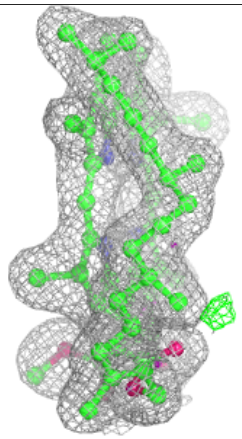


Electron density around PHO A 408:

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

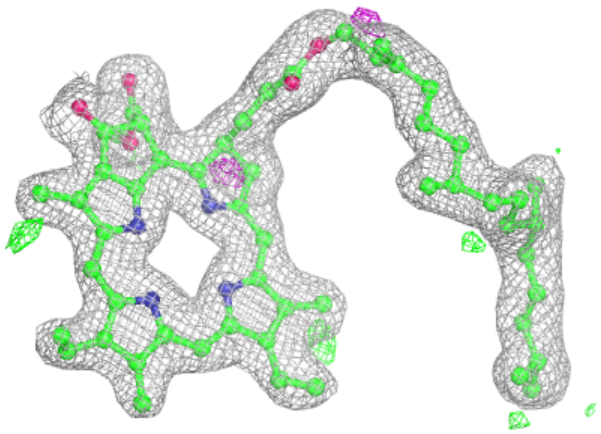


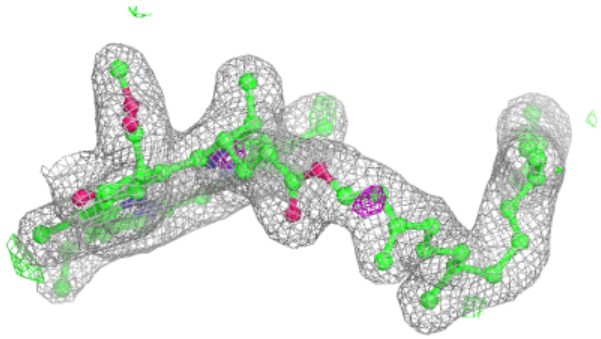


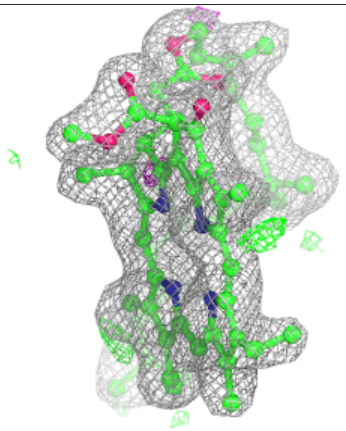


Electron density around PHO A 409 (A):

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

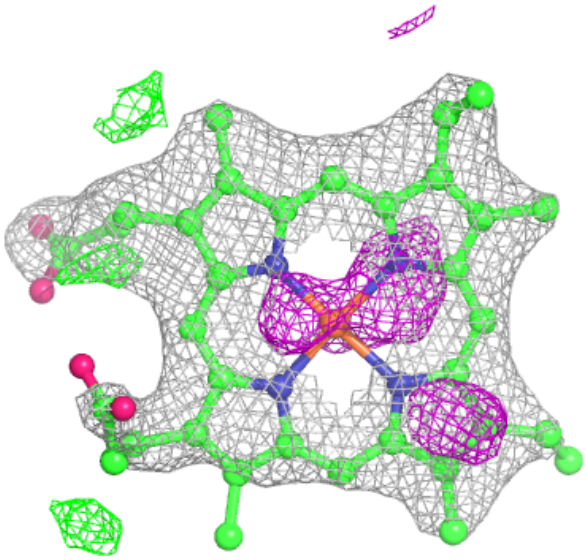


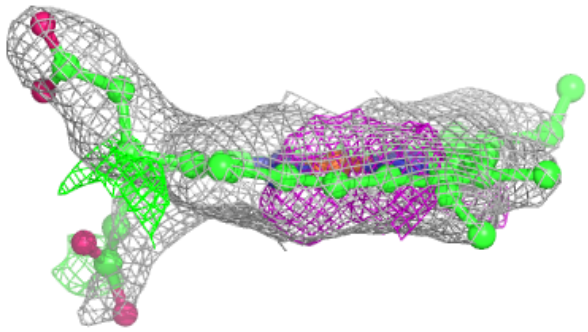


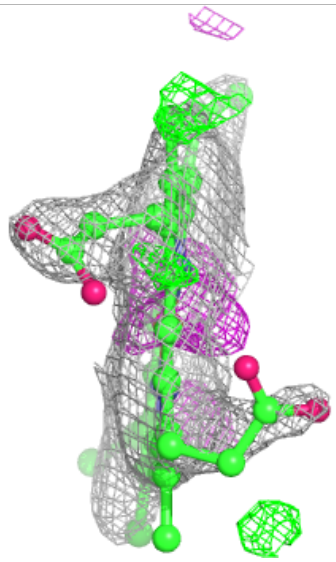


Electron density around HEM e 102:

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

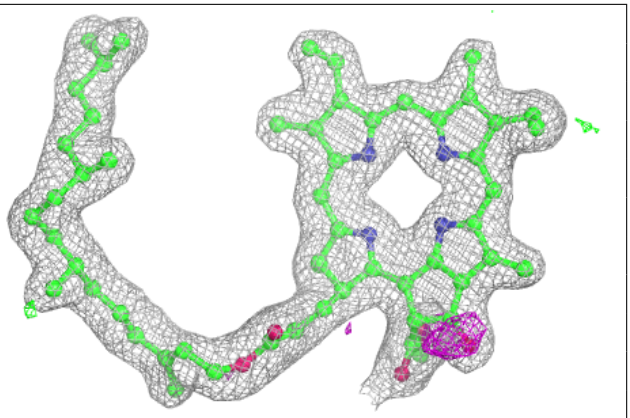


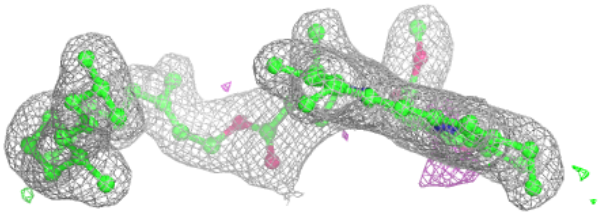


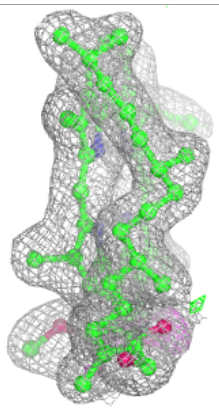


Electron density around PHO a 411:

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

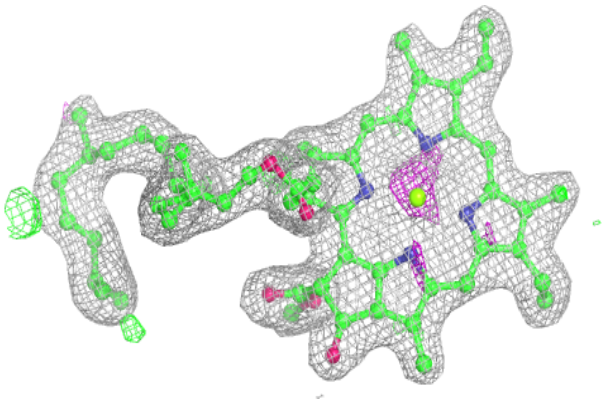


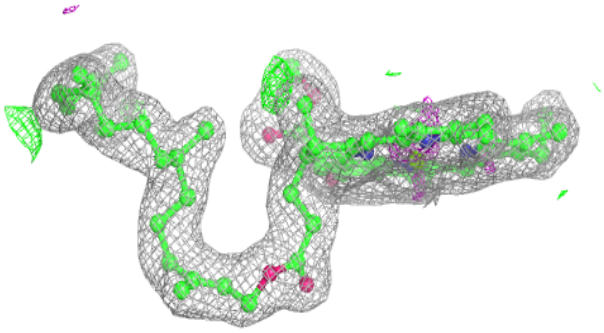


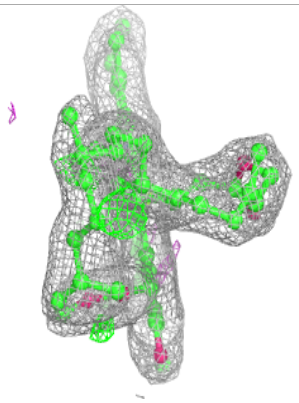


Electron density around CLA B 613:

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

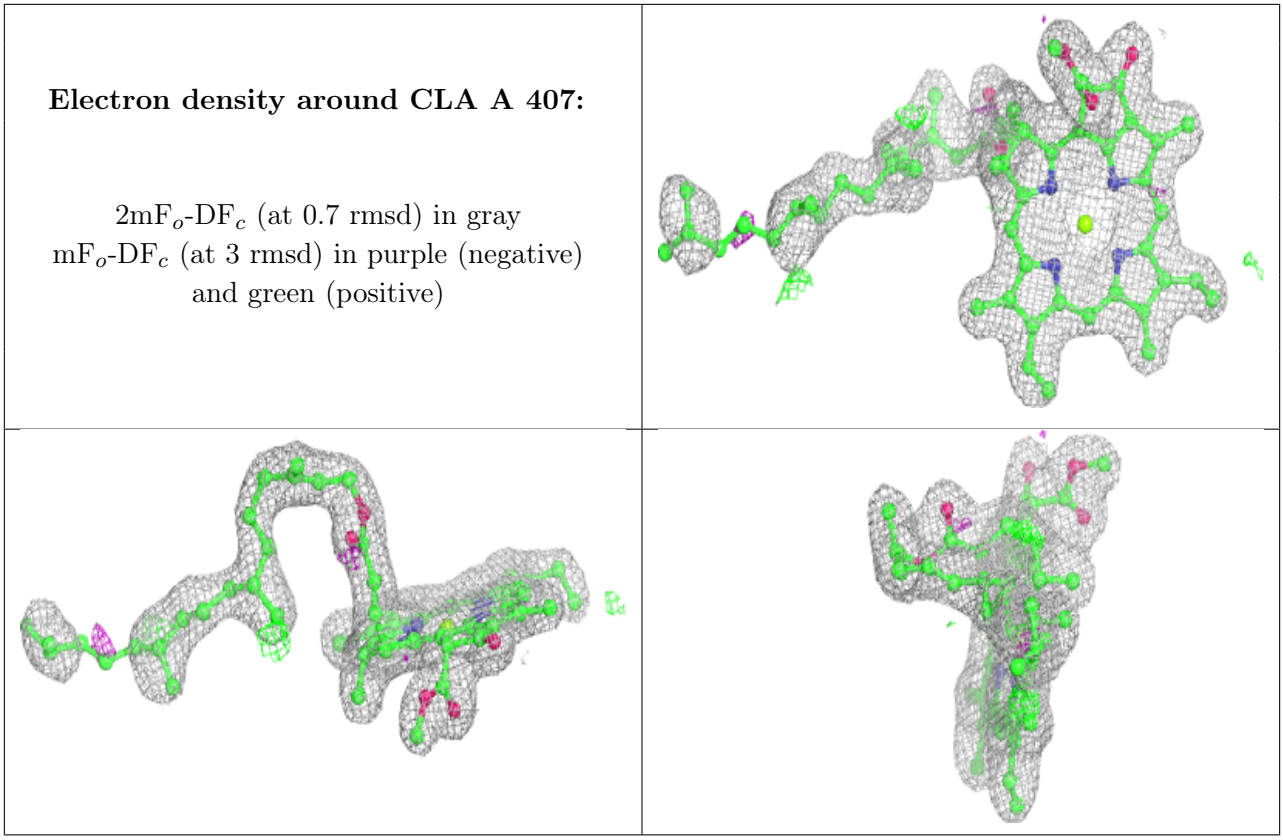






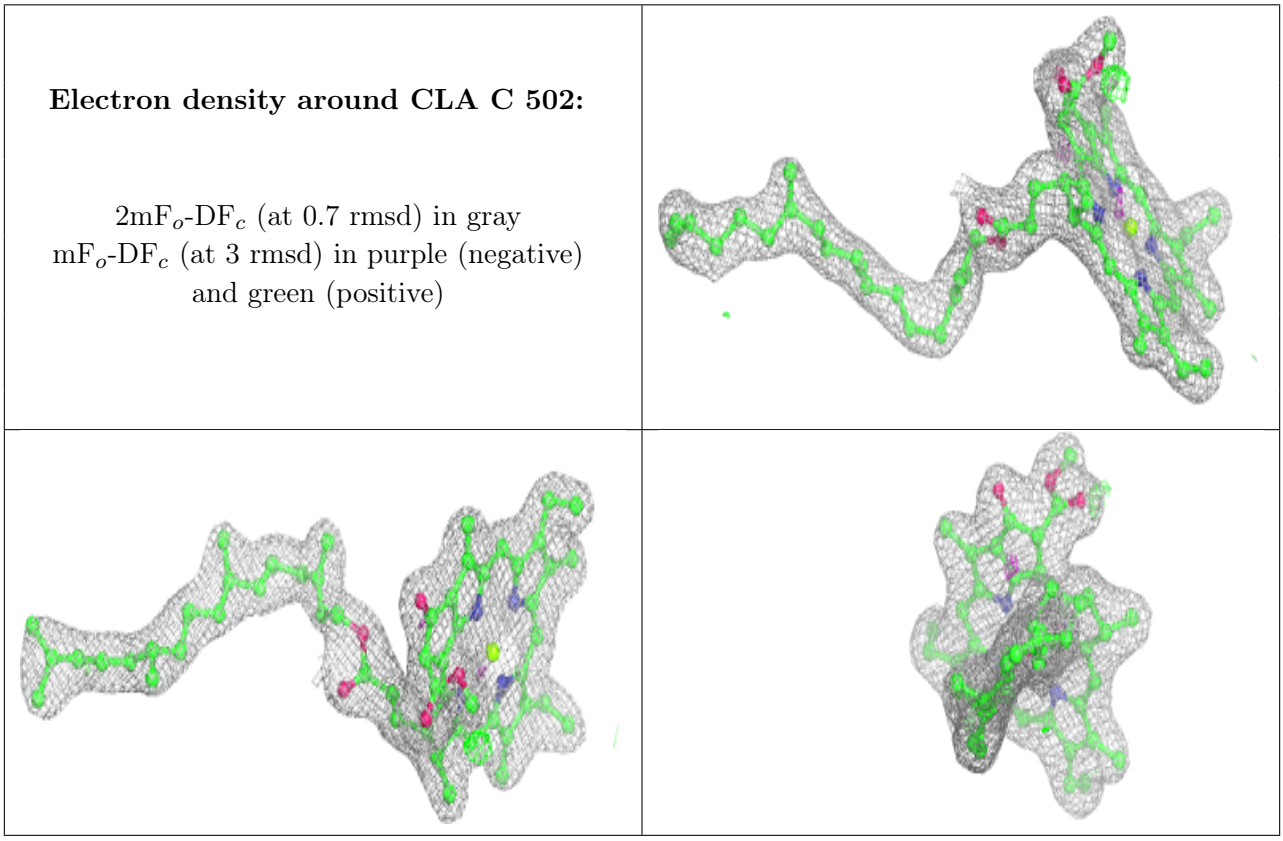
Electron density around CLA A 407:

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



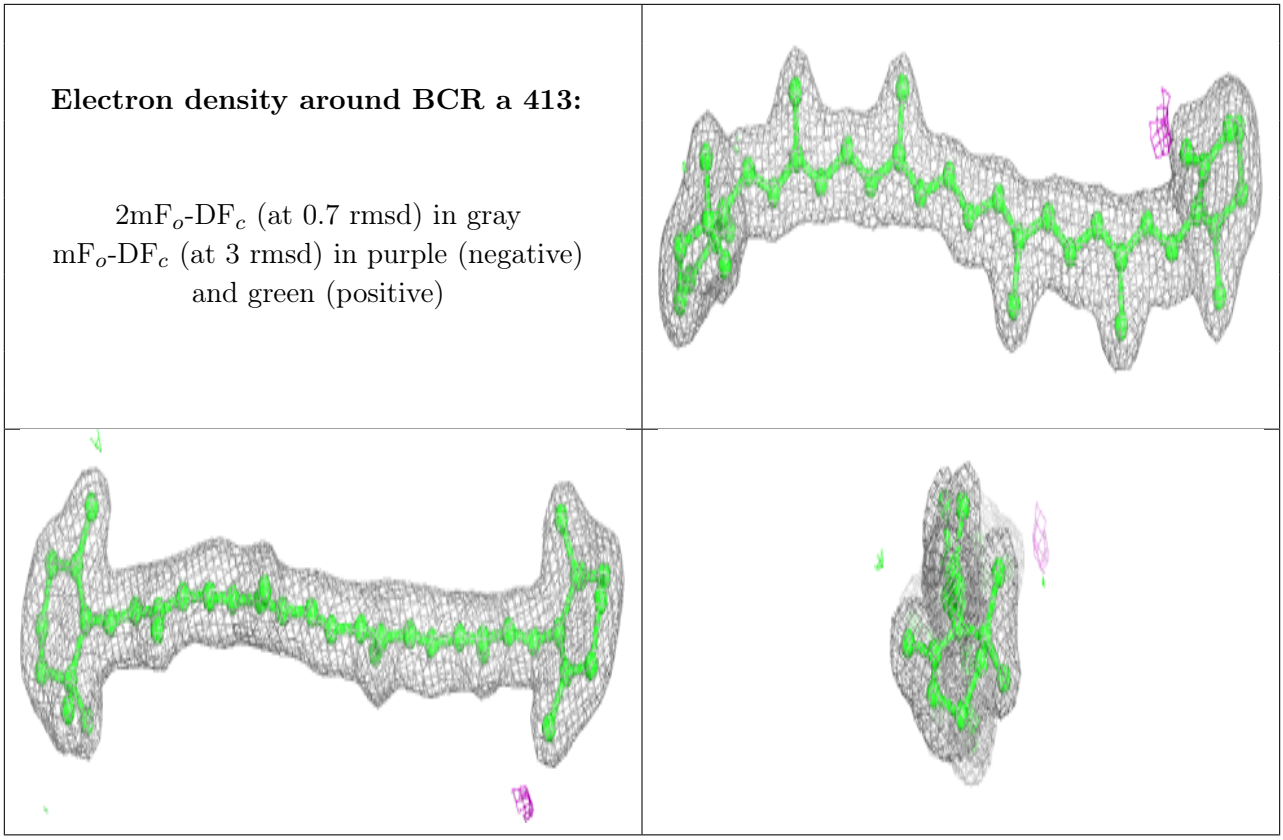
Electron density around CLA C 502:

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



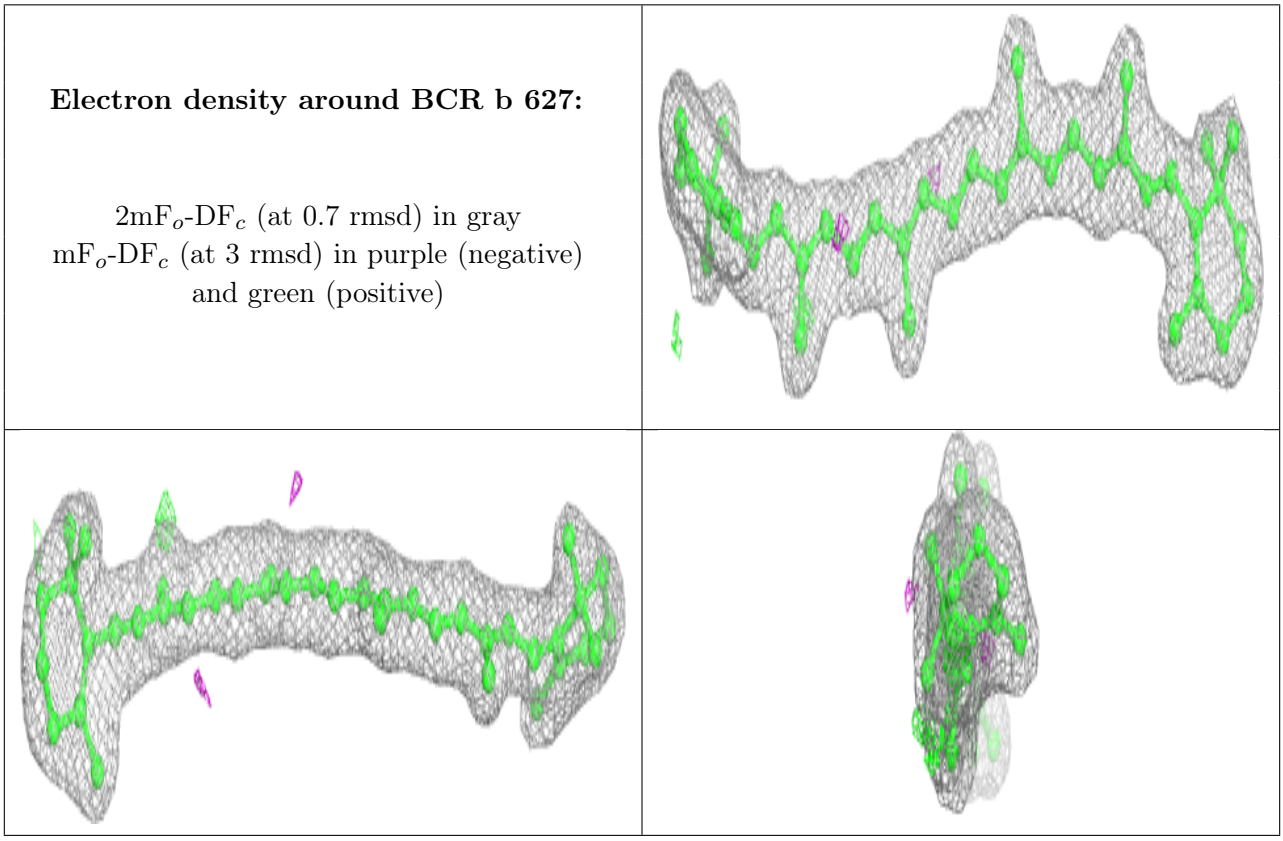
Electron density around BCR a 413:

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



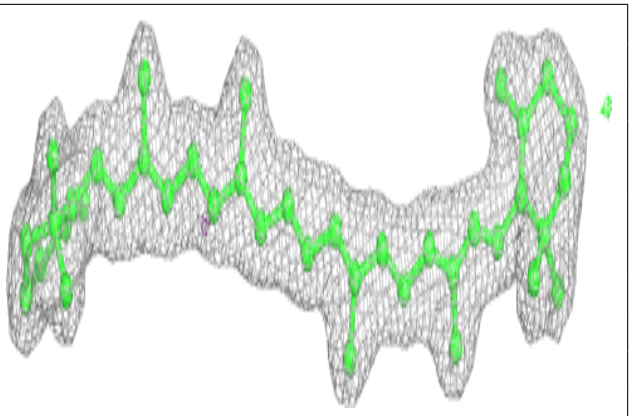
Electron density around BCR b 627:

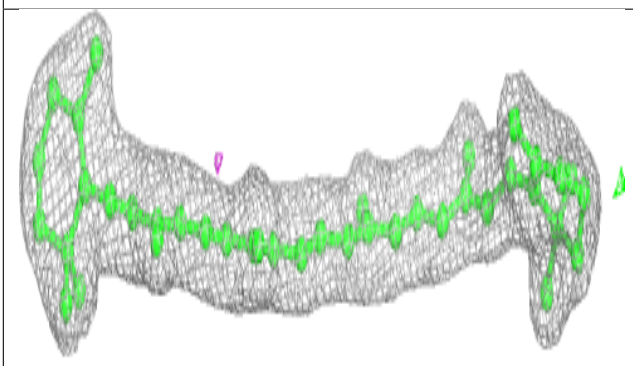
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

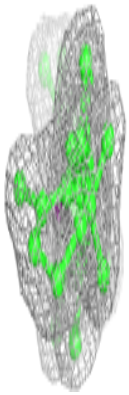


Electron density around BCR B 618:

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

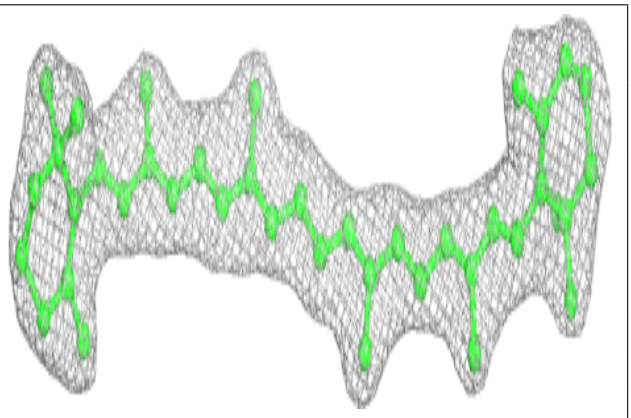


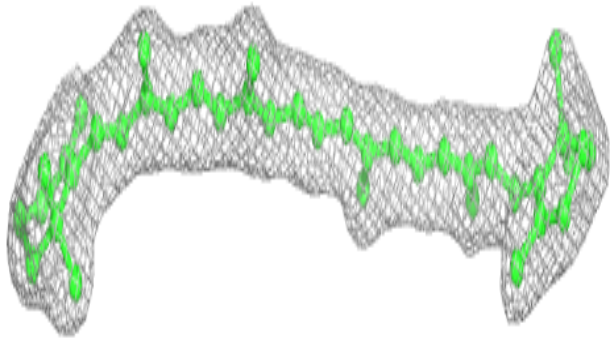


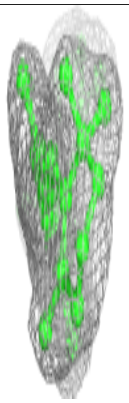


Electron density around BCR b 629:

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

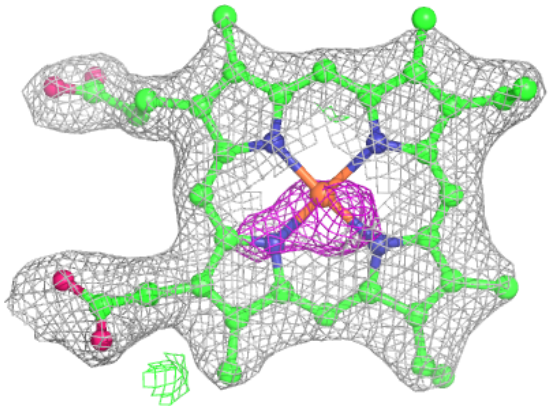


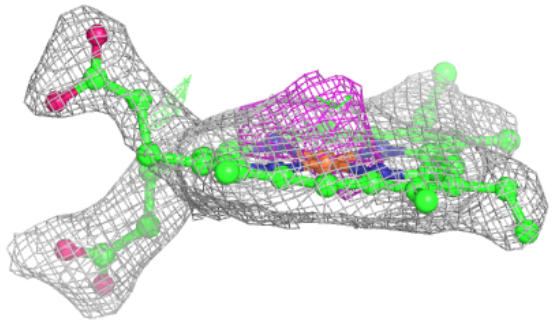


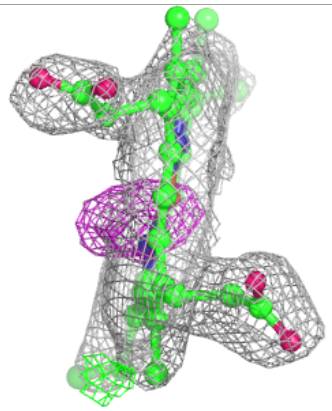


Electron density around HEM F 102:

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

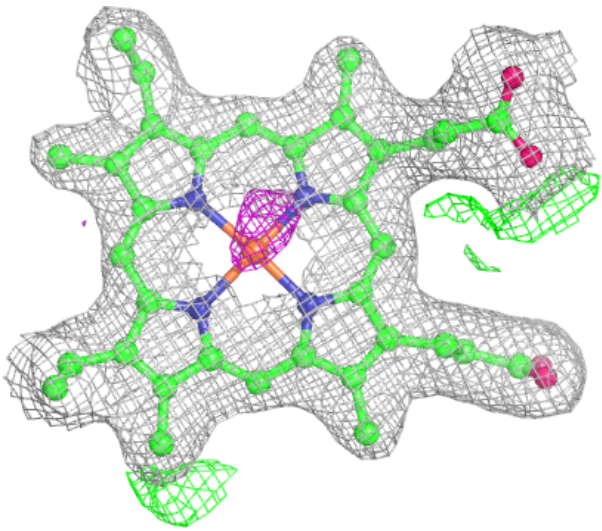


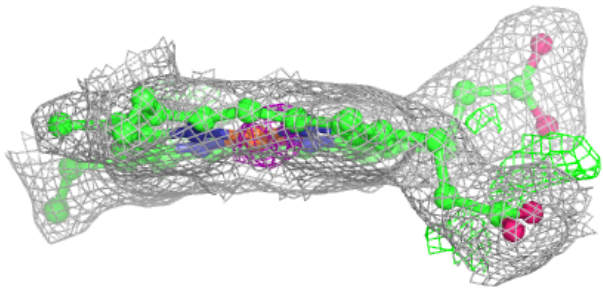


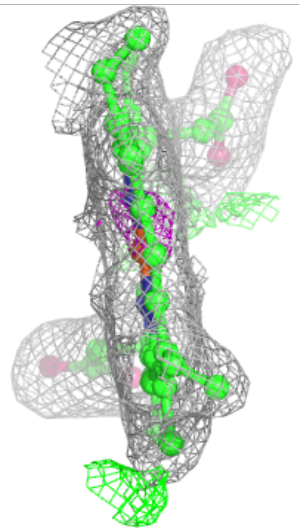


Electron density around HEM V 206:

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

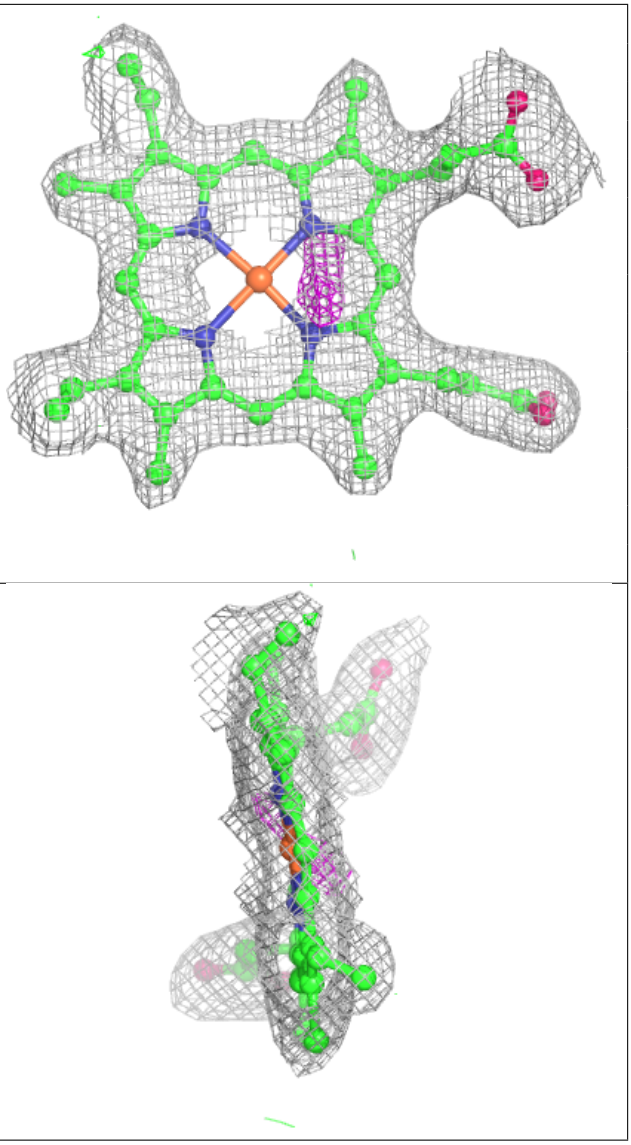






Electron density around HEM v 205:

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



6.5 Other polymers (i)

There are no such residues in this entry.