Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 12:16 PM JST

PDB ID	:	7CJI
Title	:	Photosystem II structure in the S1 state
Authors	:	Li, H.; Shen, J.-R.; Suga, M.
Deposited on	:	2020-07-11
Resolution	:	2.35 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:

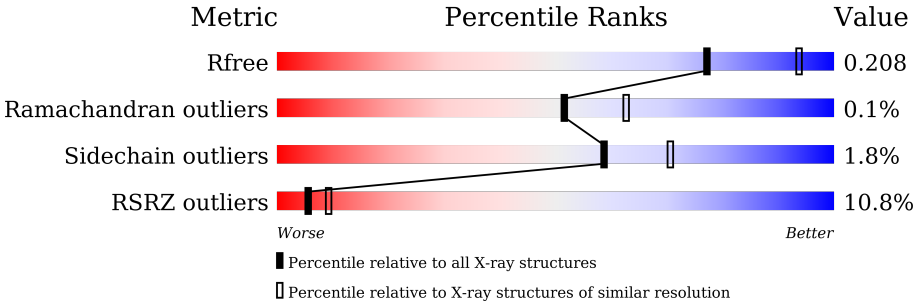
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.35 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	1164 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	6% 96%
1	a	344	8% 96%
2	B	505	6% 99%
2	b	505	12% 98%
3	C	455	8% 98%
3	c	455	10% 99%
4	D	342	6% 99%

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Mol	Chain	Length	Quality of chain
4	d	342	8% 99%
5	E	84	20% 93%
5	e	84	19% 92% 6%
6	F	44	5% 77% 23%
6	f	44	7% 70% 30%
7	H	65	2% 94% 5%
7	h	65	9% 94% 5%
8	I	38	5% 100%
8	i	38	5% 95% 5%
9	J	39	23% 95%
9	j	39	13% 100%
10	K	37	92% 8%
10	k	37	11% 92% 8%
11	L	37	5% 97%
11	l	37	3% 97%
12	M	36	3% 89% 8%
12	m	36	6% 89% 6% 6%
13	O	244	13% 98%
13	o	244	23% 97%
14	T	32	3% 91% 6%
14	t	32	6% 91% 6%
15	U	104	3% 90% 8%
15	u	104	92% 7%
16	V	137	% 99%
16	v	137	11% 98%

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Mol	Chain	Length	Quality of chain
17	X	40	12% 92% 5%
17	x	40	20% 95% 5%
18	Y	30	47% 97%
18	y	30	17% 90% 7%
19	Z	62	32% 97%
19	z	62	47% 97%
20	R	34	100% 100%

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
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
27	SQD	f	102	-	-	-	X
30	UNL	A	414	-	-	-	X
30	UNL	j	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	LMG	C	521	-	-	-	X
33	HTG	B	622	-	-	-	X
33	HTG	b	622	-	-	-	X
34	LMT	C	525	-	-	-	X
34	LMT	a	412	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	e	101	-	-	-	X
34	LMT	m	103	-	-	-	X

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 53071 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	2634	1725	433	461	15	0	2	0
1	a	334	2642	1731	434	462	15	0	3	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	4050	2650	677	710	13	0	10	0
2	b	504	3998	2622	665	698	13	0	4	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	3513	2295	588	617	13	0	4	0
3	c	455	3534	2311	591	619	13	0	2	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	342	2726	1805	445	464	12	0	0	0
4	d	341	2717	1800	444	461	12	0	0	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	435	108	125	0	1	0
5	e	79	648	424	105	119	0	0	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	31	250	170	42	37	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	64	517	345	85	85	2	0	1	0
7	h	64	506	339	81	84	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	277	185	43	48	1	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			
11	L	36	304	203	48	53	0	1	0
11	l	36	304	203	48	53	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	33	268	179	39	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	1886	1177	318	386	5	0	3	0
			Total	C	N	O	S			
13	o	243	1879	1173	317	384	5	0	2	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	258	181	36	39	2	0	0	0
			Total	C	N	O	S			
14	t	30	258	181	36	39	2	0	0	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	96	765	486	128	151	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	1064	675	177	208	4	0	0	0
			Total	C	N	O	S			
16	v	137	1064	675	177	208	4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Y	29	215	142	37	33	3	0	0	0
18	y	29	215	142	37	33	3	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	34	273	186	47	40	0	0	0

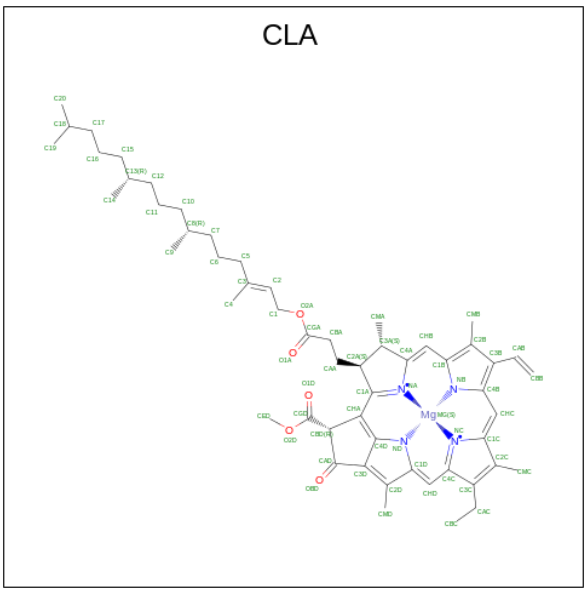
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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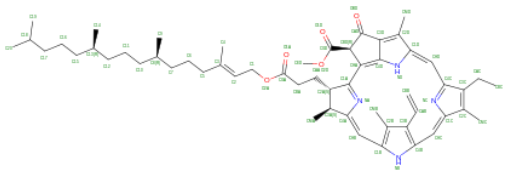
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
23	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
23	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
23	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
23	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
23	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
23	c	1	65	55	1	4	5	0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

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

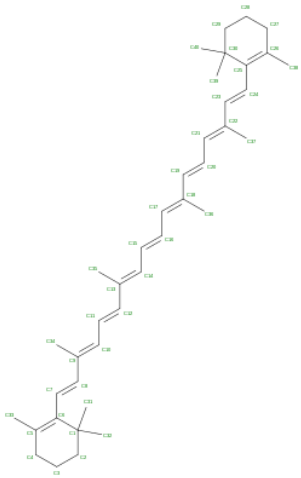
PHO



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

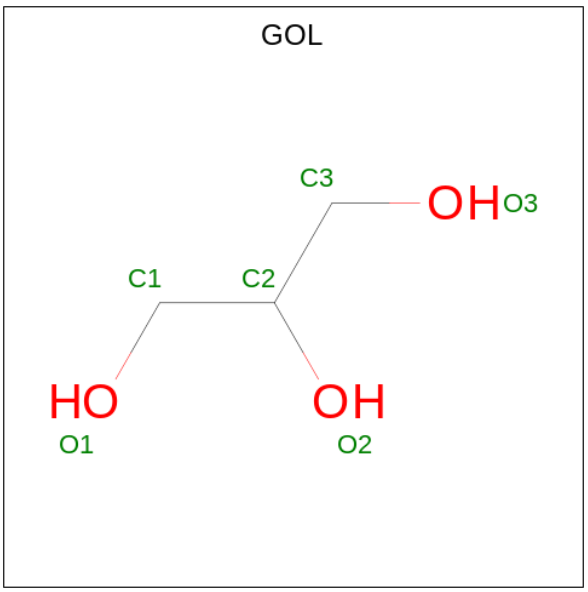
- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR



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

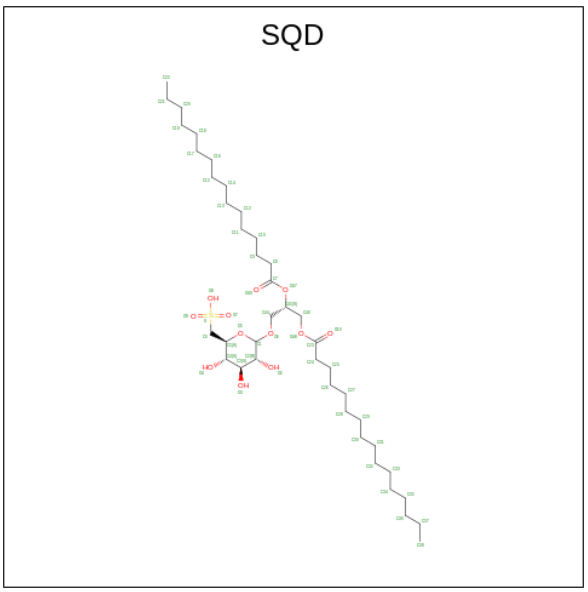
- Molecule 26 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
26	A	1	6	3	3	0	0
26	B	1	6	3	3	0	0
26	B	1	6	3	3	0	0
26	B	1	6	3	3	0	0
26	C	1	6	3	3	0	0
26	O	1	6	3	3	0	0
26	a	1	6	3	3	0	0
26	b	1	6	3	3	0	0
26	b	1	6	3	3	0	0
26	c	1	6	3	3	0	0
26	c	1	6	3	3	0	0
26	v	1	6	3	3	0	0

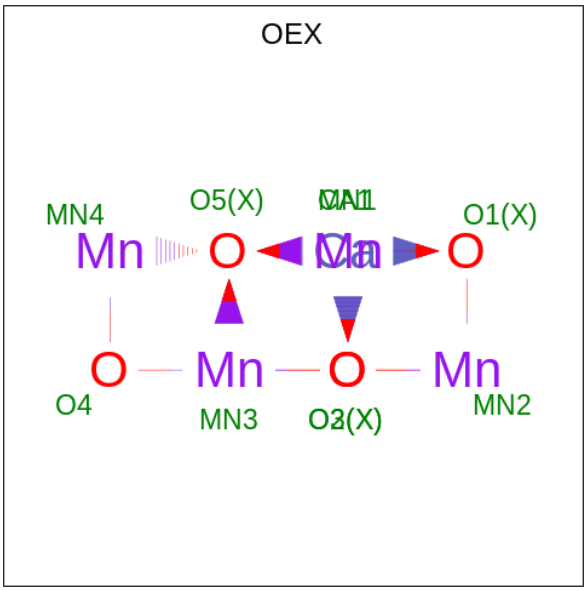
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



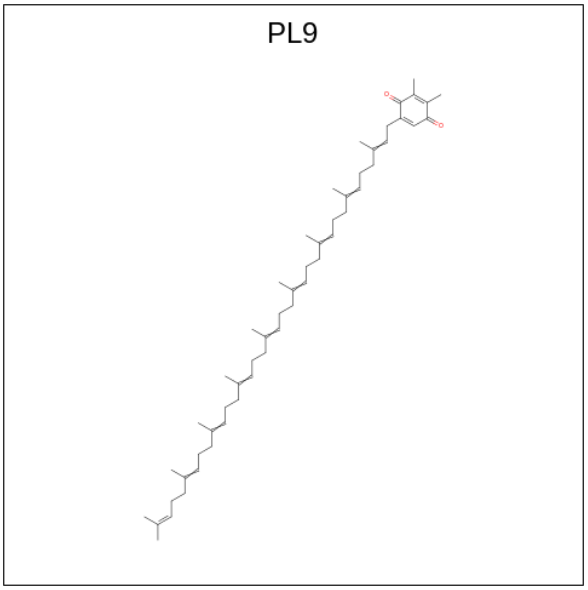
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
27	A	1	54	41	12	1	0	0
27	B	1	54	41	12	1	0	0
27	C	1	54	41	12	1	0	0
27	D	1	43	30	12	1	0	0
27	L	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	a	1	54	41	12	1	0	0
27	f	1	43	30	12	1	0	0

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).

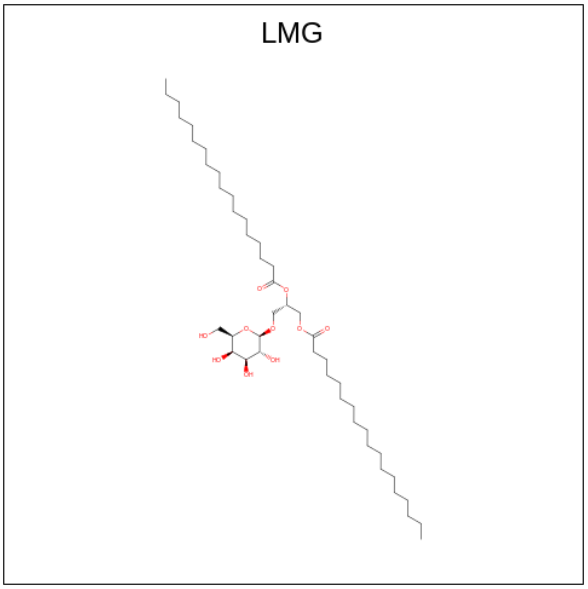


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 55 53 2	0	0
29	D	1	Total C O 55 53 2	0	0
29	a	1	Total C O 55 53 2	0	0
29	d	1	Total C O 55 53 2	0	0

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

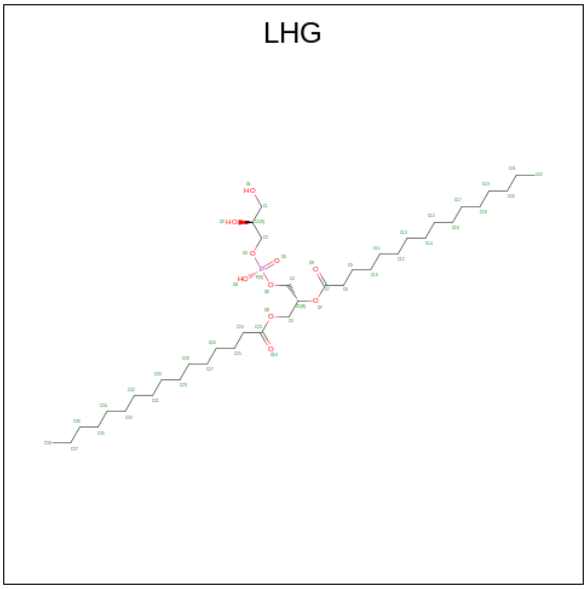
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	C	1	Total C O 34 29 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	M	1	Total C 10 10	0	0
30	X	1	Total C O 18 16 2	0	0
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 32 27 5	0	0
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



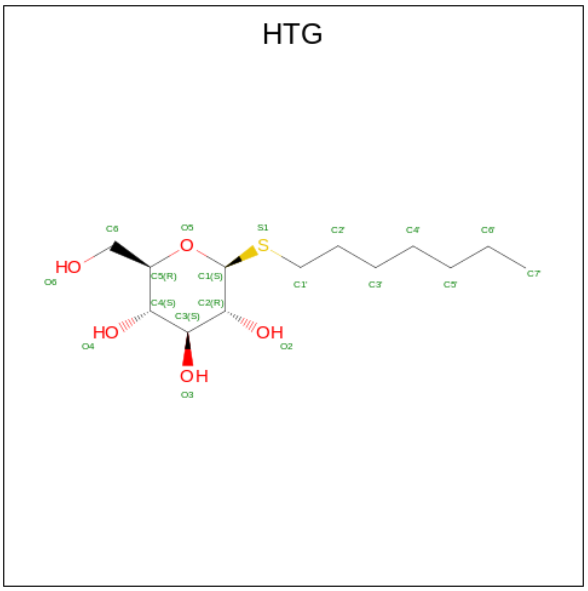
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
31	A	1	51	41	10	0	0
31	C	1	51	41	10	0	0
31	C	1	51	41	10	0	0
31	D	1	51	41	10	0	0
31	M	1	51	41	10	0	0
31	Z	1	37	27	10	0	0
31	a	1	51	41	10	0	0
31	c	1	51	41	10	0	0
31	c	1	51	41	10	0	0
31	d	1	51	41	10	0	0
31	m	1	51	41	10	0	0
31	z	1	39	29	10	0	0

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



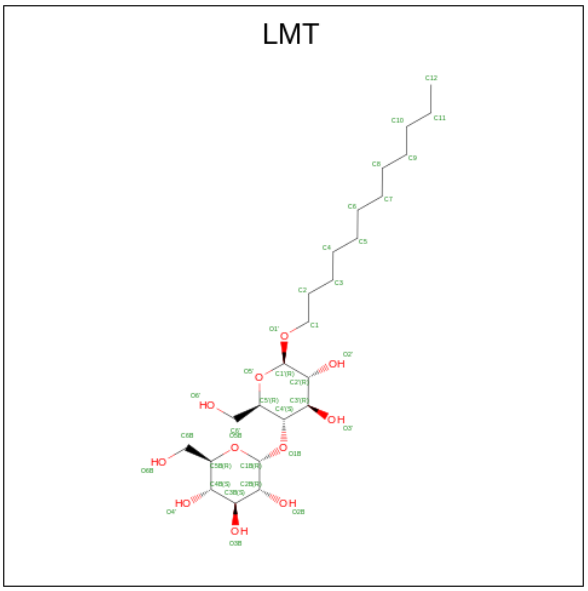
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
32	A	1	49	38	10	1	0	0
32	D	1	49	38	10	1	0	0
32	D	1	49	38	10	1	0	0
32	E	1	42	31	10	1	0	0
32	L	1	49	38	10	1	0	0
32	a	1	42	31	10	1	0	0
32	b	1	49	38	10	1	0	0
32	d	1	49	38	10	1	0	0
32	d	1	49	38	10	1	0	0
32	d	1	49	38	10	1	0	0

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



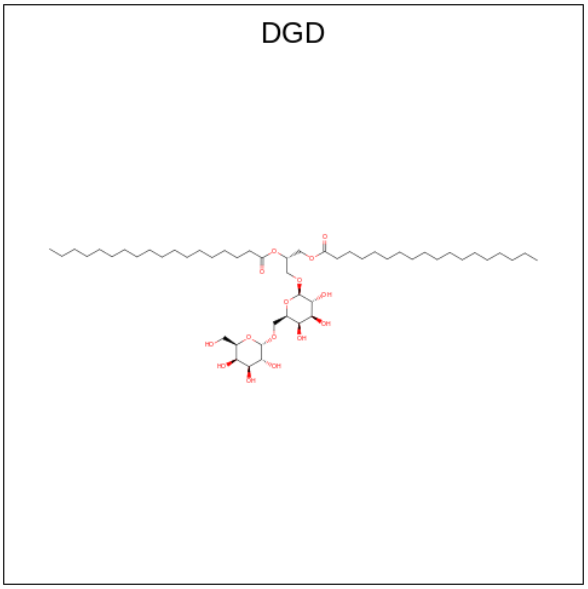
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	B	1	Total C O S 19 13 5 1	0	0
33	C	1	Total C O S 19 13 5 1	0	0
33	D	1	Total C O S 16 10 5 1	0	0
33	V	1	Total C O 11 6 5	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33	b	1	Total C O S 19 13 5 1	0	0
33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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	B	1	25	19	6	0	0
			Total	C	O		
34	C	1	35	24	11	0	0
			Total	C	O		
34	D	1	35	24	11	0	0
			Total	C	O		
34	D	1	35	24	11	0	0
			Total	C	O		
34	E	1	35	24	11	0	0
			Total	C	O		
34	M	1	35	24	11	0	0
			Total	C	O		
34	M	1	35	24	11	0	0
			Total	C	O		
34	a	1	35	24	11	0	0
			Total	C	O		
34	a	1	35	24	11	0	0
			Total	C	O		
34	b	1	25	19	6	0	0
			Total	C	O		
34	b	1	25	19	6	0	0
			Total	C	O		
34	e	1	35	24	11	0	0
			Total	C	O		
34	m	1	35	24	11	0	0
			Total	C	O		
34	t	1	26	19	7	0	0

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



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

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
36	C	1	1	1	0	0
36	F	1	Total	Ca	0	0
			1	1		

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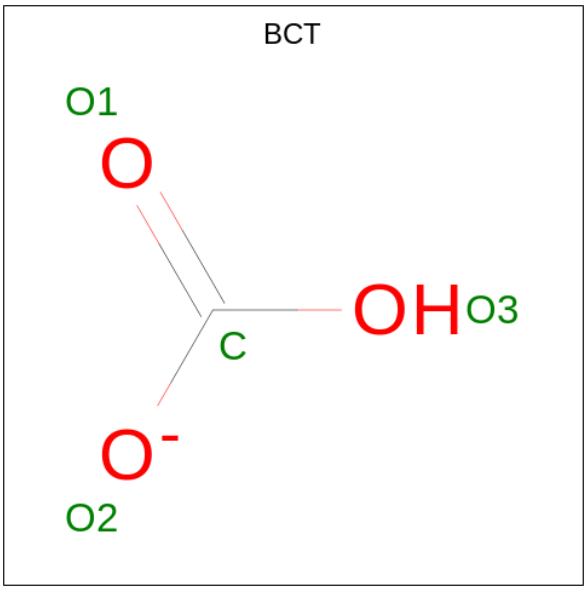
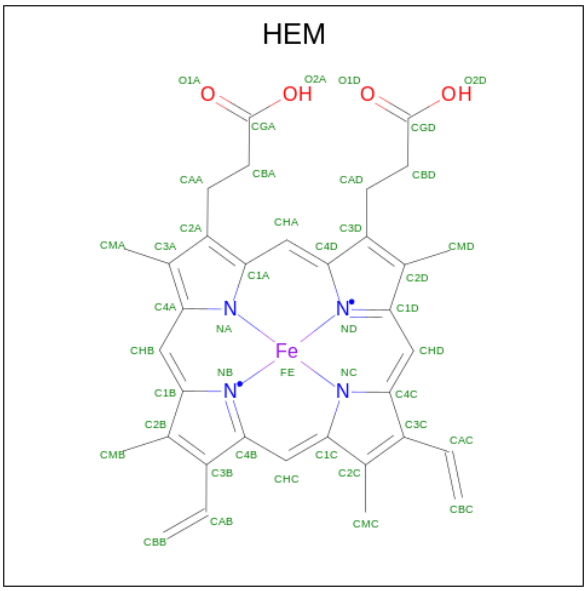
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
36	O	1	1	1	0	0
			Total	Ca		
36	c	2	2	2	0	0
			Total	Ca		
36	o	1	1	1	0	0
			Total	Ca		
36	v	1	1	1	0	0

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
37	D	1	4	1	3	0	0
			Total	C	O		
37	d	1	4	1	3	0	0

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

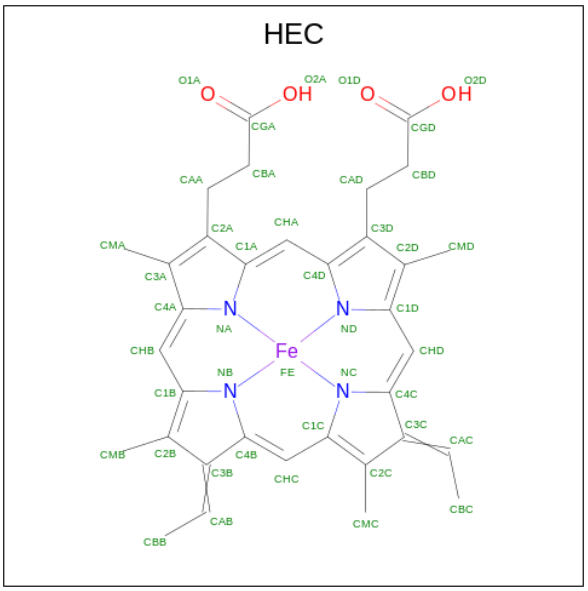


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
38	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
38	f	1	43	34	1	4	4	0	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	A	147	147	147	0	0
			Total	O		
41	B	207	207	207	0	0
			Total	O		
41	C	186	186	186	0	0
			Total	O		
41	D	132	132	132	0	0
			Total	O		
41	E	24	24	24	0	0
			Total	O		
41	F	8	8	8	0	0
			Total	O		
41	H	30	30	30	0	0
			Total	O		
41	I	3	3	3	0	0
			Total	O		
41	J	6	6	6	0	0
			Total	O		
41	K	6	6	6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	8	Total O 8 8	0	0
41	M	16	Total O 16 16	0	0
41	O	122	Total O 122 122	0	0
41	T	15	Total O 15 15	0	0
41	U	58	Total O 58 58	0	0
41	V	93	Total O 93 93	0	0
41	X	10	Total O 10 10	0	0
41	Y	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	144	Total O 144 144	0	0
41	b	222	Total O 222 222	0	0
41	c	166	Total O 166 166	0	0
41	d	127	Total O 127 127	0	0
41	e	13	Total O 13 13	0	0
41	f	5	Total O 5 5	0	0
41	h	24	Total O 24 24	0	0
41	i	2	Total O 2 2	0	0
41	j	3	Total O 3 3	0	0
41	k	5	Total O 5 5	0	0
41	l	7	Total O 7 7	0	0
41	m	11	Total O 11 11	0	0

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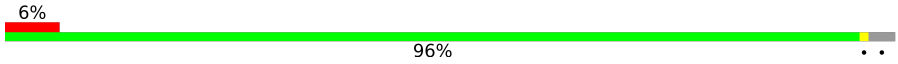
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
41	o	102	102	102	0	0
			Total	O		
41	t	11	11	11	0	0
			Total	O		
41	u	67	67	67	0	0
			Total	O		
41	v	56	56	56	0	0
			Total	O		
41	x	10	10	10	0	0
			Total	O		
41	y	3	3	3	0	0

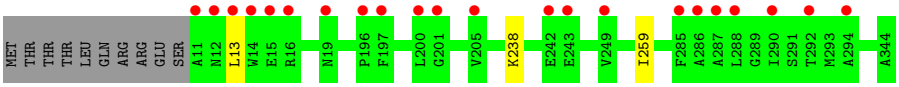
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

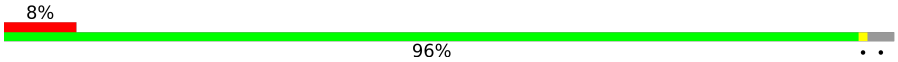
Chain A:

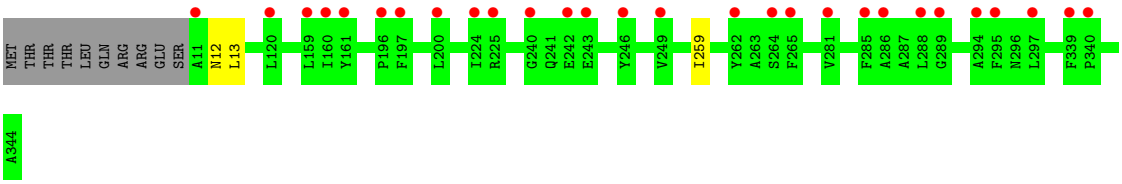




• Molecule 1: Photosystem II protein D1

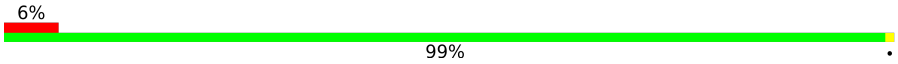
Chain a:

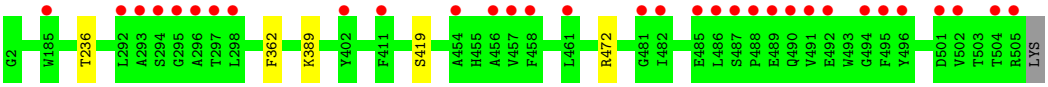




• Molecule 2: Photosystem II CP47 reaction center protein

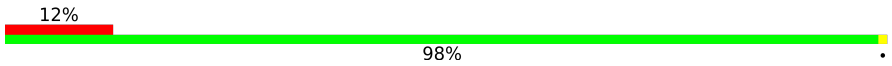
Chain B:

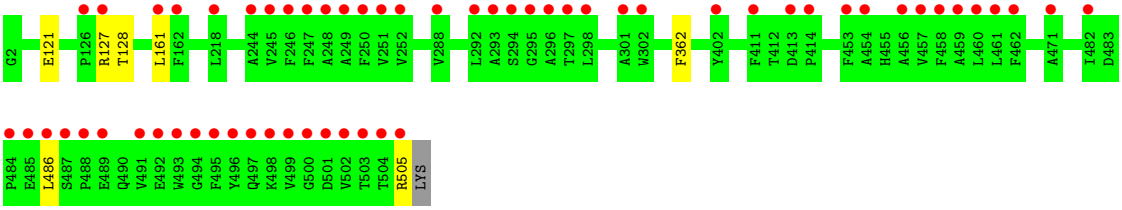




• Molecule 2: Photosystem II CP47 reaction center protein

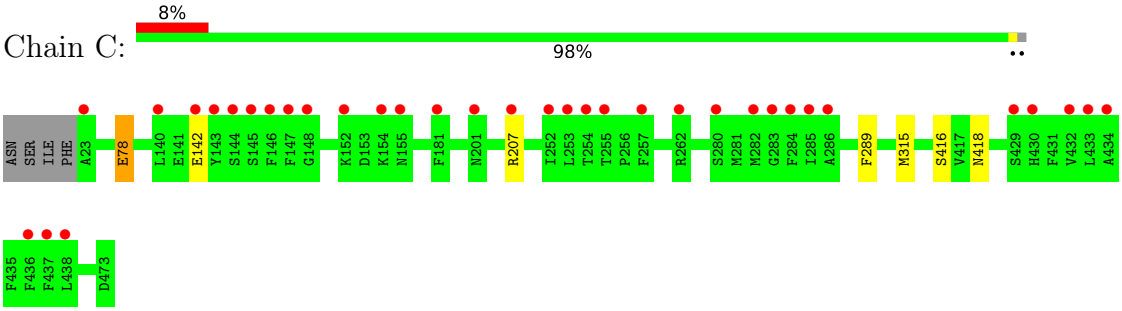
Chain b:





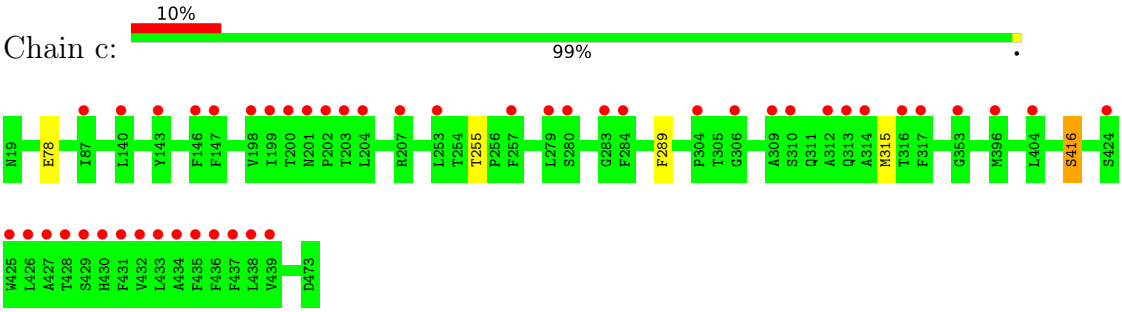
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



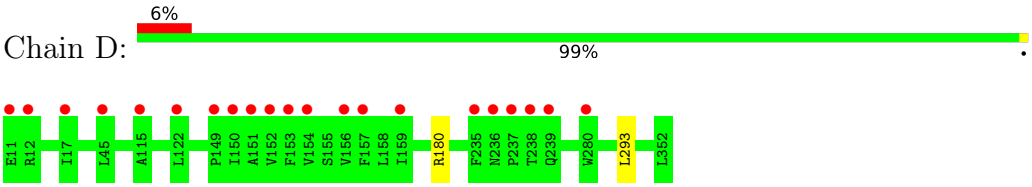
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



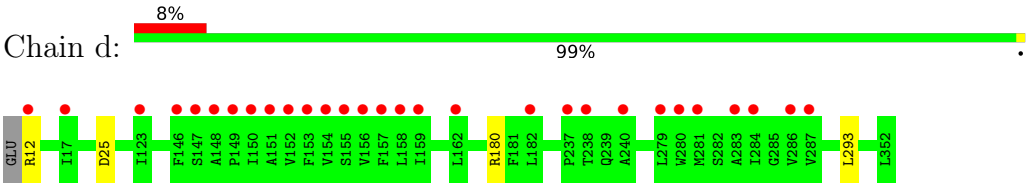
- Molecule 4: Photosystem II D2 protein

Chain D:



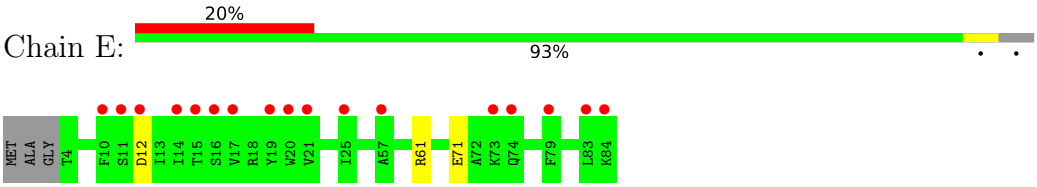
- Molecule 4: Photosystem II D2 protein

Chain d:



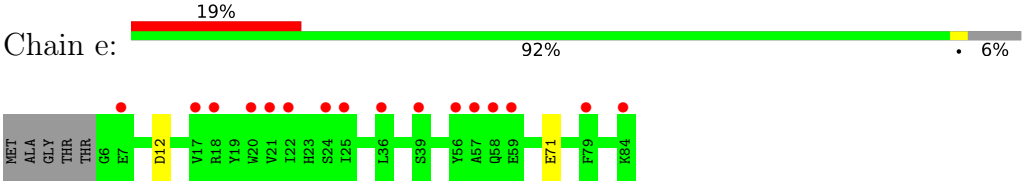
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:



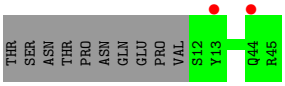
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:



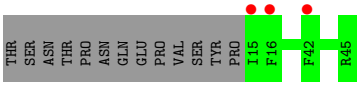
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



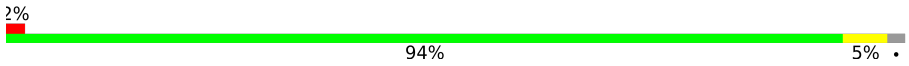
• Molecule 6: Cytochrome b559 subunit beta

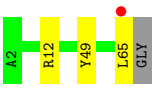
Chain f:



• Molecule 7: Photosystem II reaction center protein H

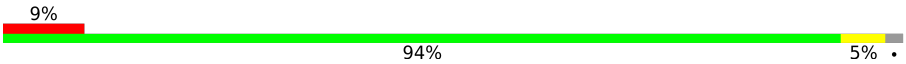
Chain H:

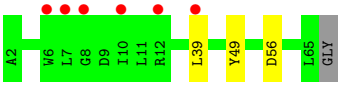




• Molecule 7: Photosystem II reaction center protein H

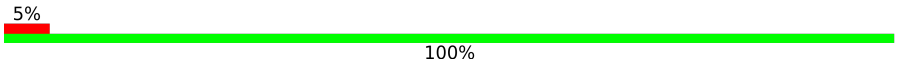
Chain h:





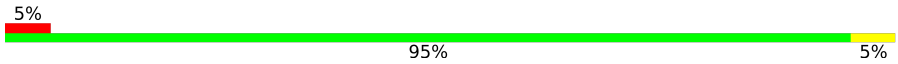
• Molecule 8: Photosystem II reaction center protein I

Chain I:



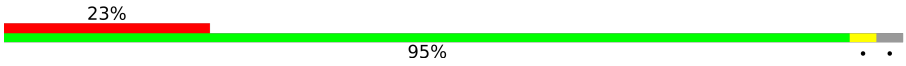
• Molecule 8: Photosystem II reaction center protein I

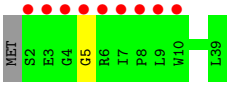
Chain i:



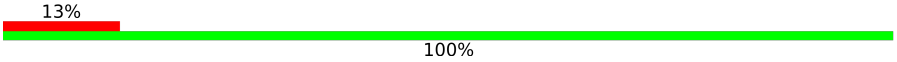
• Molecule 9: Photosystem II reaction center protein J

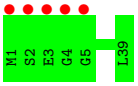
Chain J:





• Molecule 9: Photosystem II reaction center protein J

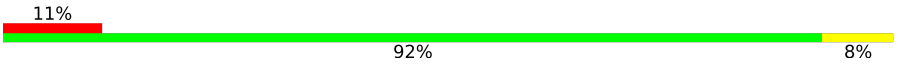
Chain j: 

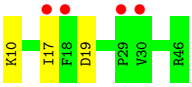


• Molecule 10: Photosystem II reaction center protein K

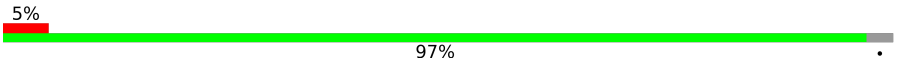
Chain K:

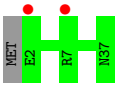
• Molecule 10: Photosystem II reaction center protein K

Chain k: 

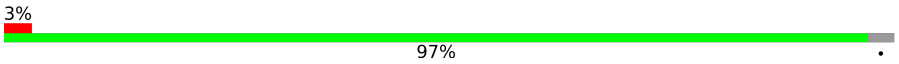


• Molecule 11: Photosystem II reaction center protein L

Chain L: 

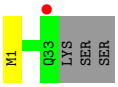


• Molecule 11: Photosystem II reaction center protein L

Chain l: 

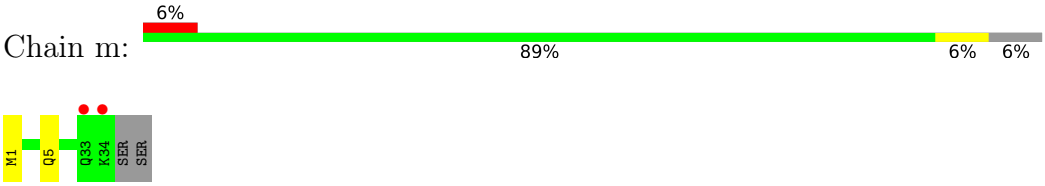
• Molecule 12: Photosystem II reaction center protein M

Chain M:



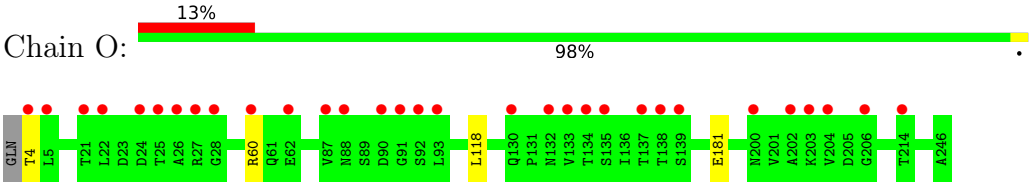
• Molecule 12: Photosystem II reaction center protein M

Chain m:



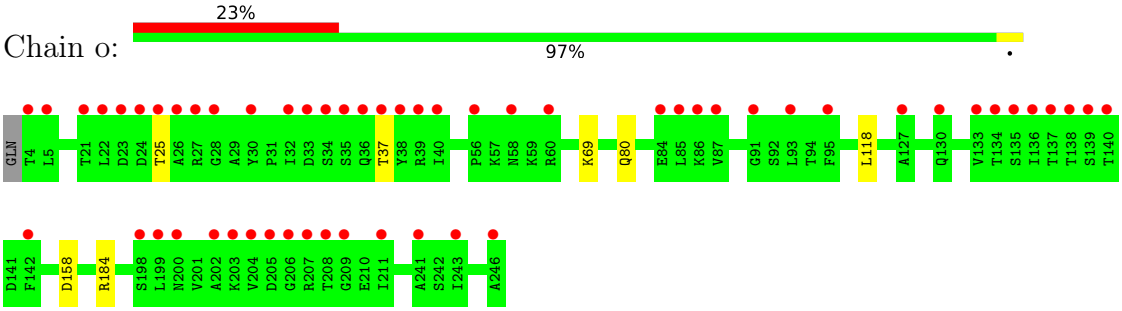
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



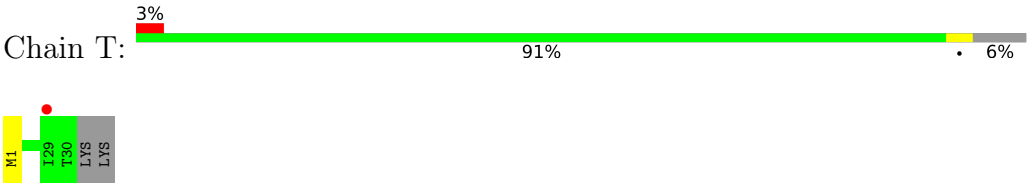
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



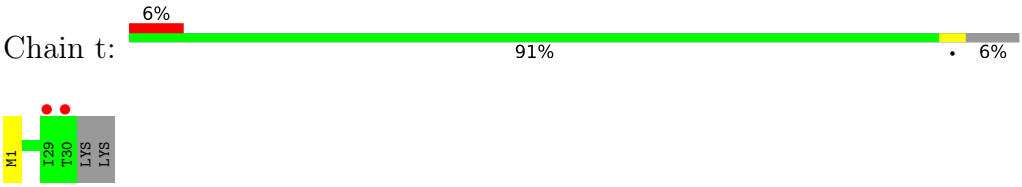
• Molecule 14: Photosystem II reaction center protein T

Chain T:



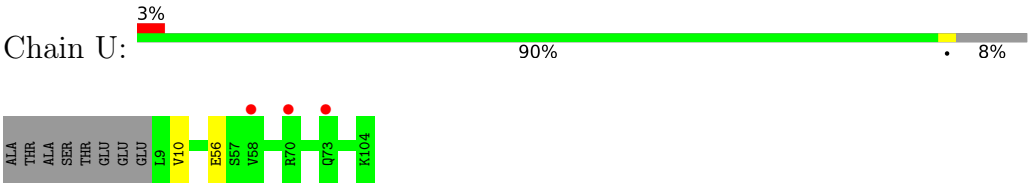
• Molecule 14: Photosystem II reaction center protein T

Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

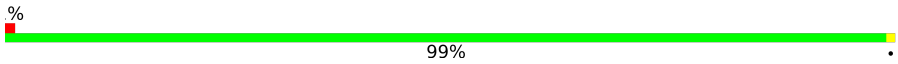


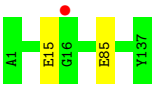
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

• Molecule 16: Cytochrome c-550

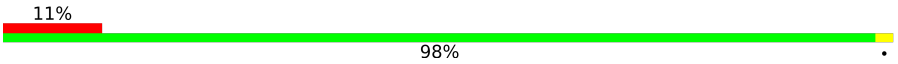
Chain V:

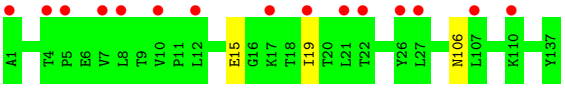




• Molecule 16: Cytochrome c-550

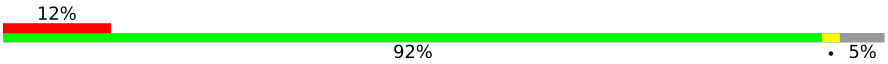
Chain v:

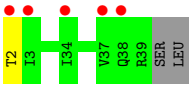




• Molecule 17: Photosystem II reaction center protein X

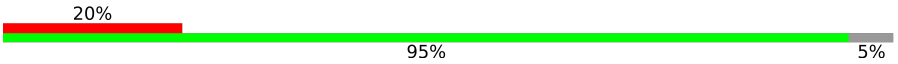
Chain X:

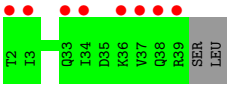




• Molecule 17: Photosystem II reaction center protein X

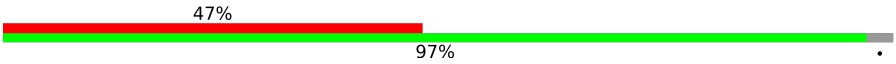
Chain x:

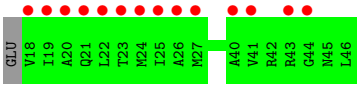




• Molecule 18: Photosystem II reaction center protein Ycf12

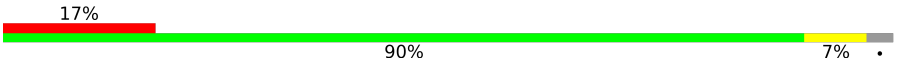
Chain Y:

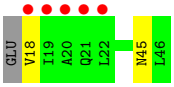




• Molecule 18: Photosystem II reaction center protein Ycf12

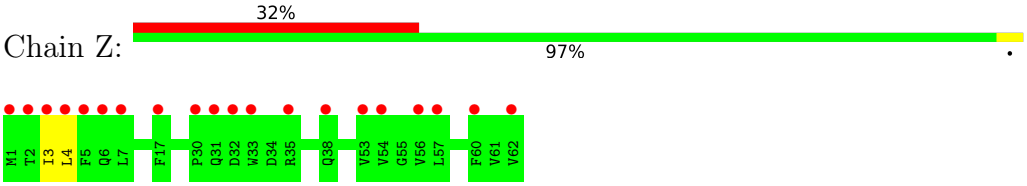
Chain y:





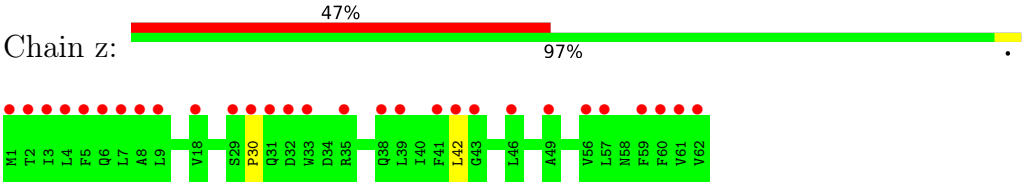
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



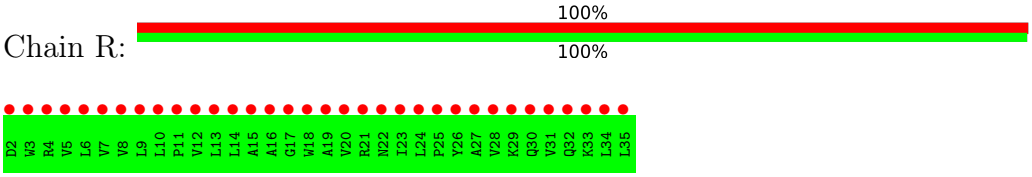
- Molecule 19: Photosystem II reaction center protein Z

Chain z:



- Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.02Å 231.70Å 288.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 2.35 52.70 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (39.93-2.35) 84.6 (52.70-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.160 , 0.208 0.162 , 0.208	Depositor DCC
R_{free} test set	17532 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 77.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	53071	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, HEC, LHG, PL9, BCT, GOL, CL, BCR, CA, LMT, PHO, DGD, HTG, FE2, HEM, FME, LMG, OEX, UNL, SQD, MG

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	0.42	0/2719	0.55	0/3708
1	a	0.40	0/2727	0.53	0/3719
2	B	0.42	0/4190	0.54	0/5708
2	b	0.40	0/4138	0.52	0/5640
3	C	0.39	1/3626 (0.0%)	0.51	0/4936
3	c	0.35	0/3648	0.49	0/4966
4	D	0.43	0/2821	0.56	0/3844
4	d	0.41	0/2812	0.53	0/3832
5	E	0.35	0/687	0.48	0/936
5	e	0.35	0/667	0.47	0/908
6	F	0.35	0/284	0.45	0/387
6	f	0.31	0/257	0.47	0/349
7	H	0.36	0/530	0.54	0/723
7	h	0.34	0/519	0.54	0/708
8	I	0.35	0/311	0.50	0/419
8	i	0.33	0/311	0.47	0/419
9	J	0.32	0/278	0.49	0/376
9	j	0.33	0/283	0.49	0/383
10	K	0.35	0/303	0.49	0/416
10	k	0.34	0/303	0.51	0/416
11	L	0.46	0/311	0.49	0/423
11	l	0.38	0/311	0.49	0/423
12	M	0.41	0/261	0.55	0/357
12	m	0.39	0/262	0.51	0/357
13	O	0.38	0/1917	0.58	0/2599
13	o	0.37	0/1910	0.58	1/2589 (0.0%)
14	T	0.47	0/257	0.50	0/349
14	t	0.45	0/257	0.45	0/349
15	U	0.38	0/776	0.54	0/1052
15	u	0.36	0/785	0.59	0/1064
16	V	0.35	0/1085	0.53	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.35	0/1085	0.51	0/1473
17	X	0.31	0/284	0.48	0/384
17	x	0.29	0/284	0.44	0/384
18	Y	0.29	0/216	0.43	0/289
18	y	0.27	0/216	0.43	0/289
19	Z	0.30	0/490	0.38	0/669
19	z	0.28	0/490	0.39	0/669
20	R	0.27	0/279	0.42	0/383
All	All	0.39	1/42890 (0.0%)	0.52	1/58368 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	78	GLU	C-N	5.08	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	o	158	ASP	CB-CG-OD1	5.39	123.16	118.30

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	334/344 (97%)	330 (99%)	3 (1%)	1 (0%)	41 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	41	47
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	443 (98%)	8 (2%)	2 (0%)	34	38
3	c	455/455 (100%)	446 (98%)	8 (2%)	1 (0%)	47	56
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	329 (97%)	10 (3%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	31 (86%)	4 (11%)	1 (3%)	5	2
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	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	244/244 (100%)	237 (97%)	7 (3%)	0	100	100
13	o	243/244 (100%)	236 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	7
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5246/5384 (97%)	5124 (98%)	115 (2%)	7 (0%)	51	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
1	a	259	ILE
19	z	30	PRO
9	J	5	GLY
1	A	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/279 (97%)	269 (99%)	2 (1%)	84	91
1	a	272/279 (98%)	270 (99%)	2 (1%)	84	91
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	82
2	b	406/403 (101%)	399 (98%)	7 (2%)	60	72
3	C	356/356 (100%)	350 (98%)	6 (2%)	60	72
3	c	358/356 (101%)	353 (99%)	5 (1%)	67	78
4	D	277/277 (100%)	275 (99%)	2 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	276/277 (100%)	272 (99%)	4 (1%)	67	78
5	E	73/73 (100%)	70 (96%)	3 (4%)	30	37
5	e	70/73 (96%)	68 (97%)	2 (3%)	42	52
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	51 (93%)	4 (7%)	14	14
7	h	54/54 (100%)	51 (94%)	3 (6%)	21	23
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	52
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	6
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	6
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	46
13	O	209/207 (101%)	205 (98%)	4 (2%)	57	68
13	o	208/207 (100%)	202 (97%)	6 (3%)	42	52
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	59
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	82
16	V	117/117 (100%)	115 (98%)	2 (2%)	60	72
16	v	117/117 (100%)	114 (97%)	3 (3%)	46	56
17	X	31/33 (94%)	30 (97%)	1 (3%)	39	47
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	8
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	41
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	R	29/29 (100%)	29 (100%)	0	100 100
All	All	4352/4403 (99%)	4275 (98%)	77 (2%)	59 70

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	238	LYS
2	B	236	THR
2	B	362	PHE
2	B	389	LYS
2	B	419	SER
2	B	472	ARG
3	C	78	GLU
3	C	142	GLU
3	C	207	ARG
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
4	D	180	ARG
4	D	293	LEU
5	E	12	ASP
5	E	61	ARG
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
7	H	65	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
13	O	4	THR
13	O	60	ARG
13	O	118	LEU
13	O	181	GLU
15	U	10	VAL
15	U	56	GLU
16	V	15	GLU
16	V	85	GLU
17	X	2	THR
19	Z	3	ILE
19	Z	4	LEU

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Mol	Chain	Res	Type
1	a	12	ASN
1	a	13	LEU
2	b	121	GLU
2	b	127	ARG
2	b	128	THR
2	b	161	LEU
2	b	362	PHE
2	b	486	LEU
2	b	505	ARG
3	c	78	GLU
3	c	255	THR
3	c	289	PHE
3	c	315	MET
3	c	416	SER
4	d	12	ARG
4	d	25	ASP
4	d	180	ARG
4	d	293	LEU
5	e	12	ASP
5	e	71	GLU
7	h	39	LEU
7	h	49	TYR
7	h	56	ASP
8	i	36	ASP
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
13	o	25	THR
13	o	37	THR
13	o	69	LYS
13	o	80	GLN
13	o	118	LEU
13	o	184	ARG
15	u	86	GLU
16	v	15	GLU
16	v	19	ILE
16	v	106	ASN
18	y	18	VAL
18	y	45	ASN
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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	0.63	0	7,9,11	1.91	2 (28%)
8	FME	i	1	8	8,9,10	0.57	0	7,9,11	1.09	1 (14%)
14	FME	T	1	14	8,9,10	0.66	0	7,9,11	1.40	1 (14%)
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	0.97	0
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.65	3 (42%)
12	FME	m	1	12	8,9,10	0.60	0	7,9,11	1.29	1 (14%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-3.48	117.47	122.82
12	M	1	FME	CA-N-CN	-2.93	118.32	122.82
14	T	1	FME	O-C-CA	-2.73	117.63	124.78
14	t	1	FME	O-C-CA	-2.39	118.52	124.78
12	M	1	FME	O-C-CA	-2.26	118.87	124.78
12	m	1	FME	O-C-CA	-2.16	119.12	124.78
12	M	1	FME	O1-CN-N	-2.12	119.68	125.27
8	i	1	FME	O-C-CA	-2.01	119.52	124.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	O-C-CA-CB
14	t	1	FME	O1-CN-N-CA
8	I	1	FME	CB-CA-N-CN
12	M	1	FME	CB-CA-N-CN
12	m	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 216 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 183 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	$\#\|Z\| > 2$
35	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	1.10	7 (9%)
40	HEC	V	201	16	32,50,50	2.04	4 (12%)	24,82,82	2.01	7 (29%)
23	CLA	b	604	-	65,73,73	2.00	15 (23%)	76,113,113	2.70	28 (36%)
26	GOL	b	623	-	5,5,5	0.97	0	5,5,5	1.09	0
33	HTG	B	624	-	19,19,19	1.06	2 (10%)	23,24,24	1.45	5 (21%)
23	CLA	c	503	-	65,73,73	2.00	15 (23%)	76,113,113	2.76	25 (32%)
31	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	7 (11%)
27	SQD	C	501	-	53,54,54	0.97	3 (5%)	62,65,65	1.98	11 (17%)
25	BCR	K	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	10 (17%)
23	CLA	c	507	-	65,73,73	2.07	17 (26%)	76,113,113	2.73	30 (39%)
23	CLA	D	405	-	65,73,73	2.01	16 (24%)	76,113,113	2.91	29 (38%)
23	CLA	B	605	-	65,73,73	2.04	17 (26%)	76,113,113	2.79	26 (34%)
23	CLA	a	407	-	65,73,73	2.02	15 (23%)	76,113,113	2.77	28 (36%)
34	LMT	b	626	-	25,25,36	0.56	1 (4%)	30,30,47	1.25	3 (10%)
29	PL9	A	413	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
23	CLA	B	610	41	65,73,73	2.07	17 (26%)	76,113,113	2.75	27 (35%)
23	CLA	b	607	41	65,73,73	1.96	17 (26%)	76,113,113	2.83	26 (34%)
34	LMT	t	101	-	26,26,36	0.50	0	31,31,47	1.03	2 (6%)
32	LHG	A	416	-	48,48,48	0.89	2 (4%)	51,54,54	1.21	5 (9%)
23	CLA	b	616	-	65,73,73	2.00	15 (23%)	76,113,113	2.90	28 (36%)
29	PL9	d	406	-	55,55,55	0.71	2 (3%)	68,69,69	1.65	18 (26%)
23	CLA	b	615	-	65,73,73	2.03	15 (23%)	76,113,113	2.75	25 (32%)
34	LMT	E	102	-	36,36,36	0.55	1 (2%)	47,47,47	1.09	4 (8%)
23	CLA	d	403	-	65,73,73	1.93	17 (26%)	76,113,113	2.74	30 (39%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.54	9 (16%)
25	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.69	12 (21%)
34	LMT	M	102	-	36,36,36	0.47	0	47,47,47	0.92	3 (6%)
23	CLA	b	614	-	65,73,73	2.03	15 (23%)	76,113,113	2.84	29 (38%)
25	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.24	5 (8%)
23	CLA	c	510	-	65,73,73	2.12	17 (26%)	76,113,113	2.75	27 (35%)
33	HTG	b	624	-	19,19,19	1.05	2 (10%)	23,24,24	1.38	2 (8%)
23	CLA	c	509	-	65,73,73	2.14	16 (24%)	76,113,113	2.72	26 (34%)
23	CLA	a	405	41	65,73,73	1.93	15 (23%)	76,113,113	2.85	27 (35%)
27	SQD	a	411	-	53,54,54	1.02	3 (5%)	62,65,65	1.31	8 (12%)
23	CLA	C	510	-	65,73,73	2.14	16 (24%)	76,113,113	2.75	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	DGD	c	517	-	63,63,67	0.91	2 (3%)	77,77,81	1.02	3 (3%)
23	CLA	b	605	-	65,73,73	1.98	17 (26%)	76,113,113	2.98	27 (35%)
26	GOL	B	627	-	5,5,5	1.04	0	5,5,5	0.87	0
31	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
23	CLA	c	511	-	65,73,73	1.99	16 (24%)	76,113,113	2.73	28 (36%)
28	OEX	A	412	1,41,3	0,15,15	-	-	-		
31	LMG	m	101	-	51,51,55	0.90	2 (3%)	59,59,63	1.13	3 (5%)
24	PHO	a	416	-	51,69,69	1.82	8 (15%)	47,99,99	1.91	9 (19%)
31	LMG	A	415	-	51,51,55	0.92	2 (3%)	59,59,63	1.12	5 (8%)
23	CLA	C	505	41	65,73,73	2.02	17 (26%)	76,113,113	2.73	29 (38%)
23	CLA	C	511	-	65,73,73	2.06	17 (26%)	76,113,113	2.79	27 (35%)
23	CLA	c	514	-	65,73,73	2.09	16 (24%)	76,113,113	2.72	29 (38%)
25	BCR	B	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.27	9 (16%)
23	CLA	C	503	-	65,73,73	2.02	16 (24%)	76,113,113	2.63	27 (35%)
23	CLA	C	513	-	65,73,73	2.12	16 (24%)	76,113,113	2.72	30 (39%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.68	12 (21%)
35	DGD	C	517	-	63,63,67	0.86	2 (3%)	77,77,81	1.18	6 (7%)
23	CLA	B	602	-	65,73,73	2.07	16 (24%)	76,113,113	2.86	29 (38%)
31	LMG	M	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.22	7 (11%)
33	HTG	b	622	-	19,19,19	1.00	1 (5%)	23,24,24	1.69	3 (13%)
23	CLA	A	408	-	65,73,73	2.05	16 (24%)	76,113,113	2.78	29 (38%)
27	SQD	L	102	-	53,54,54	1.02	3 (5%)	62,65,65	1.62	10 (16%)
32	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
23	CLA	b	601	41	65,73,73	2.14	16 (24%)	76,113,113	2.70	25 (32%)
23	CLA	B	601	41	65,73,73	2.11	16 (24%)	76,113,113	2.74	28 (36%)
23	CLA	b	610	41	65,73,73	2.02	18 (27%)	76,113,113	2.79	28 (36%)
25	BCR	D	407	-	41,41,41	1.02	1 (2%)	56,56,56	1.78	14 (25%)
34	LMT	D	403	-	36,36,36	0.52	1 (2%)	47,47,47	0.81	2 (4%)
32	LHG	a	419	-	41,41,48	1.04	2 (4%)	44,47,54	0.97	2 (4%)
35	DGD	c	519	-	63,63,67	0.87	3 (4%)	77,77,81	0.98	4 (5%)
23	CLA	c	512	3	65,73,73	2.05	15 (23%)	76,113,113	2.82	29 (38%)
23	CLA	b	603	-	65,73,73	2.10	16 (24%)	76,113,113	2.83	28 (36%)
23	CLA	a	404	-	65,73,73	2.06	15 (23%)	76,113,113	2.81	33 (43%)
23	CLA	B	609	-	65,73,73	1.98	16 (24%)	76,113,113	2.75	23 (30%)
23	CLA	C	514	-	65,73,73	2.03	15 (23%)	76,113,113	2.76	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	LMG	C	520	-	51,51,55	0.99	2 (3%)	59,59,63	0.99	4 (6%)
40	HEC	v	203	16	32,50,50	2.07	4 (12%)	24,82,82	1.77	5 (20%)
34	LMT	b	620	-	25,25,36	0.51	0	30,30,47	0.62	0
26	GOL	v	202	-	5,5,5	0.98	0	5,5,5	0.92	0
38	HEM	E	103	5,6	41,50,50	1.31	7 (17%)	45,82,82	1.89	14 (31%)
31	LMG	c	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.05	4 (6%)
23	CLA	D	406	-	65,73,73	2.04	15 (23%)	76,113,113	2.76	28 (36%)
23	CLA	b	606	-	65,73,73	1.99	16 (24%)	76,113,113	2.89	30 (39%)
33	HTG	V	202	-	11,11,19	0.21	0	15,15,24	1.12	1 (6%)
25	BCR	b	619	-	41,41,41	1.13	1 (2%)	56,56,56	1.55	12 (21%)
25	BCR	B	618	-	41,41,41	0.90	1 (2%)	56,56,56	1.53	12 (21%)
23	CLA	B	608	-	65,73,73	2.00	16 (24%)	76,113,113	2.77	29 (38%)
23	CLA	b	602	-	65,73,73	2.10	16 (24%)	76,113,113	2.83	29 (38%)
23	CLA	C	502	-	65,73,73	2.00	16 (24%)	76,113,113	2.89	26 (34%)
23	CLA	c	506	-	65,73,73	2.03	16 (24%)	76,113,113	2.65	25 (32%)
33	HTG	D	413	-	16,16,19	1.11	2 (12%)	20,21,24	1.33	1 (5%)
25	BCR	A	409	-	41,41,41	1.00	1 (2%)	56,56,56	1.41	8 (14%)
25	BCR	a	408	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	10 (17%)
23	CLA	B	612	-	65,73,73	1.94	17 (26%)	76,113,113	2.94	28 (36%)
24	PHO	A	407	-	51,69,69	1.82	7 (13%)	47,99,99	1.81	10 (21%)
23	CLA	c	502	-	65,73,73	2.00	17 (26%)	76,113,113	2.73	28 (36%)
25	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.60	11 (19%)
34	LMT	m	103	-	36,36,36	0.44	0	47,47,47	1.02	3 (6%)
27	SQD	D	415	-	42,43,54	1.15	3 (7%)	51,54,65	1.84	10 (19%)
33	HTG	B	622	-	19,19,19	0.84	1 (5%)	23,24,24	1.45	1 (4%)
25	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.52	14 (25%)
23	CLA	C	508	41	65,73,73	2.04	16 (24%)	76,113,113	2.71	28 (36%)
34	LMT	M	104	-	36,36,36	0.50	0	47,47,47	1.16	3 (6%)
27	SQD	a	409	-	53,54,54	0.98	3 (5%)	62,65,65	1.66	11 (17%)
23	CLA	c	508	41	65,73,73	2.08	15 (23%)	76,113,113	2.86	26 (34%)
33	HTG	B	621	-	19,19,19	0.97	1 (5%)	23,24,24	1.55	4 (17%)
23	CLA	C	509	-	65,73,73	2.08	15 (23%)	76,113,113	2.79	24 (31%)
32	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.10	5 (9%)
32	LHG	D	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.03	4 (7%)
25	BCR	d	405	-	41,41,41	1.14	1 (2%)	56,56,56	1.82	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	4 (5%)
34	LMT	C	525	-	36,36,36	0.53	1 (2%)	47,47,47	1.14	3 (6%)
26	GOL	c	526	-	5,5,5	0.80	0	5,5,5	1.05	0
31	LMG	d	412	39	51,51,55	0.92	2 (3%)	59,59,63	0.90	3 (5%)
27	SQD	B	620	-	53,54,54	1.02	3 (5%)	62,65,65	1.55	11 (17%)
37	BCT	d	401	21	2,3,3	0.54	0	2,3,3	1.93	1 (50%)
24	PHO	a	406	-	51,69,69	1.88	8 (15%)	47,99,99	1.91	10 (21%)
35	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	1.15	6 (7%)
23	CLA	B	603	-	65,73,73	2.05	16 (24%)	76,113,113	2.92	26 (34%)
25	BCR	b	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.36	10 (17%)
35	DGD	C	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.02	3 (3%)
25	BCR	c	516	-	41,41,41	1.07	1 (2%)	56,56,56	1.49	11 (19%)
38	HEM	f	101	5,6	41,50,50	1.30	6 (14%)	45,82,82	1.82	10 (22%)
23	CLA	b	608	-	65,73,73	2.06	16 (24%)	76,113,113	2.76	28 (36%)
32	LHG	d	409	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	3 (5%)
23	CLA	c	513	-	65,73,73	2.04	16 (24%)	76,113,113	2.71	29 (38%)
23	CLA	b	613	-	65,73,73	2.10	15 (23%)	76,113,113	2.71	28 (36%)
34	LMT	D	404	-	36,36,36	0.43	0	47,47,47	1.11	4 (8%)
23	CLA	b	612	-	65,73,73	2.05	17 (26%)	76,113,113	2.84	28 (36%)
23	CLA	A	406	41	65,73,73	1.99	16 (24%)	76,113,113	2.76	25 (32%)
23	CLA	c	505	41	65,73,73	2.12	17 (26%)	76,113,113	2.81	32 (42%)
23	CLA	B	611	-	65,73,73	2.01	15 (23%)	76,113,113	2.82	27 (35%)
23	CLA	C	506	-	65,73,73	1.99	17 (26%)	76,113,113	2.65	25 (32%)
28	OEX	a	413	1,41,3	0,15,15	-	-	-		
32	LHG	D	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
37	BCT	D	401	21	2,3,3	0.56	0	2,3,3	1.16	0
23	CLA	b	609	-	65,73,73	2.07	18 (27%)	76,113,113	2.76	28 (36%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.44	9 (16%)
34	LMT	a	418	-	36,36,36	0.50	1 (2%)	47,47,47	0.93	2 (4%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.02	5 (6%)
34	LMT	e	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.86	1 (2%)
23	CLA	C	507	-	65,73,73	2.07	17 (26%)	76,113,113	2.79	30 (39%)
26	GOL	A	410	-	5,5,5	1.11	0	5,5,5	0.74	0
33	HTG	b	621	-	19,19,19	0.99	1 (5%)	23,24,24	1.38	2 (8%)
29	PL9	a	414	-	55,55,55	0.64	1 (1%)	68,69,69	2.01	21 (30%)
26	GOL	B	626	-	5,5,5	0.83	0	5,5,5	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	GOL	B	623	-	5,5,5	0.98	0	5,5,5	1.10	0
23	CLA	d	402	41	65,73,73	2.06	16 (24%)	76,113,113	2.72	30 (39%)
24	PHO	D	402	-	51,69,69	1.86	8 (15%)	47,99,99	1.88	12 (25%)
23	CLA	A	404	-	65,73,73	2.04	17 (26%)	76,113,113	2.80	32 (42%)
23	CLA	B	606	-	65,73,73	2.01	17 (26%)	76,113,113	2.83	28 (36%)
25	BCR	k	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.61	12 (21%)
23	CLA	C	504	-	65,73,73	2.04	16 (24%)	76,113,113	2.81	25 (32%)
33	HTG	c	522	-	19,19,19	0.99	2 (10%)	23,24,24	1.39	1 (4%)
23	CLA	c	504	-	65,73,73	2.02	16 (24%)	76,113,113	2.80	26 (34%)
23	CLA	B	607	41	65,73,73	1.96	17 (26%)	76,113,113	2.74	26 (34%)
26	GOL	a	410	-	5,5,5	0.83	0	5,5,5	1.00	0
33	HTG	C	522	-	19,19,19	0.91	1 (5%)	23,24,24	1.36	1 (4%)
23	CLA	b	611	-	65,73,73	1.98	16 (24%)	76,113,113	2.85	27 (35%)
32	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.14	4 (7%)
26	GOL	b	627	-	5,5,5	0.97	0	5,5,5	1.03	0
23	CLA	B	604	-	65,73,73	2.00	16 (24%)	76,113,113	2.76	30 (39%)
25	BCR	h	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	7 (12%)
26	GOL	O	302	-	5,5,5	0.85	0	5,5,5	1.02	0
23	CLA	B	613	-	65,73,73	2.02	17 (26%)	76,113,113	2.83	25 (32%)
25	BCR	Y	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.85	16 (28%)
27	SQD	f	102	-	42,43,54	1.16	3 (7%)	51,54,65	1.29	6 (11%)
34	LMT	a	412	-	36,36,36	0.63	1 (2%)	47,47,47	1.24	3 (6%)
23	CLA	B	614	-	65,73,73	1.93	16 (24%)	76,113,113	3.00	29 (38%)
26	GOL	c	501	-	5,5,5	1.02	0	5,5,5	0.88	0
31	LMG	C	521	-	51,51,55	1.02	3 (5%)	59,59,63	1.35	7 (11%)
23	CLA	A	405	41	65,73,73	2.03	17 (26%)	76,113,113	2.83	30 (39%)
27	SQD	A	411	-	53,54,54	1.06	3 (5%)	62,65,65	1.33	8 (12%)
31	LMG	Z	101	-	37,37,55	1.02	3 (8%)	45,45,63	1.51	7 (15%)
31	LMG	c	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.20	6 (10%)
23	CLA	d	404	-	65,73,73	2.09	16 (24%)	76,113,113	2.84	28 (36%)
32	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.05	2 (4%)
32	LHG	b	628	-	48,48,48	0.94	2 (4%)	51,54,54	1.02	3 (5%)
26	GOL	C	523	-	5,5,5	1.16	0	5,5,5	0.93	0
25	BCR	b	617	-	41,41,41	1.12	1 (2%)	56,56,56	1.43	6 (10%)
33	HTG	h	101	-	16,16,19	1.14	2 (12%)	20,21,24	2.13	7 (35%)
34	LMT	B	628	-	25,25,36	0.46	0	30,30,47	1.01	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	B	615	-	65,73,73	1.94	15 (23%)	76,113,113	2.89	27 (35%)
29	PL9	D	408	-	55,55,55	0.66	2 (3%)	68,69,69	1.72	19 (27%)
23	CLA	C	512	3	65,73,73	2.08	19 (29%)	76,113,113	2.71	28 (36%)
25	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	B	616	-	65,73,73	1.97	15 (23%)	76,113,113	2.82	27 (35%)
31	LMG	D	414	39	51,51,55	0.85	3 (5%)	59,59,63	0.98	3 (5%)

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
35	DGD	H	102	-	-	17/51/91/95	0/2/2/2
40	HEC	V	201	16	-	2/10/54/54	-
23	CLA	b	604	-	1/1/15/20	8/37/115/115	-
26	GOL	b	623	-	-	2/4/4/4	-
33	HTG	B	624	-	-	4/10/30/30	0/1/1/1
23	CLA	c	503	-	1/1/15/20	2/37/115/115	-
31	LMG	a	417	-	-	13/46/66/70	0/1/1/1
27	SQD	C	501	-	-	13/49/69/69	0/1/1/1
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
23	CLA	c	507	-	1/1/15/20	11/37/115/115	-
23	CLA	D	405	-	1/1/15/20	4/37/115/115	-
23	CLA	B	605	-	1/1/15/20	7/37/115/115	-
23	CLA	a	407	-	1/1/15/20	9/37/115/115	-
34	LMT	b	626	-	-	9/17/37/61	0/1/1/2
29	PL9	A	413	-	-	17/53/73/73	0/1/1/1
23	CLA	B	610	41	1/1/15/20	7/37/115/115	-
23	CLA	b	607	41	1/1/15/20	2/37/115/115	-
34	LMT	t	101	-	-	6/17/38/61	0/1/1/2
32	LHG	A	416	-	-	15/53/53/53	-
23	CLA	b	616	-	1/1/15/20	10/37/115/115	-
29	PL9	d	406	-	-	6/53/73/73	0/1/1/1
23	CLA	b	615	-	1/1/15/20	11/37/115/115	-
34	LMT	E	102	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	403	-	1/1/15/20	6/37/115/115	-
25	BCR	c	515	-	-	3/29/63/63	0/2/2/2
25	BCR	k	102	-	-	6/29/63/63	0/2/2/2
34	LMT	M	102	-	-	5/21/61/61	0/2/2/2
23	CLA	b	614	-	1/1/15/20	12/37/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	c	510	-	1/1/15/20	10/37/115/115	-
33	HTG	b	624	-	-	2/10/30/30	0/1/1/1
23	CLA	c	509	-	1/1/15/20	8/37/115/115	-
23	CLA	a	405	41	-	7/37/115/115	-
27	SQD	a	411	-	-	16/49/69/69	0/1/1/1
23	CLA	C	510	-	1/1/15/20	4/37/115/115	-
35	DGD	c	517	-	-	17/51/91/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	8/37/115/115	-
26	GOL	B	627	-	-	0/4/4/4	-
31	LMG	z	101	-	-	8/34/54/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	7/37/115/115	-
31	LMG	m	101	-	-	11/46/66/70	0/1/1/1
24	PHO	a	416	-	-	7/37/103/103	0/5/6/6
31	LMG	A	415	-	-	24/46/66/70	0/1/1/1
23	CLA	C	505	41	1/1/15/20	6/37/115/115	-
23	CLA	C	511	-	1/1/15/20	10/37/115/115	-
23	CLA	c	514	-	1/1/15/20	11/37/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	C	503	-	-	8/37/115/115	-
23	CLA	C	513	-	1/1/15/20	13/37/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
35	DGD	C	517	-	-	14/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	10/37/115/115	-
31	LMG	M	101	-	-	10/46/66/70	0/1/1/1
33	HTG	b	622	-	-	3/10/30/30	0/1/1/1
23	CLA	A	408	-	1/1/15/20	10/37/115/115	-
27	SQD	L	102	-	-	19/49/69/69	0/1/1/1
32	LHG	d	408	-	-	20/53/53/53	-
23	CLA	b	601	41	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	601	41	1/1/15/20	11/37/115/115	-
23	CLA	b	610	41	1/1/15/20	9/37/115/115	-
25	BCR	D	407	-	-	8/29/63/63	0/2/2/2
34	LMT	D	403	-	-	8/21/61/61	0/2/2/2
32	LHG	a	419	-	-	15/46/46/53	-
35	DGD	c	519	-	-	8/51/91/95	0/2/2/2
23	CLA	c	512	3	1/1/15/20	4/37/115/115	-
23	CLA	b	603	-	1/1/15/20	7/37/115/115	-
23	CLA	a	404	-	1/1/15/20	6/37/115/115	-
23	CLA	B	609	-	1/1/15/20	6/37/115/115	-
23	CLA	C	514	-	1/1/15/20	10/37/115/115	-
31	LMG	C	520	-	-	13/46/66/70	0/1/1/1
40	HEC	v	203	16	-	2/10/54/54	-
34	LMT	b	620	-	-	7/17/37/61	0/1/1/2
26	GOL	v	202	-	-	2/4/4/4	-
38	HEM	E	103	5,6	-	3/12/54/54	-
31	LMG	c	520	-	-	10/46/66/70	0/1/1/1
23	CLA	D	406	-	1/1/15/20	8/37/115/115	-
23	CLA	b	606	-	1/1/15/20	8/37/115/115	-
33	HTG	V	202	-	-	1/2/19/30	0/1/1/1
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	B	608	-	-	2/37/115/115	-
23	CLA	b	602	-	1/1/15/20	3/37/115/115	-
23	CLA	C	502	-	1/1/15/20	4/37/115/115	-
23	CLA	c	506	-	1/1/15/20	5/37/115/115	-
33	HTG	D	413	-	-	1/7/27/30	0/1/1/1
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	a	408	-	-	1/29/63/63	0/2/2/2
23	CLA	B	612	-	1/1/15/20	4/37/115/115	-
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
23	CLA	c	502	-	1/1/15/20	4/37/115/115	-
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
34	LMT	m	103	-	-	5/21/61/61	0/2/2/2
27	SQD	D	415	-	-	14/38/58/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HTG	B	622	-	-	4/10/30/30	0/1/1/1
25	BCR	t	102	-	-	6/29/63/63	0/2/2/2
23	CLA	C	508	41	1/1/15/20	6/37/115/115	-
34	LMT	M	104	-	-	8/21/61/61	0/2/2/2
27	SQD	a	409	-	-	13/49/69/69	0/1/1/1
23	CLA	c	508	41	1/1/15/20	9/37/115/115	-
33	HTG	B	621	-	-	4/10/30/30	0/1/1/1
23	CLA	C	509	-	1/1/15/20	7/37/115/115	-
32	LHG	d	407	-	-	17/53/53/53	-
32	LHG	D	409	-	-	16/53/53/53	-
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2
34	LMT	C	525	-	-	9/21/61/61	0/2/2/2
26	GOL	c	526	-	-	0/4/4/4	-
31	LMG	d	412	39	-	8/46/66/70	0/1/1/1
27	SQD	B	620	-	-	16/49/69/69	0/1/1/1
24	PHO	a	406	-	-	4/37/103/103	0/5/6/6
35	DGD	C	518	-	-	17/51/91/95	0/2/2/2
23	CLA	B	603	-	1/1/15/20	8/37/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
35	DGD	C	519	-	-	9/51/91/95	0/2/2/2
25	BCR	c	516	-	-	2/29/63/63	0/2/2/2
38	HEM	f	101	5,6	-	2/12/54/54	-
23	CLA	b	608	-	-	3/37/115/115	-
32	LHG	d	409	-	-	10/53/53/53	-
23	CLA	c	513	-	1/1/15/20	11/37/115/115	-
23	CLA	b	613	-	1/1/15/20	7/37/115/115	-
34	LMT	D	404	-	-	9/21/61/61	0/2/2/2
23	CLA	b	612	-	1/1/15/20	4/37/115/115	-
23	CLA	A	406	41	-	6/37/115/115	-
23	CLA	c	505	41	1/1/15/20	4/37/115/115	-
23	CLA	B	611	-	1/1/15/20	4/37/115/115	-
23	CLA	C	506	-	1/1/15/20	7/37/115/115	-
32	LHG	D	410	-	-	14/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	609	-	1/1/15/20	7/37/115/115	-
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
34	LMT	a	418	-	-	4/21/61/61	0/2/2/2
35	DGD	h	103	-	-	12/51/91/95	0/2/2/2
34	LMT	e	101	-	-	10/21/61/61	0/2/2/2
23	CLA	C	507	-	1/1/15/20	13/37/115/115	-
26	GOL	A	410	-	-	3/4/4/4	-
33	HTG	b	621	-	-	4/10/30/30	0/1/1/1
29	PL9	a	414	-	-	18/53/73/73	0/1/1/1
26	GOL	B	626	-	-	2/4/4/4	-
26	GOL	B	623	-	-	2/4/4/4	-
23	CLA	d	402	41	1/1/15/20	10/37/115/115	-
24	PHO	D	402	-	-	1/37/103/103	0/5/6/6
23	CLA	A	404	-	1/1/15/20	2/37/115/115	-
23	CLA	B	606	-	1/1/15/20	13/37/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	C	504	-	-	5/37/115/115	-
33	HTG	c	522	-	-	3/10/30/30	0/1/1/1
23	CLA	c	504	-	1/1/15/20	1/37/115/115	-
23	CLA	B	607	41	1/1/15/20	4/37/115/115	-
26	GOL	a	410	-	-	4/4/4/4	-
33	HTG	C	522	-	-	1/10/30/30	0/1/1/1
23	CLA	b	611	-	1/1/15/20	5/37/115/115	-
32	LHG	L	101	-	-	12/53/53/53	-
26	GOL	b	627	-	-	0/4/4/4	-
23	CLA	B	604	-	1/1/15/20	8/37/115/115	-
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
26	GOL	O	302	-	-	4/4/4/4	-
23	CLA	B	613	-	1/1/15/20	8/37/115/115	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
34	LMT	a	412	-	-	7/21/61/61	0/2/2/2
23	CLA	B	614	-	1/1/15/20	11/37/115/115	-
26	GOL	c	501	-	-	1/4/4/4	-
31	LMG	C	521	-	-	14/46/66/70	0/1/1/1
23	CLA	A	405	41	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	411	-	-	15/49/69/69	0/1/1/1
31	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
31	LMG	c	521	-	-	9/46/66/70	0/1/1/1
23	CLA	d	404	-	1/1/15/20	7/37/115/115	-
32	LHG	E	101	-	-	16/46/46/53	-
32	LHG	b	628	-	-	17/53/53/53	-
26	GOL	C	523	-	-	0/4/4/4	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
33	HTG	h	101	-	-	2/7/27/30	0/1/1/1
34	LMT	B	628	-	-	2/17/37/61	0/1/1/2
23	CLA	B	615	-	1/1/15/20	8/37/115/115	-
29	PL9	D	408	-	-	9/53/73/73	0/1/1/1
23	CLA	C	512	3	1/1/15/20	3/37/115/115	-
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/15/20	7/37/115/115	-
31	LMG	D	414	39	-	9/46/66/70	0/1/1/1

All (1324) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C3B-C2B	7.16	1.50	1.40
23	C	509	CLA	C3B-C2B	6.67	1.49	1.40
23	A	404	CLA	C3B-C2B	6.65	1.49	1.40
23	C	510	CLA	C3B-C2B	6.64	1.49	1.40
23	c	509	CLA	C3B-C2B	6.63	1.49	1.40
23	b	603	CLA	C3B-C2B	6.58	1.49	1.40
23	b	613	CLA	C3B-C2B	6.51	1.49	1.40
23	D	405	CLA	C3B-C2B	6.51	1.49	1.40
23	a	404	CLA	C3B-C2B	6.47	1.49	1.40
23	b	612	CLA	C3B-C2B	6.47	1.49	1.40
23	c	510	CLA	C3B-C2B	6.45	1.49	1.40
23	B	603	CLA	C3B-C2B	6.36	1.49	1.40
23	B	613	CLA	C3B-C2B	6.35	1.49	1.40
23	c	512	CLA	C3B-C2B	6.32	1.49	1.40
23	B	604	CLA	C3B-C2B	6.30	1.49	1.40
23	C	513	CLA	C3B-C2B	6.28	1.49	1.40
40	v	203	HEC	C2B-C3B	-6.26	1.34	1.40
23	b	614	CLA	C3B-C2B	6.26	1.49	1.40
23	C	512	CLA	C3B-C2B	6.24	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	PHO	C3B-C2B	6.23	1.49	1.40
23	b	609	CLA	C3B-C2B	6.20	1.49	1.40
23	c	503	CLA	C3B-C2B	6.17	1.48	1.40
23	b	604	CLA	C3B-C2B	6.14	1.48	1.40
24	D	402	PHO	C3B-C2B	6.13	1.48	1.40
23	B	612	CLA	C3B-C2B	6.11	1.48	1.40
23	b	602	CLA	C3B-C2B	6.09	1.48	1.40
24	A	407	PHO	C3B-C2B	6.09	1.48	1.40
23	b	611	CLA	C3B-C2B	6.07	1.48	1.40
23	B	601	CLA	C3B-C2B	6.05	1.48	1.40
23	d	403	CLA	C3B-C2B	6.04	1.48	1.40
23	C	511	CLA	C3B-C2B	6.02	1.48	1.40
24	a	406	PHO	C3D-C2D	6.00	1.50	1.39
23	c	507	CLA	C3B-C2B	5.98	1.48	1.40
23	b	601	CLA	C3B-C2B	5.98	1.48	1.40
40	V	201	HEC	C2B-C3B	-5.96	1.34	1.40
23	B	610	CLA	C3B-C2B	5.95	1.48	1.40
23	A	408	CLA	C3B-C2B	5.94	1.48	1.40
23	c	511	CLA	C3B-C2B	5.93	1.48	1.40
23	B	608	CLA	C3B-C2B	5.92	1.48	1.40
23	b	608	CLA	C3B-C2B	5.91	1.48	1.40
23	C	508	CLA	C3B-C2B	5.91	1.48	1.40
23	B	610	CLA	C3C-C2C	5.90	1.49	1.36
23	B	606	CLA	C3B-C2B	5.83	1.48	1.40
23	B	611	CLA	C3B-C2B	5.80	1.48	1.40
23	d	404	CLA	C1D-ND	5.79	1.44	1.37
23	C	514	CLA	C3B-C2B	5.79	1.48	1.40
24	a	416	PHO	C3B-C2B	5.78	1.48	1.40
23	c	514	CLA	C3B-C2B	5.77	1.48	1.40
23	C	509	CLA	C3C-C2C	5.76	1.49	1.36
23	C	503	CLA	C3B-C2B	5.71	1.48	1.40
23	b	616	CLA	C3B-C2B	5.68	1.48	1.40
23	C	502	CLA	C3B-C2B	5.68	1.48	1.40
23	d	402	CLA	C1D-ND	5.68	1.44	1.37
23	b	601	CLA	C3C-C2C	5.67	1.48	1.36
23	B	616	CLA	C3B-C2B	5.67	1.48	1.40
23	b	605	CLA	C3B-C2B	5.66	1.48	1.40
23	b	601	CLA	C1D-ND	5.66	1.44	1.37
23	C	513	CLA	C3C-C2C	5.65	1.48	1.36
23	B	602	CLA	CHC-C1C	5.64	1.49	1.35
23	B	614	CLA	C3C-C2C	5.61	1.48	1.36
23	C	505	CLA	C3B-C2B	5.60	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C3C-C2C	5.59	1.48	1.36
23	C	507	CLA	C3B-C2B	5.58	1.48	1.40
23	c	508	CLA	C1D-ND	5.58	1.44	1.37
24	D	402	PHO	C3D-C2D	5.57	1.49	1.39
23	c	509	CLA	C3C-C2C	5.56	1.48	1.36
23	b	610	CLA	C3B-C2B	5.56	1.48	1.40
40	v	203	HEC	C3D-C2D	5.55	1.54	1.37
23	B	602	CLA	C3B-C2B	5.55	1.48	1.40
23	B	601	CLA	C3C-C2C	5.55	1.48	1.36
23	b	606	CLA	C3B-C2B	5.51	1.48	1.40
23	b	607	CLA	C3C-C2C	5.51	1.48	1.36
23	b	613	CLA	C3C-C2C	5.51	1.48	1.36
23	D	406	CLA	C1D-ND	5.51	1.44	1.37
23	B	607	CLA	C3B-C2B	5.51	1.48	1.40
23	b	615	CLA	C3C-C2C	5.50	1.48	1.36
23	b	604	CLA	C1D-ND	5.48	1.44	1.37
23	B	614	CLA	C3B-C2B	5.48	1.48	1.40
23	b	613	CLA	C1D-ND	5.45	1.44	1.37
23	b	605	CLA	C3C-C2C	5.44	1.48	1.36
23	C	502	CLA	C3C-C2C	5.44	1.48	1.36
23	C	506	CLA	C3B-C2B	5.44	1.47	1.40
23	c	509	CLA	C1D-ND	5.43	1.44	1.37
23	b	606	CLA	C3C-C2C	5.43	1.48	1.36
23	c	514	CLA	C1D-ND	5.42	1.44	1.37
23	C	504	CLA	C3C-C2C	5.42	1.48	1.36
23	C	504	CLA	C1D-ND	5.41	1.44	1.37
23	a	407	CLA	C3B-C2B	5.41	1.47	1.40
23	c	502	CLA	C3B-C2B	5.41	1.47	1.40
23	A	406	CLA	C3C-C2C	5.41	1.48	1.36
23	c	508	CLA	CHC-C1C	5.40	1.48	1.35
23	d	404	CLA	CHC-C1C	5.40	1.48	1.35
23	C	512	CLA	O2D-CGD	5.40	1.46	1.33
23	A	408	CLA	C3C-C2C	5.39	1.48	1.36
23	C	506	CLA	CHC-C1C	5.39	1.48	1.35
23	d	402	CLA	C3C-C2C	5.38	1.48	1.36
23	B	602	CLA	C3C-C2C	5.38	1.48	1.36
23	c	513	CLA	C3C-C2C	5.38	1.48	1.36
23	a	407	CLA	CHC-C1C	5.36	1.48	1.35
23	A	405	CLA	C3C-C2C	5.36	1.48	1.36
23	b	609	CLA	CHC-C1C	5.36	1.48	1.35
23	a	407	CLA	C3C-C2C	5.36	1.48	1.36
23	B	603	CLA	C3C-C2C	5.36	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C1D-ND	5.35	1.44	1.37
23	b	612	CLA	C3C-C2C	5.35	1.48	1.36
24	a	416	PHO	C3D-C2D	5.35	1.49	1.39
23	D	405	CLA	C3C-C2C	5.35	1.48	1.36
23	C	504	CLA	C3B-C2B	5.34	1.47	1.40
23	C	510	CLA	C3C-C2C	5.33	1.48	1.36
23	c	504	CLA	C1D-ND	5.32	1.44	1.37
23	C	510	CLA	C1D-ND	5.32	1.44	1.37
23	C	508	CLA	C3C-C2C	5.32	1.48	1.36
25	d	405	BCR	C23-C22	-5.32	1.34	1.45
23	C	511	CLA	C1D-ND	5.32	1.44	1.37
23	B	605	CLA	C3C-C2C	5.32	1.48	1.36
23	b	614	CLA	O2D-CGD	5.31	1.46	1.33
23	C	506	CLA	C3C-C2C	5.31	1.48	1.36
23	b	602	CLA	O2D-CGD	5.30	1.46	1.33
40	V	201	HEC	C3C-C2C	-5.30	1.35	1.40
23	b	615	CLA	C1D-ND	5.30	1.44	1.37
23	B	605	CLA	CHC-C1C	5.29	1.48	1.35
23	a	404	CLA	C3C-C2C	5.29	1.48	1.36
23	b	603	CLA	C1D-ND	5.29	1.44	1.37
23	c	503	CLA	C3C-C2C	5.28	1.48	1.36
23	a	405	CLA	C3B-C2B	5.28	1.47	1.40
23	b	609	CLA	C3C-C2C	5.28	1.47	1.36
23	C	514	CLA	C1D-ND	5.28	1.44	1.37
23	C	503	CLA	CHC-C1C	5.28	1.48	1.35
23	c	509	CLA	O2D-CGD	5.27	1.46	1.33
23	C	513	CLA	C1D-ND	5.27	1.44	1.37
23	B	611	CLA	C3C-C2C	5.26	1.47	1.36
23	c	508	CLA	C3B-C2B	5.25	1.47	1.40
23	b	610	CLA	C3C-C2C	5.25	1.47	1.36
23	C	513	CLA	CHC-C1C	5.25	1.48	1.35
23	D	406	CLA	C3C-C2C	5.24	1.47	1.36
23	b	614	CLA	C3C-C2C	5.24	1.47	1.36
23	B	601	CLA	O2D-CGD	5.24	1.46	1.33
23	A	405	CLA	C3B-C2B	5.24	1.47	1.40
23	b	614	CLA	CHC-C1C	5.23	1.48	1.35
23	c	513	CLA	CHC-C1C	5.23	1.48	1.35
23	b	615	CLA	C3B-C2B	5.22	1.47	1.40
23	B	604	CLA	CHC-C1C	5.22	1.48	1.35
23	B	616	CLA	C3C-C2C	5.22	1.47	1.36
23	d	404	CLA	C3C-C2C	5.21	1.47	1.36
23	c	505	CLA	O2D-CGD	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C3C-C2C	5.20	1.47	1.36
23	d	404	CLA	C3B-C2B	5.20	1.47	1.40
23	c	504	CLA	C3C-C2C	5.20	1.47	1.36
23	B	601	CLA	C1D-ND	5.20	1.44	1.37
23	A	406	CLA	CHC-C1C	5.19	1.48	1.35
23	B	608	CLA	C3C-C2C	5.18	1.47	1.36
23	c	507	CLA	C1D-ND	5.18	1.44	1.37
23	c	512	CLA	C3C-C2C	5.18	1.47	1.36
23	b	603	CLA	C3C-C2C	5.18	1.47	1.36
23	C	509	CLA	CHC-C1C	5.18	1.48	1.35
23	c	514	CLA	CHC-C1C	5.17	1.48	1.35
25	k	101	BCR	C23-C22	-5.17	1.34	1.45
23	d	402	CLA	CHC-C1C	5.17	1.48	1.35
23	c	505	CLA	C3C-C2C	5.17	1.47	1.36
23	A	408	CLA	O2D-CGD	5.16	1.45	1.33
23	B	609	CLA	O2D-CGD	5.16	1.45	1.33
23	c	505	CLA	C1D-ND	5.15	1.44	1.37
23	B	602	CLA	C1D-ND	5.15	1.44	1.37
23	C	503	CLA	O2D-CGD	5.15	1.45	1.33
23	c	506	CLA	CHC-C1C	5.14	1.48	1.35
23	C	514	CLA	C3C-C2C	5.14	1.47	1.36
23	B	602	CLA	O2D-CGD	5.13	1.45	1.33
23	b	603	CLA	O2D-CGD	5.13	1.45	1.33
23	C	511	CLA	C3C-C2C	5.13	1.47	1.36
23	c	510	CLA	C3C-C2C	5.12	1.47	1.36
24	A	407	PHO	OBD-CAD	5.12	1.29	1.22
23	A	404	CLA	C3C-C2C	5.12	1.47	1.36
23	B	606	CLA	C1D-ND	5.11	1.44	1.37
23	c	503	CLA	O2D-CGD	5.11	1.45	1.33
23	B	616	CLA	CHC-C1C	5.11	1.48	1.35
23	b	602	CLA	CHC-C1C	5.11	1.48	1.35
23	c	514	CLA	C3C-C2C	5.10	1.47	1.36
23	b	616	CLA	C3C-C2C	5.10	1.47	1.36
23	d	402	CLA	C3B-C2B	5.10	1.47	1.40
23	C	511	CLA	CHC-C1C	5.10	1.48	1.35
23	C	507	CLA	C1D-ND	5.09	1.44	1.37
40	V	201	HEC	C3D-C2D	5.09	1.52	1.37
23	C	504	CLA	CHC-C1C	5.08	1.48	1.35
23	A	404	CLA	C1D-ND	5.08	1.44	1.37
23	C	505	CLA	CHC-C1C	5.08	1.48	1.35
23	a	407	CLA	C1D-ND	5.08	1.44	1.37
23	c	502	CLA	C3C-C2C	5.08	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	CHC-C1C	5.08	1.48	1.35
23	c	512	CLA	C1D-ND	5.08	1.44	1.37
23	C	502	CLA	CHC-C1C	5.08	1.48	1.35
23	B	605	CLA	C3B-C2B	5.07	1.47	1.40
23	c	512	CLA	CHC-C1C	5.07	1.48	1.35
25	K	101	BCR	C23-C22	-5.07	1.35	1.45
23	B	605	CLA	C1D-ND	5.07	1.44	1.37
23	B	615	CLA	C1D-ND	5.06	1.44	1.37
23	b	608	CLA	C3C-C2C	5.06	1.47	1.36
23	A	408	CLA	CHC-C1C	5.06	1.47	1.35
23	b	615	CLA	O2D-CGD	5.05	1.45	1.33
23	C	503	CLA	C3C-C2C	5.04	1.47	1.36
23	c	513	CLA	C3B-C2B	5.04	1.47	1.40
23	c	514	CLA	O2D-CGD	5.04	1.45	1.33
23	B	615	CLA	CHC-C1C	5.04	1.47	1.35
23	b	610	CLA	CHC-C1C	5.03	1.47	1.35
23	B	611	CLA	O2D-CGD	5.03	1.45	1.33
23	c	506	CLA	C3B-C2B	5.02	1.47	1.40
23	c	513	CLA	O2D-CGD	5.02	1.45	1.33
23	a	405	CLA	CHC-C1C	5.02	1.47	1.35
25	c	516	BCR	C23-C22	-5.02	1.35	1.45
23	B	606	CLA	C3C-C2C	5.02	1.47	1.36
24	A	407	PHO	C3D-C2D	5.02	1.48	1.39
23	C	508	CLA	CHC-C1C	5.01	1.47	1.35
23	B	603	CLA	CHC-C1C	5.01	1.47	1.35
23	b	606	CLA	C1D-ND	5.01	1.43	1.37
23	B	601	CLA	CHC-C1C	5.01	1.47	1.35
23	c	502	CLA	C1D-ND	5.01	1.43	1.37
23	b	613	CLA	O2D-CGD	5.01	1.45	1.33
23	C	507	CLA	C3C-C2C	5.01	1.47	1.36
23	b	615	CLA	CHC-C1C	5.00	1.47	1.35
23	c	503	CLA	CHC-C1C	5.00	1.47	1.35
23	c	508	CLA	O2D-CGD	5.00	1.45	1.33
23	B	607	CLA	CHC-C1C	5.00	1.47	1.35
23	b	613	CLA	CHC-C1C	5.00	1.47	1.35
25	b	617	BCR	C23-C22	-4.99	1.35	1.45
25	b	619	BCR	C23-C22	-4.99	1.35	1.45
23	c	511	CLA	C3C-C2C	4.99	1.47	1.36
23	b	608	CLA	CHC-C1C	4.99	1.47	1.35
23	B	611	CLA	C1D-ND	4.99	1.43	1.37
23	c	507	CLA	O2D-CGD	4.98	1.45	1.33
23	b	616	CLA	CHC-C1C	4.98	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	406	CLA	O2D-CGD	4.98	1.45	1.33
23	B	613	CLA	CHC-C1C	4.98	1.47	1.35
23	b	604	CLA	CHC-C1C	4.98	1.47	1.35
23	b	603	CLA	CHC-C1C	4.98	1.47	1.35
23	b	616	CLA	C1D-ND	4.98	1.43	1.37
24	A	407	PHO	O2D-CGD	4.97	1.45	1.33
23	c	502	CLA	CHC-C1C	4.97	1.47	1.35
23	c	506	CLA	O2D-CGD	4.97	1.45	1.33
24	a	416	PHO	O2D-CGD	4.97	1.45	1.33
23	C	507	CLA	O2D-CGD	4.97	1.45	1.33
23	B	605	CLA	O2D-CGD	4.96	1.45	1.33
23	B	604	CLA	C3C-C2C	4.96	1.47	1.36
23	b	602	CLA	C3C-C2C	4.96	1.47	1.36
23	c	510	CLA	O2D-CGD	4.96	1.45	1.33
23	B	615	CLA	C3C-C2C	4.96	1.47	1.36
23	C	514	CLA	CHC-C1C	4.96	1.47	1.35
23	c	504	CLA	C3B-C2B	4.96	1.47	1.40
23	b	616	CLA	O2D-CGD	4.96	1.45	1.33
23	c	504	CLA	CHC-C1C	4.95	1.47	1.35
23	c	507	CLA	CHC-C1C	4.95	1.47	1.35
23	A	406	CLA	C3B-C2B	4.95	1.47	1.40
23	c	509	CLA	CHC-C1C	4.95	1.47	1.35
23	a	404	CLA	C1D-ND	4.95	1.43	1.37
23	b	606	CLA	CHC-C1C	4.94	1.47	1.35
23	B	608	CLA	CHC-C1C	4.94	1.47	1.35
23	D	406	CLA	CHC-C1C	4.93	1.47	1.35
23	B	610	CLA	CHC-C1C	4.93	1.47	1.35
23	B	603	CLA	O2D-CGD	4.93	1.45	1.33
24	D	402	PHO	O2D-CGD	4.93	1.45	1.33
23	D	405	CLA	CHC-C1C	4.93	1.47	1.35
23	c	511	CLA	C1D-ND	4.92	1.43	1.37
23	A	405	CLA	CHC-C1C	4.92	1.47	1.35
23	A	405	CLA	O2D-CGD	4.92	1.45	1.33
23	b	612	CLA	C1D-ND	4.92	1.43	1.37
23	b	604	CLA	C3C-C2C	4.92	1.47	1.36
23	b	611	CLA	C3C-C2C	4.92	1.47	1.36
25	C	515	BCR	C23-C22	-4.92	1.35	1.45
23	C	512	CLA	C1D-ND	4.92	1.43	1.37
23	b	609	CLA	O2D-CGD	4.91	1.45	1.33
23	B	607	CLA	C3C-C2C	4.91	1.47	1.36
23	a	405	CLA	C3C-C2C	4.91	1.47	1.36
23	B	614	CLA	C1D-ND	4.91	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3C-C2C	4.91	1.47	1.36
23	D	406	CLA	C3B-C2B	4.90	1.47	1.40
23	B	609	CLA	CHC-C1C	4.90	1.47	1.35
23	B	613	CLA	C1D-ND	4.90	1.43	1.37
23	C	510	CLA	CHC-C1C	4.90	1.47	1.35
23	b	610	CLA	O2D-CGD	4.89	1.45	1.33
23	a	404	CLA	CHC-C1C	4.89	1.47	1.35
23	b	601	CLA	O2D-CGD	4.89	1.45	1.33
23	C	507	CLA	CHC-C1C	4.89	1.47	1.35
23	A	406	CLA	O2D-CGD	4.89	1.45	1.33
23	B	609	CLA	C3C-C2C	4.88	1.47	1.36
23	A	405	CLA	C1D-ND	4.88	1.43	1.37
23	b	608	CLA	O2D-CGD	4.88	1.45	1.33
25	H	101	BCR	C23-C22	-4.87	1.35	1.45
23	B	606	CLA	CHC-C1C	4.87	1.47	1.35
23	A	404	CLA	CHC-C1C	4.87	1.47	1.35
23	C	512	CLA	CHC-C1C	4.86	1.47	1.35
23	b	611	CLA	CHC-C1C	4.85	1.47	1.35
23	c	511	CLA	CHC-C1C	4.84	1.47	1.35
25	k	102	BCR	C23-C22	-4.84	1.35	1.45
23	c	505	CLA	CHC-C1C	4.84	1.47	1.35
23	C	511	CLA	O2D-CGD	4.84	1.45	1.33
23	C	507	CLA	CHD-C1D	4.84	1.47	1.38
23	B	612	CLA	CHC-C1C	4.83	1.47	1.35
23	b	605	CLA	C1D-ND	4.83	1.43	1.37
23	c	510	CLA	CHC-C1C	4.83	1.47	1.35
23	d	402	CLA	O2D-CGD	4.82	1.45	1.33
24	a	406	PHO	O2D-CGD	4.81	1.44	1.33
23	C	505	CLA	O2D-CGD	4.81	1.44	1.33
25	B	619	BCR	C23-C22	-4.80	1.35	1.45
23	B	616	CLA	C1D-ND	4.80	1.43	1.37
23	c	513	CLA	C1D-ND	4.79	1.43	1.37
23	b	602	CLA	C1D-ND	4.79	1.43	1.37
23	C	510	CLA	O2D-CGD	4.79	1.44	1.33
23	B	611	CLA	CHC-C1C	4.79	1.47	1.35
23	d	403	CLA	C3C-C2C	4.79	1.46	1.36
23	B	616	CLA	O2D-CGD	4.78	1.44	1.33
23	B	615	CLA	O2D-CGD	4.78	1.44	1.33
23	C	512	CLA	C3C-C2C	4.77	1.46	1.36
23	C	509	CLA	C1D-ND	4.76	1.43	1.37
23	b	611	CLA	O2D-CGD	4.76	1.44	1.33
23	B	609	CLA	C3B-C2B	4.76	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CHC-C1C	4.76	1.47	1.35
25	T	101	BCR	C23-C22	-4.76	1.35	1.45
23	C	508	CLA	O2D-CGD	4.75	1.44	1.33
23	d	403	CLA	CHC-C1C	4.75	1.47	1.35
23	C	502	CLA	C1D-ND	4.74	1.43	1.37
23	b	604	CLA	O2D-CGD	4.74	1.44	1.33
23	c	508	CLA	C3C-C2C	4.73	1.46	1.36
23	b	607	CLA	C1D-ND	4.73	1.43	1.37
23	b	612	CLA	CHC-C1C	4.73	1.47	1.35
23	B	610	CLA	C1D-ND	4.72	1.43	1.37
23	B	609	CLA	C1D-ND	4.72	1.43	1.37
25	c	515	BCR	C23-C22	-4.72	1.35	1.45
23	B	604	CLA	O2D-CGD	4.72	1.44	1.33
23	b	607	CLA	C3B-C2B	4.72	1.46	1.40
23	C	504	CLA	O2D-CGD	4.72	1.44	1.33
23	B	613	CLA	C3C-C2C	4.72	1.46	1.36
23	C	506	CLA	O2D-CGD	4.71	1.44	1.33
23	A	408	CLA	C1D-ND	4.71	1.43	1.37
23	a	407	CLA	O2D-CGD	4.71	1.44	1.33
23	b	607	CLA	CHC-C1C	4.71	1.47	1.35
23	c	503	CLA	C1D-ND	4.70	1.43	1.37
23	b	601	CLA	CHD-C1D	4.70	1.47	1.38
23	b	605	CLA	CHC-C1C	4.69	1.47	1.35
23	b	607	CLA	O2D-CGD	4.69	1.44	1.33
23	b	614	CLA	C1D-ND	4.69	1.43	1.37
23	B	613	CLA	O2D-CGD	4.67	1.44	1.33
23	B	601	CLA	O2A-CGA	4.67	1.47	1.33
25	b	618	BCR	C23-C22	-4.66	1.35	1.45
23	B	612	CLA	O2D-CGD	4.66	1.44	1.33
23	C	513	CLA	O2D-CGD	4.65	1.44	1.33
23	b	610	CLA	C1D-ND	4.65	1.43	1.37
40	v	203	HEC	C3C-C2C	-4.65	1.35	1.40
23	B	612	CLA	C3C-C2C	4.65	1.46	1.36
23	C	503	CLA	C1D-ND	4.65	1.43	1.37
23	c	514	CLA	CHD-C1D	4.65	1.47	1.38
25	B	617	BCR	C23-C22	-4.64	1.36	1.45
23	c	512	CLA	O2D-CGD	4.64	1.44	1.33
23	d	403	CLA	O2D-CGD	4.64	1.44	1.33
23	a	405	CLA	O2D-CGD	4.63	1.44	1.33
25	t	102	BCR	C23-C22	-4.63	1.36	1.45
23	b	612	CLA	O2D-CGD	4.62	1.44	1.33
25	h	102	BCR	C23-C22	-4.62	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C1D-ND	4.62	1.43	1.37
23	C	508	CLA	C1D-ND	4.62	1.43	1.37
25	D	407	BCR	C23-C22	-4.61	1.36	1.45
23	c	507	CLA	CHD-C1D	4.61	1.47	1.38
23	b	601	CLA	O2A-CGA	4.61	1.46	1.33
23	c	502	CLA	O2D-CGD	4.60	1.44	1.33
23	d	404	CLA	O2D-CGD	4.59	1.44	1.33
23	C	509	CLA	O2D-CGD	4.59	1.44	1.33
23	a	404	CLA	O2D-CGD	4.58	1.44	1.33
23	C	514	CLA	O2D-CGD	4.58	1.44	1.33
23	c	504	CLA	O2D-CGD	4.57	1.44	1.33
23	B	606	CLA	O2D-CGD	4.56	1.44	1.33
23	b	605	CLA	O2D-CGD	4.55	1.44	1.33
25	C	516	BCR	C23-C22	-4.54	1.36	1.45
23	A	406	CLA	CHD-C1D	4.54	1.47	1.38
25	a	408	BCR	C23-C22	-4.52	1.36	1.45
24	D	402	PHO	OBD-CAD	4.52	1.28	1.22
24	a	406	PHO	OBD-CAD	4.52	1.28	1.22
23	B	615	CLA	C3B-C2B	4.51	1.46	1.40
23	C	510	CLA	CHD-C1D	4.51	1.47	1.38
23	B	602	CLA	CHD-C1D	4.51	1.47	1.38
27	A	411	SQD	O48-C23	4.51	1.46	1.33
23	b	602	CLA	CHD-C1D	4.50	1.47	1.38
23	b	609	CLA	C1D-ND	4.49	1.43	1.37
23	A	404	CLA	O2D-CGD	4.49	1.44	1.33
23	b	611	CLA	C1D-ND	4.49	1.43	1.37
23	B	605	CLA	CHD-C1D	4.49	1.47	1.38
23	c	511	CLA	O2D-CGD	4.49	1.44	1.33
23	A	408	CLA	CHD-C1D	4.48	1.47	1.38
23	B	603	CLA	C1D-ND	4.48	1.43	1.37
25	A	409	BCR	C23-C22	-4.48	1.36	1.45
23	C	513	CLA	CHD-C1D	4.47	1.47	1.38
27	D	415	SQD	O47-C7	4.47	1.46	1.34
23	d	404	CLA	O2A-CGA	4.45	1.46	1.33
23	d	404	CLA	CHD-C1D	4.45	1.47	1.38
32	E	101	LHG	O8-C23	4.45	1.46	1.33
23	C	505	CLA	C1D-ND	4.45	1.43	1.37
23	c	506	CLA	CHD-C1D	4.43	1.47	1.38
23	c	506	CLA	C1D-ND	4.43	1.43	1.37
23	c	504	CLA	CHD-C1D	4.43	1.47	1.38
23	B	608	CLA	O2D-CGD	4.43	1.44	1.33
23	c	513	CLA	O2A-CGA	4.43	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	O2A-CGA	4.42	1.46	1.33
23	b	608	CLA	C1D-ND	4.41	1.43	1.37
31	C	520	LMG	O8-C28	4.41	1.46	1.33
23	B	615	CLA	C3D-C2D	4.41	1.51	1.39
23	b	611	CLA	O2A-CGA	4.41	1.46	1.33
31	C	521	LMG	O8-C28	4.40	1.46	1.33
31	C	521	LMG	O7-C10	4.40	1.46	1.34
23	C	502	CLA	O2D-CGD	4.39	1.43	1.33
31	z	101	LMG	O8-C28	4.38	1.46	1.33
32	a	419	LHG	O8-C23	4.38	1.46	1.33
23	D	405	CLA	O2D-CGD	4.38	1.43	1.33
23	d	402	CLA	C3D-C2D	4.37	1.51	1.39
23	c	513	CLA	CHD-C1D	4.37	1.46	1.38
23	b	612	CLA	CHD-C1D	4.37	1.46	1.38
23	C	506	CLA	CHD-C1D	4.37	1.46	1.38
31	c	520	LMG	O8-C28	4.37	1.46	1.33
23	B	609	CLA	O2A-CGA	4.36	1.46	1.33
23	a	407	CLA	O2A-CGA	4.36	1.46	1.33
35	c	517	DGD	O1G-C1A	4.36	1.46	1.33
31	Z	101	LMG	O7-C10	4.35	1.46	1.34
23	B	609	CLA	CHD-C1D	4.34	1.46	1.38
23	b	602	CLA	O2A-CGA	4.34	1.46	1.33
23	B	614	CLA	O2D-CGD	4.34	1.43	1.33
27	B	620	SQD	O47-C7	4.34	1.46	1.34
31	m	101	LMG	O8-C28	4.34	1.46	1.33
35	c	519	DGD	O1G-C1A	4.33	1.46	1.33
32	a	419	LHG	O7-C7	4.33	1.46	1.34
31	C	520	LMG	O7-C10	4.32	1.46	1.34
23	b	603	CLA	CHD-C1D	4.32	1.46	1.38
23	c	508	CLA	CHD-C4C	4.31	1.49	1.39
27	f	102	SQD	O47-C7	4.31	1.46	1.34
23	B	606	CLA	CHD-C1D	4.30	1.46	1.38
23	b	601	CLA	CHD-C4C	4.30	1.49	1.39
31	c	521	LMG	O8-C28	4.30	1.45	1.33
23	b	608	CLA	CHD-C1D	4.30	1.46	1.38
27	L	102	SQD	O48-C23	4.29	1.45	1.33
23	a	404	CLA	CHD-C1D	4.28	1.46	1.38
31	c	521	LMG	O7-C10	4.28	1.46	1.34
23	C	507	CLA	O2A-CGA	4.28	1.45	1.33
23	B	607	CLA	O2D-CGD	4.28	1.43	1.33
23	B	607	CLA	C1D-ND	4.28	1.43	1.37
23	d	402	CLA	O2A-CGA	4.27	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	CHD-C1D	4.27	1.46	1.38
23	d	402	CLA	CHD-C1D	4.27	1.46	1.38
23	c	509	CLA	O2A-CGA	4.27	1.45	1.33
24	a	416	PHO	OBD-CAD	4.26	1.28	1.22
23	b	609	CLA	CHD-C1D	4.26	1.46	1.38
27	A	411	SQD	O47-C7	4.26	1.46	1.34
23	c	514	CLA	O2A-CGA	4.25	1.45	1.33
23	c	514	CLA	CHD-C4C	4.25	1.48	1.39
27	a	411	SQD	O48-C23	4.25	1.45	1.33
23	c	508	CLA	CHD-C1D	4.24	1.46	1.38
23	b	613	CLA	C3D-C2D	4.24	1.50	1.39
23	b	615	CLA	CHD-C1D	4.24	1.46	1.38
23	b	606	CLA	O2D-CGD	4.24	1.43	1.33
23	c	509	CLA	CHD-C1D	4.24	1.46	1.38
23	c	507	CLA	CHD-C4C	4.24	1.48	1.39
23	c	508	CLA	O2A-CGA	4.24	1.45	1.33
31	d	412	LMG	O8-C28	4.22	1.45	1.33
23	b	608	CLA	O2A-CGA	4.22	1.45	1.33
23	C	514	CLA	O2A-CGA	4.21	1.45	1.33
23	C	513	CLA	O2A-CGA	4.21	1.45	1.33
27	B	620	SQD	O48-C23	4.21	1.45	1.33
23	A	408	CLA	O2A-CGA	4.21	1.45	1.33
23	c	510	CLA	CHD-C1D	4.21	1.46	1.38
31	A	415	LMG	O8-C28	4.21	1.45	1.33
23	D	405	CLA	CHD-C4C	4.20	1.48	1.39
23	d	404	CLA	CHD-C4C	4.20	1.48	1.39
23	B	601	CLA	CHD-C1D	4.20	1.46	1.38
23	D	405	CLA	O2A-CGA	4.20	1.45	1.33
23	C	512	CLA	O2A-CGA	4.20	1.45	1.33
25	Y	101	BCR	C23-C22	-4.19	1.36	1.45
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
23	C	509	CLA	O2A-CGA	4.18	1.45	1.33
27	L	102	SQD	O47-C7	4.18	1.46	1.34
23	A	405	CLA	CHD-C1D	4.18	1.46	1.38
23	B	604	CLA	C1D-ND	4.18	1.42	1.37
23	C	503	CLA	CHD-C1D	4.17	1.46	1.38
23	b	601	CLA	C3D-C2D	4.17	1.50	1.39
23	B	606	CLA	O2A-CGA	4.17	1.45	1.33
35	C	517	DGD	O1G-C1A	4.16	1.45	1.33
32	E	101	LHG	O7-C7	4.16	1.46	1.34
35	c	517	DGD	O2G-C1B	4.16	1.46	1.34
23	C	506	CLA	C1D-ND	4.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	CHD-C4C	4.15	1.48	1.39
32	L	101	LHG	O8-C23	4.15	1.45	1.33
23	c	510	CLA	O2A-CGA	4.15	1.45	1.33
23	c	508	CLA	OBD-CAD	4.15	1.29	1.22
27	a	411	SQD	O47-C7	4.14	1.46	1.34
32	b	628	LHG	O7-C7	4.14	1.46	1.34
32	d	409	LHG	O7-C7	4.14	1.46	1.34
23	d	404	CLA	C3D-C2D	4.14	1.50	1.39
23	B	608	CLA	CHD-C1D	4.14	1.46	1.38
23	C	502	CLA	CHD-C1D	4.14	1.46	1.38
23	a	404	CLA	CHD-C4C	4.13	1.48	1.39
23	B	610	CLA	O2D-CGD	4.13	1.43	1.33
35	h	103	DGD	O1G-C1A	4.13	1.45	1.33
23	C	508	CLA	CHD-C1D	4.13	1.46	1.38
23	B	603	CLA	O2A-CGA	4.13	1.45	1.33
23	b	607	CLA	CHD-C1D	4.12	1.46	1.38
23	D	405	CLA	CHD-C1D	4.12	1.46	1.38
24	A	407	PHO	O2A-CGA	4.12	1.45	1.33
23	a	405	CLA	C1D-ND	4.11	1.42	1.37
23	C	509	CLA	C3D-C2D	4.11	1.50	1.39
32	b	628	LHG	O8-C23	4.09	1.45	1.33
31	a	417	LMG	O8-C28	4.09	1.45	1.33
23	A	405	CLA	O2A-CGA	4.09	1.45	1.33
23	D	406	CLA	CHD-C1D	4.09	1.46	1.38
23	c	512	CLA	CHD-C1D	4.09	1.46	1.38
27	a	409	SQD	O47-C7	4.08	1.45	1.34
35	c	518	DGD	O1G-C1A	4.08	1.45	1.33
31	z	101	LMG	O7-C10	4.08	1.45	1.34
23	c	503	CLA	O2A-CGA	4.08	1.45	1.33
23	b	602	CLA	CHD-C4C	4.08	1.48	1.39
23	B	615	CLA	O2A-CGA	4.07	1.45	1.33
32	d	409	LHG	O8-C23	4.07	1.45	1.33
23	B	612	CLA	O2A-CGA	4.07	1.45	1.33
27	f	102	SQD	O48-C23	4.07	1.45	1.33
23	B	610	CLA	CHD-C1D	4.07	1.46	1.38
35	C	519	DGD	O1G-C1A	4.07	1.45	1.33
23	C	502	CLA	O2A-CGA	4.07	1.45	1.33
23	c	511	CLA	CHD-C4C	4.07	1.48	1.39
23	B	613	CLA	CHD-C1D	4.06	1.46	1.38
31	c	520	LMG	O7-C10	4.06	1.45	1.34
23	C	505	CLA	O2A-CGA	4.06	1.45	1.33
23	B	610	CLA	CHD-C4C	4.06	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	518	DGD	O1G-C1A	4.06	1.45	1.33
23	b	614	CLA	O2A-CGA	4.06	1.45	1.33
27	D	415	SQD	O48-C23	4.06	1.45	1.33
23	b	604	CLA	CHD-C1D	4.06	1.46	1.38
27	a	409	SQD	O48-C23	4.06	1.45	1.33
23	b	612	CLA	O2A-CGA	4.05	1.45	1.33
23	c	511	CLA	CHD-C1D	4.05	1.46	1.38
35	h	103	DGD	O2G-C1B	4.05	1.45	1.34
23	c	510	CLA	CHD-C4C	4.05	1.48	1.39
23	c	502	CLA	CHD-C4C	4.04	1.48	1.39
23	c	502	CLA	O2A-CGA	4.04	1.45	1.33
23	C	503	CLA	C3D-C2D	4.04	1.50	1.39
23	C	504	CLA	O2A-CGA	4.04	1.45	1.33
23	A	406	CLA	CHD-C4C	4.04	1.48	1.39
31	A	415	LMG	O7-C10	4.04	1.45	1.34
23	a	405	CLA	O2A-CGA	4.04	1.45	1.33
23	B	613	CLA	O2A-CGA	4.04	1.45	1.33
23	d	403	CLA	O2A-CGA	4.03	1.45	1.33
23	B	604	CLA	CHD-C1D	4.03	1.46	1.38
23	C	513	CLA	C3D-C2D	4.03	1.50	1.39
23	C	511	CLA	C3D-C2D	4.03	1.50	1.39
23	a	404	CLA	OBD-CAD	4.02	1.29	1.22
23	b	614	CLA	CHD-C1D	4.02	1.46	1.38
23	c	505	CLA	CHD-C1D	4.02	1.46	1.38
23	C	510	CLA	CHD-C4C	4.02	1.48	1.39
23	c	506	CLA	O2A-CGA	4.01	1.45	1.33
23	C	510	CLA	O2A-CGA	4.01	1.45	1.33
23	C	512	CLA	CHD-C4C	4.01	1.48	1.39
23	A	405	CLA	C3D-C2D	4.01	1.50	1.39
23	C	510	CLA	OBD-CAD	4.01	1.29	1.22
23	c	505	CLA	C3D-C2D	4.00	1.50	1.39
23	c	504	CLA	O2A-CGA	4.00	1.45	1.33
23	c	505	CLA	O2A-CGA	4.00	1.45	1.33
23	c	504	CLA	CHD-C4C	3.99	1.48	1.39
23	c	506	CLA	CHD-C4C	3.99	1.48	1.39
27	C	501	SQD	O48-C23	3.99	1.45	1.33
23	D	406	CLA	OBD-CAD	3.99	1.29	1.22
23	b	608	CLA	CHD-C4C	3.98	1.48	1.39
23	B	615	CLA	OBD-CAD	3.98	1.29	1.22
31	a	417	LMG	O7-C10	3.98	1.45	1.34
23	C	512	CLA	CHD-C1D	3.98	1.46	1.38
23	b	613	CLA	CHD-C1D	3.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C3D-C2D	3.97	1.50	1.39
23	a	404	CLA	C3D-C2D	3.97	1.50	1.39
23	b	603	CLA	OBD-CAD	3.97	1.29	1.22
23	b	610	CLA	CHD-C1D	3.97	1.46	1.38
23	B	602	CLA	CHD-C4C	3.97	1.48	1.39
32	D	410	LHG	O7-C7	3.96	1.45	1.34
23	C	505	CLA	C3D-C2D	3.96	1.49	1.39
31	M	101	LMG	O8-C28	3.96	1.44	1.33
35	C	518	DGD	O2G-C1B	3.96	1.45	1.34
23	C	514	CLA	C3D-C2D	3.96	1.49	1.39
24	D	402	PHO	C3C-C2C	3.96	1.49	1.37
23	c	503	CLA	CHD-C1D	3.96	1.46	1.38
32	L	101	LHG	O7-C7	3.95	1.45	1.34
23	C	514	CLA	CHD-C4C	3.95	1.48	1.39
23	b	606	CLA	CHD-C1D	3.95	1.46	1.38
23	b	616	CLA	CHD-C1D	3.95	1.46	1.38
23	b	615	CLA	CHD-C4C	3.94	1.48	1.39
23	c	514	CLA	C3D-C2D	3.94	1.49	1.39
24	a	406	PHO	C3C-C2C	3.94	1.49	1.37
32	d	408	LHG	O7-C7	3.94	1.45	1.34
23	C	504	CLA	CHD-C4C	3.94	1.48	1.39
23	B	611	CLA	C3D-C2D	3.93	1.49	1.39
23	B	616	CLA	O2A-CGA	3.93	1.44	1.33
24	a	416	PHO	O2A-CGA	3.93	1.44	1.33
23	b	609	CLA	CHD-C4C	3.93	1.48	1.39
23	B	607	CLA	CHD-C4C	3.93	1.48	1.39
23	c	509	CLA	C3D-C2D	3.92	1.49	1.39
23	b	602	CLA	C3D-C2D	3.92	1.49	1.39
23	c	509	CLA	CHD-C4C	3.92	1.48	1.39
23	b	615	CLA	O2A-CGA	3.92	1.44	1.33
23	D	406	CLA	C3D-C2D	3.92	1.49	1.39
31	M	101	LMG	O7-C10	3.91	1.45	1.34
23	C	505	CLA	CHD-C1D	3.91	1.46	1.38
23	b	605	CLA	OBD-CAD	3.91	1.29	1.22
23	C	510	CLA	C3D-C2D	3.91	1.49	1.39
23	d	402	CLA	CHD-C4C	3.91	1.48	1.39
23	C	513	CLA	CHD-C4C	3.91	1.48	1.39
23	B	610	CLA	OBD-CAD	3.90	1.29	1.22
23	c	502	CLA	CHD-C1D	3.89	1.45	1.38
23	C	503	CLA	O2A-CGA	3.89	1.44	1.33
23	B	607	CLA	CHD-C1D	3.89	1.45	1.38
23	a	405	CLA	C3D-C2D	3.89	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	O2A-CGA	3.89	1.44	1.33
23	b	609	CLA	C3D-C2D	3.88	1.49	1.39
31	d	412	LMG	O7-C10	3.88	1.45	1.34
23	c	512	CLA	CHD-C4C	3.88	1.48	1.39
35	C	519	DGD	O2G-C1B	3.88	1.45	1.34
35	C	517	DGD	O2G-C1B	3.88	1.45	1.34
23	c	503	CLA	C3D-C2D	3.88	1.49	1.39
23	C	506	CLA	CHD-C4C	3.88	1.48	1.39
23	B	614	CLA	O2A-CGA	3.86	1.44	1.33
23	c	509	CLA	OBD-CAD	3.86	1.29	1.22
23	c	513	CLA	C3D-C2D	3.86	1.49	1.39
23	C	508	CLA	CHD-C4C	3.86	1.48	1.39
23	C	511	CLA	O2A-CGA	3.86	1.44	1.33
27	C	501	SQD	O47-C7	3.86	1.45	1.34
23	B	601	CLA	C3D-C2D	3.86	1.49	1.39
23	b	606	CLA	OBD-CAD	3.85	1.29	1.22
23	C	509	CLA	CHD-C1D	3.85	1.45	1.38
23	c	513	CLA	CHD-C4C	3.85	1.48	1.39
23	b	603	CLA	CHD-C4C	3.85	1.48	1.39
23	b	610	CLA	CHD-C4C	3.85	1.48	1.39
23	C	504	CLA	C3D-C2D	3.85	1.49	1.39
32	D	409	LHG	O8-C23	3.85	1.44	1.33
23	B	609	CLA	CHD-C4C	3.85	1.48	1.39
23	a	407	CLA	CHD-C4C	3.84	1.48	1.39
23	D	406	CLA	O2A-CGA	3.84	1.44	1.33
23	b	611	CLA	CHD-C4C	3.84	1.48	1.39
23	A	406	CLA	C1D-ND	3.84	1.42	1.37
23	c	508	CLA	C3D-C2D	3.83	1.49	1.39
23	B	607	CLA	O2A-CGA	3.83	1.44	1.33
35	c	518	DGD	O2G-C1B	3.83	1.45	1.34
32	A	416	LHG	O7-C7	3.83	1.45	1.34
23	B	608	CLA	CHD-C4C	3.83	1.48	1.39
31	m	101	LMG	O7-C10	3.83	1.45	1.34
23	b	613	CLA	CHD-C4C	3.82	1.48	1.39
23	a	407	CLA	CHD-C1D	3.82	1.45	1.38
23	B	604	CLA	O2A-CGA	3.82	1.44	1.33
23	b	604	CLA	O2A-CGA	3.82	1.44	1.33
23	c	505	CLA	CHD-C4C	3.82	1.47	1.39
23	C	511	CLA	CHD-C1D	3.81	1.45	1.38
23	c	512	CLA	C3D-C2D	3.81	1.49	1.39
23	c	507	CLA	C3D-C2D	3.80	1.49	1.39
23	C	511	CLA	CHD-C4C	3.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C3D-C2D	3.80	1.49	1.39
23	B	601	CLA	CHD-C4C	3.80	1.47	1.39
23	b	615	CLA	C3D-C2D	3.79	1.49	1.39
23	C	505	CLA	CHD-C4C	3.79	1.47	1.39
23	C	505	CLA	OBD-CAD	3.79	1.29	1.22
23	B	616	CLA	C3D-C2D	3.79	1.49	1.39
23	B	608	CLA	O2A-CGA	3.79	1.44	1.33
23	B	611	CLA	O2A-CGA	3.79	1.44	1.33
24	a	406	PHO	O2A-CGA	3.78	1.44	1.33
23	A	406	CLA	O2A-CGA	3.78	1.44	1.33
23	b	610	CLA	C3D-C2D	3.78	1.49	1.39
23	B	605	CLA	C3D-C2D	3.78	1.49	1.39
23	C	508	CLA	C3D-C2D	3.78	1.49	1.39
23	c	506	CLA	C3D-C2D	3.78	1.49	1.39
23	b	608	CLA	C3D-C2D	3.78	1.49	1.39
23	b	616	CLA	O2A-CGA	3.77	1.44	1.33
32	D	410	LHG	O8-C23	3.77	1.44	1.33
32	d	407	LHG	O8-C23	3.76	1.44	1.33
23	c	510	CLA	C3D-C2D	3.76	1.49	1.39
23	b	614	CLA	C3D-C2D	3.76	1.49	1.39
32	A	416	LHG	O8-C23	3.76	1.44	1.33
23	c	502	CLA	C3D-C2D	3.76	1.49	1.39
23	B	605	CLA	O2A-CGA	3.76	1.44	1.33
32	d	408	LHG	O8-C23	3.75	1.44	1.33
23	b	605	CLA	CHD-C1D	3.75	1.45	1.38
23	b	611	CLA	CHD-C1D	3.75	1.45	1.38
23	a	405	CLA	OBD-CAD	3.75	1.28	1.22
23	B	610	CLA	C3D-C2D	3.75	1.49	1.39
23	b	603	CLA	O2A-CGA	3.75	1.44	1.33
23	b	606	CLA	O2A-CGA	3.74	1.44	1.33
23	C	502	CLA	CHD-C4C	3.74	1.47	1.39
31	D	414	LMG	O8-C28	3.74	1.44	1.33
23	b	616	CLA	C3D-C2D	3.74	1.49	1.39
23	A	408	CLA	CHD-C4C	3.73	1.47	1.39
23	c	507	CLA	O2A-CGA	3.73	1.44	1.33
23	b	613	CLA	O2A-CGA	3.73	1.44	1.33
23	b	613	CLA	OBD-CAD	3.73	1.28	1.22
35	c	519	DGD	O2G-C1B	3.72	1.44	1.34
23	B	605	CLA	CHD-C4C	3.71	1.47	1.39
23	b	612	CLA	C3D-C2D	3.71	1.49	1.39
35	H	102	DGD	O1G-C1A	3.71	1.44	1.33
23	b	616	CLA	CHD-C4C	3.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	O2A-CGA	3.71	1.44	1.33
23	c	510	CLA	OBD-CAD	3.70	1.28	1.22
23	b	616	CLA	OBD-CAD	3.70	1.28	1.22
23	C	503	CLA	OBD-CAD	3.70	1.28	1.22
32	D	409	LHG	O7-C7	3.70	1.44	1.34
23	C	504	CLA	OBD-CAD	3.69	1.28	1.22
23	c	503	CLA	CHD-C4C	3.69	1.47	1.39
32	d	407	LHG	O7-C7	3.69	1.44	1.34
23	b	604	CLA	C3D-C2D	3.69	1.49	1.39
23	a	407	CLA	C3D-C2D	3.68	1.49	1.39
23	B	611	CLA	CHD-C1D	3.68	1.45	1.38
23	B	606	CLA	C3D-C2D	3.68	1.49	1.39
23	c	513	CLA	OBD-CAD	3.68	1.28	1.22
23	b	614	CLA	CHD-C4C	3.68	1.47	1.39
23	C	513	CLA	OBD-CAD	3.68	1.28	1.22
23	b	604	CLA	CHD-C4C	3.67	1.47	1.39
23	A	404	CLA	C3D-C2D	3.67	1.49	1.39
23	B	609	CLA	C3D-C2D	3.67	1.49	1.39
23	b	608	CLA	OBD-CAD	3.67	1.28	1.22
23	B	603	CLA	OBD-CAD	3.66	1.28	1.22
23	A	404	CLA	O2A-CGA	3.66	1.44	1.33
23	B	611	CLA	OBD-CAD	3.66	1.28	1.22
23	d	403	CLA	C1D-ND	3.66	1.42	1.37
23	b	607	CLA	C3D-C2D	3.66	1.49	1.39
23	B	603	CLA	CHD-C4C	3.66	1.47	1.39
24	D	402	PHO	O2A-CGA	3.65	1.44	1.33
23	D	406	CLA	CHD-C4C	3.65	1.47	1.39
23	b	603	CLA	C3D-C2D	3.65	1.49	1.39
23	A	406	CLA	OBD-CAD	3.65	1.28	1.22
23	B	601	CLA	OBD-CAD	3.65	1.28	1.22
23	C	507	CLA	C3D-C2D	3.65	1.49	1.39
33	h	101	HTG	C1'-S1	-3.64	1.76	1.81
23	b	602	CLA	OBD-CAD	3.64	1.28	1.22
23	A	408	CLA	C3D-C2D	3.63	1.49	1.39
23	B	602	CLA	O2A-CGA	3.62	1.43	1.33
23	C	506	CLA	C3D-C2D	3.61	1.49	1.39
23	A	406	CLA	C3D-C2D	3.61	1.49	1.39
23	B	603	CLA	C3D-C2D	3.61	1.49	1.39
23	c	507	CLA	OBD-CAD	3.60	1.28	1.22
23	d	404	CLA	OBD-CAD	3.60	1.28	1.22
23	B	604	CLA	CHD-C4C	3.60	1.47	1.39
23	B	602	CLA	C3D-C2D	3.60	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CHD-C1D	3.59	1.45	1.38
23	b	605	CLA	CHD-C4C	3.59	1.47	1.39
25	B	618	BCR	C23-C22	-3.58	1.38	1.45
23	C	504	CLA	CHD-C1D	3.58	1.45	1.38
23	B	612	CLA	CHD-C1D	3.58	1.45	1.38
33	b	622	HTG	C1'-S1	-3.57	1.76	1.81
23	b	615	CLA	OBD-CAD	3.57	1.28	1.22
23	B	610	CLA	O2A-CGA	3.57	1.43	1.33
23	B	604	CLA	C3D-C2D	3.57	1.48	1.39
23	a	405	CLA	CHD-C4C	3.57	1.47	1.39
23	B	608	CLA	C3D-C2D	3.57	1.48	1.39
23	c	504	CLA	C3D-C2D	3.56	1.48	1.39
23	C	502	CLA	C3D-C2D	3.56	1.48	1.39
23	C	509	CLA	CHD-C4C	3.56	1.47	1.39
23	b	606	CLA	CHD-C4C	3.56	1.47	1.39
23	C	503	CLA	CHD-C4C	3.56	1.47	1.39
23	b	611	CLA	C3D-C2D	3.55	1.48	1.39
23	d	403	CLA	C3D-C2D	3.54	1.48	1.39
23	B	614	CLA	C3D-C2D	3.54	1.48	1.39
23	b	601	CLA	OBD-CAD	3.54	1.28	1.22
23	D	405	CLA	C3D-C2D	3.54	1.48	1.39
23	B	602	CLA	OBD-CAD	3.53	1.28	1.22
23	B	606	CLA	CHD-C4C	3.52	1.47	1.39
23	c	511	CLA	OBD-CAD	3.52	1.28	1.22
23	D	405	CLA	C1D-ND	3.52	1.42	1.37
23	a	405	CLA	CHD-C1D	3.51	1.45	1.38
23	A	405	CLA	CHD-C4C	3.50	1.47	1.39
23	b	607	CLA	O2A-CGA	3.49	1.43	1.33
23	B	613	CLA	CHD-C4C	3.49	1.47	1.39
33	B	624	HTG	C1'-S1	-3.49	1.77	1.81
23	b	614	CLA	OBD-CAD	3.49	1.28	1.22
23	B	616	CLA	CHD-C1D	3.49	1.45	1.38
23	B	612	CLA	C3D-C2D	3.48	1.48	1.39
23	B	605	CLA	OBD-CAD	3.48	1.28	1.22
23	b	610	CLA	OBD-CAD	3.48	1.28	1.22
23	c	511	CLA	C3D-C2D	3.48	1.48	1.39
23	C	507	CLA	OBD-CAD	3.48	1.28	1.22
23	b	612	CLA	OBD-CAD	3.47	1.28	1.22
23	C	509	CLA	OBD-CAD	3.47	1.28	1.22
23	b	612	CLA	CHD-C4C	3.47	1.47	1.39
24	a	416	PHO	C3C-C2C	3.47	1.48	1.37
38	f	101	HEM	C4D-ND	-3.47	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	OBD-CAD	3.47	1.28	1.22
23	B	614	CLA	CHD-C4C	3.47	1.47	1.39
23	b	605	CLA	C3D-C2D	3.47	1.48	1.39
23	C	512	CLA	OBD-CAD	3.46	1.28	1.22
23	C	506	CLA	OBD-CAD	3.46	1.28	1.22
23	B	612	CLA	C1D-ND	3.46	1.42	1.37
23	c	512	CLA	OBD-CAD	3.46	1.28	1.22
23	B	611	CLA	CHD-C4C	3.46	1.47	1.39
31	D	414	LMG	O7-C10	3.45	1.44	1.34
23	B	607	CLA	C3D-C2D	3.45	1.48	1.39
23	A	404	CLA	CHD-C1D	3.45	1.45	1.38
23	B	615	CLA	CHD-C4C	3.45	1.47	1.39
23	b	606	CLA	C3D-C2D	3.44	1.48	1.39
23	b	607	CLA	CHD-C4C	3.44	1.47	1.39
23	c	506	CLA	OBD-CAD	3.43	1.28	1.22
38	E	103	HEM	C4D-ND	-3.43	1.34	1.40
23	B	612	CLA	C1C-C2C	3.43	1.51	1.44
23	b	610	CLA	O2A-CGA	3.42	1.43	1.33
23	B	616	CLA	CHD-C4C	3.42	1.47	1.39
23	B	604	CLA	OBD-CAD	3.41	1.28	1.22
33	b	624	HTG	C1'-S1	-3.41	1.77	1.81
33	D	413	HTG	C1'-S1	-3.41	1.77	1.81
23	c	511	CLA	O2A-CGA	3.41	1.43	1.33
23	B	613	CLA	OBD-CAD	3.40	1.28	1.22
23	A	404	CLA	CHD-C4C	3.38	1.47	1.39
23	B	615	CLA	CHD-C1D	3.38	1.45	1.38
23	C	511	CLA	OBD-CAD	3.38	1.28	1.22
38	E	103	HEM	C1B-NB	-3.37	1.34	1.40
23	b	604	CLA	OBD-CAD	3.37	1.28	1.22
23	B	609	CLA	OBD-CAD	3.36	1.28	1.22
33	B	621	HTG	C1'-S1	-3.36	1.77	1.81
23	C	508	CLA	OBD-CAD	3.35	1.28	1.22
23	A	404	CLA	C1C-C2C	3.35	1.51	1.44
23	c	505	CLA	OBD-CAD	3.35	1.28	1.22
23	B	616	CLA	OBD-CAD	3.34	1.28	1.22
23	A	405	CLA	OBD-CAD	3.33	1.28	1.22
33	c	522	HTG	C1'-S1	-3.33	1.77	1.81
23	d	403	CLA	OBD-CAD	3.32	1.28	1.22
23	b	605	CLA	O2A-CGA	3.32	1.43	1.33
23	d	403	CLA	CHD-C1D	3.31	1.44	1.38
23	A	408	CLA	OBD-CAD	3.28	1.28	1.22
35	H	102	DGD	O2G-C1B	3.26	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	OBD-CAD	3.24	1.28	1.22
23	B	607	CLA	OBD-CAD	3.22	1.28	1.22
33	b	621	HTG	C1'-S1	-3.22	1.77	1.81
24	D	402	PHO	CHA-CBD	-3.21	1.48	1.52
23	C	502	CLA	OBD-CAD	3.21	1.28	1.22
23	B	602	CLA	C1C-C2C	3.20	1.50	1.44
23	B	608	CLA	OBD-CAD	3.20	1.28	1.22
23	c	514	CLA	OBD-CAD	3.18	1.28	1.22
23	a	404	CLA	O2A-CGA	3.16	1.42	1.33
23	C	514	CLA	OBD-CAD	3.14	1.27	1.22
23	c	502	CLA	OBD-CAD	3.14	1.27	1.22
23	d	403	CLA	CHD-C4C	3.13	1.46	1.39
24	A	407	PHO	C3C-C2C	3.13	1.46	1.37
23	B	612	CLA	CHD-C4C	3.12	1.46	1.39
33	C	522	HTG	C1'-S1	-3.12	1.77	1.81
23	c	504	CLA	OBD-CAD	3.09	1.27	1.22
23	c	504	CLA	C4C-C3C	3.08	1.50	1.45
23	d	402	CLA	OBD-CAD	3.08	1.27	1.22
38	f	101	HEM	C1B-NB	-3.07	1.35	1.40
23	C	502	CLA	C1C-C2C	3.07	1.50	1.44
23	b	611	CLA	OBD-CAD	3.07	1.27	1.22
23	c	503	CLA	OBD-CAD	3.06	1.27	1.22
23	c	510	CLA	C4C-C3C	3.06	1.50	1.45
23	b	607	CLA	OBD-CAD	3.05	1.27	1.22
23	A	405	CLA	C1C-C2C	3.04	1.50	1.44
23	C	510	CLA	C1C-C2C	3.04	1.50	1.44
23	b	607	CLA	C1B-NB	-3.04	1.32	1.35
23	c	508	CLA	C1C-C2C	3.04	1.50	1.44
23	B	603	CLA	C1C-C2C	3.01	1.50	1.44
23	a	407	CLA	OBD-CAD	3.00	1.27	1.22
23	c	512	CLA	C1B-CHB	2.98	1.49	1.41
23	B	602	CLA	C4B-CHC	2.97	1.49	1.41
23	c	502	CLA	C1B-CHB	2.96	1.49	1.41
23	B	611	CLA	C1C-C2C	2.94	1.50	1.44
23	B	605	CLA	C4B-CHC	2.93	1.49	1.41
38	E	103	HEM	FE-NB	2.93	2.11	1.96
23	C	505	CLA	C1C-C2C	2.92	1.50	1.44
23	D	406	CLA	C1C-C2C	2.92	1.50	1.44
27	f	102	SQD	C6-S	-2.92	1.66	1.77
23	B	612	CLA	C1B-CHB	2.92	1.49	1.41
38	f	101	HEM	FE-NB	2.92	2.11	1.96
23	B	614	CLA	CHD-C1D	2.91	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	OBD-CAD	2.90	1.27	1.22
23	B	606	CLA	OBD-CAD	2.90	1.27	1.22
23	b	604	CLA	C4D-CHA	2.88	1.48	1.38
23	b	602	CLA	C4C-C3C	2.87	1.50	1.45
23	C	512	CLA	C4D-CHA	2.87	1.48	1.38
23	d	402	CLA	C1C-C2C	2.86	1.50	1.44
23	D	405	CLA	OBD-CAD	2.86	1.27	1.22
23	b	603	CLA	C1C-C2C	2.86	1.50	1.44
23	C	508	CLA	C4D-CHA	2.86	1.48	1.38
23	c	506	CLA	C4C-C3C	2.83	1.49	1.45
27	C	501	SQD	C6-S	-2.83	1.66	1.77
23	B	612	CLA	C1B-NB	-2.83	1.32	1.35
33	B	622	HTG	C1'-S1	-2.83	1.77	1.81
27	a	409	SQD	C6-S	-2.81	1.67	1.77
23	B	604	CLA	C4D-CHA	2.80	1.48	1.38
33	b	624	HTG	C1-S1	-2.80	1.76	1.80
23	A	408	CLA	C1C-C2C	2.79	1.50	1.44
23	D	406	CLA	C1B-CHB	2.79	1.48	1.41
23	c	504	CLA	C1C-C2C	2.78	1.49	1.44
23	c	513	CLA	C4B-CHC	2.78	1.48	1.41
23	b	615	CLA	C4D-CHA	2.78	1.48	1.38
23	d	403	CLA	C1C-C2C	2.78	1.49	1.44
23	C	514	CLA	C1C-C2C	2.77	1.49	1.44
23	B	607	CLA	C4D-CHA	2.77	1.48	1.38
23	C	505	CLA	C4D-CHA	2.77	1.48	1.38
23	B	608	CLA	C4D-CHA	2.77	1.48	1.38
24	a	416	PHO	C3A-C2A	-2.76	1.52	1.54
23	A	404	CLA	OBD-CAD	2.75	1.27	1.22
23	c	504	CLA	C4D-CHA	2.75	1.48	1.38
23	C	507	CLA	C4C-C3C	2.75	1.49	1.45
23	c	510	CLA	C4D-CHA	2.75	1.48	1.38
23	c	514	CLA	C4C-C3C	2.74	1.49	1.45
23	c	506	CLA	C1C-C2C	2.74	1.49	1.44
23	c	509	CLA	C4C-C3C	2.74	1.49	1.45
23	c	506	CLA	C4D-CHA	2.73	1.48	1.38
23	C	507	CLA	C4D-CHA	2.73	1.48	1.38
23	A	405	CLA	C4B-CHC	2.73	1.48	1.41
23	c	508	CLA	C4B-CHC	2.73	1.48	1.41
23	B	615	CLA	C1C-C2C	2.72	1.49	1.44
23	c	508	CLA	C4D-CHA	2.72	1.48	1.38
23	C	506	CLA	C4C-C3C	2.71	1.49	1.45
23	C	502	CLA	C4B-CHC	2.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1C-C2C	2.71	1.49	1.44
23	A	404	CLA	C4C-C3C	2.70	1.49	1.45
23	c	505	CLA	C4D-CHA	2.70	1.48	1.38
23	C	513	CLA	C4D-CHA	2.70	1.48	1.38
27	B	620	SQD	C6-S	-2.70	1.67	1.77
23	a	405	CLA	C1C-C2C	2.70	1.49	1.44
23	b	602	CLA	C1C-C2C	2.70	1.49	1.44
23	b	603	CLA	C4C-C3C	2.70	1.49	1.45
23	C	512	CLA	C4C-C3C	2.70	1.49	1.45
23	b	607	CLA	C1B-CHB	2.70	1.48	1.41
27	A	411	SQD	C6-S	-2.70	1.67	1.77
27	a	411	SQD	C6-S	-2.70	1.67	1.77
23	B	614	CLA	C4D-CHA	2.69	1.48	1.38
23	b	606	CLA	C1C-C2C	2.69	1.49	1.44
23	c	511	CLA	C4D-CHA	2.69	1.47	1.38
23	B	611	CLA	C1B-CHB	2.68	1.48	1.41
23	B	601	CLA	C4B-CHC	2.68	1.48	1.41
23	C	511	CLA	C4D-CHA	2.68	1.47	1.38
23	C	504	CLA	C1C-C2C	2.68	1.49	1.44
23	c	514	CLA	C1C-C2C	2.68	1.49	1.44
23	C	511	CLA	C1C-C2C	2.67	1.49	1.44
23	c	511	CLA	C1B-CHB	2.67	1.48	1.41
29	A	413	PL9	C6-C5	2.66	1.49	1.35
23	c	513	CLA	C4D-CHA	2.66	1.47	1.38
23	C	503	CLA	C1C-C2C	2.66	1.49	1.44
23	B	613	CLA	C1B-CHB	2.66	1.48	1.41
23	D	405	CLA	C1B-CHB	2.66	1.48	1.41
23	C	506	CLA	C4D-CHA	2.65	1.47	1.38
23	B	606	CLA	C4D-CHA	2.65	1.47	1.38
23	b	610	CLA	C1C-C2C	2.65	1.49	1.44
23	C	509	CLA	C4D-CHA	2.65	1.47	1.38
23	C	513	CLA	C1C-C2C	2.64	1.49	1.44
29	a	414	PL9	C6-C5	2.64	1.49	1.35
23	c	506	CLA	C4B-CHC	2.64	1.48	1.41
23	B	604	CLA	C1B-CHB	2.64	1.48	1.41
23	B	610	CLA	C3D-C4D	-2.63	1.38	1.44
23	b	610	CLA	C4B-CHC	2.63	1.48	1.41
23	b	602	CLA	C4D-CHA	2.63	1.47	1.38
33	B	624	HTG	C1-S1	-2.63	1.76	1.80
23	B	610	CLA	C4C-C3C	2.63	1.49	1.45
23	C	514	CLA	C4D-CHA	2.63	1.47	1.38
23	c	513	CLA	C1C-C2C	2.63	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C1B-CHB	2.63	1.48	1.41
23	b	609	CLA	C1C-C2C	2.63	1.49	1.44
23	B	607	CLA	C1B-CHB	2.62	1.48	1.41
23	b	616	CLA	C1C-C2C	2.62	1.49	1.44
23	C	512	CLA	C1B-CHB	2.62	1.48	1.41
23	b	608	CLA	C4D-CHA	2.62	1.47	1.38
23	c	509	CLA	C4D-CHA	2.62	1.47	1.38
23	B	607	CLA	C4C-C3C	2.62	1.49	1.45
23	b	609	CLA	C4D-CHA	2.62	1.47	1.38
23	d	403	CLA	C4C-C3C	2.62	1.49	1.45
23	B	615	CLA	C1B-CHB	2.62	1.48	1.41
23	d	403	CLA	C4D-CHA	2.61	1.47	1.38
23	C	511	CLA	C1B-CHB	2.61	1.48	1.41
23	B	613	CLA	C4D-CHA	2.61	1.47	1.38
23	b	608	CLA	C1B-CHB	2.60	1.48	1.41
23	b	605	CLA	C1B-NB	-2.60	1.32	1.35
23	A	408	CLA	C4D-CHA	2.60	1.47	1.38
23	c	512	CLA	C4D-CHA	2.59	1.47	1.38
23	D	405	CLA	C1C-C2C	2.59	1.49	1.44
38	f	101	HEM	C1D-ND	-2.59	1.33	1.38
35	h	103	DGD	O5D-C1E	2.59	1.44	1.40
23	a	407	CLA	C1B-CHB	2.58	1.48	1.41
23	C	510	CLA	C4C-C3C	2.58	1.49	1.45
24	a	416	PHO	CHA-CBD	-2.58	1.49	1.52
23	b	610	CLA	C4D-CHA	2.58	1.47	1.38
23	A	404	CLA	C4D-CHA	2.58	1.47	1.38
23	b	608	CLA	C3D-C4D	-2.57	1.38	1.44
34	a	412	LMT	O1'-C1'	2.57	1.44	1.40
23	C	502	CLA	C4D-CHA	2.57	1.47	1.38
31	Z	101	LMG	O8-C28	2.57	1.46	1.33
23	C	512	CLA	C1C-C2C	2.57	1.49	1.44
23	A	408	CLA	C4B-CHC	2.57	1.48	1.41
23	C	514	CLA	C1B-CHB	2.57	1.48	1.41
23	b	614	CLA	C4D-CHA	2.57	1.47	1.38
23	b	616	CLA	C4D-CHA	2.57	1.47	1.38
23	c	511	CLA	C1C-C2C	2.57	1.49	1.44
27	D	415	SQD	C6-S	-2.56	1.67	1.77
27	L	102	SQD	C6-S	-2.56	1.67	1.77
23	B	604	CLA	C1C-C2C	2.56	1.49	1.44
23	b	606	CLA	C4D-CHA	2.56	1.47	1.38
23	B	611	CLA	C4D-CHA	2.55	1.47	1.38
23	d	402	CLA	C4B-CHC	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	C1C-C2C	2.55	1.49	1.44
23	A	406	CLA	C1B-NB	-2.55	1.32	1.35
23	c	502	CLA	C3D-C4D	-2.55	1.38	1.44
23	A	405	CLA	C4D-CHA	2.55	1.47	1.38
24	a	406	PHO	CHA-CBD	-2.55	1.49	1.52
23	c	514	CLA	C4D-CHA	2.54	1.47	1.38
23	B	607	CLA	C1B-NB	-2.54	1.32	1.35
23	C	508	CLA	C1C-C2C	2.54	1.49	1.44
23	c	502	CLA	C1C-C2C	2.54	1.49	1.44
23	b	601	CLA	C4D-CHA	2.54	1.47	1.38
23	a	407	CLA	C4D-CHA	2.54	1.47	1.38
23	b	604	CLA	C4B-CHC	2.54	1.48	1.41
23	C	508	CLA	C3D-C4D	-2.54	1.38	1.44
23	C	512	CLA	C1C-NC	-2.53	1.34	1.37
23	b	611	CLA	C1B-CHB	2.53	1.48	1.41
23	c	502	CLA	C4D-CHA	2.53	1.47	1.38
23	B	603	CLA	C4B-CHC	2.53	1.48	1.41
23	C	509	CLA	C1B-CHB	2.53	1.48	1.41
23	B	607	CLA	C1C-C2C	2.53	1.49	1.44
23	C	505	CLA	C3D-C4D	-2.53	1.38	1.44
23	C	510	CLA	C4D-CHA	2.53	1.47	1.38
23	B	605	CLA	C4D-CHA	2.53	1.47	1.38
23	B	616	CLA	C4B-CHC	2.53	1.48	1.41
23	C	504	CLA	C4B-CHC	2.52	1.48	1.41
23	c	513	CLA	C4C-C3C	2.52	1.49	1.45
23	b	608	CLA	C1C-C2C	2.52	1.49	1.44
23	c	505	CLA	C4C-C3C	2.52	1.49	1.45
23	C	510	CLA	C4B-CHC	2.52	1.48	1.41
23	B	613	CLA	C4C-C3C	2.52	1.49	1.45
23	D	405	CLA	C4C-C3C	2.51	1.49	1.45
23	C	504	CLA	C1B-CHB	2.51	1.48	1.41
23	B	603	CLA	C4D-CHA	2.51	1.47	1.38
23	b	602	CLA	C4B-CHC	2.51	1.48	1.41
23	c	505	CLA	C1B-CHB	2.51	1.48	1.41
23	C	503	CLA	C1B-CHB	2.51	1.48	1.41
23	c	510	CLA	C1C-C2C	2.51	1.49	1.44
23	A	406	CLA	C4C-C3C	2.50	1.49	1.45
23	B	614	CLA	C4B-CHC	2.50	1.47	1.41
33	D	413	HTG	C1-S1	-2.50	1.76	1.80
23	b	603	CLA	C4D-CHA	2.50	1.47	1.38
23	B	609	CLA	C1B-CHB	2.50	1.47	1.41
23	B	610	CLA	C4B-CHC	2.50	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C1B-CHB	2.50	1.47	1.41
23	B	601	CLA	C4D-CHA	2.50	1.47	1.38
23	C	505	CLA	C1B-CHB	2.49	1.47	1.41
23	B	601	CLA	C1C-C2C	2.49	1.49	1.44
23	C	506	CLA	C1C-C2C	2.49	1.49	1.44
23	D	406	CLA	C4D-CHA	2.49	1.47	1.38
23	A	405	CLA	C1B-CHB	2.48	1.47	1.41
23	b	616	CLA	C4B-CHC	2.48	1.47	1.41
23	b	611	CLA	C4D-CHA	2.48	1.47	1.38
23	B	614	CLA	C3D-C4D	-2.48	1.38	1.44
23	D	405	CLA	C4D-CHA	2.48	1.47	1.38
23	B	609	CLA	C4D-CHA	2.48	1.47	1.38
23	b	613	CLA	C4D-CHA	2.48	1.47	1.38
23	B	616	CLA	C4D-CHA	2.47	1.47	1.38
23	B	610	CLA	C4D-CHA	2.47	1.47	1.38
23	b	611	CLA	C1C-C2C	2.47	1.49	1.44
23	b	609	CLA	C4B-CHC	2.47	1.47	1.41
23	C	506	CLA	C1B-CHB	2.46	1.47	1.41
23	D	405	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	507	CLA	C1D-C2D	2.46	1.50	1.45
23	b	605	CLA	C4B-CHC	2.46	1.47	1.41
23	C	504	CLA	C4D-CHA	2.46	1.47	1.38
23	B	606	CLA	C1B-CHB	2.46	1.47	1.41
23	b	612	CLA	C1B-CHB	2.46	1.47	1.41
23	B	612	CLA	C4D-CHA	2.46	1.47	1.38
23	C	510	CLA	C1B-CHB	2.46	1.47	1.41
23	c	512	CLA	C4B-CHC	2.46	1.47	1.41
23	B	606	CLA	C3D-C4D	-2.45	1.38	1.44
29	d	406	PL9	C6-C5	2.45	1.48	1.35
23	B	607	CLA	C4B-CHC	2.45	1.47	1.41
23	b	609	CLA	C1B-CHB	2.45	1.47	1.41
23	b	615	CLA	C4C-C3C	2.45	1.49	1.45
23	d	404	CLA	C4B-CHC	2.45	1.47	1.41
23	b	602	CLA	C3D-C4D	-2.45	1.38	1.44
23	B	608	CLA	C1C-C2C	2.45	1.49	1.44
23	D	406	CLA	C4B-CHC	2.45	1.47	1.41
23	C	511	CLA	C4B-CHC	2.45	1.47	1.41
23	a	405	CLA	C1B-CHB	2.45	1.47	1.41
23	C	508	CLA	C4B-CHC	2.44	1.47	1.41
23	b	610	CLA	C1B-CHB	2.44	1.47	1.41
23	C	503	CLA	C4D-CHA	2.44	1.47	1.38
23	d	404	CLA	C1C-C2C	2.44	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C4D-CHA	2.43	1.47	1.38
23	b	603	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	609	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	608	CLA	C4B-CHC	2.43	1.47	1.41
23	a	404	CLA	C4D-CHA	2.42	1.47	1.38
23	c	511	CLA	C3D-C4D	-2.42	1.38	1.44
23	c	503	CLA	C4D-CHA	2.42	1.47	1.38
23	b	614	CLA	C1C-C2C	2.42	1.49	1.44
23	A	406	CLA	C4D-CHA	2.42	1.47	1.38
23	A	404	CLA	C1B-CHB	2.42	1.47	1.41
23	c	507	CLA	C4C-C3C	2.42	1.49	1.45
23	b	613	CLA	C4C-C3C	2.42	1.49	1.45
23	C	513	CLA	C4B-CHC	2.41	1.47	1.41
23	B	603	CLA	C1B-CHB	2.41	1.47	1.41
23	C	503	CLA	C3D-C4D	-2.41	1.38	1.44
23	C	504	CLA	C4C-C3C	2.40	1.49	1.45
23	C	511	CLA	C1B-NB	-2.40	1.33	1.35
23	a	404	CLA	C1C-C2C	2.40	1.49	1.44
23	d	403	CLA	C1B-CHB	2.40	1.47	1.41
23	B	603	CLA	C4C-C3C	2.40	1.49	1.45
23	a	407	CLA	C4B-CHC	2.40	1.47	1.41
23	B	605	CLA	C1C-C2C	2.40	1.49	1.44
23	c	511	CLA	C4B-CHC	2.40	1.47	1.41
23	a	405	CLA	C4D-CHA	2.40	1.46	1.38
23	B	608	CLA	C3D-C4D	-2.40	1.38	1.44
23	b	616	CLA	C1B-CHB	2.40	1.47	1.41
23	d	404	CLA	C3D-C4D	-2.39	1.38	1.44
23	c	510	CLA	C1B-NB	-2.39	1.33	1.35
23	b	603	CLA	C1B-CHB	2.39	1.47	1.41
23	A	405	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	608	CLA	C1B-CHB	2.39	1.47	1.41
23	d	402	CLA	C4D-CHA	2.39	1.46	1.38
23	C	514	CLA	C4B-CHC	2.38	1.47	1.41
23	c	512	CLA	C4C-C3C	2.38	1.49	1.45
23	b	612	CLA	C4C-C3C	2.38	1.49	1.45
23	c	502	CLA	C4B-CHC	2.38	1.47	1.41
23	C	503	CLA	C4B-CHC	2.37	1.47	1.41
23	B	612	CLA	C4B-CHC	2.37	1.47	1.41
23	c	504	CLA	C4B-CHC	2.37	1.47	1.41
23	c	507	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	605	CLA	C1B-CHB	2.37	1.47	1.41
23	a	404	CLA	C1B-CHB	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C3D-C4D	-2.37	1.38	1.44
23	B	616	CLA	C1B-CHB	2.37	1.47	1.41
23	b	610	CLA	C3D-C4D	-2.37	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.37	1.38	1.44
23	A	406	CLA	C4B-CHC	2.37	1.47	1.41
23	B	602	CLA	C4D-CHA	2.37	1.46	1.38
23	b	614	CLA	C4B-CHC	2.37	1.47	1.41
23	b	612	CLA	C4D-CHA	2.37	1.46	1.38
23	C	509	CLA	C4B-CHC	2.37	1.47	1.41
23	d	403	CLA	C1B-NB	-2.36	1.33	1.35
23	C	502	CLA	C1B-CHB	2.36	1.47	1.41
23	C	508	CLA	C4C-C3C	2.36	1.49	1.45
23	B	605	CLA	C3D-C4D	-2.35	1.38	1.44
23	B	613	CLA	C1C-C2C	2.35	1.49	1.44
23	c	505	CLA	C1C-C2C	2.35	1.49	1.44
23	b	607	CLA	C1C-C2C	2.35	1.49	1.44
23	c	506	CLA	C1B-CHB	2.35	1.47	1.41
23	c	507	CLA	C4B-CHC	2.35	1.47	1.41
23	d	403	CLA	C4B-CHC	2.35	1.47	1.41
29	D	408	PL9	C6-C5	2.35	1.47	1.35
23	c	504	CLA	C3D-C4D	-2.35	1.38	1.44
23	c	507	CLA	C1B-CHB	2.34	1.47	1.41
23	c	509	CLA	C1C-C2C	2.34	1.49	1.44
23	c	514	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	505	CLA	C4B-CHC	2.34	1.47	1.41
23	C	513	CLA	C4C-C3C	2.34	1.49	1.45
23	b	605	CLA	C4D-CHA	2.34	1.46	1.38
23	b	611	CLA	C4B-CHC	2.33	1.47	1.41
23	c	503	CLA	C1B-CHB	2.33	1.47	1.41
23	c	503	CLA	C1C-C2C	2.33	1.49	1.44
23	c	502	CLA	C4C-C3C	2.33	1.49	1.45
23	b	605	CLA	C1C-C2C	2.33	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.32	1.38	1.44
23	b	612	CLA	C4B-CHC	2.32	1.47	1.41
23	b	607	CLA	C4D-CHA	2.32	1.46	1.38
23	d	404	CLA	C4D-CHA	2.32	1.46	1.38
23	d	404	CLA	C1B-CHB	2.31	1.47	1.41
23	B	609	CLA	C4B-CHC	2.31	1.47	1.41
23	C	507	CLA	C1C-C2C	2.31	1.49	1.44
23	b	609	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	611	CLA	C3D-C4D	-2.31	1.39	1.44
23	c	510	CLA	C1B-CHB	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C4B-CHC	2.31	1.47	1.41
23	A	408	CLA	C3D-C4D	-2.31	1.39	1.44
23	C	508	CLA	C1B-CHB	2.31	1.47	1.41
23	d	403	CLA	C3D-C4D	-2.30	1.39	1.44
23	b	608	CLA	C4C-C3C	2.30	1.49	1.45
23	c	508	CLA	C1D-C2D	2.30	1.49	1.45
23	c	503	CLA	C4B-CHC	2.30	1.47	1.41
23	b	605	CLA	C3D-C4D	-2.30	1.39	1.44
23	b	612	CLA	C1C-C2C	2.30	1.49	1.44
23	b	610	CLA	C1C-NC	-2.30	1.34	1.37
23	b	605	CLA	C1D-C2D	2.30	1.49	1.45
23	B	609	CLA	C1C-C2C	2.30	1.49	1.44
23	b	603	CLA	C4B-CHC	2.29	1.47	1.41
23	C	509	CLA	C1C-C2C	2.29	1.49	1.44
23	A	404	CLA	C3D-C4D	-2.29	1.39	1.44
35	H	102	DGD	O5D-C1E	2.29	1.44	1.40
23	C	506	CLA	C4B-CHC	2.29	1.47	1.41
34	C	525	LMT	O1'-C1'	2.29	1.44	1.40
23	c	513	CLA	C1B-CHB	2.29	1.47	1.41
23	B	601	CLA	C4C-C3C	2.29	1.49	1.45
23	b	613	CLA	C1B-CHB	2.28	1.47	1.41
23	C	502	CLA	C4C-C3C	2.28	1.49	1.45
23	c	509	CLA	C1B-CHB	2.28	1.47	1.41
23	b	601	CLA	C4B-CHC	2.27	1.47	1.41
23	c	514	CLA	C1B-CHB	2.27	1.47	1.41
23	C	505	CLA	C4C-C3C	2.27	1.49	1.45
23	B	604	CLA	C3D-C4D	-2.27	1.39	1.44
23	C	511	CLA	C4C-C3C	2.27	1.49	1.45
23	C	514	CLA	C4C-C3C	2.27	1.49	1.45
23	C	513	CLA	C1B-CHB	2.27	1.47	1.41
23	A	404	CLA	C1B-NB	-2.27	1.33	1.35
23	b	613	CLA	C1C-C2C	2.27	1.49	1.44
23	C	507	CLA	C3D-C4D	-2.27	1.39	1.44
31	Z	101	LMG	O1-C1	2.26	1.44	1.40
23	b	616	CLA	C3D-C4D	-2.26	1.39	1.44
33	c	522	HTG	C1-S1	-2.26	1.77	1.80
23	c	507	CLA	C1C-C2C	2.25	1.48	1.44
23	B	614	CLA	C4C-C3C	2.25	1.48	1.45
23	B	602	CLA	C4C-C3C	2.25	1.48	1.45
23	a	404	CLA	C3D-C4D	-2.25	1.39	1.44
23	b	606	CLA	C4B-CHC	2.25	1.47	1.41
23	B	610	CLA	C1B-CHB	2.25	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C1C-C2C	2.24	1.48	1.44
23	a	405	CLA	C1C-NC	-2.24	1.34	1.37
23	c	505	CLA	C4B-CHC	2.24	1.47	1.41
23	c	509	CLA	C4B-CHC	2.24	1.47	1.41
23	B	606	CLA	MG-NA	2.24	2.11	2.06
23	c	505	CLA	C3D-C4D	-2.24	1.39	1.44
23	d	402	CLA	C1B-CHB	2.24	1.47	1.41
23	A	408	CLA	C4C-C3C	2.24	1.48	1.45
23	C	509	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	604	CLA	C1B-CHB	2.24	1.47	1.41
23	A	408	CLA	C1B-CHB	2.23	1.47	1.41
23	A	405	CLA	C4C-C3C	2.23	1.48	1.45
23	B	615	CLA	C4D-CHA	2.23	1.46	1.38
23	c	506	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	602	CLA	C3D-C4D	-2.23	1.39	1.44
23	b	607	CLA	C4C-C3C	2.22	1.48	1.45
23	b	606	CLA	C3D-C4D	-2.22	1.39	1.44
23	b	601	CLA	C1B-CHB	2.22	1.47	1.41
31	C	521	LMG	O1-C1	2.22	1.44	1.40
23	B	609	CLA	C4C-C3C	2.22	1.48	1.45
24	D	402	PHO	C3A-C2A	-2.22	1.52	1.54
29	A	413	PL9	C2-C3	2.21	1.40	1.34
23	c	510	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	608	CLA	C4C-C3C	2.21	1.48	1.45
23	C	507	CLA	C1B-CHB	2.21	1.47	1.41
32	D	409	LHG	O7-C5	-2.21	1.41	1.46
23	c	514	CLA	C4B-CHC	2.21	1.47	1.41
23	B	604	CLA	C4B-CHC	2.21	1.47	1.41
23	B	615	CLA	C4B-CHC	2.21	1.47	1.41
23	B	612	CLA	C4C-C3C	2.21	1.48	1.45
23	D	406	CLA	C1B-NB	-2.21	1.33	1.35
23	B	610	CLA	C1B-NB	-2.20	1.33	1.35
23	a	407	CLA	C3D-C4D	-2.20	1.39	1.44
34	D	403	LMT	O1'-C1'	2.20	1.44	1.40
23	b	602	CLA	C1B-CHB	2.20	1.47	1.41
23	b	615	CLA	C1B-CHB	2.20	1.47	1.41
33	h	101	HTG	C1-S1	-2.20	1.77	1.80
23	A	404	CLA	C4B-CHC	2.20	1.47	1.41
23	C	504	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	613	CLA	C4B-CHC	2.19	1.47	1.41
23	c	513	CLA	C3D-C4D	-2.19	1.39	1.44
23	A	405	CLA	C1B-NB	-2.19	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	CHA-CBD	-2.19	1.49	1.52
23	B	613	CLA	C1B-NB	-2.19	1.33	1.35
23	C	513	CLA	C3D-C4D	-2.19	1.39	1.44
23	B	602	CLA	C1B-CHB	2.19	1.47	1.41
23	C	510	CLA	C3D-C4D	-2.19	1.39	1.44
23	b	614	CLA	C1B-CHB	2.18	1.47	1.41
23	B	611	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	614	CLA	C1C-C2C	2.18	1.48	1.44
23	C	506	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	601	CLA	C3D-C4D	-2.18	1.39	1.44
23	c	511	CLA	C4C-C3C	2.18	1.48	1.45
23	c	509	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	616	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	614	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	508	CLA	C1B-CHB	2.17	1.47	1.41
23	B	604	CLA	C4C-C3C	2.16	1.48	1.45
23	b	601	CLA	C1C-C2C	2.16	1.48	1.44
23	b	606	CLA	C1B-CHB	2.15	1.47	1.41
34	E	102	LMT	O1'-C1'	2.15	1.43	1.40
23	C	512	CLA	C3D-C4D	-2.15	1.39	1.44
23	c	503	CLA	C3D-C4D	-2.15	1.39	1.44
23	d	404	CLA	C1D-C2D	2.14	1.49	1.45
23	B	613	CLA	C1D-C2D	2.14	1.49	1.45
23	b	611	CLA	C4C-C3C	2.14	1.48	1.45
23	C	512	CLA	C4B-NB	-2.14	1.33	1.35
23	D	405	CLA	C4B-CHC	2.14	1.46	1.41
23	b	609	CLA	C4C-C3C	2.13	1.48	1.45
23	B	611	CLA	C4B-CHC	2.13	1.46	1.41
23	A	406	CLA	C1C-C2C	2.13	1.48	1.44
23	C	503	CLA	C4C-C3C	2.13	1.48	1.45
23	a	405	CLA	C3D-C4D	-2.13	1.39	1.44
23	B	605	CLA	C4C-C3C	2.12	1.48	1.45
34	b	626	LMT	O1'-C1'	2.12	1.43	1.40
23	d	402	CLA	C4C-C3C	2.11	1.48	1.45
23	C	512	CLA	C4B-CHC	2.11	1.46	1.41
23	b	612	CLA	C1B-NB	-2.11	1.33	1.35
23	B	605	CLA	C1B-NB	-2.11	1.33	1.35
23	b	604	CLA	C1C-C2C	2.11	1.48	1.44
23	b	601	CLA	C3D-C4D	-2.11	1.39	1.44
23	B	606	CLA	C4B-CHC	2.10	1.46	1.41
24	a	406	PHO	CBD-CGD	-2.10	1.49	1.52
23	b	615	CLA	C4B-CHC	2.10	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C4B-CHC	2.10	1.46	1.41
38	E	103	HEM	CHB-C1B	2.10	1.40	1.35
23	b	607	CLA	C4B-CHC	2.09	1.46	1.41
34	e	101	LMT	O1'-C1'	2.09	1.43	1.40
38	E	103	HEM	C1D-ND	-2.09	1.34	1.38
23	B	601	CLA	C1B-CHB	2.09	1.46	1.41
23	C	507	CLA	C4B-CHC	2.08	1.46	1.41
23	B	606	CLA	C1C-C2C	2.08	1.48	1.44
35	c	519	DGD	O2G-C2G	-2.08	1.41	1.46
38	f	101	HEM	CHB-C1B	2.08	1.40	1.35
29	D	408	PL9	C2-C3	2.07	1.40	1.34
23	B	612	CLA	C3D-C4D	-2.07	1.39	1.44
23	d	402	CLA	C3D-C4D	-2.07	1.39	1.44
23	c	507	CLA	C1B-NB	-2.06	1.33	1.35
23	b	609	CLA	C1C-NC	-2.06	1.34	1.37
23	b	601	CLA	C1C-NC	-2.05	1.34	1.37
23	b	612	CLA	C1C-NC	-2.05	1.34	1.37
23	b	607	CLA	C1A-CHA	2.05	1.51	1.43
23	b	606	CLA	C4C-C3C	2.05	1.48	1.45
23	b	609	CLA	C1D-C2D	2.05	1.49	1.45
23	B	610	CLA	C1C-C2C	2.05	1.48	1.44
23	C	512	CLA	C1A-CHA	2.05	1.51	1.43
29	d	406	PL9	C2-C3	2.05	1.40	1.34
40	v	203	HEC	C4D-ND	2.05	1.40	1.36
23	c	505	CLA	C4B-NB	-2.04	1.33	1.35
23	B	607	CLA	C3D-C4D	-2.04	1.39	1.44
31	D	414	LMG	O7-C8	-2.04	1.41	1.46
23	b	610	CLA	C1B-NB	-2.04	1.33	1.35
23	b	610	CLA	C4C-C3C	2.04	1.48	1.45
34	a	418	LMT	O1'-C1'	2.03	1.43	1.40
23	C	506	CLA	C1B-NB	-2.03	1.33	1.35
23	A	406	CLA	C3D-C4D	-2.02	1.39	1.44
23	B	603	CLA	C1B-NB	-2.02	1.33	1.35
40	V	201	HEC	C3C-C4C	2.02	1.46	1.43
38	f	101	HEM	C3B-C4B	2.01	1.48	1.44
23	C	505	CLA	C1A-CHA	2.01	1.51	1.43
38	E	103	HEM	C4B-NB	-2.01	1.34	1.38
23	B	615	CLA	C3D-C4D	-2.01	1.39	1.44
23	a	404	CLA	C4B-CHC	2.01	1.46	1.41
23	b	604	CLA	C1A-CHA	2.01	1.51	1.43
23	c	502	CLA	C1C-NC	-2.01	1.34	1.37
23	B	606	CLA	C1B-NB	-2.01	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	103	HEM	C3B-C4B	2.01	1.48	1.44
23	B	605	CLA	C1B-CHB	2.00	1.46	1.41
23	B	613	CLA	C1A-CHA	2.00	1.51	1.43

All (2597) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405	CLA	C1D-ND-C4D	-10.67	98.76	106.33
23	b	605	CLA	C1D-ND-C4D	-10.57	98.82	106.33
23	c	503	CLA	C1D-ND-C4D	-10.01	99.22	106.33
23	B	614	CLA	C1D-ND-C4D	-10.01	99.23	106.33
23	c	512	CLA	C1D-ND-C4D	-9.97	99.25	106.33
23	a	405	CLA	C2D-C1D-ND	9.93	117.42	110.10
23	B	603	CLA	C1D-ND-C4D	-9.88	99.32	106.33
23	B	612	CLA	C1D-ND-C4D	-9.87	99.32	106.33
23	B	612	CLA	C2D-C1D-ND	9.80	117.33	110.10
23	B	615	CLA	C1D-ND-C4D	-9.80	99.38	106.33
23	C	502	CLA	C1D-ND-C4D	-9.76	99.40	106.33
23	B	613	CLA	C1D-ND-C4D	-9.75	99.41	106.33
23	B	614	CLA	C2D-C1D-ND	9.73	117.27	110.10
23	B	615	CLA	C2D-C1D-ND	9.69	117.25	110.10
23	C	504	CLA	C1D-ND-C4D	-9.68	99.46	106.33
23	D	406	CLA	C1D-ND-C4D	-9.67	99.47	106.33
23	B	601	CLA	C1D-ND-C4D	-9.60	99.51	106.33
23	B	608	CLA	C1D-ND-C4D	-9.60	99.52	106.33
23	A	406	CLA	C1D-ND-C4D	-9.59	99.53	106.33
23	b	607	CLA	C2D-C1D-ND	9.54	117.14	110.10
23	a	407	CLA	C1D-ND-C4D	-9.53	99.56	106.33
23	b	614	CLA	C1D-ND-C4D	-9.49	99.59	106.33
23	c	504	CLA	C1D-ND-C4D	-9.49	99.59	106.33
23	b	607	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	B	609	CLA	C1D-ND-C4D	-9.47	99.60	106.33
23	B	613	CLA	C2D-C1D-ND	9.45	117.07	110.10
23	A	405	CLA	C1D-ND-C4D	-9.43	99.63	106.33
23	B	602	CLA	C1D-ND-C4D	-9.43	99.64	106.33
23	D	405	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	B	607	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	d	404	CLA	C1D-ND-C4D	-9.39	99.66	106.33
23	B	605	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	B	616	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	C	514	CLA	C1D-ND-C4D	-9.35	99.70	106.33
23	c	505	CLA	C1D-ND-C4D	-9.28	99.74	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	408	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	b	616	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	b	611	CLA	C1D-ND-C4D	-9.22	99.79	106.33
23	c	508	CLA	C1D-ND-C4D	-9.20	99.80	106.33
23	c	502	CLA	C1D-ND-C4D	-9.20	99.80	106.33
23	C	509	CLA	C1D-ND-C4D	-9.15	99.84	106.33
23	B	611	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	B	603	CLA	C2D-C1D-ND	9.12	116.82	110.10
23	b	609	CLA	C1D-ND-C4D	-9.11	99.87	106.33
23	b	606	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	C	510	CLA	C1D-ND-C4D	-9.07	99.89	106.33
23	B	616	CLA	C2D-C1D-ND	9.06	116.78	110.10
23	b	615	CLA	C1D-ND-C4D	-9.05	99.91	106.33
23	B	611	CLA	C2D-C1D-ND	9.04	116.77	110.10
23	C	512	CLA	C1D-ND-C4D	-9.04	99.92	106.33
23	C	506	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	b	603	CLA	C1D-ND-C4D	-8.99	99.95	106.33
23	c	510	CLA	C1D-ND-C4D	-8.96	99.97	106.33
23	c	512	CLA	C2D-C1D-ND	8.96	116.70	110.10
23	b	602	CLA	C1D-ND-C4D	-8.95	99.97	106.33
23	c	503	CLA	C2D-C1D-ND	8.95	116.70	110.10
23	A	404	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	B	607	CLA	C2D-C1D-ND	8.92	116.68	110.10
23	c	511	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	b	608	CLA	C1D-ND-C4D	-8.90	100.01	106.33
23	A	405	CLA	C2D-C1D-ND	8.89	116.66	110.10
23	C	504	CLA	C2D-C1D-ND	8.89	116.66	110.10
23	C	511	CLA	C1D-ND-C4D	-8.88	100.03	106.33
23	b	612	CLA	C1D-ND-C4D	-8.87	100.04	106.33
23	d	402	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	C	507	CLA	C1D-ND-C4D	-8.79	100.09	106.33
23	b	610	CLA	C1D-ND-C4D	-8.79	100.09	106.33
23	c	513	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	c	514	CLA	C1D-ND-C4D	-8.73	100.13	106.33
23	C	505	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	b	616	CLA	C2D-C1D-ND	8.70	116.52	110.10
23	C	509	CLA	C2D-C1D-ND	8.68	116.50	110.10
23	b	614	CLA	C2D-C1D-ND	8.66	116.49	110.10
23	b	601	CLA	C1D-ND-C4D	-8.63	100.20	106.33
23	C	503	CLA	C1D-ND-C4D	-8.61	100.22	106.33
23	c	506	CLA	C1D-ND-C4D	-8.61	100.22	106.33
23	c	507	CLA	C1D-ND-C4D	-8.58	100.24	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C1D-ND-C4D	-8.58	100.24	106.33
23	d	403	CLA	C1D-ND-C4D	-8.57	100.24	106.33
23	b	604	CLA	C1D-ND-C4D	-8.57	100.25	106.33
23	a	404	CLA	C1D-ND-C4D	-8.53	100.27	106.33
23	C	502	CLA	C2D-C1D-ND	8.45	116.33	110.10
23	D	405	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	b	605	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	a	407	CLA	C2D-C1D-ND	8.38	116.28	110.10
23	c	509	CLA	C1D-ND-C4D	-8.36	100.40	106.33
23	c	505	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	B	610	CLA	C1D-ND-C4D	-8.32	100.43	106.33
23	D	406	CLA	C2D-C1D-ND	8.30	116.22	110.10
23	b	613	CLA	C1D-ND-C4D	-8.28	100.45	106.33
23	b	611	CLA	C2D-C1D-ND	8.27	116.20	110.10
23	C	508	CLA	C1D-ND-C4D	-8.27	100.46	106.33
23	d	403	CLA	C2D-C1D-ND	8.25	116.19	110.10
23	A	408	CLA	C2D-C1D-ND	8.24	116.18	110.10
23	b	604	CLA	C2D-C1D-ND	8.23	116.17	110.10
23	C	514	CLA	C2D-C1D-ND	8.21	116.16	110.10
23	C	505	CLA	C2D-C1D-ND	8.21	116.16	110.10
23	d	402	CLA	C2D-C1D-ND	8.21	116.16	110.10
23	c	504	CLA	C2D-C1D-ND	8.19	116.14	110.10
23	B	606	CLA	C1D-ND-C4D	-8.18	100.52	106.33
23	C	513	CLA	C1D-ND-C4D	-8.18	100.52	106.33
23	c	502	CLA	C2D-C1D-ND	8.18	116.13	110.10
24	a	406	PHO	O2D-CGD-CBD	8.14	121.31	111.00
23	C	512	CLA	C2D-C1D-ND	8.14	116.10	110.10
23	B	609	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	B	601	CLA	C2D-C1D-ND	8.09	116.06	110.10
23	B	608	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	D	405	CLA	C4A-NA-C1A	-8.06	103.08	106.71
23	c	508	CLA	C2D-C1D-ND	8.03	116.03	110.10
23	b	609	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	C	503	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	c	509	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	A	406	CLA	C2D-C1D-ND	7.89	115.92	110.10
23	b	613	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	C	511	CLA	C2D-C1D-ND	7.83	115.87	110.10
23	b	606	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	b	610	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	B	604	CLA	C2D-C1D-ND	7.78	115.84	110.10
23	b	612	CLA	C2D-C1D-ND	7.77	115.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C2D-C1D-ND	7.76	115.83	110.10
23	C	510	CLA	C2D-C1D-ND	7.76	115.82	110.10
23	d	404	CLA	C2D-C1D-ND	7.74	115.81	110.10
23	B	606	CLA	C2D-C1D-ND	7.73	115.80	110.10
23	C	508	CLA	C2D-C1D-ND	7.72	115.79	110.10
23	b	615	CLA	C2D-C1D-ND	7.68	115.77	110.10
23	c	510	CLA	C2D-C1D-ND	7.68	115.76	110.10
23	B	602	CLA	C2D-C1D-ND	7.67	115.75	110.10
23	c	513	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	B	602	CLA	C4A-NA-C1A	-7.43	103.37	106.71
23	c	514	CLA	C2D-C1D-ND	7.42	115.57	110.10
23	b	606	CLA	C4A-NA-C1A	-7.39	103.38	106.71
23	b	602	CLA	C2D-C1D-ND	7.38	115.55	110.10
23	C	506	CLA	C2D-C1D-ND	7.37	115.54	110.10
23	A	404	CLA	C2D-C1D-ND	7.35	115.52	110.10
23	B	615	CLA	CHD-C4C-C3C	-7.33	114.07	124.84
24	a	416	PHO	O2D-CGD-CBD	7.32	120.27	111.00
23	C	507	CLA	CMD-C2D-C1D	7.31	137.59	124.71
23	c	508	CLA	CMD-C2D-C1D	7.31	137.59	124.71
23	B	610	CLA	CMD-C2D-C1D	7.27	137.53	124.71
23	c	508	CLA	CHD-C1D-ND	-7.26	117.78	124.45
23	B	610	CLA	C2D-C1D-ND	7.26	115.45	110.10
23	C	513	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	c	507	CLA	C2D-C1D-ND	7.23	115.43	110.10
23	c	511	CLA	C2D-C1D-ND	7.23	115.43	110.10
23	b	608	CLA	C2D-C1D-ND	7.21	115.42	110.10
23	b	603	CLA	C2D-C1D-ND	7.19	115.41	110.10
23	b	611	CLA	CMD-C2D-C1D	7.18	137.36	124.71
23	b	601	CLA	C2D-C1D-ND	7.15	115.38	110.10
23	B	616	CLA	CHD-C4C-C3C	-7.13	114.36	124.84
24	A	407	PHO	O2D-CGD-CBD	7.11	120.01	111.00
23	B	606	CLA	CMD-C2D-C1D	7.09	137.22	124.71
23	A	406	CLA	CHD-C1D-ND	-7.05	117.97	124.45
23	c	506	CLA	C2D-C1D-ND	7.00	115.27	110.10
23	d	404	CLA	CHD-C1D-ND	-7.00	118.02	124.45
23	b	605	CLA	CMD-C2D-C1D	6.96	136.98	124.71
23	b	615	CLA	CMD-C2D-C1D	6.92	136.91	124.71
23	B	611	CLA	CHD-C4C-C3C	-6.89	114.71	124.84
23	b	616	CLA	C4A-NA-C1A	-6.89	103.61	106.71
23	C	502	CLA	C4A-NA-C1A	-6.88	103.61	106.71
23	B	614	CLA	CMD-C2D-C1D	6.85	136.79	124.71
23	C	507	CLA	C2D-C1D-ND	6.81	115.12	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	C4A-NA-C1A	-6.80	103.65	106.71
23	a	404	CLA	C2D-C1D-ND	6.80	115.11	110.10
23	C	507	CLA	CHD-C1D-ND	-6.77	118.23	124.45
23	B	606	CLA	CHD-C1D-ND	-6.77	118.23	124.45
23	b	605	CLA	CHD-C1D-ND	-6.76	118.24	124.45
23	B	602	CLA	CMD-C2D-C1D	6.76	136.62	124.71
23	b	606	CLA	CMD-C2D-C1D	6.75	136.60	124.71
23	C	508	CLA	CMD-C2D-C1D	6.74	136.59	124.71
23	b	616	CLA	CHD-C4C-C3C	-6.74	114.94	124.84
24	D	402	PHO	O2D-CGD-CBD	6.71	119.50	111.00
23	B	606	CLA	C4A-NA-C1A	-6.69	103.70	106.71
23	B	614	CLA	CHD-C4C-C3C	-6.69	115.01	124.84
23	B	614	CLA	O2D-CGD-CBD	6.67	123.12	111.27
23	b	616	CLA	O2D-CGD-CBD	6.64	123.08	111.27
33	b	622	HTG	C1'-S1-C1	6.64	112.50	100.09
23	b	605	CLA	CHD-C4C-C3C	-6.63	115.09	124.84
23	C	511	CLA	CMD-C2D-C1D	6.63	136.40	124.71
23	b	602	CLA	O2D-CGD-CBD	6.63	123.04	111.27
23	B	609	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	b	602	CLA	C4A-NA-C1A	-6.62	103.73	106.71
23	a	405	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
23	B	612	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	a	405	CLA	CHD-C1D-ND	-6.61	118.38	124.45
23	c	511	CLA	CMD-C2D-C1D	6.59	136.32	124.71
23	D	405	CLA	CHD-C1D-ND	-6.58	118.41	124.45
23	c	504	CLA	CMD-C2D-C1D	6.57	136.29	124.71
27	C	501	SQD	O6-C1-C2	6.57	118.56	108.30
23	A	408	CLA	CMD-C2D-C1D	6.56	136.28	124.71
23	D	405	CLA	C2C-C1C-NC	6.56	116.12	109.97
23	d	404	CLA	C4A-NA-C1A	-6.54	103.77	106.71
23	b	609	CLA	CHD-C1D-ND	-6.54	118.44	124.45
23	B	604	CLA	O2D-CGD-CBD	6.54	122.88	111.27
23	c	509	CLA	C2C-C1C-NC	6.51	116.08	109.97
23	b	609	CLA	C4A-NA-C1A	-6.50	103.78	106.71
23	c	514	CLA	CMD-C2D-C1D	6.50	136.16	124.71
23	d	404	CLA	CMD-C2D-C1D	6.49	136.16	124.71
23	C	504	CLA	CMD-C2D-C1D	6.49	136.15	124.71
23	C	502	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	C	504	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
23	C	512	CLA	CMD-C2D-C1D	6.43	136.04	124.71
23	b	603	CLA	CMD-C2D-C1D	6.43	136.04	124.71
23	C	513	CLA	O2D-CGD-CBD	6.42	122.67	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	CHD-C1D-ND	-6.40	118.58	124.45
23	c	508	CLA	O2D-CGD-CBD	6.39	122.63	111.27
23	c	502	CLA	CMD-C2D-C1D	6.38	135.96	124.71
23	b	611	CLA	CHD-C1D-ND	-6.38	118.59	124.45
23	b	608	CLA	CMD-C2D-C1D	6.37	135.94	124.71
23	A	404	CLA	CMD-C2D-C1D	6.37	135.93	124.71
23	d	403	CLA	C2C-C1C-NC	6.36	115.93	109.97
23	B	603	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
23	C	514	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
23	c	507	CLA	CMD-C2D-C1D	6.35	135.90	124.71
23	B	605	CLA	C4A-NA-C1A	-6.34	103.85	106.71
23	c	506	CLA	O2D-CGD-CBD	6.34	122.53	111.27
23	b	616	CLA	CMD-C2D-C1D	6.33	135.87	124.71
23	a	407	CLA	CHD-C4C-C3C	-6.32	115.54	124.84
23	B	602	CLA	CHD-C1D-ND	-6.32	118.64	124.45
23	b	608	CLA	C4A-NA-C1A	-6.31	103.87	106.71
23	B	612	CLA	O2D-CGD-CBD	6.29	122.45	111.27
23	c	514	CLA	CHD-C1D-ND	-6.29	118.67	124.45
23	b	610	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
23	C	502	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	b	613	CLA	C2C-C1C-NC	6.27	115.85	109.97
23	B	615	CLA	CHD-C1D-ND	-6.27	118.69	124.45
23	B	616	CLA	C4A-NA-C1A	-6.27	103.89	106.71
23	C	509	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	c	505	CLA	CMD-C2D-C1D	6.24	135.71	124.71
23	b	609	CLA	CMD-C2D-C1D	6.24	135.71	124.71
23	c	505	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	c	510	CLA	CMD-C2D-C1D	6.22	135.68	124.71
23	B	616	CLA	O2D-CGD-CBD	6.22	122.33	111.27
23	c	503	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	B	613	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	c	512	CLA	CHD-C1D-ND	-6.21	118.75	124.45
23	c	512	CLA	CMD-C2D-C1D	6.20	135.64	124.71
23	B	606	CLA	O2D-CGD-CBD	6.19	122.27	111.27
25	D	407	BCR	C7-C8-C9	-6.18	116.89	126.23
23	B	614	CLA	CHD-C1D-ND	-6.18	118.78	124.45
23	b	614	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
23	B	608	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
23	b	606	CLA	CHD-C1D-ND	-6.17	118.78	124.45
23	B	605	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	C	505	CLA	C2C-C1C-NC	6.16	115.75	109.97
23	A	405	CLA	CHD-C4C-C3C	-6.16	115.78	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	406	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	B	602	CLA	CHD-C4C-C3C	-6.15	115.81	124.84
23	b	615	CLA	C4A-NA-C1A	-6.14	103.95	106.71
23	C	509	CLA	O2D-CGD-CBD	6.13	122.16	111.27
23	b	601	CLA	CMD-C2D-C1D	6.13	135.51	124.71
23	b	614	CLA	O2D-CGD-CBD	6.13	122.16	111.27
23	A	404	CLA	CHD-C1D-ND	-6.13	118.82	124.45
23	C	502	CLA	CHD-C1D-ND	-6.12	118.83	124.45
23	c	507	CLA	C4A-NA-C1A	-6.12	103.95	106.71
23	c	507	CLA	CHD-C1D-ND	-6.11	118.83	124.45
23	B	603	CLA	CHD-C1D-ND	-6.11	118.84	124.45
23	b	611	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
23	C	508	CLA	O2D-CGD-CBD	6.09	122.09	111.27
23	b	608	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	B	603	CLA	O2D-CGD-CBD	6.07	122.06	111.27
23	c	512	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
23	A	408	CLA	CHD-C1D-ND	-6.06	118.88	124.45
23	A	406	CLA	C4A-NA-C1A	-6.06	103.98	106.71
23	B	604	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
23	c	503	CLA	CHD-C1D-ND	-6.04	118.90	124.45
23	A	405	CLA	CMD-C2D-C1D	6.03	135.34	124.71
23	b	604	CLA	O2D-CGD-CBD	6.03	121.98	111.27
23	C	513	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	A	408	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
23	a	404	CLA	CMD-C2D-C1D	5.99	135.28	124.71
23	B	609	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	B	608	CLA	CMD-C2D-C1D	5.98	135.25	124.71
23	c	508	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
23	b	601	CLA	O2D-CGD-CBD	5.96	121.86	111.27
23	C	511	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	c	509	CLA	O2D-CGD-CBD	5.96	121.86	111.27
23	b	602	CLA	CMD-C2D-C1D	5.96	135.22	124.71
23	c	502	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	B	601	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	c	513	CLA	C4A-NA-C1A	-5.96	104.03	106.71
23	B	607	CLA	C2C-C1C-NC	5.96	115.55	109.97
23	B	608	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	C	513	CLA	C4A-NA-C1A	-5.96	104.03	106.71
23	B	610	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	C	508	CLA	CHD-C1D-ND	-5.95	118.98	124.45
23	b	606	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	b	613	CLA	CMD-C2D-C1D	5.94	135.18	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	611	CLA	C4A-NA-C1A	-5.94	104.04	106.71
23	B	601	CLA	CMD-C2D-C1D	5.93	135.17	124.71
23	b	615	CLA	CHD-C1D-ND	-5.93	119.00	124.45
23	C	502	CLA	O2D-CGD-CBD	5.92	121.79	111.27
23	C	503	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	b	601	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	C	510	CLA	CMD-C2D-C1D	5.91	135.13	124.71
23	b	607	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
23	D	406	CLA	CMD-C2D-C1D	5.91	135.12	124.71
23	b	612	CLA	C4A-NA-C1A	-5.90	104.05	106.71
27	C	501	SQD	C1-O5-C5	-5.90	102.11	113.69
23	A	406	CLA	CMD-C2D-C1D	5.90	135.11	124.71
23	D	405	CLA	CMD-C2D-C1D	5.88	135.08	124.71
23	c	510	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	B	601	CLA	O2D-CGD-CBD	5.88	121.72	111.27
23	C	506	CLA	O2D-CGD-CBD	5.88	121.71	111.27
23	c	502	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	c	504	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	a	404	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	c	508	CLA	C4A-NA-C1A	-5.86	104.07	106.71
23	C	508	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
23	b	601	CLA	CHD-C1D-ND	-5.84	119.08	124.45
23	c	504	CLA	C4A-NA-C1A	-5.84	104.08	106.71
23	B	604	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	b	614	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	b	612	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	d	402	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	C	503	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	B	603	CLA	CMD-C2D-C1D	5.84	135.00	124.71
23	b	601	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	b	610	CLA	O2D-CGD-CBD	5.83	121.62	111.27
23	B	613	CLA	CHD-C1D-ND	-5.82	119.10	124.45
23	c	511	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	b	604	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
23	b	603	CLA	O2D-CGD-CBD	5.82	121.60	111.27
23	a	404	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
23	C	507	CLA	C2C-C1C-NC	5.81	115.42	109.97
23	C	504	CLA	CHD-C1D-ND	-5.81	119.12	124.45
23	A	405	CLA	CHD-C1D-ND	-5.81	119.12	124.45
23	C	510	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
27	D	415	SQD	O6-C1-C2	5.80	117.36	108.30
23	b	612	CLA	C2C-C1C-NC	5.80	115.41	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	C2C-C1C-NC	5.79	115.40	109.97
23	B	601	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	b	603	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	c	509	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
23	C	511	CLA	O2D-CGD-CBD	5.78	121.53	111.27
23	d	404	CLA	O2D-CGD-CBD	5.78	121.53	111.27
23	B	611	CLA	CMD-C2D-C1D	5.77	134.89	124.71
23	b	612	CLA	O2D-CGD-CBD	5.76	121.50	111.27
23	B	615	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	c	513	CLA	O2D-CGD-CBD	5.76	121.50	111.27
23	C	512	CLA	CHD-C1D-ND	-5.75	119.17	124.45
23	c	507	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	b	607	CLA	C2C-C1C-NC	5.74	115.35	109.97
23	b	614	CLA	CHD-C1D-ND	-5.74	119.18	124.45
23	b	603	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
23	B	603	CLA	C4A-NA-C1A	-5.74	104.13	106.71
23	B	614	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
23	c	505	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
23	c	505	CLA	C2C-C1C-NC	5.73	115.34	109.97
23	B	605	CLA	CMD-C2D-C1D	5.72	134.80	124.71
23	b	612	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	c	506	CLA	CMD-C2D-C1D	5.72	134.79	124.71
23	B	606	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	C	514	CLA	CMD-C2D-C1D	5.70	134.75	124.71
23	b	609	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
23	B	610	CLA	O2D-CGD-CBD	5.67	121.34	111.27
23	d	404	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
23	C	506	CLA	CMD-C2D-C1D	5.65	134.68	124.71
23	C	512	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
23	B	609	CLA	C4A-NA-C1A	-5.65	104.17	106.71
23	b	606	CLA	O2D-CGD-CBD	5.64	121.30	111.27
23	c	513	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	b	616	CLA	CHD-C1D-ND	-5.64	119.27	124.45
23	C	510	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	C	507	CLA	C4A-NA-C1A	-5.63	104.17	106.71
29	a	414	PL9	C7-C3-C4	5.63	121.45	116.88
23	b	610	CLA	C4A-NA-C1A	-5.63	104.18	106.71
23	d	403	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
23	C	505	CLA	CMD-C2D-C1D	5.62	134.61	124.71
23	B	614	CLA	C2C-C1C-NC	5.61	115.23	109.97
23	c	514	CLA	C4A-NA-C1A	-5.61	104.18	106.71
23	C	505	CLA	CHD-C4C-C3C	-5.61	116.59	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	514	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	B	607	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	C	509	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	c	506	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	B	605	CLA	CHD-C1D-ND	-5.59	119.31	124.45
23	b	607	CLA	CHD-C1D-ND	-5.59	119.32	124.45
23	b	615	CLA	C2C-C1C-NC	5.59	115.20	109.97
23	A	404	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	C	506	CLA	CHD-C1D-ND	-5.58	119.33	124.45
33	c	522	HTG	C1'-S1-C1	5.57	110.52	100.09
33	B	622	HTG	C1'-S1-C1	5.57	110.50	100.09
40	V	201	HEC	CBD-CAD-C3D	-5.57	103.12	112.62
23	C	511	CLA	C2C-C1C-NC	5.57	115.19	109.97
33	h	101	HTG	C1'-S1-C1	5.55	110.48	100.09
23	d	403	CLA	CMD-C2D-C1D	5.55	134.50	124.71
23	b	604	CLA	CMD-C2D-C1D	5.55	134.49	124.71
23	b	607	CLA	CMD-C2D-C1D	5.54	134.48	124.71
25	Y	101	BCR	C33-C5-C6	-5.53	118.31	124.53
25	k	102	BCR	C33-C5-C6	-5.53	118.32	124.53
23	C	505	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	C	511	CLA	CHD-C1D-ND	-5.53	119.38	124.45
23	C	506	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	c	510	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	c	504	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
23	B	607	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
23	B	612	CLA	C3C-C4C-NC	5.50	116.74	110.57
23	B	606	CLA	C2C-C1C-NC	5.49	115.11	109.97
23	c	503	CLA	C2C-C1C-NC	5.49	115.11	109.97
23	D	406	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	b	610	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	C	514	CLA	C2C-C1C-NC	5.48	115.10	109.97
23	b	613	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
23	c	506	CLA	C4A-NA-C1A	-5.48	104.24	106.71
23	C	510	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	B	604	CLA	C2C-C1C-NC	5.47	115.10	109.97
23	c	506	CLA	C2C-C1C-NC	5.47	115.10	109.97
23	c	509	CLA	CMD-C2D-C1D	5.46	134.33	124.71
23	B	603	CLA	C2C-C1C-NC	5.46	115.08	109.97
23	b	611	CLA	O2D-CGD-CBD	5.45	120.96	111.27
23	b	602	CLA	CHD-C1D-ND	-5.45	119.44	124.45
23	c	504	CLA	CHD-C1D-ND	-5.45	119.45	124.45
23	b	615	CLA	CHD-C4C-C3C	-5.45	116.84	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	CMD-C2D-C1D	5.44	134.31	124.71
23	C	512	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	B	609	CLA	C2C-C1C-NC	5.44	115.07	109.97
27	B	620	SQD	O47-C7-C8	5.44	123.22	111.50
23	b	611	CLA	C2C-C1C-NC	5.42	115.05	109.97
33	D	413	HTG	C1'-S1-C1	5.42	110.22	100.09
23	a	407	CLA	CMD-C2D-C1D	5.41	134.26	124.71
23	C	503	CLA	CHD-C1D-ND	-5.40	119.49	124.45
23	b	608	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
23	A	405	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
23	c	507	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
23	a	404	CLA	CHD-C1D-ND	-5.39	119.50	124.45
23	B	612	CLA	CHD-C1D-ND	-5.39	119.50	124.45
23	B	605	CLA	O2D-CGD-CBD	5.39	120.84	111.27
23	b	607	CLA	C3D-C2D-C1D	-5.38	98.48	105.83
23	b	602	CLA	C2C-C1C-NC	5.38	115.02	109.97
23	d	402	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	C	508	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	c	504	CLA	O2D-CGD-CBD	5.36	120.79	111.27
23	B	613	CLA	CMD-C2D-C1D	5.36	134.16	124.71
23	B	616	CLA	CMD-C2D-C1D	5.36	134.15	124.71
23	C	506	CLA	C2C-C1C-NC	5.35	114.99	109.97
27	L	102	SQD	O6-C1-C2	5.35	116.66	108.30
23	B	611	CLA	CHD-C1D-ND	-5.35	119.54	124.45
23	c	511	CLA	CHD-C1D-ND	-5.34	119.54	124.45
23	c	511	CLA	C2C-C1C-NC	5.34	114.97	109.97
23	c	502	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	A	406	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
23	b	610	CLA	C2C-C1C-NC	5.33	114.96	109.97
33	C	522	HTG	C1'-S1-C1	5.32	110.05	100.09
23	C	505	CLA	O2D-CGD-CBD	5.32	120.72	111.27
23	d	402	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	B	604	CLA	C4A-NA-C1A	-5.32	104.32	106.71
29	A	413	PL9	C7-C3-C4	5.31	121.19	116.88
23	C	506	CLA	C4A-NA-C1A	-5.30	104.32	106.71
23	b	602	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
23	B	613	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
27	C	501	SQD	C1-C2-C3	-5.28	98.99	110.00
23	A	405	CLA	C2C-C1C-NC	5.28	114.92	109.97
23	c	505	CLA	O2D-CGD-CBD	5.28	120.65	111.27
23	B	611	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	B	611	CLA	C3D-C2D-C1D	-5.27	98.64	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C4A-NA-C1A	-5.27	104.34	106.71
23	B	608	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	B	613	CLA	C1-C2-C3	-5.26	116.94	126.04
23	A	404	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
23	B	615	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
23	c	513	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	d	402	CLA	CMD-C2D-C1D	5.23	133.93	124.71
23	b	608	CLA	C2C-C1C-NC	5.22	114.86	109.97
23	c	506	CLA	CHD-C1D-ND	-5.22	119.66	124.45
23	b	603	CLA	C4A-NA-C1A	-5.22	104.36	106.71
23	C	510	CLA	O2D-CGD-CBD	5.22	120.54	111.27
23	c	512	CLA	C2C-C1C-NC	5.19	114.84	109.97
23	A	408	CLA	C2C-C1C-NC	5.19	114.84	109.97
23	B	613	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	A	406	CLA	C2C-C1C-NC	5.18	114.83	109.97
23	a	405	CLA	CMD-C2D-C1D	5.18	133.84	124.71
23	c	502	CLA	O2D-CGD-CBD	5.18	120.46	111.27
23	a	405	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
23	b	601	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	b	616	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
23	B	610	CLA	C4A-NA-C1A	-5.16	104.39	106.71
23	d	402	CLA	CHD-C1D-ND	-5.15	119.72	124.45
23	C	504	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
23	B	606	CLA	C3D-C2D-C1D	-5.15	98.81	105.83
27	a	409	SQD	O6-C1-C2	5.15	116.34	108.30
23	b	605	CLA	C4A-NA-C1A	-5.14	104.39	106.71
23	D	405	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
23	C	513	CLA	C2C-C1C-NC	5.14	114.79	109.97
23	c	514	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	b	612	CLA	C1-C2-C3	-5.13	117.18	126.04
23	a	407	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	b	614	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	b	612	CLA	CHD-C1D-ND	-5.12	119.75	124.45
23	A	408	CLA	C4A-NA-C1A	-5.11	104.41	106.71
23	c	510	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
23	b	603	CLA	CHD-C1D-ND	-5.10	119.77	124.45
23	c	513	CLA	CMD-C2D-C1D	5.10	133.70	124.71
27	C	501	SQD	O9-S-C6	5.09	112.99	106.94
23	C	503	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	A	405	CLA	O2D-CGD-CBD	5.09	120.32	111.27
23	c	514	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	d	403	CLA	C4A-NA-C1A	-5.09	104.42	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	C3C-C4C-NC	5.08	116.27	110.57
23	C	510	CLA	C4A-NA-C1A	-5.08	104.42	106.71
23	b	613	CLA	CHD-C1D-ND	-5.08	119.78	124.45
27	f	102	SQD	O47-C7-C8	5.08	122.44	111.50
23	B	616	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
23	B	612	CLA	C2C-C1C-NC	5.06	114.71	109.97
27	L	102	SQD	O47-C7-C8	5.05	122.38	111.50
24	a	416	PHO	C1-C2-C3	-5.04	117.33	126.04
23	a	404	CLA	C4A-NA-C1A	-5.03	104.44	106.71
23	B	611	CLA	C3C-C4C-NC	5.03	116.22	110.57
23	b	605	CLA	O2D-CGD-CBD	5.03	120.20	111.27
23	b	607	CLA	O2D-CGD-CBD	5.02	120.20	111.27
23	d	403	CLA	CHD-C1D-ND	-5.02	119.84	124.45
23	A	406	CLA	O2D-CGD-CBD	5.02	120.18	111.27
23	B	612	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
23	a	407	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	D	406	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	C	503	CLA	C2C-C1C-NC	4.99	114.65	109.97
23	B	615	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	A	406	CLA	C3D-C4D-ND	4.98	118.30	110.24
23	B	610	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	c	509	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	D	406	CLA	C4A-NA-C1A	-4.97	104.47	106.71
23	B	607	CLA	CMD-C2D-C1D	4.97	133.48	124.71
23	a	407	CLA	CHD-C1D-ND	-4.97	119.89	124.45
23	C	502	CLA	C2C-C1C-NC	4.97	114.63	109.97
23	C	504	CLA	C2C-C1C-NC	4.96	114.62	109.97
23	A	408	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	c	505	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	B	603	CLA	C3C-C4C-NC	4.94	116.11	110.57
23	b	606	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	C	503	CLA	O2D-CGD-CBD	4.94	120.05	111.27
27	D	415	SQD	O47-C7-C8	4.94	122.14	111.50
23	b	608	CLA	O2D-CGD-CBD	4.94	120.04	111.27
23	b	605	CLA	C3D-C4D-ND	4.93	118.22	110.24
23	C	513	CLA	CHD-C1D-ND	-4.93	119.92	124.45
23	B	603	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
23	B	604	CLA	C3C-C4C-NC	4.93	116.09	110.57
23	d	402	CLA	O2D-CGD-CBD	4.91	120.00	111.27
23	D	405	CLA	C1C-C2C-C3C	-4.91	101.80	106.96
23	B	615	CLA	C4A-NA-C1A	-4.91	104.50	106.71
23	c	504	CLA	C3D-C2D-C1D	-4.90	99.14	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	611	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	b	605	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	B	607	CLA	O2D-CGD-CBD	4.89	119.96	111.27
23	C	507	CLA	O2D-CGD-CBD	4.89	119.96	111.27
23	c	510	CLA	O2D-CGD-CBD	4.89	119.96	111.27
23	B	607	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
38	E	103	HEM	CAD-CBD-CGD	4.89	124.12	113.60
23	d	402	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	B	612	CLA	CMD-C2D-C1D	4.87	133.30	124.71
23	c	502	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	C	505	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
25	b	617	BCR	C7-C8-C9	-4.86	118.89	126.23
23	B	616	CLA	CHD-C1D-ND	-4.86	119.99	124.45
23	c	503	CLA	CMD-C2D-C1D	4.85	133.27	124.71
23	C	507	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
23	C	509	CLA	CHD-C1D-ND	-4.84	120.00	124.45
23	c	508	CLA	CMC-C2C-C1C	4.83	132.40	125.04
25	T	101	BCR	C15-C16-C17	-4.82	113.59	123.47
23	A	404	CLA	CAA-C2A-C3A	-4.82	99.59	112.78
24	D	402	PHO	C1-C2-C3	-4.82	117.71	126.04
23	a	405	CLA	C3D-C4D-ND	4.81	118.03	110.24
23	B	608	CLA	O2D-CGD-CBD	4.80	119.80	111.27
23	B	611	CLA	O2D-CGD-CBD	4.80	119.80	111.27
23	C	509	CLA	CMD-C2D-C1D	4.80	133.17	124.71
23	C	512	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	b	614	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
23	b	614	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	a	404	CLA	C1D-CHD-C4C	-4.79	115.72	126.06
23	C	502	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	609	CLA	O2D-CGD-CBD	4.78	119.77	111.27
23	c	512	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	c	508	CLA	C3D-C2D-C1D	-4.77	99.31	105.83
23	b	604	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	B	610	CLA	CHD-C4C-C3C	-4.76	117.85	124.84
23	B	610	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	b	612	CLA	C3C-C4C-NC	4.75	115.89	110.57
23	a	407	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	B	601	CLA	C2C-C1C-NC	4.74	114.42	109.97
23	c	503	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	d	404	CLA	C3D-C2D-C1D	-4.74	99.37	105.83
23	c	513	CLA	CHD-C1D-ND	-4.74	120.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	C2C-C1C-NC	4.73	114.40	109.97
23	c	503	CLA	C3D-C4D-ND	4.72	117.88	110.24
23	B	609	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	B	601	CLA	C4A-NA-C1A	-4.72	104.58	106.71
23	C	509	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
23	b	613	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	C	511	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	b	615	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	509	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	b	605	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	A	408	CLA	O2D-CGD-CBD	4.68	119.59	111.27
23	B	612	CLA	O2D-CGD-O1D	-4.68	114.68	123.84
29	a	414	PL9	C15-C14-C16	4.68	123.14	115.27
23	D	405	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	B	605	CLA	C2C-C1C-NC	4.67	114.35	109.97
23	c	505	CLA	C4A-NA-C1A	-4.67	104.61	106.71
25	d	405	BCR	C7-C8-C9	-4.67	119.18	126.23
23	B	614	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	b	609	CLA	C3D-C2D-C1D	-4.66	99.46	105.83
23	C	503	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	d	403	CLA	C3C-C4C-NC	4.66	115.80	110.57
23	c	511	CLA	O2D-CGD-CBD	4.66	119.55	111.27
23	B	605	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	C	503	CLA	C3C-C4C-NC	4.65	115.79	110.57
33	b	624	HTG	C1'-S1-C1	4.65	108.79	100.09
23	c	510	CLA	C1-C2-C3	-4.65	118.01	126.04
23	c	503	CLA	O2D-CGD-CBD	4.64	119.52	111.27
23	b	606	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	B	605	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	c	506	CLA	C3C-C4C-NC	4.63	115.77	110.57
23	B	602	CLA	O2D-CGD-CBD	4.63	119.50	111.27
23	C	514	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	C	505	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
23	b	610	CLA	CHD-C1D-ND	-4.61	120.21	124.45
23	D	406	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
23	C	514	CLA	C4A-NA-C1A	-4.61	104.63	106.71
23	c	512	CLA	O2D-CGD-CBD	4.60	119.45	111.27
34	b	626	LMT	C1'-O5'-C5'	4.60	122.72	113.69
23	c	510	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	a	407	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	B	609	CLA	C3C-C4C-NC	4.58	115.71	110.57
38	f	101	HEM	CAD-CBD-CGD	4.57	123.44	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C3C-C4C-NC	4.57	115.70	110.57
23	c	503	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
29	a	414	PL9	C37-C38-C39	-4.57	116.66	127.66
23	C	510	CLA	C3C-C4C-NC	4.57	115.69	110.57
23	C	514	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	c	514	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	d	403	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	C	508	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	c	510	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	c	511	CLA	C4A-NA-C1A	-4.54	104.66	106.71
23	d	403	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
23	C	514	CLA	C3C-C4C-NC	4.53	115.66	110.57
23	a	407	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	d	404	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	B	601	CLA	C3D-C4D-ND	4.52	117.56	110.24
23	C	509	CLA	O2D-CGD-O1D	-4.52	115.00	123.84
23	b	602	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	B	601	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	B	605	CLA	C3C-C4C-NC	4.51	115.63	110.57
25	d	405	BCR	C15-C14-C13	-4.51	120.88	127.31
23	B	602	CLA	C3D-C4D-ND	4.51	117.53	110.24
23	b	610	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	D	406	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	D	405	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	b	607	CLA	C3C-C4C-NC	4.48	115.59	110.57
31	Z	101	LMG	O7-C10-C11	4.47	121.14	111.50
27	B	620	SQD	O6-C1-C2	4.47	115.29	108.30
33	h	101	HTG	O5-C5-C4	4.47	117.82	109.69
23	a	405	CLA	C3C-C4C-NC	4.47	115.58	110.57
23	c	509	CLA	CHD-C1D-ND	-4.47	120.35	124.45
23	B	607	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
38	f	101	HEM	CHC-C4B-NB	4.46	129.28	124.43
23	D	406	CLA	C3D-C4D-ND	4.46	117.45	110.24
23	a	405	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	c	504	CLA	C3C-C4C-NC	4.45	115.56	110.57
23	b	613	CLA	C1-C2-C3	-4.45	118.35	126.04
23	B	607	CLA	C4A-NA-C1A	-4.45	104.71	106.71
23	b	613	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	B	602	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	C	508	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	C	510	CLA	C3D-C2D-C1D	-4.44	99.77	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C3D-C4D-ND	4.43	117.41	110.24
23	b	616	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	B	608	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
23	A	404	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
23	B	610	CLA	CAC-C3C-C4C	4.42	130.55	124.81
31	C	521	LMG	O6-C5-C4	4.42	117.72	109.69
23	b	603	CLA	C1D-CHD-C4C	-4.42	116.53	126.06
23	b	609	CLA	C3D-C4D-ND	4.42	117.38	110.24
23	C	511	CLA	C4A-NA-C1A	-4.42	104.72	106.71
23	B	608	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	c	509	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	B	613	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
23	b	609	CLA	C2C-C1C-NC	4.40	114.10	109.97
23	B	612	CLA	CMC-C2C-C1C	4.40	131.74	125.04
23	b	601	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	b	610	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	B	609	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	C	502	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	D	406	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	C	506	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	B	604	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	c	512	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	B	611	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	a	405	CLA	C2C-C1C-NC	4.39	114.09	109.97
29	A	413	PL9	C15-C14-C16	4.39	122.66	115.27
23	b	611	CLA	C3C-C4C-NC	4.39	115.49	110.57
23	b	604	CLA	CHD-C1D-ND	-4.39	120.42	124.45
34	C	525	LMT	C1'-O5'-C5'	4.39	122.30	113.69
23	b	613	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	d	404	CLA	C2C-C1C-NC	4.39	114.08	109.97
23	A	404	CLA	C3D-C4D-ND	4.38	117.32	110.24
27	C	501	SQD	O47-C7-C8	4.37	120.93	111.50
27	a	409	SQD	O47-C7-C8	4.37	120.93	111.50
23	c	508	CLA	C2C-C1C-NC	4.37	114.07	109.97
23	a	404	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	c	504	CLA	C1D-CHD-C4C	-4.36	116.64	126.06
23	b	605	CLA	C4-C3-C5	4.36	122.60	115.27
23	A	408	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	B	613	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	D	405	CLA	C1-C2-C3	-4.35	118.51	126.04
23	C	512	CLA	O2D-CGD-CBD	4.35	119.00	111.27
24	a	416	PHO	C4-C3-C5	4.35	122.59	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	514	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	b	607	CLA	C4A-NA-C1A	-4.35	104.75	106.71
23	C	504	CLA	C1D-CHD-C4C	-4.35	116.67	126.06
23	C	513	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
23	b	601	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
23	b	609	CLA	C3C-C4C-NC	4.34	115.44	110.57
23	b	602	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
23	B	613	CLA	CAC-C3C-C4C	4.34	130.44	124.81
23	a	404	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
23	B	603	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	b	608	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	c	506	CLA	C3D-C4D-ND	4.32	117.23	110.24
23	c	509	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	B	604	CLA	CHD-C1D-ND	-4.32	120.48	124.45
38	E	103	HEM	CHC-C4B-NB	4.32	129.12	124.43
23	C	512	CLA	CAC-C3C-C4C	4.31	130.41	124.81
23	C	502	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	b	605	CLA	C3C-C4C-NC	4.31	115.40	110.57
23	B	614	CLA	O2D-CGD-O1D	-4.31	115.42	123.84
23	B	613	CLA	C3B-C4B-NB	4.31	114.78	109.21
27	D	415	SQD	C44-O6-C1	-4.31	105.33	113.74
23	A	405	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
23	c	505	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	d	402	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	c	513	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
23	b	606	CLA	C3C-C4C-NC	4.28	115.38	110.57
23	b	607	CLA	C3B-C4B-NB	4.28	114.75	109.21
23	b	606	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
23	B	615	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	b	603	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	c	514	CLA	O2D-CGD-CBD	4.27	118.85	111.27
31	M	101	LMG	O7-C10-C11	4.27	120.70	111.50
23	b	604	CLA	C3C-C4C-NC	4.27	115.36	110.57
25	t	102	BCR	C33-C5-C6	-4.27	119.74	124.53
23	b	614	CLA	C3D-C4D-ND	4.26	117.13	110.24
23	C	507	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	B	616	CLA	C2C-C1C-NC	4.25	113.96	109.97
23	C	510	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	A	408	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	c	507	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	B	606	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	A	405	CLA	C3D-C4D-ND	4.25	117.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	407	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	b	603	CLA	C3D-C4D-ND	4.24	117.10	110.24
23	c	514	CLA	C3D-C4D-ND	4.24	117.10	110.24
23	B	611	CLA	C1-C2-C3	-4.24	118.72	126.04
23	a	404	CLA	CAA-C2A-C3A	-4.23	101.18	112.78
23	C	513	CLA	C3C-C4C-NC	4.23	115.32	110.57
29	d	406	PL9	C42-C43-C44	-4.23	117.47	127.66
23	c	513	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	c	507	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
25	C	516	BCR	C7-C8-C9	-4.22	119.85	126.23
23	b	603	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
23	C	506	CLA	C3C-C4C-NC	4.22	115.31	110.57
27	A	411	SQD	C3-C4-C5	4.22	117.77	110.24
23	C	504	CLA	C3C-C4C-NC	4.22	115.30	110.57
23	c	511	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	c	502	CLA	C3C-C4C-NC	4.21	115.30	110.57
23	b	612	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	b	615	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	b	616	CLA	C2C-C1C-NC	4.20	113.91	109.97
23	c	504	CLA	C3D-C4D-ND	4.20	117.04	110.24
23	B	613	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	C	512	CLA	C3B-C4B-NB	4.20	114.64	109.21
34	M	104	LMT	O5'-C5'-C4'	4.20	118.60	109.75
23	c	511	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	b	610	CLA	O2A-CGA-CBA	4.19	125.06	111.91
23	C	509	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	c	502	CLA	C3D-C4D-ND	4.18	116.99	110.24
23	B	607	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	b	610	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	b	611	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	C	511	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	d	402	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	C	511	CLA	C1-C2-C3	-4.16	118.85	126.04
23	b	613	CLA	O2A-CGA-O1A	-4.16	113.10	123.59
23	B	602	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	B	608	CLA	C3C-C4C-NC	4.15	115.22	110.57
33	B	621	HTG	O5-C1-C2	4.15	115.53	110.31
23	C	507	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	c	502	CLA	C4A-NA-C1A	-4.14	104.84	106.71
25	T	101	BCR	C11-C10-C9	-4.14	121.41	127.31
23	b	616	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
23	C	511	CLA	C1C-C2C-C3C	-4.13	102.61	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	C3D-C4D-ND	4.13	116.92	110.24
32	A	416	LHG	O7-C7-C8	4.13	120.40	111.50
23	A	406	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
23	c	512	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	B	616	CLA	C1D-CHD-C4C	-4.13	117.16	126.06
23	A	404	CLA	C3C-C4C-NC	4.12	115.20	110.57
23	C	513	CLA	C1D-CHD-C4C	-4.12	117.16	126.06
23	C	512	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	D	405	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	b	610	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	C	504	CLA	O2D-CGD-CBD	4.12	118.58	111.27
25	Y	101	BCR	C16-C17-C18	-4.11	121.45	127.31
23	c	508	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	C	504	CLA	C3D-C4D-ND	4.10	116.87	110.24
25	k	102	BCR	C15-C14-C13	-4.10	121.46	127.31
23	c	510	CLA	C3D-C4D-ND	4.09	116.86	110.24
23	c	510	CLA	CAC-C3C-C4C	4.09	130.12	124.81
31	C	521	LMG	O7-C10-C11	4.09	120.32	111.50
23	b	604	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	A	405	CLA	C3C-C4C-NC	4.09	115.16	110.57
23	C	503	CLA	C3D-C4D-ND	4.09	116.85	110.24
23	c	502	CLA	O2D-CGD-O1D	-4.09	115.85	123.84
23	b	608	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
23	b	614	CLA	C3C-C4C-NC	4.08	115.15	110.57
27	a	411	SQD	O47-C7-C8	4.08	120.29	111.50
23	B	604	CLA	C1D-CHD-C4C	-4.08	117.27	126.06
23	c	504	CLA	CAC-C3C-C4C	4.07	130.09	124.81
29	a	414	PL9	C7-C3-C2	-4.07	117.95	123.30
23	B	615	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
40	v	203	HEC	CBD-CAD-C3D	-4.06	105.68	112.62
23	C	511	CLA	C3C-C4C-NC	4.06	115.13	110.57
31	a	417	LMG	O7-C10-C11	4.06	120.26	111.50
23	B	612	CLA	C3D-C4D-ND	4.06	116.81	110.24
23	C	502	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
23	c	513	CLA	C3C-C4C-NC	4.06	115.12	110.57
38	E	103	HEM	CBA-CAA-C2A	-4.06	105.69	112.62
25	b	619	BCR	C38-C26-C25	-4.06	119.97	124.53
23	C	512	CLA	C3C-C4C-NC	4.05	115.12	110.57
23	c	512	CLA	C4A-NA-C1A	-4.05	104.89	106.71
23	b	612	CLA	C3D-C4D-ND	4.05	116.78	110.24
35	C	517	DGD	O1G-C1A-C2A	4.05	124.61	111.91
23	c	511	CLA	C1C-C2C-C3C	-4.04	102.71	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	415	LMG	O7-C10-C11	4.04	120.20	111.50
23	C	509	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
23	B	607	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	b	601	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
23	b	603	CLA	CAA-C2A-C3A	-4.03	101.74	112.78
23	C	507	CLA	CAC-C3C-C4C	4.03	130.04	124.81
23	C	505	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	a	404	CLA	C3B-C4B-NB	4.02	114.41	109.21
23	b	606	CLA	C4-C3-C5	4.02	122.04	115.27
27	a	409	SQD	C1-O5-C5	-4.02	105.79	113.69
23	A	404	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
23	c	509	CLA	C1-C2-C3	-4.01	119.10	126.04
23	b	612	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
23	B	610	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	b	614	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	b	615	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
32	E	101	LHG	O7-C7-C8	4.01	120.14	111.50
23	d	404	CLA	O2D-CGD-O1D	-4.01	116.01	123.84
25	d	405	BCR	C38-C26-C25	-4.00	120.03	124.53
40	v	203	HEC	CMC-C2C-C1C	-4.00	122.31	128.46
25	K	101	BCR	C7-C8-C9	-4.00	120.19	126.23
23	b	607	CLA	C3D-C4D-ND	4.00	116.71	110.24
23	D	406	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
25	C	515	BCR	C7-C8-C9	-4.00	120.20	126.23
23	b	613	CLA	C3B-C4B-NB	3.99	114.37	109.21
23	C	513	CLA	C3D-C4D-ND	3.99	116.69	110.24
23	c	511	CLA	C3B-C4B-NB	3.98	114.36	109.21
23	c	503	CLA	C4A-NA-C1A	-3.98	104.92	106.71
23	c	505	CLA	C3C-C4C-NC	3.98	115.03	110.57
23	C	509	CLA	C3B-C4B-NB	3.97	114.35	109.21
23	c	507	CLA	O2D-CGD-CBD	3.97	118.33	111.27
23	b	616	CLA	C3D-C4D-ND	3.97	116.67	110.24
23	C	509	CLA	C4A-NA-C1A	-3.97	104.92	106.71
23	b	606	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	b	613	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	B	604	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	c	513	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
23	b	602	CLA	C3C-C4C-NC	3.96	115.01	110.57
29	A	413	PL9	C37-C38-C39	-3.96	118.13	127.66
23	B	613	CLA	O2D-CGD-CBD	3.96	118.30	111.27
23	c	509	CLA	C3B-C4B-NB	3.95	114.32	109.21
23	b	607	CLA	C1C-C2C-C3C	-3.95	102.80	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	b	606	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
23	b	612	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	d	402	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	602	CLA	CAC-C3C-C4C	3.95	129.93	124.81
23	b	613	CLA	O2A-CGA-CBA	3.94	124.27	111.91
23	c	510	CLA	C3B-C4B-NB	3.94	114.30	109.21
23	C	514	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
23	c	503	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	B	614	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
23	B	605	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
29	A	413	PL9	C27-C28-C29	-3.94	118.18	127.66
23	A	405	CLA	CBC-CAC-C3C	-3.93	101.59	112.43
23	c	505	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
23	b	603	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
23	B	601	CLA	C3C-C4C-NC	3.93	114.98	110.57
23	b	610	CLA	C1-C2-C3	-3.93	119.24	126.04
23	B	612	CLA	C4A-NA-C1A	-3.93	104.94	106.71
23	b	613	CLA	C4A-NA-C1A	-3.93	104.94	106.71
25	d	405	BCR	C33-C5-C6	-3.92	120.12	124.53
23	B	616	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	d	402	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
23	C	509	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
23	C	505	CLA	C4A-NA-C1A	-3.91	104.95	106.71
23	B	603	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
34	a	412	LMT	C1B-O5B-C5B	3.91	121.37	113.69
27	a	409	SQD	O8-S-C6	3.91	111.97	105.74
31	Z	101	LMG	C1-C2-C3	3.91	118.14	110.00
25	h	102	BCR	C7-C8-C9	-3.91	120.33	126.23
40	V	201	HEC	C1D-C2D-C3D	-3.91	104.28	107.00
23	B	611	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
23	b	605	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
23	a	407	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
23	B	614	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	c	509	CLA	C3D-C4D-ND	3.90	116.55	110.24
31	c	521	LMG	O7-C10-C11	3.90	119.90	111.50
23	a	404	CLA	C3D-C2D-C1D	-3.89	100.52	105.83
23	A	404	CLA	O2A-CGA-CBA	3.89	124.12	111.91
23	A	408	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	c	509	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
23	b	616	CLA	O2D-CGD-O1D	-3.88	116.24	123.84
23	A	405	CLA	C1D-CHD-C4C	-3.88	117.70	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C3D-C4D-ND	3.87	116.51	110.24
23	c	510	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
23	c	511	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
23	B	601	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
23	C	510	CLA	C1-C2-C3	-3.86	119.37	126.04
23	c	511	CLA	CBC-CAC-C3C	-3.86	101.79	112.43
27	a	409	SQD	C1-C2-C3	-3.86	101.97	110.00
23	b	608	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	B	612	CLA	C1-C2-C3	-3.85	119.38	126.04
23	c	514	CLA	CAC-C3C-C4C	3.84	129.79	124.81
23	b	614	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
23	C	511	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
29	D	408	PL9	C42-C43-C44	-3.83	118.45	127.66
23	B	613	CLA	CMC-C2C-C1C	3.82	130.86	125.04
23	c	502	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
27	B	620	SQD	C3-C4-C5	3.82	117.06	110.24
23	B	602	CLA	CMC-C2C-C1C	3.82	130.86	125.04
23	B	609	CLA	O2D-CGD-CBD	3.82	118.06	111.27
23	B	606	CLA	C3B-C4B-NB	3.82	114.14	109.21
23	b	612	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
23	B	602	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
25	c	515	BCR	C15-C14-C13	-3.81	121.88	127.31
23	B	611	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
23	B	608	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
23	C	508	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
23	A	406	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
23	b	608	CLA	C3C-C4C-NC	3.79	114.83	110.57
23	b	604	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
23	c	508	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
23	b	615	CLA	O2D-CGD-CBD	3.79	118.00	111.27
23	b	611	CLA	C3B-C4B-NB	3.79	114.11	109.21
32	d	409	LHG	O7-C7-C8	3.79	119.67	111.50
23	b	607	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
31	C	521	LMG	C3-C4-C5	3.79	117.00	110.24
23	c	507	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
23	C	512	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
23	B	606	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
38	E	103	HEM	C1B-NB-C4B	3.77	108.97	105.07
32	L	101	LHG	O7-C7-C8	3.77	119.63	111.50
23	c	514	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	a	407	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
25	C	515	BCR	C33-C5-C6	-3.76	120.30	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	611	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
32	D	410	LHG	O7-C7-C8	3.76	119.61	111.50
27	D	415	SQD	C1-C2-C3	-3.76	102.16	110.00
23	a	404	CLA	O2D-CGD-CBD	3.76	117.95	111.27
23	b	602	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
34	M	104	LMT	C1'-O5'-C5'	3.76	121.06	113.69
23	C	507	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
31	c	520	LMG	O7-C10-C11	3.75	119.59	111.50
23	C	513	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	c	506	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	B	615	CLA	CED-O2D-CGD	3.75	124.42	115.94
23	A	404	CLA	C3B-C4B-NB	3.74	114.05	109.21
31	z	101	LMG	O7-C10-C11	3.74	119.57	111.50
23	b	612	CLA	CAC-C3C-C4C	3.74	129.67	124.81
23	C	505	CLA	C3B-C4B-NB	3.74	114.05	109.21
23	B	602	CLA	C2C-C1C-NC	3.74	113.48	109.97
23	B	606	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	C	502	CLA	C1-C2-C3	-3.74	119.58	126.04
23	c	510	CLA	C3C-C4C-NC	3.74	114.76	110.57
23	b	615	CLA	C3C-C4C-NC	3.74	114.76	110.57
29	D	408	PL9	C25-C24-C26	3.73	121.55	115.27
23	b	601	CLA	C3C-C4C-NC	3.73	114.75	110.57
23	c	506	CLA	C3D-C2D-C1D	-3.73	100.75	105.83
23	a	404	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	c	511	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	C	514	CLA	C1-C2-C3	-3.72	119.61	126.04
23	c	514	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
23	C	505	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
23	b	605	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
23	B	614	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	A	406	CLA	C3C-C4C-NC	3.71	114.73	110.57
35	c	517	DGD	O2G-C1B-C2B	3.71	119.50	111.50
23	A	408	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
23	c	505	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
25	Y	101	BCR	C15-C14-C13	-3.70	122.03	127.31
25	C	515	BCR	C15-C14-C13	-3.70	122.03	127.31
23	B	605	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
23	b	613	CLA	O2D-CGD-CBD	3.70	117.84	111.27
35	C	518	DGD	O2G-C1B-C2B	3.70	119.47	111.50
29	a	414	PL9	C27-C28-C29	-3.69	118.76	127.66
23	b	610	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
23	C	508	CLA	C3D-C4D-ND	3.69	116.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C3D-C2D-C1D	-3.69	100.79	105.83
23	D	405	CLA	O2D-CGD-CBD	3.69	117.83	111.27
23	B	603	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	B	611	CLA	C3B-C4B-NB	3.69	113.98	109.21
23	d	403	CLA	O2D-CGD-CBD	3.69	117.82	111.27
23	b	604	CLA	C3B-C4B-NB	3.68	113.97	109.21
25	D	407	BCR	C38-C26-C25	-3.68	120.40	124.53
27	C	501	SQD	C44-O6-C1	-3.68	106.56	113.74
23	C	502	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
23	C	510	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
25	K	101	BCR	C38-C26-C25	-3.66	120.41	124.53
23	B	612	CLA	CAC-C3C-C4C	3.66	129.56	124.81
23	C	502	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
23	b	604	CLA	C3D-C4D-ND	3.66	116.16	110.24
23	b	603	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
23	B	608	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
23	B	612	CLA	C1D-CHD-C4C	-3.65	118.17	126.06
23	c	508	CLA	C3C-C4C-NC	3.65	114.67	110.57
23	c	513	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	d	403	CLA	C3B-C4B-NB	3.65	113.93	109.21
23	b	603	CLA	C3B-C4B-NB	3.65	113.93	109.21
31	C	520	LMG	O7-C10-C11	3.64	119.35	111.50
23	B	604	CLA	C1-C2-C3	-3.64	119.75	126.04
25	k	101	BCR	C15-C14-C13	-3.64	122.11	127.31
23	b	608	CLA	C3B-C4B-NB	3.64	113.92	109.21
23	b	606	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
23	C	505	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	c	512	CLA	C1-C2-C3	-3.63	119.76	126.04
23	C	510	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	c	510	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
32	d	407	LHG	O7-C7-C8	3.62	119.31	111.50
23	b	608	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	a	407	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	D	406	CLA	C3B-C4B-NB	3.61	113.88	109.21
23	C	514	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	B	602	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
23	B	616	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
25	C	516	BCR	C11-C10-C9	-3.61	122.16	127.31
23	A	404	CLA	CMB-C2B-C3B	3.60	131.42	124.68
23	C	506	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	B	615	CLA	O2D-CGD-CBD	3.60	117.67	111.27
23	B	608	CLA	C3B-C4B-NB	3.60	113.86	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	C4-C3-C5	3.60	121.32	115.27
34	E	102	LMT	C1B-O5B-C5B	3.59	120.73	113.69
35	C	519	DGD	O2G-C1B-C2B	3.59	119.24	111.50
23	b	601	CLA	C3B-C4B-NB	3.59	113.85	109.21
27	a	411	SQD	O7-S-C6	3.59	111.20	106.94
23	B	610	CLA	C4C-C3C-C2C	-3.58	101.67	106.90
23	C	506	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	C	510	CLA	C3B-C4B-NB	3.58	113.84	109.21
23	a	405	CLA	O2D-CGD-CBD	3.58	117.62	111.27
23	C	508	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
23	b	603	CLA	C4-C3-C5	3.58	121.28	115.27
25	C	516	BCR	C33-C5-C6	-3.57	120.52	124.53
25	H	101	BCR	C38-C26-C25	-3.57	120.52	124.53
24	A	407	PHO	C1A-C2A-C3A	-3.57	99.44	102.84
23	b	612	CLA	C4-C3-C5	3.56	121.27	115.27
25	k	101	BCR	C24-C23-C22	-3.56	120.85	126.23
23	c	502	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
35	c	518	DGD	O2G-C1B-C2B	3.56	119.18	111.50
24	a	406	PHO	CMA-C3A-C4A	-3.56	106.58	114.38
23	B	605	CLA	O2A-CGA-O1A	-3.56	114.61	123.59
23	c	513	CLA	C1-C2-C3	-3.56	119.89	126.04
23	c	505	CLA	C3B-C4B-NB	3.56	113.81	109.21
23	B	613	CLA	C4A-NA-C1A	-3.55	105.11	106.71
33	B	624	HTG	C1'-S1-C1	3.55	106.74	100.09
23	c	512	CLA	C3B-C4B-NB	3.55	113.80	109.21
23	D	405	CLA	C3B-C4B-NB	3.55	113.80	109.21
23	B	608	CLA	C4A-NA-C1A	-3.55	105.11	106.71
29	A	413	PL9	C20-C19-C21	3.55	121.24	115.27
23	B	614	CLA	C3B-C4B-NB	3.55	113.80	109.21
29	A	413	PL9	C25-C24-C26	3.54	121.23	115.27
25	A	409	BCR	C24-C23-C22	-3.54	120.88	126.23
23	b	601	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
25	B	618	BCR	C29-C30-C25	3.54	115.92	110.48
23	c	514	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
27	a	411	SQD	O48-C23-C24	3.53	123.00	111.91
23	C	511	CLA	C3B-C4B-NB	3.53	113.78	109.21
23	b	605	CLA	O2A-CGA-O1A	-3.53	114.67	123.59
23	C	513	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
23	b	602	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
23	B	615	CLA	CHD-C4C-NC	3.53	129.77	124.20
23	c	507	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	B	604	CLA	O2D-CGD-O1D	-3.53	116.94	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	514	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	C	513	CLA	CMB-C2B-C3B	3.52	131.27	124.68
23	b	614	CLA	C3B-C4B-NB	3.52	113.77	109.21
27	a	409	SQD	C44-O6-C1	-3.52	106.86	113.74
23	C	514	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
27	D	415	SQD	O8-S-C6	3.52	111.35	105.74
23	D	406	CLA	CAC-C3C-C4C	3.52	129.37	124.81
23	B	610	CLA	O2A-CGA-CBA	3.52	122.94	111.91
23	b	610	CLA	O2A-CGA-O1A	-3.51	114.73	123.59
23	a	405	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
23	a	407	CLA	C3B-C4B-NB	3.51	113.75	109.21
23	B	607	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
23	b	609	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
23	b	612	CLA	C4C-C3C-C2C	-3.50	101.79	106.90
23	A	404	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
31	c	521	LMG	O6-C5-C4	3.50	116.05	109.69
24	D	402	PHO	C1A-C2A-C3A	-3.50	99.51	102.84
23	d	403	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
32	a	419	LHG	O7-C7-C8	3.49	119.03	111.50
25	k	102	BCR	C38-C26-C25	-3.49	120.61	124.53
23	b	612	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	b	615	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	B	606	CLA	C3D-C4D-ND	3.48	115.87	110.24
23	B	606	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	B	608	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	b	604	CLA	C1-C2-C3	-3.48	120.03	126.04
23	b	608	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
29	d	406	PL9	C40-C39-C41	3.47	121.11	115.27
23	d	404	CLA	C3C-C4C-NC	3.47	114.46	110.57
23	B	610	CLA	CAA-C2A-C3A	-3.47	103.29	112.78
25	a	408	BCR	C7-C8-C9	-3.46	121.00	126.23
25	B	617	BCR	C33-C5-C6	-3.46	120.64	124.53
23	B	605	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
25	d	405	BCR	C28-C27-C26	-3.46	107.91	114.08
27	A	411	SQD	O47-C7-C8	3.46	118.95	111.50
23	c	512	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
23	C	510	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
23	c	510	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
23	b	609	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
23	B	609	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
25	b	617	BCR	C33-C5-C6	-3.45	120.65	124.53
23	B	605	CLA	CAC-C3C-C4C	3.45	129.29	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
27	D	415	SQD	C1-O5-C5	-3.44	106.94	113.69
25	H	101	BCR	C16-C17-C18	-3.44	122.40	127.31
23	C	507	CLA	C3B-C4B-NB	3.44	113.66	109.21
23	B	603	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
24	A	407	PHO	CMA-C3A-C4A	-3.44	106.85	114.38
23	d	404	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	A	404	CLA	O2A-CGA-O1A	-3.43	114.93	123.59
23	B	604	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	b	602	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	c	506	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
23	C	513	CLA	C3B-C4B-NB	3.43	113.65	109.21
25	c	516	BCR	C7-C8-C9	-3.43	121.06	126.23
23	B	615	CLA	C1C-C2C-C3C	-3.43	103.36	106.96
23	b	604	CLA	CMC-C2C-C1C	3.42	130.25	125.04
23	b	614	CLA	C1-C2-C3	-3.42	120.13	126.04
27	a	411	SQD	C3-C4-C5	3.42	116.34	110.24
23	c	509	CLA	C4A-NA-C1A	-3.42	105.17	106.71
23	B	602	CLA	CAC-C3C-C4C	3.42	129.24	124.81
29	D	408	PL9	C53-C6-C1	3.42	121.97	114.99
23	c	504	CLA	C3B-C4B-NB	3.41	113.62	109.21
23	c	512	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
23	b	615	CLA	C3B-C4B-NB	3.41	113.62	109.21
23	c	507	CLA	O2A-CGA-O1A	-3.41	114.99	123.59
23	b	611	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
23	C	506	CLA	C1D-CHD-C4C	-3.40	118.71	126.06
23	B	614	CLA	O2A-CGA-O1A	-3.40	115.00	123.59
23	d	403	CLA	C1-C2-C3	-3.40	120.16	126.04
23	b	616	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
27	L	102	SQD	C1-O5-C5	-3.40	107.02	113.69
23	B	612	CLA	C3B-C4B-NB	3.39	113.60	109.21
23	c	504	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
23	b	603	CLA	O2A-CGA-O1A	-3.39	115.03	123.59
23	B	607	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
23	C	503	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
23	C	514	CLA	C3B-C4B-NB	3.38	113.58	109.21
23	B	612	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
32	A	416	LHG	O8-C23-O10	-3.38	115.06	123.59
33	b	621	HTG	C1-O5-C5	3.38	118.81	112.58
23	b	616	CLA	CHD-C4C-NC	3.38	129.53	124.20
25	B	618	BCR	C37-C22-C21	-3.38	118.19	122.92
25	Y	101	BCR	C37-C22-C23	3.38	123.40	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	CMC-C2C-C1C	3.38	130.18	125.04
23	A	404	CLA	CAC-C3C-C4C	3.37	129.18	124.81
25	c	515	BCR	C11-C10-C9	-3.37	122.50	127.31
23	d	404	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
23	B	612	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
29	A	413	PL9	C7-C3-C2	-3.37	118.87	123.30
23	C	512	CLA	C4A-NA-C1A	-3.37	105.19	106.71
38	f	101	HEM	C1B-NB-C4B	3.36	108.55	105.07
23	b	606	CLA	C1-C2-C3	-3.36	120.23	126.04
23	c	512	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	b	605	CLA	CHD-C4C-NC	3.36	129.50	124.20
23	C	507	CLA	CBC-CAC-C3C	-3.36	103.17	112.43
23	d	402	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
23	B	604	CLA	C3B-C4B-NB	3.36	113.55	109.21
23	C	507	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
23	c	506	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
23	c	504	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
23	C	511	CLA	C4-C3-C5	3.35	120.90	115.27
23	B	611	CLA	CMC-C2C-C1C	3.35	130.14	125.04
23	c	507	CLA	C3C-C4C-NC	3.35	114.32	110.57
25	K	101	BCR	C24-C23-C22	-3.34	121.18	126.23
23	b	610	CLA	CAA-C2A-C3A	-3.34	103.62	112.78
23	C	503	CLA	C1-C2-C3	-3.34	120.26	126.04
23	c	503	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	B	609	CLA	C3B-C4B-NB	3.34	113.52	109.21
23	a	405	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
23	A	408	CLA	C4-C3-C5	3.33	120.88	115.27
33	b	621	HTG	C1'-S1-C1	3.33	106.32	100.09
29	a	414	PL9	C37-C36-C34	-3.33	102.02	112.98
23	c	503	CLA	CBC-CAC-C3C	-3.33	103.25	112.43
23	A	405	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
23	b	605	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
25	b	619	BCR	C24-C23-C22	-3.32	121.21	126.23
23	c	506	CLA	C4C-C3C-C2C	-3.32	102.05	106.90
23	b	604	CLA	C4A-NA-C1A	-3.32	105.22	106.71
23	B	607	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
23	c	511	CLA	CMC-C2C-C1C	3.31	130.09	125.04
23	b	615	CLA	CHC-C1C-C2C	-3.31	117.57	126.72
23	B	609	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
23	C	506	CLA	C3B-C4B-NB	3.31	113.48	109.21
23	B	604	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
23	d	404	CLA	CMC-C2C-C1C	3.30	130.06	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
35	C	517	DGD	O2G-C1B-C2B	3.29	118.60	111.50
23	A	404	CLA	C2A-C1A-CHA	-3.29	118.10	123.86
23	b	609	CLA	C1-C2-C3	-3.29	120.36	126.04
25	C	515	BCR	C16-C17-C18	-3.29	122.62	127.31
23	C	508	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
35	C	517	DGD	O1G-C1A-O1A	-3.28	115.31	123.59
23	b	616	CLA	C1-C2-C3	-3.28	120.37	126.04
23	B	604	CLA	C4-C3-C5	3.28	120.79	115.27
35	C	518	DGD	O1G-C1A-C2A	3.28	122.20	111.91
23	C	512	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	B	615	CLA	C3B-C4B-NB	3.28	113.45	109.21
23	A	405	CLA	C4A-NA-C1A	-3.28	105.23	106.71
23	B	616	CLA	CHD-C4C-NC	3.28	129.37	124.20
23	B	601	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	c	513	CLA	CAC-C3C-C4C	3.28	129.06	124.81
23	A	406	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
25	b	619	BCR	C7-C8-C9	-3.27	121.29	126.23
23	C	504	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
23	b	606	CLA	C3B-C4B-NB	3.27	113.44	109.21
23	a	404	CLA	CMB-C2B-C3B	3.27	130.80	124.68
29	A	413	PL9	C53-C6-C1	3.27	121.67	114.99
33	h	101	HTG	C1-O5-C5	3.26	118.60	112.58
23	a	404	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
24	a	416	PHO	O2D-CGD-O1D	-3.26	117.46	123.84
23	b	607	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
29	a	414	PL9	C7-C8-C9	-3.26	121.36	126.79
29	D	408	PL9	C22-C23-C24	-3.26	119.81	127.66
23	C	512	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	A	408	CLA	C1-C2-C3	-3.26	120.41	126.04
23	C	504	CLA	CHD-C4C-NC	3.26	129.33	124.20
25	c	515	BCR	C16-C17-C18	-3.25	122.67	127.31
23	b	601	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
23	b	608	CLA	CAC-C3C-C4C	3.25	129.03	124.81
34	C	525	LMT	O1B-C4'-C3'	3.25	115.94	107.28
25	B	618	BCR	C2-C1-C6	3.25	115.49	110.48
23	B	612	CLA	CMB-C2B-C3B	3.25	130.76	124.68
27	L	102	SQD	C1-C2-C3	-3.25	103.23	110.00
31	D	414	LMG	O7-C10-C11	3.25	118.50	111.50
23	b	602	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
23	C	512	CLA	C4-C3-C5	3.25	120.73	115.27
23	B	604	CLA	O2A-CGA-O1A	-3.25	115.40	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C4-C3-C5	3.25	120.73	115.27
23	c	503	CLA	CHD-C4C-NC	3.24	129.31	124.20
23	B	603	CLA	C3B-C4B-NB	3.24	113.40	109.21
23	A	405	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
23	c	505	CLA	CAC-C3C-C4C	3.24	129.02	124.81
23	b	608	CLA	CMC-C2C-C1C	3.24	129.98	125.04
23	C	509	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
40	V	201	HEC	CMB-C2B-C1B	-3.24	123.48	128.46
23	B	615	CLA	C4-C3-C5	3.24	120.72	115.27
29	A	413	PL9	C10-C9-C11	3.24	120.72	115.27
23	a	405	CLA	CHD-C4C-NC	3.24	129.30	124.20
23	C	509	CLA	C4-C3-C5	3.24	120.71	115.27
23	a	404	CLA	O2A-CGA-O1A	-3.24	115.43	123.59
23	c	506	CLA	CAC-C3C-C4C	3.23	129.01	124.81
23	b	608	CLA	CBC-CAC-C3C	-3.23	103.52	112.43
23	d	403	CLA	O2A-CGA-CBA	3.23	122.04	111.91
23	c	504	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
23	B	607	CLA	C3B-C4B-NB	3.23	113.39	109.21
23	b	605	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	b	605	CLA	C2A-C1A-CHA	-3.23	118.21	123.86
27	L	102	SQD	O8-S-C6	3.23	110.88	105.74
23	C	503	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	C	510	CLA	CAC-C3C-C4C	3.22	128.99	124.81
23	B	603	CLA	CAA-C2A-C3A	-3.22	103.95	112.78
25	H	101	BCR	C7-C8-C9	-3.22	121.36	126.23
25	c	515	BCR	C38-C26-C25	-3.22	120.91	124.53
23	a	404	CLA	C1-C2-C3	-3.22	120.47	126.04
23	c	509	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
23	a	404	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
25	T	101	BCR	C15-C14-C13	3.22	131.90	127.31
31	Z	101	LMG	O6-C1-C2	3.22	117.16	110.35
25	k	101	BCR	C36-C18-C19	3.22	123.14	118.08
23	d	404	CLA	O2A-CGA-CBA	3.21	121.99	111.91
23	C	510	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
23	A	404	CLA	O2D-CGD-CBD	3.21	116.97	111.27
23	c	508	CLA	CHD-C4C-NC	3.21	129.26	124.20
23	B	606	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
23	A	406	CLA	O2A-CGA-O1A	-3.21	115.50	123.59
29	a	414	PL9	C25-C24-C26	3.21	120.66	115.27
38	f	101	HEM	C4D-ND-C1D	3.21	108.38	105.07
25	D	407	BCR	C37-C22-C23	3.21	123.13	118.08
23	C	507	CLA	C3C-C4C-NC	3.20	114.16	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	628	LHG	O7-C7-C8	3.20	118.40	111.50
23	C	511	CLA	CBC-CAC-C3C	-3.20	103.61	112.43
23	b	607	CLA	CHC-C1C-C2C	-3.20	117.88	126.72
23	C	502	CLA	CMC-C2C-C1C	3.20	129.91	125.04
23	b	611	CLA	CMC-C2C-C1C	3.20	129.91	125.04
23	b	604	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
23	C	505	CLA	CMC-C2C-C1C	3.19	129.90	125.04
25	B	618	BCR	C15-C14-C13	-3.19	122.75	127.31
27	A	411	SQD	O5-C5-C4	3.19	115.49	109.69
23	a	405	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	A	405	CLA	C3B-C4B-NB	3.19	113.33	109.21
23	B	603	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	c	510	CLA	O2A-CGA-CBA	3.19	121.91	111.91
23	B	614	CLA	CHC-C1C-C2C	-3.19	117.91	126.72
32	d	407	LHG	O8-C23-O10	-3.19	115.55	123.59
23	a	407	CLA	CMA-C3A-C2A	-3.19	100.98	113.83
25	b	617	BCR	C29-C30-C25	3.18	115.38	110.48
23	c	509	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
24	D	402	PHO	C4-C3-C5	3.18	120.62	115.27
23	B	614	CLA	C4-C3-C5	3.18	120.61	115.27
23	b	613	CLA	C1D-CHD-C4C	-3.18	119.21	126.06
23	b	611	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
23	c	508	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
31	C	521	LMG	O8-C28-C29	3.17	121.86	111.91
23	C	508	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	c	502	CLA	C3B-C4B-NB	3.17	113.31	109.21
23	C	507	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
23	d	402	CLA	CAA-C2A-C3A	-3.17	104.11	112.78
23	B	610	CLA	CAA-CBA-CGA	-3.17	104.00	113.25
23	B	615	CLA	C4C-C3C-C2C	-3.16	102.28	106.90
23	a	407	CLA	C4C-C3C-C2C	-3.16	102.28	106.90
31	m	101	LMG	O7-C10-C11	3.16	118.32	111.50
25	C	516	BCR	C3-C4-C5	-3.16	108.43	114.08
23	b	610	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	c	505	CLA	CMB-C2B-C3B	3.15	130.58	124.68
23	B	615	CLA	CMC-C2C-C1C	3.15	129.84	125.04
23	B	609	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
25	b	619	BCR	C11-C10-C9	-3.15	122.82	127.31
23	B	601	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
23	B	609	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
23	b	613	CLA	C4-C3-C5	3.15	120.56	115.27
23	c	504	CLA	C1-C2-C3	-3.14	120.60	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	CAA-C2A-C3A	-3.14	104.17	112.78
23	B	603	CLA	C4-C3-C5	3.14	120.56	115.27
23	B	614	CLA	CHD-C4C-NC	3.14	129.15	124.20
23	A	408	CLA	C3B-C4B-NB	3.14	113.27	109.21
23	c	508	CLA	C4-C3-C5	3.14	120.55	115.27
23	b	602	CLA	C3B-C4B-NB	3.14	113.27	109.21
25	d	405	BCR	C40-C30-C25	-3.13	105.22	110.30
29	D	408	PL9	C51-C49-C50	3.13	121.52	114.60
23	D	406	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
23	c	511	CLA	C4-C3-C5	3.13	120.53	115.27
27	C	501	SQD	O48-C23-C24	3.12	121.71	111.91
23	C	510	CLA	CMB-C2B-C3B	3.12	130.52	124.68
23	B	610	CLA	C3B-C4B-NB	3.12	113.25	109.21
23	B	609	CLA	CMB-C2B-C1B	3.12	133.26	128.46
23	B	614	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	d	404	CLA	C3B-C4B-NB	3.12	113.24	109.21
23	B	611	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	C	504	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	D	405	CLA	CAA-C2A-C3A	-3.12	104.25	112.78
38	f	101	HEM	CHA-C4D-ND	3.12	128.23	124.38
23	D	406	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
23	c	514	CLA	C1-C2-C3	-3.11	120.66	126.04
23	B	608	CLA	CMB-C2B-C3B	3.11	130.50	124.68
23	C	514	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	A	404	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	C	513	CLA	C4-C3-C5	3.10	120.49	115.27
23	b	604	CLA	O2A-CGA-O1A	-3.10	115.77	123.59
23	b	613	CLA	CHC-C1C-C2C	-3.10	118.16	126.72
23	C	513	CLA	C4C-C3C-C2C	-3.10	102.39	106.90
35	h	103	DGD	O1G-C1A-C2A	3.09	121.62	111.91
23	D	406	CLA	CMC-C2C-C1C	3.09	129.75	125.04
31	M	101	LMG	O8-C28-C29	3.09	121.61	111.91
23	b	602	CLA	CMC-C2C-C1C	3.09	129.74	125.04
23	a	404	CLA	O2A-CGA-CBA	3.09	121.59	111.91
23	b	614	CLA	CHD-C4C-NC	3.08	129.06	124.20
31	C	520	LMG	O8-C28-C29	3.08	121.58	111.91
23	b	614	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
32	b	628	LHG	O8-C23-C24	3.08	121.58	111.91
23	B	614	CLA	O2A-CGA-CBA	3.08	121.57	111.91
23	A	405	CLA	CHD-C4C-NC	3.07	129.05	124.20
23	B	611	CLA	CHD-C4C-NC	3.07	129.04	124.20
23	B	602	CLA	C4C-C3C-C2C	-3.07	102.43	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402	CLA	CBC-CAC-C3C	-3.07	103.98	112.43
23	c	507	CLA	CBC-CAC-C3C	-3.06	103.99	112.43
23	D	405	CLA	CMB-C2B-C3B	3.06	130.41	124.68
23	C	506	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	C	506	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	C	507	CLA	C1-C2-C3	-3.06	120.75	126.04
23	d	403	CLA	C4-C3-C5	3.06	120.42	115.27
23	C	507	CLA	CMC-C2C-C1C	3.06	129.70	125.04
38	f	101	HEM	CHD-C1D-ND	3.06	127.75	124.43
23	d	404	CLA	CHD-C4C-NC	3.06	129.02	124.20
31	a	417	LMG	O6-C5-C4	3.06	115.24	109.69
23	B	610	CLA	CHC-C1C-C2C	-3.06	118.27	126.72
23	c	512	CLA	C4C-C3C-C2C	-3.05	102.44	106.90
23	c	513	CLA	C4-C3-C5	3.05	120.41	115.27
33	V	202	HTG	C1-O5-C5	3.05	116.33	112.19
23	b	616	CLA	O2A-CGA-CBA	3.05	121.49	111.91
25	k	102	BCR	C24-C23-C22	-3.05	121.62	126.23
23	b	604	CLA	CAC-C3C-C4C	3.05	128.77	124.81
23	B	608	CLA	CHD-C4C-NC	3.05	129.01	124.20
29	a	414	PL9	C42-C43-C44	-3.05	120.32	127.66
25	b	618	BCR	C15-C14-C13	-3.05	122.96	127.31
33	B	624	HTG	O5-C5-C4	3.05	115.23	109.69
23	D	405	CLA	CBC-CAC-C3C	-3.05	104.03	112.43
24	a	406	PHO	C1A-C2A-C3A	-3.05	99.94	102.84
29	A	413	PL9	C42-C43-C44	-3.04	120.33	127.66
23	b	604	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
27	L	102	SQD	C3-C4-C5	3.04	115.67	110.24
23	b	612	CLA	O2A-CGA-CBA	3.04	121.45	111.91
23	B	610	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
23	c	509	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	a	407	CLA	O2A-CGA-CBA	3.04	121.45	111.91
38	f	101	HEM	CBD-CAD-C3D	-3.04	104.18	112.63
23	b	607	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	A	408	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
23	C	505	CLA	CBC-CAC-C3C	-3.04	104.06	112.43
23	b	601	CLA	CHD-C4C-NC	3.04	128.99	124.20
23	C	502	CLA	CHD-C4C-NC	3.03	128.99	124.20
23	b	601	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
25	k	101	BCR	C16-C17-C18	-3.03	122.98	127.31
25	b	618	BCR	C29-C30-C25	3.03	115.15	110.48
23	c	510	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
23	a	405	CLA	C3B-C4B-NB	3.03	113.13	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	101	BCR	C28-C27-C26	-3.03	108.67	114.08
23	B	602	CLA	CHD-C4C-NC	3.03	128.97	124.20
32	d	409	LHG	O8-C23-C24	3.02	121.40	111.91
23	b	602	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
23	A	406	CLA	C3B-C4B-NB	3.02	113.12	109.21
23	c	506	CLA	C3B-C4B-NB	3.02	113.12	109.21
23	c	511	CLA	CHD-C4C-NC	3.02	128.97	124.20
23	C	504	CLA	C4-C3-C5	3.02	120.35	115.27
29	d	406	PL9	C53-C6-C1	3.02	121.17	114.99
23	b	612	CLA	CMB-C2B-C3B	3.02	130.33	124.68
32	d	408	LHG	O8-C23-O10	-3.02	115.97	123.59
25	A	409	BCR	C11-C10-C9	-3.02	123.00	127.31
23	b	615	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	b	607	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
25	c	516	BCR	C15-C16-C17	-3.01	117.30	123.47
31	m	101	LMG	O8-C28-C29	3.01	121.36	111.91
23	B	601	CLA	C3B-C4B-NB	3.01	113.11	109.21
23	c	502	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	a	404	CLA	CHD-C4C-NC	3.01	128.94	124.20
23	B	606	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	C	511	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	c	505	CLA	CMC-C2C-C1C	3.01	129.62	125.04
23	B	601	CLA	CHD-C4C-NC	3.01	128.94	124.20
29	a	414	PL9	C32-C33-C34	-3.00	120.42	127.66
23	C	510	CLA	CMC-C2C-C1C	3.00	129.61	125.04
23	B	607	CLA	CBC-CAC-C3C	-3.00	104.16	112.43
23	C	511	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	b	603	CLA	O2A-CGA-CBA	3.00	121.31	111.91
23	b	601	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
23	b	615	CLA	CAC-C3C-C4C	2.99	128.69	124.81
23	B	606	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
23	c	508	CLA	O2A-CGA-CBA	2.99	121.30	111.91
23	b	602	CLA	C2A-C1A-CHA	-2.99	118.63	123.86
23	c	503	CLA	C3B-C4B-NB	2.99	113.08	109.21
23	C	510	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
23	B	612	CLA	C4-C3-C5	2.99	120.30	115.27
33	B	621	HTG	C1-C2-C3	2.99	116.49	110.59
23	c	512	CLA	C4-C3-C5	2.99	120.30	115.27
23	c	514	CLA	CMC-C2C-C1C	2.99	129.59	125.04
23	D	405	CLA	O2A-CGA-CBA	2.99	121.29	111.91
23	B	608	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
29	a	414	PL9	C22-C23-C24	-2.99	120.46	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CMC-C2C-C1C	2.99	129.59	125.04
23	b	616	CLA	C3B-C4B-NB	2.99	113.07	109.21
23	A	406	CLA	CAA-C2A-C3A	-2.98	104.61	112.78
23	A	406	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	c	507	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
23	C	503	CLA	C3B-C4B-NB	2.98	113.07	109.21
23	b	611	CLA	C1-C2-C3	-2.98	120.89	126.04
23	b	607	CLA	CBC-CAC-C3C	-2.98	104.21	112.43
23	b	610	CLA	CHD-C4C-NC	2.98	128.90	124.20
23	D	405	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
27	C	501	SQD	C45-O47-C7	-2.97	110.47	117.79
29	D	408	PL9	C42-C41-C39	-2.97	103.19	112.98
40	v	203	HEC	CBA-CAA-C2A	-2.97	107.59	112.60
23	b	606	CLA	CMB-C2B-C3B	2.97	130.23	124.68
23	d	404	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
23	C	509	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
24	a	406	PHO	O1D-CGD-CBD	-2.97	119.80	124.74
23	d	402	CLA	C3B-C4B-NB	2.96	113.04	109.21
23	c	512	CLA	CHD-C4C-NC	2.96	128.87	124.20
25	B	618	BCR	C37-C22-C23	2.96	122.75	118.08
23	b	613	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	B	613	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
24	a	406	PHO	O2A-CGA-CBA	2.96	121.20	111.91
23	b	614	CLA	O2A-CGA-CBA	2.96	121.20	111.91
25	k	101	BCR	C29-C30-C25	2.96	115.04	110.48
23	a	407	CLA	CAA-C2A-C3A	-2.96	104.68	112.78
29	D	408	PL9	C32-C33-C34	-2.96	120.54	127.66
29	D	408	PL9	C45-C44-C46	2.96	120.24	115.27
23	B	616	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
29	d	406	PL9	C10-C9-C11	2.95	120.24	115.27
24	D	402	PHO	O2D-CGD-O1D	-2.95	118.07	123.84
23	B	616	CLA	O2A-CGA-CBA	2.95	121.16	111.91
23	D	406	CLA	CAA-C2A-C3A	-2.95	104.70	112.78
23	B	610	CLA	C1D-CHD-C4C	-2.95	119.70	126.06
23	B	614	CLA	C4A-NA-C1A	-2.94	105.38	106.71
23	c	507	CLA	CMB-C2B-C3B	2.94	130.19	124.68
23	C	514	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	B	607	CLA	C4-C3-C5	2.94	120.22	115.27
23	d	404	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
23	b	614	CLA	CMB-C2B-C3B	2.94	130.18	124.68
23	C	512	CLA	CHC-C1C-C2C	-2.94	118.60	126.72
23	c	505	CLA	C4C-C3C-C2C	-2.93	102.62	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	619	BCR	C29-C30-C25	2.93	114.99	110.48
31	c	520	LMG	O8-C28-C29	2.93	121.11	111.91
23	B	606	CLA	CMB-C2B-C3B	2.93	130.16	124.68
23	C	502	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
29	d	406	PL9	C36-C37-C38	-2.93	102.26	111.88
23	B	607	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	c	507	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	a	404	CLA	CHB-C4A-NA	2.93	128.56	124.51
34	E	102	LMT	C4B-C3B-C2B	-2.93	105.71	110.82
27	A	411	SQD	O48-C23-C24	2.93	121.09	111.91
35	H	102	DGD	O1G-C1A-O1A	-2.92	116.21	123.59
23	b	610	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
25	k	101	BCR	C3-C4-C5	-2.92	108.86	114.08
23	C	507	CLA	CGD-CBD-CAD	-2.92	101.29	110.73
23	C	509	CLA	CMB-C2B-C3B	2.92	130.13	124.68
29	A	413	PL9	C17-C18-C19	-2.91	120.64	127.66
23	B	601	CLA	O2A-CGA-CBA	2.91	121.05	111.91
23	C	511	CLA	CHD-C4C-NC	2.91	128.79	124.20
25	A	409	BCR	C31-C1-C6	-2.91	105.58	110.30
23	A	405	CLA	C4-C3-C5	2.91	120.17	115.27
23	B	613	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
23	b	611	CLA	O2A-CGA-CBA	2.91	121.04	111.91
31	c	521	LMG	O8-C28-C29	2.91	121.04	111.91
23	A	404	CLA	CAA-C2A-C1A	-2.91	102.44	111.97
32	A	416	LHG	O8-C23-C24	2.91	121.03	111.91
23	b	603	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
23	C	511	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	A	406	CLA	C1D-CHD-C4C	-2.91	119.79	126.06
31	c	521	LMG	C3-C4-C5	2.91	115.42	110.24
23	B	615	CLA	C11-C10-C8	-2.90	106.53	115.92
35	H	102	DGD	O1G-C1A-C2A	2.90	121.02	111.91
32	D	410	LHG	O8-C23-O10	-2.90	116.27	123.59
23	c	511	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
23	C	502	CLA	C3B-C4B-NB	2.90	112.96	109.21
23	D	406	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
35	c	519	DGD	O1G-C1A-C2A	2.90	121.01	111.91
23	c	514	CLA	O2A-CGA-CBA	2.90	121.01	111.91
23	B	601	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	b	608	CLA	CMB-C2B-C3B	2.90	130.10	124.68
25	b	619	BCR	C15-C14-C13	-2.90	123.18	127.31
23	c	507	CLA	CHD-C4C-NC	2.90	128.77	124.20
25	T	101	BCR	C12-C13-C14	-2.90	114.50	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C4-C3-C5	2.89	120.14	115.27
23	b	607	CLA	O2A-CGA-O1A	-2.89	116.29	123.59
23	b	611	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	b	616	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
23	b	606	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	c	505	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
23	C	504	CLA	C1-C2-C3	-2.89	121.05	126.04
23	c	513	CLA	CMC-C2C-C1C	2.89	129.44	125.04
25	T	101	BCR	C33-C5-C6	-2.89	121.29	124.53
25	a	408	BCR	C33-C5-C6	-2.89	121.29	124.53
23	C	504	CLA	C3B-C4B-NB	2.89	112.94	109.21
23	a	405	CLA	CMC-C2C-C1C	2.89	129.43	125.04
23	B	614	CLA	C1-C2-C3	-2.89	121.05	126.04
23	a	404	CLA	CMA-C3A-C4A	-2.89	104.02	111.77
23	d	402	CLA	CHD-C4C-NC	2.88	128.75	124.20
25	k	101	BCR	C11-C10-C9	-2.88	123.19	127.31
23	B	613	CLA	C4-C3-C5	2.88	120.12	115.27
23	c	512	CLA	CAC-C3C-C4C	2.88	128.55	124.81
23	c	510	CLA	CMB-C2B-C3B	2.88	130.06	124.68
23	B	616	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
23	d	403	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
23	b	614	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
25	B	617	BCR	C7-C8-C9	-2.87	121.89	126.23
23	D	405	CLA	C1D-CHD-C4C	-2.87	119.86	126.06
23	c	513	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	c	512	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	a	407	CLA	CHD-C4C-NC	2.87	128.73	124.20
23	B	605	CLA	C3B-C4B-NB	2.87	112.92	109.21
32	E	101	LHG	O8-C23-C24	2.87	120.92	111.91
23	b	612	CLA	CMC-C2C-C1C	2.87	129.41	125.04
25	a	408	BCR	C38-C26-C25	-2.87	121.31	124.53
23	A	408	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
25	B	619	BCR	C24-C23-C22	-2.87	121.90	126.23
25	C	515	BCR	C38-C26-C25	-2.87	121.31	124.53
23	b	609	CLA	CMB-C2B-C3B	2.87	130.04	124.68
23	b	609	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
35	C	518	DGD	O1G-C1A-O1A	-2.86	116.37	123.59
23	c	509	CLA	C4-C3-C5	2.86	120.09	115.27
23	c	514	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
23	B	602	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
23	B	608	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
23	c	510	CLA	C4C-C3C-C2C	-2.86	102.73	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	413	PL9	C22-C23-C24	-2.86	120.77	127.66
23	c	510	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	C	513	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
23	A	405	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
23	B	610	CLA	C1-C2-C3	-2.86	121.10	126.04
23	b	609	CLA	CAC-C3C-C4C	2.85	128.51	124.81
23	c	513	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	D	406	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	b	605	CLA	C3B-C4B-NB	2.85	112.89	109.21
23	c	511	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
25	D	407	BCR	C3-C4-C5	-2.85	109.00	114.08
23	B	615	CLA	CMB-C2B-C1B	2.85	132.84	128.46
23	b	610	CLA	C3B-C4B-NB	2.85	112.89	109.21
38	E	103	HEM	CBD-CAD-C3D	-2.84	104.72	112.63
27	a	409	SQD	O9-S-C6	2.84	110.32	106.94
23	c	502	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
23	B	611	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	D	402	PHO	C6-C5-C3	-2.84	106.01	113.45
25	D	407	BCR	C24-C23-C22	-2.84	121.94	126.23
29	d	406	PL9	C20-C19-C21	2.84	120.05	115.27
23	b	604	CLA	O2A-CGA-CBA	2.84	120.82	111.91
23	a	405	CLA	CAA-C2A-C3A	-2.84	105.01	112.78
25	D	407	BCR	C33-C5-C6	-2.84	121.34	124.53
23	b	603	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	c	503	CLA	C1-C2-C3	-2.84	121.14	126.04
25	b	618	BCR	C37-C22-C21	-2.84	118.95	122.92
27	a	411	SQD	O48-C23-O10	-2.84	116.43	123.59
23	C	513	CLA	CHD-C4C-NC	2.84	128.67	124.20
23	b	606	CLA	C1-O2A-CGA	2.84	123.88	116.44
23	c	508	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
23	B	608	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
23	B	614	CLA	CAC-C3C-C4C	2.83	128.48	124.81
23	c	506	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
23	B	613	CLA	O2A-CGA-CBA	2.83	120.78	111.91
23	b	610	CLA	CAA-CBA-CGA	-2.83	104.99	113.25
25	c	516	BCR	C33-C5-C6	-2.82	121.36	124.53
25	t	102	BCR	C3-C4-C5	-2.82	109.03	114.08
29	a	414	PL9	C10-C9-C11	2.82	120.02	115.27
23	c	504	CLA	C4-C3-C5	2.82	120.02	115.27
25	D	407	BCR	C21-C20-C19	-2.82	114.41	123.22
23	B	616	CLA	C3B-C4B-NB	2.82	112.86	109.21
23	c	514	CLA	CHC-C1C-C2C	-2.82	118.92	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	CMC-C2C-C1C	2.82	129.33	125.04
23	b	612	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
23	c	513	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
23	c	508	CLA	CAC-C3C-C4C	2.82	128.47	124.81
29	a	414	PL9	C20-C19-C21	2.82	120.01	115.27
29	D	408	PL9	C10-C9-C11	2.81	120.00	115.27
23	b	614	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
23	A	408	CLA	CHD-C4C-NC	2.81	128.64	124.20
31	D	414	LMG	O8-C28-O10	-2.81	116.50	123.59
23	C	503	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	B	605	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
23	C	510	CLA	O2A-CGA-CBA	2.81	120.72	111.91
23	B	602	CLA	CED-O2D-CGD	2.81	122.28	115.94
23	C	506	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
23	C	508	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	b	611	CLA	CHD-C4C-NC	2.80	128.62	124.20
23	C	502	CLA	C4-C3-C5	2.80	119.98	115.27
24	A	407	PHO	C4-C3-C5	2.80	119.98	115.27
29	A	413	PL9	C32-C33-C34	-2.80	120.92	127.66
23	B	604	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
23	c	508	CLA	O1D-CGD-CBD	-2.80	118.76	124.48
23	b	611	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
32	D	409	LHG	O8-C23-O10	-2.79	116.54	123.59
34	a	412	LMT	O5'-C5'-C4'	2.79	115.64	109.75
23	C	508	CLA	C3B-C4B-NB	2.79	112.82	109.21
29	D	408	PL9	C30-C29-C31	2.79	119.96	115.27
23	B	605	CLA	CHD-C4C-NC	2.79	128.60	124.20
23	b	614	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
23	d	403	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
40	V	201	HEC	CMC-C2C-C1C	-2.79	124.18	128.46
23	b	615	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
23	C	507	CLA	O2A-CGA-CBA	2.79	120.65	111.91
23	B	605	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
23	C	511	CLA	O2A-CGA-CBA	2.79	120.65	111.91
32	D	410	LHG	O8-C23-C24	2.79	120.65	111.91
35	h	103	DGD	O2G-C1B-C2B	2.79	117.50	111.50
23	B	603	CLA	CMB-C2B-C3B	2.78	129.89	124.68
23	b	609	CLA	C1D-CHD-C4C	-2.78	120.05	126.06
23	b	608	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
34	b	626	LMT	O5'-C5'-C4'	2.78	115.61	109.75
32	D	409	LHG	O8-C23-C24	2.78	120.62	111.91
27	L	102	SQD	O7-S-C6	2.78	110.24	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
25	k	102	BCR	C28-C27-C26	-2.78	109.12	114.08
23	C	511	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
25	b	619	BCR	C39-C30-C25	-2.78	105.80	110.30
23	b	611	CLA	O2A-CGA-O1A	-2.78	116.59	123.59
23	A	406	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
23	b	603	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
25	Y	101	BCR	C34-C9-C8	2.77	122.45	118.08
23	C	513	CLA	C1-C2-C3	-2.77	121.25	126.04
23	a	407	CLA	C1-C2-C3	-2.77	121.25	126.04
24	A	407	PHO	C1-C2-C3	-2.77	121.25	126.04
38	E	103	HEM	CHB-C1B-NB	2.77	127.80	124.38
23	a	404	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
23	b	616	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
23	c	502	CLA	CMC-C2C-C1C	2.76	129.25	125.04
25	H	101	BCR	C24-C23-C22	-2.76	122.06	126.23
27	f	102	SQD	O48-C23-C24	2.76	120.58	111.91
23	b	612	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
27	D	415	SQD	O7-S-C6	2.76	110.22	106.94
23	c	505	CLA	CHD-C4C-NC	2.76	128.55	124.20
23	B	612	CLA	O2A-CGA-CBA	2.76	120.56	111.91
23	b	606	CLA	CMC-C2C-C1C	2.76	129.24	125.04
23	C	504	CLA	CHC-C1C-C2C	-2.76	119.10	126.72
23	b	614	CLA	CMC-C2C-C1C	2.75	129.23	125.04
24	D	402	PHO	CMB-C2B-C3B	2.75	129.83	124.68
23	b	610	CLA	C4-C3-C5	2.75	119.90	115.27
23	b	602	CLA	C1-C2-C3	-2.75	121.28	126.04
23	C	514	CLA	O2A-CGA-CBA	2.75	120.54	111.91
23	B	614	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	a	407	CLA	C4-C3-C5	2.75	119.90	115.27
25	a	408	BCR	C24-C23-C22	-2.75	122.08	126.23
23	d	404	CLA	C1-C2-C3	-2.75	121.29	126.04
38	f	101	HEM	CHB-C1B-NB	2.75	127.78	124.38
23	B	603	CLA	CMC-C2C-C1C	2.75	129.22	125.04
27	L	102	SQD	C44-O6-C1	-2.75	108.37	113.74
23	C	509	CLA	CHD-C4C-NC	2.74	128.53	124.20
23	b	614	CLA	C4-C3-C5	2.74	119.89	115.27
31	m	101	LMG	C7-O1-C1	-2.74	108.38	113.74
23	b	606	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	c	507	CLA	O2A-CGA-CBA	2.74	120.51	111.91
31	M	101	LMG	C9-C8-C7	-2.74	105.31	111.79
24	A	407	PHO	CMB-C2B-C3B	2.74	129.80	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
23	d	403	CLA	CMC-C2C-C1C	2.74	129.21	125.04
23	A	406	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
23	B	614	CLA	CMC-C2C-C1C	2.74	129.21	125.04
23	A	408	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
23	c	502	CLA	O2A-CGA-O1A	-2.74	116.69	123.59
23	c	508	CLA	CBC-CAC-C3C	-2.73	104.89	112.43
32	d	409	LHG	O8-C23-O10	-2.73	116.70	123.59
23	a	407	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
23	d	403	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	c	513	CLA	O2A-CGA-CBA	2.73	120.47	111.91
23	B	607	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
23	B	608	CLA	CMC-C2C-C1C	2.73	129.19	125.04
35	c	519	DGD	O2G-C1B-C2B	2.73	117.38	111.50
23	c	502	CLA	CHD-C4C-NC	2.72	128.50	124.20
23	A	404	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
25	D	407	BCR	C28-C27-C26	-2.72	109.21	114.08
23	a	404	CLA	CAA-C2A-C1A	-2.72	103.06	111.97
23	b	606	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
27	L	102	SQD	O48-C23-C24	2.72	120.44	111.91
23	C	514	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
31	A	415	LMG	C1-O6-C5	2.72	119.03	113.69
23	a	405	CLA	C1-C2-C3	-2.72	121.34	126.04
38	E	103	HEM	CHD-C1D-ND	2.72	127.39	124.43
29	A	413	PL9	C40-C39-C41	2.72	119.84	115.27
23	d	403	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
23	A	408	CLA	CMC-C2C-C1C	2.71	129.17	125.04
32	d	408	LHG	O7-C7-C8	2.71	117.35	111.50
23	c	512	CLA	CMC-C2C-C1C	2.71	129.17	125.04
31	z	101	LMG	O8-C28-C29	2.71	120.42	111.91
23	B	609	CLA	O2A-CGA-CBA	2.71	120.42	111.91
23	B	608	CLA	C1-C2-C3	-2.71	121.35	126.04
23	b	612	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
25	B	617	BCR	C38-C26-C25	-2.71	121.48	124.53
23	B	603	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
23	B	605	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
29	A	413	PL9	C30-C29-C31	2.71	119.82	115.27
23	C	513	CLA	O2A-CGA-CBA	2.71	120.40	111.91
27	f	102	SQD	O7-S-C6	2.71	110.15	106.94
23	D	405	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
29	D	408	PL9	C37-C38-C39	-2.70	121.15	127.66
25	t	102	BCR	C2-C1-C6	2.70	114.64	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
33	B	621	HTG	O2-C2-C3	-2.70	104.11	110.35
23	b	603	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
23	B	603	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
35	H	102	DGD	O2G-C1B-C2B	2.70	117.31	111.50
32	d	408	LHG	O8-C23-C24	2.70	120.37	111.91
23	B	608	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	C	506	CLA	CMC-C2C-C1C	2.70	129.14	125.04
25	b	619	BCR	C34-C9-C10	-2.69	119.15	122.92
29	a	414	PL9	C53-C6-C1	2.69	120.50	114.99
23	d	402	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	C	505	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
23	c	508	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	C	516	BCR	C15-C16-C17	-2.69	117.96	123.47
23	c	511	CLA	C11-C10-C8	-2.69	107.22	115.92
25	B	619	BCR	C21-C20-C19	-2.69	114.82	123.22
23	b	608	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
23	b	616	CLA	OBD-CAD-C3D	-2.69	122.05	128.52
29	D	408	PL9	C40-C39-C41	2.69	119.79	115.27
27	a	409	SQD	O48-C23-C24	2.69	120.34	111.91
40	v	203	HEC	C1D-C2D-C3D	-2.69	105.13	107.00
23	c	507	CLA	CAC-C3C-C4C	2.69	128.30	124.81
23	C	507	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
25	c	515	BCR	C33-C5-C6	-2.68	121.52	124.53
23	c	514	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	C	505	CLA	C1-C2-C3	-2.68	121.41	126.04
31	Z	101	LMG	C4-C3-C2	2.68	115.50	110.82
23	b	615	CLA	O2A-CGA-CBA	2.67	120.30	111.91
24	A	407	PHO	CBA-CAA-C2A	-2.67	106.00	113.81
23	B	601	CLA	CAC-C3C-C4C	2.67	128.28	124.81
29	d	406	PL9	C37-C38-C39	-2.67	121.22	127.66
23	B	604	CLA	C11-C12-C13	-2.67	107.28	115.92
23	d	402	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
27	C	501	SQD	O48-C23-O10	-2.67	116.85	123.59
23	c	503	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
23	B	613	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
25	K	101	BCR	C15-C14-C13	-2.67	123.50	127.31
25	c	516	BCR	C15-C14-C13	-2.67	123.50	127.31
23	c	512	CLA	O2A-CGA-CBA	2.67	120.28	111.91
23	A	408	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
23	b	615	CLA	CHD-C4C-NC	2.67	128.40	124.20
23	A	406	CLA	O2A-CGA-CBA	2.66	120.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C11-C12-C13	-2.66	107.31	115.92
25	Y	101	BCR	C40-C30-C25	-2.66	105.98	110.30
29	A	413	PL9	C45-C44-C46	2.66	119.75	115.27
23	c	506	CLA	O2A-CGA-CBA	2.66	120.26	111.91
23	c	511	CLA	O2A-CGA-CBA	2.66	120.26	111.91
23	c	507	CLA	C1-C2-C3	-2.66	121.44	126.04
23	C	514	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	C	505	CLA	C1-O2A-CGA	2.66	123.42	116.44
23	c	509	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	b	607	CLA	C4-C3-C5	2.66	119.74	115.27
25	D	407	BCR	C37-C22-C21	-2.66	119.20	122.92
23	B	616	CLA	CMC-C2C-C1C	2.66	129.08	125.04
23	c	504	CLA	CMC-C2C-C1C	2.66	129.08	125.04
23	B	607	CLA	C1-O2A-CGA	2.65	123.41	116.44
23	b	613	CLA	CMB-C2B-C3B	2.65	129.64	124.68
23	b	608	CLA	O2A-CGA-CBA	2.65	120.23	111.91
33	B	624	HTG	C3-C4-C5	2.65	114.97	110.24
23	d	402	CLA	CMC-C2C-C1C	2.65	129.07	125.04
23	d	403	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
23	B	603	CLA	CHD-C4C-NC	2.65	128.38	124.20
25	t	102	BCR	C21-C20-C19	-2.65	114.96	123.22
23	c	504	CLA	O2A-CGA-O1A	-2.65	116.92	123.59
23	A	405	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	B	601	CLA	CMB-C2B-C3B	2.64	129.62	124.68
34	D	404	LMT	C1-O1'-C1'	-2.64	109.47	113.84
23	b	604	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	c	502	CLA	CAC-C3C-C4C	2.63	128.23	124.81
31	D	414	LMG	O8-C28-C29	2.63	120.17	111.91
23	d	404	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	b	601	CLA	O2A-CGA-CBA	2.63	120.17	111.91
23	a	404	CLA	CMC-C2C-C1C	2.63	129.05	125.04
25	b	619	BCR	C16-C17-C18	-2.63	123.56	127.31
23	b	614	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
25	D	407	BCR	C29-C30-C25	2.63	114.53	110.48
33	h	101	HTG	C1-C2-C3	-2.63	105.39	110.59
23	C	512	CLA	CHD-C4C-NC	2.63	128.35	124.20
23	a	407	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
25	T	101	BCR	C16-C17-C18	-2.63	123.56	127.31
29	a	414	PL9	C17-C18-C19	-2.62	121.34	127.66
23	B	603	CLA	O2A-CGA-CBA	2.62	120.14	111.91
23	B	601	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
23	C	503	CLA	CHC-C1C-C2C	-2.62	119.47	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
25	t	102	BCR	C7-C8-C9	-2.62	122.28	126.23
23	c	513	CLA	CHD-C4C-NC	2.62	128.33	124.20
27	B	620	SQD	O48-C23-C24	2.62	120.12	111.91
25	H	101	BCR	C31-C1-C6	-2.62	106.05	110.30
29	d	406	PL9	C30-C29-C31	2.62	119.67	115.27
34	a	412	LMT	O5B-C5B-C4B	2.62	114.45	109.69
23	B	608	CLA	CHC-C1C-C2C	-2.62	119.49	126.72
23	C	504	CLA	CMC-C2C-C1C	2.62	129.02	125.04
35	c	519	DGD	O3G-C3G-C2G	-2.61	104.59	110.90
23	b	614	CLA	CED-O2D-CGD	2.61	121.84	115.94
25	d	405	BCR	C29-C30-C25	2.61	114.50	110.48
23	A	408	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
23	b	610	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
31	Z	101	LMG	C9-C8-C7	-2.61	105.62	111.79
25	d	405	BCR	C16-C17-C18	-2.61	123.59	127.31
23	c	503	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
23	a	407	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
23	C	509	CLA	C1-C2-C3	-2.60	121.54	126.04
35	C	517	DGD	C2G-O2G-C1B	-2.60	111.38	117.79
25	h	102	BCR	C38-C26-C25	-2.60	121.61	124.53
23	C	508	CLA	O2A-CGA-CBA	2.60	120.06	111.91
23	a	404	CLA	CAC-C3C-C4C	2.60	128.18	124.81
25	B	619	BCR	C2-C3-C4	-2.60	105.57	111.38
23	b	605	CLA	CED-O2D-CGD	2.60	121.81	115.94
29	A	413	PL9	C7-C8-C9	-2.60	122.47	126.79
32	D	409	LHG	O7-C7-C8	2.60	117.09	111.50
27	B	620	SQD	O9-S-C6	2.59	110.02	106.94
32	d	407	LHG	O8-C23-C24	2.59	120.05	111.91
23	c	503	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	c	511	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	b	613	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	c	508	CLA	C1-C2-C3	-2.59	121.56	126.04
25	a	408	BCR	C3-C4-C5	-2.59	109.45	114.08
29	a	414	PL9	C45-C44-C46	2.59	119.62	115.27
23	C	510	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
23	b	603	CLA	CAC-C3C-C4C	2.58	128.16	124.81
24	a	416	PHO	CMB-C2B-C3B	2.58	129.51	124.68
23	B	602	CLA	C1-C2-C3	-2.58	121.57	126.04
23	b	616	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
25	H	101	BCR	C10-C11-C12	-2.58	115.16	123.22
23	b	608	CLA	CHD-C4C-NC	2.58	128.27	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	515	BCR	C23-C24-C25	-2.58	119.96	127.20
23	b	602	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
27	B	620	SQD	O5-C5-C4	2.58	114.38	109.69
23	B	606	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
23	C	505	CLA	C4C-C3C-C2C	-2.57	103.14	106.90
23	B	601	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
35	h	103	DGD	O1G-C1A-O1A	-2.57	117.10	123.59
38	E	103	HEM	C4D-ND-C1D	2.57	107.73	105.07
24	a	416	PHO	C1A-C2A-C3A	-2.57	100.39	102.84
23	a	405	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
23	A	406	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	C	511	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	b	609	CLA	C3B-C4B-NB	2.57	112.53	109.21
23	B	609	CLA	CHD-C4C-NC	2.57	128.25	124.20
24	a	406	PHO	CMC-C2C-C3C	2.57	129.78	124.94
27	A	411	SQD	O6-C1-C2	2.57	112.31	108.30
23	b	607	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	c	509	CLA	CMB-C2B-C3B	2.57	129.48	124.68
23	b	610	CLA	CMC-C2C-C1C	2.57	128.95	125.04
23	c	513	CLA	C3B-C4B-NB	2.56	112.52	109.21
32	a	419	LHG	O8-C23-C24	2.56	119.95	111.91
25	t	102	BCR	C29-C28-C27	-2.56	105.65	111.38
23	b	604	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
23	B	605	CLA	C1-C2-C3	-2.56	121.61	126.04
23	d	404	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
29	D	408	PL9	C25-C24-C23	-2.56	117.11	123.68
23	b	609	CLA	C7-C6-C5	-2.56	106.41	113.36
29	D	408	PL9	C17-C18-C19	-2.56	121.50	127.66
23	D	406	CLA	O2A-CGA-CBA	2.56	119.94	111.91
23	C	509	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
23	C	512	CLA	CMB-C2B-C3B	2.55	129.46	124.68
23	d	403	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
35	C	519	DGD	O1G-C1A-C2A	2.55	119.92	111.91
23	C	502	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
32	d	408	LHG	C6-C5-C4	-2.55	105.75	111.79
23	b	603	CLA	CHD-C4C-NC	2.55	128.23	124.20
23	D	406	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
23	d	404	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
23	B	606	CLA	C4-C3-C5	2.55	119.56	115.27
23	C	503	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	d	403	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	b	603	CLA	CMC-C2C-C1C	2.55	128.92	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	516	BCR	C38-C26-C25	-2.55	121.67	124.53
23	B	611	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
23	B	606	CLA	CHD-C4C-NC	2.55	128.22	124.20
29	d	406	PL9	C36-C34-C33	-2.54	115.97	121.12
23	b	608	CLA	C4-C3-C5	2.54	119.55	115.27
23	B	604	CLA	CAC-C3C-C4C	2.54	128.11	124.81
23	b	615	CLA	C4-C3-C5	2.54	119.55	115.27
23	B	615	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
23	B	601	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
31	Z	101	LMG	C1-O6-C5	2.54	118.67	113.69
23	b	613	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
31	d	412	LMG	O7-C10-C11	2.54	116.97	111.50
23	B	613	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
24	a	406	PHO	O2D-CGD-O1D	-2.54	118.88	123.84
23	C	508	CLA	CHD-C4C-NC	2.54	128.20	124.20
23	b	606	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
23	D	405	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
23	d	402	CLA	C1-O2A-CGA	2.53	123.09	116.44
23	b	615	CLA	C11-C12-C13	-2.53	107.73	115.92
23	A	408	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	b	608	CLA	C1-C2-C3	-2.53	121.67	126.04
23	B	602	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	B	611	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	A	404	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
23	B	608	CLA	O2A-CGA-CBA	2.53	119.84	111.91
23	c	503	CLA	O2A-CGA-CBA	2.53	119.83	111.91
25	k	101	BCR	C34-C9-C8	2.52	122.05	118.08
23	a	407	CLA	OBD-CAD-C3D	-2.52	122.45	128.52
23	B	611	CLA	C4-C3-C5	2.52	119.52	115.27
23	d	404	CLA	CAC-C3C-C4C	2.52	128.08	124.81
23	C	511	CLA	CAC-C3C-C4C	2.52	128.08	124.81
23	b	609	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
23	B	604	CLA	C6-C7-C8	-2.52	107.78	115.92
27	D	415	SQD	O48-C23-C24	2.52	119.81	111.91
23	B	603	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
25	D	407	BCR	C10-C11-C12	-2.52	115.36	123.22
23	B	606	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
23	b	616	CLA	C4-C3-C5	2.52	119.50	115.27
25	C	516	BCR	C36-C18-C19	2.51	122.04	118.08
23	d	402	CLA	CAA-CBA-CGA	2.51	120.59	113.25
23	a	404	CLA	C4C-C3C-C2C	-2.51	103.24	106.90
23	b	615	CLA	CBC-CAC-C3C	-2.51	105.51	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	CBC-CAC-C3C	-2.51	105.51	112.43
23	B	602	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	b	616	CLA	CHC-C1C-C2C	-2.51	119.79	126.72
23	B	607	CLA	CHD-C4C-NC	2.51	128.15	124.20
23	C	505	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
23	B	607	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
23	b	610	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
32	d	407	LHG	C5-O7-C7	-2.50	111.64	117.79
23	c	509	CLA	CHD-C4C-NC	2.50	128.14	124.20
25	t	102	BCR	C37-C22-C23	2.50	122.02	118.08
25	B	617	BCR	C11-C10-C9	-2.50	123.74	127.31
23	c	502	CLA	O2A-CGA-CBA	2.50	119.75	111.91
35	H	102	DGD	O4D-C4D-C5D	-2.50	103.09	109.30
23	C	514	CLA	C4-C3-C5	2.50	119.47	115.27
23	c	514	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
23	C	502	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
33	h	101	HTG	C6-C5-C4	-2.49	107.16	113.00
32	L	101	LHG	O8-C23-C24	2.49	119.72	111.91
23	c	511	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	D	408	PL9	C36-C37-C38	-2.49	103.70	111.88
23	B	607	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
27	A	411	SQD	O8-S-C6	2.49	109.71	105.74
23	B	611	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
25	b	617	BCR	C39-C30-C25	-2.49	106.26	110.30
23	c	514	CLA	CAA-C2A-C3A	-2.49	105.97	112.78
25	t	102	BCR	C1-C6-C7	2.49	122.81	115.78
40	v	203	HEC	CMB-C2B-C1B	-2.48	124.64	128.46
23	C	507	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
23	C	507	CLA	CHD-C4C-NC	2.48	128.12	124.20
23	d	402	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
23	b	605	CLA	CMC-C2C-C1C	2.48	128.81	125.04
23	b	608	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
23	c	512	CLA	CMB-C2B-C3B	2.48	129.31	124.68
23	C	505	CLA	OBD-CAD-C3D	-2.48	122.56	128.52
23	c	514	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
31	d	412	LMG	O8-C28-C29	2.48	119.68	111.91
23	B	612	CLA	CHD-C4C-NC	2.48	128.10	124.20
23	c	502	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
25	T	101	BCR	C16-C15-C14	2.47	128.54	123.47
23	A	405	CLA	CED-O2D-CGD	2.47	121.53	115.94
23	B	615	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	c	506	CLA	CMC-C2C-C1C	2.47	128.80	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	m	103	LMT	C1-O1'-C1'	-2.47	109.75	113.84
23	D	406	CLA	C4-C3-C5	2.47	119.42	115.27
23	c	513	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
25	k	101	BCR	C36-C18-C17	-2.47	119.47	122.92
23	b	604	CLA	C11-C12-C13	-2.46	107.95	115.92
23	C	506	CLA	C4-C3-C5	2.46	119.42	115.27
23	d	404	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
23	c	503	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
23	B	602	CLA	O2A-CGA-CBA	2.46	119.62	111.91
23	b	609	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	D	402	PHO	C4A-C3A-C2A	-2.46	100.50	102.84
25	d	405	BCR	C10-C11-C12	-2.46	115.55	123.22
23	a	405	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	h	102	BCR	C24-C23-C22	-2.46	122.52	126.23
25	T	101	BCR	C2-C1-C6	2.45	114.26	110.48
23	c	513	CLA	CHB-C4A-NA	2.45	127.91	124.51
23	B	605	CLA	O2A-CGA-CBA	2.45	119.61	111.91
23	c	504	CLA	O2A-CGA-CBA	2.45	119.61	111.91
32	A	416	LHG	O7-C7-O9	-2.45	117.77	123.70
24	a	406	PHO	O2A-CGA-O1A	-2.45	117.41	123.59
23	c	505	CLA	CBC-CAC-C3C	-2.45	105.67	112.43
29	D	408	PL9	C27-C28-C29	-2.45	121.76	127.66
23	C	505	CLA	C4-C3-C5	2.45	119.39	115.27
23	d	402	CLA	CMA-C3A-C2A	-2.45	103.95	113.83
23	c	502	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
25	h	102	BCR	C36-C18-C17	-2.45	119.49	122.92
23	b	602	CLA	O2A-CGA-CBA	2.45	119.59	111.91
23	C	503	CLA	CHD-C4C-NC	2.45	128.06	124.20
23	b	601	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
27	A	411	SQD	O7-S-C6	2.45	109.84	106.94
23	b	616	CLA	CMC-C2C-C1C	2.44	128.76	125.04
23	b	609	CLA	CMC-C2C-C1C	2.44	128.76	125.04
23	b	609	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	b	611	CLA	CAC-C3C-C4C	2.44	127.97	124.81
23	c	505	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
27	C	501	SQD	O9-S-O7	-2.44	105.52	113.95
23	B	610	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	C	509	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	C	514	CLA	CAC-C3C-C4C	2.43	127.97	124.81
25	B	617	BCR	C31-C1-C6	-2.43	106.35	110.30
23	C	507	CLA	C4-C3-C5	2.43	119.36	115.27
38	E	103	HEM	O2D-CGD-CBD	2.43	121.84	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	405	BCR	C24-C23-C22	-2.43	122.56	126.23
25	B	619	BCR	C29-C30-C25	2.43	114.22	110.48
23	C	508	CLA	C1-C2-C3	-2.43	121.84	126.04
24	a	406	PHO	C1-C2-C3	-2.43	121.84	126.04
27	a	409	SQD	C45-O47-C7	-2.43	111.81	117.79
25	H	101	BCR	C11-C10-C9	-2.43	123.85	127.31
23	A	408	CLA	CMA-C3A-C2A	-2.42	104.05	113.83
23	A	405	CLA	CAA-CBA-CGA	2.42	120.33	113.25
23	D	405	CLA	CMC-C2C-C1C	2.42	128.73	125.04
25	b	618	BCR	C38-C26-C25	-2.42	121.81	124.53
31	z	101	LMG	C8-O7-C10	-2.42	111.83	117.79
27	a	411	SQD	O5-C5-C4	2.42	114.09	109.69
23	c	507	CLA	C4-C3-C5	2.42	119.34	115.27
25	B	618	BCR	C7-C8-C9	-2.42	122.58	126.23
23	A	408	CLA	O2A-CGA-CBA	2.42	119.50	111.91
29	d	406	PL9	C51-C49-C50	2.42	119.95	114.60
25	b	617	BCR	C24-C23-C22	-2.42	122.58	126.23
25	B	619	BCR	C38-C26-C25	-2.42	121.81	124.53
29	A	413	PL9	C16-C14-C13	-2.42	116.22	121.12
29	d	406	PL9	C27-C28-C29	-2.42	121.84	127.66
25	t	102	BCR	C11-C10-C9	-2.41	123.86	127.31
38	E	103	HEM	CHA-C4D-ND	2.41	127.36	124.38
23	c	511	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
23	B	604	CLA	O2A-CGA-CBA	2.41	119.48	111.91
23	a	405	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
23	b	611	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
23	B	611	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
23	c	507	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
35	c	518	DGD	O1G-C1A-C2A	2.41	119.46	111.91
23	B	610	CLA	CMA-C3A-C4A	-2.41	105.30	111.77
23	a	404	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
23	C	508	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
35	c	517	DGD	O1G-C1A-C2A	2.40	119.45	111.91
23	B	604	CLA	CMB-C2B-C3B	2.40	129.18	124.68
23	A	405	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	C	510	CLA	CHD-C4C-NC	2.40	127.99	124.20
23	c	505	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
23	d	402	CLA	C1-C2-C3	-2.40	121.89	126.04
23	b	611	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
32	b	628	LHG	O8-C23-O10	-2.40	117.53	123.59
23	b	607	CLA	CAC-C3C-C4C	2.40	127.92	124.81
25	B	618	BCR	C31-C1-C6	-2.40	106.41	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	C1-C2-C3	-2.40	121.90	126.04
23	b	605	CLA	C6-C7-C8	-2.40	108.17	115.92
31	M	101	LMG	O8-C28-O10	-2.40	117.54	123.59
40	V	201	HEC	CAD-CBD-CGD	-2.39	107.05	113.76
24	A	407	PHO	O1D-CGD-CBD	-2.39	120.75	124.74
23	B	611	CLA	CED-O2D-CGD	2.39	121.35	115.94
25	Y	101	BCR	C38-C26-C25	-2.39	121.84	124.53
27	f	102	SQD	O8-S-C6	2.39	109.55	105.74
23	a	405	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
23	B	606	CLA	O2A-CGA-CBA	2.39	119.40	111.91
23	b	613	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	B	604	CLA	CHD-C4C-NC	2.39	127.96	124.20
23	C	512	CLA	CED-O2D-CGD	2.38	121.33	115.94
23	C	508	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
23	B	613	CLA	CMB-C2B-C3B	2.38	129.14	124.68
23	B	616	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
23	C	506	CLA	CHD-C4C-NC	2.38	127.95	124.20
33	b	622	HTG	O5-C1-C2	2.38	113.31	110.31
25	a	408	BCR	C29-C30-C25	2.38	114.14	110.48
23	a	405	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
23	c	505	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
31	C	520	LMG	O6-C5-C6	2.38	112.34	106.44
23	d	403	CLA	CMB-C2B-C3B	2.38	129.12	124.68
25	k	102	BCR	C10-C11-C12	-2.37	115.81	123.22
23	B	606	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
25	h	102	BCR	C16-C17-C18	-2.37	123.93	127.31
24	a	406	PHO	CBA-CAA-C2A	-2.37	106.89	113.81
23	c	512	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
27	B	620	SQD	O7-S-C6	2.37	109.75	106.94
24	a	416	PHO	C4A-C3A-C2A	-2.36	100.59	102.84
25	b	618	BCR	C3-C4-C5	-2.36	109.86	114.08
23	b	601	CLA	CMB-C2B-C3B	2.36	129.10	124.68
23	B	612	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
25	b	618	BCR	C15-C16-C17	-2.36	118.63	123.47
23	C	508	CLA	CMB-C2B-C3B	2.36	129.10	124.68
23	b	602	CLA	CHD-C4C-NC	2.36	127.93	124.20
25	B	619	BCR	C7-C8-C9	-2.36	122.67	126.23
25	K	101	BCR	C2-C1-C6	2.36	114.12	110.48
25	D	407	BCR	C16-C17-C18	-2.36	123.94	127.31
25	b	618	BCR	C8-C7-C6	-2.36	120.58	127.20
25	C	515	BCR	C11-C10-C9	-2.36	123.94	127.31
29	a	414	PL9	C30-C29-C31	2.36	119.24	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CMA-C3A-C2A	-2.36	104.32	113.83
31	c	521	LMG	O8-C28-O10	-2.36	117.64	123.59
23	d	403	CLA	C6-C5-C3	2.36	119.63	113.45
25	T	101	BCR	C34-C9-C8	2.36	121.79	118.08
25	k	101	BCR	C7-C8-C9	-2.35	122.68	126.23
25	C	515	BCR	C37-C22-C23	2.35	121.78	118.08
23	c	507	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
24	A	407	PHO	O2D-CGD-O1D	-2.35	119.24	123.84
23	C	507	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
23	B	609	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	a	405	CLA	O2A-CGA-CBA	2.35	119.28	111.91
23	B	611	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	b	611	CLA	CMB-C2B-C3B	2.35	129.07	124.68
37	d	401	BCT	O2-C-O1	2.35	125.64	119.55
25	c	516	BCR	C37-C22-C23	2.35	121.78	118.08
25	c	516	BCR	C11-C10-C9	-2.35	123.96	127.31
34	C	525	LMT	O5'-C5'-C4'	2.35	114.70	109.75
23	c	510	CLA	CHD-C4C-NC	2.35	127.90	124.20
32	A	416	LHG	C5-O7-C7	-2.35	112.02	117.79
34	t	101	LMT	C1'-O5'-C5'	2.35	118.29	113.69
23	c	505	CLA	O2A-CGA-CBA	2.35	119.27	111.91
23	B	602	CLA	CMB-C2B-C3B	2.35	129.07	124.68
23	B	609	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
35	C	517	DGD	O5D-C6D-C5D	-2.34	104.71	109.05
23	B	611	CLA	OBD-CAD-C3D	-2.34	122.88	128.52
23	B	616	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
23	b	602	CLA	C1-O2A-CGA	2.34	122.59	116.44
23	C	502	CLA	CAC-C3C-C4C	2.34	127.85	124.81
25	D	407	BCR	C40-C30-C25	-2.34	106.50	110.30
31	A	415	LMG	O8-C28-C29	2.34	119.25	111.91
23	c	510	CLA	C1-O2A-CGA	2.34	122.58	116.44
23	c	514	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	d	402	CLA	C4-C3-C5	2.34	119.21	115.27
25	c	515	BCR	C35-C13-C14	-2.34	119.65	122.92
25	T	101	BCR	C21-C20-C19	-2.34	115.92	123.22
33	h	101	HTG	C3-C4-C5	2.34	114.41	110.24
25	K	101	BCR	C16-C17-C18	-2.34	123.97	127.31
24	a	416	PHO	C4-C3-C2	-2.34	117.68	123.68
23	C	508	CLA	C16-C15-C13	-2.34	108.36	115.92
23	b	607	CLA	C1-O2A-CGA	2.34	122.58	116.44
24	a	416	PHO	CBA-CAA-C2A	-2.34	106.99	113.81
23	b	614	CLA	C2A-C1A-CHA	-2.34	119.78	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	CMC-C2C-C1C	2.33	128.59	125.04
23	c	509	CLA	CAC-C3C-C4C	2.33	127.84	124.81
23	B	603	CLA	CMA-C3A-C2A	-2.33	104.42	113.83
23	D	405	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
23	C	503	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	A	404	CLA	CMA-C3A-C2A	-2.32	104.45	113.83
23	C	504	CLA	O2A-CGA-CBA	2.32	119.20	111.91
23	B	606	CLA	OBD-CAD-C3D	-2.32	122.93	128.52
35	H	102	DGD	C3G-O3G-C1D	-2.32	109.20	113.74
23	c	511	CLA	CMB-C2B-C3B	2.32	129.02	124.68
27	C	501	SQD	O8-S-C6	2.32	109.44	105.74
23	b	609	CLA	C16-C15-C13	-2.32	108.42	115.92
23	B	608	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
23	c	508	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
25	Y	101	BCR	C29-C30-C25	2.31	114.04	110.48
29	A	413	PL9	C47-C48-C49	-2.31	119.86	127.75
23	D	405	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
23	C	512	CLA	O2A-CGA-CBA	2.31	119.15	111.91
23	C	514	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
23	B	602	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	c	514	CLA	C4-C3-C5	2.31	119.15	115.27
25	A	409	BCR	C38-C26-C25	-2.31	121.94	124.53
23	C	506	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
23	B	608	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
38	E	103	HEM	C4B-C3B-C2B	-2.30	105.29	107.11
25	b	619	BCR	C21-C20-C19	-2.30	116.04	123.22
23	b	606	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	A	405	CLA	OBD-CAD-C3D	-2.30	122.99	128.52
23	b	613	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
25	Y	101	BCR	C8-C7-C6	-2.30	120.75	127.20
25	b	619	BCR	C8-C9-C10	2.30	122.46	118.94
35	c	519	DGD	C2G-O2G-C1B	-2.29	112.14	117.79
23	B	614	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
23	c	512	CLA	C1-O2A-CGA	2.29	122.46	116.44
23	c	512	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
35	C	518	DGD	O5D-C1E-C2E	2.29	111.88	108.30
23	a	407	CLA	CMC-C2C-C1C	2.29	128.53	125.04
23	d	404	CLA	C4-C3-C5	2.29	119.12	115.27
31	d	412	LMG	O8-C28-O10	-2.29	117.81	123.59
25	h	102	BCR	C10-C11-C12	-2.29	116.08	123.22
23	B	602	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
34	D	404	LMT	O1B-C4'-C3'	2.29	113.36	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	502	CLA	C1-C2-C3	-2.29	122.09	126.04
25	A	409	BCR	C40-C30-C25	-2.29	106.59	110.30
23	b	607	CLA	C1-C2-C3	-2.29	122.09	126.04
25	K	101	BCR	C33-C5-C6	-2.29	121.96	124.53
25	k	102	BCR	C21-C20-C19	-2.28	116.09	123.22
23	b	606	CLA	CAC-C3C-C4C	2.28	127.77	124.81
23	A	405	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
25	B	618	BCR	C15-C16-C17	-2.28	118.80	123.47
23	C	513	CLA	CHB-C4A-NA	2.28	127.67	124.51
35	C	517	DGD	O6E-C5E-C4E	2.28	113.83	109.69
31	C	520	LMG	O8-C28-O10	-2.28	117.84	123.59
25	k	102	BCR	C29-C28-C27	-2.28	106.29	111.38
23	c	505	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
23	A	405	CLA	CMC-C2C-C1C	2.27	128.50	125.04
23	C	507	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
25	a	408	BCR	C10-C11-C12	-2.27	116.12	123.22
23	b	603	CLA	C6-C7-C8	-2.27	108.58	115.92
23	c	511	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
23	c	506	CLA	C1-C2-C3	-2.27	122.12	126.04
29	d	406	PL9	C31-C32-C33	-2.27	104.42	111.88
31	C	521	LMG	C1-C2-C3	-2.27	105.27	110.00
23	b	602	CLA	CMB-C2B-C3B	2.27	128.92	124.68
23	C	508	CLA	CAC-C3C-C4C	2.27	127.75	124.81
31	c	520	LMG	O1-C7-C8	-2.27	105.43	110.90
23	C	502	CLA	CBC-CAC-C3C	-2.27	106.19	112.43
23	b	616	CLA	CMB-C2B-C3B	2.26	128.91	124.68
27	D	415	SQD	O48-C23-O10	-2.26	117.88	123.59
23	b	605	CLA	O2A-C1-C2	-2.26	102.69	108.64
23	b	609	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
24	D	402	PHO	O2A-CGA-CBA	2.26	119.00	111.91
25	k	102	BCR	C16-C15-C14	-2.26	118.85	123.47
23	a	405	CLA	C4-C3-C5	2.26	119.06	115.27
29	D	408	PL9	C20-C19-C21	2.25	119.06	115.27
27	A	411	SQD	O48-C23-O10	-2.25	117.91	123.59
29	a	414	PL9	C47-C48-C49	-2.25	120.06	127.75
32	d	407	LHG	O7-C7-O9	-2.25	118.26	123.70
25	Y	101	BCR	C11-C10-C9	-2.25	124.10	127.31
23	c	505	CLA	C1-O2A-CGA	2.25	122.35	116.44
25	t	102	BCR	C33-C5-C4	2.25	117.94	113.62
25	K	101	BCR	C36-C18-C19	2.25	121.62	118.08
25	d	405	BCR	C21-C20-C19	-2.25	116.20	123.22
25	a	408	BCR	C15-C16-C17	-2.25	118.87	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	415	SQD	O47-C7-O49	-2.25	118.27	123.70
33	b	622	HTG	C1-O5-C5	2.25	116.72	112.58
23	B	608	CLA	C11-C12-C13	-2.25	108.66	115.92
32	L	101	LHG	O4-P-O5	2.24	123.33	112.24
23	C	507	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
23	A	406	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
23	C	503	CLA	CMB-C2B-C1B	2.24	131.91	128.46
23	C	503	CLA	O2A-CGA-CBA	2.24	118.94	111.91
25	A	409	BCR	C33-C5-C6	-2.24	122.01	124.53
23	C	512	CLA	C11-C10-C8	-2.24	108.68	115.92
23	B	613	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
23	B	615	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
23	c	514	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
23	c	510	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
31	a	417	LMG	C3-C4-C5	2.24	114.23	110.24
25	k	102	BCR	C37-C22-C23	2.24	121.60	118.08
24	D	402	PHO	O2A-CGA-O1A	-2.24	117.95	123.59
23	B	607	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
35	c	517	DGD	C2G-O2G-C1B	-2.23	112.29	117.79
31	a	417	LMG	C30-C29-C28	-2.23	105.50	113.62
27	B	620	SQD	O8-S-C6	2.23	109.29	105.74
23	d	404	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
23	c	512	CLA	C11-C10-C8	-2.23	108.72	115.92
23	A	404	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
23	b	602	CLA	CMA-C3A-C2A	-2.22	104.86	113.83
23	C	505	CLA	CHD-C4C-NC	2.22	127.71	124.20
23	c	510	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
25	H	101	BCR	C2-C1-C6	2.22	113.90	110.48
23	C	502	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
23	b	614	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
23	c	507	CLA	CGD-CBD-CAD	-2.22	103.55	110.73
23	B	605	CLA	CMC-C2C-C1C	2.22	128.42	125.04
29	d	406	PL9	C22-C23-C24	-2.22	122.32	127.66
23	C	504	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
29	A	413	PL9	C51-C49-C50	2.22	119.50	114.60
23	b	606	CLA	C4-C3-C2	-2.22	118.00	123.68
23	B	610	CLA	CMB-C2B-C3B	2.21	128.82	124.68
23	c	504	CLA	CHD-C4C-NC	2.21	127.69	124.20
23	C	504	CLA	CAC-C3C-C4C	2.21	127.68	124.81
25	C	515	BCR	C20-C21-C22	-2.21	124.15	127.31
23	C	510	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
23	B	612	CLA	O2A-CGA-O1A	-2.21	118.02	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	C1-O2A-CGA	2.21	122.24	116.44
23	b	610	CLA	CMB-C2B-C1B	2.21	131.86	128.46
25	H	101	BCR	C16-C15-C14	-2.21	118.95	123.47
34	D	403	LMT	O5'-C5'-C4'	2.20	114.40	109.75
27	a	411	SQD	C1-O5-C5	2.20	118.01	113.69
29	d	406	PL9	C7-C8-C9	-2.20	123.12	126.79
23	A	404	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
23	c	511	CLA	C1-C2-C3	-2.20	122.23	126.04
25	k	101	BCR	C10-C11-C12	-2.20	116.35	123.22
23	b	612	CLA	CHD-C4C-NC	2.20	127.67	124.20
23	c	514	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	Y	101	BCR	C37-C22-C21	-2.20	119.84	122.92
25	B	618	BCR	C30-C25-C26	-2.20	119.52	122.61
23	b	602	CLA	C4-C3-C5	2.20	118.97	115.27
23	c	504	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
27	a	411	SQD	O8-S-C6	2.20	109.24	105.74
34	t	101	LMT	O1'-C1'-C2'	2.20	111.73	108.30
35	H	102	DGD	C3E-C4E-C5E	-2.20	106.32	110.24
23	A	405	CLA	CMA-C3A-C4A	-2.20	105.87	111.77
40	V	201	HEC	CAA-CBA-CGA	-2.20	107.61	113.76
29	A	413	PL9	C35-C34-C36	2.19	118.96	115.27
24	D	402	PHO	CMC-C2C-C3C	2.19	129.08	124.94
23	b	608	CLA	C11-C10-C8	-2.19	108.83	115.92
23	A	404	CLA	CHD-C4C-NC	2.19	127.66	124.20
25	T	101	BCR	C29-C28-C27	-2.19	106.48	111.38
23	b	613	CLA	CHD-C4C-NC	2.19	127.66	124.20
25	B	619	BCR	C3-C4-C5	-2.19	110.16	114.08
23	B	605	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
29	a	414	PL9	C47-C46-C44	-2.19	105.78	112.98
25	B	619	BCR	C37-C22-C21	-2.19	119.86	122.92
23	b	609	CLA	C4-C3-C5	2.19	118.95	115.27
34	E	102	LMT	O5'-C5'-C4'	2.19	114.36	109.75
23	c	508	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
25	h	102	BCR	C34-C9-C8	2.19	121.52	118.08
31	C	521	LMG	O8-C28-O10	-2.19	118.07	123.59
25	c	516	BCR	C38-C26-C25	-2.19	122.07	124.53
25	b	617	BCR	C20-C21-C22	-2.18	124.19	127.31
25	t	102	BCR	C7-C6-C5	-2.18	116.17	121.46
23	B	613	CLA	CHD-C4C-NC	2.18	127.64	124.20
23	B	612	CLA	OBD-CAD-C3D	-2.18	123.27	128.52
27	f	102	SQD	O47-C7-O49	-2.18	118.43	123.70
23	c	513	CLA	CBA-CAA-C2A	-2.18	107.43	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	O2A-CGA-CBA	2.18	118.75	111.91
23	C	508	CLA	CMC-C2C-C1C	2.18	128.36	125.04
38	f	101	HEM	C3C-C4C-NC	-2.18	106.83	110.94
23	c	508	CLA	C3B-C4B-NB	2.18	112.03	109.21
25	C	516	BCR	C29-C30-C25	2.18	113.83	110.48
23	A	405	CLA	CHB-C4A-NA	2.18	127.52	124.51
23	c	509	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
38	E	103	HEM	CMD-C2D-C1D	2.18	128.35	125.04
23	B	616	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
23	C	504	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
34	m	103	LMT	O5B-C5B-C6B	2.17	111.84	106.44
23	C	508	CLA	C4-C3-C5	2.17	118.93	115.27
33	b	624	HTG	C4-C3-C2	-2.17	107.03	110.82
27	B	620	SQD	C1-C2-C3	-2.17	105.47	110.00
23	B	604	CLA	C11-C10-C8	-2.17	108.90	115.92
23	b	604	CLA	C4-C3-C5	2.17	118.92	115.27
23	b	606	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
23	B	602	CLA	C11-C12-C13	-2.17	108.91	115.92
31	a	417	LMG	C7-O1-C1	-2.17	109.50	113.74
25	K	101	BCR	C10-C11-C12	-2.17	116.45	123.22
23	A	406	CLA	CMA-C3A-C2A	-2.17	105.08	113.83
23	B	614	CLA	CMB-C2B-C3B	2.17	128.74	124.68
25	C	516	BCR	C36-C18-C17	-2.17	119.89	122.92
23	b	601	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
23	c	506	CLA	CHD-C4C-NC	2.17	127.62	124.20
23	c	514	CLA	CED-O2D-CGD	2.17	120.84	115.94
23	B	610	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	c	506	CLA	C4-C3-C5	2.17	118.92	115.27
23	d	403	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
32	L	101	LHG	O8-C23-O10	-2.17	118.12	123.59
23	C	506	CLA	C1-C2-C3	-2.17	122.30	126.04
31	M	101	LMG	O1-C7-C8	-2.17	105.67	110.90
34	M	102	LMT	O1B-C1B-C2B	2.17	113.71	108.10
23	b	616	CLA	CAC-C3C-C4C	2.16	127.62	124.81
23	B	608	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
23	d	403	CLA	CHD-C4C-NC	2.16	127.61	124.20
23	C	507	CLA	CMB-C2B-C3B	2.16	128.73	124.68
23	C	506	CLA	O2A-CGA-CBA	2.16	118.70	111.91
23	b	612	CLA	OBD-CAD-C3D	-2.16	123.31	128.52
29	d	406	PL9	C45-C44-C46	2.16	118.91	115.27
23	B	602	CLA	CHC-C1C-C2C	-2.16	120.74	126.72
23	B	612	CLA	CHC-C1C-C2C	-2.16	120.74	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	f	101	HEM	O2D-CGD-CBD	2.16	120.97	114.03
25	c	516	BCR	C21-C20-C19	-2.16	116.49	123.22
25	B	618	BCR	C3-C4-C5	-2.16	110.23	114.08
25	C	516	BCR	C39-C30-C25	-2.16	106.80	110.30
34	D	404	LMT	O1B-C4'-C5'	-2.15	103.54	109.45
31	a	417	LMG	O7-C10-O9	-2.15	118.50	123.70
32	D	409	LHG	C6-C5-C4	-2.15	106.69	111.79
24	D	402	PHO	CMA-C3A-C4A	-2.15	109.66	114.38
33	B	621	HTG	C1-O5-C5	2.15	116.55	112.58
23	B	615	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
23	C	508	CLA	C6-C7-C8	-2.15	108.97	115.92
23	C	514	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
23	B	616	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
23	b	611	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
23	c	509	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
23	D	405	CLA	CMA-C3A-C2A	-2.15	105.17	113.83
23	b	604	CLA	C7-C6-C5	-2.15	107.53	113.36
29	D	408	PL9	O2-C1-C6	-2.14	116.88	120.59
23	B	604	CLA	CMC-C2C-C1C	2.14	128.30	125.04
25	Y	101	BCR	C21-C20-C19	-2.14	116.53	123.22
34	M	102	LMT	O5B-C5B-C6B	2.14	111.76	106.44
27	a	409	SQD	O48-C23-O10	-2.14	118.19	123.59
31	M	101	LMG	O6-C5-C4	2.14	113.58	109.69
29	d	406	PL9	C47-C48-C49	-2.14	120.44	127.75
23	B	601	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
27	f	102	SQD	O48-C23-O10	-2.14	118.20	123.59
31	A	415	LMG	O6-C1-C2	2.14	114.87	110.35
23	c	502	CLA	C4-C3-C5	2.14	118.86	115.27
23	C	513	CLA	CAC-C3C-C4C	2.14	127.58	124.81
34	M	102	LMT	O1'-C1'-C2'	2.14	111.64	108.30
25	B	618	BCR	C28-C27-C26	-2.14	110.26	114.08
23	c	505	CLA	C11-C10-C8	-2.13	109.02	115.92
23	D	406	CLA	CMA-C3A-C4A	-2.13	106.04	111.77
35	H	102	DGD	O2G-C1B-O1B	-2.13	118.55	123.70
23	D	405	CLA	C11-C12-C13	-2.13	109.03	115.92
23	b	613	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
34	e	101	LMT	C4B-C3B-C2B	2.13	114.54	110.82
23	B	614	CLA	OBD-CAD-C3D	-2.13	123.40	128.52
23	B	606	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	a	414	PL9	C40-C39-C41	2.13	118.85	115.27
25	t	102	BCR	C35-C13-C12	2.13	121.43	118.08
23	B	604	CLA	O1D-CGD-CBD	-2.13	120.13	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
23	d	402	CLA	O2A-CGA-CBA	2.13	118.58	111.91
23	c	509	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
27	L	102	SQD	O47-C7-O49	-2.13	118.56	123.70
35	c	518	DGD	C2G-O2G-C1B	-2.12	112.56	117.79
35	C	519	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
25	Y	101	BCR	C10-C11-C12	-2.12	116.59	123.22
23	a	404	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
23	B	615	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
24	A	407	PHO	O2A-CGA-CBA	2.12	118.56	111.91
23	A	404	CLA	CHB-C4A-NA	2.12	127.44	124.51
25	b	618	BCR	C37-C22-C23	2.12	121.41	118.08
25	c	516	BCR	C37-C22-C21	-2.12	119.96	122.92
23	C	503	CLA	CMC-C2C-C1C	2.12	128.26	125.04
23	b	605	CLA	CAC-C3C-C4C	2.12	127.56	124.81
25	D	407	BCR	C15-C14-C13	-2.12	124.29	127.31
25	b	618	BCR	C11-C10-C9	-2.12	124.29	127.31
23	D	406	CLA	CHB-C4A-NA	2.12	127.44	124.51
34	b	626	LMT	O5'-C1'-C2'	2.11	114.83	110.35
35	C	518	DGD	C1E-O6E-C5E	-2.11	109.54	113.69
25	A	409	BCR	C36-C18-C19	2.11	121.41	118.08
29	d	406	PL9	C25-C24-C26	2.11	118.82	115.27
23	C	503	CLA	C4-C3-C5	2.11	118.82	115.27
23	D	405	CLA	CHD-C4C-NC	2.11	127.53	124.20
35	h	103	DGD	O4D-C4D-C3D	-2.11	105.47	110.35
34	M	104	LMT	O1B-C1B-C2B	2.11	113.56	108.10
23	b	614	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
23	C	505	CLA	O2A-CGA-CBA	2.11	118.52	111.91
23	A	405	CLA	CMA-C3A-C2A	-2.11	105.33	113.83
23	C	506	CLA	C2A-C1A-CHA	-2.11	120.18	123.86
25	k	102	BCR	C40-C30-C25	-2.11	106.88	110.30
34	a	418	LMT	O5B-C5B-C4B	2.10	113.51	109.69
23	A	404	CLA	O2A-C1-C2	2.10	114.16	108.64
33	h	101	HTG	O5-C1-C2	-2.10	107.67	110.31
35	c	518	DGD	O1G-C1A-O1A	-2.10	118.28	123.59
23	b	609	CLA	O2A-CGA-CBA	2.10	118.51	111.91
25	b	618	BCR	C20-C21-C22	-2.10	124.31	127.31
23	A	406	CLA	C1-C2-C3	-2.10	122.41	126.04
25	K	101	BCR	C3-C4-C5	-2.10	110.33	114.08
23	c	505	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
23	C	504	CLA	CBC-CAC-C3C	-2.10	106.66	112.43
23	B	607	CLA	O2A-CGA-CBA	2.09	118.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	405	CLA	C4-C3-C5	2.09	118.79	115.27
23	B	604	CLA	CHA-C1A-NA	-2.09	121.60	126.40
38	E	103	HEM	C3C-C4C-NC	-2.09	106.99	110.94
23	c	506	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	D	406	CLA	C1-O2A-CGA	2.09	121.93	116.44
23	A	404	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
29	d	406	PL9	C45-C44-C43	-2.09	118.32	123.68
34	B	628	LMT	C1-O1'-C1'	-2.09	110.38	113.84
23	A	404	CLA	CAA-CBA-CGA	-2.09	107.15	113.25
23	C	505	CLA	CAC-C3C-C4C	2.09	127.52	124.81
27	a	409	SQD	O47-C7-O49	-2.09	118.66	123.70
23	b	615	CLA	CHA-C1A-NA	-2.09	121.62	126.40
23	C	513	CLA	CBA-CAA-C2A	-2.09	107.70	113.86
25	C	516	BCR	C21-C20-C19	-2.09	116.71	123.22
23	c	513	CLA	CHA-C1A-NA	-2.09	121.62	126.40
34	m	103	LMT	O6'-C6'-C5'	-2.09	104.14	111.29
23	A	408	CLA	CHB-C4A-NA	2.08	127.39	124.51
31	c	520	LMG	C8-O7-C10	-2.08	112.66	117.79
25	Y	101	BCR	C16-C15-C14	-2.08	119.21	123.47
23	A	408	CLA	CAC-C3C-C4C	2.08	127.51	124.81
23	b	616	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
38	E	103	HEM	O2A-CGA-CBA	2.08	120.72	114.03
33	B	624	HTG	C1-O5-C5	2.08	116.42	112.58
23	D	406	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	d	402	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	b	615	CLA	C6-C5-C3	-2.08	108.01	113.45
23	B	616	CLA	CAC-C3C-C2C	2.07	131.08	127.53
23	b	606	CLA	C2A-C3A-C4A	-2.07	98.52	101.87
23	c	513	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
23	c	505	CLA	C4-C3-C5	2.07	118.76	115.27
29	a	414	PL9	C16-C14-C13	-2.07	116.92	121.12
25	Y	101	BCR	C29-C28-C27	-2.07	106.75	111.38
23	c	512	CLA	C11-C12-C13	-2.07	109.23	115.92
34	E	102	LMT	O5B-C5B-C4B	2.07	113.45	109.69
23	b	610	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
23	d	403	CLA	C4-C3-C2	-2.07	118.38	123.68
23	C	512	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
33	B	624	HTG	C6-C5-C4	-2.07	108.16	113.00
23	d	402	CLA	CMB-C2B-C1B	2.07	131.64	128.46
23	B	616	CLA	C1-O2A-CGA	2.07	121.86	116.44
23	a	404	CLA	CMA-C3A-C2A	-2.07	105.50	113.83
23	b	604	CLA	C6-C7-C8	-2.07	109.24	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	618	BCR	C10-C11-C12	-2.07	116.77	123.22
23	B	614	CLA	CHB-C4A-NA	2.07	127.37	124.51
23	C	505	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
23	C	514	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
34	D	404	LMT	C3B-C4B-C5B	2.06	113.92	110.24
23	c	510	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
25	d	405	BCR	C35-C13-C14	-2.06	120.03	122.92
23	b	601	CLA	C1-O2A-CGA	2.06	121.85	116.44
31	c	521	LMG	C1-O6-C5	2.06	117.73	113.69
25	A	409	BCR	C34-C9-C10	-2.06	120.04	122.92
25	c	516	BCR	C20-C21-C22	-2.06	124.37	127.31
23	B	601	CLA	C1-O2A-CGA	2.06	121.84	116.44
25	k	101	BCR	C34-C9-C10	-2.06	120.04	122.92
23	c	507	CLA	C2A-C1A-CHA	-2.06	120.27	123.86
35	h	103	DGD	C3G-O3G-C1D	-2.06	109.72	113.74
25	a	408	BCR	C11-C10-C9	-2.06	124.38	127.31
23	a	407	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
23	c	507	CLA	CED-O2D-CGD	2.05	120.58	115.94
23	c	502	CLA	C7-C6-C5	-2.05	107.78	113.36
31	C	521	LMG	C9-C8-C7	-2.05	106.93	111.79
23	C	513	CLA	CMC-C2C-C1C	2.05	128.16	125.04
23	B	615	CLA	C1-C2-C3	-2.05	122.50	126.04
23	c	504	CLA	CMB-C2B-C1B	2.05	131.62	128.46
23	c	503	CLA	C1-O2A-CGA	2.05	121.82	116.44
25	a	408	BCR	C39-C30-C25	-2.05	106.97	110.30
25	c	515	BCR	C3-C4-C5	-2.05	110.42	114.08
25	T	101	BCR	C34-C9-C10	-2.05	120.05	122.92
25	c	515	BCR	C8-C7-C6	-2.05	121.45	127.20
23	B	609	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
23	B	601	CLA	CHB-C4A-NA	2.05	127.34	124.51
25	b	619	BCR	C2-C1-C6	2.05	113.63	110.48
23	B	616	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
34	B	628	LMT	C3'-C4'-C5'	-2.04	106.24	110.93
23	B	606	CLA	CMC-C2C-C1C	2.04	128.15	125.04
23	c	513	CLA	C1-O2A-CGA	2.04	121.81	116.44
23	C	512	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
23	B	610	CLA	C11-C12-C13	-2.04	109.32	115.92
23	B	609	CLA	C4-C3-C5	2.04	118.70	115.27
25	t	102	BCR	C19-C18-C17	-2.04	115.81	118.94
23	b	606	CLA	C6-C7-C8	-2.04	109.33	115.92
23	B	602	CLA	C4-C3-C5	2.04	118.70	115.27
25	c	515	BCR	C34-C9-C10	-2.04	120.07	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	406	CLA	CBC-CAC-C3C	-2.03	106.82	112.43
23	C	503	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
23	B	616	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	B	619	BCR	C39-C30-C25	-2.03	107.00	110.30
23	B	601	CLA	C4-C3-C5	2.03	118.69	115.27
23	c	503	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
34	a	418	LMT	C1B-O1B-C4'	-2.03	112.94	117.96
23	b	613	CLA	C16-C15-C13	-2.03	109.36	115.92
25	C	515	BCR	C3-C4-C5	-2.03	110.46	114.08
23	c	502	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
23	C	513	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
23	C	509	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
34	D	403	LMT	C1'-O5'-C5'	2.02	117.66	113.69
25	d	405	BCR	C38-C26-C27	2.02	117.50	113.62
31	M	101	LMG	O1-C1-C2	-2.02	105.15	108.30
23	C	512	CLA	C1-C2-C3	-2.02	122.55	126.04
23	C	505	CLA	CMB-C2B-C3B	2.02	128.46	124.68
23	B	612	CLA	C11-C12-C13	-2.02	109.39	115.92
23	b	612	CLA	C11-C10-C8	-2.02	109.39	115.92
29	D	408	PL9	C15-C14-C16	2.02	118.67	115.27
23	C	513	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
25	t	102	BCR	C28-C27-C26	-2.02	110.47	114.08
25	k	102	BCR	C35-C13-C14	-2.02	120.09	122.92
35	C	518	DGD	C3A-C2A-C1A	-2.02	106.28	113.62
23	A	408	CLA	CMB-C2B-C3B	2.02	128.45	124.68
27	B	620	SQD	O48-C23-O10	-2.02	118.50	123.59
23	C	513	CLA	CMA-C3A-C4A	-2.02	106.36	111.77
23	c	505	CLA	C1-C2-C3	-2.02	122.56	126.04
29	A	413	PL9	C37-C36-C34	-2.01	106.35	112.98
23	C	511	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
23	b	604	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	b	607	CLA	CMC-C2C-C1C	2.01	128.10	125.04
40	V	201	HEC	CMB-C2B-C3B	2.01	128.18	125.82
27	B	620	SQD	O47-C7-O49	-2.01	118.84	123.70
23	a	405	CLA	C1-O2A-CGA	2.01	121.72	116.44
23	C	503	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
31	A	415	LMG	C7-O1-C1	-2.01	109.82	113.74
31	Z	101	LMG	O6-C5-C6	2.01	111.42	106.44
23	b	601	CLA	C5-C3-C2	-2.01	117.06	121.12
23	c	505	CLA	C6-C7-C8	-2.00	109.44	115.92
31	a	417	LMG	C8-O7-C10	-2.00	112.86	117.79
25	c	516	BCR	C29-C30-C25	2.00	113.56	110.48

All (64) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	405	CLA	ND
23	D	406	CLA	ND
23	a	404	CLA	ND
23	a	407	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND
23	d	404	CLA	ND

All (1289) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	C14-C13-C15-C16
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	C	509	CLA	CHA-CBD-CGD-O1D
23	D	406	CLA	C2-C3-C5-C6
23	D	406	CLA	C4-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	610	CLA	C11-C12-C13-C14
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	C6-C7-C8-C9
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	514	CLA	C2-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
23	d	404	CLA	C2-C3-C5-C6
23	d	404	CLA	C4-C3-C5-C6
25	D	407	BCR	C21-C22-C23-C24
25	D	407	BCR	C37-C22-C23-C24
25	D	407	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	d	405	BCR	C23-C24-C25-C30
25	k	102	BCR	C1-C6-C7-C8
25	k	102	BCR	C5-C6-C7-C8
25	t	102	BCR	C11-C12-C13-C14
25	t	102	BCR	C11-C12-C13-C35
26	B	623	GOL	C1-C2-C3-O3
26	b	623	GOL	C1-C2-C3-O3
26	v	202	GOL	O1-C1-C2-C3
27	A	411	SQD	O6-C44-C45-O47
27	B	620	SQD	O49-C7-O47-C45
27	B	620	SQD	C8-C7-O47-C45
27	D	415	SQD	O49-C7-O47-C45
27	D	415	SQD	C8-C7-O47-C45
27	L	102	SQD	O49-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
27	a	411	SQD	C5-C6-S-O7
27	a	411	SQD	C5-C6-S-O8
27	a	411	SQD	C5-C6-S-O9
27	f	102	SQD	C2-C1-O6-C44
27	f	102	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C8-C7-O47-C45
29	A	413	PL9	C19-C21-C22-C23
29	A	413	PL9	C23-C24-C26-C27
29	A	413	PL9	C25-C24-C26-C27
29	a	414	PL9	C13-C14-C16-C17
29	a	414	PL9	C15-C14-C16-C17
29	a	414	PL9	C19-C21-C22-C23
31	C	521	LMG	C11-C10-O7-C8
31	Z	101	LMG	O9-C10-O7-C8
31	Z	101	LMG	C11-C10-O7-C8
31	a	417	LMG	O9-C10-O7-C8
31	a	417	LMG	C11-C10-O7-C8
31	c	521	LMG	C11-C10-O7-C8
31	z	101	LMG	O6-C1-O1-C7
31	z	101	LMG	C11-C10-O7-C8
32	D	409	LHG	C3-O3-P-O4
32	E	101	LHG	C3-O3-P-O4
32	E	101	LHG	C3-O3-P-O5
32	E	101	LHG	C3-O3-P-O6
32	L	101	LHG	C4-O6-P-O4
32	a	419	LHG	C3-O3-P-O4
32	a	419	LHG	O10-C23-O8-C6
32	a	419	LHG	C24-C23-O8-C6
32	b	628	LHG	C4-O6-P-O3
32	b	628	LHG	C4-O6-P-O4
32	b	628	LHG	C4-O6-P-O5
32	d	407	LHG	C3-O3-P-O4
32	d	407	LHG	C3-O3-P-O5
32	d	407	LHG	C3-O3-P-O6
32	d	408	LHG	O2-C2-C3-O3
32	d	408	LHG	C3-O3-P-O4
33	b	621	HTG	C2'-C1'-S1-C1
34	C	525	LMT	C2'-C1'-O1'-C1
34	C	525	LMT	O5'-C1'-O1'-C1
34	D	403	LMT	C2'-C1'-O1'-C1
34	D	403	LMT	O5'-C1'-O1'-C1
34	E	102	LMT	C2'-C1'-O1'-C1
34	E	102	LMT	O5'-C1'-O1'-C1
34	M	104	LMT	C2'-C1'-O1'-C1
34	M	104	LMT	O5'-C1'-O1'-C1
34	a	412	LMT	C2'-C1'-O1'-C1
34	a	412	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
34	a	418	LMT	C2'-C1'-O1'-C1
34	a	418	LMT	O5'-C1'-O1'-C1
34	b	620	LMT	O5'-C1'-O1'-C1
34	b	626	LMT	C2'-C1'-O1'-C1
34	b	626	LMT	O5'-C1'-O1'-C1
34	b	626	LMT	C2-C1-O1'-C1'
34	e	101	LMT	C2'-C1'-O1'-C1
34	e	101	LMT	O5'-C1'-O1'-C1
34	t	101	LMT	O5'-C1'-O1'-C1
34	t	101	LMT	C2-C1-O1'-C1'
34	C	525	LMT	C3'-C4'-O1B-C1B
32	E	101	LHG	O10-C23-O8-C6
32	E	101	LHG	C24-C23-O8-C6
27	f	102	SQD	O49-C7-O47-C45
31	c	521	LMG	O9-C10-O7-C8
23	B	604	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	C	507	CLA	C3-C5-C6-C7
23	b	615	CLA	C13-C15-C16-C17
23	B	603	CLA	C4-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6
29	A	413	PL9	C13-C14-C16-C17
23	C	502	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	a	407	CLA	C3-C5-C6-C7
23	c	507	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	404	CLA	C3-C5-C6-C7
27	f	102	SQD	C24-C23-O48-C46
34	M	104	LMT	O5'-C5'-C6'-O6'
31	C	521	LMG	O9-C10-O7-C8
31	z	101	LMG	O9-C10-O7-C8
25	T	101	BCR	C13-C14-C15-C16
31	c	521	LMG	O6-C5-C6-O5
23	b	613	CLA	CBD-CGD-O2D-CED
33	c	522	HTG	C4-C5-C6-O6
34	E	102	LMT	O5'-C5'-C6'-O6'
31	C	521	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
31	A	415	LMG	C4-C5-C6-O5
34	D	404	LMT	O5B-C5B-C6B-O6B
34	e	101	LMT	O5'-C5'-C6'-O6'
33	B	624	HTG	O5-C5-C6-O6
33	c	522	HTG	O5-C5-C6-O6
23	A	408	CLA	C4-C3-C5-C6
23	B	616	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
29	A	413	PL9	C15-C14-C16-C17
29	a	414	PL9	C25-C24-C26-C27
23	A	408	CLA	C2-C3-C5-C6
23	B	616	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	a	414	PL9	C23-C24-C26-C27
32	b	628	LHG	C7-C8-C9-C10
23	c	510	CLA	O1A-CGA-O2A-C1
27	f	102	SQD	O10-C23-O48-C46
27	B	620	SQD	O5-C1-O6-C44
31	c	521	LMG	O6-C1-O1-C7
34	M	102	LMT	O5'-C1'-O1'-C1
29	a	414	PL9	C24-C26-C27-C28
29	a	414	PL9	C29-C31-C32-C33
29	d	406	PL9	C39-C41-C42-C43
23	c	510	CLA	CBA-CGA-O2A-C1
31	M	101	LMG	C32-C33-C34-C35
34	D	404	LMT	C4'-C5'-C6'-O6'
23	b	604	CLA	CBD-CGD-O2D-CED
34	D	404	LMT	C5'-C4'-O1B-C1B
34	M	104	LMT	C4'-C5'-C6'-O6'
23	A	405	CLA	C15-C16-C17-C18
23	A	408	CLA	C5-C6-C7-C8
23	C	513	CLA	C15-C16-C17-C18
23	b	604	CLA	C8-C10-C11-C12
23	c	507	CLA	C15-C16-C17-C18
32	d	407	LHG	O2-C2-C3-O3
34	b	620	LMT	C2'-C1'-O1'-C1
34	t	101	LMT	C2'-C1'-O1'-C1
27	a	411	SQD	O6-C44-C45-O47
27	C	501	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	A	415	LMG	O6-C5-C6-O5
29	A	413	PL9	C12-C11-C9-C10
23	B	603	CLA	C2-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C12-C13-C14
23	C	514	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
25	D	407	BCR	C7-C8-C9-C34
25	Y	101	BCR	C37-C22-C23-C24
25	d	405	BCR	C7-C8-C9-C34
32	d	407	LHG	C23-C24-C25-C26
23	C	507	CLA	C10-C11-C12-C13
34	C	525	LMT	O5B-C5B-C6B-O6B
23	B	601	CLA	CBA-CGA-O2A-C1
23	B	606	CLA	C15-C16-C17-C18
23	B	614	CLA	C8-C10-C11-C12
23	C	509	CLA	C10-C11-C12-C13
23	b	606	CLA	C10-C11-C12-C13
23	c	508	CLA	C8-C10-C11-C12
27	B	620	SQD	C7-C8-C9-C10
31	Z	101	LMG	C10-C11-C12-C13
34	D	404	LMT	C3'-C4'-O1B-C1B
34	m	103	LMT	O5'-C5'-C6'-O6'
23	B	602	CLA	C15-C16-C17-C18
23	B	615	CLA	C5-C6-C7-C8
23	C	503	CLA	C13-C15-C16-C17
23	C	506	CLA	C8-C10-C11-C12
23	C	506	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8
23	b	616	CLA	C13-C15-C16-C17
23	c	513	CLA	C15-C16-C17-C18
26	O	302	GOL	O2-C2-C3-O3
26	v	202	GOL	O1-C1-C2-O2
27	D	415	SQD	C7-C8-C9-C10
34	b	626	LMT	C11-C10-C9-C8
34	D	404	LMT	C4B-C5B-C6B-O6B
23	A	408	CLA	C15-C16-C17-C18
23	B	614	CLA	C10-C11-C12-C13
23	C	510	CLA	C13-C15-C16-C17
23	d	404	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	M	101	LMG	C15-C16-C17-C18
23	d	402	CLA	C15-C16-C17-C18
35	c	518	DGD	C1B-C2B-C3B-C4B
23	c	509	CLA	C10-C11-C12-C13
23	D	406	CLA	C11-C10-C8-C7
23	a	405	CLA	C11-C12-C13-C15
23	B	601	CLA	O1A-CGA-O2A-C1
23	b	610	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C10-C11-C12-C13
33	B	624	HTG	C4-C5-C6-O6
34	e	101	LMT	C4'-C5'-C6'-O6'
35	C	518	DGD	O6E-C1E-O5D-C6D
29	A	413	PL9	C24-C26-C27-C28
29	D	408	PL9	C39-C41-C42-C43
31	a	417	LMG	O6-C5-C6-O5
34	C	525	LMT	O1'-C1-C2-C3
23	d	404	CLA	O1A-CGA-O2A-C1
23	B	603	CLA	C8-C10-C11-C12
23	C	507	CLA	C8-C10-C11-C12
23	C	511	CLA	C8-C10-C11-C12
23	b	603	CLA	C13-C15-C16-C17
23	b	606	CLA	C13-C15-C16-C17
27	C	501	SQD	C18-C19-C20-C21
34	D	404	LMT	O5'-C5'-C6'-O6'
23	A	406	CLA	C15-C16-C17-C18
23	B	601	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
23	b	605	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
23	b	616	CLA	C10-C11-C12-C13
32	D	409	LHG	C3-O3-P-O6
32	L	101	LHG	C4-O6-P-O3
32	a	419	LHG	C3-O3-P-O6
32	d	408	LHG	C3-O3-P-O6
31	Z	101	LMG	O6-C5-C6-O5
33	B	622	HTG	C1'-C2'-C3'-C4'
35	C	518	DGD	C5A-C6A-C7A-C8A
32	d	408	LHG	C1-C2-C3-O3
24	a	406	PHO	C4-C3-C5-C6
29	D	408	PL9	C15-C14-C16-C17
23	B	610	CLA	C2A-CAA-CBA-CGA
35	c	517	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
32	E	101	LHG	C23-C24-C25-C26
23	B	604	CLA	C8-C10-C11-C12
27	A	411	SQD	C17-C18-C19-C20
27	C	501	SQD	C9-C10-C11-C12
31	A	415	LMG	C16-C17-C18-C19
31	C	520	LMG	C30-C31-C32-C33
31	C	521	LMG	C36-C37-C38-C39
31	d	412	LMG	C21-C22-C23-C24
32	d	408	LHG	C32-C33-C34-C35
35	C	517	DGD	C4B-C5B-C6B-C7B
35	c	518	DGD	C7A-C8A-C9A-CAA
23	d	402	CLA	C16-C17-C18-C20
32	d	409	LHG	C29-C30-C31-C32
35	H	102	DGD	C5B-C6B-C7B-C8B
35	c	517	DGD	C8B-C9B-CAB-CBB
27	B	620	SQD	C46-C45-O47-C7
31	M	101	LMG	O9-C10-O7-C8
23	C	504	CLA	CBD-CGD-O2D-CED
27	a	411	SQD	C25-C26-C27-C28
32	b	628	LHG	C14-C15-C16-C17
32	b	628	LHG	C25-C26-C27-C28
32	d	408	LHG	C33-C34-C35-C36
35	c	518	DGD	C7B-C8B-C9B-CAB
31	A	415	LMG	C12-C13-C14-C15
32	D	410	LHG	C28-C29-C30-C31
31	c	521	LMG	C4-C5-C6-O5
31	z	101	LMG	C4-C5-C6-O5
23	C	513	CLA	C13-C15-C16-C17
31	a	417	LMG	C21-C22-C23-C24
27	f	102	SQD	C23-C24-C25-C26
31	d	412	LMG	C10-C11-C12-C13
27	D	415	SQD	C2-C1-O6-C44
31	A	415	LMG	C2-C1-O1-C7
34	M	102	LMT	C2'-C1'-O1'-C1
35	C	518	DGD	C2E-C1E-O5D-C6D
27	a	409	SQD	C30-C31-C32-C33
31	C	520	LMG	C21-C22-C23-C24
31	C	520	LMG	C37-C38-C39-C40
31	c	521	LMG	C30-C31-C32-C33
32	D	410	LHG	C32-C33-C34-C35
23	C	508	CLA	C5-C6-C7-C8
23	C	502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C4-C3-C5-C6
23	b	601	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
27	C	501	SQD	C12-C13-C14-C15
27	D	415	SQD	C30-C31-C32-C33
35	c	518	DGD	C9A-CAA-CBA-CCA
23	C	506	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
23	B	606	CLA	C11-C10-C8-C9
23	a	404	CLA	C14-C13-C15-C16
27	a	409	SQD	C9-C10-C11-C12
32	d	407	LHG	C34-C35-C36-C37
32	d	409	LHG	C28-C29-C30-C31
35	C	518	DGD	C8B-C9B-CAB-CBB
27	C	501	SQD	C15-C16-C17-C18
31	D	414	LMG	C19-C20-C21-C22
26	A	410	GOL	O1-C1-C2-C3
26	A	410	GOL	C1-C2-C3-O3
26	B	626	GOL	C1-C2-C3-O3
26	O	302	GOL	O1-C1-C2-C3
26	O	302	GOL	C1-C2-C3-O3
26	a	410	GOL	O1-C1-C2-C3
26	a	410	GOL	C1-C2-C3-O3
32	A	416	LHG	O1-C1-C2-C3
32	D	410	LHG	O1-C1-C2-C3
32	d	407	LHG	O1-C1-C2-C3
23	b	614	CLA	C3-C5-C6-C7
31	M	101	LMG	C11-C10-O7-C8
32	D	409	LHG	C12-C13-C14-C15
34	D	403	LMT	C5-C6-C7-C8
23	d	402	CLA	CBD-CGD-O2D-CED
31	A	415	LMG	C17-C18-C19-C20
31	M	101	LMG	C36-C37-C38-C39
32	D	410	LHG	C12-C13-C14-C15
32	D	410	LHG	C29-C30-C31-C32
32	d	407	LHG	C33-C34-C35-C36
35	h	103	DGD	CAB-CBB-CCB-CDB
23	B	615	CLA	C16-C17-C18-C20
23	a	407	CLA	C16-C17-C18-C19
23	a	407	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	A	415	LMG	O6-C1-O1-C7
23	b	611	CLA	C15-C16-C17-C18
29	A	413	PL9	C14-C16-C17-C18
27	L	102	SQD	C13-C14-C15-C16
27	a	411	SQD	C16-C17-C18-C19
31	A	415	LMG	C14-C15-C16-C17
32	D	410	LHG	C33-C34-C35-C36
35	c	517	DGD	C4D-C5D-C6D-O5D
27	A	411	SQD	C24-C25-C26-C27
32	L	101	LHG	C17-C18-C19-C20
33	B	622	HTG	C2'-C3'-C4'-C5'
34	B	628	LMT	O1'-C1-C2-C3
32	E	101	LHG	C7-C8-C9-C10
27	A	411	SQD	C26-C27-C28-C29
31	D	414	LMG	C35-C36-C37-C38
32	E	101	LHG	C24-C25-C26-C27
31	C	521	LMG	C17-C18-C19-C20
35	h	103	DGD	CCB-CDB-CEB-CFB
34	a	412	LMT	C1-C2-C3-C4
34	e	101	LMT	C2-C1-O1'-C1'
27	B	620	SQD	C30-C31-C32-C33
27	D	415	SQD	C28-C29-C30-C31
31	A	415	LMG	C18-C19-C20-C21
31	A	415	LMG	C34-C35-C36-C37
32	E	101	LHG	C10-C11-C12-C13
23	B	615	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C19
27	B	620	SQD	C11-C10-C9-C8
31	Z	101	LMG	C16-C17-C18-C19
27	C	501	SQD	O6-C44-C45-C46
31	A	415	LMG	C38-C39-C40-C41
23	b	604	CLA	C3-C5-C6-C7
35	C	518	DGD	CBB-CCB-CDB-CEB
23	B	614	CLA	C5-C6-C7-C8
23	c	513	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	C4E-C5E-C6E-O5E
23	b	601	CLA	C2-C3-C5-C6
23	b	609	CLA	C2-C3-C5-C6
24	a	406	PHO	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
27	C	501	SQD	C8-C7-O47-C45
34	D	403	LMT	C3-C4-C5-C6
32	A	416	LHG	C23-C24-C25-C26
23	b	609	CLA	C16-C17-C18-C20
35	c	518	DGD	CBB-CCB-CDB-CEB
32	d	409	LHG	C11-C10-C9-C8
34	b	626	LMT	C5-C6-C7-C8
27	C	501	SQD	O49-C7-O47-C45
23	b	601	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C2-C1-O2A-CGA
31	A	415	LMG	C37-C38-C39-C40
31	d	412	LMG	C38-C39-C40-C41
34	e	101	LMT	C5-C6-C7-C8
31	C	520	LMG	C17-C18-C19-C20
32	A	416	LHG	C26-C27-C28-C29
23	b	601	CLA	C3-C5-C6-C7
25	D	407	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	d	405	BCR	C23-C24-C25-C26
31	C	520	LMG	C29-C30-C31-C32
32	L	101	LHG	C25-C26-C27-C28
32	d	409	LHG	C24-C23-O8-C6
23	c	512	CLA	C8-C10-C11-C12
34	b	620	LMT	C5-C6-C7-C8
34	m	103	LMT	O1'-C1-C2-C3
34	b	626	LMT	C1-C2-C3-C4
31	d	412	LMG	O6-C5-C6-O5
27	B	620	SQD	C10-C11-C12-C13
31	C	520	LMG	C31-C32-C33-C34
31	m	101	LMG	C14-C15-C16-C17
23	B	604	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
29	D	408	PL9	C30-C29-C31-C32
23	B	606	CLA	C11-C10-C8-C7
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C2-C3-C5-C6
23	D	405	CLA	C12-C13-C15-C16
23	a	404	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	c	511	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
29	D	408	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
29	d	406	PL9	C13-C14-C16-C17
23	c	513	CLA	O1A-CGA-O2A-C1
27	L	102	SQD	C27-C28-C29-C30
32	a	419	LHG	C23-C24-C25-C26
32	d	408	LHG	C34-C35-C36-C37
23	c	509	CLA	C5-C6-C7-C8
35	H	102	DGD	CBA-CCA-CDA-CEA
35	c	517	DGD	C1A-C2A-C3A-C4A
23	c	510	CLA	C15-C16-C17-C18
27	A	411	SQD	C29-C30-C31-C32
32	L	101	LHG	C24-C25-C26-C27
34	B	628	LMT	C11-C10-C9-C8
31	C	521	LMG	C18-C19-C20-C21
31	c	520	LMG	C32-C33-C34-C35
31	m	101	LMG	C38-C39-C40-C41
32	d	409	LHG	O10-C23-O8-C6
32	D	410	LHG	C24-C23-O8-C6
27	D	415	SQD	O5-C1-O6-C44
34	m	103	LMT	O5'-C1'-O1'-C1
35	c	518	DGD	O6E-C1E-O5D-C6D
23	B	613	CLA	C15-C16-C17-C18
29	A	413	PL9	C9-C11-C12-C13
29	a	414	PL9	C39-C41-C42-C43
32	E	101	LHG	C11-C10-C9-C8
32	b	628	LHG	C16-C17-C18-C19
31	m	101	LMG	C11-C10-O7-C8
31	m	101	LMG	C39-C40-C41-C42
32	D	409	LHG	C16-C17-C18-C19
34	M	104	LMT	C2B-C1B-O1B-C4'
23	D	406	CLA	C3-C5-C6-C7
31	D	414	LMG	C30-C31-C32-C33
32	d	409	LHG	C9-C10-C11-C12
34	m	103	LMT	C2'-C1'-O1'-C1
23	C	508	CLA	C10-C11-C12-C13
27	C	501	SQD	O6-C44-C45-O47
35	c	517	DGD	O6E-C5E-C6E-O5E
27	L	102	SQD	C12-C13-C14-C15
31	a	417	LMG	C36-C37-C38-C39
35	h	103	DGD	CAA-CBA-CCA-CDA
31	D	414	LMG	C12-C13-C14-C15
32	b	628	LHG	C31-C32-C33-C34
23	C	511	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	413	PL9	C4-C3-C7-C8
29	a	414	PL9	C4-C3-C7-C8
23	C	510	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	D	406	CLA	C11-C10-C8-C9
23	a	405	CLA	C11-C12-C13-C14
23	c	506	CLA	C11-C12-C13-C14
35	C	519	DGD	O6E-C5E-C6E-O5E
32	a	419	LHG	C13-C14-C15-C16
27	B	620	SQD	C14-C15-C16-C17
35	C	518	DGD	C5B-C6B-C7B-C8B
25	b	619	BCR	C37-C22-C23-C24
25	t	102	BCR	C7-C8-C9-C34
34	m	103	LMT	C4'-C5'-C6'-O6'
25	Y	101	BCR	C21-C22-C23-C24
23	C	502	CLA	C1A-C2A-CAA-CBA
23	b	610	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
31	A	415	LMG	O9-C10-O7-C8
31	m	101	LMG	O9-C10-O7-C8
31	A	415	LMG	C11-C10-O7-C8
32	d	407	LHG	C29-C30-C31-C32
35	C	519	DGD	C6B-C7B-C8B-C9B
34	M	104	LMT	O1'-C1-C2-C3
32	L	101	LHG	C23-C24-C25-C26
23	b	613	CLA	O1D-CGD-O2D-CED
34	t	101	LMT	C6-C7-C8-C9
32	A	416	LHG	C18-C19-C20-C21
35	C	518	DGD	CCB-CDB-CEB-CFB
27	A	411	SQD	C7-C8-C9-C10
23	B	605	CLA	C5-C6-C7-C8
27	L	102	SQD	C28-C29-C30-C31
35	C	517	DGD	O6D-C5D-C6D-O5D
31	c	520	LMG	C36-C37-C38-C39
35	H	102	DGD	C9A-CAA-CBA-CCA
35	c	518	DGD	C6A-C7A-C8A-C9A
27	L	102	SQD	C24-C23-O48-C46
31	D	414	LMG	O6-C5-C6-O5
29	D	408	PL9	C13-C14-C16-C17
23	A	408	CLA	C8-C10-C11-C12
27	A	411	SQD	C30-C31-C32-C33
32	d	408	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
33	b	622	HTG	O5-C5-C6-O6
27	A	411	SQD	C16-C17-C18-C19
27	B	620	SQD	C44-C45-C46-O48
27	a	411	SQD	O6-C44-C45-C46
31	Z	101	LMG	C7-C8-C9-O8
33	h	101	HTG	O5-C5-C6-O6
35	C	518	DGD	C8A-C9A-CAA-CBA
32	D	410	LHG	O10-C23-O8-C6
35	c	518	DGD	C5D-C6D-O5D-C1E
31	c	520	LMG	C30-C31-C32-C33
32	a	419	LHG	C18-C19-C20-C21
35	C	517	DGD	C6B-C7B-C8B-C9B
23	c	502	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	C15-C16-C17-C18
23	B	615	CLA	C8-C10-C11-C12
34	e	101	LMT	C2B-C1B-O1B-C4'
33	B	621	HTG	C3'-C4'-C5'-C6'
35	C	518	DGD	CDA-CEA-CFA-CGA
34	b	620	LMT	C3'-C4'-O1B-C1B
23	B	603	CLA	C16-C17-C18-C20
23	c	514	CLA	CBD-CGD-O2D-CED
26	B	623	GOL	O2-C2-C3-O3
26	O	302	GOL	O1-C1-C2-O2
26	a	410	GOL	O2-C2-C3-O3
32	d	407	LHG	O1-C1-C2-O2
35	c	518	DGD	CCA-CDA-CEA-CFA
23	C	511	CLA	O1A-CGA-O2A-C1
32	d	407	LHG	C16-C17-C18-C19
32	d	408	LHG	C31-C32-C33-C34
35	C	518	DGD	C6A-C7A-C8A-C9A
23	B	602	CLA	C13-C15-C16-C17
23	B	611	CLA	C8-C10-C11-C12
29	a	414	PL9	C30-C29-C31-C32
29	d	406	PL9	C15-C14-C16-C17
32	D	409	LHG	C11-C12-C13-C14
23	b	610	CLA	C16-C17-C18-C20
23	C	511	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
35	C	517	DGD	O6E-C5E-C6E-O5E
23	C	513	CLA	C10-C11-C12-C13
31	A	415	LMG	C40-C41-C42-C43
31	M	101	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	D	406	CLA	C10-C11-C12-C13
23	B	616	CLA	C2-C1-O2A-CGA
33	B	624	HTG	C3'-C4'-C5'-C6'
35	h	103	DGD	CDB-CEB-CFB-CGB
31	D	414	LMG	C38-C39-C40-C41
23	c	512	CLA	CBA-CGA-O2A-C1
23	a	404	CLA	C16-C17-C18-C19
23	b	609	CLA	C16-C17-C18-C19
23	c	512	CLA	O1A-CGA-O2A-C1
23	C	514	CLA	C13-C15-C16-C17
35	c	518	DGD	C2E-C1E-O5D-C6D
27	L	102	SQD	O47-C45-C46-O48
23	c	508	CLA	C5-C6-C7-C8
31	c	521	LMG	C29-C30-C31-C32
34	a	418	LMT	C4-C5-C6-C7
27	D	415	SQD	C29-C30-C31-C32
35	C	517	DGD	C3A-C4A-C5A-C6A
23	C	503	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C12-C13-C15-C16
23	b	610	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
23	c	511	CLA	C11-C10-C8-C7
23	B	614	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	a	405	CLA	C14-C13-C15-C16
23	b	610	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
27	L	102	SQD	C15-C16-C17-C18
27	D	415	SQD	C24-C23-O48-C46
35	c	517	DGD	C2A-C1A-O1G-C1G
23	C	507	CLA	C13-C15-C16-C17
31	C	521	LMG	C33-C34-C35-C36
31	M	101	LMG	C17-C18-C19-C20
23	b	601	CLA	O1A-CGA-O2A-C1
23	B	606	CLA	C16-C17-C18-C20
25	D	407	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
34	t	101	LMT	C3-C4-C5-C6
23	C	513	CLA	C3-C5-C6-C7
23	D	405	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
27	L	102	SQD	O10-C23-O48-C46
23	c	511	CLA	CBA-CGA-O2A-C1
27	a	411	SQD	C24-C23-O48-C46
31	a	417	LMG	C28-C29-C30-C31
23	d	402	CLA	C13-C15-C16-C17
35	C	517	DGD	CDB-CEB-CFB-CGB
23	B	606	CLA	C13-C15-C16-C17
23	b	602	CLA	C10-C11-C12-C13
32	a	419	LHG	O6-C4-C5-C6
29	a	414	PL9	C9-C11-C12-C13
34	C	525	LMT	C3-C4-C5-C6
35	c	519	DGD	CBA-CCA-CDA-CEA
23	c	508	CLA	C15-C16-C17-C18
29	a	414	PL9	C28-C29-C31-C32
35	C	517	DGD	CBB-CCB-CDB-CEB
27	D	415	SQD	C27-C28-C29-C30
35	C	517	DGD	C3B-C4B-C5B-C6B
23	B	601	CLA	C3-C5-C6-C7
23	B	608	CLA	C16-C17-C18-C20
32	d	408	LHG	C30-C31-C32-C33
31	a	417	LMG	O8-C28-C29-C30
31	d	412	LMG	C28-C29-C30-C31
35	c	517	DGD	C2A-C3A-C4A-C5A
23	B	609	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
32	D	409	LHG	C28-C29-C30-C31
27	A	411	SQD	C27-C28-C29-C30
31	z	101	LMG	O6-C5-C6-O5
27	L	102	SQD	C44-C45-C46-O48
27	a	409	SQD	O6-C44-C45-C46
32	E	101	LHG	C4-C5-C6-O8
32	a	419	LHG	C4-C5-C6-O8
23	C	514	CLA	CBD-CGD-O2D-CED
34	a	418	LMT	C2-C3-C4-C5
35	H	102	DGD	O2G-C1B-C2B-C3B
33	b	621	HTG	C3'-C4'-C5'-C6'
34	b	626	LMT	C3-C4-C5-C6
34	e	101	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
32	A	416	LHG	C32-C33-C34-C35
35	c	517	DGD	C3A-C4A-C5A-C6A
23	c	511	CLA	O1A-CGA-O2A-C1
35	C	517	DGD	C4D-C5D-C6D-O5D
27	L	102	SQD	C14-C15-C16-C17
27	a	411	SQD	C31-C32-C33-C34
23	b	604	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C10-C11-C12-C13
31	M	101	LMG	C28-C29-C30-C31
35	H	102	DGD	CAA-CBA-CCA-CDA
32	A	416	LHG	O1-C1-C2-O2
32	A	416	LHG	C30-C31-C32-C33
35	C	517	DGD	C5B-C6B-C7B-C8B
35	H	102	DGD	O6E-C5E-C6E-O5E
27	a	411	SQD	C19-C20-C21-C22
33	B	622	HTG	C4'-C5'-C6'-C7'
23	b	608	CLA	C13-C15-C16-C17
34	E	102	LMT	C4'-C5'-C6'-O6'
27	B	620	SQD	O47-C45-C46-O48
27	a	409	SQD	O6-C44-C45-O47
31	Z	101	LMG	O7-C8-C9-O8
32	E	101	LHG	O7-C5-C6-O8
32	a	419	LHG	O7-C5-C6-O8
23	a	407	CLA	CBA-CGA-O2A-C1
27	D	415	SQD	C25-C26-C27-C28
35	c	517	DGD	O6E-C1E-O5D-C6D
23	b	616	CLA	C4-C3-C5-C6
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C2-C1-O2A-CGA
35	C	518	DGD	CAB-CBB-CCB-CDB
23	C	509	CLA	C5-C6-C7-C8
23	B	605	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	b	615	CLA	C6-C7-C8-C9
33	B	621	HTG	C2'-C3'-C4'-C5'
32	D	410	LHG	C2-C3-O3-P
27	a	411	SQD	C27-C28-C29-C30
27	f	102	SQD	C29-C30-C31-C32
23	a	404	CLA	C16-C17-C18-C20
25	Y	101	BCR	C23-C24-C25-C26
25	c	515	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	c	515	BCR	C23-C24-C25-C30
25	k	102	BCR	C23-C24-C25-C26
23	A	408	CLA	C13-C15-C16-C17
23	C	506	CLA	C10-C11-C12-C13
23	b	608	CLA	C15-C16-C17-C18
27	a	409	SQD	C27-C28-C29-C30
32	L	101	LHG	C12-C13-C14-C15
35	c	519	DGD	C2B-C3B-C4B-C5B
25	c	516	BCR	C7-C8-C9-C34
31	A	415	LMG	C35-C36-C37-C38
34	C	525	LMT	C4-C5-C6-C7
27	D	415	SQD	O10-C23-O48-C46
35	c	517	DGD	O1A-C1A-O1G-C1G
25	d	405	BCR	C7-C8-C9-C10
25	d	405	BCR	C21-C22-C23-C24
23	B	610	CLA	C13-C15-C16-C17
27	B	620	SQD	C19-C20-C21-C22
33	b	624	HTG	C4'-C5'-C6'-C7'
35	H	102	DGD	CDB-CEB-CFB-CGB
34	M	104	LMT	O5B-C1B-O1B-C4'
31	C	521	LMG	C32-C33-C34-C35
27	a	411	SQD	O10-C23-O48-C46
31	a	417	LMG	C32-C33-C34-C35
23	B	606	CLA	C8-C10-C11-C12
32	b	628	LHG	O6-C4-C5-C6
33	B	624	HTG	C2'-C3'-C4'-C5'
35	h	103	DGD	C9A-CAA-CBA-CCA
23	B	614	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	D	406	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C2-C3-C5-C6
23	c	505	CLA	C12-C13-C15-C16
23	c	507	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C10-C8-C7
33	c	522	HTG	S1-C1'-C2'-C3'
23	A	404	CLA	C13-C15-C16-C17
23	B	603	CLA	C16-C17-C18-C19
27	D	415	SQD	C23-C24-C25-C26
23	C	512	CLA	CBA-CGA-O2A-C1
35	C	519	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
31	A	415	LMG	O8-C28-C29-C30
33	b	621	HTG	S1-C1'-C2'-C3'
23	B	613	CLA	C13-C15-C16-C17
23	c	509	CLA	C8-C10-C11-C12
34	D	404	LMT	C6-C7-C8-C9
23	B	604	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
24	D	402	PHO	CAD-CBD-CGD-O2D
38	f	101	HEM	C2B-C3B-CAB-CBB
34	D	403	LMT	C4'-C5'-C6'-O6'
32	a	419	LHG	C25-C26-C27-C28
23	C	503	CLA	C15-C16-C17-C18
23	b	616	CLA	C15-C16-C17-C18
32	D	409	LHG	C26-C27-C28-C29
23	B	602	CLA	C16-C17-C18-C20
23	B	608	CLA	C16-C17-C18-C19
27	a	409	SQD	C34-C35-C36-C37
31	M	101	LMG	C20-C21-C22-C23
29	A	413	PL9	C44-C46-C47-C48
27	A	411	SQD	O6-C44-C45-C46
31	C	521	LMG	C7-C8-C9-O8
32	d	409	LHG	C2-C3-O3-P
34	M	102	LMT	C9-C10-C11-C12
32	a	419	LHG	O6-C4-C5-O7
32	b	628	LHG	O6-C4-C5-O7
23	b	615	CLA	C5-C6-C7-C8
32	b	628	LHG	C34-C35-C36-C37
23	C	506	CLA	C5-C6-C7-C8
23	b	611	CLA	C10-C11-C12-C13
31	A	415	LMG	C32-C33-C34-C35
34	M	102	LMT	C2-C3-C4-C5
23	a	405	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C16-C17-C18-C19
27	A	411	SQD	O49-C7-O47-C45
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
32	D	410	LHG	C9-C10-C11-C12
23	C	512	CLA	O1A-CGA-O2A-C1
23	a	407	CLA	O1A-CGA-O2A-C1
32	b	628	LHG	C32-C33-C34-C35
35	c	517	DGD	C2E-C1E-O5D-C6D
27	a	411	SQD	C26-C27-C28-C29
23	b	604	CLA	C13-C15-C16-C17
27	B	620	SQD	C9-C10-C11-C12
32	D	409	LHG	C10-C11-C12-C13
26	B	626	GOL	O2-C2-C3-O3
26	a	410	GOL	O1-C1-C2-O2
32	D	410	LHG	O1-C1-C2-O2
27	A	411	SQD	C8-C7-O47-C45
35	C	519	DGD	C1B-C2B-C3B-C4B
23	c	514	CLA	O1D-CGD-O2D-CED
23	D	406	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	d	402	CLA	C14-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C14
31	C	520	LMG	C13-C14-C15-C16
31	m	101	LMG	C32-C33-C34-C35
35	C	519	DGD	C8A-C9A-CAA-CBA
35	c	517	DGD	C6B-C7B-C8B-C9B
23	C	504	CLA	O1D-CGD-O2D-CED
27	B	620	SQD	C12-C13-C14-C15
32	E	101	LHG	C26-C27-C28-C29
23	b	601	CLA	CAA-CBA-CGA-O2A
25	b	619	BCR	C21-C22-C23-C24
34	b	620	LMT	C3-C4-C5-C6
23	C	513	CLA	CBA-CGA-O2A-C1
31	c	521	LMG	C29-C28-O8-C9
35	h	103	DGD	C5B-C6B-C7B-C8B
32	a	419	LHG	C4-O6-P-O3
32	d	409	LHG	C10-C11-C12-C13
34	D	403	LMT	C6-C7-C8-C9
33	V	202	HTG	O5-C5-C6-O6
24	a	416	PHO	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	A	413	PL9	C3-C7-C8-C9
32	L	101	LHG	C4-O6-P-O5
23	A	406	CLA	C16-C17-C18-C20
23	b	603	CLA	C16-C17-C18-C20
32	E	101	LHG	C17-C18-C19-C20
35	C	517	DGD	C2B-C3B-C4B-C5B
23	A	408	CLA	C3-C5-C6-C7
23	b	605	CLA	C16-C17-C18-C20
31	d	412	LMG	C29-C30-C31-C32
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	C	511	CLA	C10-C11-C12-C13
34	b	626	LMT	C4-C5-C6-C7
23	c	502	CLA	O1D-CGD-O2D-CED
27	C	501	SQD	C13-C14-C15-C16
23	d	403	CLA	C16-C17-C18-C20
23	A	406	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	B	602	CLA	C11-C12-C13-C15
23	b	601	CLA	C6-C7-C8-C10
23	b	609	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C15
23	c	509	CLA	C11-C12-C13-C15
23	d	403	CLA	C11-C12-C13-C15
33	B	621	HTG	C2-C1-S1-C1'
33	h	101	HTG	C2-C1-S1-C1'
35	h	103	DGD	O2G-C1B-C2B-C3B
27	L	102	SQD	C19-C20-C21-C22
23	B	615	CLA	C13-C15-C16-C17
23	C	513	CLA	O1A-CGA-O2A-C1
23	B	612	CLA	C10-C11-C12-C13
23	B	601	CLA	CAA-CBA-CGA-O2A
27	f	102	SQD	O47-C45-C46-O48
31	C	521	LMG	O7-C8-C9-O8
23	B	604	CLA	C13-C15-C16-C17
35	H	102	DGD	C7B-C8B-C9B-CAB
34	C	525	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
35	c	519	DGD	O6E-C5E-C6E-O5E
23	D	405	CLA	C13-C15-C16-C17
23	c	510	CLA	C10-C11-C12-C13
32	A	416	LHG	C19-C20-C21-C22
27	L	102	SQD	C30-C31-C32-C33
31	c	521	LMG	O10-C28-O8-C9
29	a	414	PL9	C12-C11-C9-C10
32	b	628	LHG	C10-C11-C12-C13
34	a	412	LMT	C6-C7-C8-C9
23	B	609	CLA	C2-C3-C5-C6
33	B	622	HTG	C3'-C4'-C5'-C6'
33	b	624	HTG	C3'-C4'-C5'-C6'
35	c	518	DGD	CCB-CDB-CEB-CFB
23	c	513	CLA	C10-C11-C12-C13
23	B	616	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	b	601	CLA	C11-C10-C8-C9
23	b	605	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C9
23	c	508	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C10-C8-C9
32	d	407	LHG	C26-C27-C28-C29
35	H	102	DGD	CBB-CCB-CDB-CEB
34	e	101	LMT	C4-C5-C6-C7
26	b	623	GOL	O2-C2-C3-O3
27	a	409	SQD	C26-C27-C28-C29
32	b	628	LHG	C33-C34-C35-C36
25	k	102	BCR	C21-C22-C23-C24
27	D	415	SQD	C34-C35-C36-C37
31	a	417	LMG	C40-C41-C42-C43
23	B	609	CLA	C4-C3-C5-C6
23	B	604	CLA	C2-C3-C5-C6
29	A	413	PL9	C12-C11-C9-C8
23	a	405	CLA	O1D-CGD-O2D-CED
27	a	409	SQD	C11-C12-C13-C14
34	b	626	LMT	C7-C8-C9-C10
35	c	517	DGD	CAA-CBA-CCA-CDA
27	L	102	SQD	C46-C45-O47-C7
23	B	613	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	c	514	CLA	C2-C1-O2A-CGA
31	C	520	LMG	C12-C13-C14-C15
35	c	518	DGD	C2B-C3B-C4B-C5B
27	a	409	SQD	C33-C34-C35-C36
34	b	620	LMT	C6-C7-C8-C9
23	d	402	CLA	O1D-CGD-O2D-CED
27	L	102	SQD	C18-C19-C20-C21
35	H	102	DGD	C7A-C8A-C9A-CAA
23	a	405	CLA	C10-C11-C12-C13
31	C	520	LMG	C36-C37-C38-C39
25	C	515	BCR	C1-C6-C7-C8
25	C	516	BCR	C5-C6-C7-C8
25	Y	101	BCR	C23-C24-C25-C30
25	k	102	BCR	C23-C24-C25-C30
23	A	408	CLA	O1A-CGA-O2A-C1
23	b	605	CLA	C16-C17-C18-C19
34	a	412	LMT	C9-C10-C11-C12
23	a	404	CLA	C2A-CAA-CBA-CGA
31	A	415	LMG	O1-C7-C8-O7
23	B	606	CLA	C10-C11-C12-C13
32	E	101	LHG	C4-O6-P-O3
35	c	519	DGD	O6D-C5D-C6D-O5D
32	A	416	LHG	C11-C10-C9-C8
35	h	103	DGD	CDA-CEA-CFA-CGA
31	A	415	LMG	O1-C7-C8-C9
29	D	408	PL9	C35-C34-C36-C37
32	d	407	LHG	C27-C28-C29-C30
23	b	611	CLA	C8-C10-C11-C12
23	B	606	CLA	C12-C13-C15-C16
23	B	610	CLA	C12-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C10
23	a	405	CLA	C12-C13-C15-C16
23	b	616	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C7
32	D	410	LHG	C30-C31-C32-C33
34	b	620	LMT	C4-C5-C6-C7
23	A	406	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C14
23	C	513	CLA	C6-C7-C8-C9
23	b	609	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C14
25	H	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	d	408	LHG	C9-C10-C11-C12
32	d	408	LHG	C25-C26-C27-C28
34	E	102	LMT	C9-C10-C11-C12
35	C	519	DGD	C9A-CAA-CBA-CCA
34	e	101	LMT	C7-C8-C9-C10
35	c	518	DGD	CDA-CEA-CFA-CGA
27	C	501	SQD	C14-C15-C16-C17
23	C	512	CLA	C3-C5-C6-C7
23	A	408	CLA	CBA-CGA-O2A-C1
29	A	413	PL9	C2-C3-C7-C8
32	d	408	LHG	O10-C23-O8-C6
27	a	411	SQD	C7-C8-C9-C10
38	E	103	HEM	CAD-CBD-CGD-O1D
33	b	621	HTG	C4'-C5'-C6'-C7'
31	a	417	LMG	C18-C19-C20-C21
32	d	408	LHG	C24-C23-O8-C6
23	b	603	CLA	C16-C17-C18-C19
29	d	406	PL9	C34-C36-C37-C38
27	f	102	SQD	C25-C26-C27-C28
31	C	520	LMG	C35-C36-C37-C38
23	A	405	CLA	C2C-C3C-CAC-CBC
38	f	101	HEM	C4B-C3B-CAB-CBB
34	E	102	LMT	C6-C7-C8-C9
23	c	514	CLA	C10-C11-C12-C13
32	D	409	LHG	C32-C33-C34-C35
23	B	611	CLA	C15-C16-C17-C18
23	c	507	CLA	C10-C11-C12-C13
33	D	413	HTG	C4-C5-C6-O6
31	c	520	LMG	C39-C40-C41-C42
23	C	507	CLA	C2-C1-O2A-CGA
23	b	602	CLA	C8-C10-C11-C12
35	c	519	DGD	C2A-C1A-O1G-C1G
35	h	103	DGD	C6A-C7A-C8A-C9A
31	C	520	LMG	C15-C16-C17-C18
23	B	610	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C10-C8-C9
23	c	503	CLA	C14-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C14
23	A	406	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
24	a	416	PHO	C8-C10-C11-C12
27	a	411	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
35	c	519	DGD	C8B-C9B-CAB-CBB
35	H	102	DGD	O1G-C1G-C2G-C3G
32	d	408	LHG	C26-C27-C28-C29
35	C	519	DGD	C5B-C6B-C7B-C8B
34	D	404	LMT	O5'-C1'-O1'-C1
25	d	405	BCR	C37-C22-C23-C24
23	c	507	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	C11-C12-C13-C15
23	C	513	CLA	C12-C13-C15-C16
32	A	416	LHG	C10-C11-C12-C13
32	A	416	LHG	C29-C30-C31-C32
38	E	103	HEM	CAD-CBD-CGD-O2D
23	C	502	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
35	C	518	DGD	C9A-CAA-CBA-CCA
24	a	416	PHO	O1D-CGD-O2D-CED
40	v	203	HEC	CAD-CBD-CGD-O1D
35	C	518	DGD	C1B-C2B-C3B-C4B
29	a	414	PL9	C43-C44-C46-C47
32	d	408	LHG	C11-C10-C9-C8
40	V	201	HEC	CAD-CBD-CGD-O1D
40	V	201	HEC	CAD-CBD-CGD-O2D
23	B	609	CLA	C13-C15-C16-C17
23	C	504	CLA	C15-C16-C17-C18
23	C	505	CLA	C8-C10-C11-C12
23	c	512	CLA	C15-C16-C17-C18
31	M	101	LMG	C34-C35-C36-C37
31	Z	101	LMG	C2-C1-O1-C7
35	H	102	DGD	O1G-C1G-C2G-O2G
32	D	409	LHG	C24-C23-O8-C6
31	C	521	LMG	C12-C13-C14-C15
23	b	613	CLA	C5-C6-C7-C8
24	A	407	PHO	C10-C11-C12-C13
27	A	411	SQD	C24-C23-O48-C46
23	C	514	CLA	O1D-CGD-O2D-CED
29	a	414	PL9	C45-C44-C46-C47
27	f	102	SQD	C33-C34-C35-C36
23	C	513	CLA	C2-C1-O2A-CGA
23	c	507	CLA	C2-C1-O2A-CGA
35	c	519	DGD	O1A-C1A-O1G-C1G
23	D	405	CLA	C14-C13-C15-C16
29	a	414	PL9	C2-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
32	D	410	LHG	C11-C12-C13-C14
23	B	614	CLA	C2A-CAA-CBA-CGA
40	v	203	HEC	CAD-CBD-CGD-O2D
35	H	102	DGD	O1B-C1B-C2B-C3B
27	A	411	SQD	O10-C23-O48-C46
25	B	617	BCR	C1-C6-C7-C8
25	C	516	BCR	C1-C6-C7-C8
25	D	407	BCR	C1-C6-C7-C8
25	a	408	BCR	C1-C6-C7-C8
25	c	515	BCR	C1-C6-C7-C8
23	B	603	CLA	C13-C15-C16-C17
27	f	102	SQD	C44-C45-C46-O48
31	c	520	LMG	C40-C41-C42-C43
35	h	103	DGD	CBA-CCA-CDA-CEA
29	d	406	PL9	C45-C44-C46-C47
34	M	102	LMT	C7-C8-C9-C10
32	d	408	LHG	C13-C14-C15-C16
23	B	612	CLA	C8-C10-C11-C12
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C2G-C3G-O3G-C1D
31	m	101	LMG	C33-C34-C35-C36
32	L	101	LHG	C13-C14-C15-C16
34	a	412	LMT	O1'-C1-C2-C3
23	B	605	CLA	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C19
35	C	519	DGD	CBA-CCA-CDA-CEA
23	c	508	CLA	C2A-CAA-CBA-CGA
32	L	101	LHG	C30-C31-C32-C33
35	H	102	DGD	C5A-C6A-C7A-C8A
32	d	407	LHG	C7-C8-C9-C10
32	D	409	LHG	O10-C23-O8-C6
23	B	607	CLA	C3-C5-C6-C7
23	C	503	CLA	O1D-CGD-O2D-CED
33	b	622	HTG	C3'-C4'-C5'-C6'
29	D	408	PL9	C45-C44-C46-C47
29	a	414	PL9	C14-C16-C17-C18
23	B	613	CLA	C12-C13-C15-C16
23	a	407	CLA	C6-C7-C8-C10
29	A	413	PL9	C43-C44-C46-C47
27	B	620	SQD	C33-C34-C35-C36
27	f	102	SQD	C28-C29-C30-C31
26	A	410	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	c	520	LMG	O10-C28-O8-C9
31	C	520	LMG	C32-C33-C34-C35
31	c	520	LMG	C22-C23-C24-C25
31	a	417	LMG	O10-C28-C29-C30
23	b	601	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CAA-CBA-CGA-O2A
32	b	628	LHG	O7-C7-C8-C9
35	C	518	DGD	C2A-C3A-C4A-C5A
24	a	416	PHO	C4C-C3C-CAC-CBC
33	B	621	HTG	C2'-C1'-S1-C1
23	C	507	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	B	616	CLA	C5-C6-C7-C8
31	C	521	LMG	C35-C36-C37-C38
34	a	412	LMT	C4-C5-C6-C7
23	C	511	CLA	CAA-CBA-CGA-O2A
23	C	513	CLA	CAA-CBA-CGA-O2A
23	b	612	CLA	CAA-CBA-CGA-O2A
27	f	102	SQD	O48-C23-C24-C25
31	Z	101	LMG	C14-C15-C16-C17
34	D	404	LMT	C4-C5-C6-C7
35	h	103	DGD	C3B-C4B-C5B-C6B
23	B	601	CLA	C11-C12-C13-C14
23	B	603	CLA	C14-C13-C15-C16
23	B	605	CLA	C14-C13-C15-C16
23	b	611	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C14
23	c	513	CLA	C6-C7-C8-C9
23	d	403	CLA	C3-C5-C6-C7
35	C	518	DGD	C9B-CAB-CBB-CCB
23	c	514	CLA	C3A-C2A-CAA-CBA
35	c	519	DGD	CDB-CEB-CFB-CGB
23	C	504	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
24	a	406	PHO	CAD-CBD-CGD-O2D
23	C	504	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	C3-C5-C6-C7
31	z	101	LMG	C19-C20-C21-C22
31	D	414	LMG	O7-C10-C11-C12
31	A	415	LMG	C21-C22-C23-C24
34	D	403	LMT	C4-C5-C6-C7
35	c	517	DGD	C2B-C3B-C4B-C5B
33	C	522	HTG	C4-C5-C6-O6
23	C	507	CLA	C2-C3-C5-C6
29	a	414	PL9	C12-C11-C9-C8
23	B	613	CLA	CAA-CBA-CGA-O2A
31	z	101	LMG	C18-C19-C20-C21
25	c	516	BCR	C7-C8-C9-C10
25	t	102	BCR	C7-C8-C9-C10
24	a	416	PHO	C2C-C3C-CAC-CBC
35	c	517	DGD	CDA-CEA-CFA-CGA
27	L	102	SQD	C31-C32-C33-C34
31	Z	101	LMG	O7-C10-C11-C12
23	B	602	CLA	O2A-C1-C2-C3
23	C	510	CLA	O2A-C1-C2-C3
24	A	407	PHO	O2A-C1-C2-C3
24	a	406	PHO	O2A-C1-C2-C3
23	A	404	CLA	C2A-CAA-CBA-CGA
23	C	509	CLA	C13-C15-C16-C17
23	c	509	CLA	C13-C15-C16-C17
27	L	102	SQD	C11-C10-C9-C8
35	c	517	DGD	O2G-C1B-C2B-C3B
23	d	402	CLA	C2C-C3C-CAC-CBC
35	h	103	DGD	C8B-C9B-CAB-CBB
23	B	607	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	C4-C3-C5-C6
29	A	413	PL9	C45-C44-C46-C47
32	A	416	LHG	C11-C12-C13-C14
35	H	102	DGD	CCA-CDA-CEA-CFA
32	A	416	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
32	L	101	LHG	O7-C7-C8-C9
27	L	102	SQD	C29-C30-C31-C32
32	D	409	LHG	C34-C35-C36-C37
23	C	514	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	CAA-CBA-CGA-O2A
23	b	603	CLA	C2A-CAA-CBA-CGA
24	a	416	PHO	CHA-CBD-CGD-O1D
24	a	416	PHO	CHA-CBD-CGD-O2D
23	C	514	CLA	CBA-CGA-O2A-C1
27	A	411	SQD	C9-C10-C11-C12
23	c	513	CLA	CAA-CBA-CGA-O2A
23	B	603	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
29	D	408	PL9	C43-C44-C46-C47
23	B	602	CLA	C16-C17-C18-C19
34	D	403	LMT	C7-C8-C9-C10
35	C	517	DGD	CCA-CDA-CEA-CFA
23	B	601	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
31	m	101	LMG	C13-C14-C15-C16
32	d	407	LHG	C11-C10-C9-C8
23	b	612	CLA	C8-C10-C11-C12
32	D	409	LHG	O2-C2-C3-O3
33	b	622	HTG	S1-C1'-C2'-C3'
32	b	628	LHG	O9-C7-C8-C9
31	C	521	LMG	C4-C5-C6-O5
31	m	101	LMG	C29-C28-O8-C9
26	c	501	GOL	C1-C2-C3-O3
35	c	518	DGD	C2A-C3A-C4A-C5A
23	B	609	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
32	D	409	LHG	C25-C26-C27-C28
27	a	409	SQD	C10-C11-C12-C13
29	D	408	PL9	C46-C47-C48-C49
31	c	520	LMG	C29-C28-O8-C9
23	B	613	CLA	CAA-CBA-CGA-O1A
27	a	409	SQD	C31-C32-C33-C34
31	a	417	LMG	C20-C21-C22-C23
31	m	101	LMG	O1-C7-C8-C9
27	C	501	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C2A-CAA-CBA-CGA
23	b	612	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
27	f	102	SQD	O10-C23-C24-C25
31	Z	101	LMG	O9-C10-C11-C12
35	c	517	DGD	O1B-C1B-C2B-C3B
31	a	417	LMG	C14-C15-C16-C17
23	c	514	CLA	O1A-CGA-O2A-C1
27	a	409	SQD	C15-C16-C17-C18
35	C	519	DGD	C9B-CAB-CBB-CCB
23	B	612	CLA	CAA-CBA-CGA-O2A
32	d	407	LHG	O8-C23-C24-C25
23	a	404	CLA	C15-C16-C17-C18
31	D	414	LMG	O9-C10-C11-C12
32	D	409	LHG	C4-O6-P-O5
32	E	101	LHG	C4-O6-P-O5
32	d	408	LHG	C4-O6-P-O5
23	C	511	CLA	CAA-CBA-CGA-O1A
23	C	513	CLA	CAA-CBA-CGA-O1A
32	A	416	LHG	O10-C23-C24-C25
23	a	407	CLA	C5-C6-C7-C8
31	m	101	LMG	O10-C28-O8-C9
25	B	617	BCR	C5-C6-C7-C8
25	C	515	BCR	C5-C6-C7-C8
25	D	407	BCR	C5-C6-C7-C8
25	t	102	BCR	C1-C6-C7-C8
25	t	102	BCR	C5-C6-C7-C8
35	H	102	DGD	C8A-C9A-CAA-CBA
23	C	507	CLA	C5-C6-C7-C8
35	C	517	DGD	C6A-C7A-C8A-C9A
32	D	410	LHG	O8-C23-C24-C25
34	C	525	LMT	C2-C3-C4-C5
32	D	409	LHG	C11-C10-C9-C8
31	A	415	LMG	O7-C10-C11-C12
31	c	520	LMG	O7-C10-C11-C12
32	d	408	LHG	C29-C30-C31-C32
34	t	101	LMT	C4-C5-C6-C7
35	C	518	DGD	CCA-CDA-CEA-CFA
29	d	406	PL9	C11-C12-C13-C14
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
31	A	415	LMG	O10-C28-C29-C30
31	d	412	LMG	C19-C20-C21-C22
23	A	406	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
31	D	414	LMG	C16-C17-C18-C19
34	M	104	LMT	C9-C10-C11-C12
32	d	409	LHG	C31-C32-C33-C34
23	c	514	CLA	CBA-CGA-O2A-C1
31	d	412	LMG	O7-C10-C11-C12
31	C	521	LMG	C39-C40-C41-C42
29	A	413	PL9	C46-C47-C48-C49
23	b	615	CLA	C8-C10-C11-C12
31	A	415	LMG	O9-C10-C11-C12
23	b	611	CLA	C13-C15-C16-C17
23	d	404	CLA	C10-C11-C12-C13
32	b	628	LHG	C13-C14-C15-C16
23	A	408	CLA	C12-C13-C15-C16
23	B	601	CLA	C6-C7-C8-C10
23	B	610	CLA	C11-C12-C13-C15
23	B	611	CLA	C11-C12-C13-C15
23	C	509	CLA	C11-C10-C8-C7
23	b	610	CLA	C11-C12-C13-C15
23	c	502	CLA	C11-C12-C13-C15
23	c	514	CLA	C12-C13-C15-C16
23	d	402	CLA	C12-C13-C15-C16
23	c	513	CLA	CAA-CBA-CGA-O1A
27	C	501	SQD	O49-C7-C8-C9
32	L	101	LHG	O9-C7-C8-C9
32	A	416	LHG	C34-C35-C36-C37
25	k	102	BCR	C17-C18-C19-C20
32	a	419	LHG	O10-C23-C24-C25
27	a	409	SQD	C11-C10-C9-C8
27	a	411	SQD	C24-C25-C26-C27
32	d	408	LHG	C35-C36-C37-C38
31	C	520	LMG	O7-C10-C11-C12
23	B	604	CLA	C2C-C3C-CAC-CBC
23	B	613	CLA	C5-C6-C7-C8

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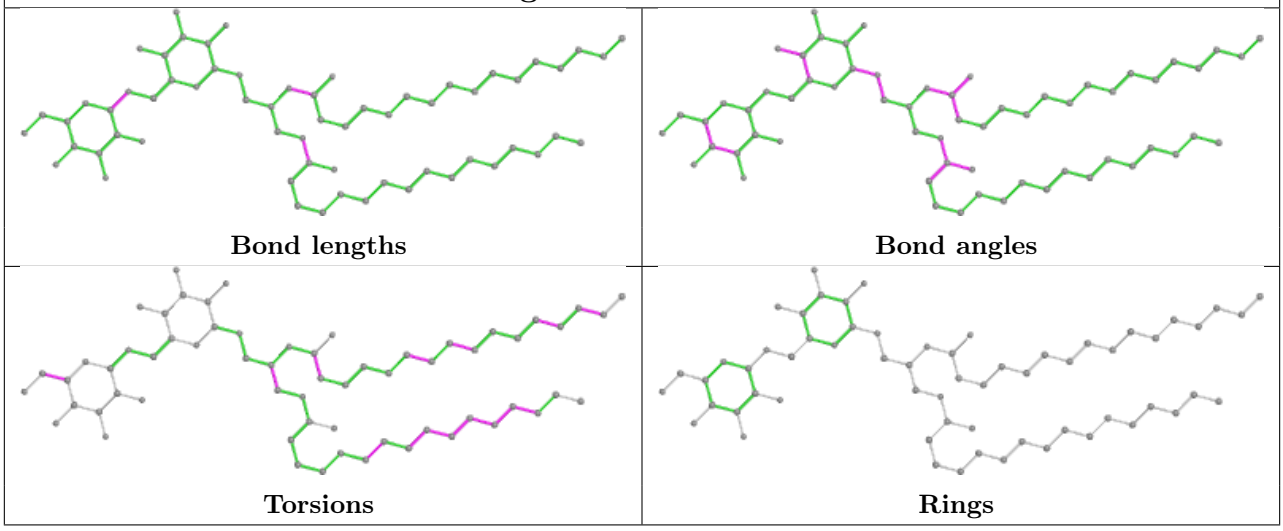
Mol	Chain	Res	Type	Atoms
35	c	518	DGD	C3B-C4B-C5B-C6B
23	B	612	CLA	CAA-CBA-CGA-O1A
23	b	613	CLA	CAA-CBA-CGA-O1A
27	B	620	SQD	C35-C36-C37-C38
23	A	405	CLA	C4C-C3C-CAC-CBC
23	B	604	CLA	C4C-C3C-CAC-CBC
32	a	419	LHG	O8-C23-C24-C25
32	d	407	LHG	O10-C23-C24-C25
38	E	103	HEM	CAA-CBA-CGA-O1A
35	C	517	DGD	C8A-C9A-CAA-CBA
31	c	520	LMG	O9-C10-C11-C12
31	z	101	LMG	O7-C10-C11-C12
32	d	409	LHG	O8-C23-C24-C25

There are no ring outliers.

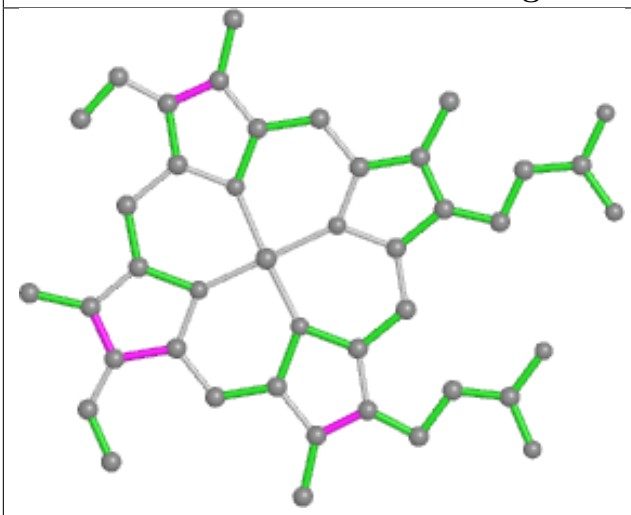
No monomer is involved in short contacts.

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.

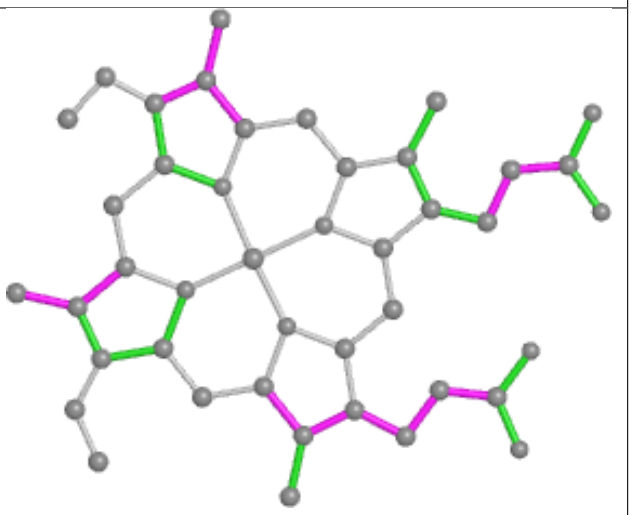
Ligand DGD H 102



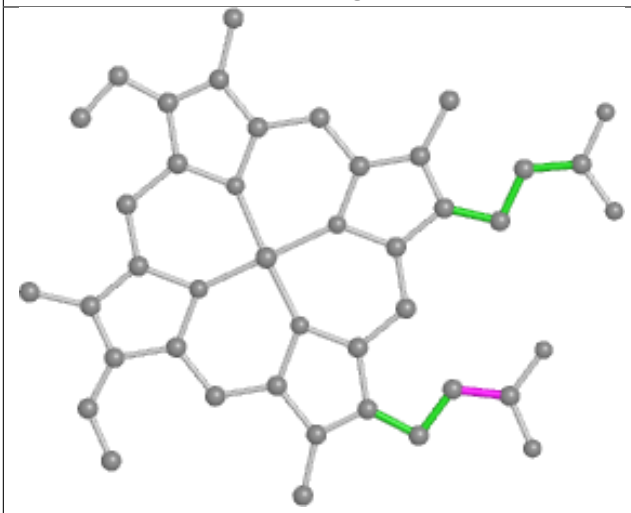
Ligand HEC V 201



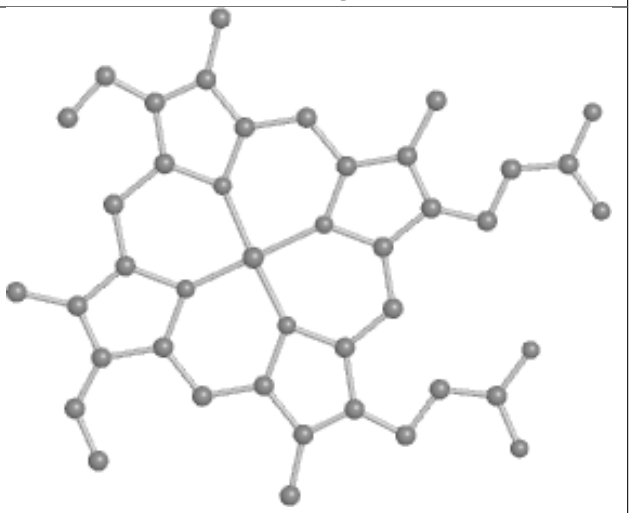
Bond lengths



Bond angles

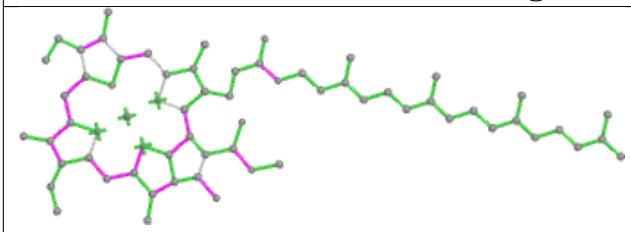


Torsions

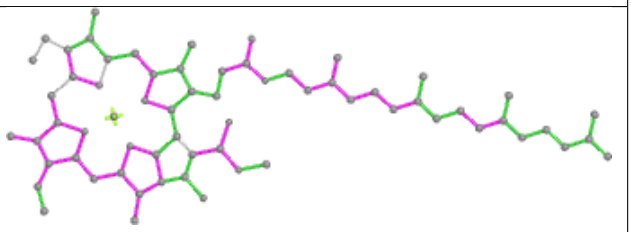


Rings

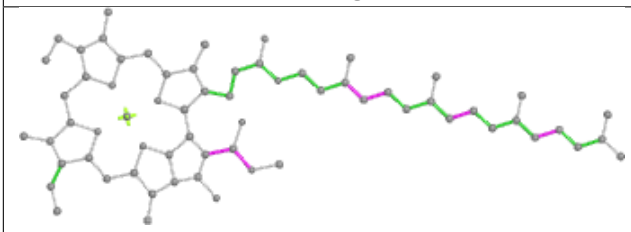
Ligand CLA b 604



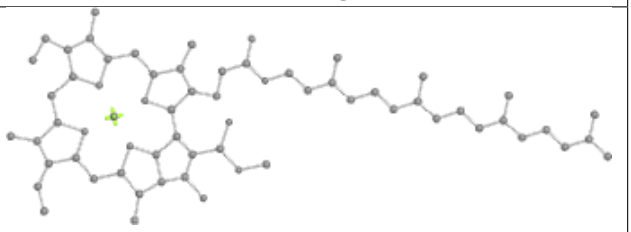
Bond lengths



Bond angles

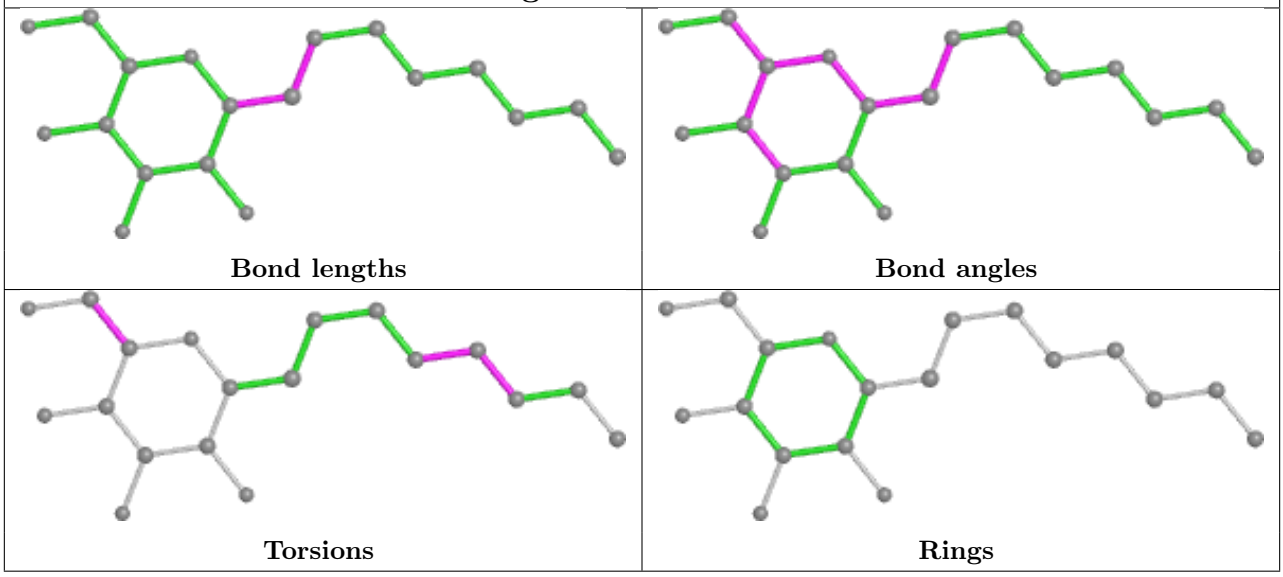


Torsions

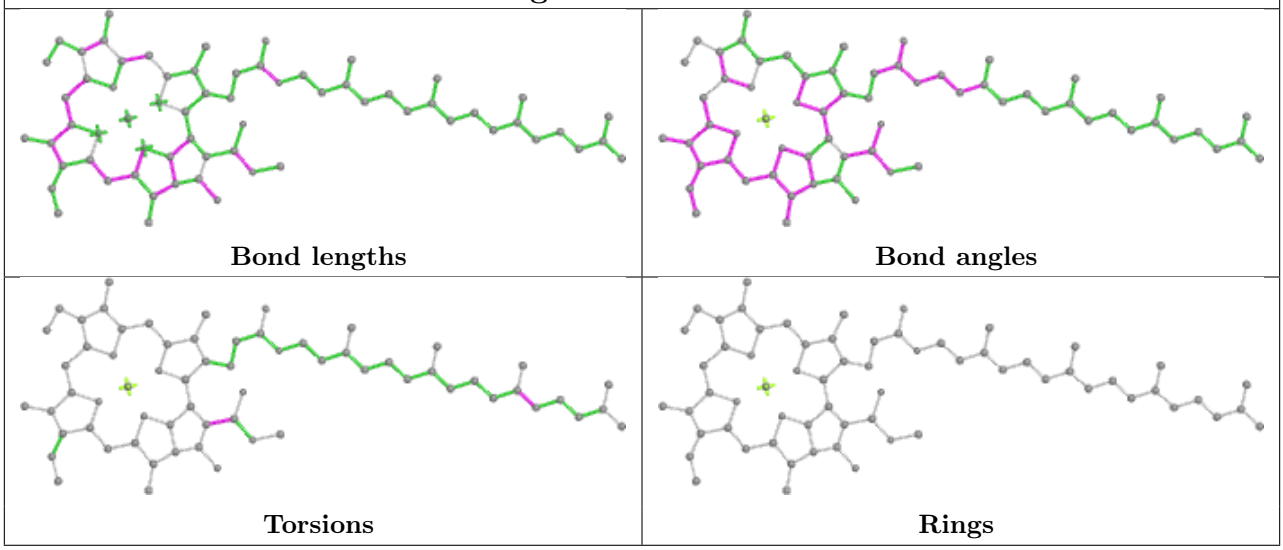


Rings

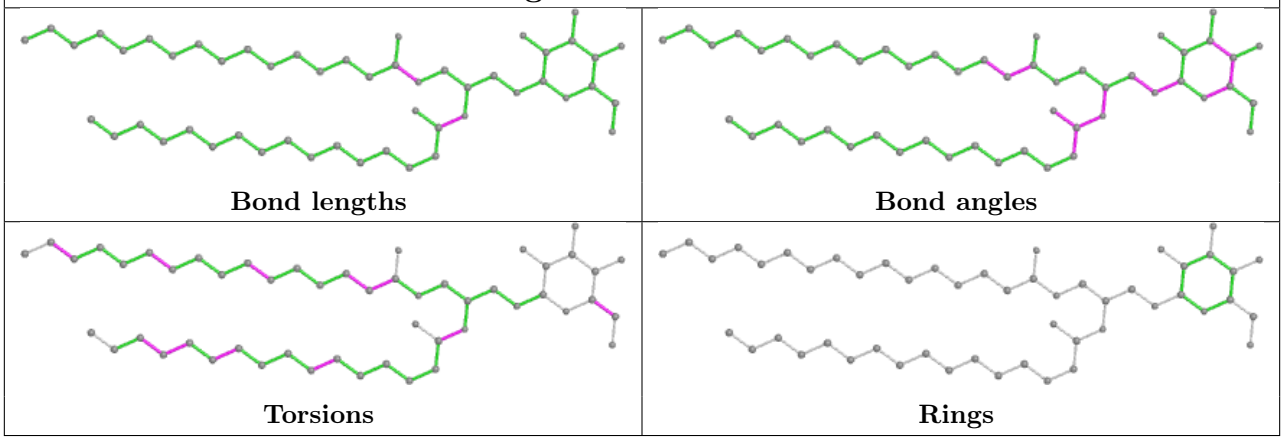
Ligand HTG B 624



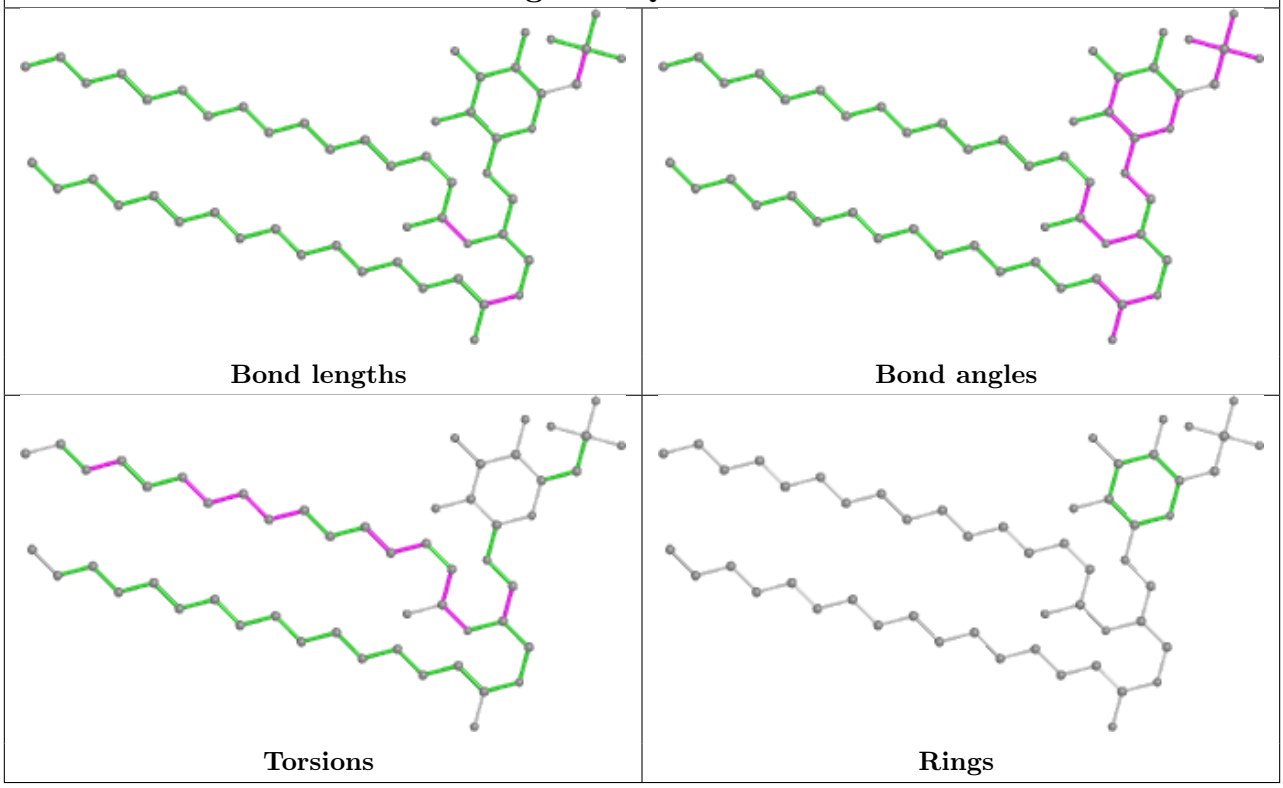
Ligand CLA c 503



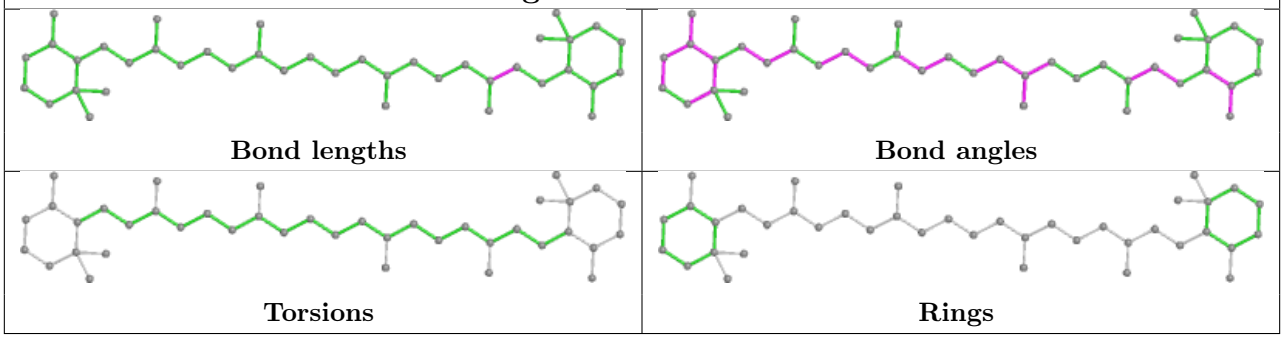
Ligand LMG a 417



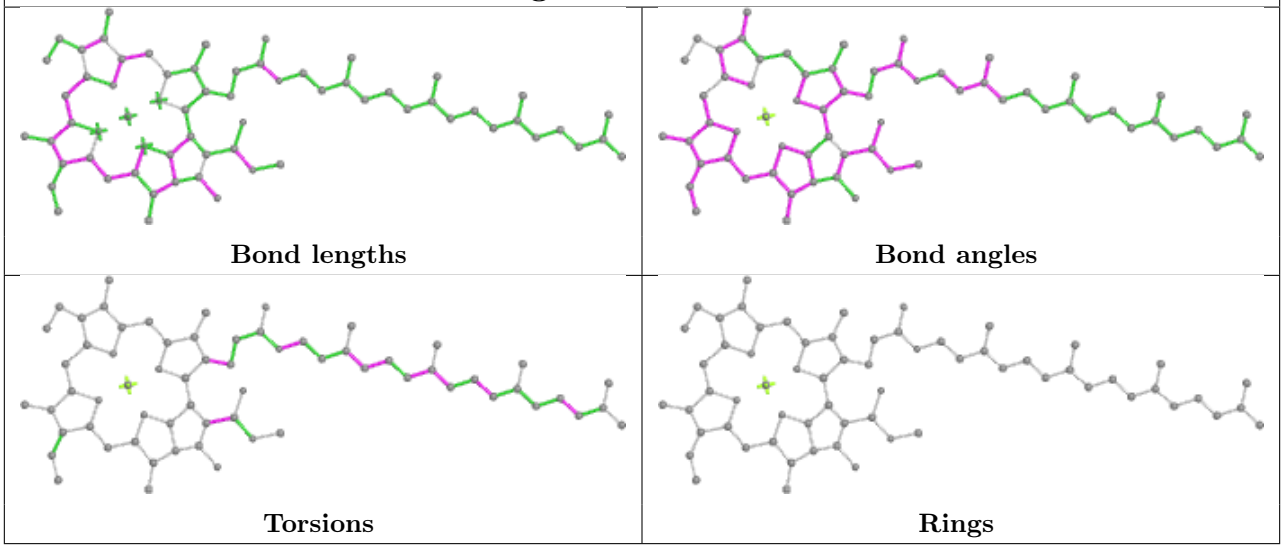
Ligand SQD C 501



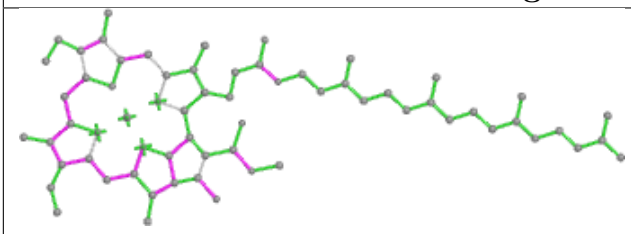
Ligand BCR K 101



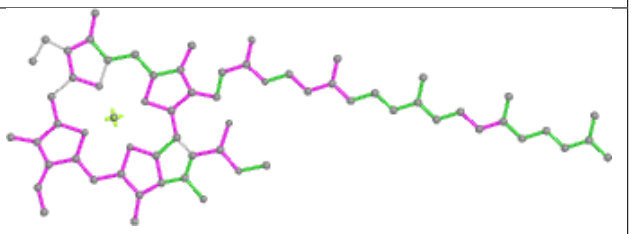
Ligand CLA c 507



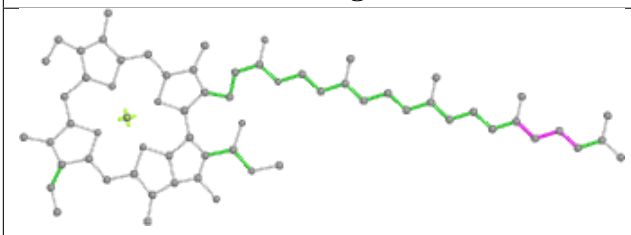
Ligand CLA D 405



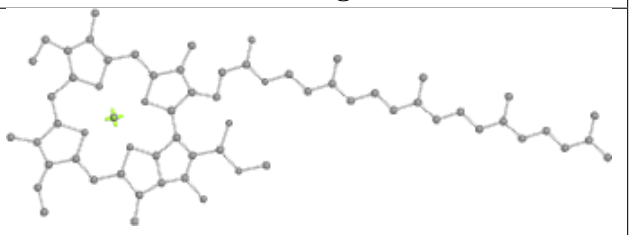
Bond lengths



Bond angles

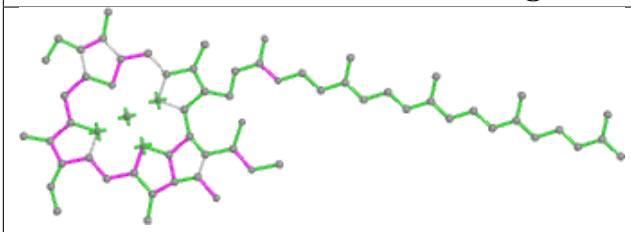


Torsions

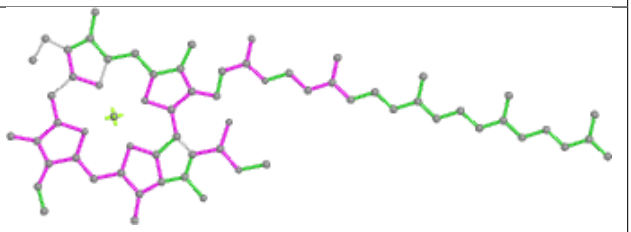


Rings

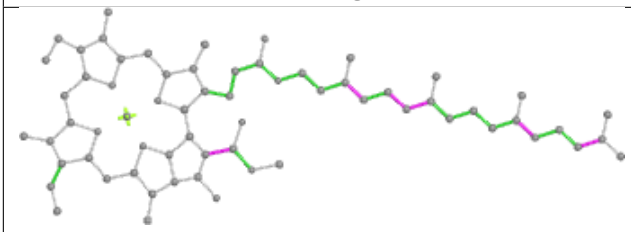
Ligand CLA B 605



Bond lengths



Bond angles



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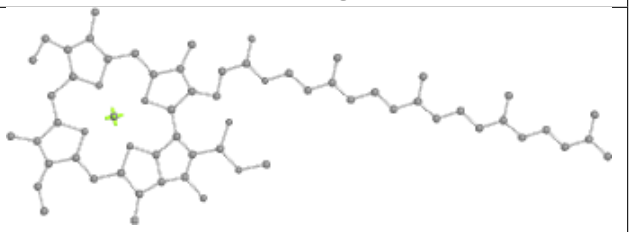
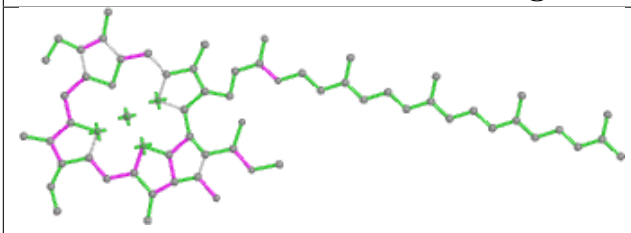
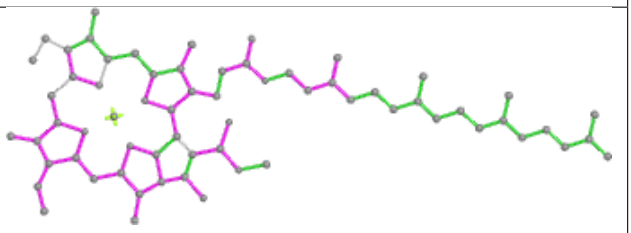


Rings

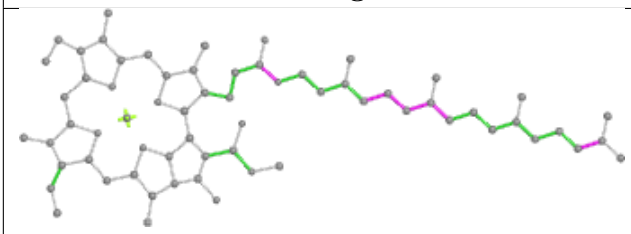
Ligand CLA a 407



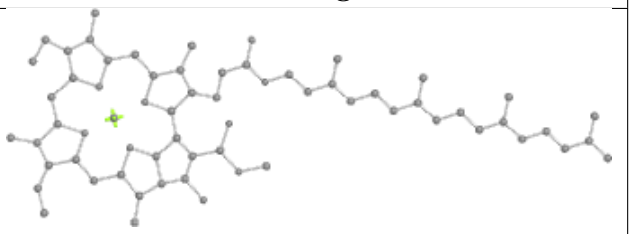
Bond lengths



Bond angles

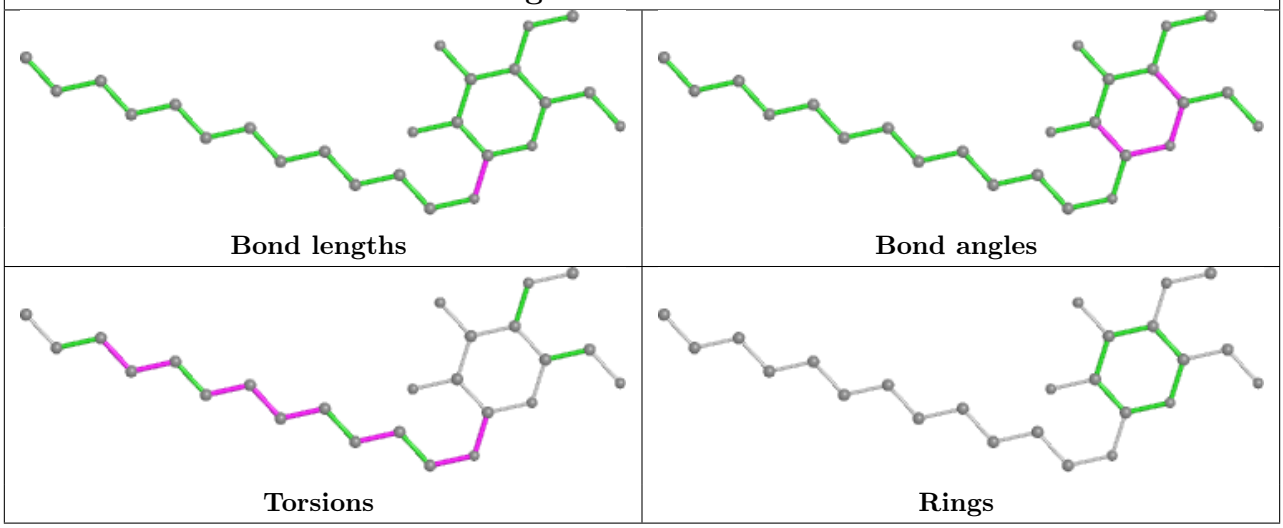


Torsions

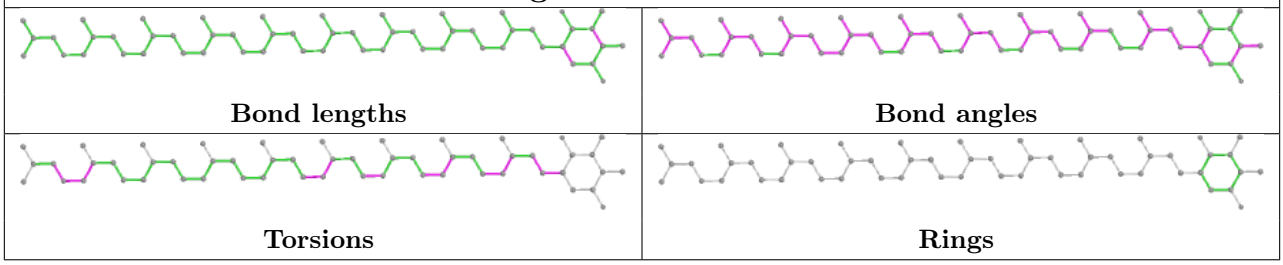


Rings

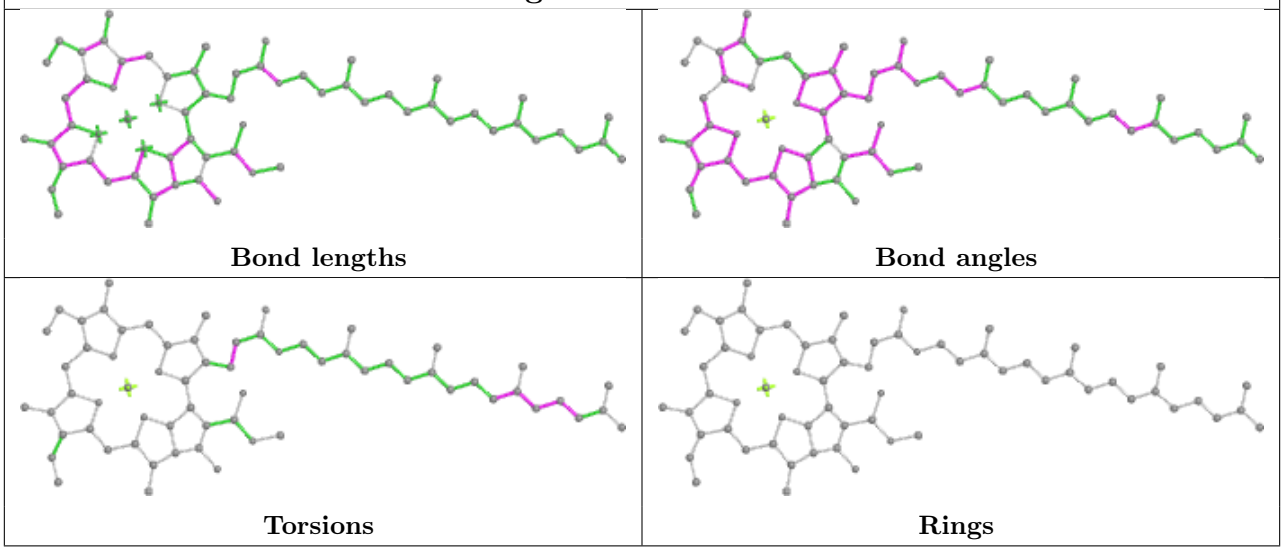
Ligand LMT b 626

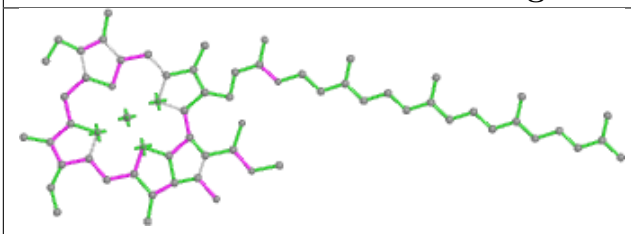
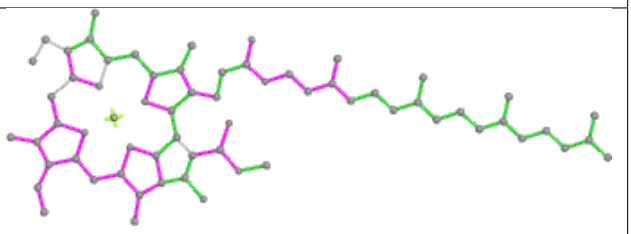
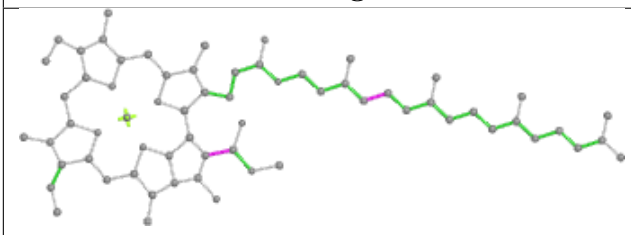
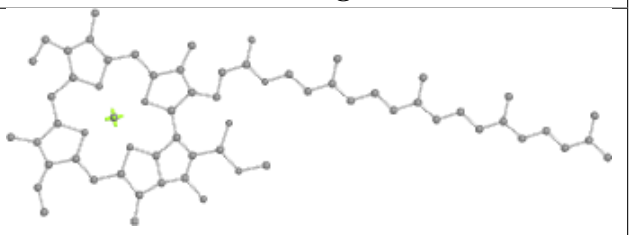


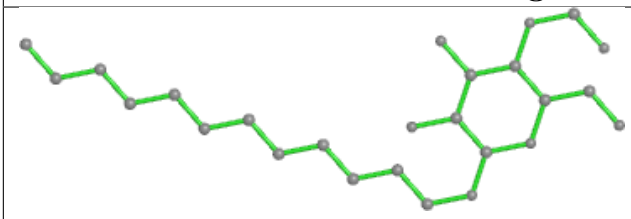
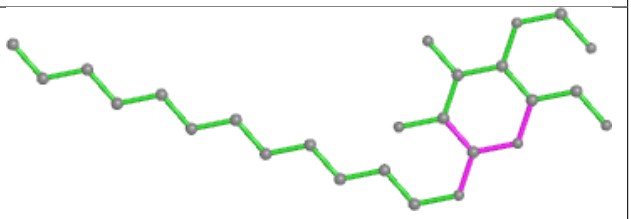
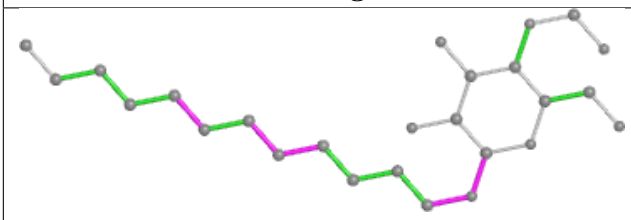
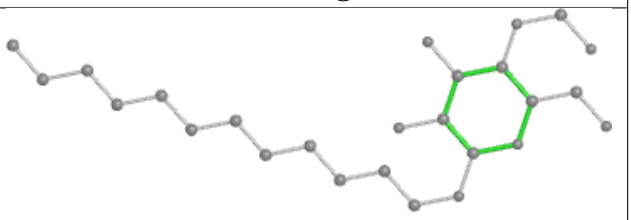
Ligand PL9 A 413



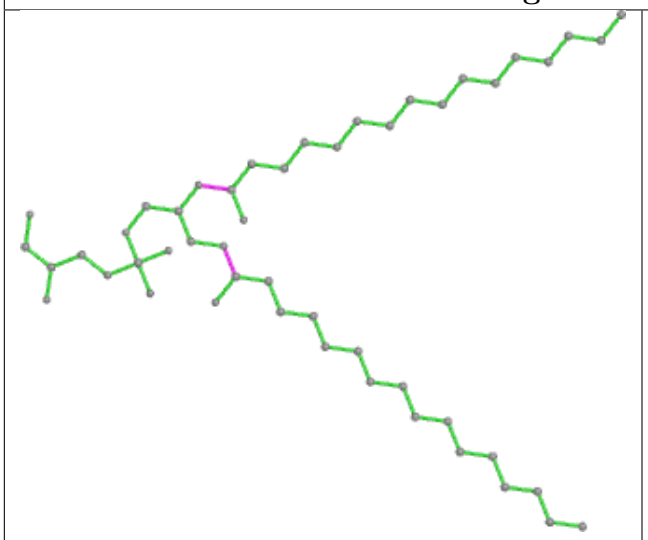
Ligand CLA B 610



Ligand CLA b 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 416



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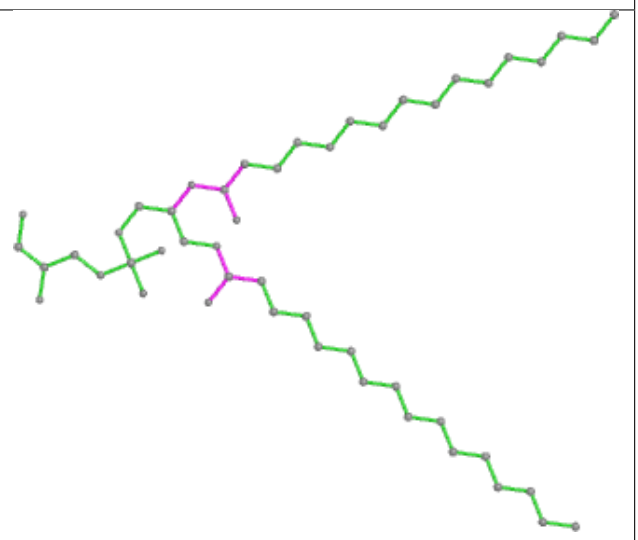
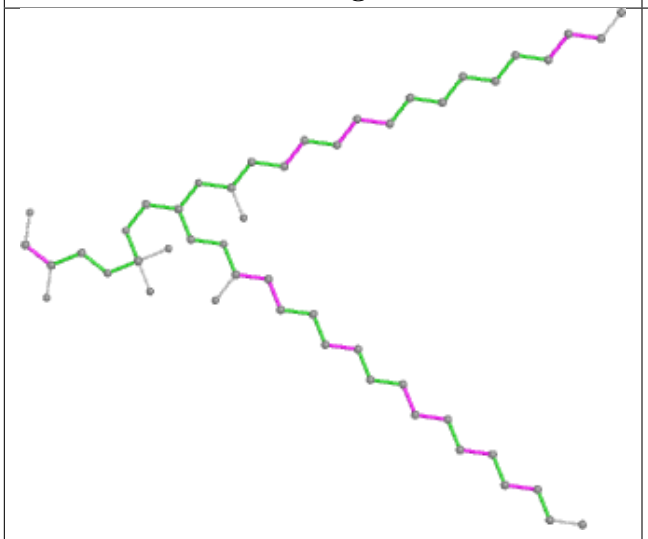
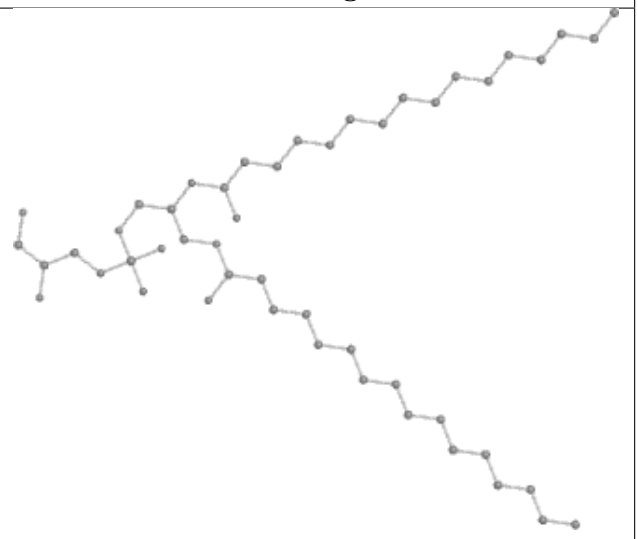


Bond angles

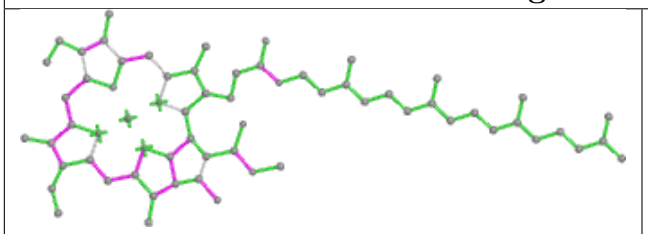


Torsions



Rings

Ligand CLA b 616



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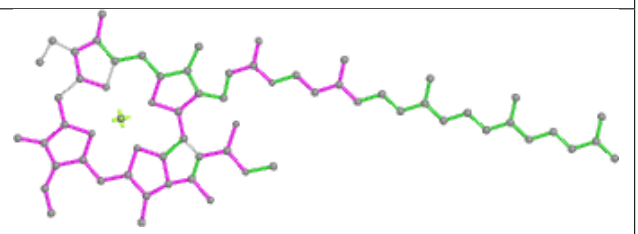

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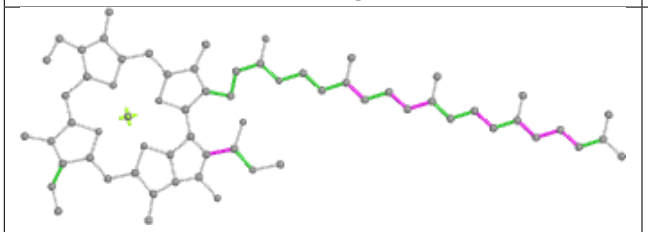

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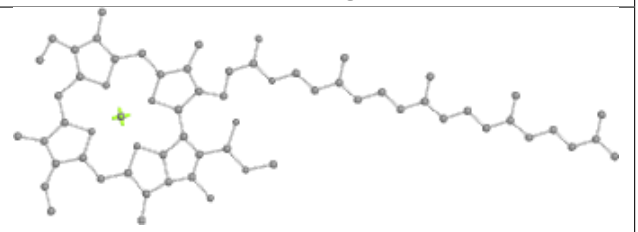
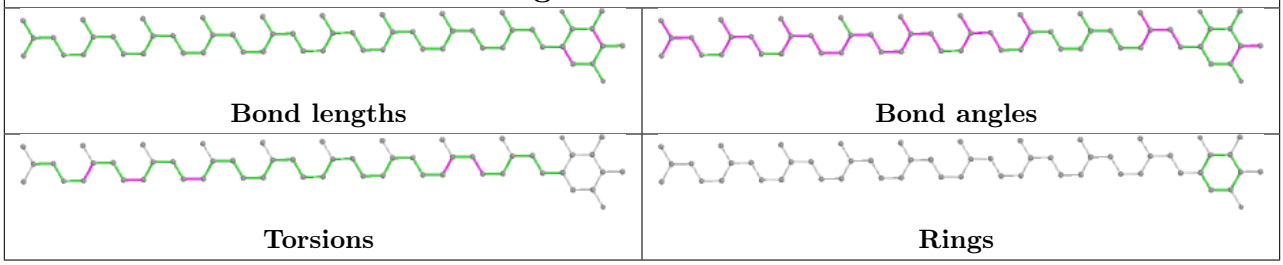


Rings

Ligand PL9 d 406



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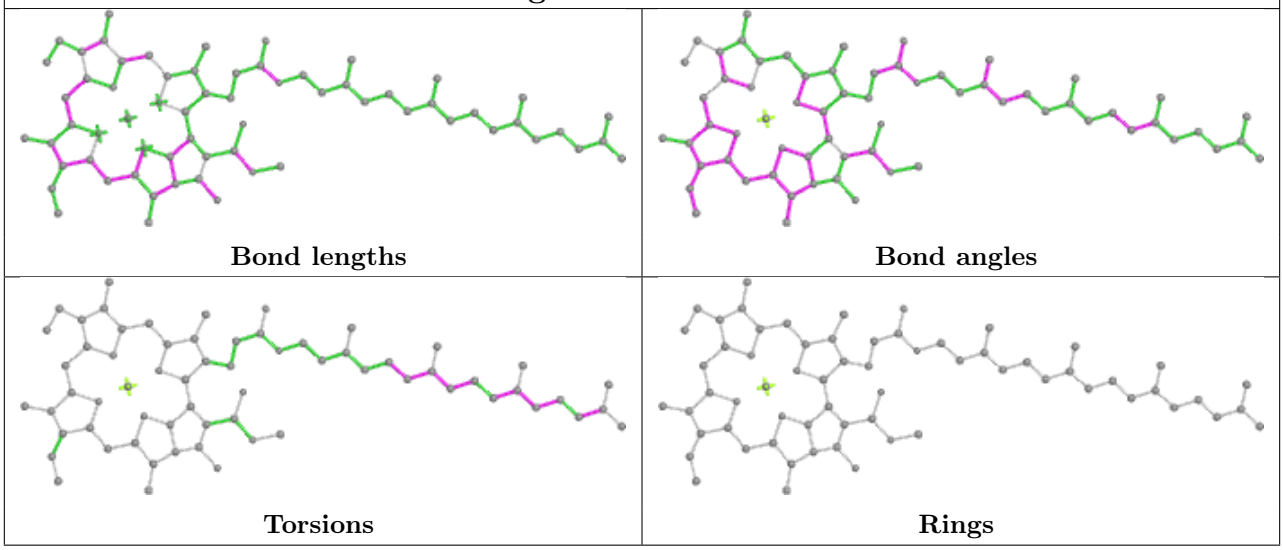
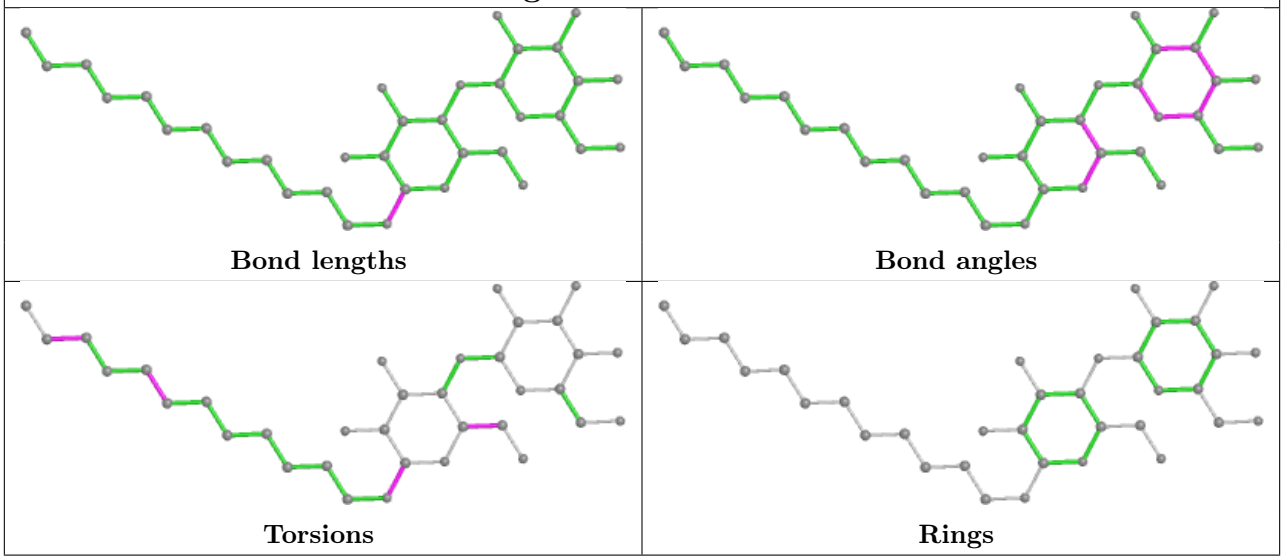


Ligand LMT E 102



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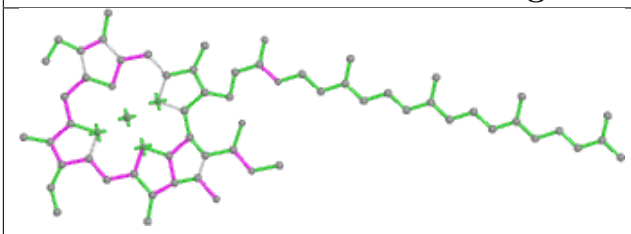
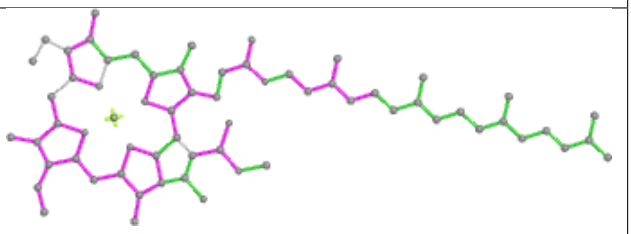
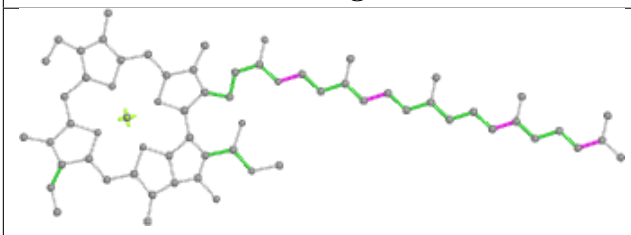


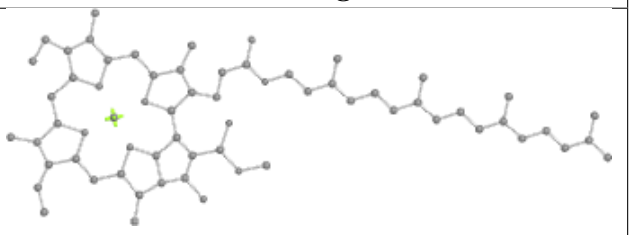
Bond lengths



Bond angles

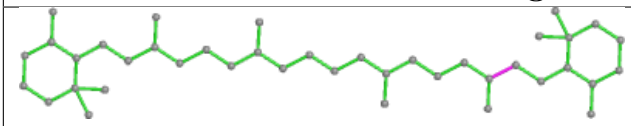


Torsions



Rings

Ligand BCR c 515



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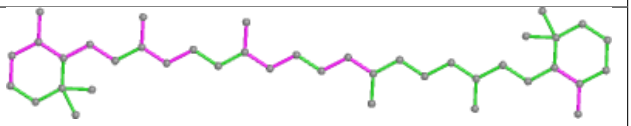

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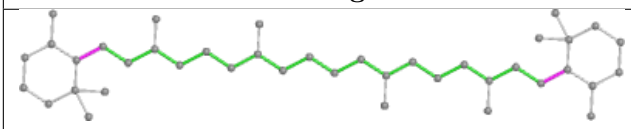

Torsions

Rings

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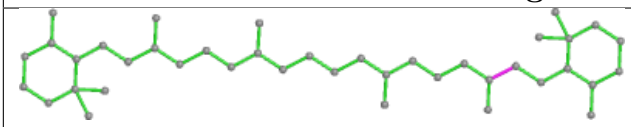

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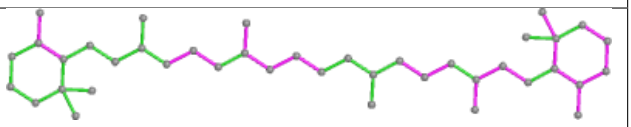

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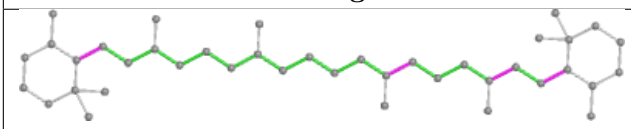
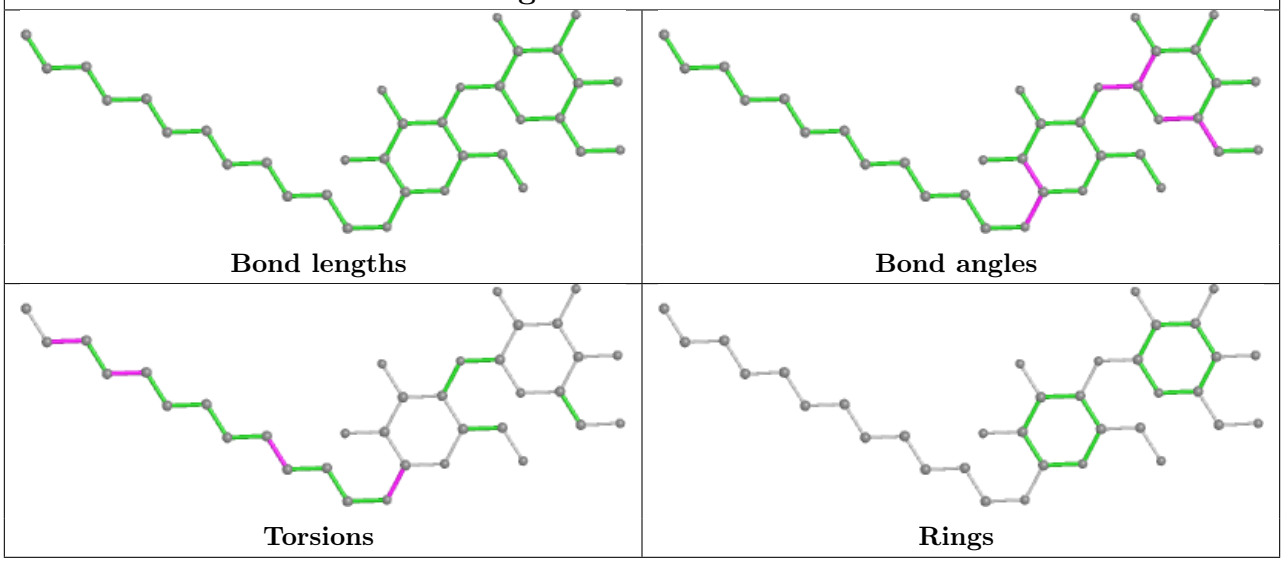


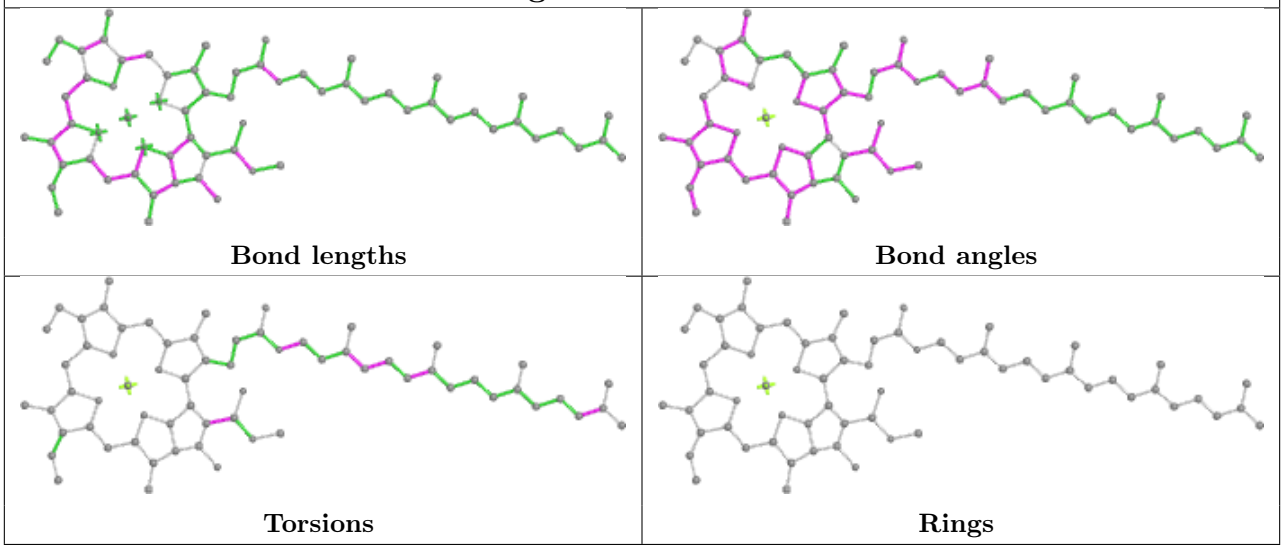
Torsions

Rings

Ligand LMT M 102



Ligand CLA b 614



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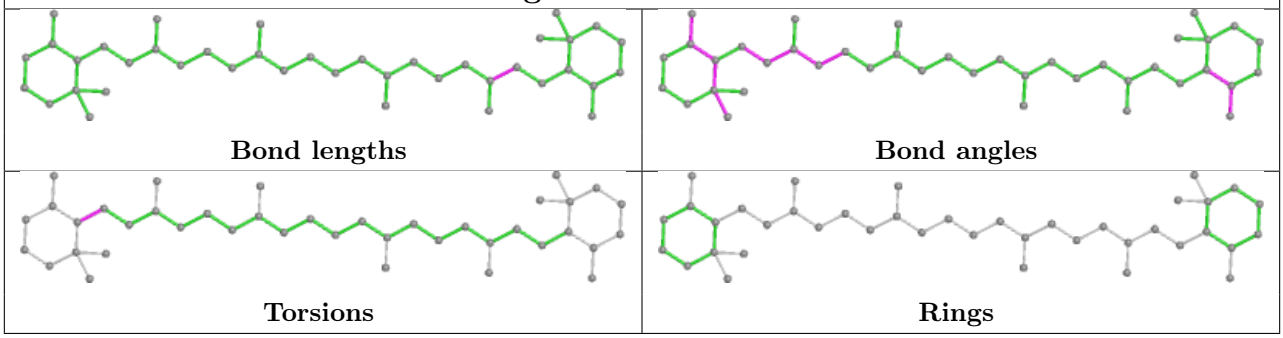

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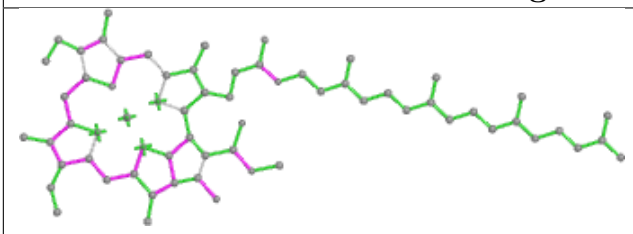

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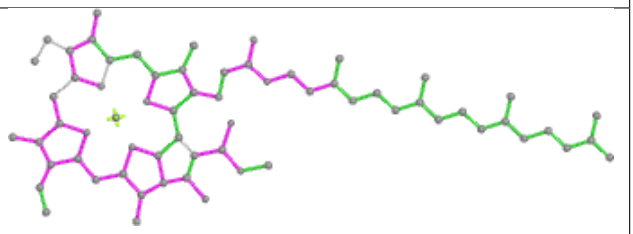
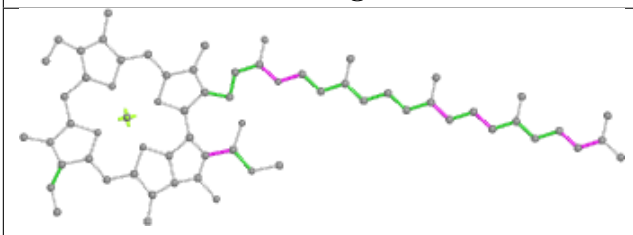


Bond angles



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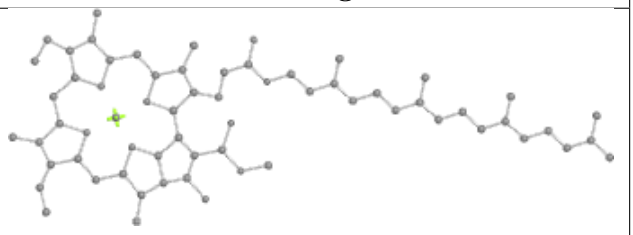
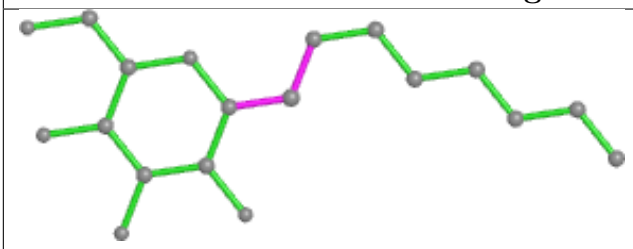


Rings

Ligand HTG b 624



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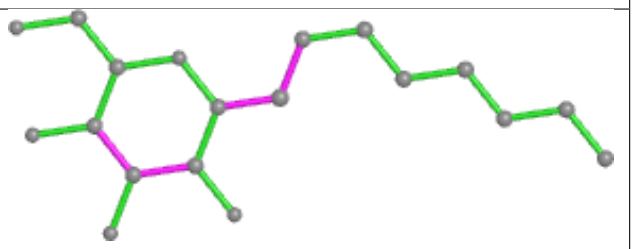

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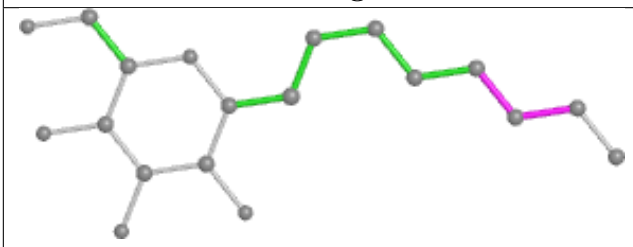

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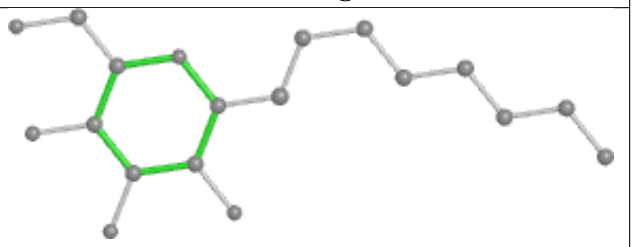
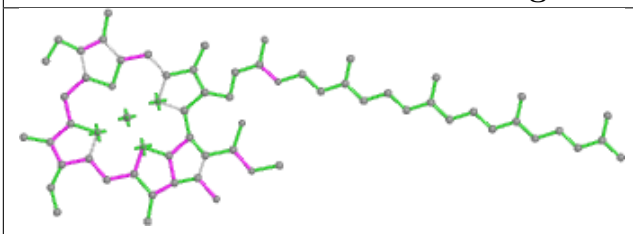


Rings

Ligand CLA c 509



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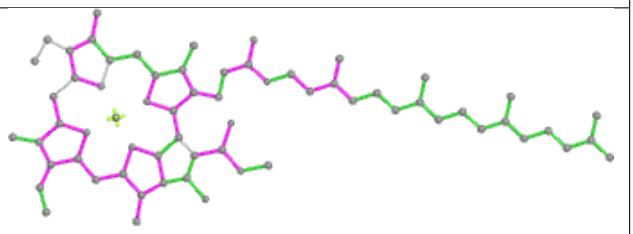
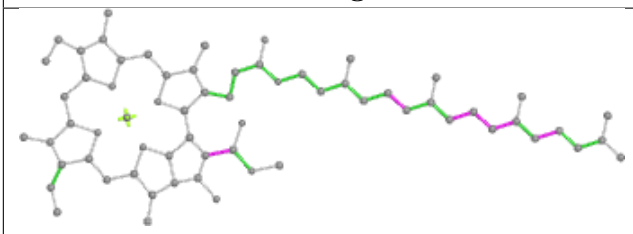


Bond angles



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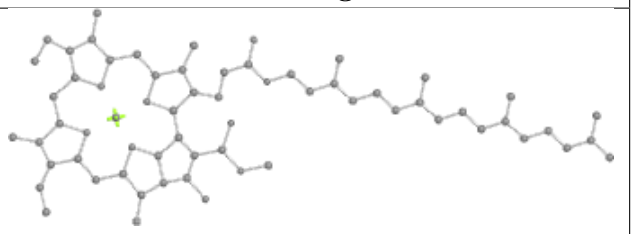
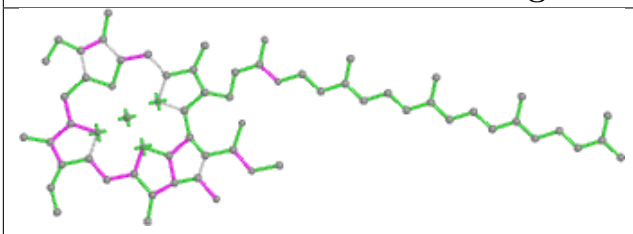
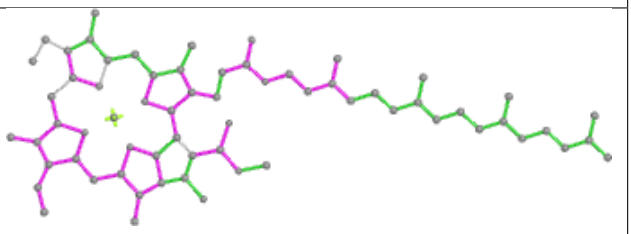


Rings

Ligand CLA a 405



Bond lengths



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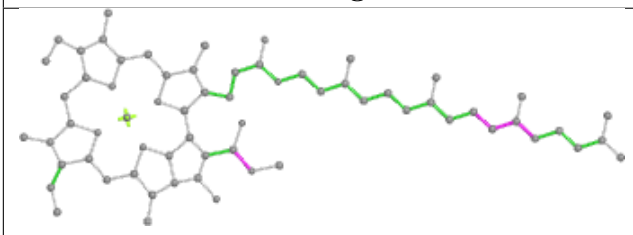

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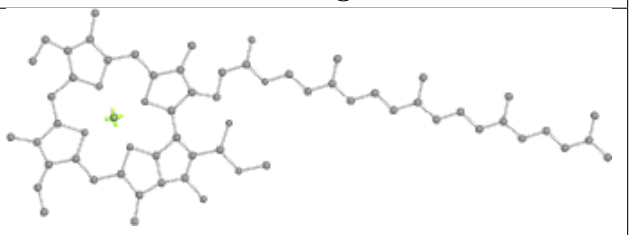
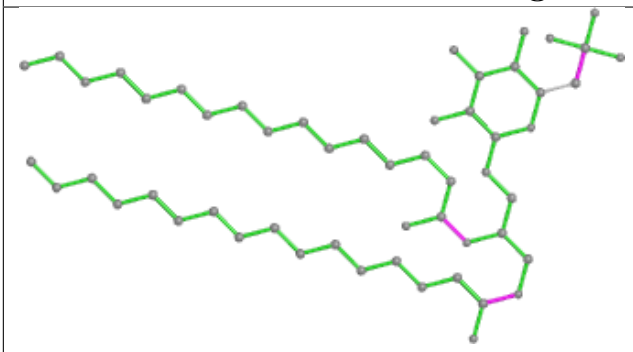


Rings

Ligand SQD a 411



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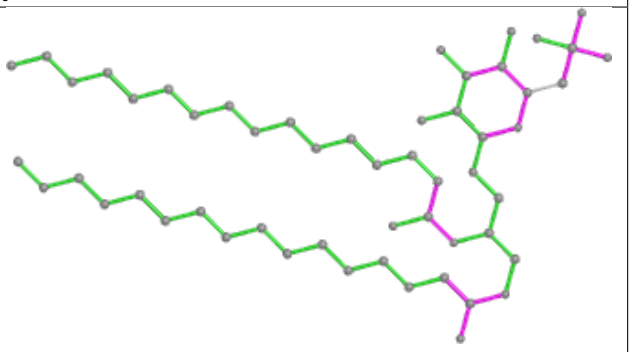
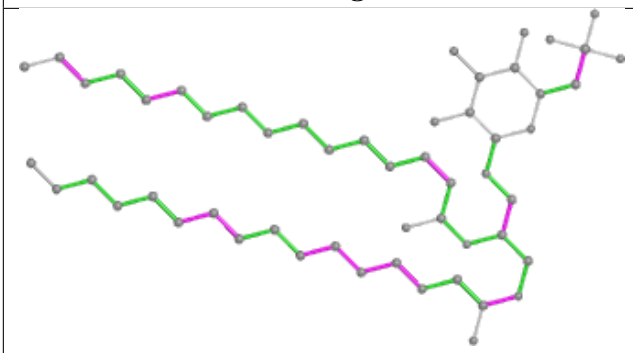
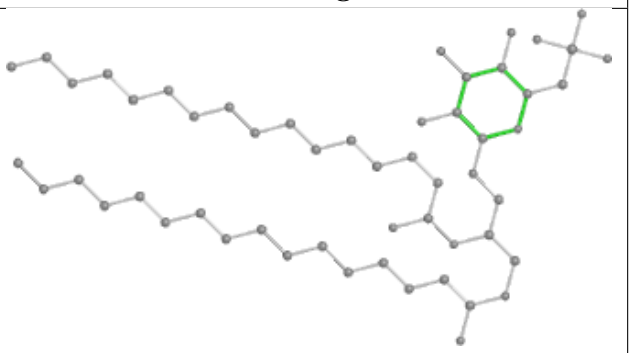


Bond angles

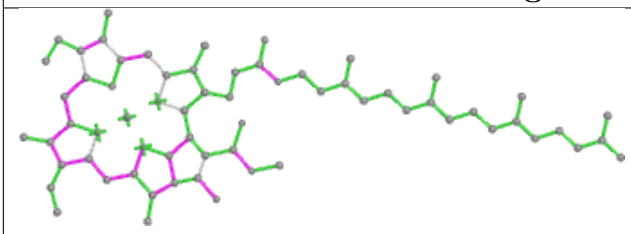


Torsions

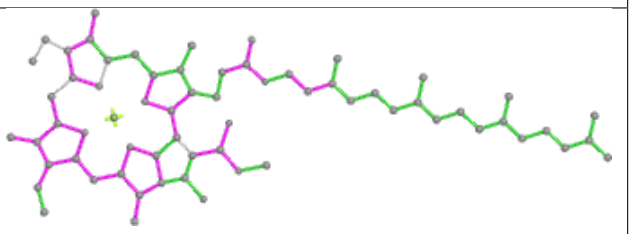


Rings

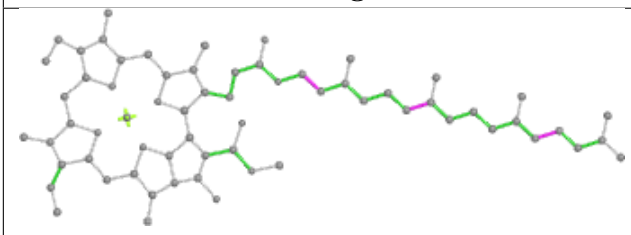
Ligand CLA C 510



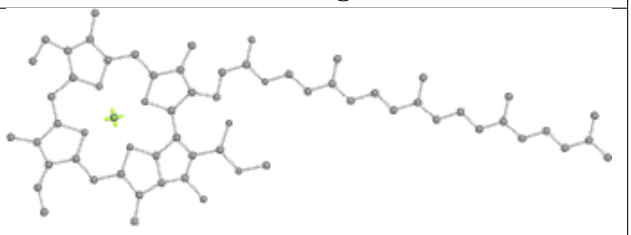
Bond lengths



Bond angles

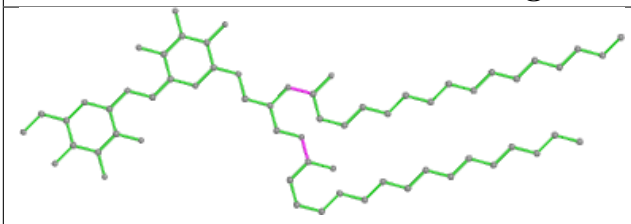


Torsions

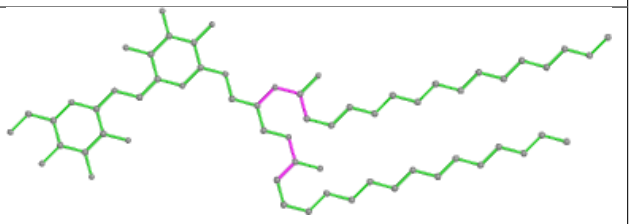


Rings

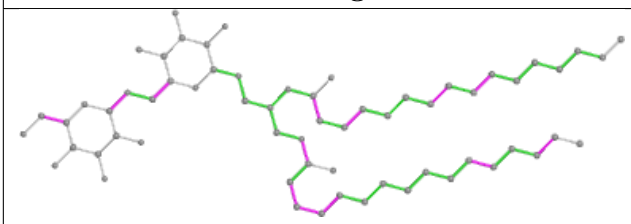
Ligand DGD c 517



Bond lengths



Bond angles



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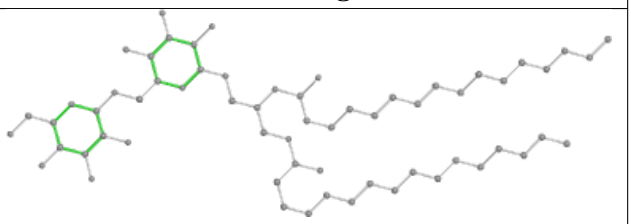
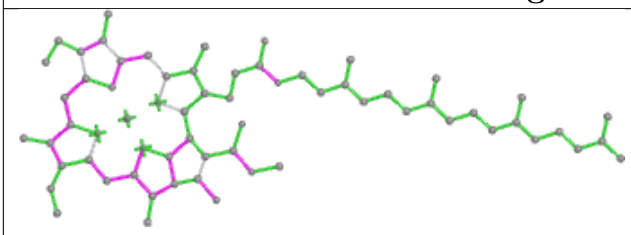


Rings

Ligand CLA b 605



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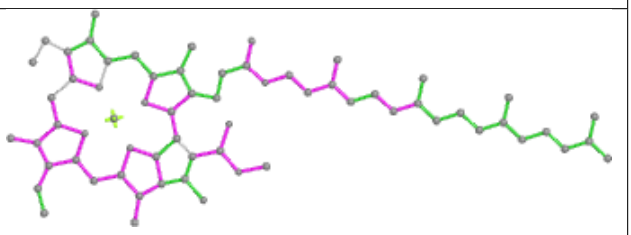
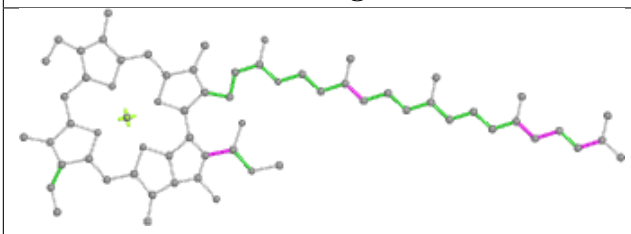
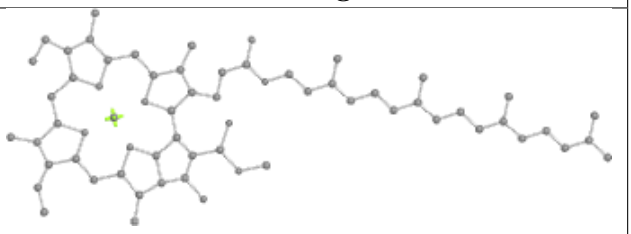


Bond angles

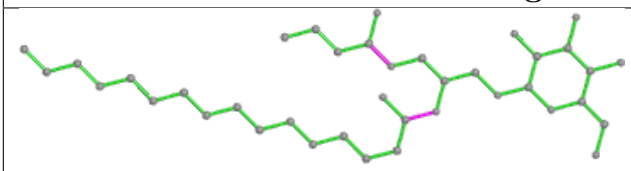


Torsions



Rings

Ligand LMG z 101



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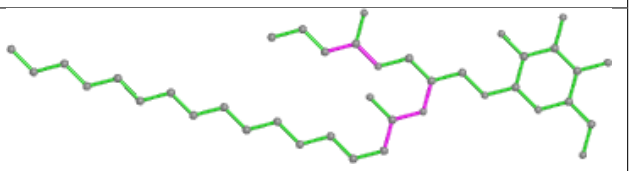
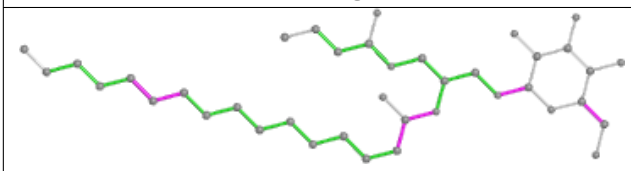


Bond angles



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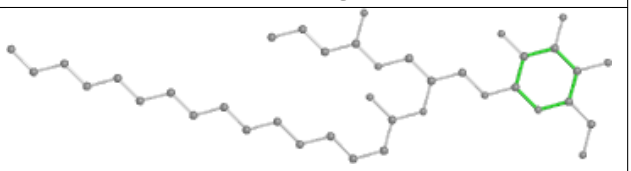
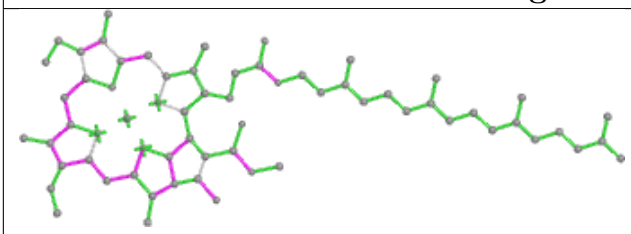
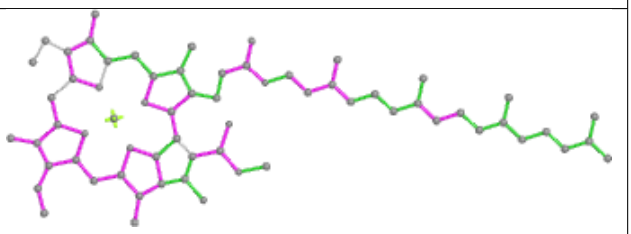


Rings

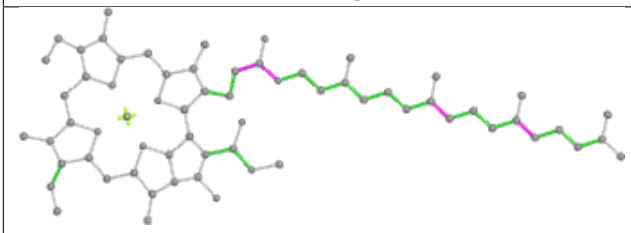
Ligand CLA c 511



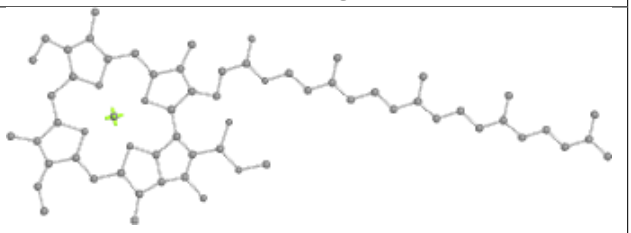
Bond lengths



Bond angles

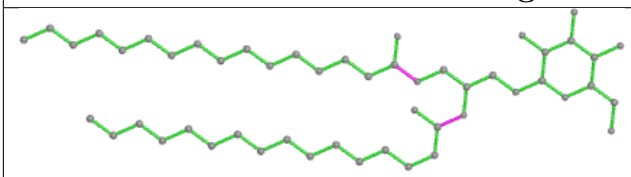


Torsions



Rings

Ligand LMG m 101



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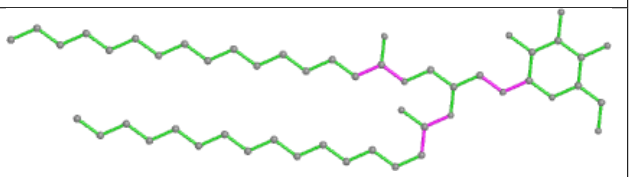
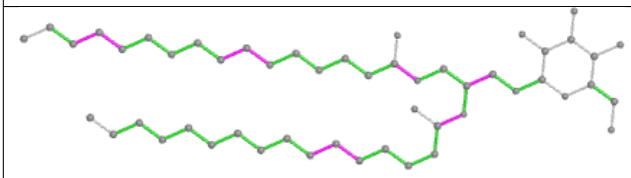
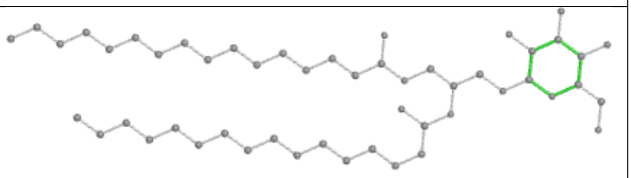


Bond angles

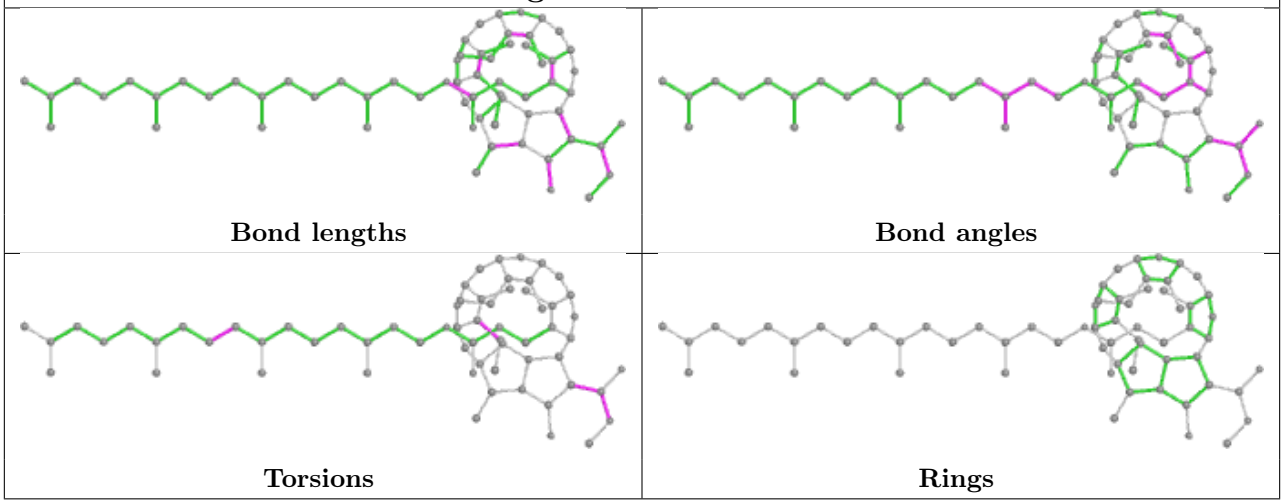


Torsions

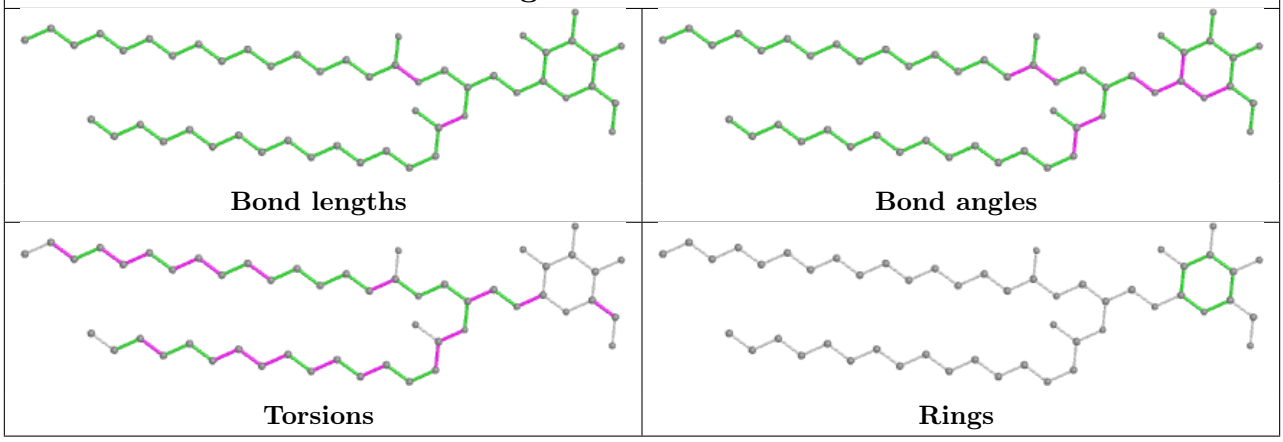


Rings

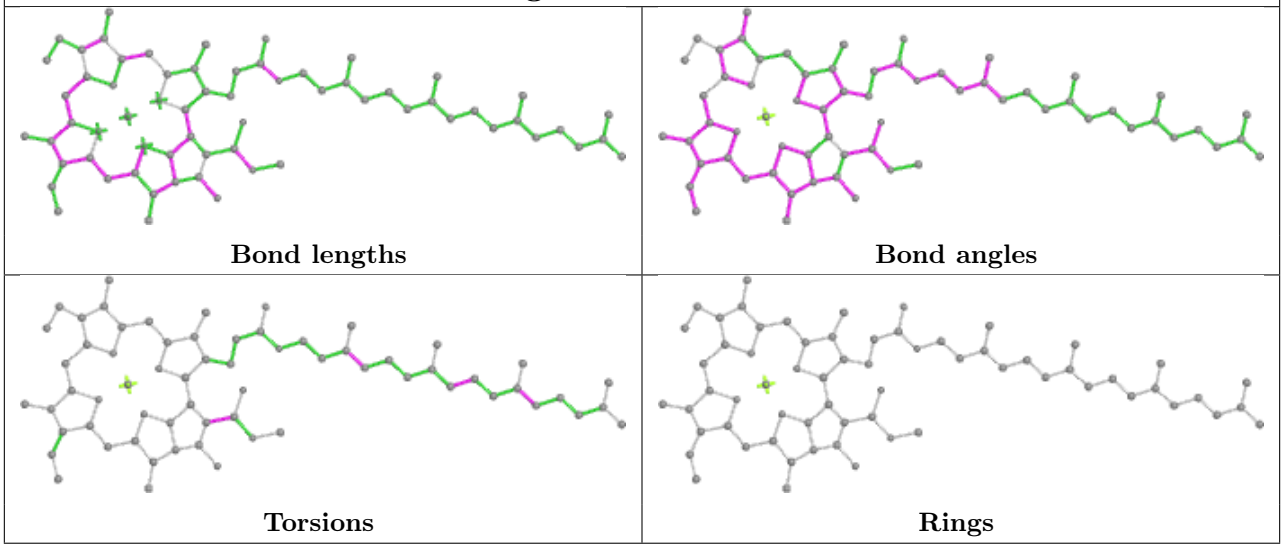
Ligand PHO a 416



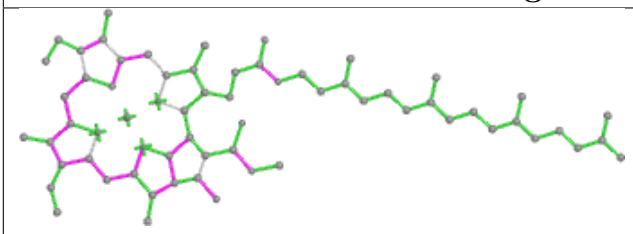
Ligand LMG A 415



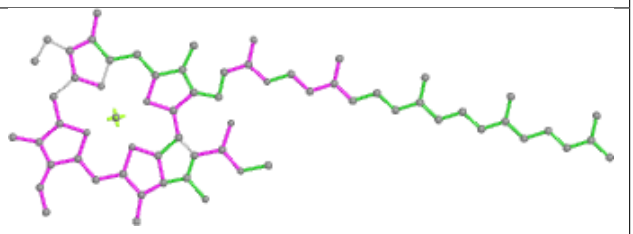
Ligand CLA C 505



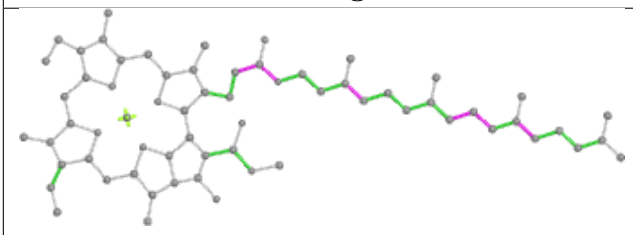
Ligand CLA C 511



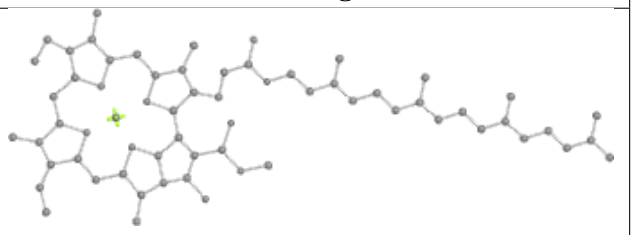
Bond lengths



Bond angles

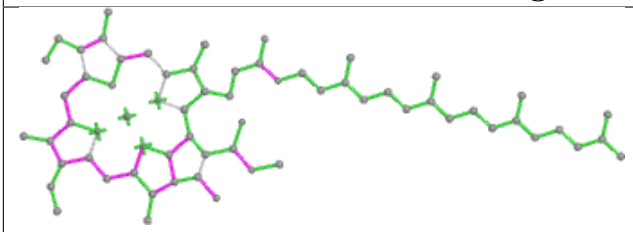


Torsions



Rings

Ligand CLA c 514



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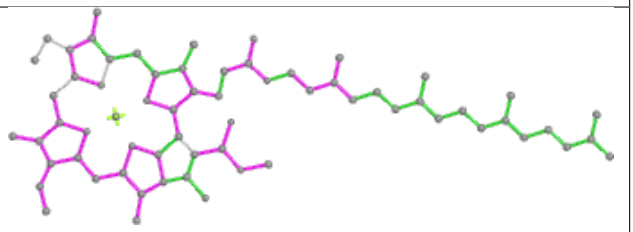
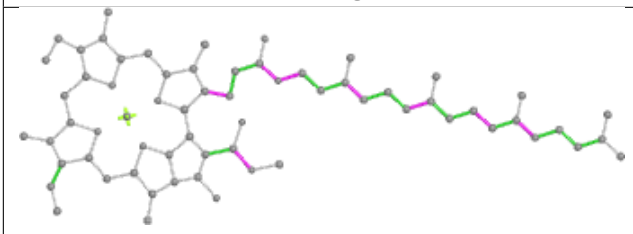
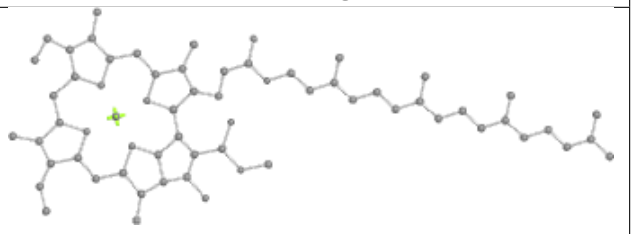


Bond angles

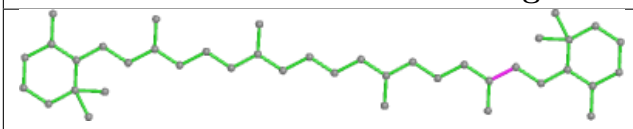


Torsions



Rings

Ligand BCR B 619



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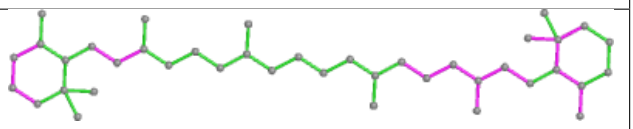
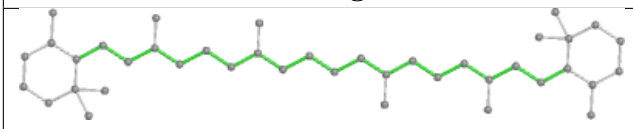


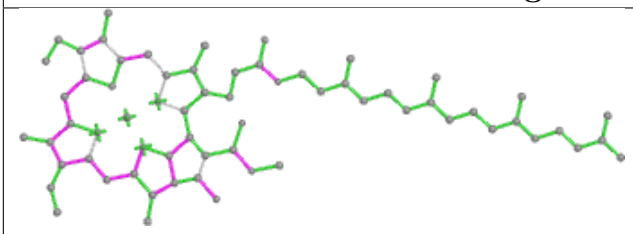
Bond angles



Torsions

Rings

Ligand CLA C 503



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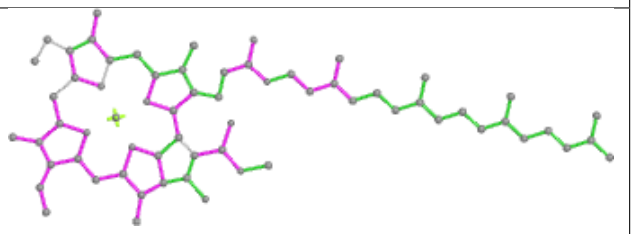
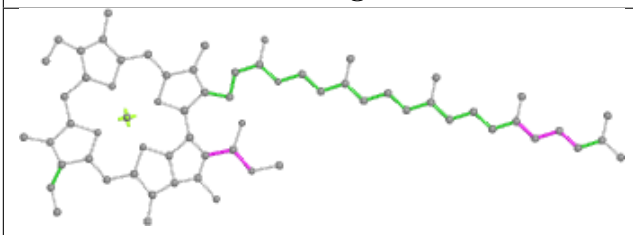
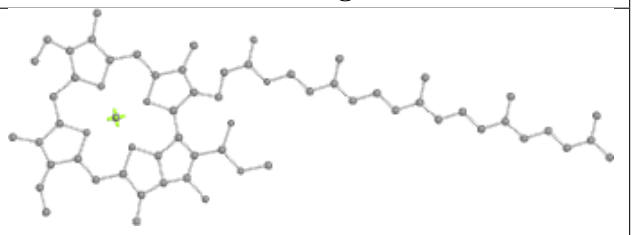


Bond angles

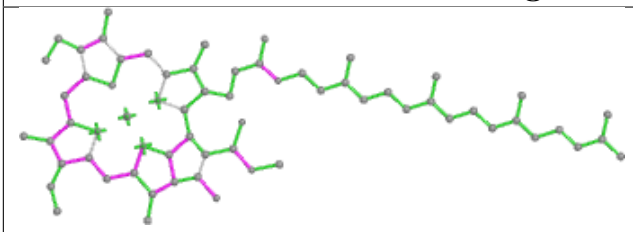


Torsions



Rings

Ligand CLA C 513



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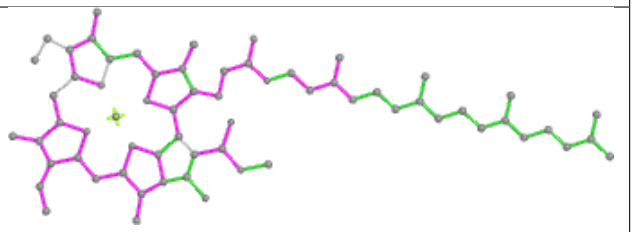
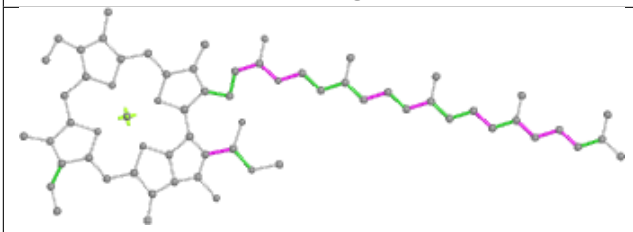
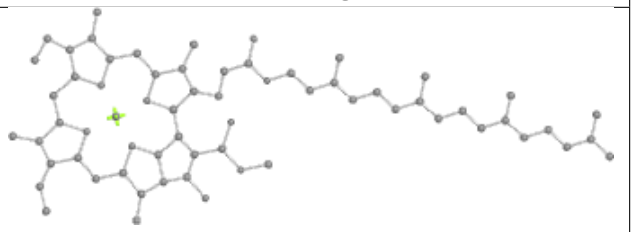


Bond angles

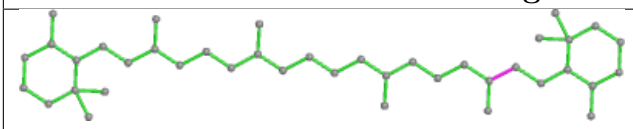


Torsions



Rings

Ligand BCR T 101



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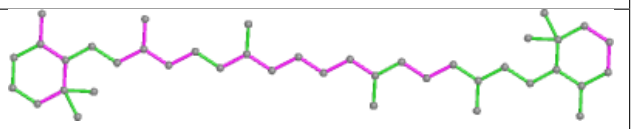
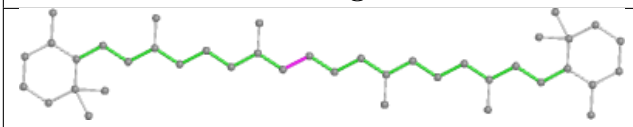


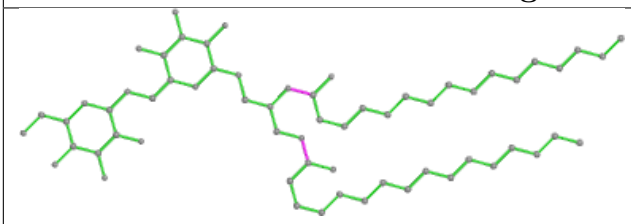
Bond angles



Torsions

Rings

Ligand DGD C 517



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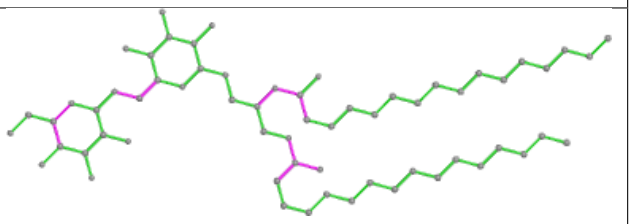
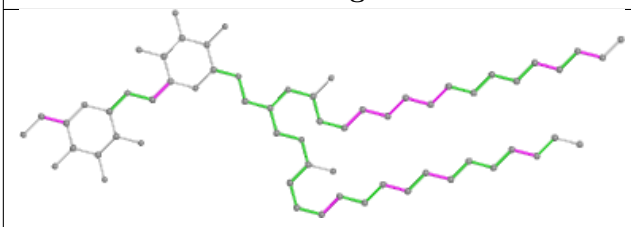
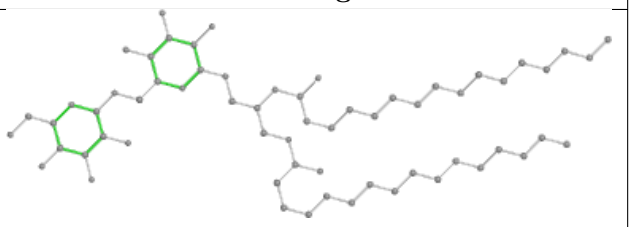


Bond angles

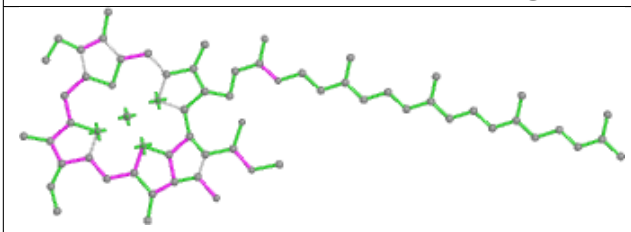


Torsions

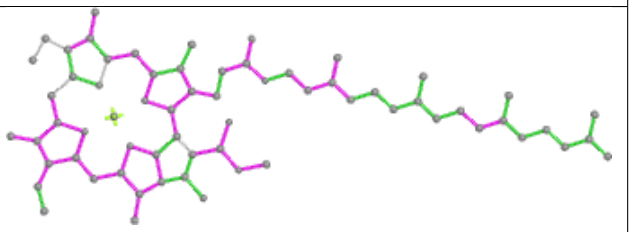


Rings

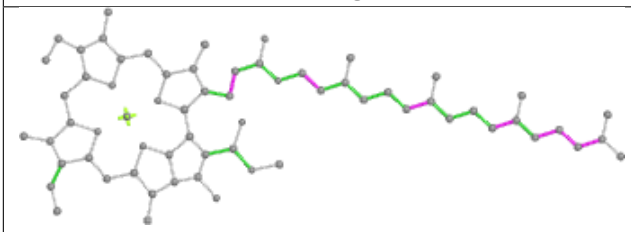
Ligand CLA B 602



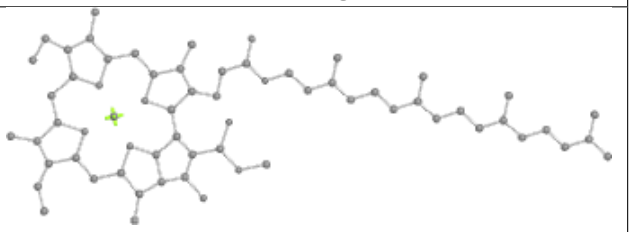
Bond lengths



Bond angles

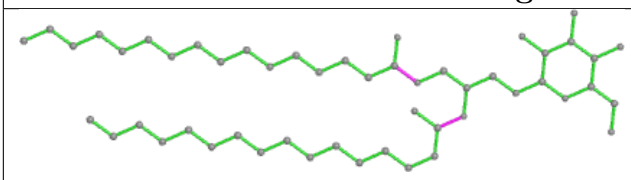


Torsions

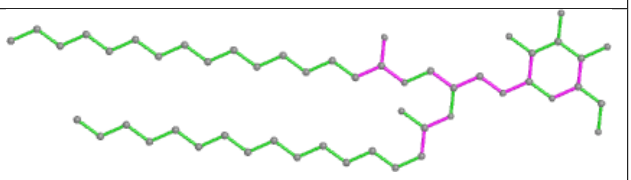


Rings

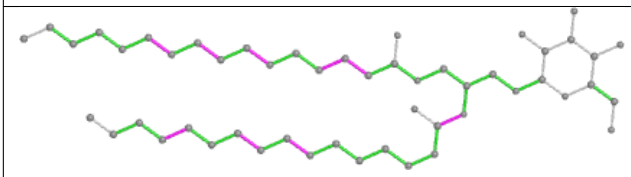
Ligand LMG M 101



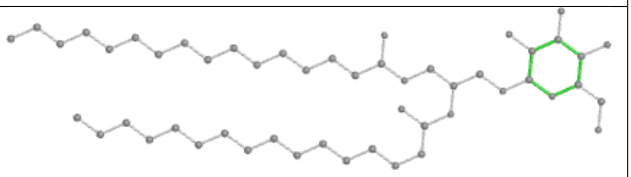
Bond lengths



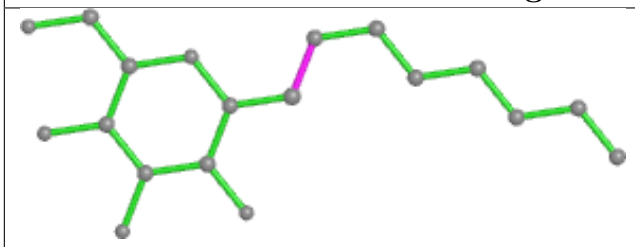
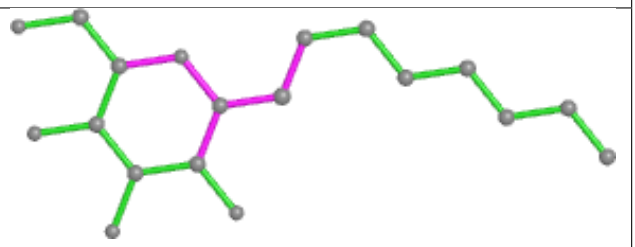
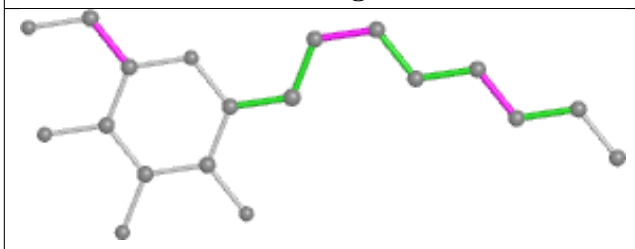
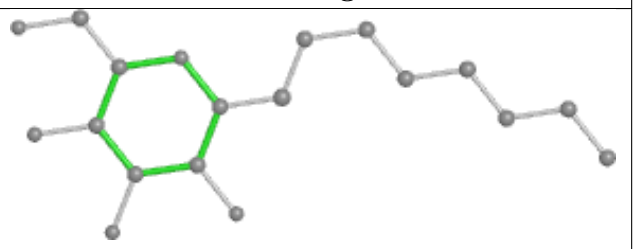
Bond angles

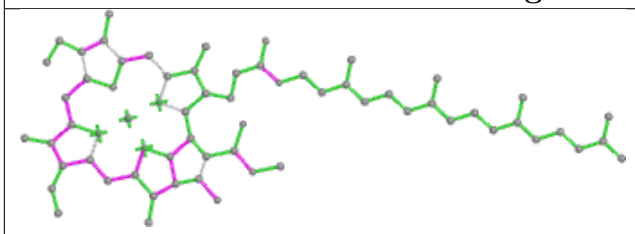
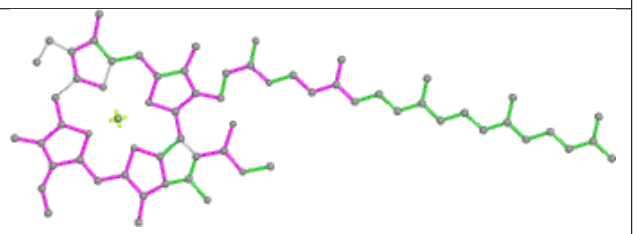
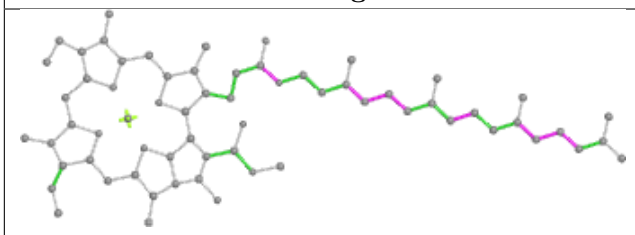
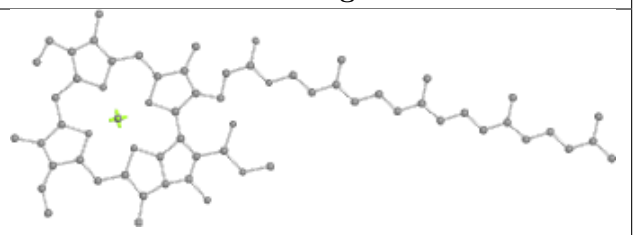


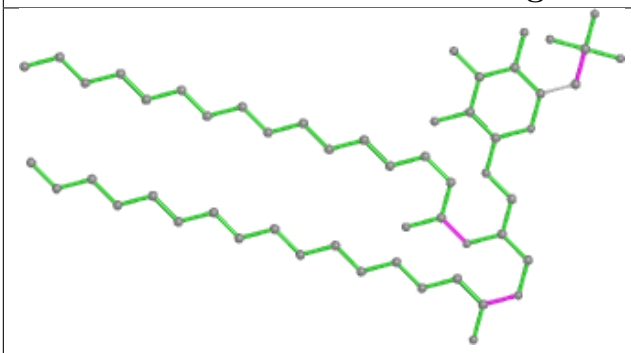
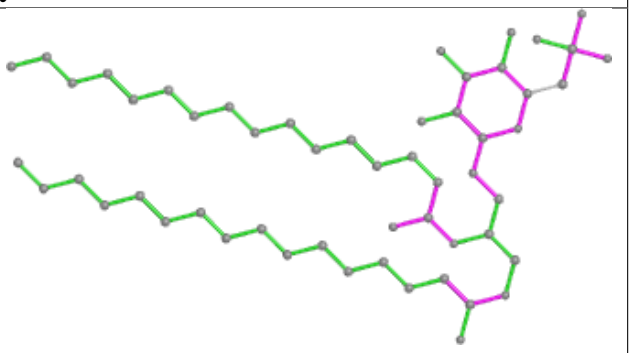
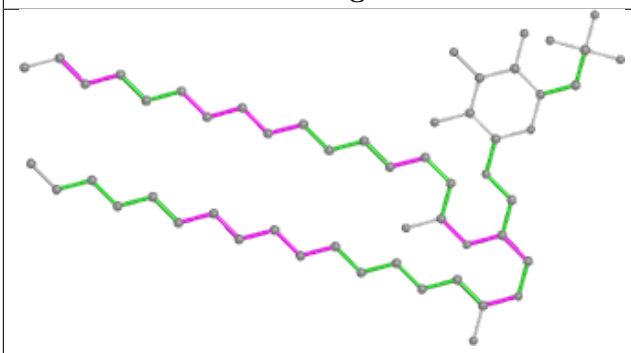
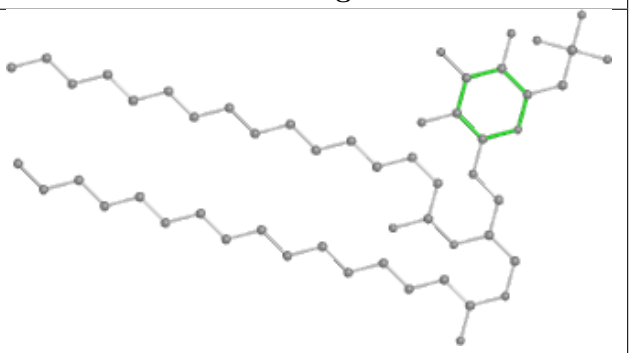
Torsions



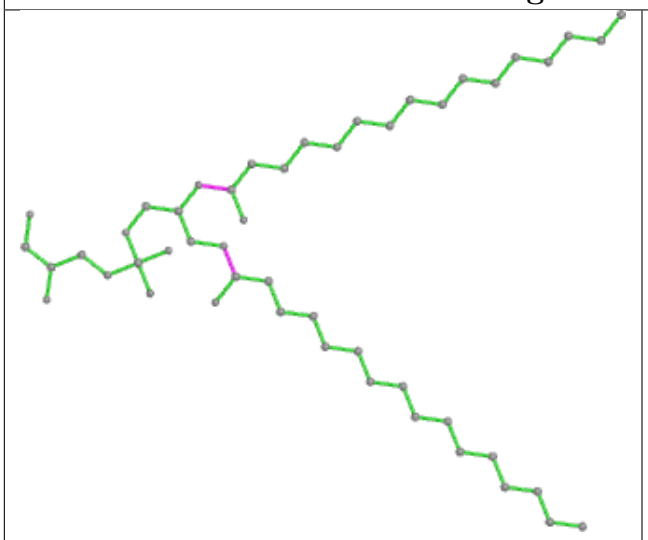
Rings

Ligand HTG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

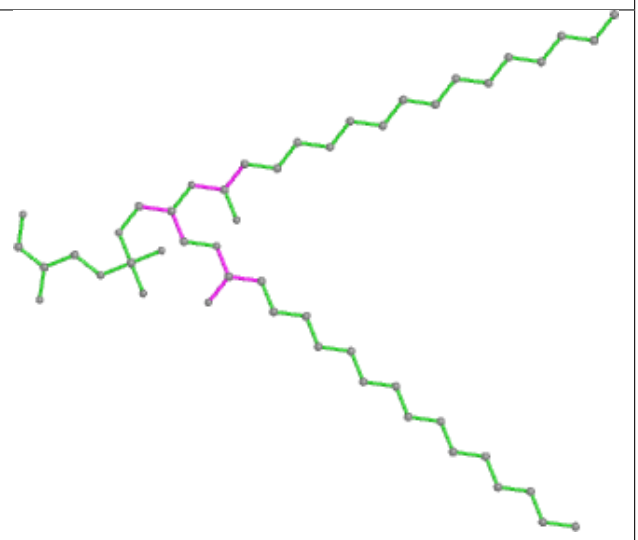
Ligand CLA A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SQD L 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

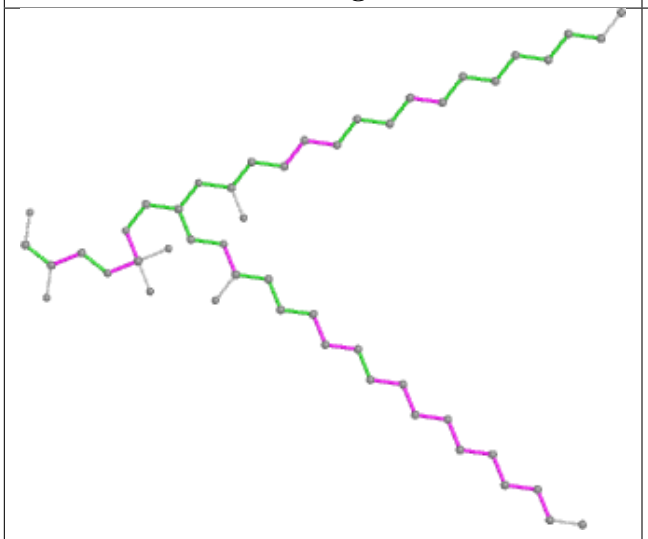
Ligand LHG d 408



Bond lengths



Bond angles



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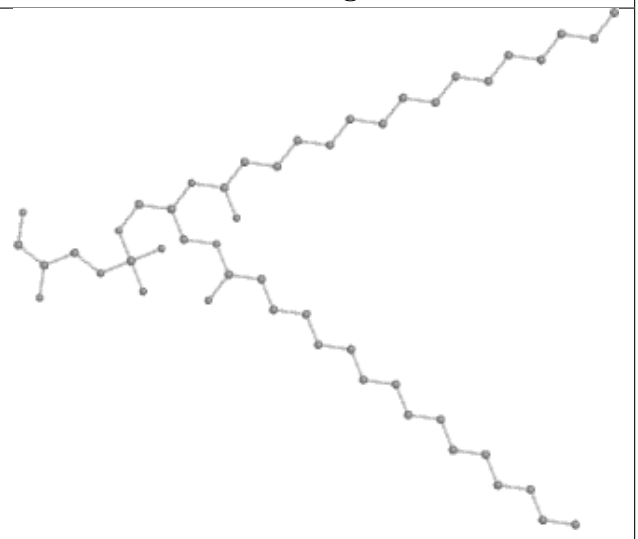
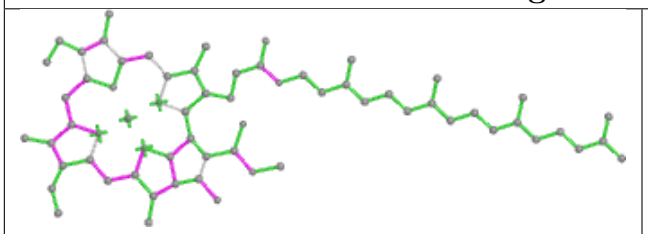


Rings

Ligand CLA b 601



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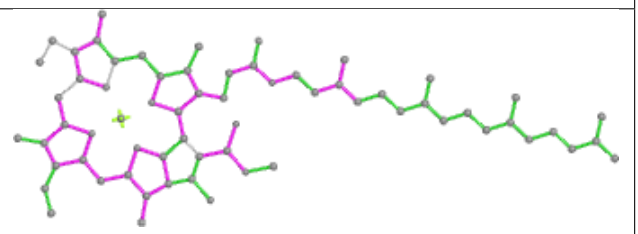
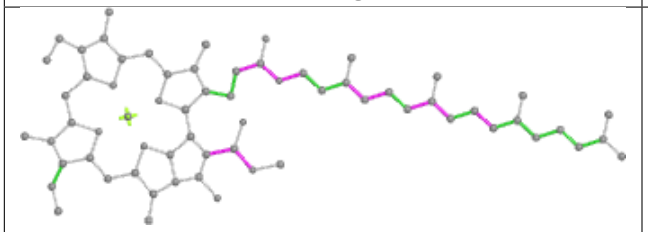


Bond angles



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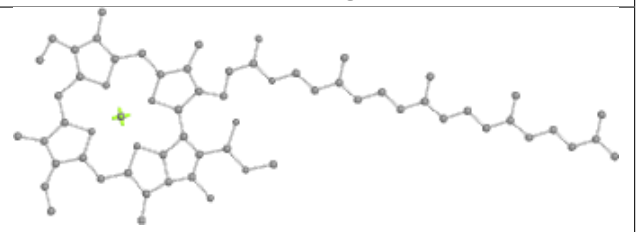
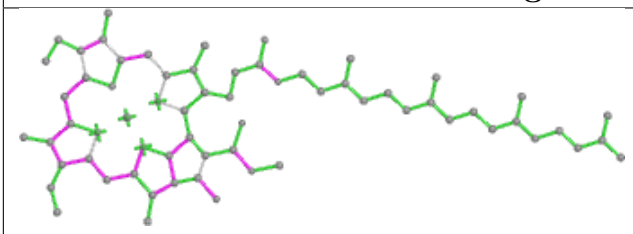


Rings

Ligand CLA B 601



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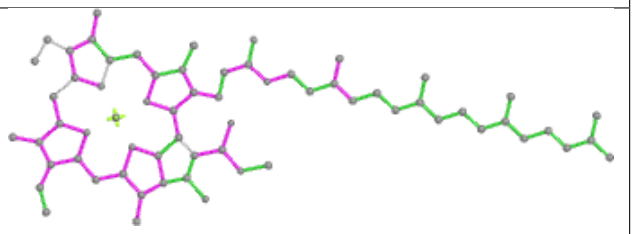

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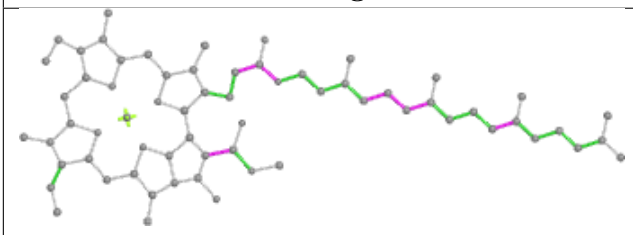

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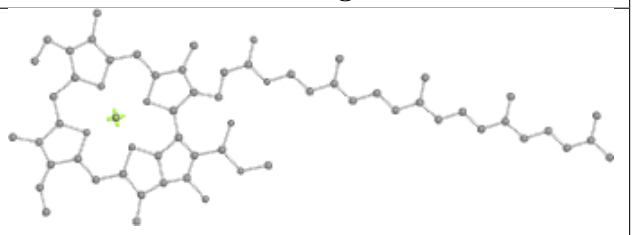
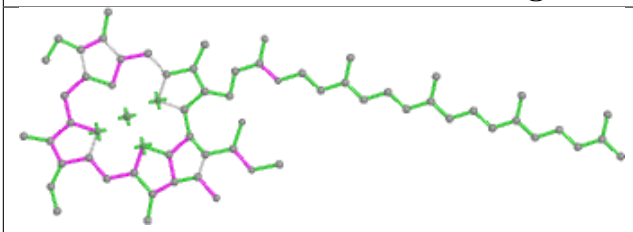


Rings

Ligand CLA b 610



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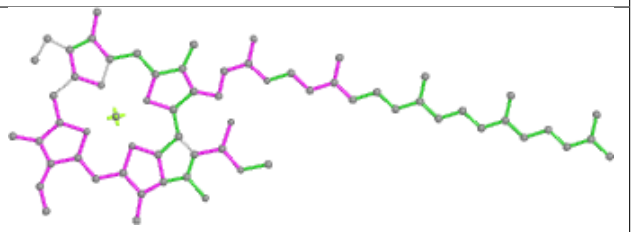
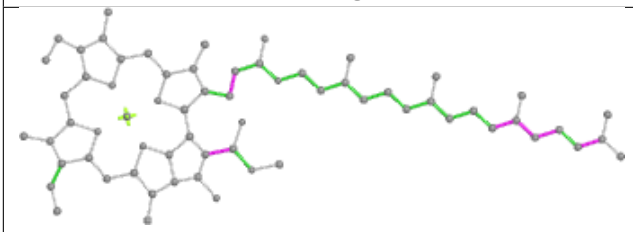


Bond angles



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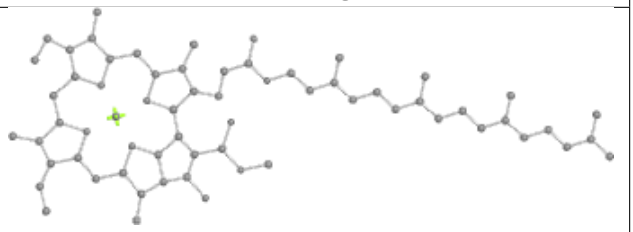
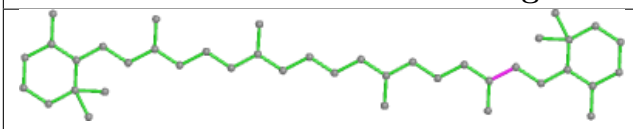


Rings

Ligand BCR D 407



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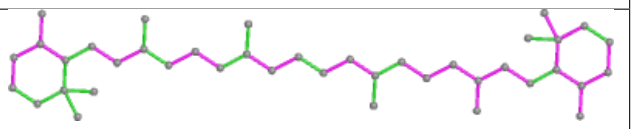
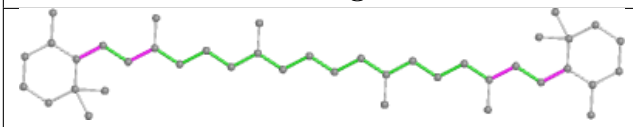


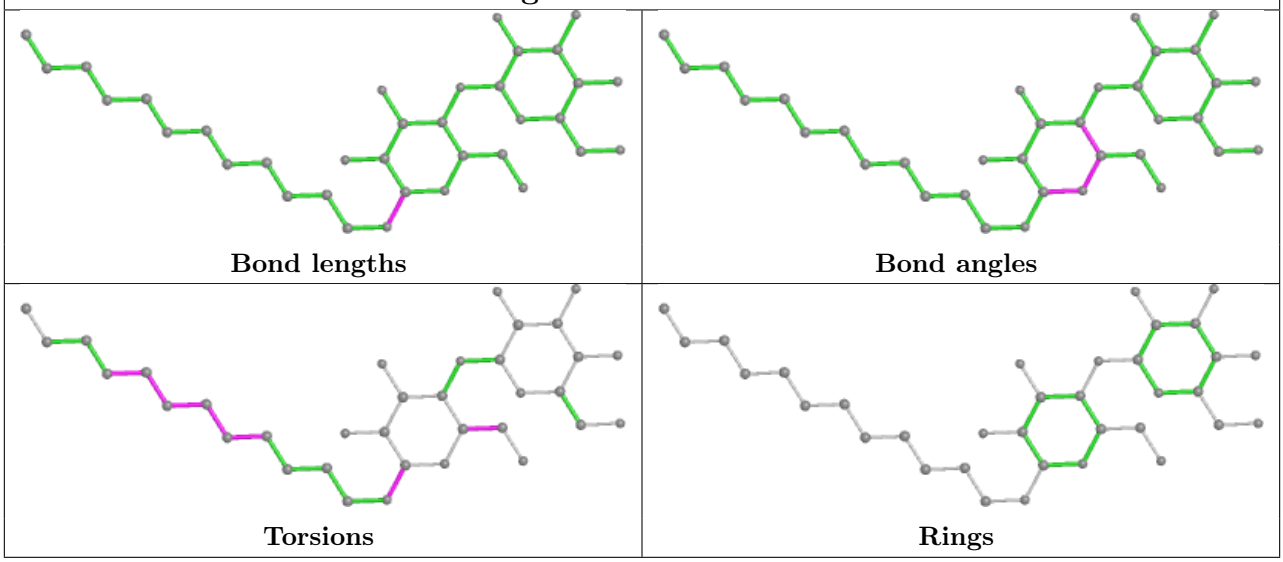
Bond angles



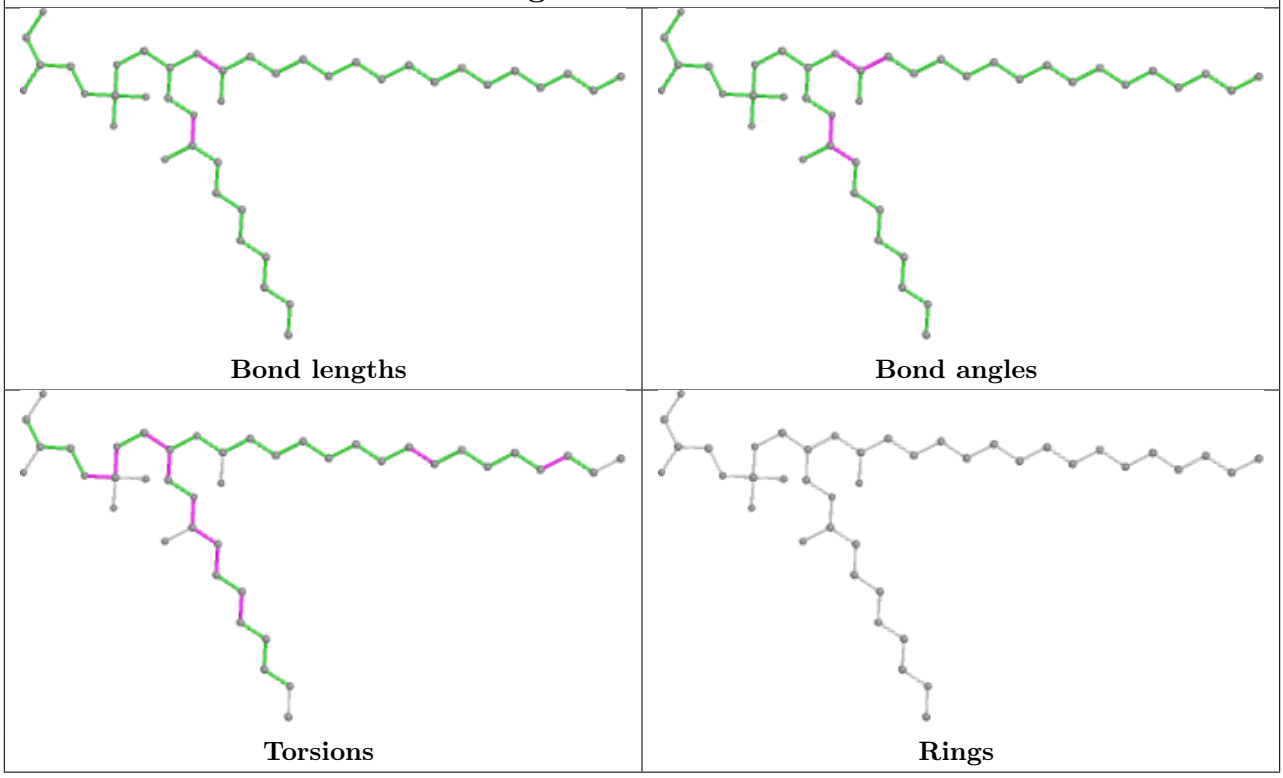
Torsions

Rings

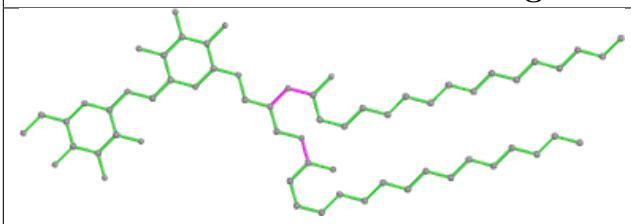
Ligand LMT D 403



Ligand LHG a 419



Ligand DGD c 519



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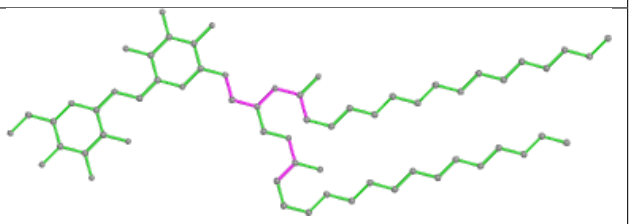
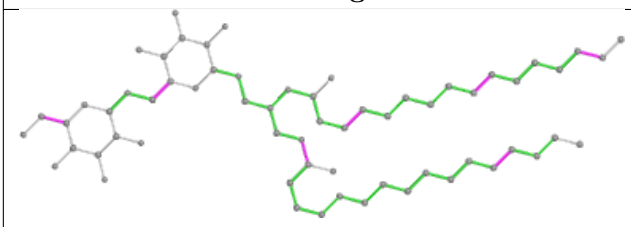


Bond angles



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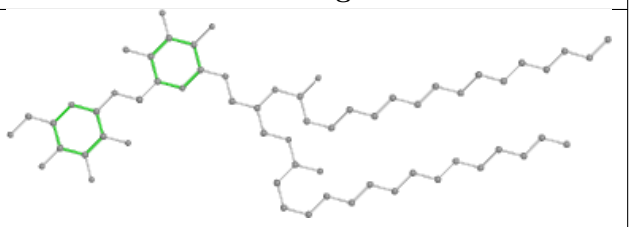
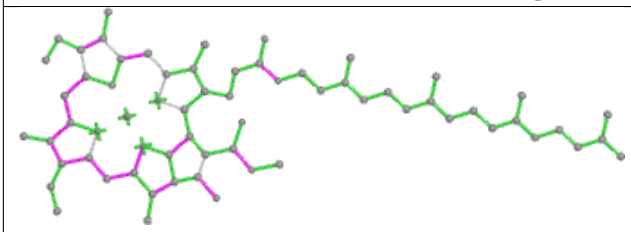


Rings

Ligand CLA c 512



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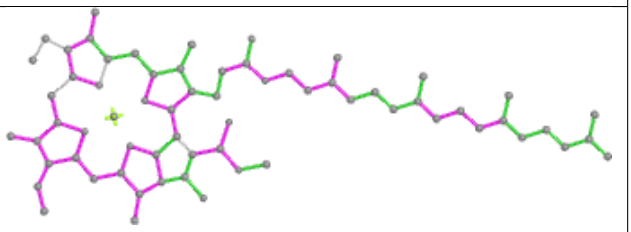
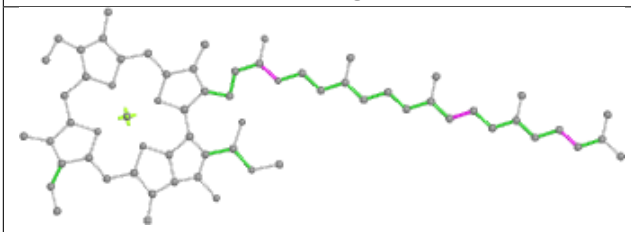


Bond angles



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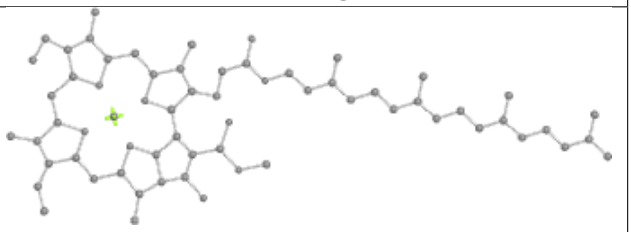
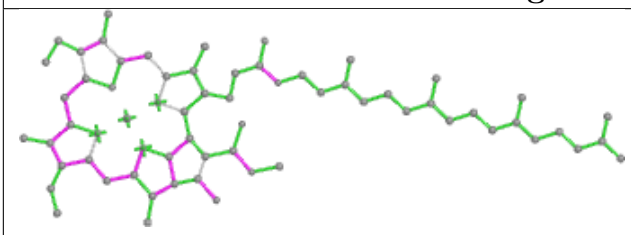


Rings

Ligand CLA b 603



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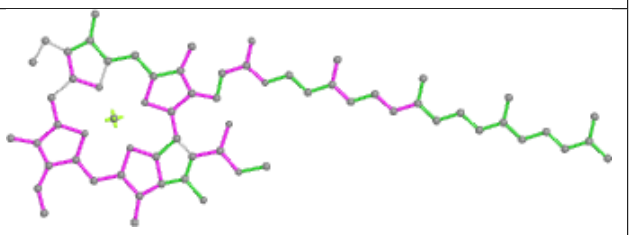
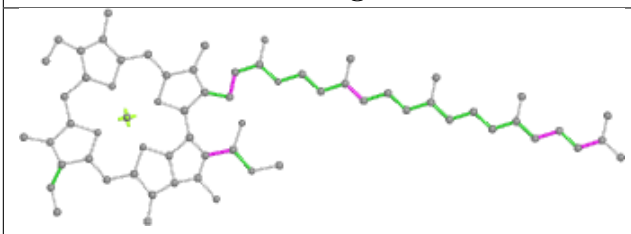


Bond angles



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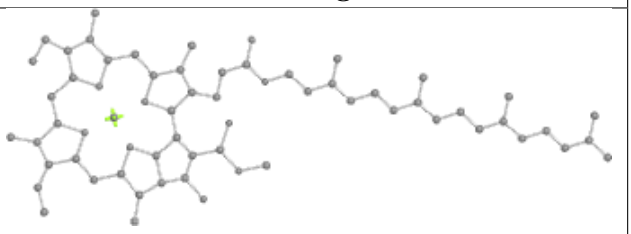
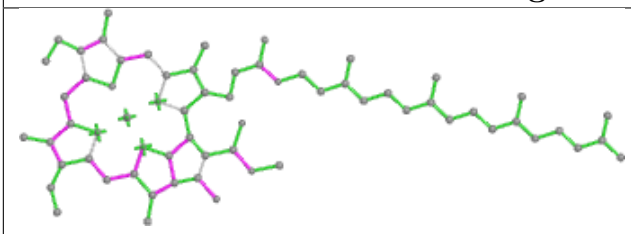
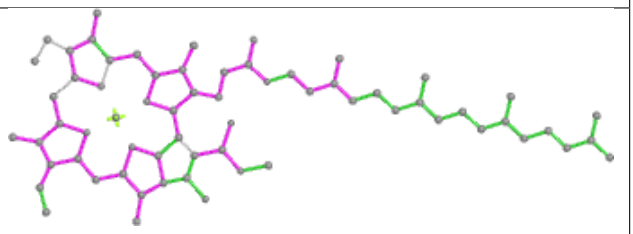


Rings

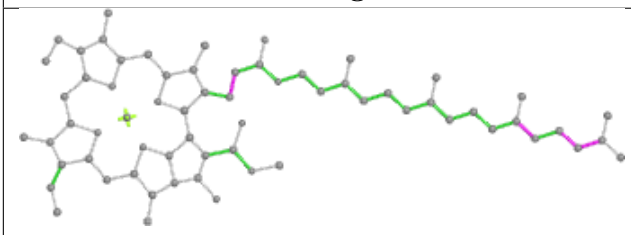
Ligand CLA a 404



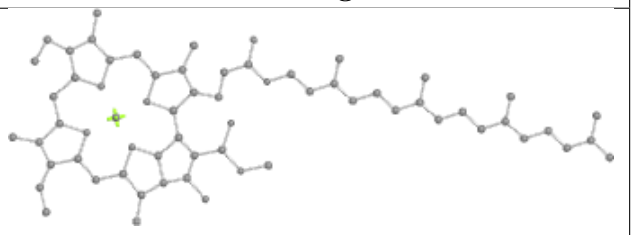
Bond lengths



Bond angles

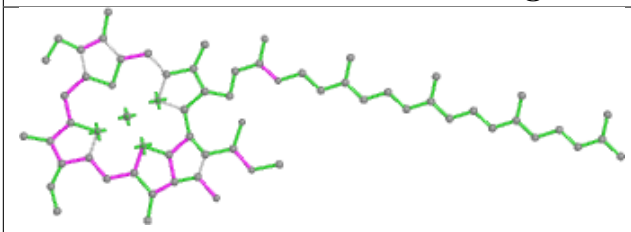


Torsions

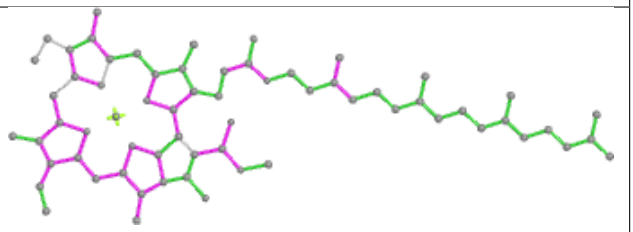


Rings

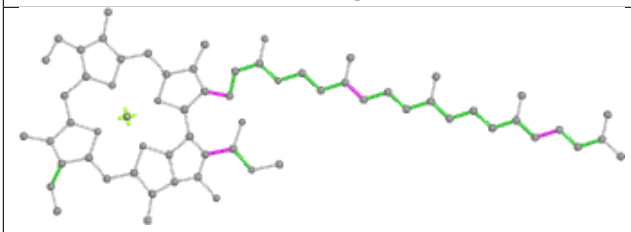
Ligand CLA B 609



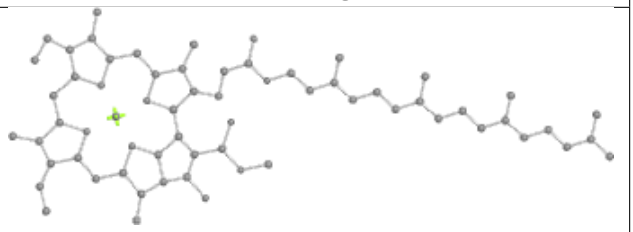
Bond lengths



Bond angles

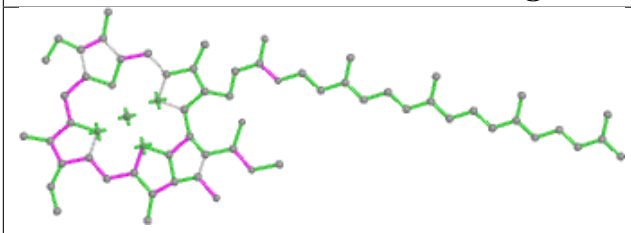


Torsions

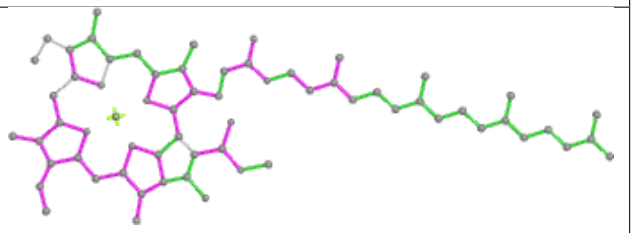


Rings

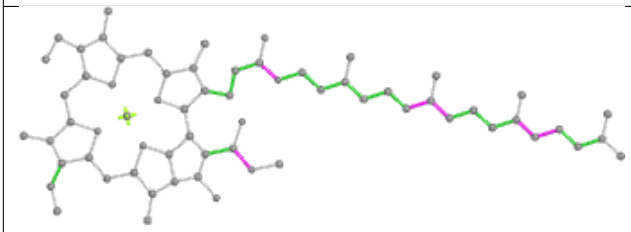
Ligand CLA C 514



Bond lengths



Bond angles



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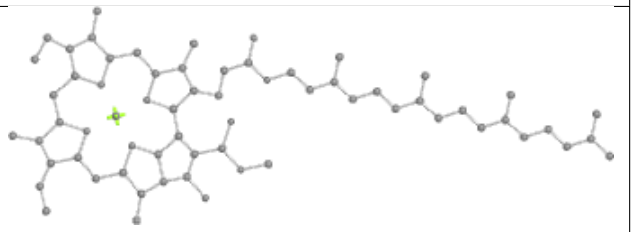
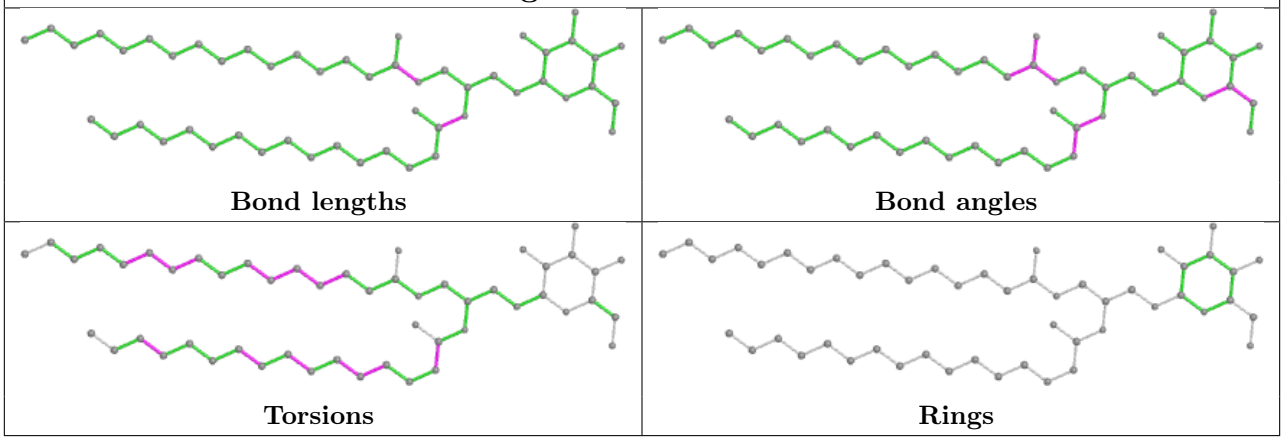
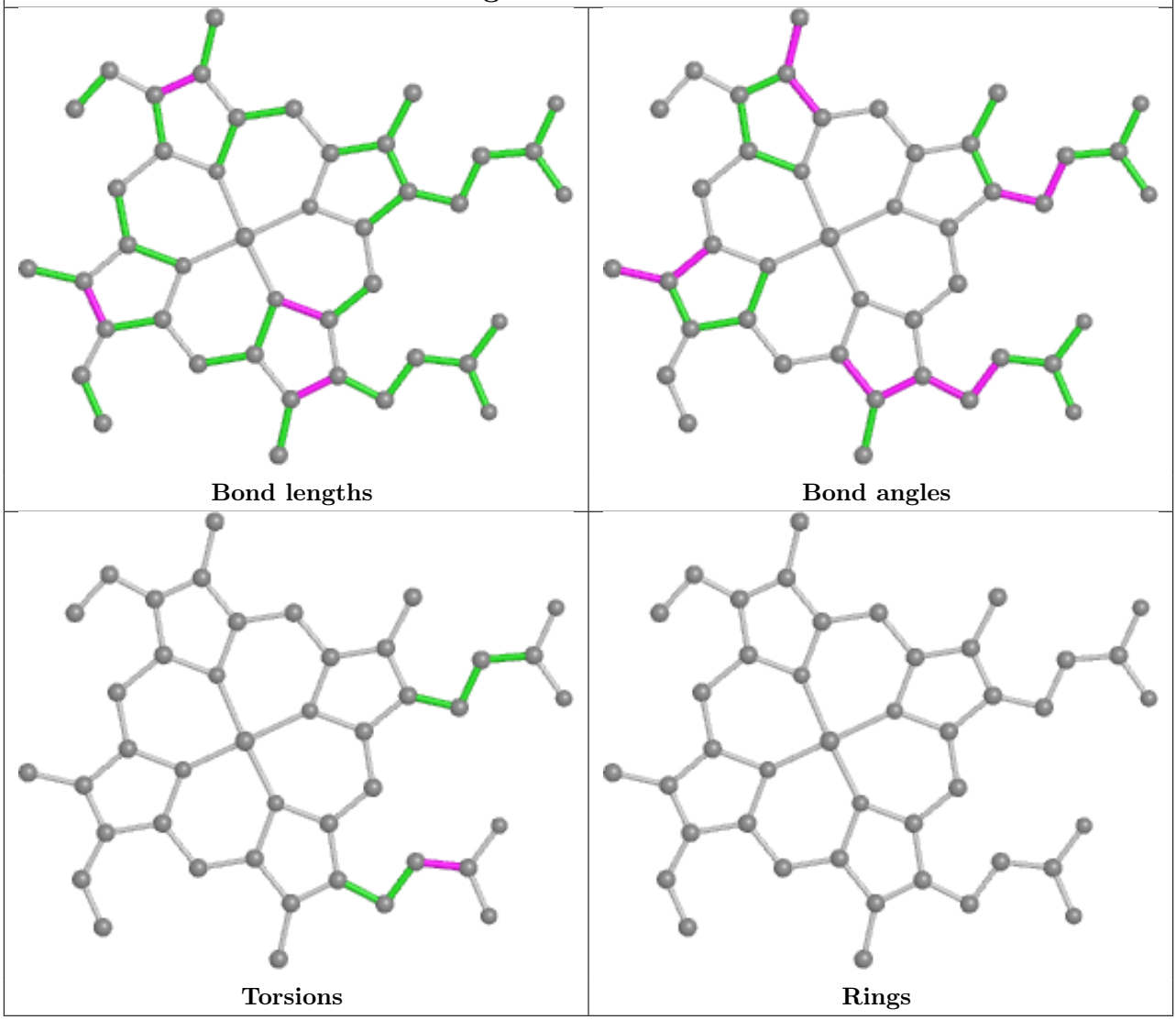


Rings

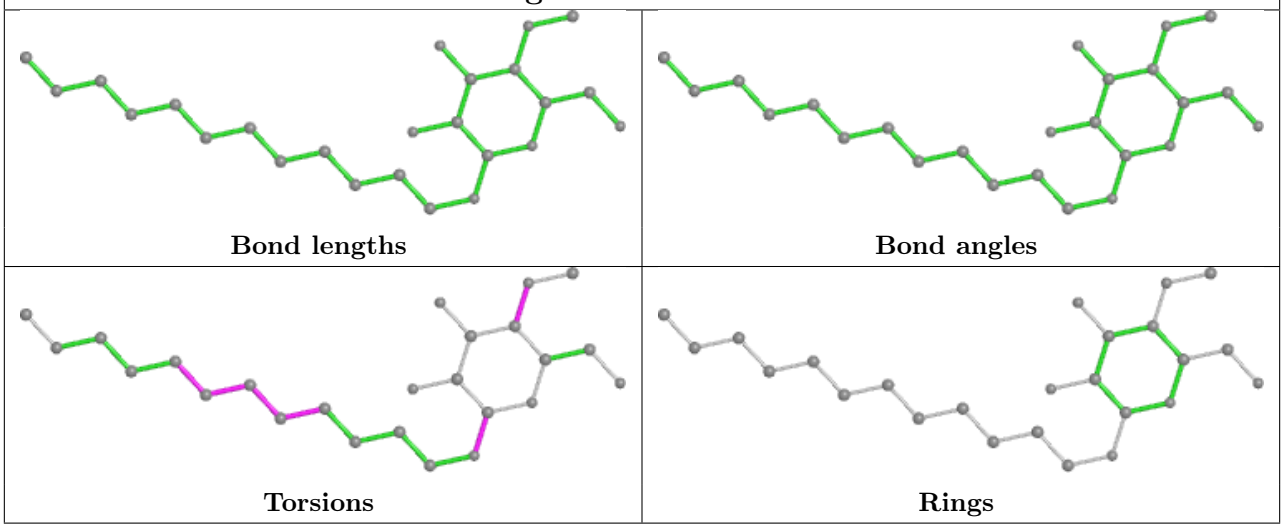
Ligand LMG C 520



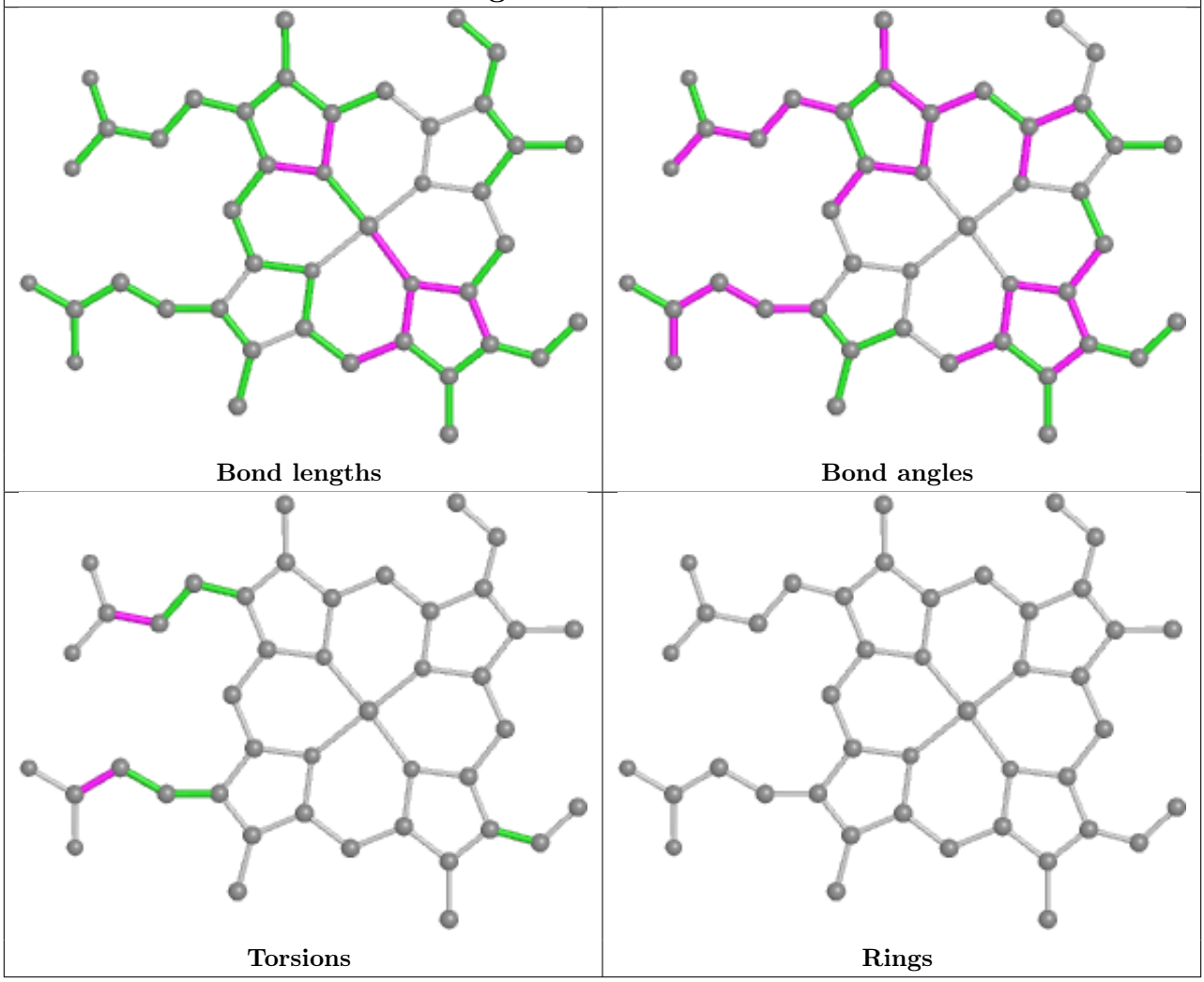
Ligand HEC v 203



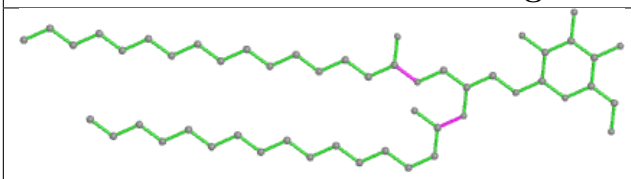
Ligand LMT b 620



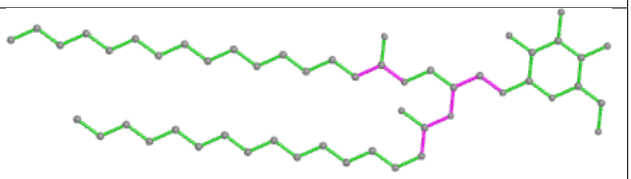
Ligand HEM E 103



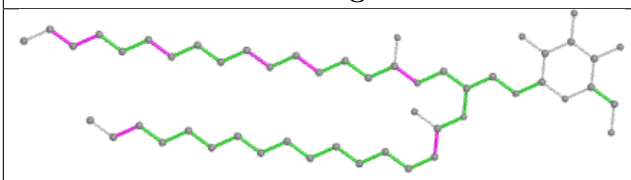
Ligand LMG c 520



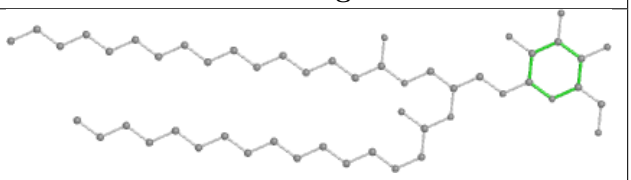
Bond lengths



Bond angles

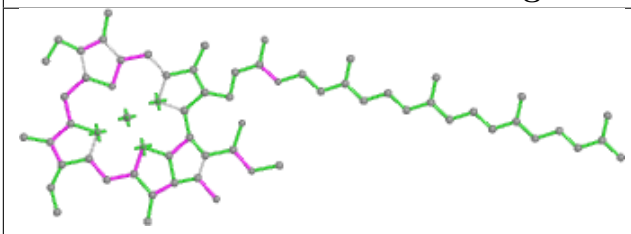


Torsions



Rings

Ligand CLA D 406



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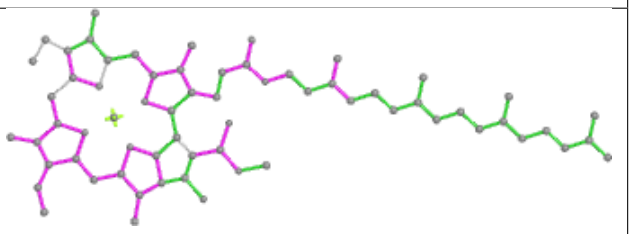
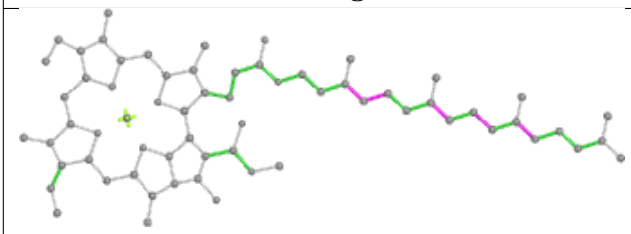


Bond angles



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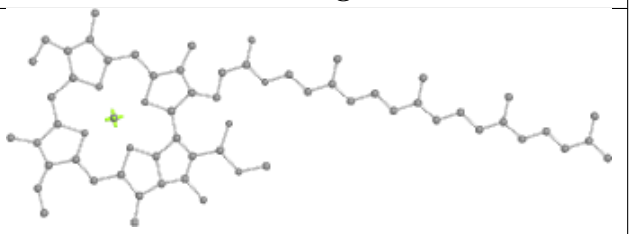
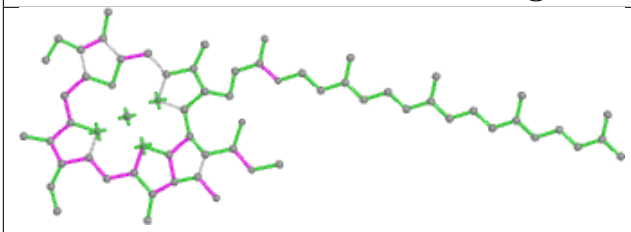
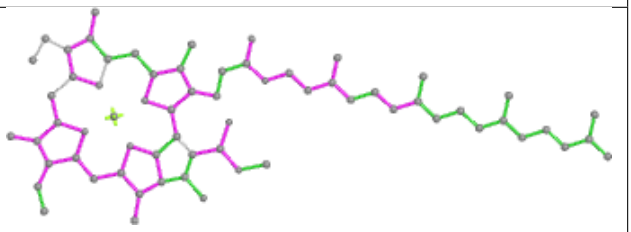


Rings

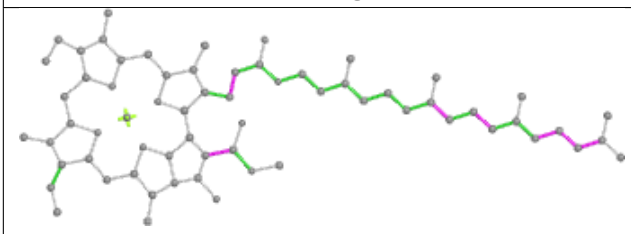
Ligand CLA b 606



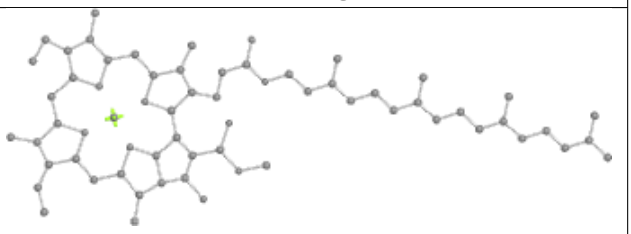
Bond lengths



Bond angles

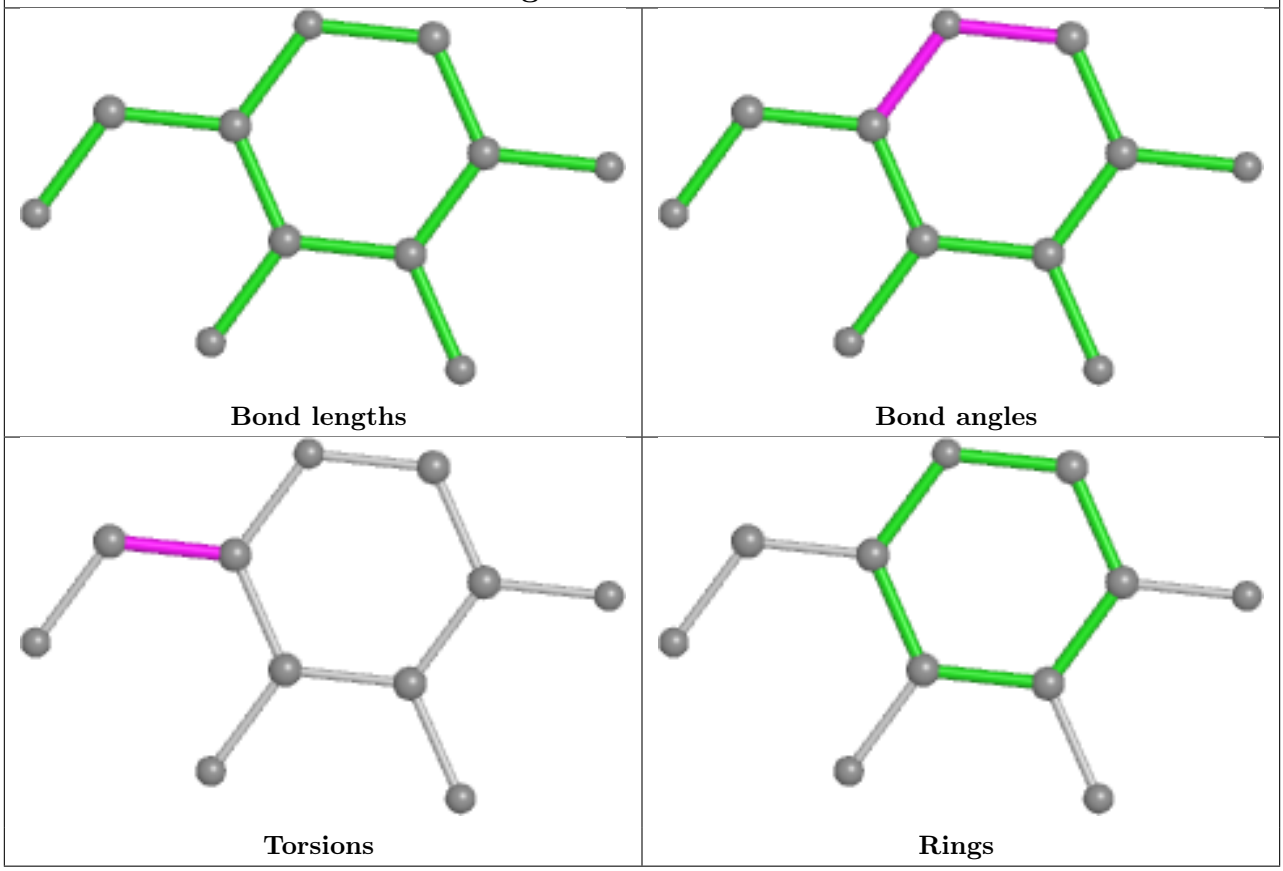


Torsions

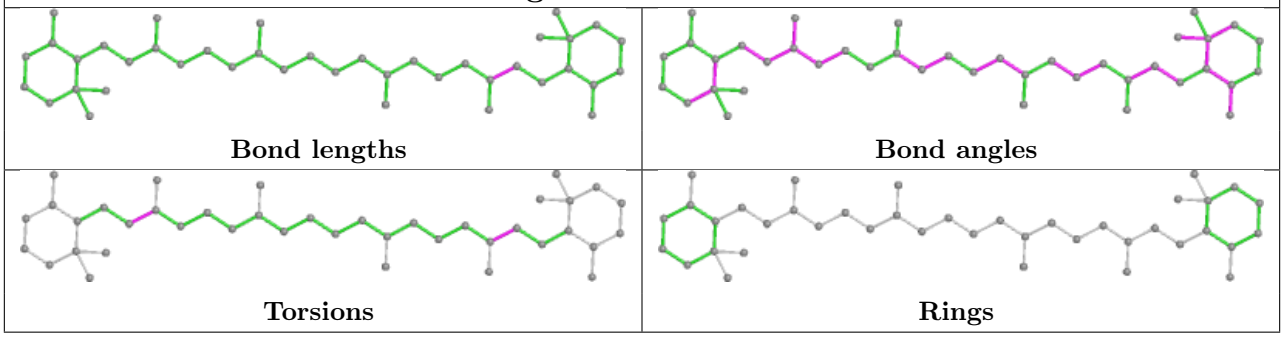


Rings

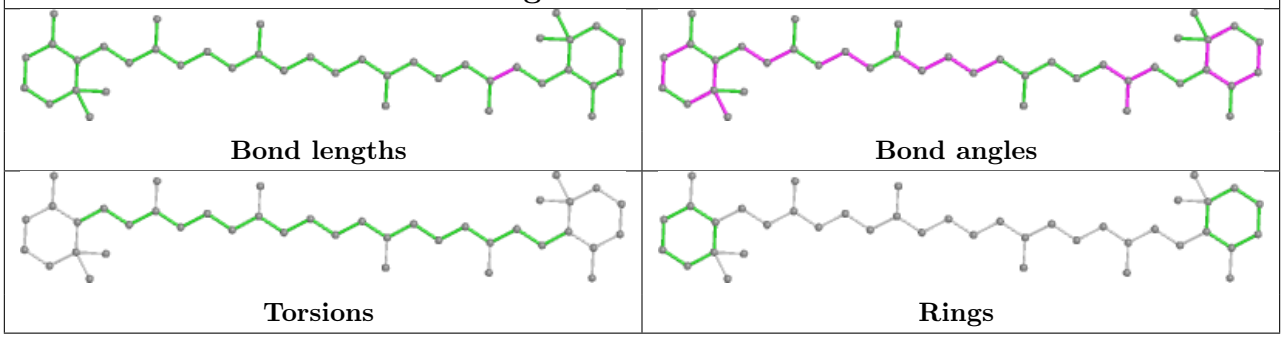
Ligand HTG V 202



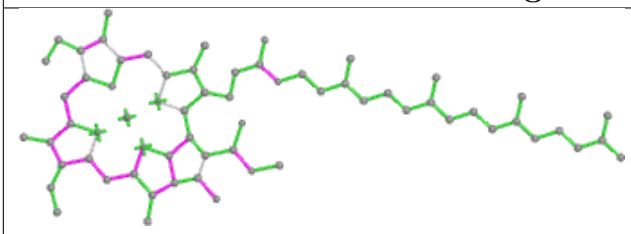
Ligand BCR b 619



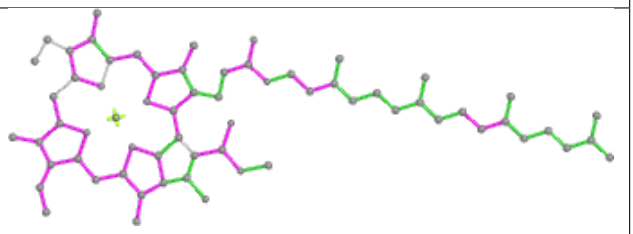
Ligand BCR B 618



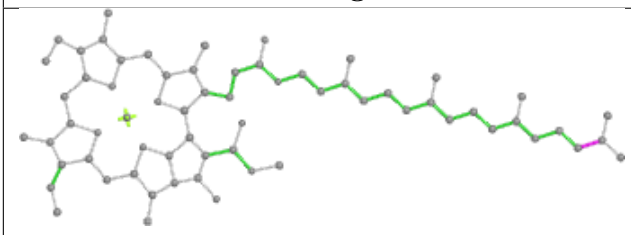
Ligand CLA B 608



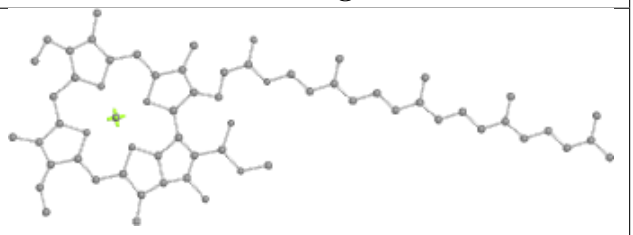
Bond lengths



Bond angles

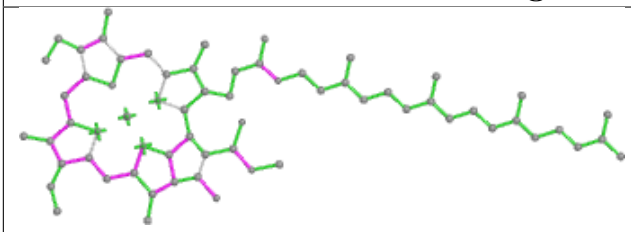


Torsions



Rings

Ligand CLA b 602



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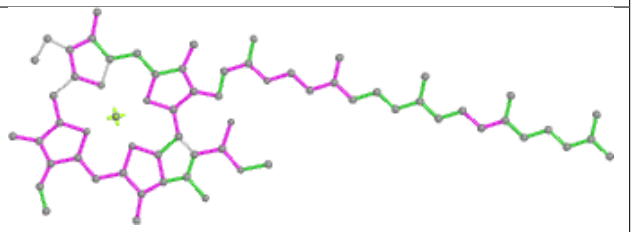
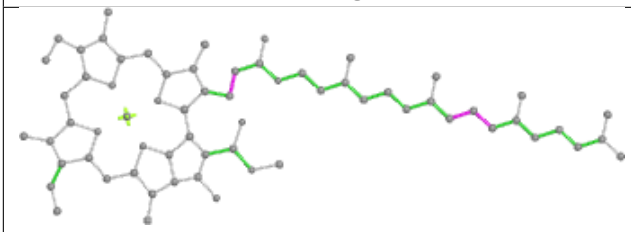


Bond angles



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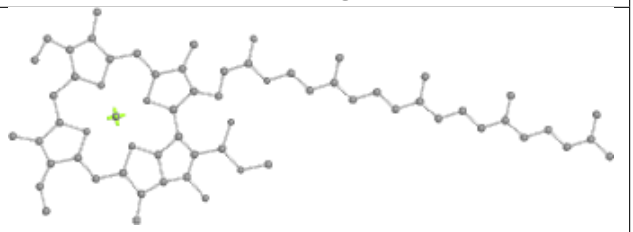
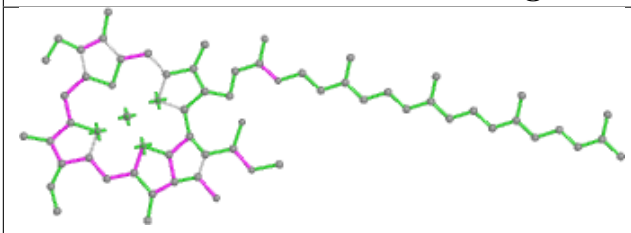


Rings

Ligand CLA C 502



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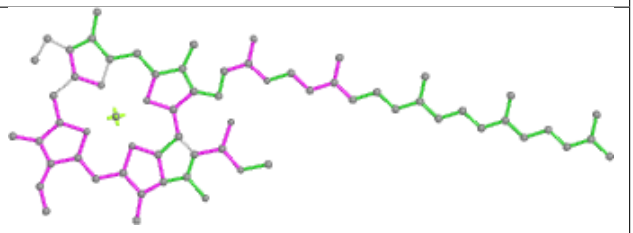
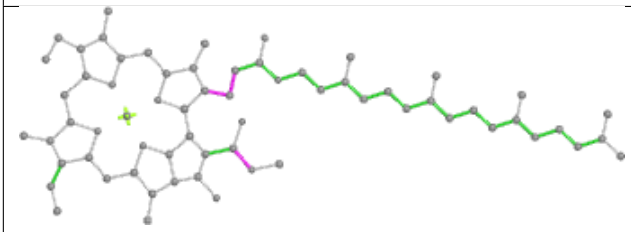


Bond angles



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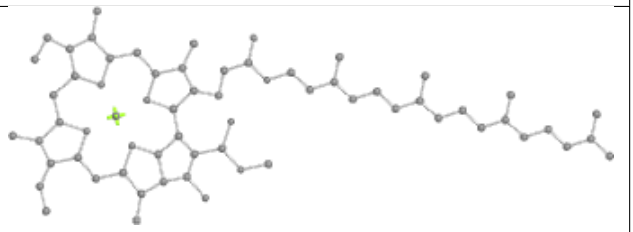
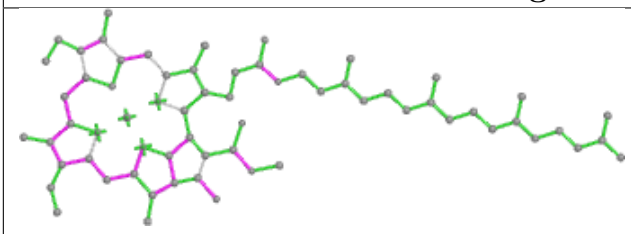


Rings

Ligand CLA c 506



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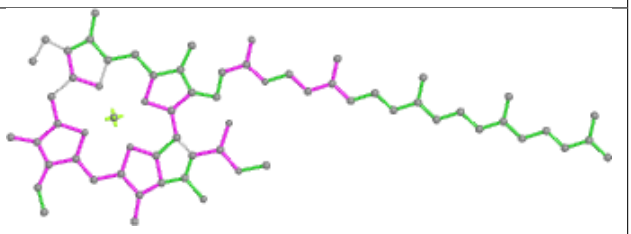
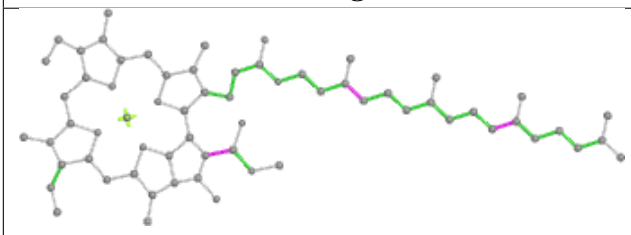


Bond angles



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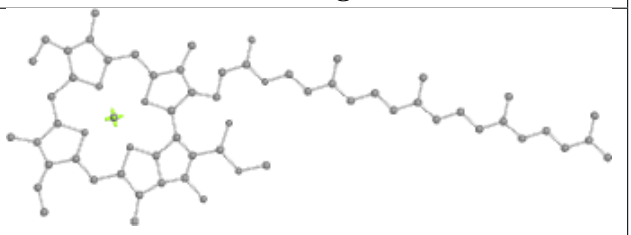
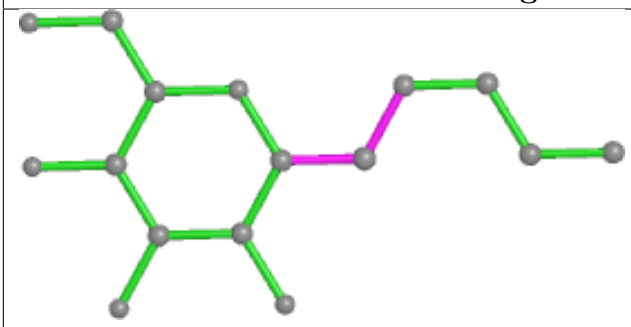


Rings

Ligand HTG D 413



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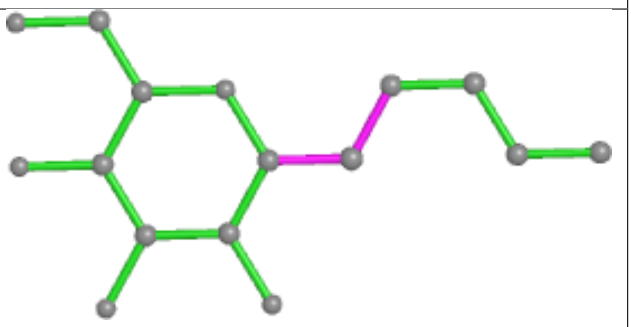
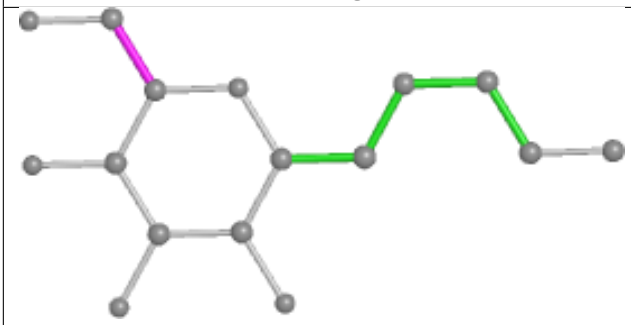
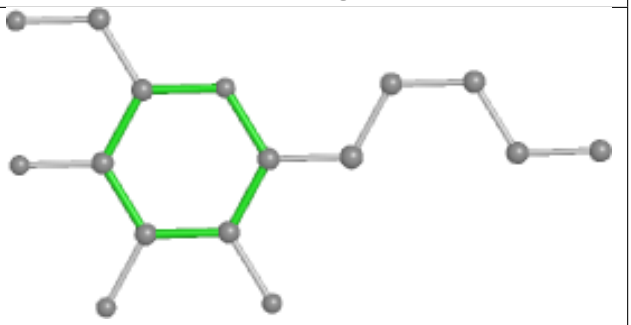


Bond angles

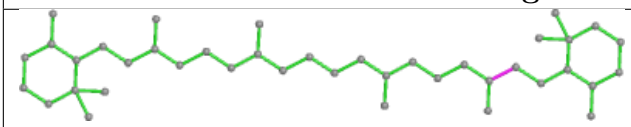


Torsions

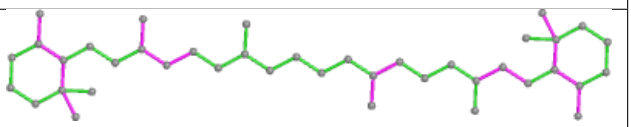


Rings

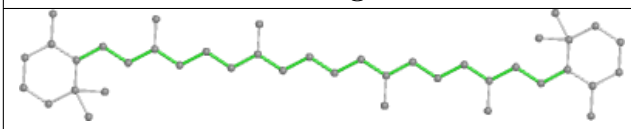
Ligand BCR A 409



Bond lengths



Bond angles



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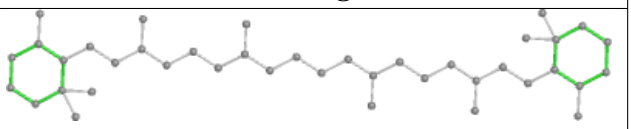
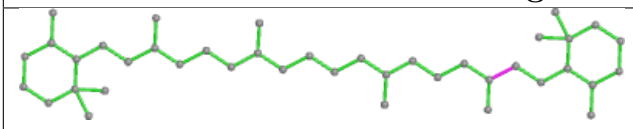
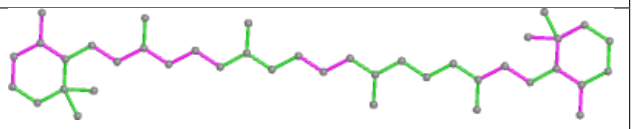


Rings

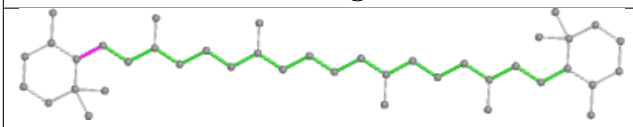
Ligand BCR a 408



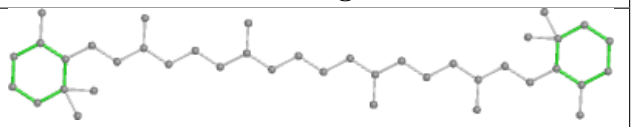
Bond lengths



Bond angles

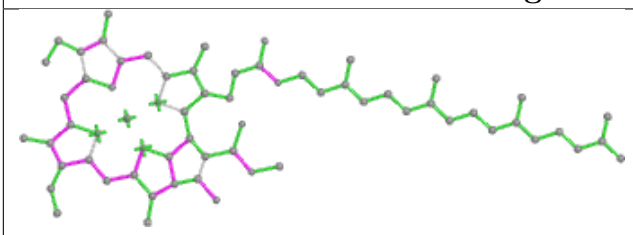


Torsions



Rings

Ligand CLA B 612



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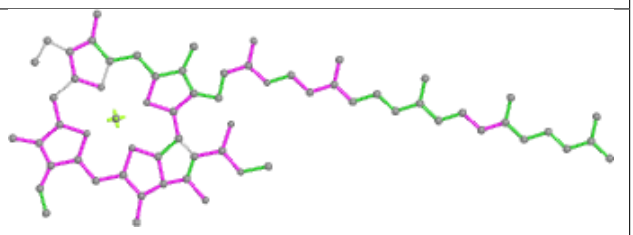
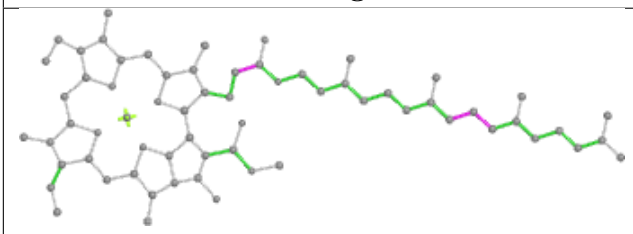
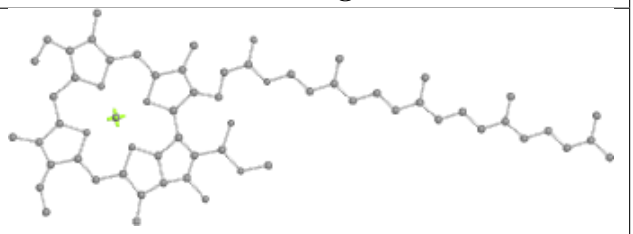


Bond angles

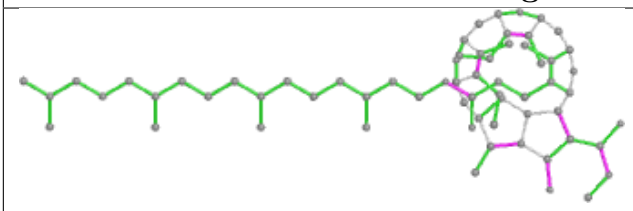


Torsions



Rings

Ligand PHO A 407



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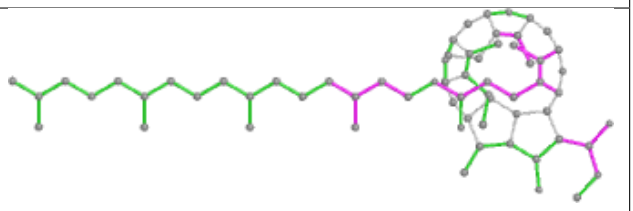
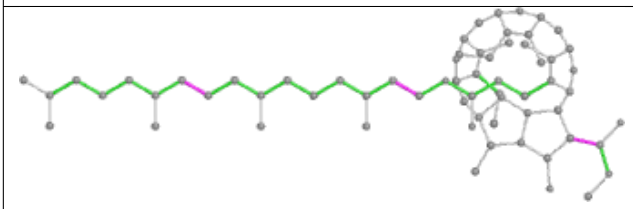


Bond angles



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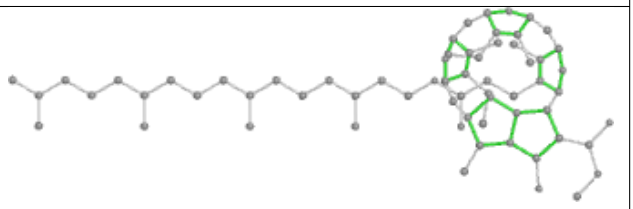
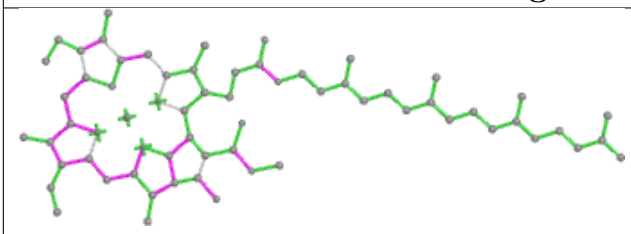


Rings

Ligand CLA c 502



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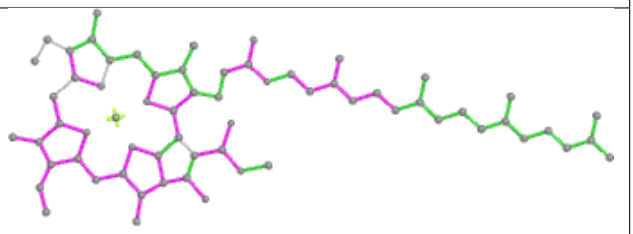

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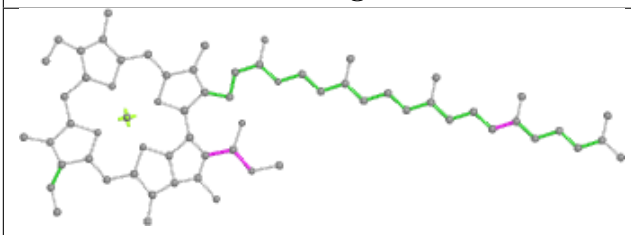

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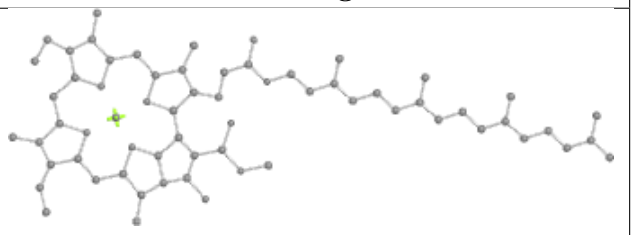
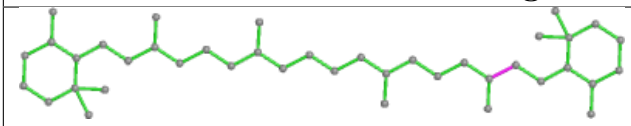


Rings

Ligand BCR C 516



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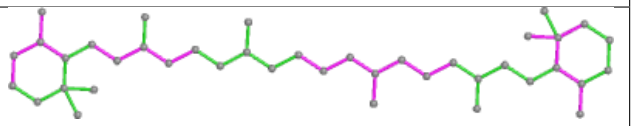
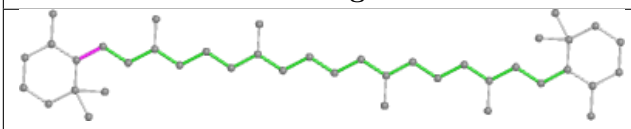


Bond angles



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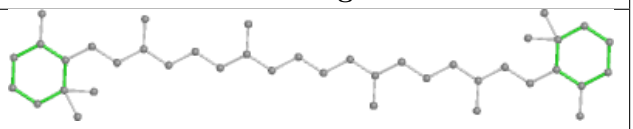
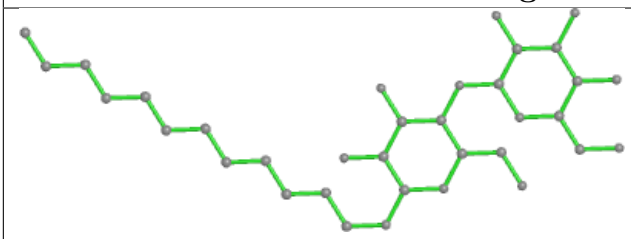


Rings

Ligand LMT m 103



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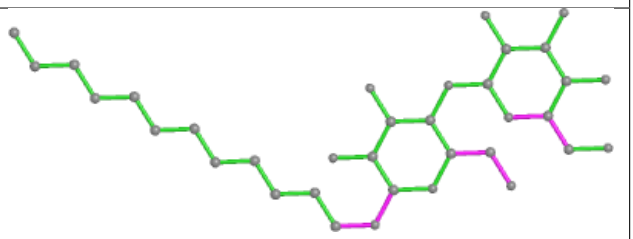

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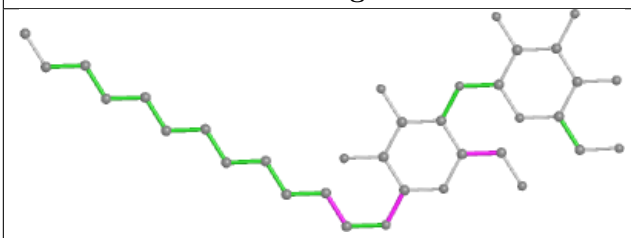

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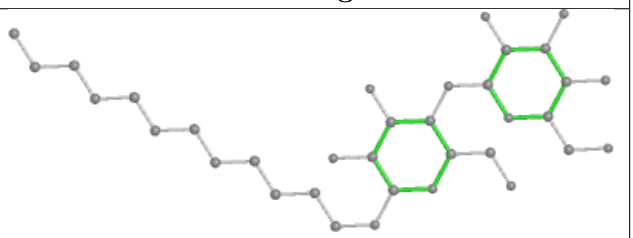
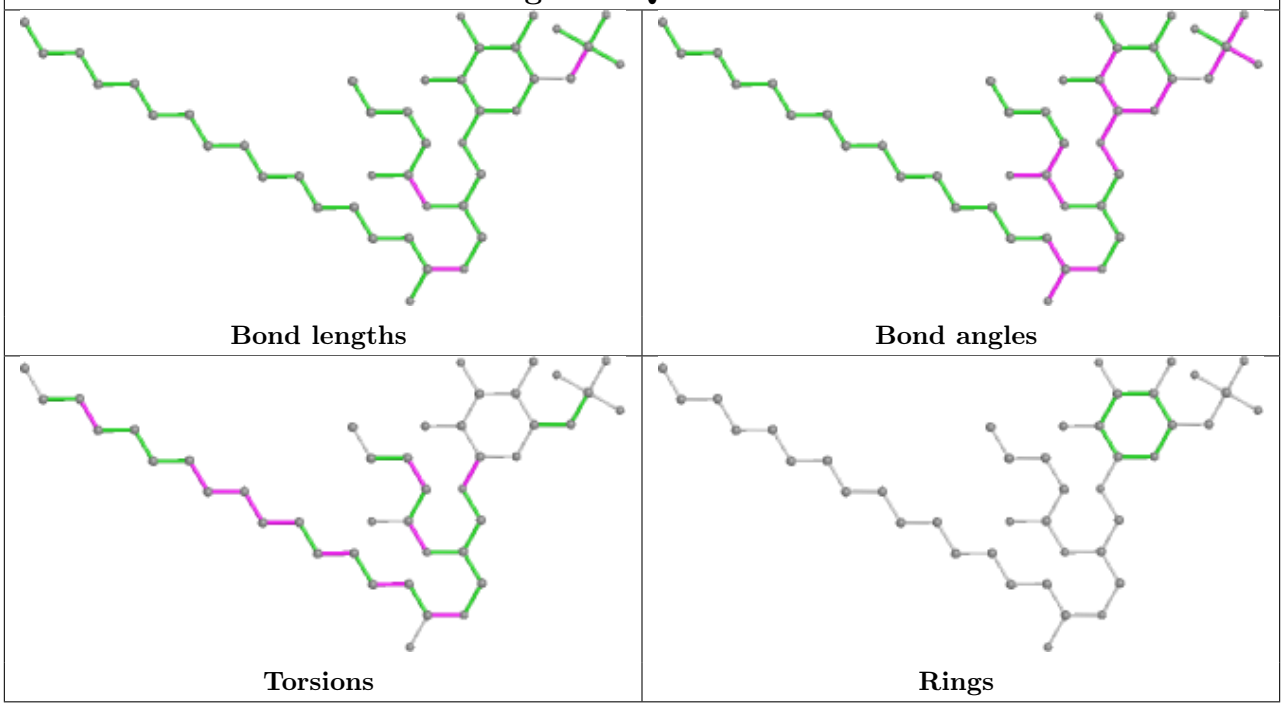
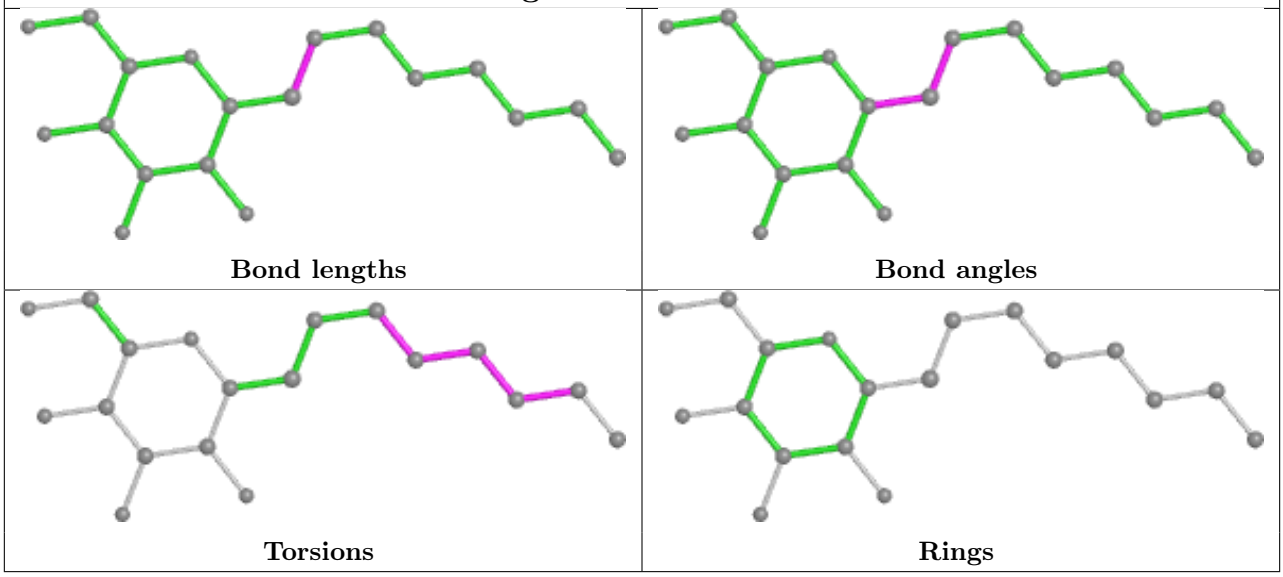


Rings

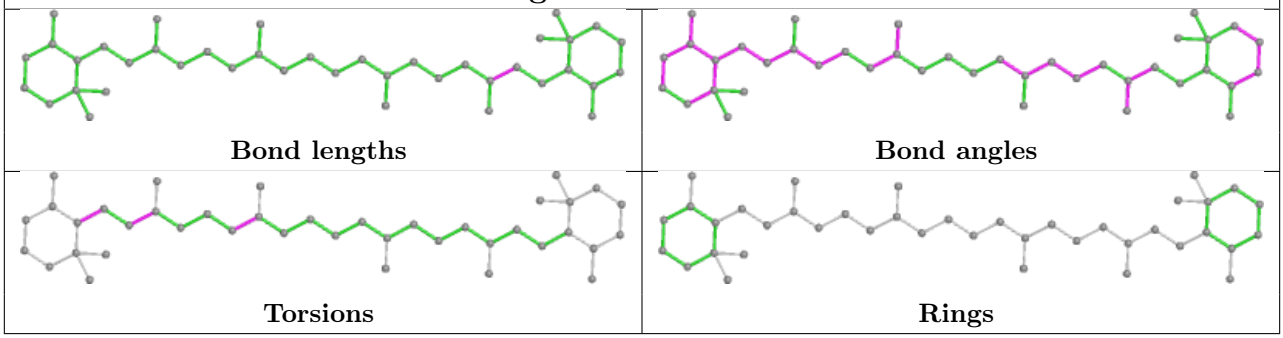
Ligand SQD D 415

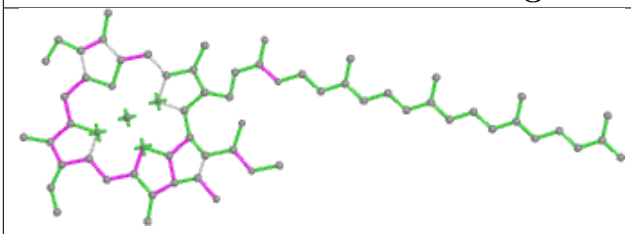
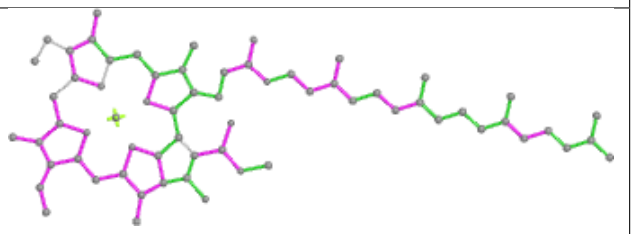
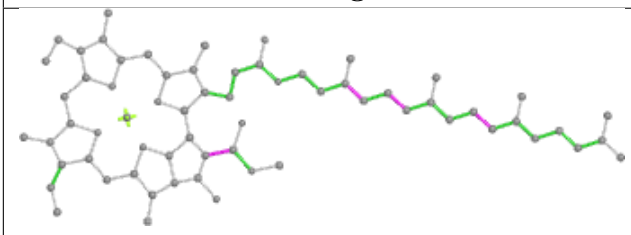
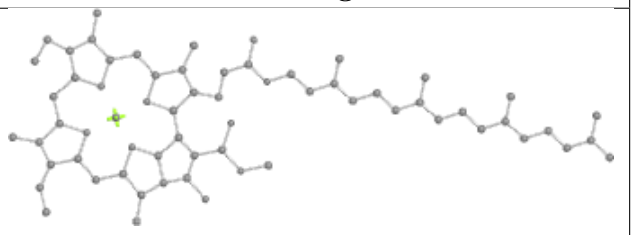


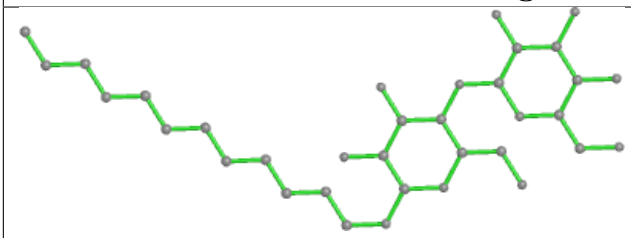
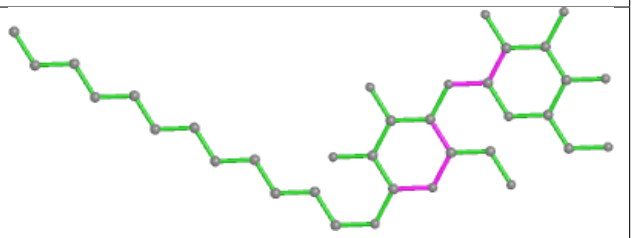
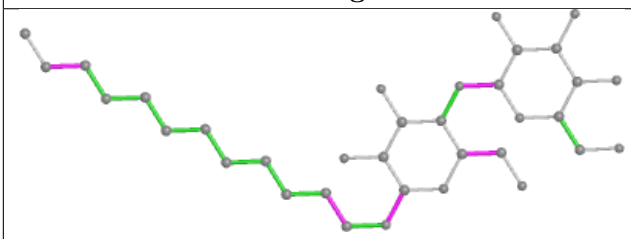
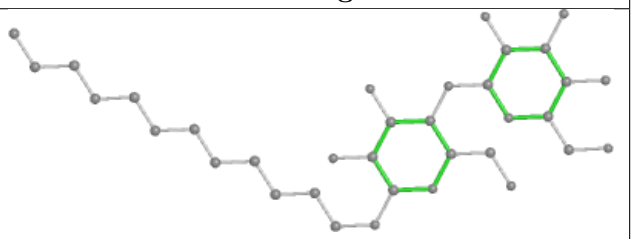
Ligand HTG B 622



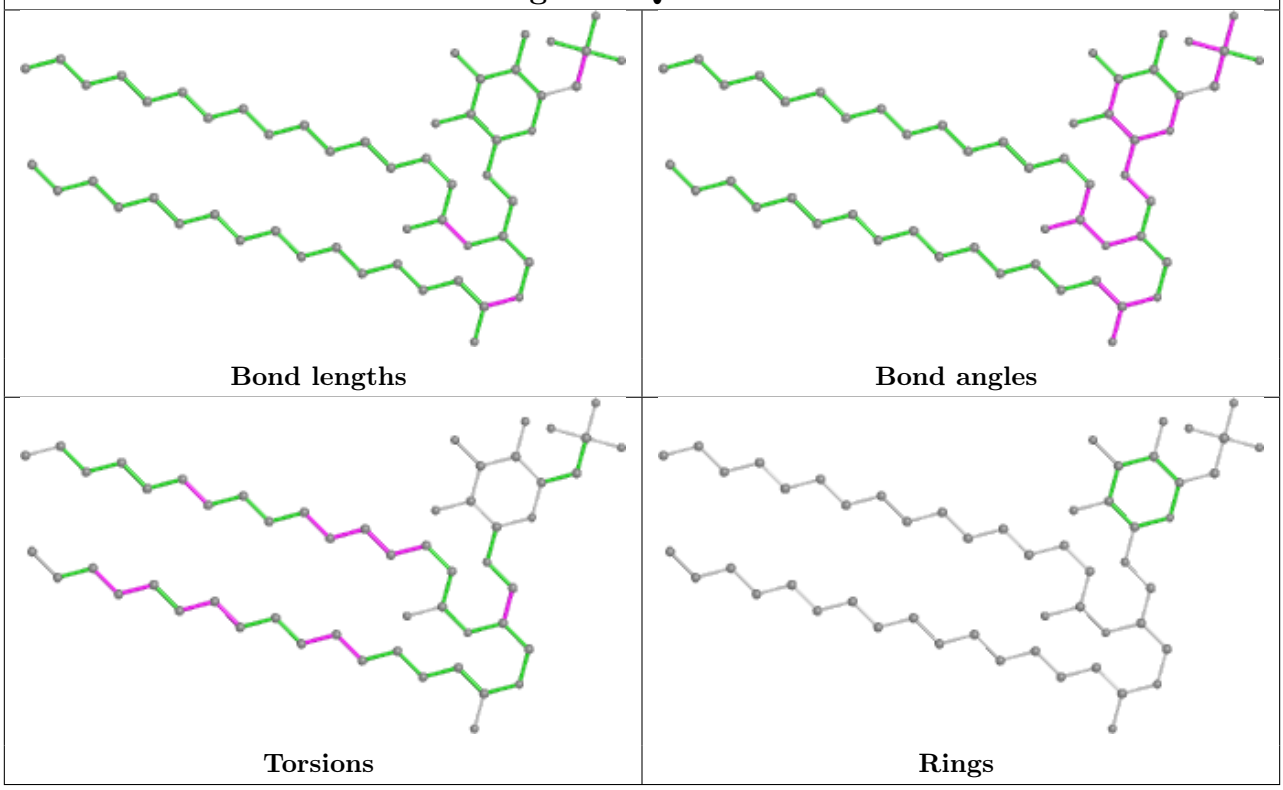
Ligand BCR t 102



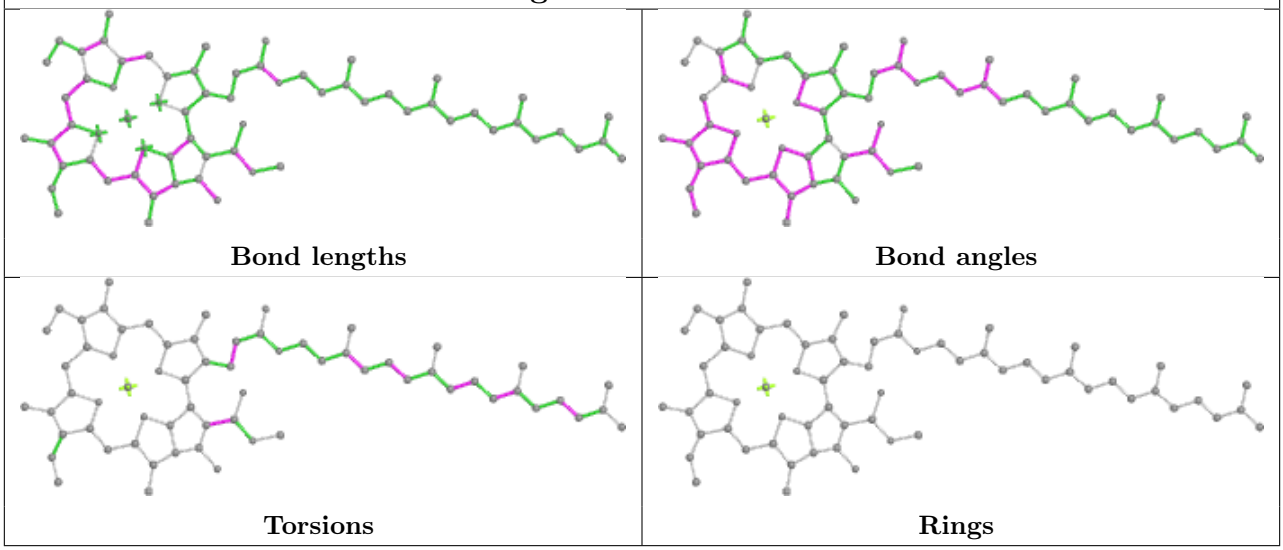
Ligand CLA C 508	
 Bond lengths	 Bond angles
 Torsions	 Rings

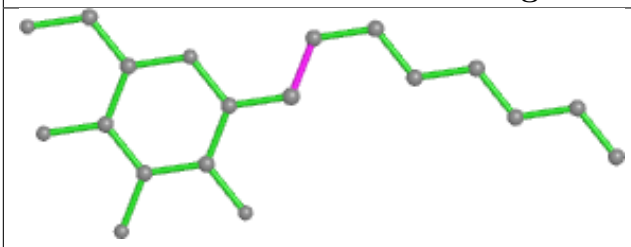
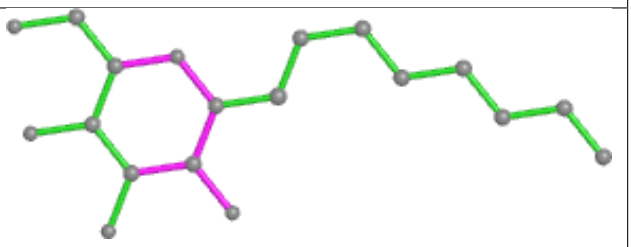
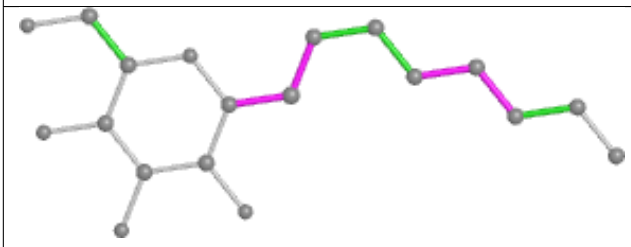
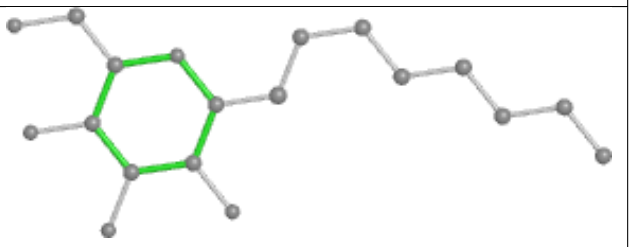
Ligand LMT M 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

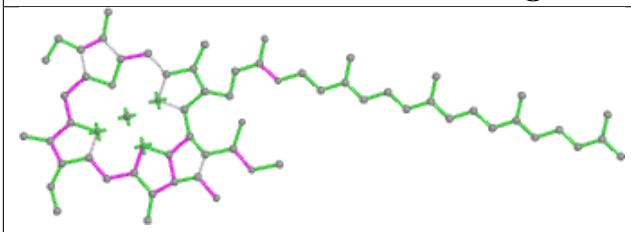
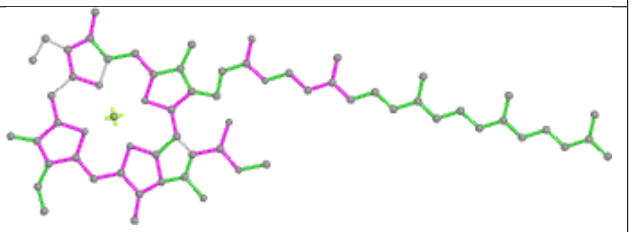
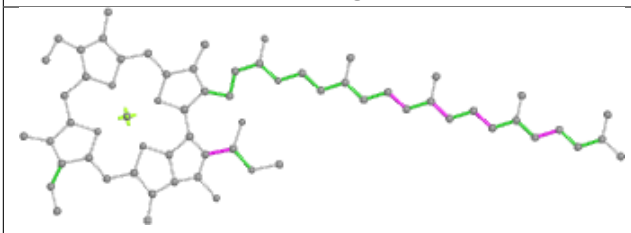
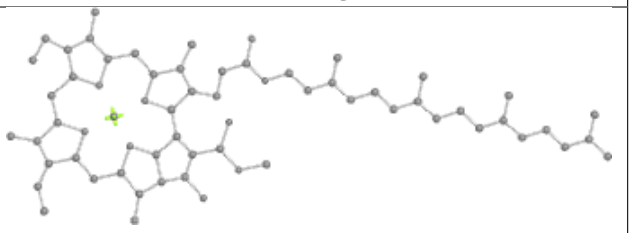
Ligand SQD a 409



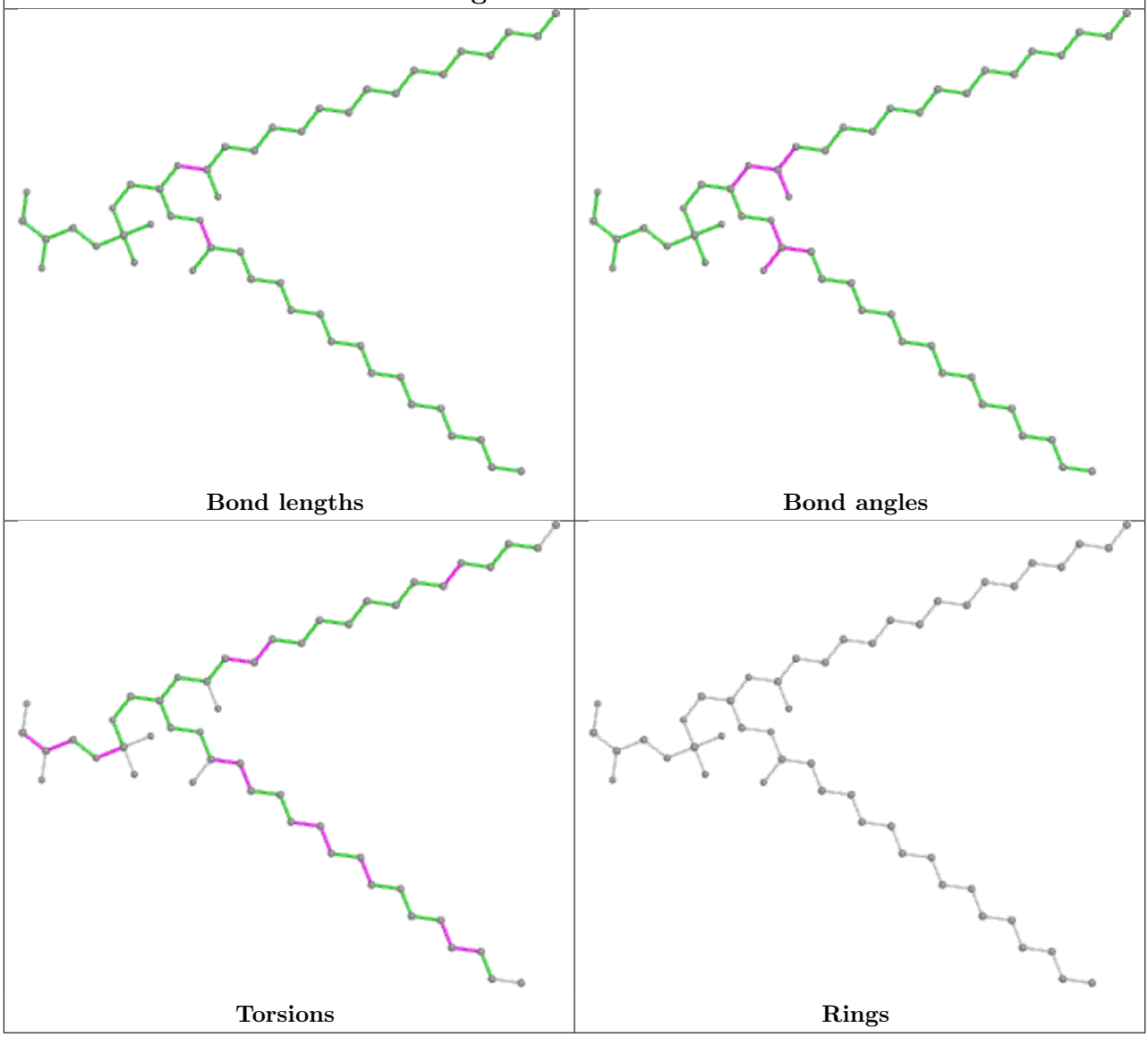
Ligand CLA c 508



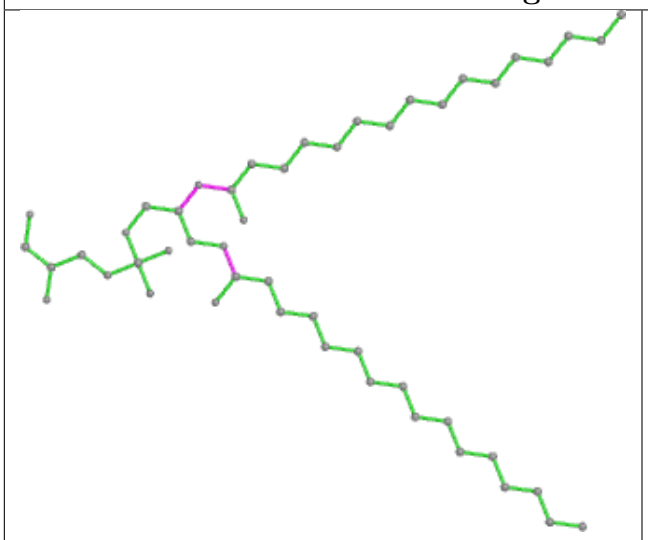
Ligand HTG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

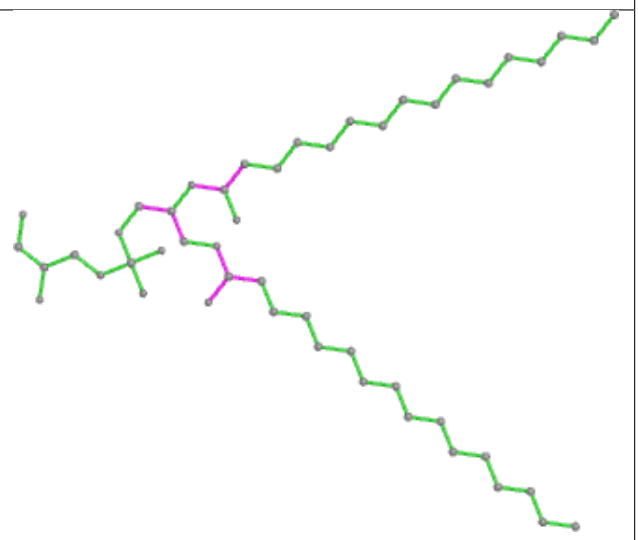
Ligand LHG d 407



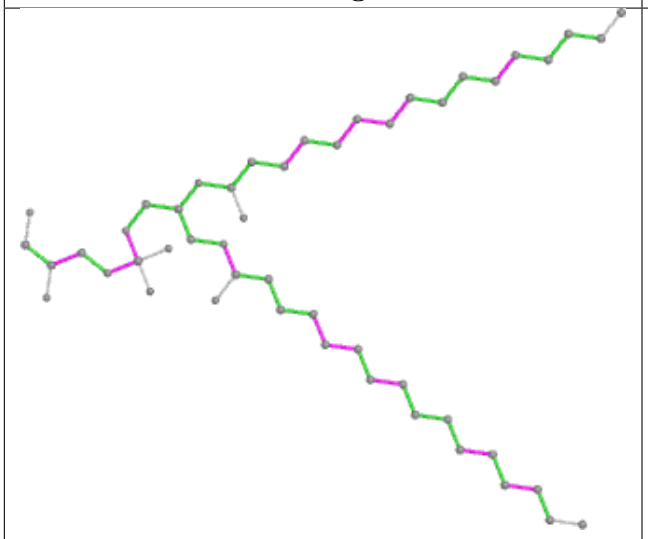
Ligand LHG D 409



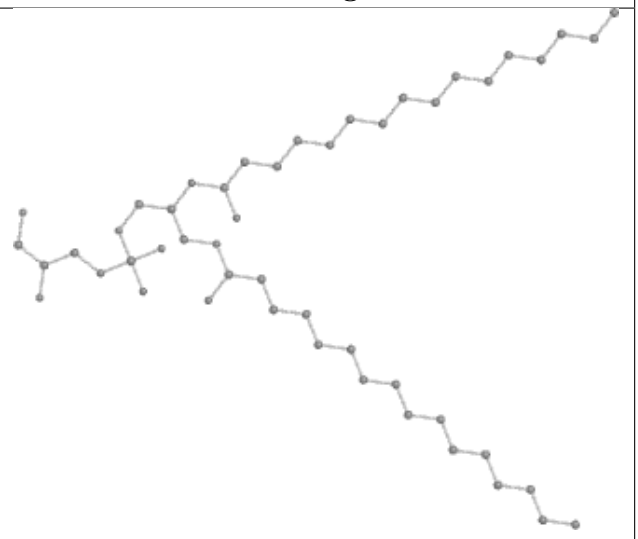
Bond lengths



Bond angles

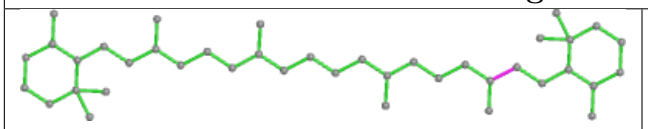


Torsions



Rings

Ligand BCR d 405



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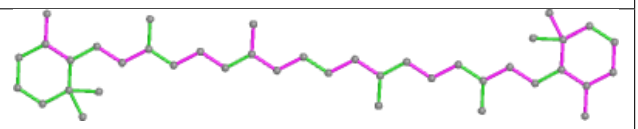
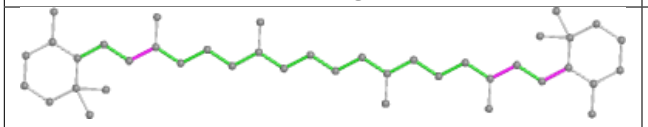
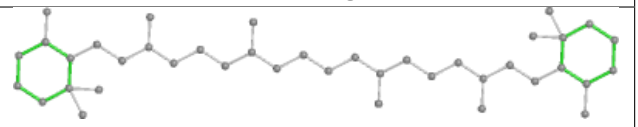


Bond angles

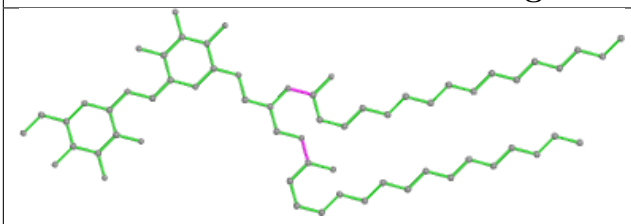


Torsions

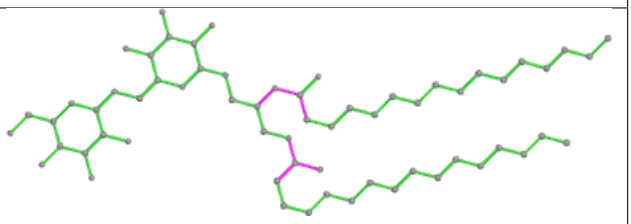


Rings

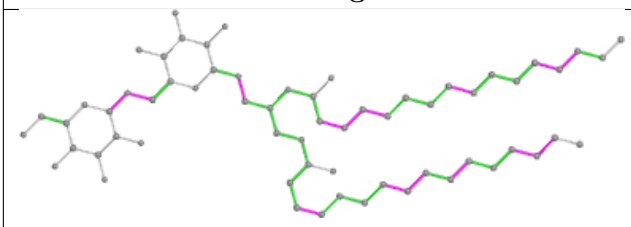
Ligand DGD c 518



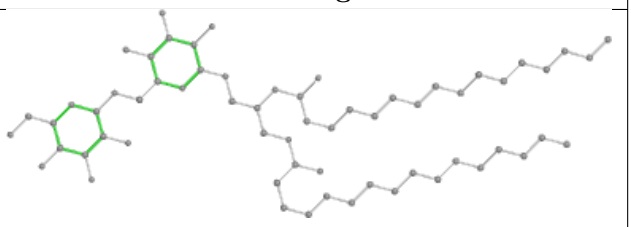
Bond lengths



Bond angles

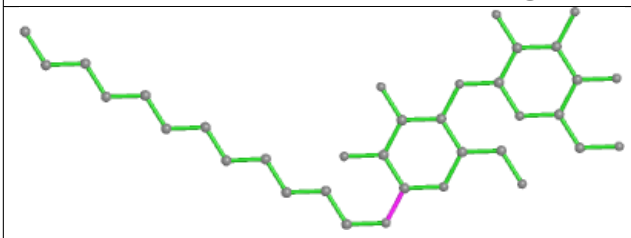


Torsions



Rings

Ligand LMT C 525



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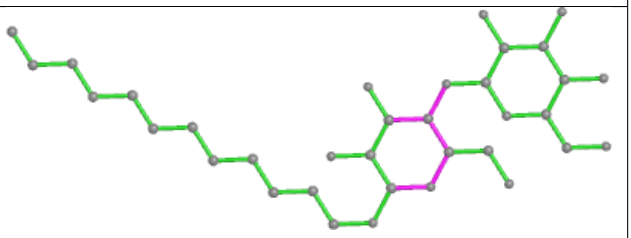

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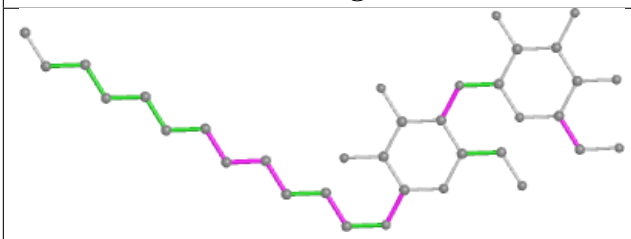

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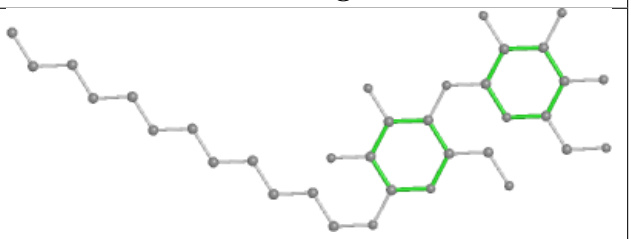
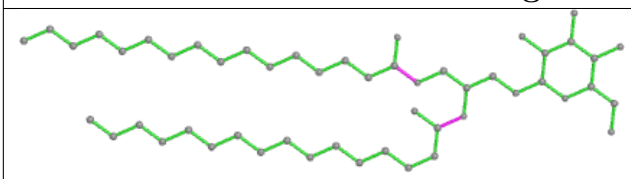


Rings

Ligand LMG d 412



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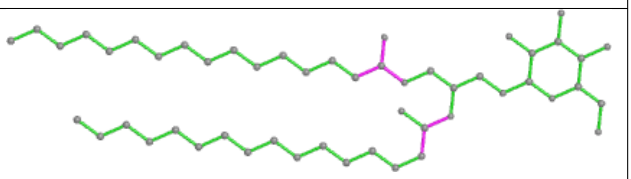
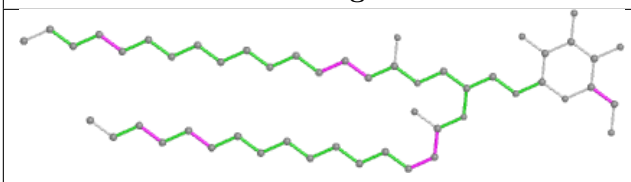


Bond angles



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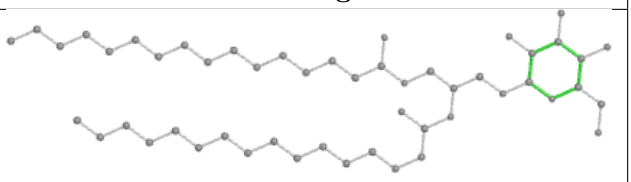
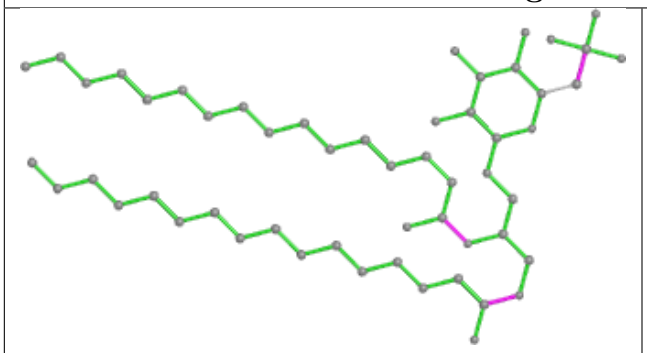


Rings

Ligand SQD B 620



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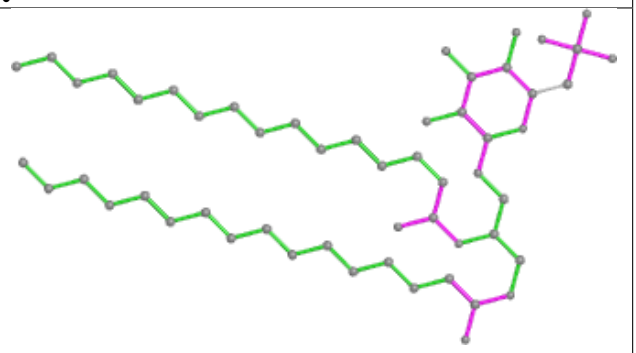
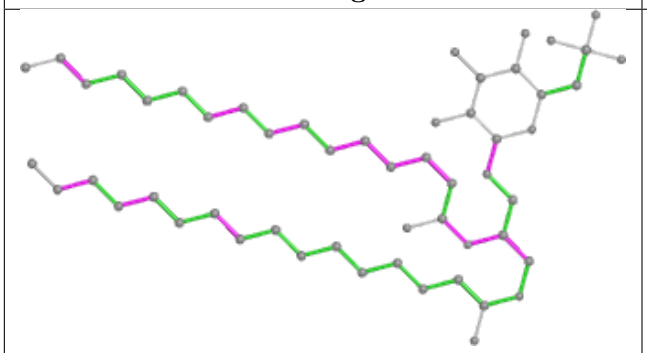


Bond angles



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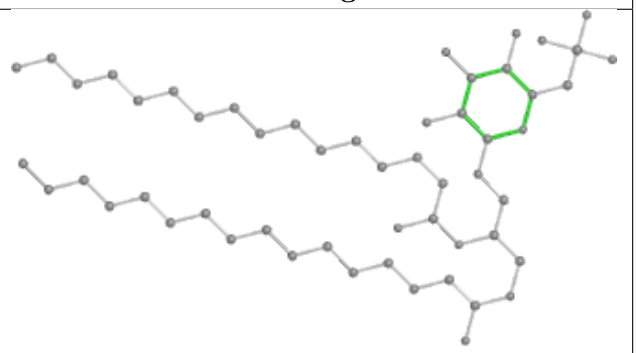
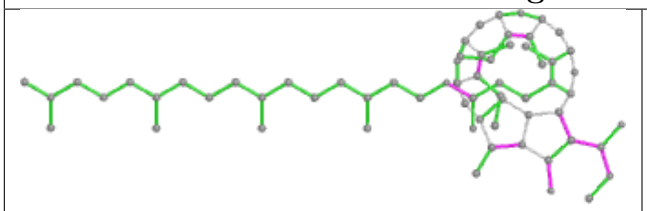


Rings

Ligand PHO a 406



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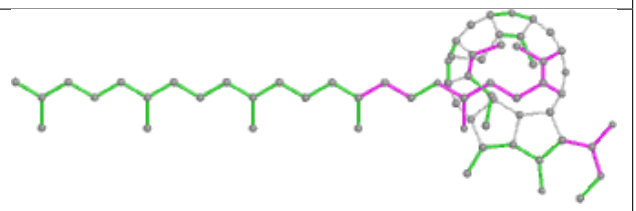
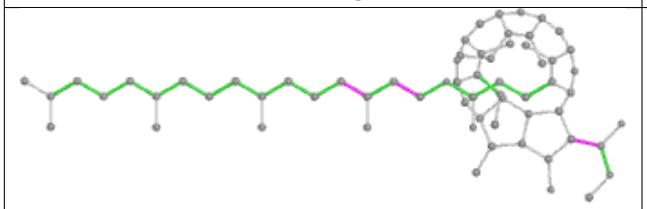


Bond angles



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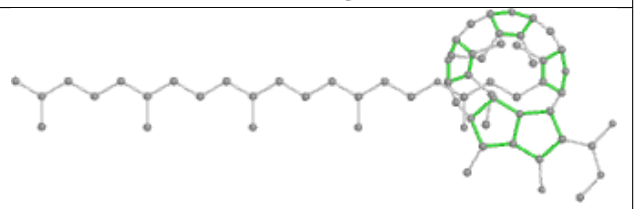
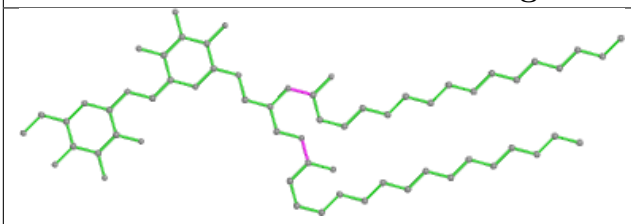


Rings

Ligand DGD C 518



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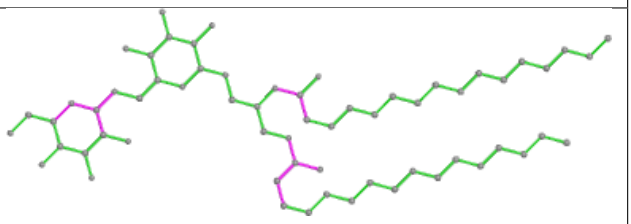
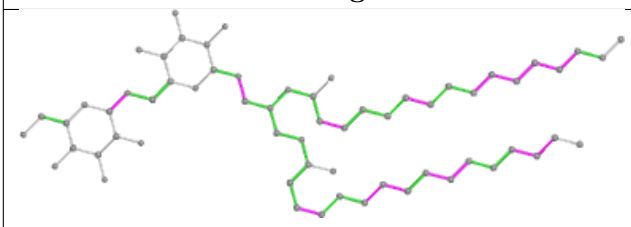


Bond angles



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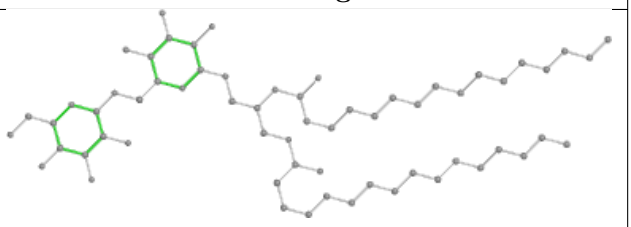
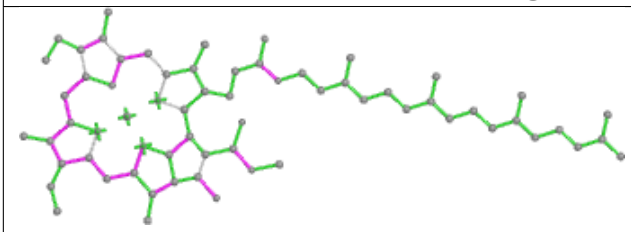


Rings

Ligand CLA B 603



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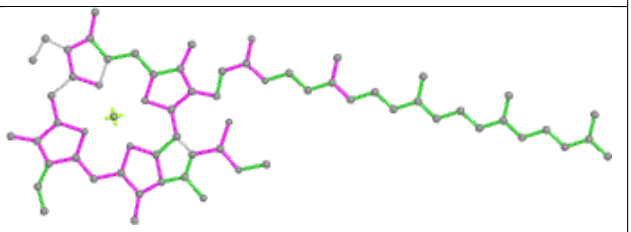
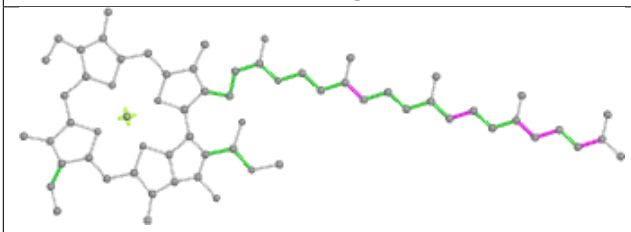


Bond angles



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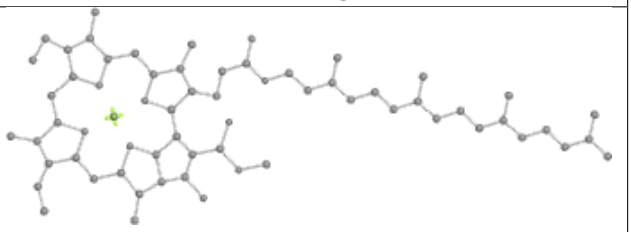
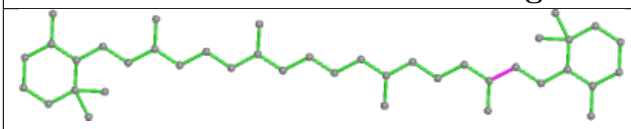


Rings

Ligand BCR b 618



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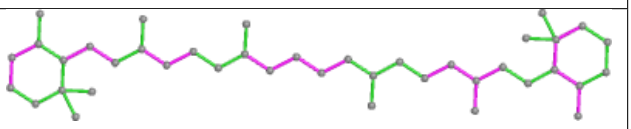
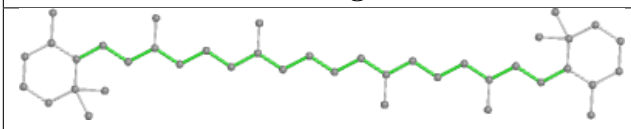
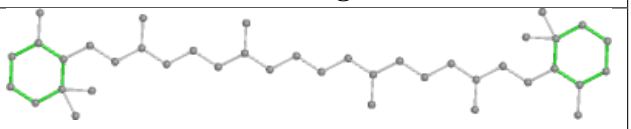


Bond angles

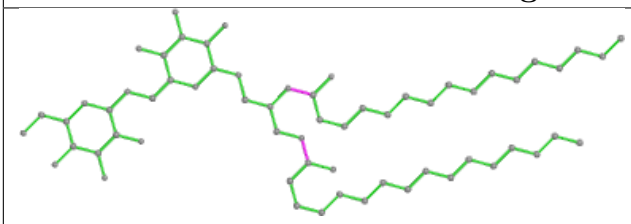


Torsions



Rings

Ligand DGD C 519



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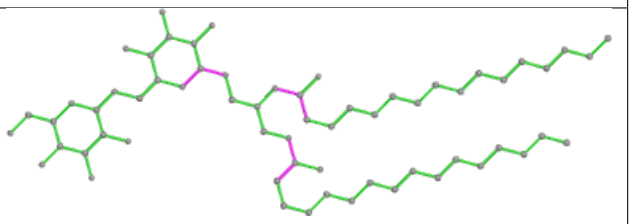
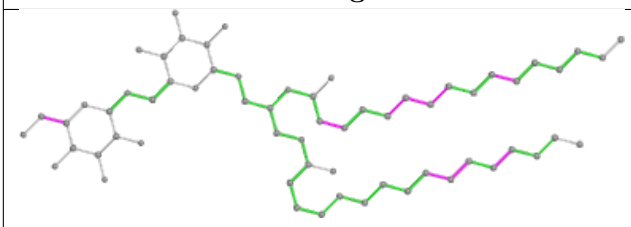


Bond angles



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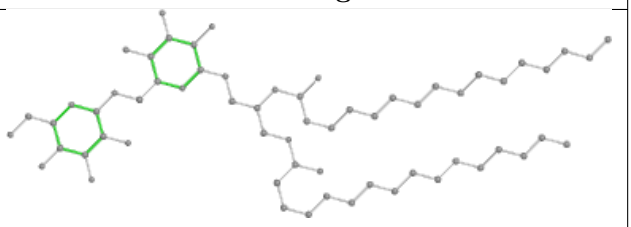

Rings

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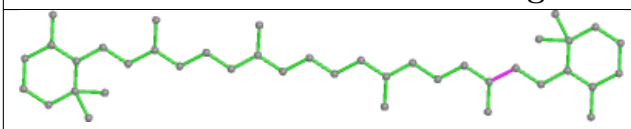

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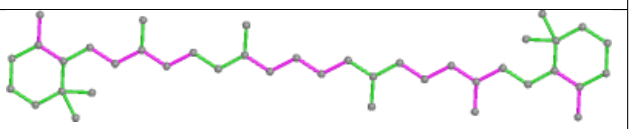

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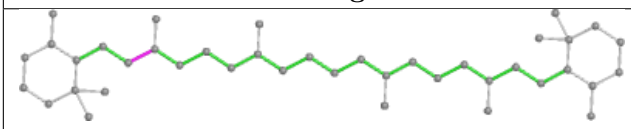

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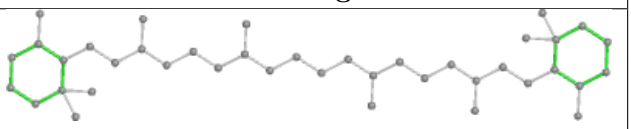
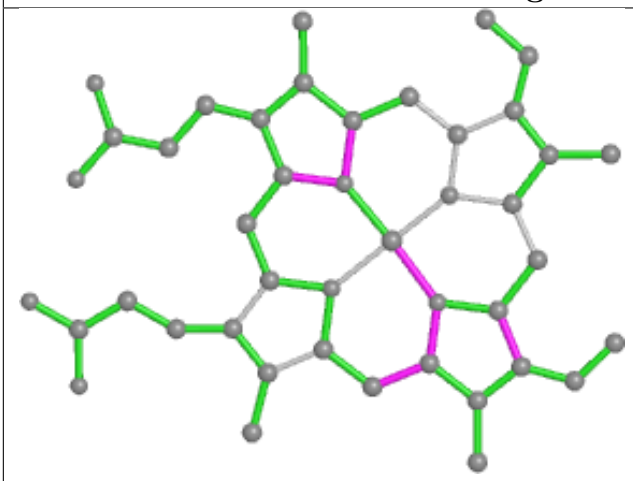


Rings

Ligand HEM f 101



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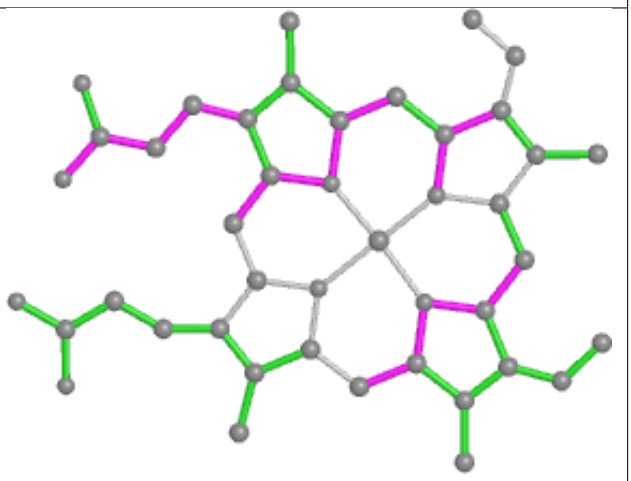
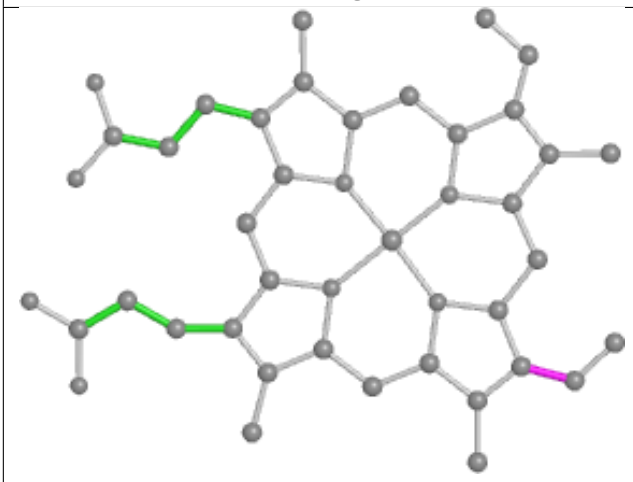


Bond angles



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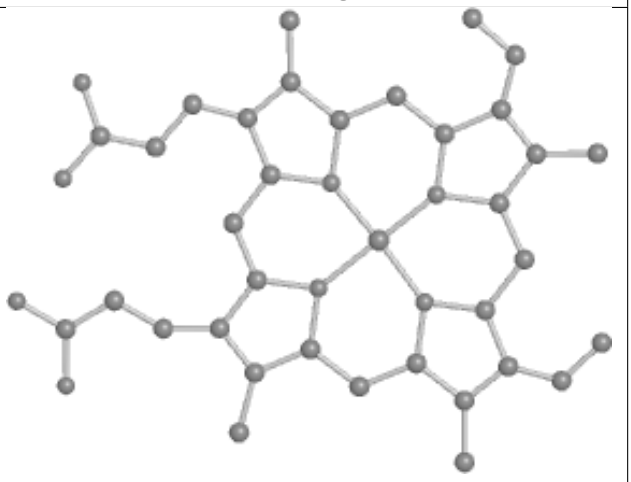
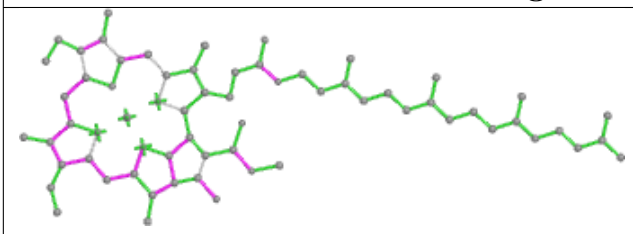


Rings

Ligand CLA b 608



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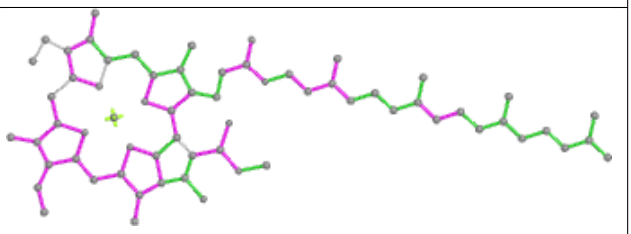
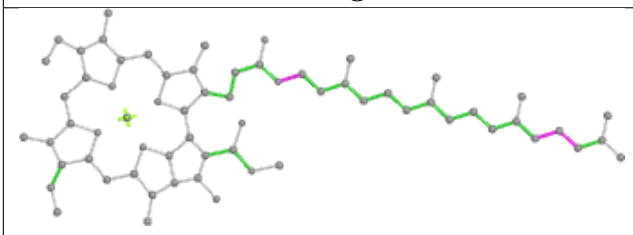


Bond angles



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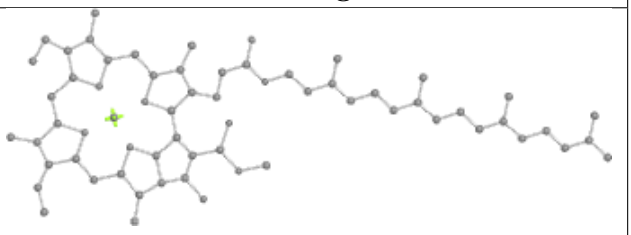
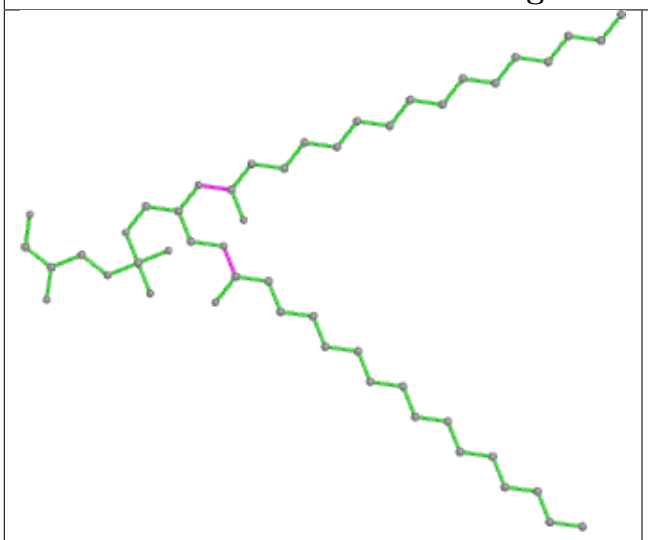


Rings

Ligand LHG d 409



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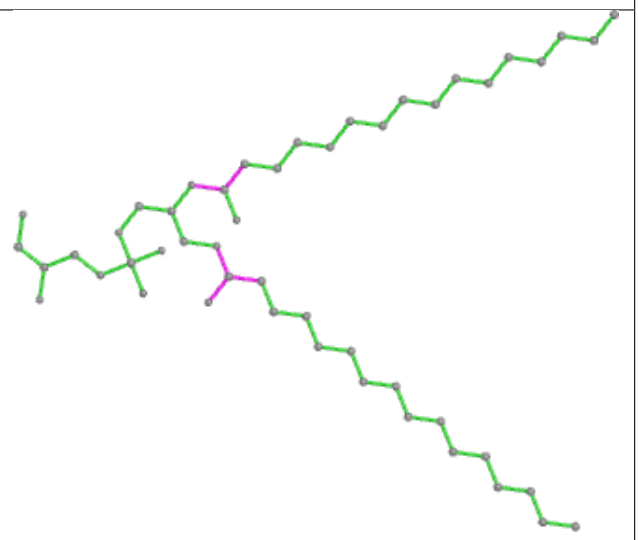
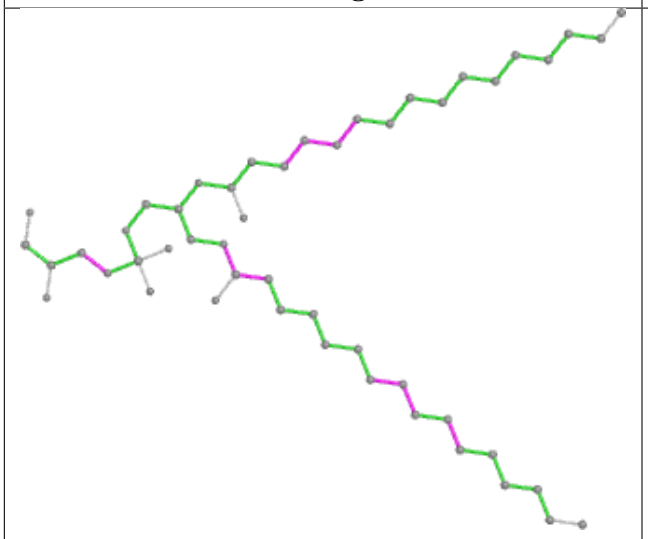


Bond angles



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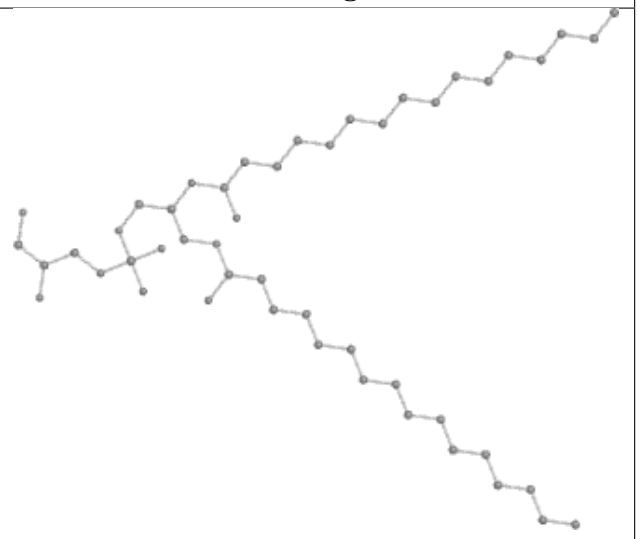
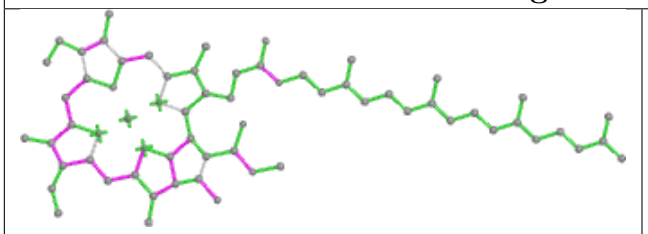


Rings

Ligand CLA c 513



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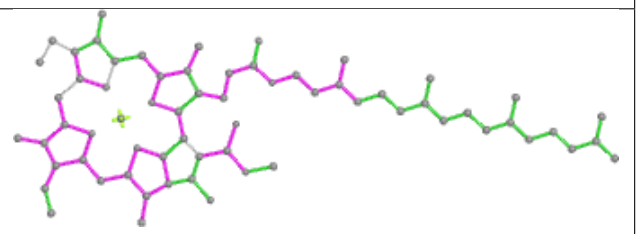
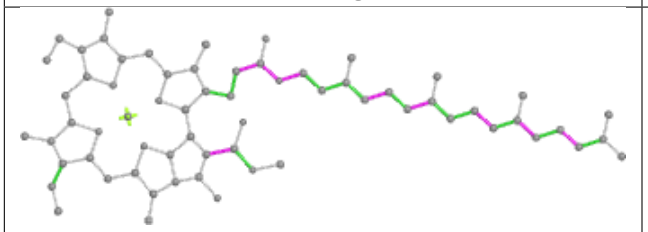
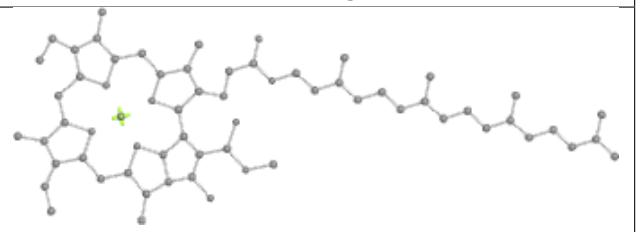


Bond angles

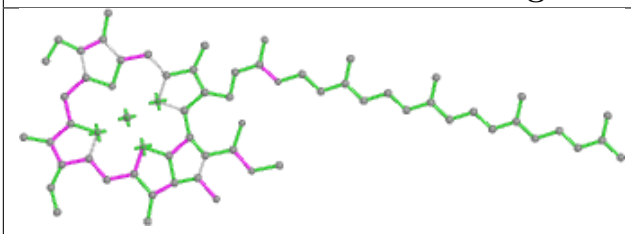


Torsions



Rings

Ligand CLA b 613



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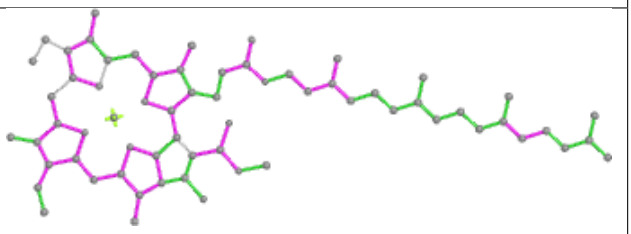

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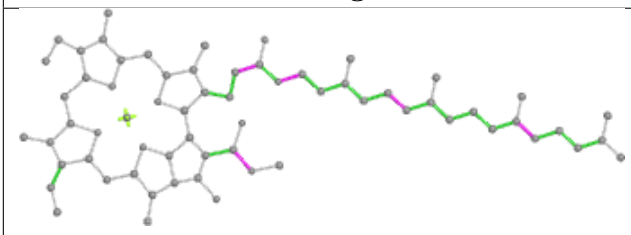

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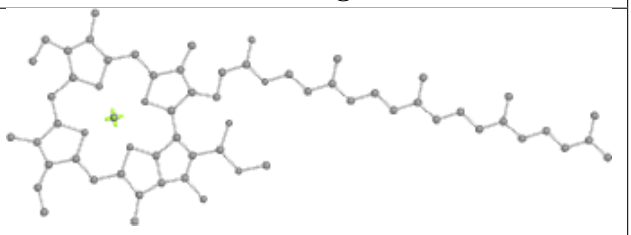
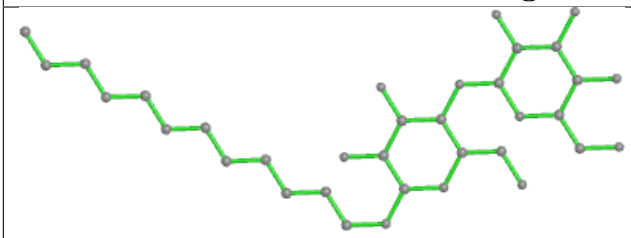


Rings

Ligand LMT D 404



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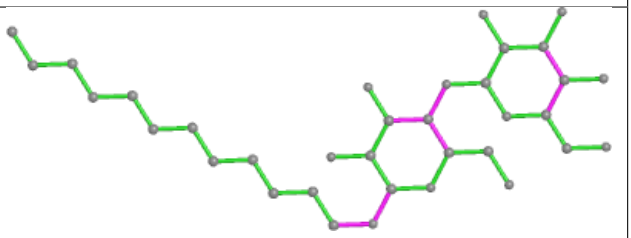

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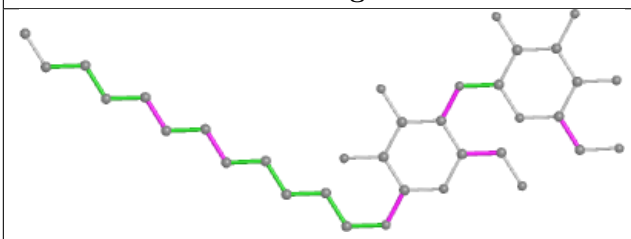

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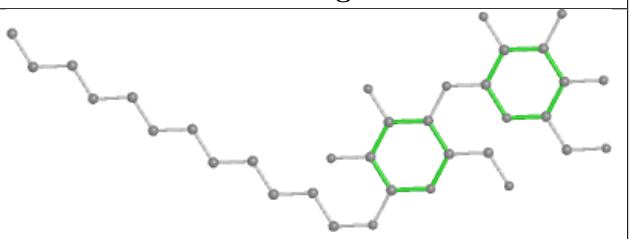
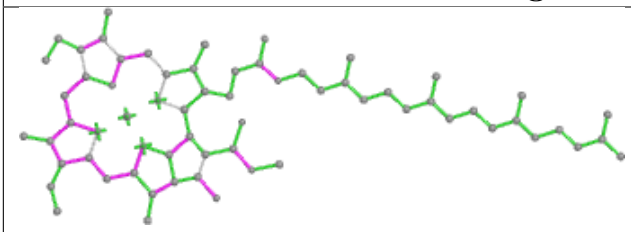


Rings

Ligand CLA b 612



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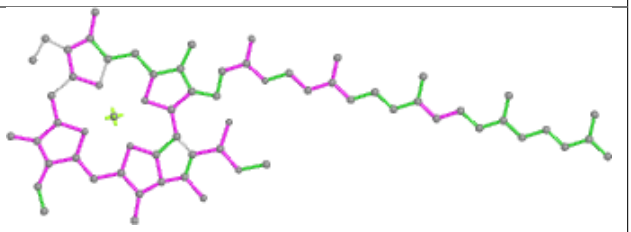
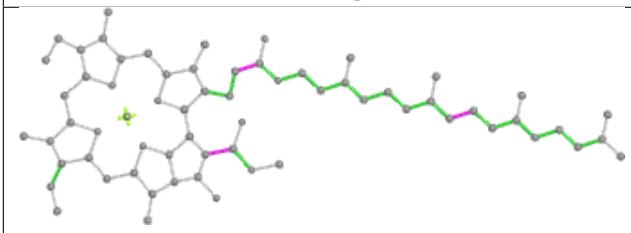


Bond angles



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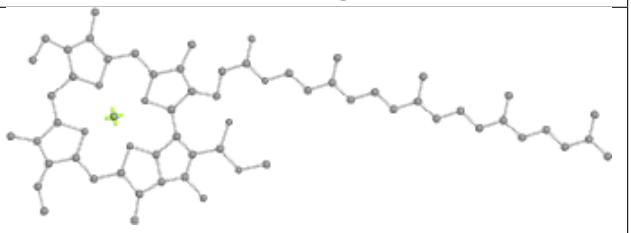
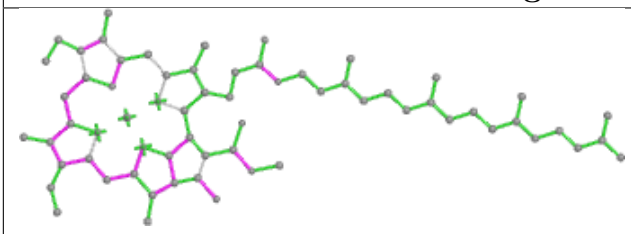


Rings

Ligand CLA A 406



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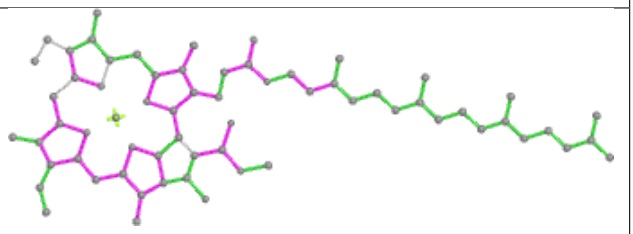

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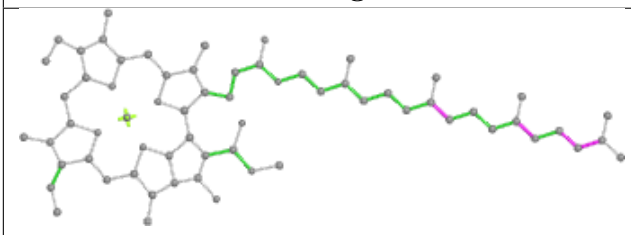

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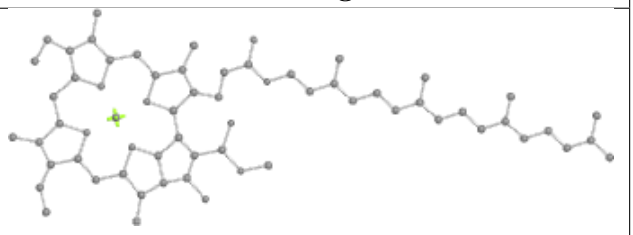
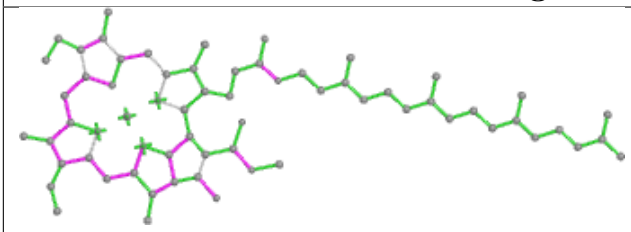


Rings

Ligand CLA c 505



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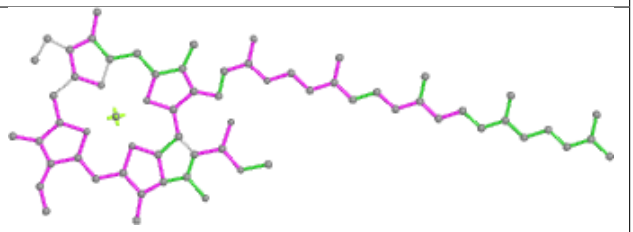
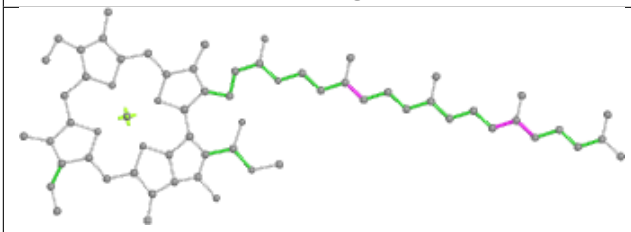


Bond angles



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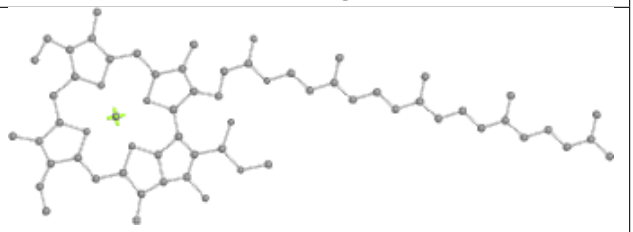
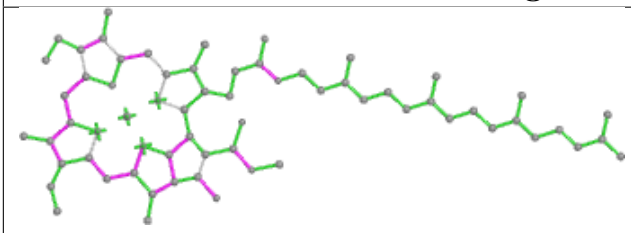


Rings

Ligand CLA B 611



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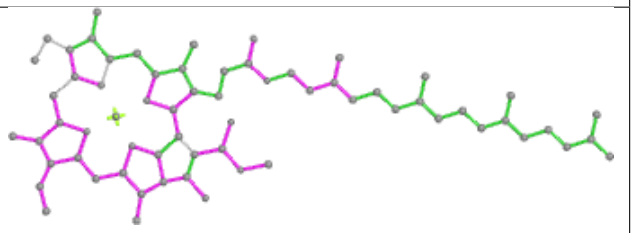

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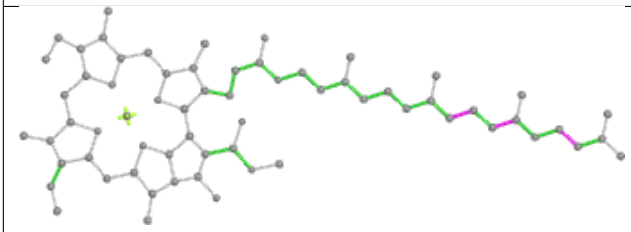

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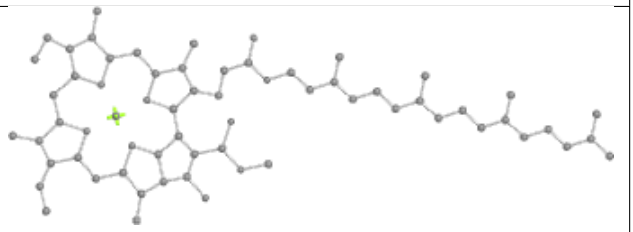

Rings

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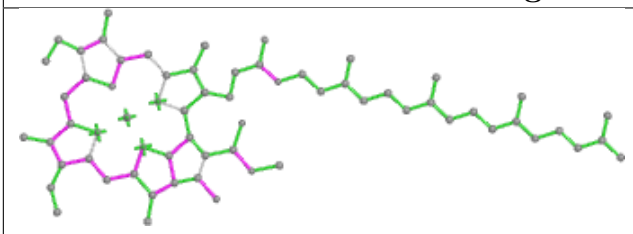

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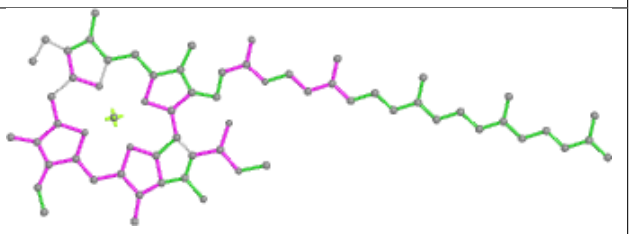

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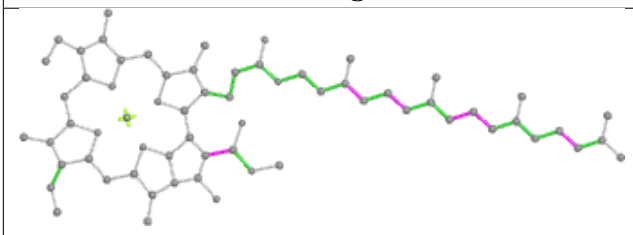

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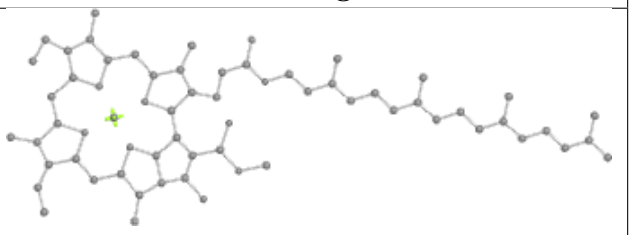
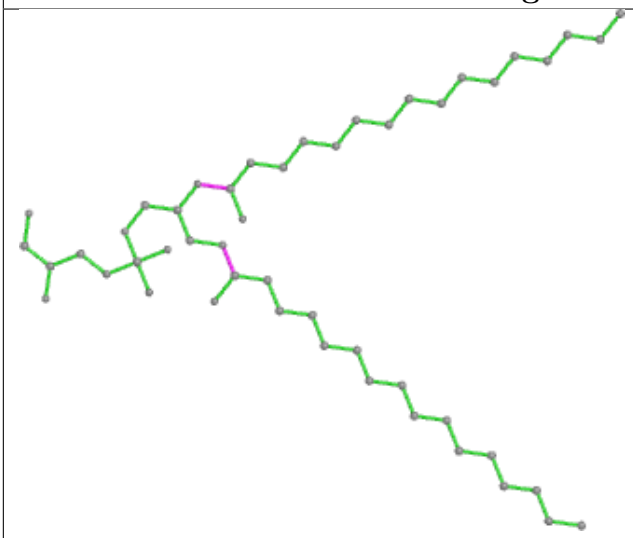


Rings

Ligand LHG D 410



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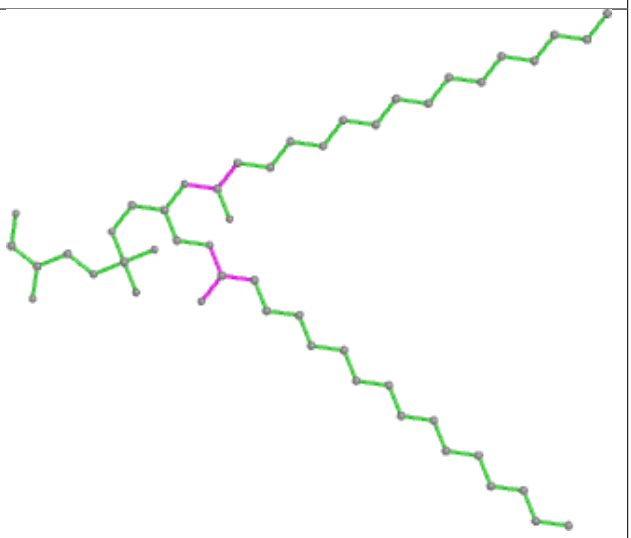
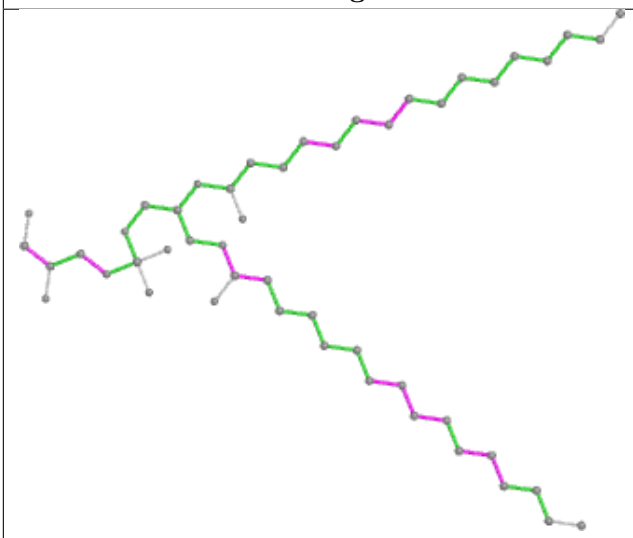


Bond angles



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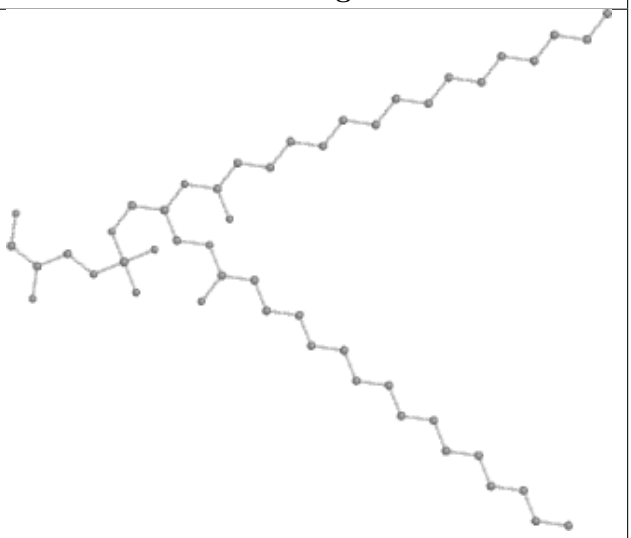
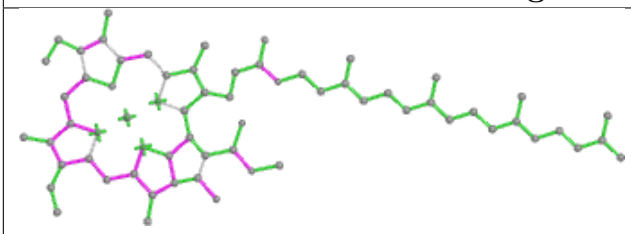


Rings

Ligand CLA b 609



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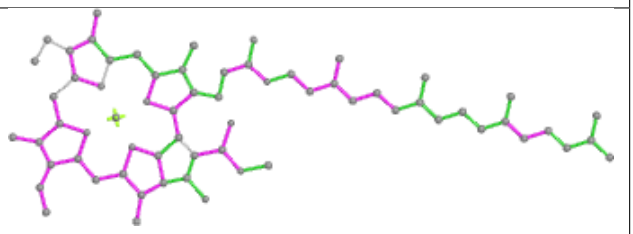

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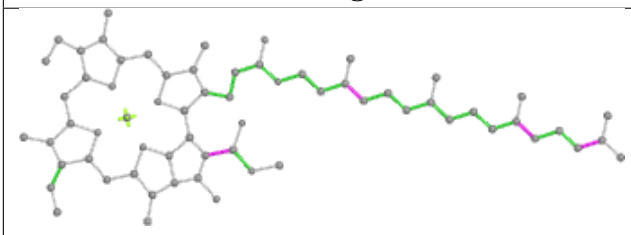

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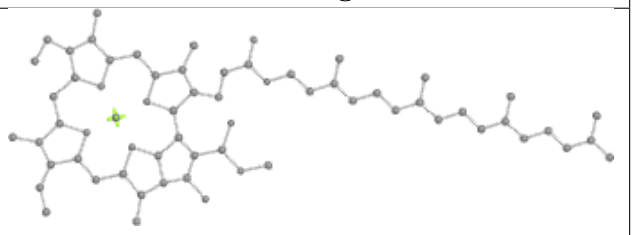
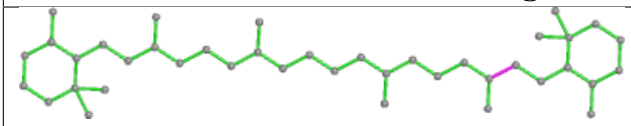


Rings

Ligand BCR H 101



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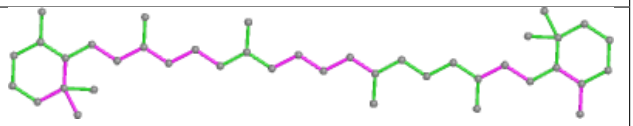
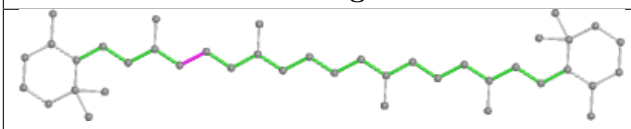


Bond angles



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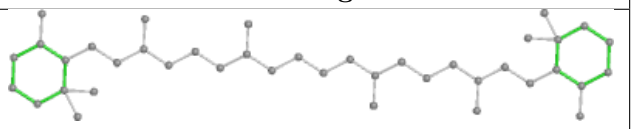
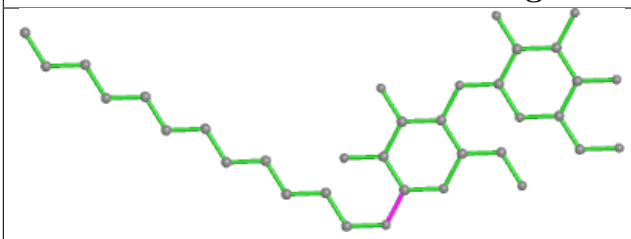


Rings

Ligand LMT a 418



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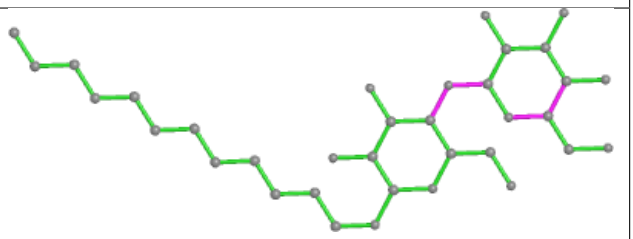
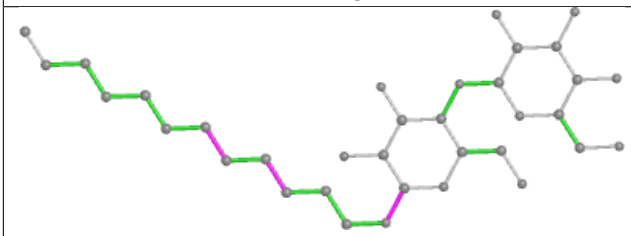


Bond angles



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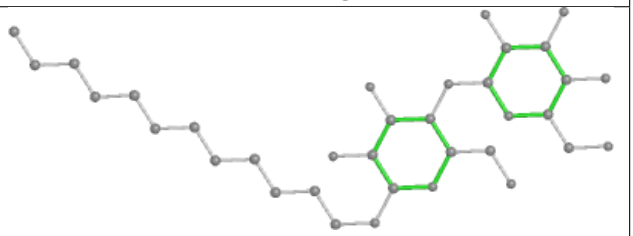

Rings

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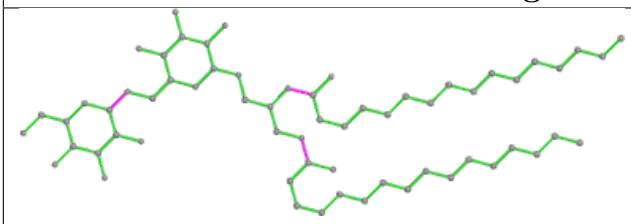

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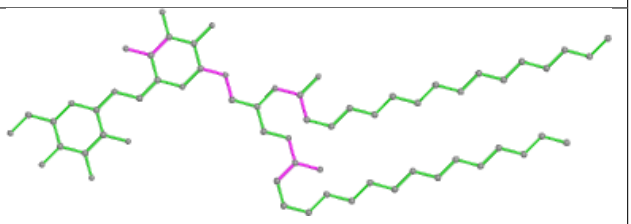
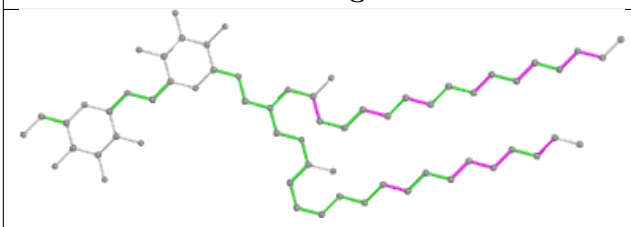


Bond angles



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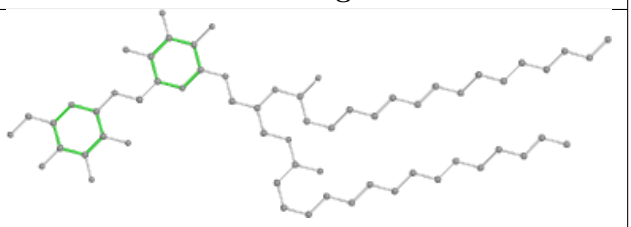
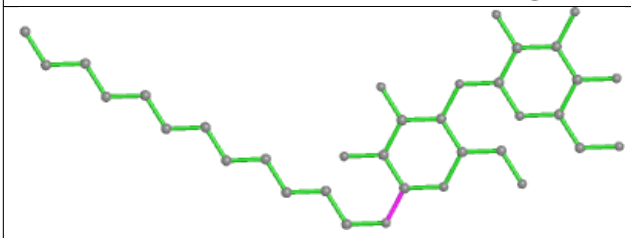


Rings

Ligand LMT e 101



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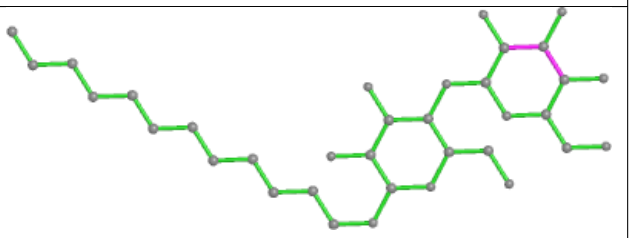
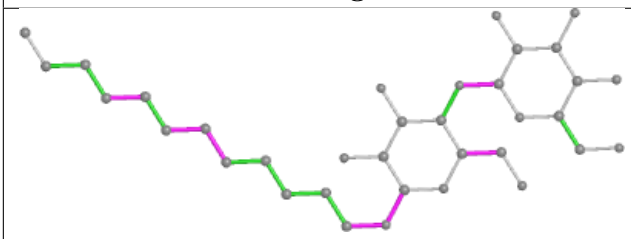
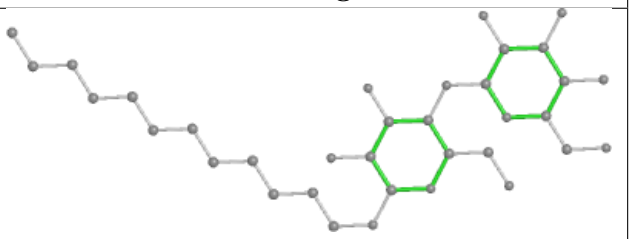


Bond angles

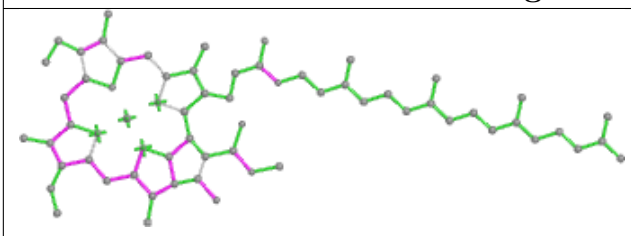


Torsions

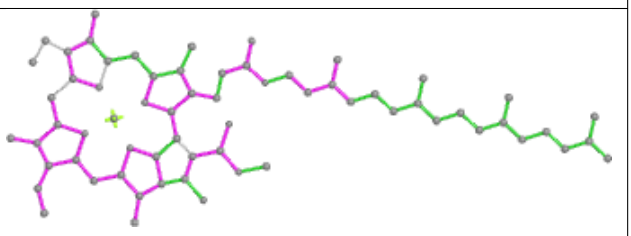


Rings

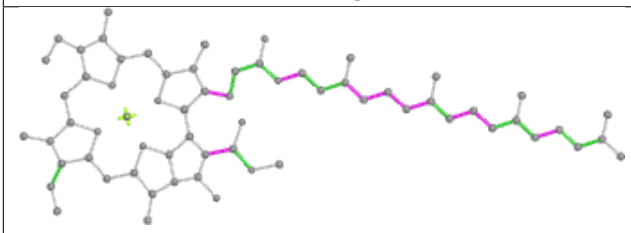
Ligand CLA C 507



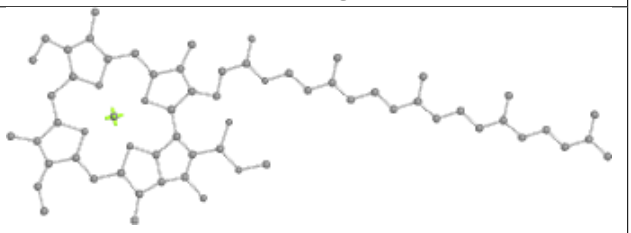
Bond lengths



Bond angles

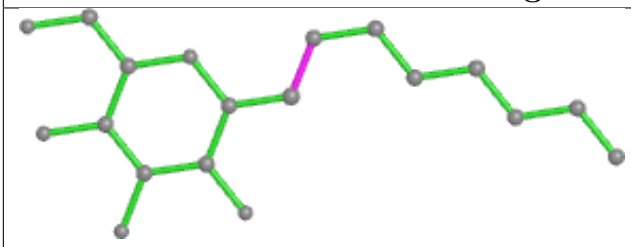


Torsions



Rings

Ligand HTG b 621



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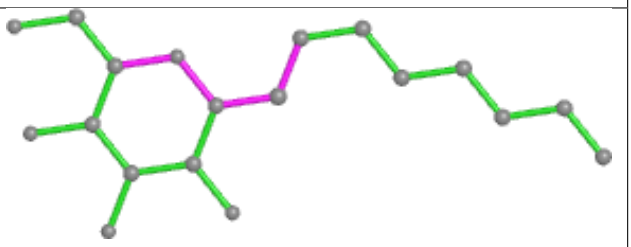
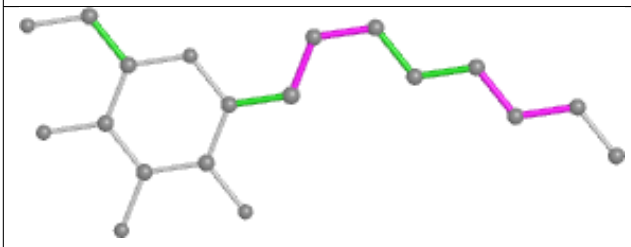
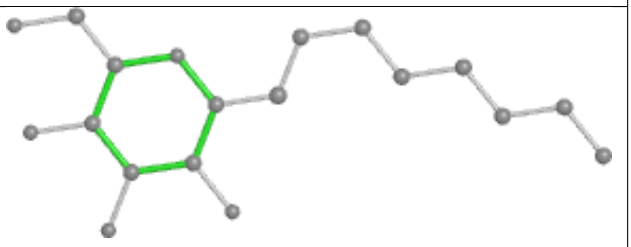


Bond angles

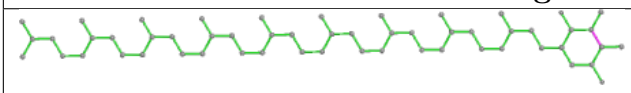


Torsions



Rings

Ligand PL9 a 414



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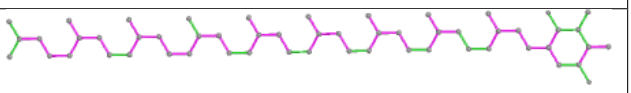
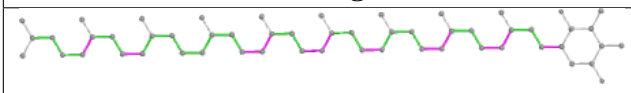


Bond angles



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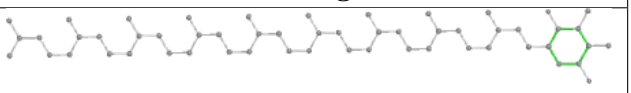
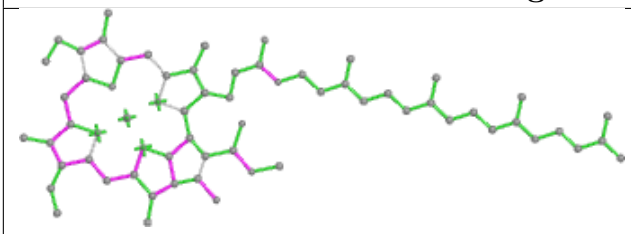


Rings

Ligand CLA d 402



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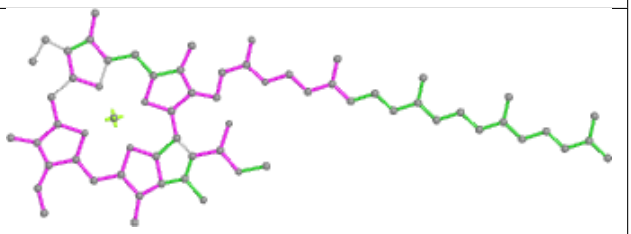
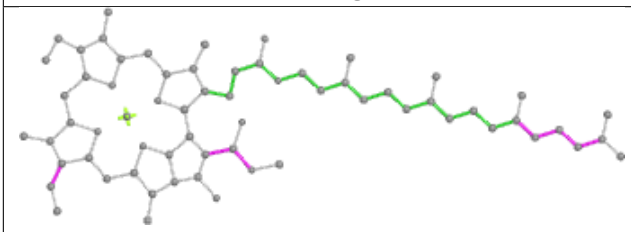


Bond angles



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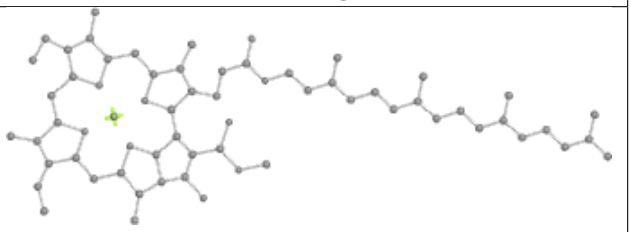
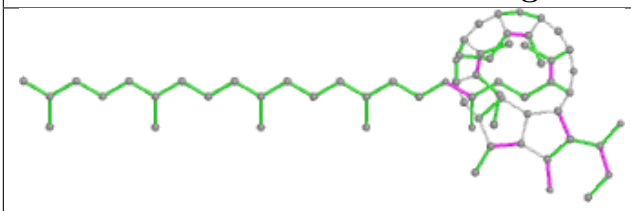


Rings

Ligand PHO D 402



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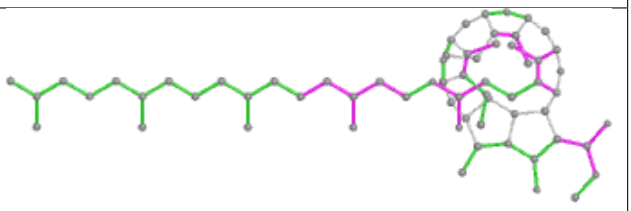

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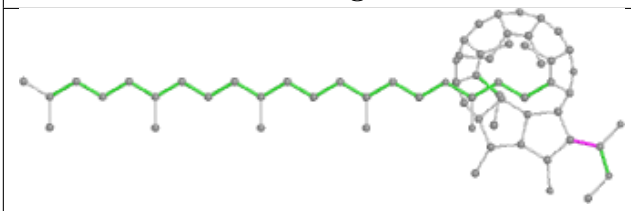

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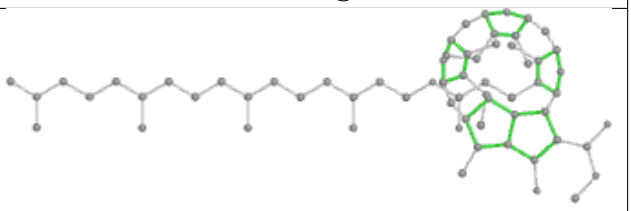
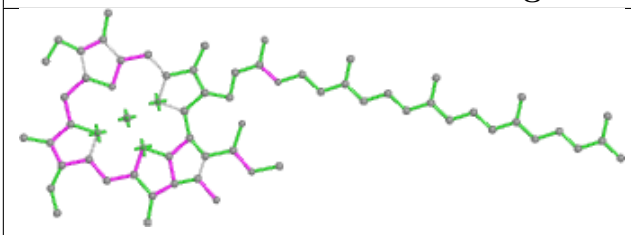


Rings

Ligand CLA A 404



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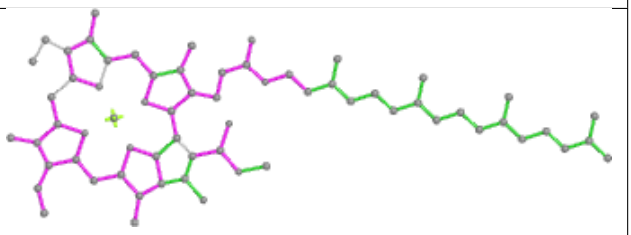
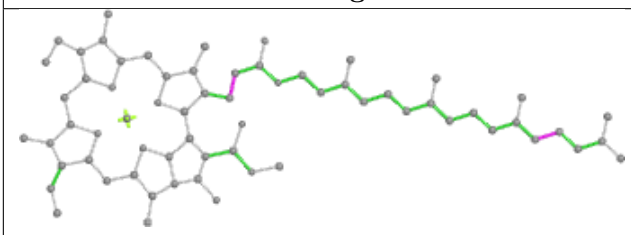


Bond angles



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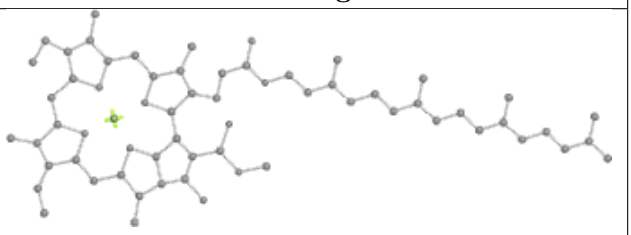
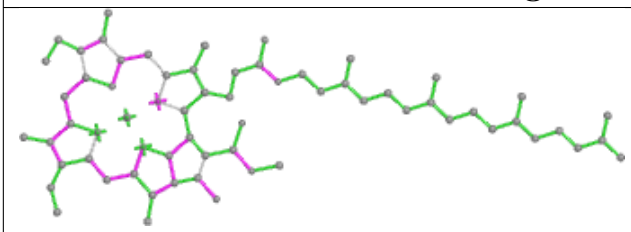


Rings

Ligand CLA B 606



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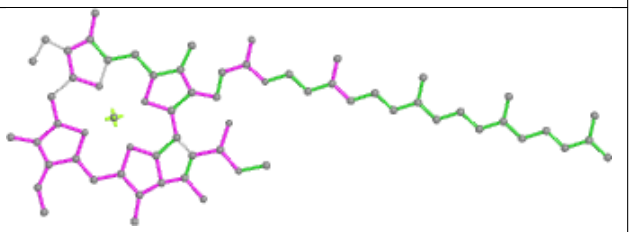
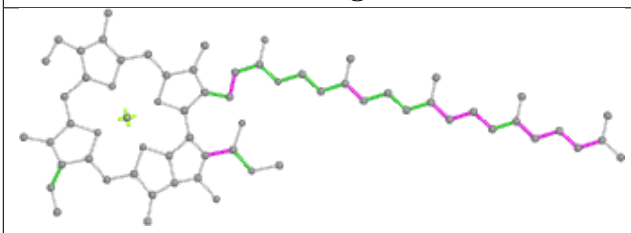


Bond angles



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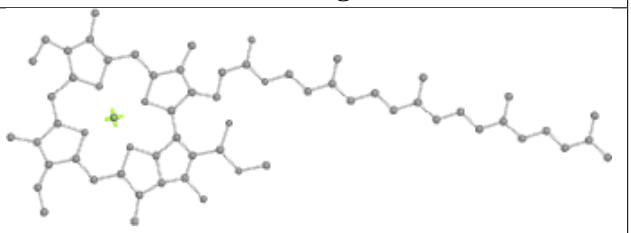
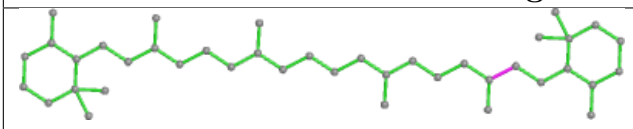


Rings

Ligand BCR k 101



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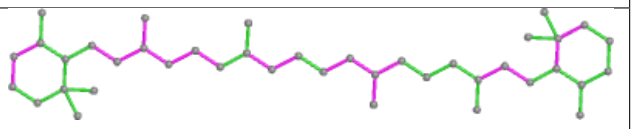
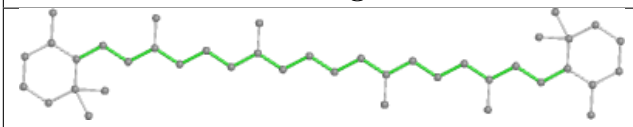


Bond angles



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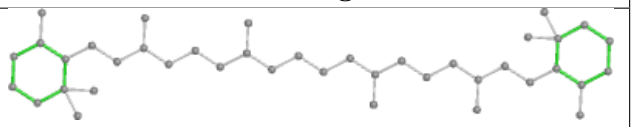
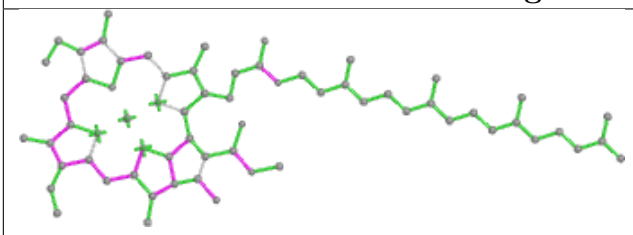


Rings

Ligand CLA C 504



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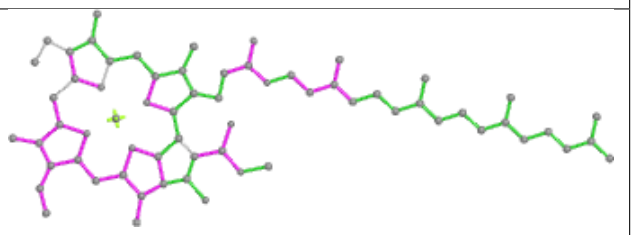
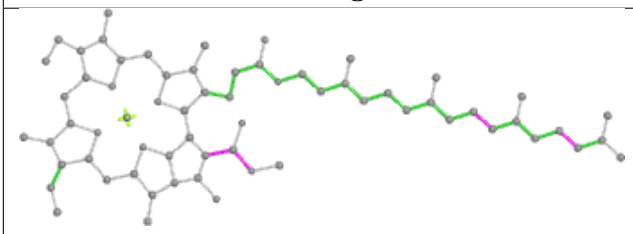


Bond angles



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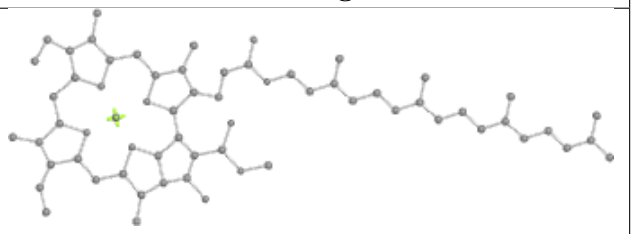
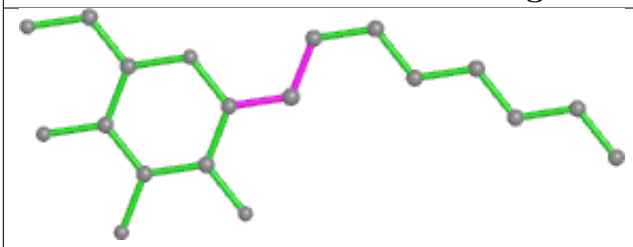


Rings

Ligand HTG c 522



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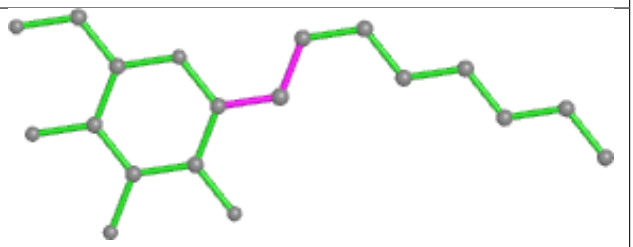

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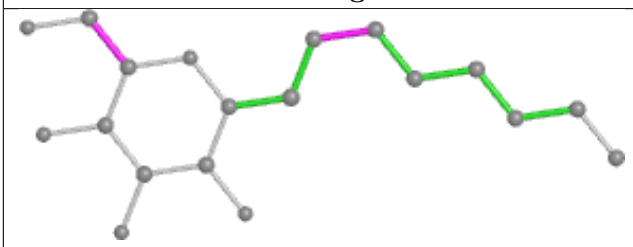

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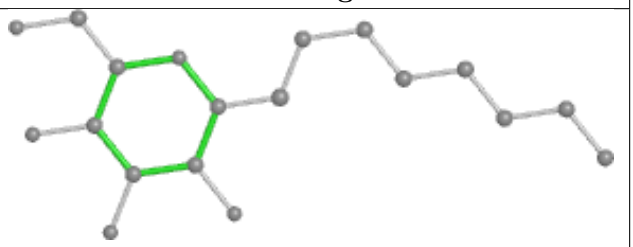

Rings

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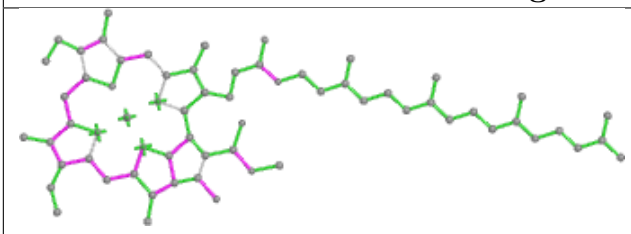

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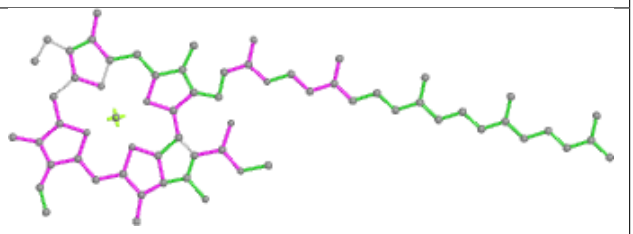
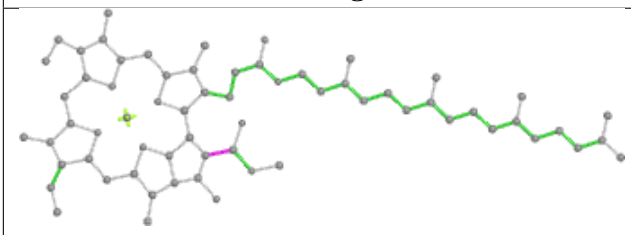


Bond angles



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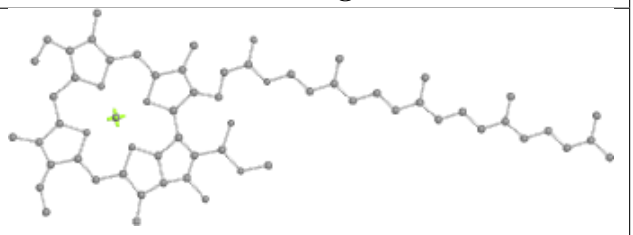
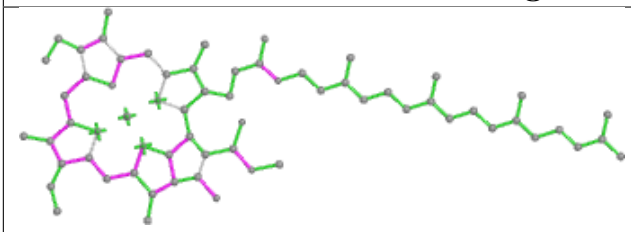


Rings

Ligand CLA B 607



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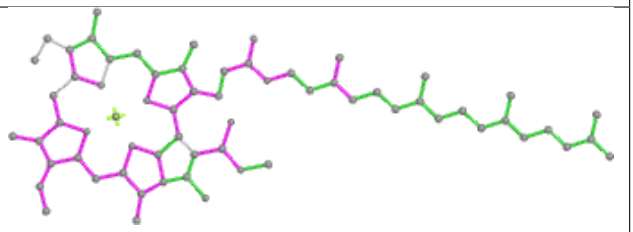
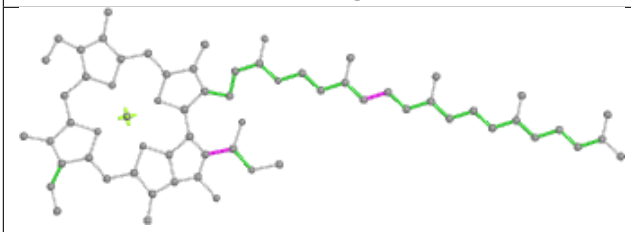


Bond angles



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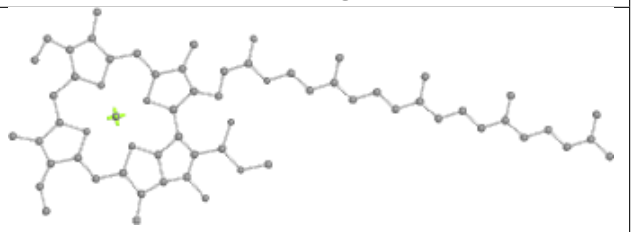
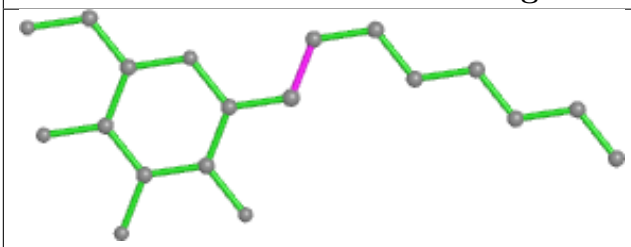


Rings

Ligand HTG C 522



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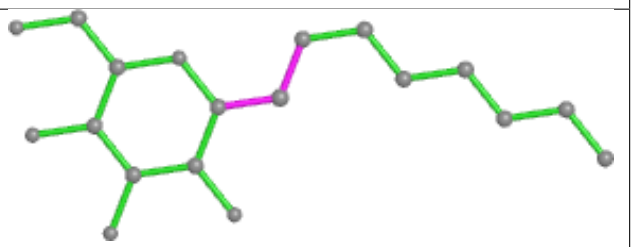
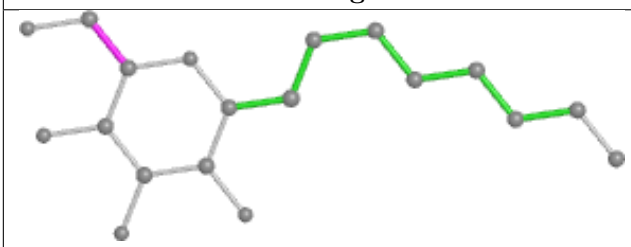


Bond angles



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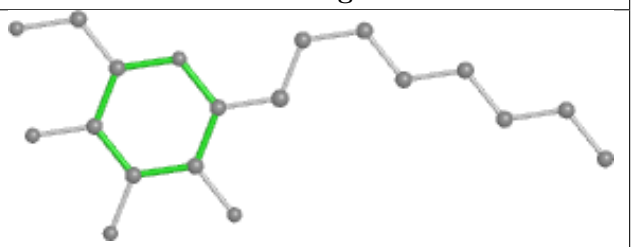
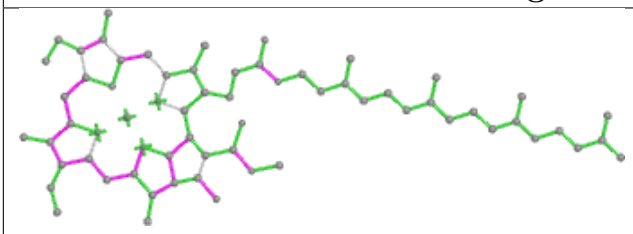
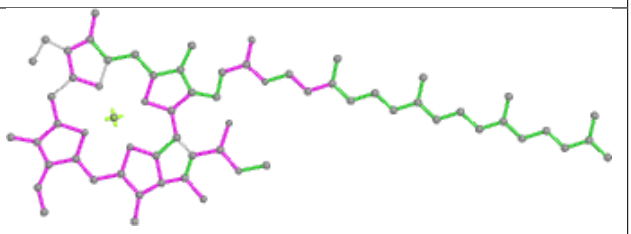


Rings

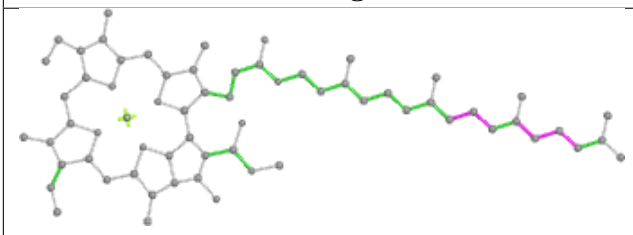
Ligand CLA b 611



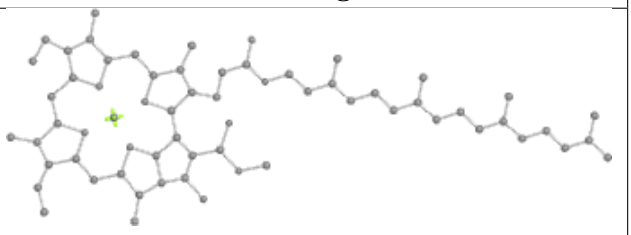
Bond lengths



Bond angles

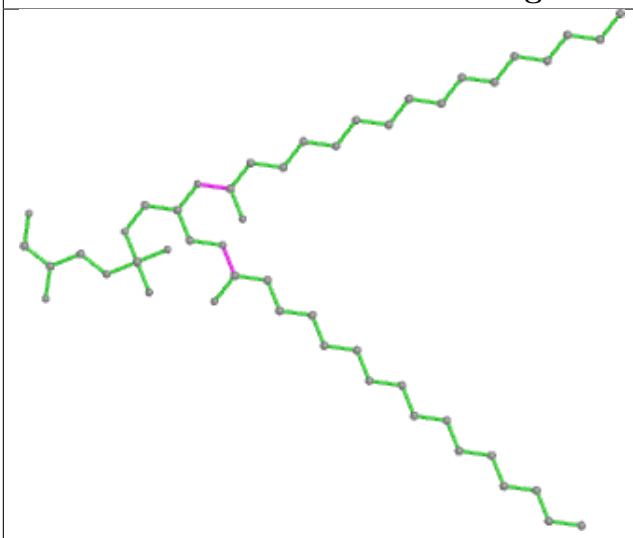


Torsions



Rings

Ligand LHG L 101



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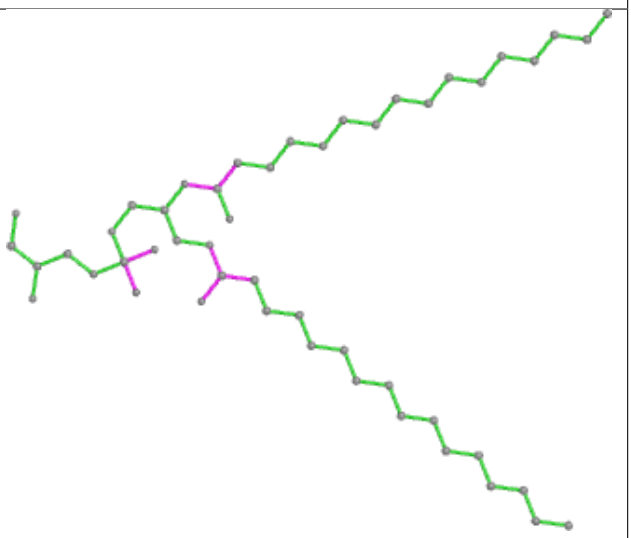

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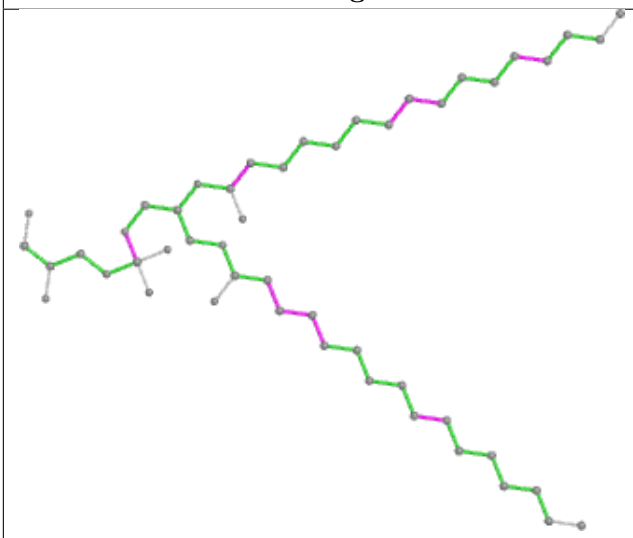

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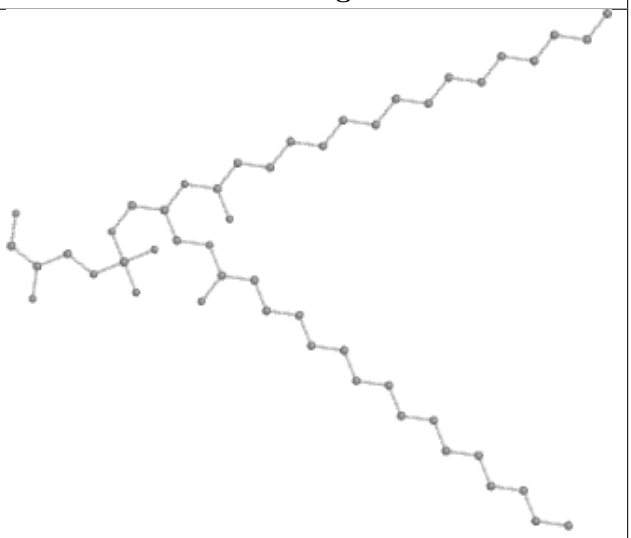
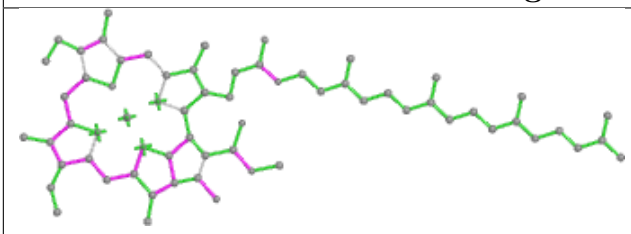


Rings

Ligand CLA B 604



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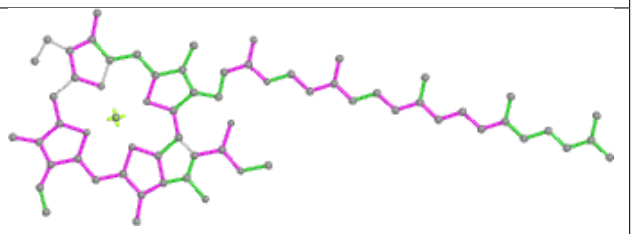
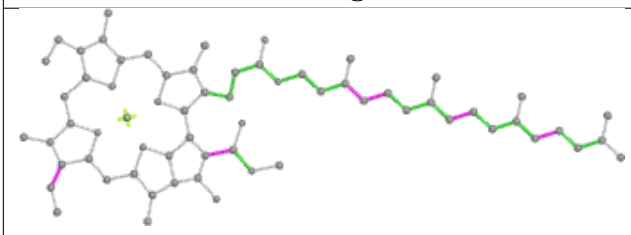


Bond angles



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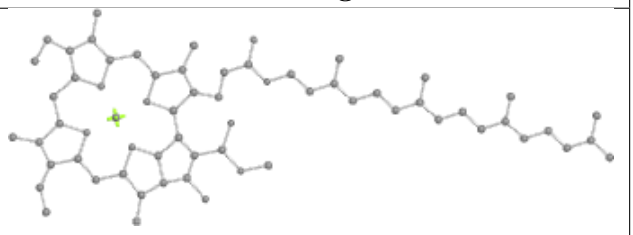
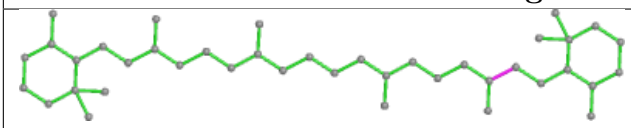


Rings

Ligand BCR h 102



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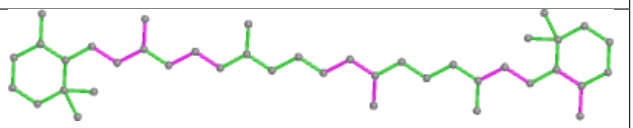

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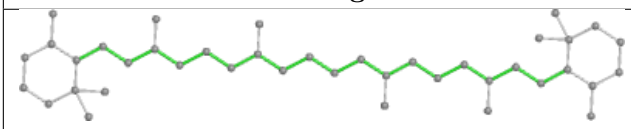

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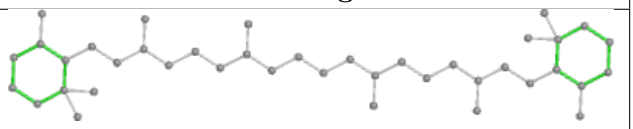
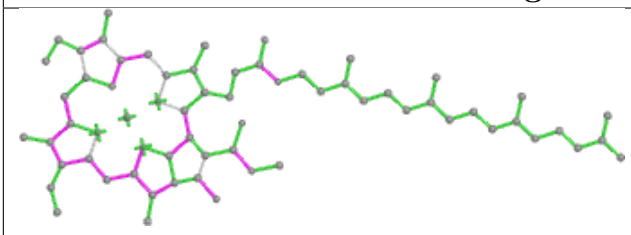


Rings

Ligand CLA B 613



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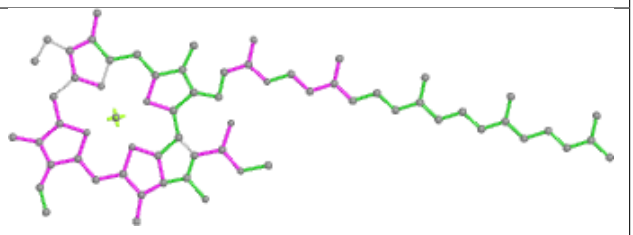

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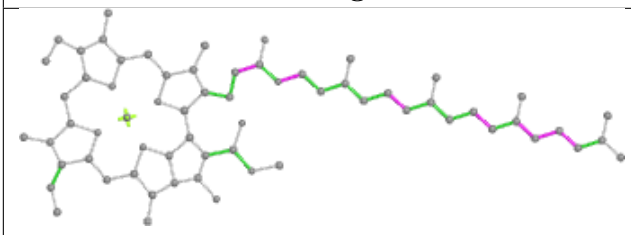

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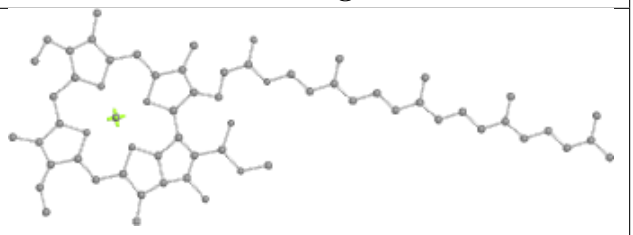
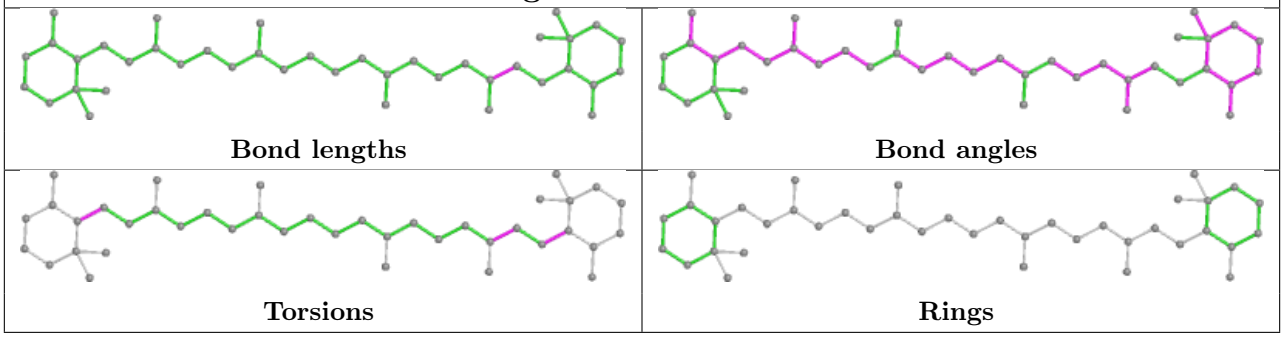
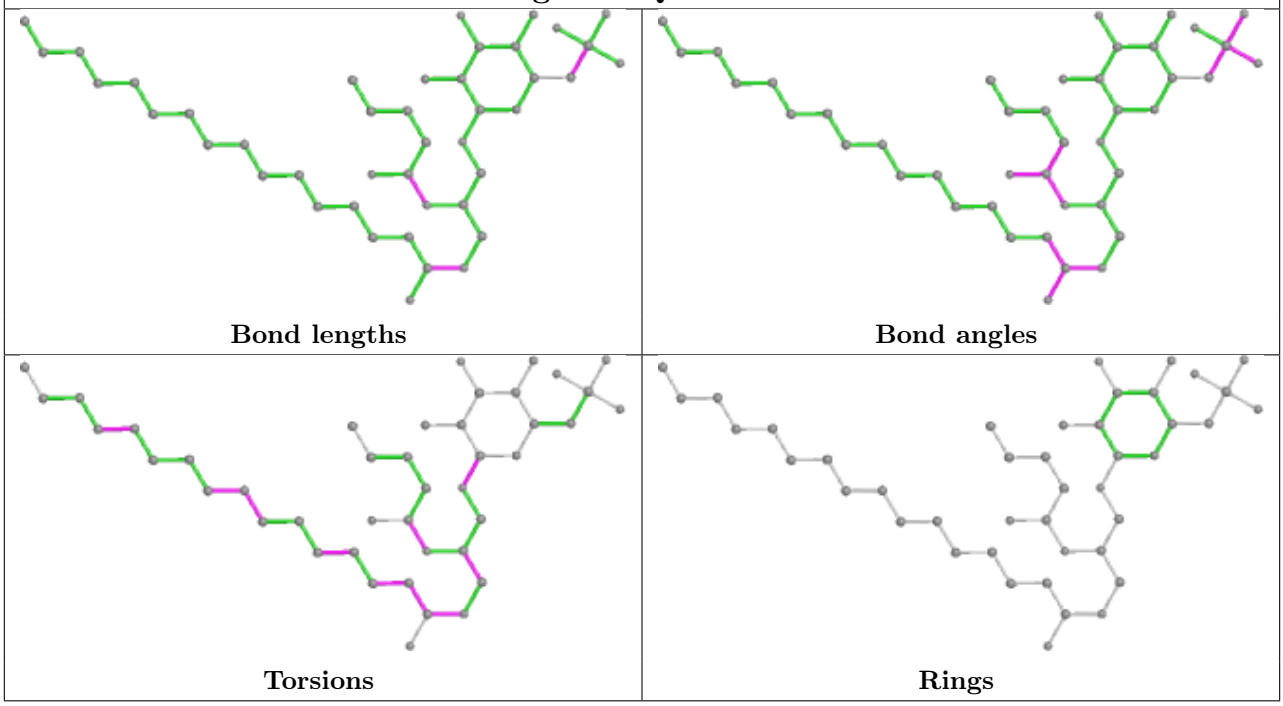


Rings

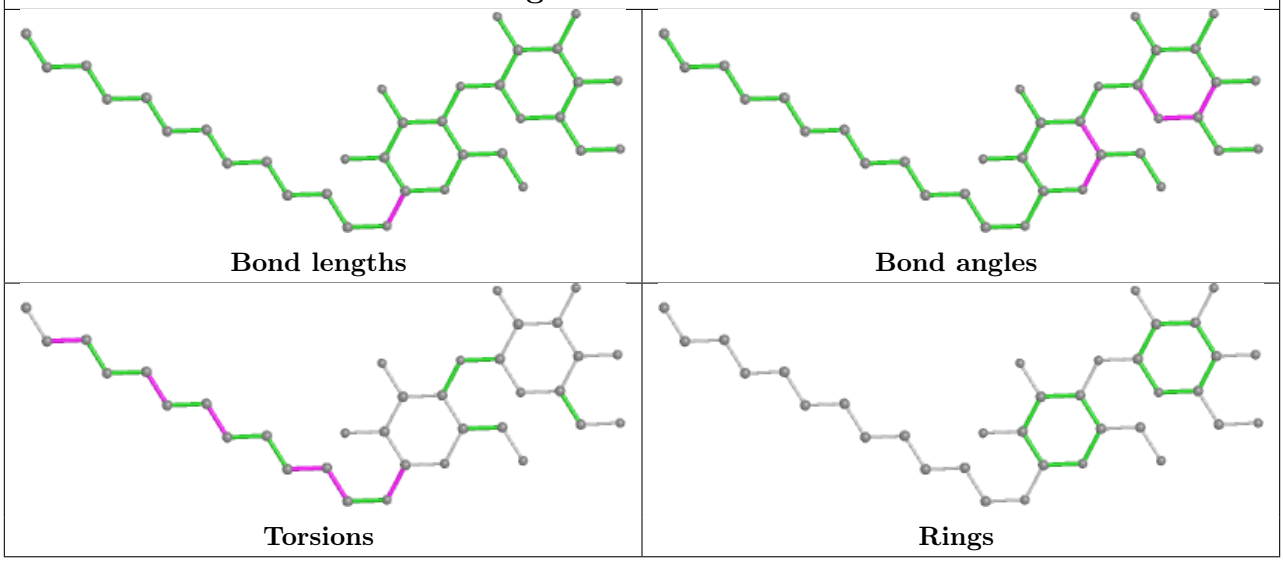
Ligand BCR Y 101



Ligand SQD f 102



Ligand LMT a 412



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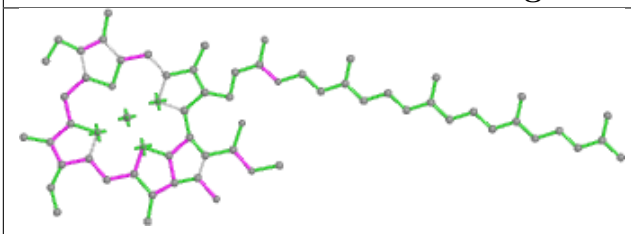
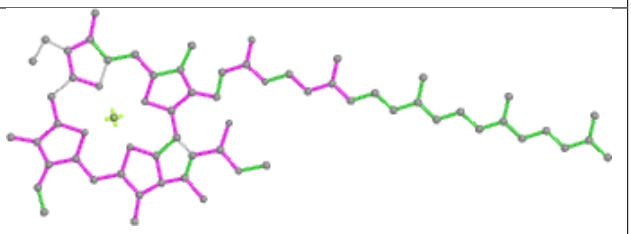
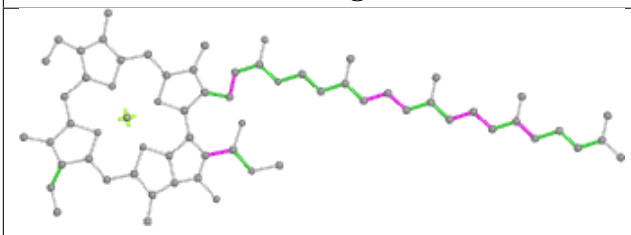


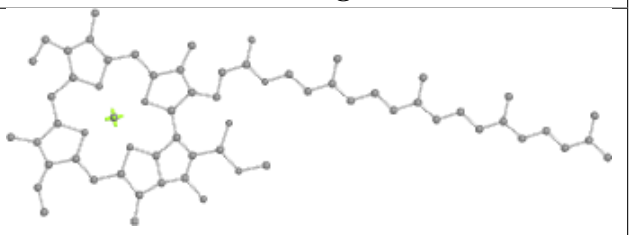
Bond lengths



Bond angles

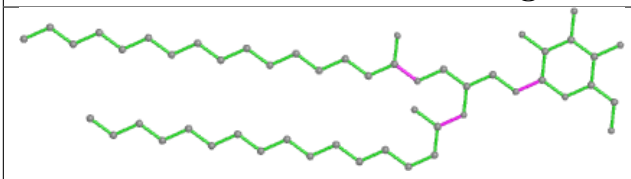


Torsions



Rings

Ligand LMG C 521



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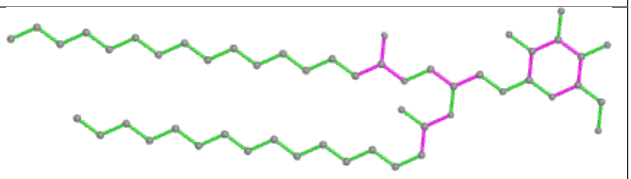
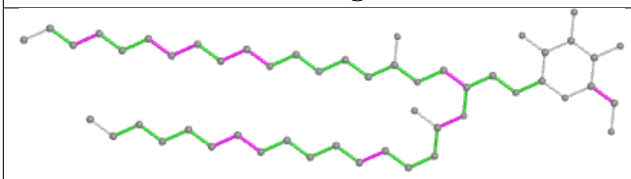


Bond angles



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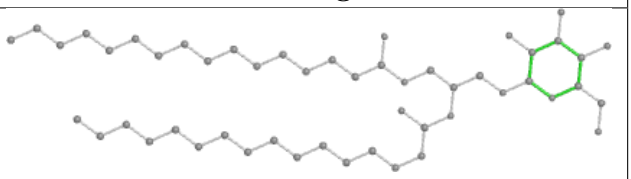
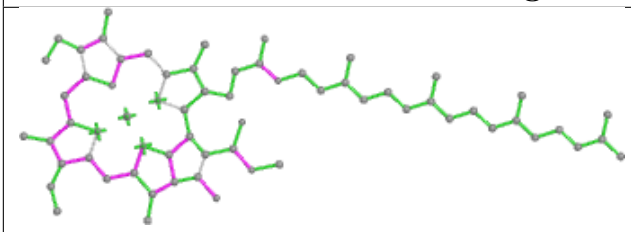


Rings

Ligand CLA A 405



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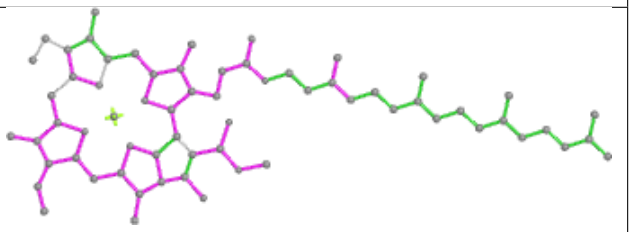
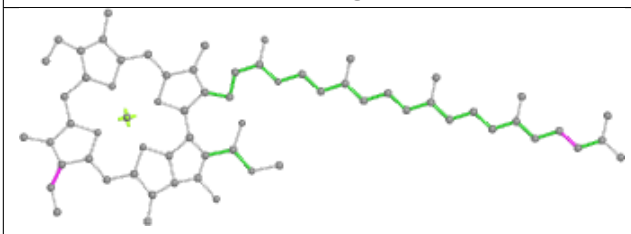


Bond angles



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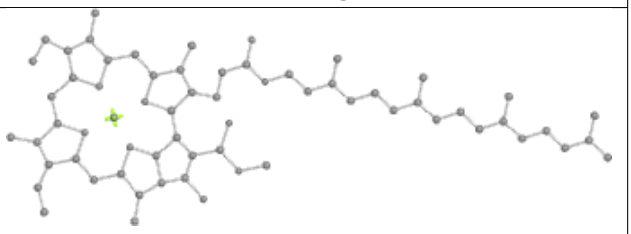
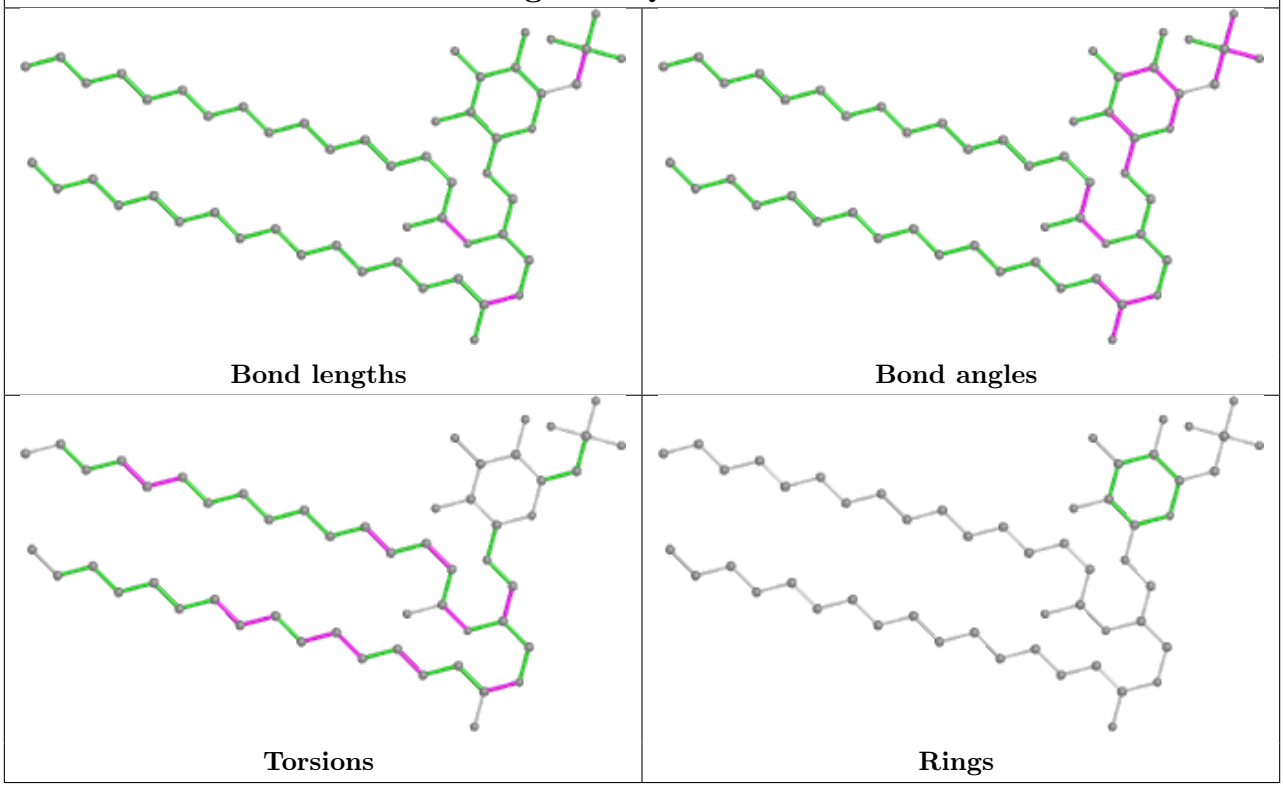
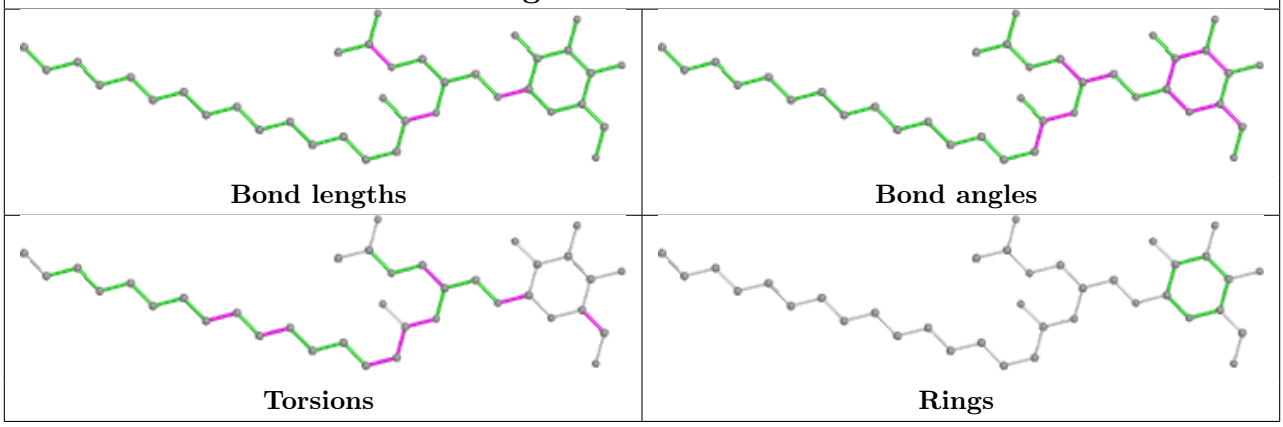


Rings

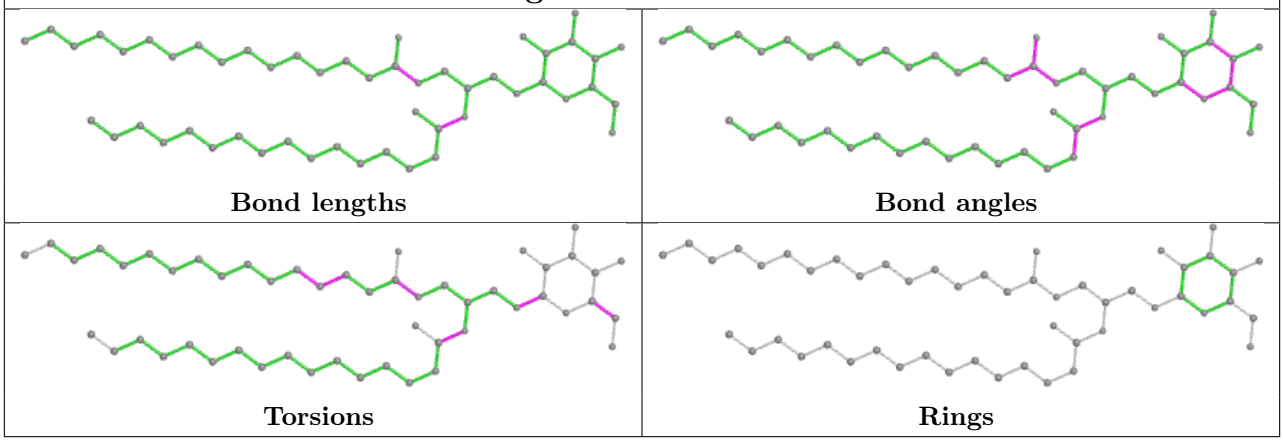
Ligand SQD A 411



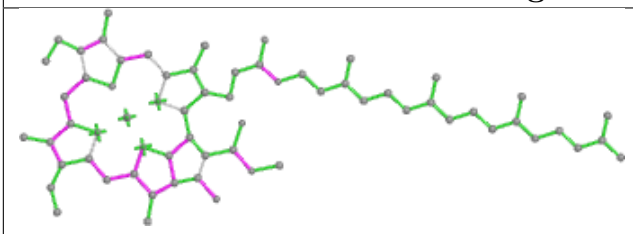
Ligand LMG Z 101



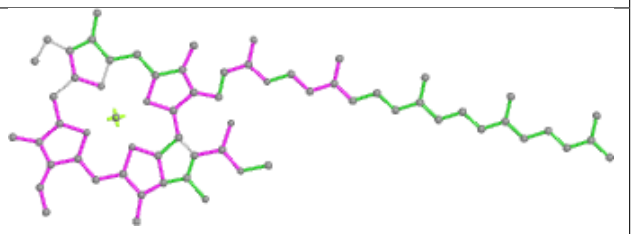
Ligand LMG c 521



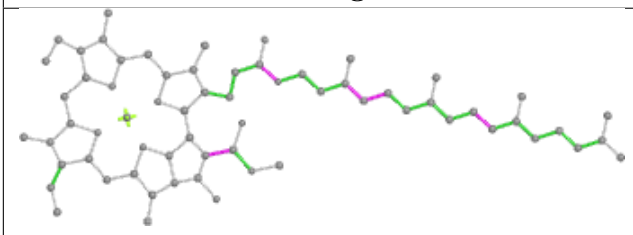
Ligand CLA d 404



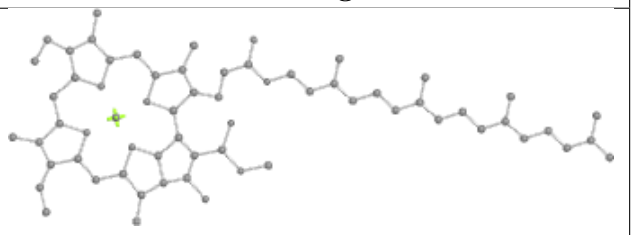
Bond lengths



Bond angles

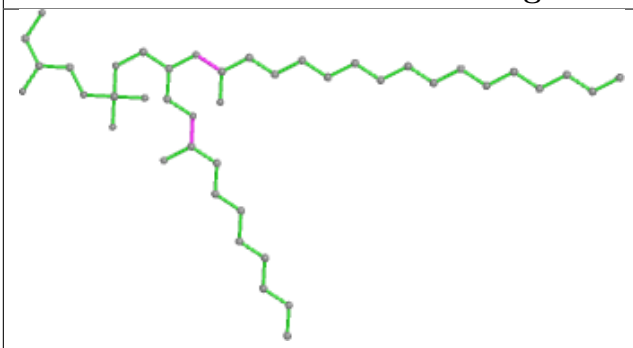


Torsions



Rings

Ligand LHG E 101



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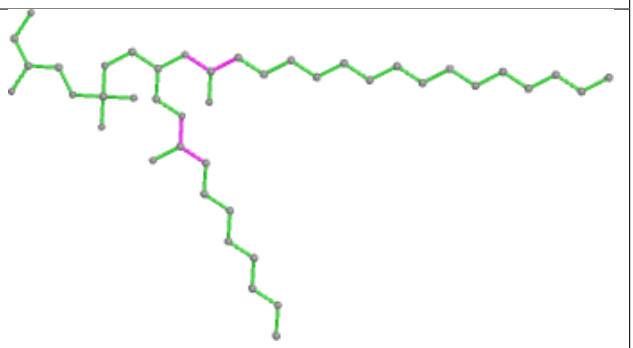
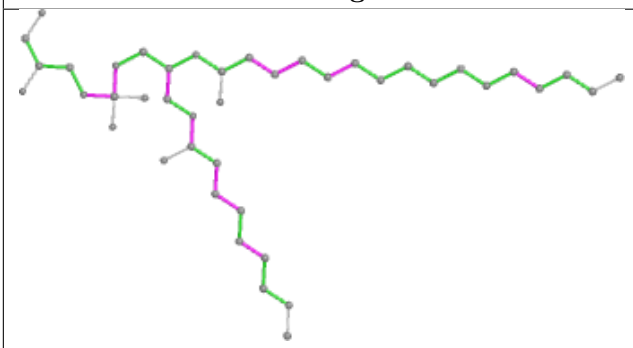
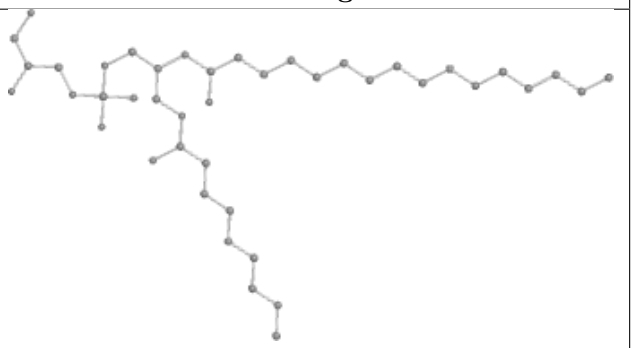


Bond angles

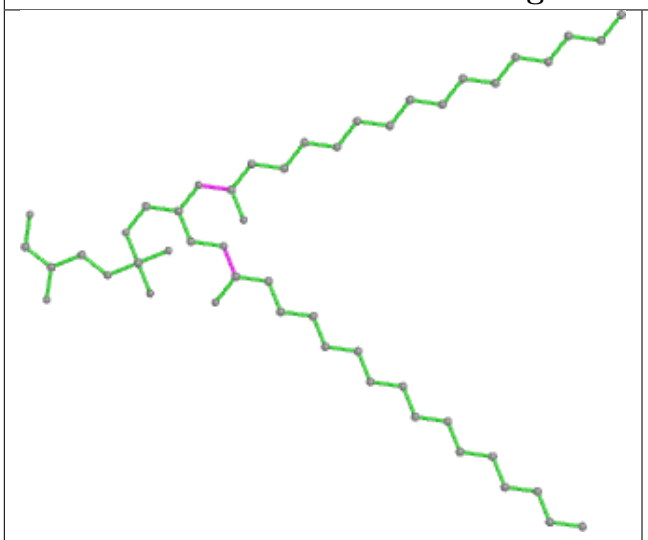


Torsions



Rings

Ligand LHG b 628



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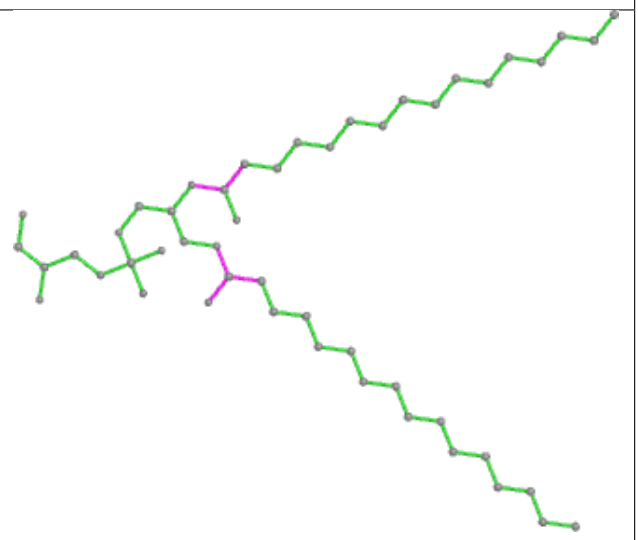
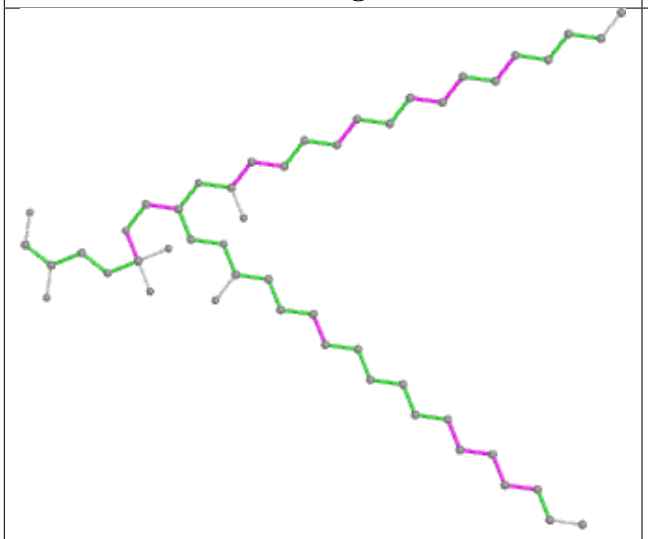
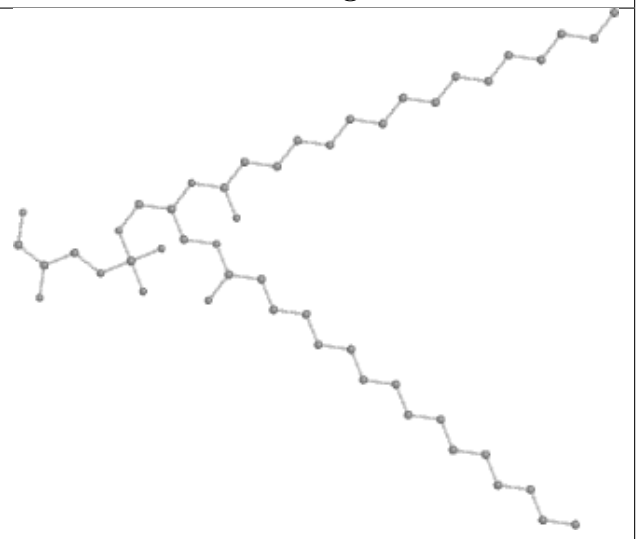


Bond angles

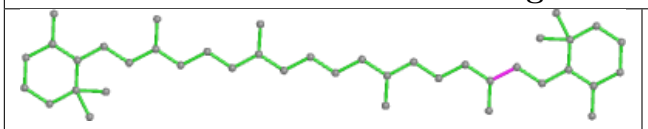


Torsions

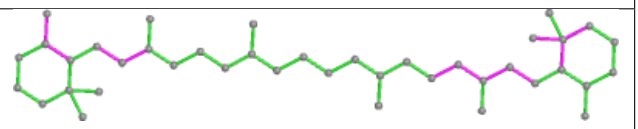


Rings

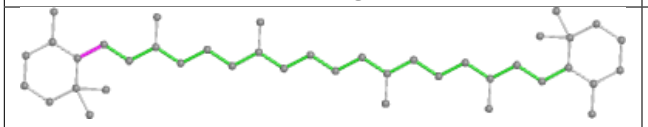
Ligand BCR b 617



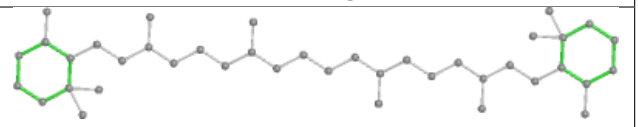
Bond lengths



Bond angles

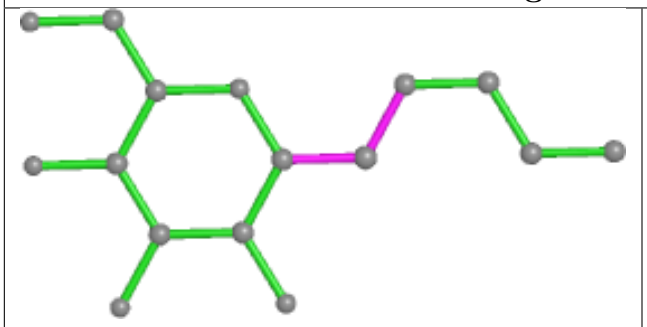


Torsions

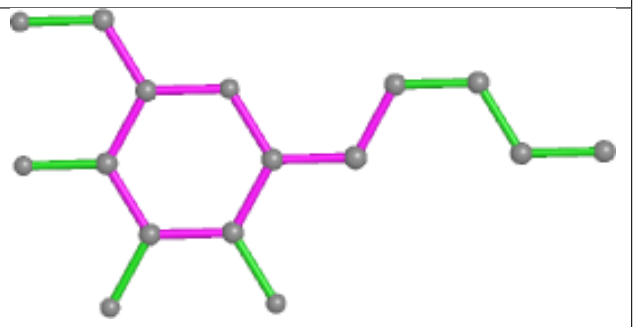


Rings

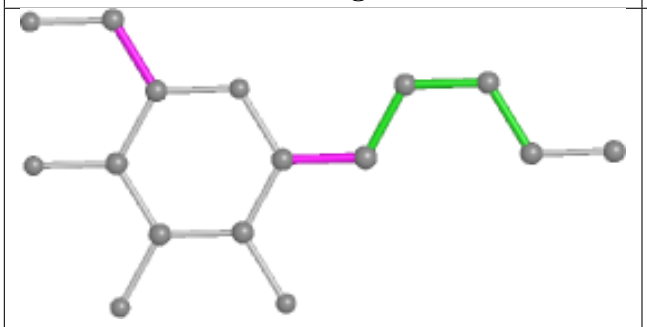
Ligand HTG h 101



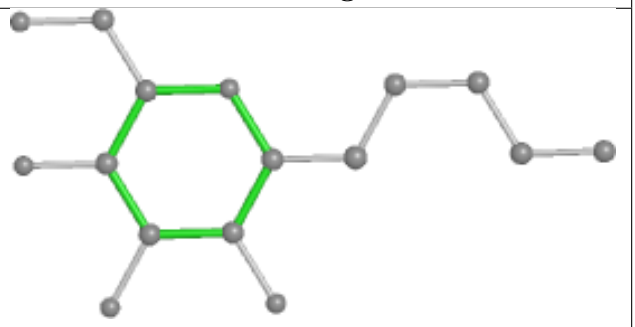
Bond lengths



Bond angles

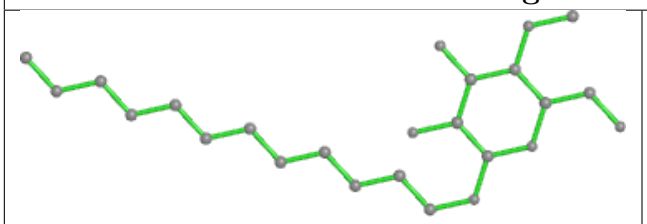


Torsions

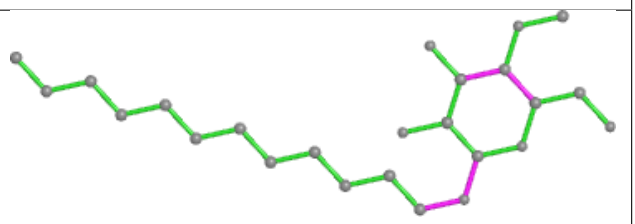


Rings

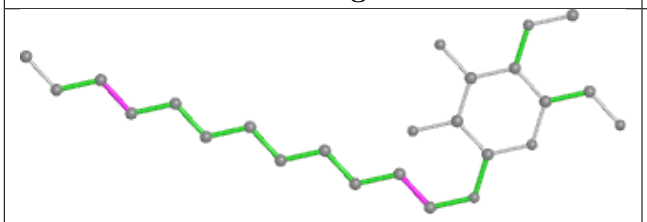
Ligand LMT B 628



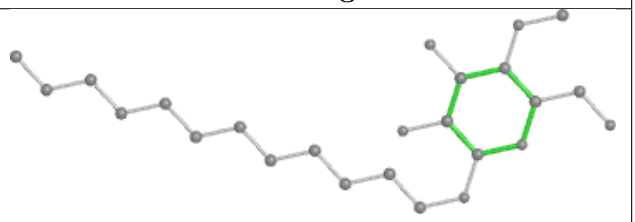
Bond lengths



Bond angles

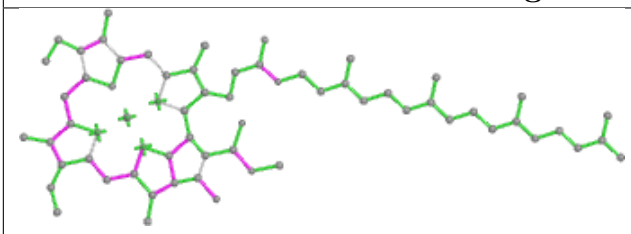


Torsions

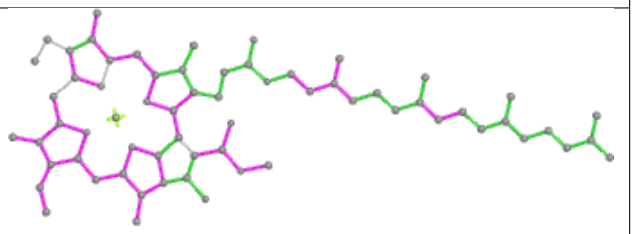


Rings

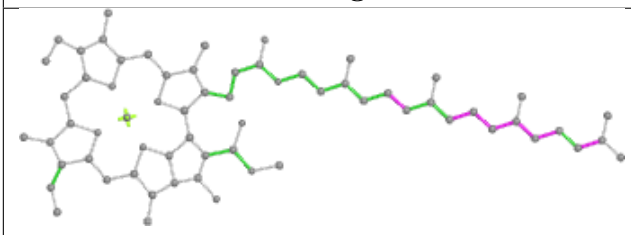
Ligand CLA B 615



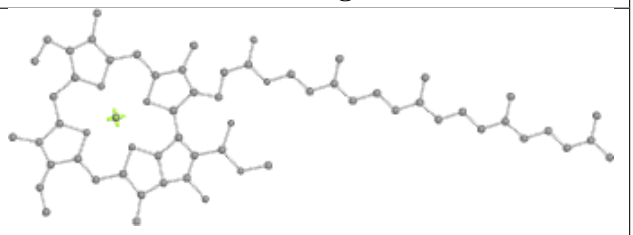
Bond lengths



Bond angles

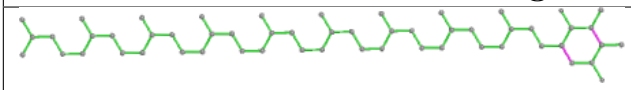


Torsions

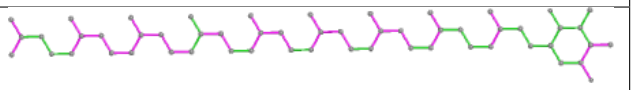


Rings

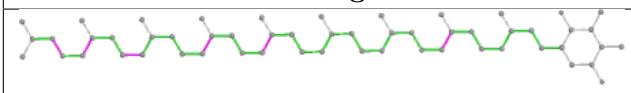
Ligand PL9 D 408



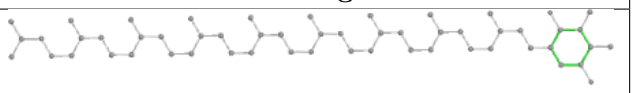
Bond lengths



Bond angles

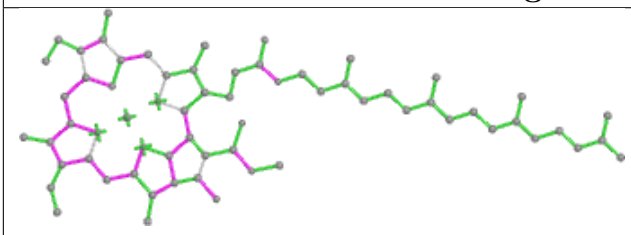


Torsions

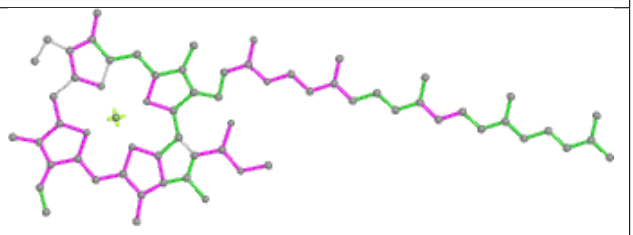


Rings

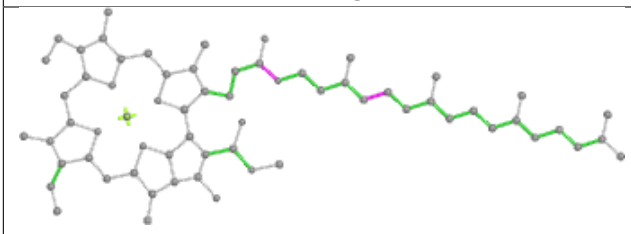
Ligand CLA C 512



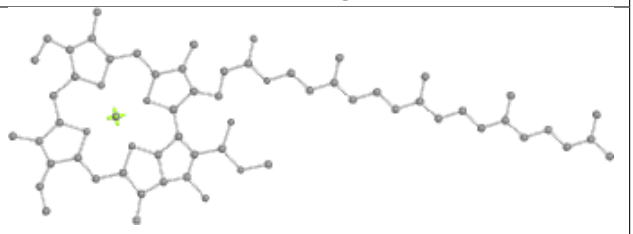
Bond lengths



Bond angles

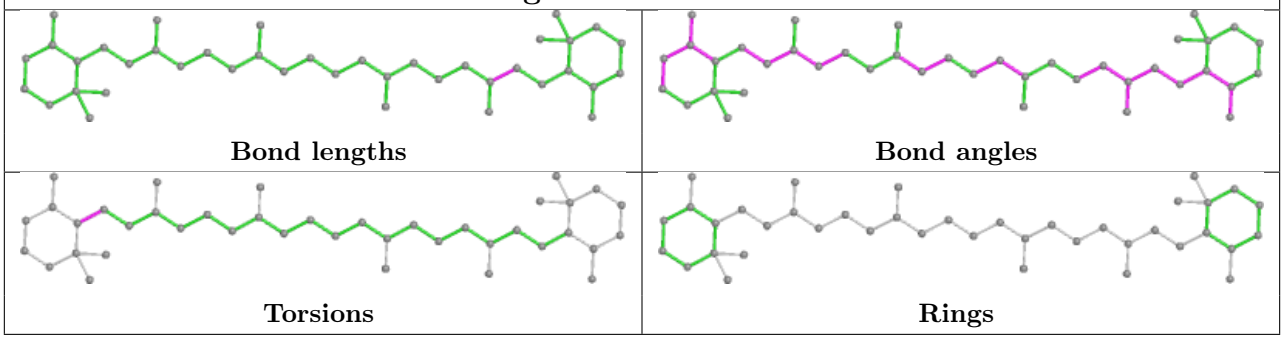


Torsions

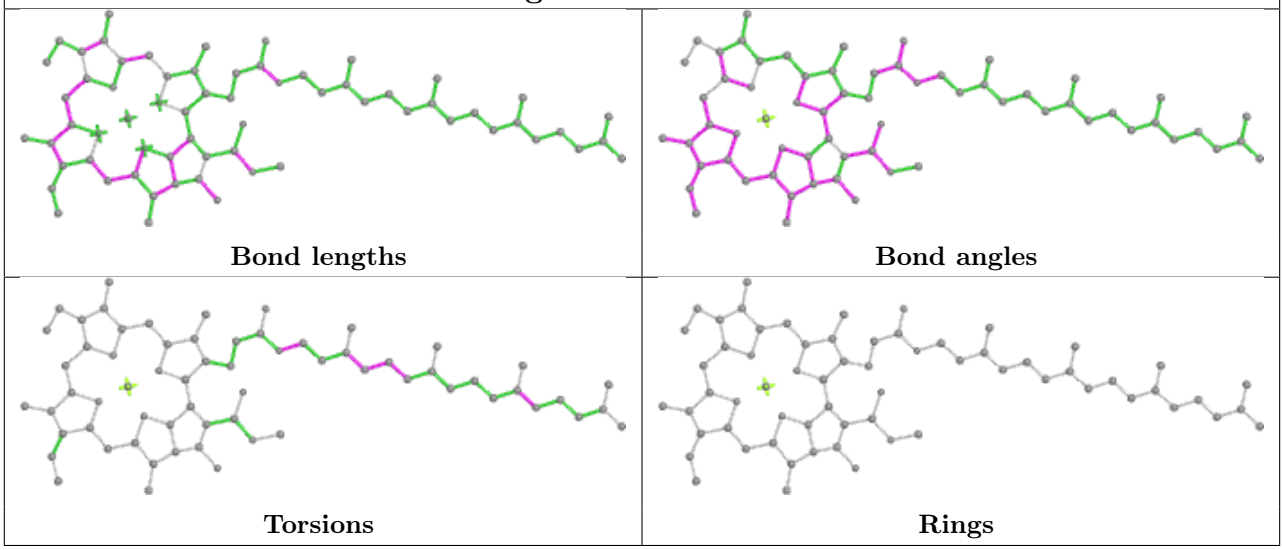


Rings

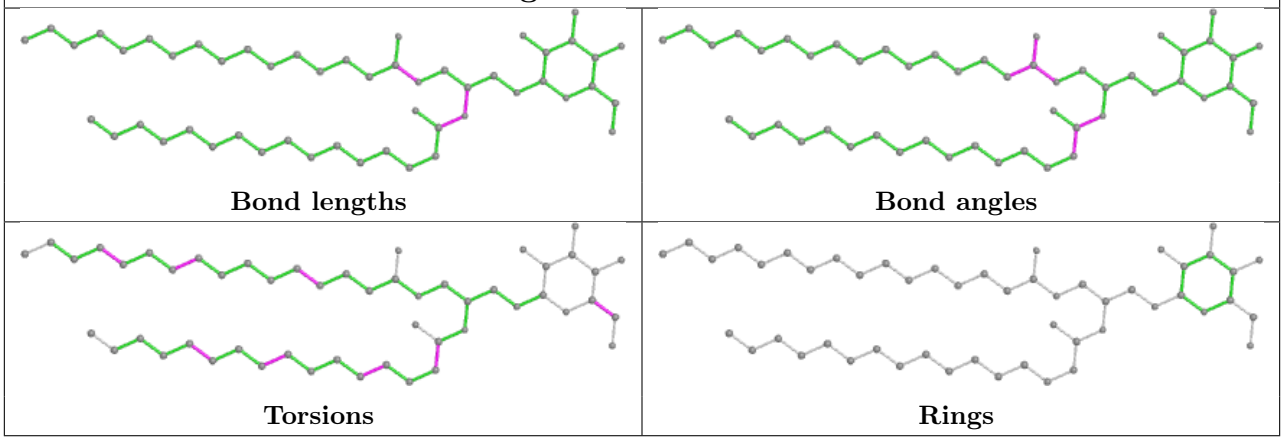
Ligand BCR C 515



Ligand CLA B 616



Ligand LMG D 414



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%)	0.29	22 (6%)	18	26	39, 48, 72, 137	0
1	a	334/344 (97%)	0.33	28 (8%)	11	16	41, 52, 80, 120	0
2	B	504/505 (99%)	-0.03	32 (6%)	20	29	41, 53, 84, 142	0
2	b	504/505 (99%)	0.20	60 (11%)	4	7	42, 56, 94, 158	0
3	C	451/455 (99%)	0.11	35 (7%)	13	19	44, 61, 87, 159	0
3	c	455/455 (100%)	0.29	47 (10%)	6	10	50, 68, 90, 125	0
4	D	342/342 (100%)	0.16	21 (6%)	21	31	39, 49, 71, 145	0
4	d	341/342 (99%)	0.18	29 (8%)	10	16	41, 54, 76, 139	0
5	E	81/84 (96%)	0.68	17 (20%)	1	1	55, 73, 102, 146	0
5	e	79/84 (94%)	0.61	16 (20%)	1	1	63, 77, 119, 148	0
6	F	34/44 (77%)	-0.15	2 (5%)	22	33	55, 66, 90, 118	0
6	f	31/44 (70%)	0.18	3 (9%)	7	12	62, 71, 101, 153	0
7	H	64/65 (98%)	-0.30	1 (1%)	72	80	49, 64, 82, 136	0
7	h	64/65 (98%)	0.37	6 (9%)	8	13	56, 68, 92, 108	0
8	I	37/38 (97%)	-0.05	2 (5%)	25	37	52, 64, 128, 151	0
8	i	37/38 (97%)	-0.18	2 (5%)	25	37	56, 64, 127, 156	0
9	J	38/39 (97%)	0.70	9 (23%)	0	1	52, 74, 136, 177	0
9	j	39/39 (100%)	0.40	5 (12%)	3	6	61, 79, 134, 165	0
10	K	37/37 (100%)	-0.43	0	100	100	61, 73, 94, 116	0
10	k	37/37 (100%)	0.22	4 (10%)	5	9	70, 77, 99, 117	0
11	L	36/37 (97%)	0.09	2 (5%)	24	35	39, 44, 100, 144	0
11	l	36/37 (97%)	0.26	1 (2%)	53	64	42, 45, 103, 123	0
12	M	32/36 (88%)	-0.01	1 (3%)	49	61	42, 47, 74, 151	0
12	m	33/36 (91%)	-0.02	2 (6%)	21	31	42, 48, 83, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	0.30	31 (12%)	3	6	40, 62, 117, 181	0
13	o	243/244 (99%)	0.74	56 (23%)	0	1	43, 65, 125, 174	0
14	T	29/32 (90%)	-0.12	1 (3%)	45	57	40, 45, 85, 116	0
14	t	29/32 (90%)	-0.05	2 (6%)	16	24	41, 48, 76, 139	0
15	U	96/104 (92%)	-0.17	3 (3%)	49	61	48, 59, 90, 98	0
15	u	97/104 (93%)	-0.35	0	100	100	52, 65, 85, 127	0
16	V	137/137 (100%)	-0.20	1 (0%)	87	92	45, 59, 86, 117	0
16	v	137/137 (100%)	0.38	15 (10%)	5	9	53, 74, 106, 131	0
17	X	38/40 (95%)	0.27	5 (13%)	3	5	62, 75, 100, 117	0
17	x	38/40 (95%)	0.80	8 (21%)	1	1	64, 80, 116, 164	0
18	Y	29/30 (96%)	2.20	14 (48%)	0	0	73, 92, 147, 178	0
18	y	29/30 (96%)	0.70	5 (17%)	1	2	80, 94, 124, 126	0
19	Z	62/62 (100%)	1.15	20 (32%)	0	0	75, 90, 136, 185	0
19	z	62/62 (100%)	2.03	29 (46%)	0	0	82, 101, 140, 175	0
20	R	34/34 (100%)	5.81	34 (100%)	0	0	91, 113, 146, 149	0
All	All	5283/5384 (98%)	0.28	571 (10%)	5	9	39, 59, 103, 185	0

All (571) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Y	19	ILE	11.8
20	R	6	LEU	11.3
1	A	11	ALA	8.4
20	R	18	TRP	8.2
17	x	38	GLN	8.0
20	R	14	LEU	7.8
20	R	19	ALA	7.5
20	R	20	VAL	7.4
20	R	5	VAL	7.2
2	b	499	VAL	7.0
20	R	8	VAL	7.0
20	R	16	ALA	6.9
3	C	143	TYR	6.8
2	b	495	PHE	6.7
20	R	15	ALA	6.7
5	E	84	LYS	6.6
13	o	4	THR	6.6

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Mol	Chain	Res	Type	RSRZ
20	R	35	LEU	6.5
17	x	37	VAL	6.4
20	R	3	TRP	6.4
6	f	15	ILE	6.2
1	A	13	LEU	6.2
20	R	12	VAL	6.2
20	R	34	LEU	6.1
20	R	10	LEU	6.1
20	R	2	ASP	6.0
2	b	504	THR	5.9
18	y	19	ILE	5.9
9	J	4	GLY	5.8
20	R	4	ARG	5.8
9	J	7	ILE	5.8
18	y	20	ALA	5.8
20	R	7	VAL	5.7
20	R	24	LEU	5.7
2	b	493	TRP	5.7
20	R	31	VAL	5.6
20	R	21	ARG	5.6
19	z	5	PHE	5.6
16	v	21	LEU	5.5
13	O	27	ARG	5.5
3	c	143	TYR	5.5
13	o	22	LEU	5.4
9	j	2	SER	5.4
20	R	9	LEU	5.4
20	R	33	LYS	5.4
20	R	23	ILE	5.4
20	R	26	TYR	5.4
13	o	133	VAL	5.3
2	b	484	PRO	5.3
2	b	486	LEU	5.3
13	O	4	THR	5.3
19	z	60	PHE	5.2
13	o	27	ARG	5.2
20	R	13	LEU	5.1
19	z	42	LEU	5.1
9	J	3	GLU	5.1
19	z	7	LEU	5.0
3	C	145[A]	SER	5.0
4	D	238	THR	5.0

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Mol	Chain	Res	Type	RSRZ
18	Y	18	VAL	4.9
5	E	83	LEU	4.9
3	C	253	LEU	4.9
17	x	39	ARG	4.9
9	j	3	GLU	4.9
9	J	2	SER	4.9
10	k	17	ILE	4.8
19	z	3	ILE	4.8
2	B	496	TYR	4.8
2	b	496	TYR	4.8
13	o	25	THR	4.8
1	a	11	ALA	4.8
18	Y	20	ALA	4.7
13	O	133	VAL	4.7
19	z	2	THR	4.7
2	b	491	VAL	4.6
13	O	5	LEU	4.6
9	J	6	ARG	4.6
19	Z	3	ILE	4.6
2	B	489	GLU	4.6
19	Z	32	ASP	4.5
2	B	490	GLN	4.5
4	d	12	ARG	4.5
2	b	492	GLU	4.5
13	o	32	ILE	4.5
20	R	17	GLY	4.5
20	R	27	ALA	4.5
20	R	25	PRO	4.4
5	E	15	THR	4.4
1	a	224	ILE	4.4
2	b	500	GLY	4.4
13	O	22	LEU	4.4
13	o	5	LEU	4.4
19	z	46	LEU	4.4
13	O	139	SER	4.3
20	R	28	VAL	4.3
2	b	488	PRO	4.3
3	c	426	LEU	4.3
13	o	134	THR	4.3
3	c	433	LEU	4.3
2	B	504	THR	4.3
3	C	257	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
10	k	18	PHE	4.2
18	y	18	VAL	4.2
9	J	5	GLY	4.2
5	e	59	GLU	4.2
13	o	58	ASN	4.2
20	R	32	GLN	4.2
2	b	459	ALA	4.2
13	o	26	ALA	4.1
13	o	243	ILE	4.1
16	v	26	TYR	4.1
2	B	293	ALA	4.1
3	C	155	ASN	4.1
4	d	152	VAL	4.1
2	b	494	GLY	4.1
13	o	206	GLY	4.1
2	b	461	LEU	4.1
8	I	37	LEU	4.0
13	o	30	TYR	4.0
2	b	460	LEU	4.0
7	h	6	TRP	4.0
12	m	34	LYS	4.0
3	c	427	ALA	4.0
19	Z	60	PHE	3.9
18	Y	25	ILE	3.9
1	A	200	LEU	3.9
19	Z	31	GLN	3.9
2	B	495	PHE	3.9
2	b	458	PHE	3.9
13	O	60	ARG	3.9
13	O	130	GLN	3.8
2	B	461	LEU	3.8
1	a	285	PHE	3.8
3	c	430	HIS	3.8
5	E	17	VAL	3.8
13	o	246	ALA	3.8
2	b	498	LYS	3.8
8	i	38	GLU	3.8
13	o	38	TYR	3.8
6	f	16	PHE	3.8
13	O	26	ALA	3.8
19	Z	53	VAL	3.8
9	j	4	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
17	x	2	THR	3.7
19	z	61	VAL	3.7
18	Y	21	GLN	3.7
19	z	9	LEU	3.7
19	z	41	PHE	3.7
8	I	38	GLU	3.7
2	b	457	VAL	3.7
13	o	36	GLN	3.7
13	O	25	THR	3.7
3	c	202	PRO	3.7
18	Y	22	LEU	3.7
3	c	428	THR	3.7
16	v	22	THR	3.7
13	o	33	ASP	3.7
2	b	248	ALA	3.7
3	c	201	ASN	3.6
20	R	22	ASN	3.6
2	b	489	GLU	3.6
4	d	156	VAL	3.6
3	C	432	VAL	3.6
3	c	429	SER	3.6
3	c	283	GLY	3.6
19	z	1	MET	3.6
3	c	198	VAL	3.6
18	Y	43	ARG	3.6
9	j	1	MET	3.6
3	c	203	THR	3.6
1	A	249	VAL	3.5
19	Z	1	MET	3.5
2	b	485	GLU	3.5
2	b	503	THR	3.5
2	B	491	VAL	3.5
4	d	154	VAL	3.5
13	o	93	LEU	3.5
18	Y	41	VAL	3.5
2	b	249	ALA	3.5
4	d	283	ALA	3.5
13	O	132	ASN	3.5
13	O	28	GLY	3.5
13	o	95	PHE	3.5
2	b	502	VAL	3.5
3	C	181	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
20	R	30	GLN	3.5
19	Z	62	VAL	3.4
20	R	29	LYS	3.4
11	l	3	PRO	3.4
13	o	37	THR	3.4
13	o	136	ILE	3.4
19	z	57	LEU	3.4
2	b	246	PHE	3.4
3	c	436	PHE	3.4
19	z	59	PHE	3.4
16	v	1	ALA	3.4
13	o	91	GLY	3.4
2	b	497	GLN	3.4
1	A	12	ASN	3.4
2	B	482	ILE	3.4
16	v	19	ILE	3.4
3	C	433	LEU	3.4
2	B	295	GLY	3.3
13	O	24	ASP	3.3
2	b	294	SER	3.3
3	C	254	THR	3.3
16	v	8	LEU	3.3
2	b	411	PHE	3.3
3	C	252	ILE	3.3
4	D	153	PHE	3.3
19	z	43	GLY	3.3
3	c	200	THR	3.3
18	Y	26	ALA	3.3
19	z	32	ASP	3.3
2	b	414	PRO	3.3
3	c	284	PHE	3.3
13	o	142	PHE	3.3
2	b	487	SER	3.3
19	Z	56	VAL	3.3
2	B	494	GLY	3.3
1	a	264	SER	3.3
4	d	155	SER	3.3
13	o	204	VAL	3.3
13	o	24	ASP	3.3
2	B	296	ALA	3.3
3	c	312	ALA	3.3
2	b	293	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
13	o	34	SER	3.2
7	h	10	ILE	3.2
2	b	298	LEU	3.2
3	C	154	LYS	3.2
18	Y	23	THR	3.2
4	d	240	ALA	3.2
2	B	486	LEU	3.2
4	D	156	VAL	3.2
5	e	21	VAL	3.2
19	z	30	PRO	3.2
6	F	13	TYR	3.2
2	b	505	ARG	3.2
2	B	185	TRP	3.1
3	C	23	ALA	3.1
13	o	60	ARG	3.1
17	X	2	THR	3.1
2	b	250	PHE	3.1
13	o	35	SER	3.1
3	c	432	VAL	3.1
19	z	31	GLN	3.1
2	B	298	LEU	3.1
16	v	17	LYS	3.1
11	L	2	GLU	3.1
4	d	148	ALA	3.1
19	Z	33	TRP	3.1
11	L	7	ARG	3.1
19	z	39	LEU	3.1
2	B	488	PRO	3.1
4	d	279	LEU	3.1
17	x	36	LYS	3.1
4	D	239	GLN	3.1
1	a	200	LEU	3.1
14	t	30	THR	3.1
13	O	87	VAL	3.0
13	o	130	GLN	3.0
18	Y	24	MET	3.0
3	C	148	GLY	3.0
13	o	199	LEU	3.0
17	X	3	ILE	3.0
5	e	79	PHE	3.0
2	B	487	SER	3.0
2	b	245	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	b	161	LEU	3.0
4	d	17	ILE	3.0
2	B	457	VAL	3.0
13	O	204	VAL	3.0
17	X	37	VAL	3.0
17	x	33	GLN	3.0
19	z	6	GLN	3.0
17	x	3	ILE	3.0
9	j	5	GLY	3.0
16	v	10	VAL	3.0
19	z	56	VAL	3.0
4	D	12	ARG	3.0
4	d	159	ILE	3.0
2	b	501	ASP	3.0
13	O	138	THR	3.0
13	o	140	THR	3.0
13	o	39	ARG	3.0
2	b	295	GLY	2.9
4	D	154	VAL	2.9
16	v	5	PRO	2.9
2	B	505	ARG	2.9
3	c	199	ILE	2.9
20	R	11	PRO	2.9
3	c	424	SER	2.9
5	E	11	SER	2.9
16	V	16	GLY	2.9
1	a	297	LEU	2.9
4	D	122	LEU	2.9
4	d	281	MET	2.9
2	b	251	VAL	2.9
12	m	33	GLN	2.9
1	A	290	ILE	2.8
17	x	34	ILE	2.8
5	e	39	SER	2.8
2	B	501	ASP	2.8
1	A	16	ARG	2.8
13	o	207	ARG	2.8
5	e	57	ALA	2.8
5	e	20	TRP	2.8
4	d	153	PHE	2.8
4	d	151	ALA	2.8
19	z	4	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
7	h	8	GLY	2.8
3	c	425	TRP	2.8
13	o	40	ILE	2.8
2	b	462	PHE	2.8
3	C	146	PHE	2.8
19	z	38	GLN	2.8
3	c	309	ALA	2.8
2	b	292	LEU	2.8
5	e	36	LEU	2.8
2	B	481	GLY	2.8
4	d	280	TRP	2.8
2	b	247	PHE	2.8
19	Z	30	PRO	2.8
1	A	243	GLU	2.8
5	e	25	ILE	2.8
1	a	246	TYR	2.8
3	C	147	PHE	2.7
3	C	140	LEU	2.7
9	J	9	LEU	2.7
2	b	296	ALA	2.7
3	C	284	PHE	2.7
3	c	280	SER	2.7
5	E	19	TYR	2.7
13	O	91	GLY	2.7
2	B	411	PHE	2.7
3	c	439	VAL	2.7
4	d	286	VAL	2.7
16	v	27	LEU	2.7
4	d	150	ILE	2.7
2	b	126	PRO	2.7
13	o	202	ALA	2.7
13	o	241	ALA	2.7
3	c	253	LEU	2.7
3	c	87	ILE	2.7
2	b	218	LEU	2.7
7	h	7	LEU	2.7
1	A	19	ASN	2.7
1	a	288	LEU	2.7
2	B	297	THR	2.7
3	C	437	PHE	2.7
4	D	157	PHE	2.7
13	O	21	THR	2.7

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Mol	Chain	Res	Type	RSRZ
13	o	138	THR	2.7
13	o	208	THR	2.7
19	Z	5	PHE	2.7
19	z	35	ARG	2.6
4	d	149	PRO	2.6
4	D	150	ILE	2.6
13	O	206	GLY	2.6
1	a	196	PRO	2.6
9	J	8	PRO	2.6
13	O	203	LYS	2.6
1	a	160	ILE	2.6
3	C	255	THR	2.6
1	a	281	VAL	2.6
2	B	292	LEU	2.6
3	c	279	LEU	2.6
3	C	144	SER	2.6
3	C	282	MET	2.6
5	E	20	TRP	2.6
4	d	284	ILE	2.6
5	E	14	ILE	2.6
13	o	23	ASP	2.6
2	B	502	VAL	2.6
4	D	152	VAL	2.6
4	d	237	PRO	2.6
18	y	22	LEU	2.6
1	a	262	TYR	2.6
7	h	12	ARG	2.6
3	C	283	GLY	2.6
4	d	238	THR	2.6
1	A	15	GLU	2.6
7	H	65	LEU	2.6
16	v	107	LEU	2.6
2	B	458	PHE	2.6
2	b	162	PHE	2.6
2	b	288	VAL	2.6
5	E	10	PHE	2.6
2	b	456	ALA	2.6
3	C	142	GLU	2.6
14	T	29	ILE	2.6
2	b	127	ARG	2.5
13	O	214	THR	2.5
3	C	438	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	c	437	PHE	2.5
4	D	235	PHE	2.5
13	O	92	SER	2.5
19	z	62	VAL	2.5
15	U	70	ARG	2.5
4	D	159	ILE	2.5
12	M	33	GLN	2.5
13	O	62	GLU	2.5
19	Z	6	GLN	2.5
3	c	257	PHE	2.5
3	c	435	PHE	2.5
6	f	42	PHE	2.5
2	B	456	ALA	2.5
4	d	147	SER	2.5
13	O	202	ALA	2.5
19	z	8	ALA	2.5
3	C	285	ILE	2.5
3	C	262	ARG	2.5
3	c	207	ARG	2.5
3	c	140	LEU	2.5
3	c	404	LEU	2.5
4	d	157	PHE	2.5
1	A	287	ALA	2.5
3	c	434	ALA	2.5
13	o	198	SER	2.5
5	E	12	ASP	2.5
2	B	492	GLU	2.5
2	B	294	SER	2.5
3	c	317	PHE	2.5
1	A	286	ALA	2.5
2	b	244	ALA	2.5
13	o	86	LYS	2.5
4	d	158	LEU	2.5
15	U	58	VAL	2.4
2	b	302	TRP	2.4
13	O	137	THR	2.4
13	o	203	LYS	2.4
19	z	33	TRP	2.4
17	X	38	GLN	2.4
1	A	197	PHE	2.4
1	a	286	ALA	2.4
2	b	454	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
13	o	127	ALA	2.4
18	Y	40	ALA	2.4
19	z	18	VAL	2.4
16	v	4	THR	2.4
2	b	402	TYR	2.4
5	E	25	ILE	2.4
5	E	73	LYS	2.4
3	c	431	PHE	2.4
2	B	454	ALA	2.4
3	C	434	ALA	2.4
3	c	146	PHE	2.4
1	a	242	GLU	2.4
3	C	201	ASN	2.4
4	D	17	ILE	2.4
1	a	249	VAL	2.4
13	o	211	ILE	2.3
3	c	438	LEU	2.3
4	D	151	ALA	2.3
5	E	57	ALA	2.3
13	o	85	LEU	2.3
1	a	295	PHE	2.3
4	d	287	VAL	2.3
4	D	149	PRO	2.3
1	A	288	LEU	2.3
5	e	7	GLU	2.3
13	o	28	GLY	2.3
1	A	294	ALA	2.3
5	e	18	ARG	2.3
19	Z	57	LEU	2.3
19	z	49	ALA	2.3
19	Z	2	THR	2.3
16	v	7	VAL	2.3
1	a	240	GLY	2.3
13	o	200	ASN	2.3
3	C	286	ALA	2.3
3	c	204	LEU	2.3
13	O	200	ASN	2.3
19	Z	35	ARG	2.3
13	o	56	PRO	2.3
3	c	310	SER	2.3
13	O	93	LEU	2.2
13	O	134	THR	2.2

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Mol	Chain	Res	Type	RSRZ
19	Z	4	LEU	2.2
3	C	430	HIS	2.2
13	O	88	ASN	2.2
1	a	265	PHE	2.2
13	O	135	SER	2.2
1	a	289	GLY	2.2
1	A	205	VAL	2.2
10	k	29	PRO	2.2
13	o	87	VAL	2.2
19	Z	17	PHE	2.2
13	o	135	SER	2.2
14	t	29	ILE	2.2
17	X	34	ILE	2.2
13	o	205	ASP	2.2
1	A	196	PRO	2.2
10	k	30	VAL	2.2
16	v	110	LYS	2.2
1	a	197	PHE	2.2
2	b	301	ALA	2.2
3	c	316	THR	2.2
4	D	115	ALA	2.2
13	o	137	THR	2.2
4	D	11	GLU	2.2
6	F	44	GLN	2.2
1	a	340	PRO	2.2
3	C	429	SER	2.2
5	E	16	SER	2.2
5	e	24	SER	2.2
1	A	285	PHE	2.2
5	e	58	GLN	2.2
18	Y	27	MET	2.2
5	e	56	TYR	2.2
13	o	21	THR	2.2
2	b	482	ILE	2.2
1	a	159	LEU	2.2
2	B	485	GLU	2.2
4	D	236	ASN	2.1
5	E	21	VAL	2.1
13	o	84	GLU	2.1
3	c	396	MET	2.1
19	z	29	SER	2.1
1	a	161	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
19	Z	54	VAL	2.1
5	E	74	GLN	2.1
15	U	73	GLN	2.1
1	a	120	LEU	2.1
19	Z	7	LEU	2.1
1	a	225	ARG	2.1
2	B	402	TYR	2.1
5	e	17	VAL	2.1
3	C	207	ARG	2.1
3	c	306	GLY	2.1
1	A	14	TRP	2.1
1	a	339	PHE	2.1
3	C	436	PHE	2.1
3	c	147	PHE	2.1
4	D	237	PRO	2.1
8	i	37	LEU	2.1
1	A	201	GLY	2.1
2	b	453	PHE	2.1
3	c	353	GLY	2.1
5	E	79	PHE	2.1
13	o	139	SER	2.1
3	c	304	PRO	2.1
4	d	123	ILE	2.1
2	b	413	ASP	2.1
13	O	90	ASP	2.1
1	a	294	ALA	2.1
5	e	84	LYS	2.1
3	C	280	SER	2.1
4	d	146	PHE	2.1
1	A	292	THR	2.0
2	b	297	THR	2.0
1	A	242	GLU	2.0
1	a	243	GLU	2.0
18	y	21	GLN	2.0
4	D	280	TRP	2.0
4	D	45	LEU	2.0
4	d	162	LEU	2.0
2	b	471	ALA	2.0
3	c	313	GLN	2.0
13	o	209	GLY	2.0
3	c	314	ALA	2.0
19	Z	38	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	b	252	VAL	2.0
3	C	152	LYS	2.0
9	J	10	TRP	2.0
4	d	182	LEU	2.0
5	e	22	ILE	2.0
7	h	39	LEU	2.0
16	v	12	LEU	2.0
18	Y	44	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.97	0.10	54,67,72,79	0
12	FME	M	1	10/11	0.98	0.12	38,58,80,89	0
14	FME	T	1	10/11	0.98	0.09	44,46,68,71	0
8	FME	I	1	10/11	0.98	0.13	56,66,73,76	0
12	FME	m	1	10/11	0.98	0.08	40,57,77,93	0
14	FME	t	1	10/11	0.98	0.08	39,46,70,75	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
31	LMG	C	521	51/55	0.44	0.48	77,131,166,170	0
33	HTG	b	622	19/19	0.47	0.57	90,147,155,155	0
34	LMT	E	102	35/35	0.49	0.39	117,161,175,176	0
30	UNL	j	101	10/-	0.50	0.43	86,94,101,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	A	414	28/-	0.51	0.43	93,105,126,127	0
34	LMT	C	525	35/35	0.56	0.55	97,149,164,168	0
34	LMT	a	412	35/35	0.56	0.45	70,139,150,152	0
34	LMT	D	403	35/35	0.57	0.40	70,135,146,152	0
34	LMT	e	101	35/35	0.59	0.60	114,176,180,181	0
34	LMT	m	103	35/35	0.61	0.43	68,104,116,119	0
29	PL9	A	413	55/55	0.62	0.39	80,108,117,118	0
30	UNL	J	101	10/-	0.63	0.31	76,91,99,100	0
33	HTG	D	413	16/19	0.64	0.33	91,119,132,136	0
31	LMG	c	521	51/55	0.64	0.39	78,133,158,163	0
34	LMT	M	102	35/35	0.65	0.29	58,107,138,142	0
34	LMT	M	104	35/35	0.66	0.29	80,152,175,176	0
30	UNL	I	101	40/-	0.69	0.28	73,109,155,156	0
32	LHG	a	419	42/49	0.69	0.38	98,142,173,177	0
30	UNL	i	101	40/-	0.69	0.31	75,103,153,163	0
32	LHG	E	101	42/49	0.70	0.27	80,126,141,143	0
31	LMG	Z	101	37/55	0.70	0.30	79,133,167,170	0
30	UNL	C	526	34/-	0.70	0.32	90,120,133,134	0
36	CA	F	101	1/1	0.70	0.05	129,129,129,129	0
30	UNL	b	625	33/-	0.71	0.39	67,101,152,154	0
30	UNL	a	415	30/-	0.73	0.28	102,114,136,145	0
34	LMT	D	404	35/35	0.74	0.30	73,118,133,134	0
34	LMT	a	418	35/35	0.74	0.51	119,152,162,163	0
26	GOL	B	626	6/6	0.74	0.25	91,105,106,108	0
26	GOL	B	627	6/6	0.74	0.33	109,114,117,119	0
26	GOL	O	302	6/6	0.74	0.26	84,85,88,89	0
30	UNL	c	525	32/-	0.75	0.39	90,115,132,135	0
33	HTG	B	621	19/19	0.76	0.26	65,82,115,116	0
33	HTG	B	622	19/19	0.76	0.41	76,96,106,106	0
27	SQD	f	102	43/54	0.76	0.47	119,138,168,171	0
30	UNL	d	411	36/-	0.77	0.26	75,100,133,136	0
30	UNL	m	102	10/-	0.77	0.26	65,72,99,100	0
34	LMT	b	620	25/35	0.78	0.22	92,128,152,154	0
34	LMT	b	626	25/35	0.78	0.25	52,77,134,137	0
29	PL9	a	414	55/55	0.78	0.31	90,117,133,138	0
30	UNL	B	625	33/-	0.78	0.23	59,113,154,157	0
33	HTG	b	621	19/19	0.78	0.24	68,82,114,118	0
31	LMG	z	101	39/55	0.79	0.31	86,136,147,149	0
27	SQD	L	102	54/54	0.80	0.22	64,92,116,121	0
31	LMG	a	417	51/55	0.80	0.23	62,96,110,122	0
33	HTG	h	101	16/19	0.81	0.30	99,136,147,148	0
30	UNL	M	103	10/-	0.82	0.27	66,78,91,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	LMT	B	628	25/35	0.82	0.22	54,82,139,141	0
34	LMT	t	101	26/35	0.82	0.21	80,119,138,141	0
33	HTG	c	522	19/19	0.82	0.31	118,141,149,151	0
30	UNL	D	412	40/-	0.83	0.24	61,93,130,131	0
27	SQD	A	411	54/54	0.83	0.17	67,87,125,127	0
25	BCR	h	102	40/40	0.84	0.18	56,67,80,84	0
26	GOL	b	623	6/6	0.84	0.21	89,99,105,112	0
31	LMG	C	520	51/55	0.85	0.23	61,92,114,119	0
26	GOL	c	526	6/6	0.85	0.53	117,120,128,129	0
25	BCR	H	101	40/40	0.85	0.18	50,69,79,81	0
31	LMG	m	101	51/55	0.86	0.23	52,72,99,103	0
27	SQD	B	620	54/54	0.86	0.18	62,94,126,130	0
33	HTG	V	202	11/19	0.87	0.47	117,124,127,128	0
30	UNL	x	101	18/-	0.87	0.19	71,80,124,127	0
31	LMG	M	101	51/55	0.87	0.20	53,72,94,115	0
33	HTG	C	522	19/19	0.87	0.29	114,127,137,138	0
23	CLA	C	514	65/65	0.87	0.21	69,80,114,116	0
36	CA	O	301	1/1	0.87	0.16	116,116,116,116	0
26	GOL	A	410	6/6	0.88	0.19	71,74,79,88	0
27	SQD	a	411	54/54	0.88	0.15	69,96,137,142	0
31	LMG	A	415	51/55	0.88	0.20	63,90,109,114	0
35	DGD	C	518	62/66	0.88	0.20	51,67,124,134	0
35	DGD	h	103	62/66	0.88	0.25	52,65,73,75	0
26	GOL	v	202	6/6	0.88	0.24	62,91,95,95	0
31	LMG	c	520	51/55	0.88	0.25	69,96,133,136	0
32	LHG	A	416	49/49	0.89	0.23	44,63,85,88	0
35	DGD	C	519	62/66	0.90	0.19	47,62,104,119	0
35	DGD	H	102	62/66	0.90	0.23	45,60,78,83	0
23	CLA	C	513	65/65	0.90	0.17	63,73,122,125	0
30	UNL	D	411	17/-	0.90	0.30	64,81,117,117	0
30	UNL	X	101	18/-	0.90	0.14	63,76,94,95	0
23	CLA	B	602	65/65	0.91	0.15	46,55,75,83	0
23	CLA	C	505	65/65	0.91	0.17	49,57,95,109	0
26	GOL	b	627	6/6	0.91	0.24	99,99,102,103	0
29	PL9	d	406	55/55	0.91	0.20	40,48,59,67	0
27	SQD	C	501	54/54	0.91	0.20	58,86,115,118	0
26	GOL	c	501	6/6	0.91	0.28	62,73,78,81	0
25	BCR	k	101	40/40	0.91	0.15	65,77,87,88	0
23	CLA	c	513	65/65	0.92	0.16	70,88,122,129	0
23	CLA	c	514	65/65	0.92	0.27	71,91,124,127	0
31	LMG	D	414	51/55	0.92	0.19	51,74,116,126	0
32	LHG	b	628	49/49	0.92	0.18	43,59,69,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	SQD	D	415	43/54	0.92	0.22	76,114,135,142	0
23	CLA	B	609	65/65	0.92	0.13	50,59,74,85	0
23	CLA	C	507	65/65	0.92	0.14	58,72,128,137	0
23	CLA	b	602	65/65	0.92	0.20	49,59,75,86	0
35	DGD	c	518	62/66	0.92	0.21	56,76,120,133	0
35	DGD	c	519	62/66	0.92	0.18	55,64,105,112	0
25	BCR	k	102	40/40	0.92	0.12	64,75,91,97	0
23	CLA	c	503	65/65	0.92	0.28	55,62,77,89	0
23	CLA	c	504	65/65	0.92	0.23	58,69,78,82	0
36	CA	c	524	1/1	0.92	0.04	90,90,90,90	0
23	CLA	c	508	65/65	0.93	0.15	58,70,81,90	0
23	CLA	C	508	65/65	0.93	0.13	55,64,78,87	0
26	GOL	a	410	6/6	0.93	0.24	66,73,88,94	0
23	CLA	b	609	65/65	0.93	0.14	53,62,76,93	0
23	CLA	d	404	65/65	0.93	0.14	54,64,120,126	0
23	CLA	c	505	65/65	0.93	0.28	56,65,106,116	0
33	HTG	b	624	19/19	0.93	0.12	68,80,100,107	0
30	UNL	d	410	17/-	0.93	0.18	69,82,99,100	0
33	HTG	B	624	19/19	0.94	0.10	68,83,91,99	0
23	CLA	b	612	65/65	0.94	0.19	44,52,64,73	0
23	CLA	b	616	65/65	0.94	0.17	47,61,122,124	0
31	LMG	d	412	51/55	0.94	0.13	57,72,117,133	0
23	CLA	b	601	65/65	0.94	0.20	65,83,126,136	0
23	CLA	B	614	65/65	0.94	0.15	38,48,100,107	0
25	BCR	C	515	40/40	0.94	0.14	67,80,90,93	0
35	DGD	C	517	62/66	0.94	0.24	48,58,103,108	0
23	CLA	D	406	65/65	0.94	0.17	50,59,132,135	0
32	LHG	L	101	49/49	0.94	0.16	42,56,69,95	0
25	BCR	Y	101	40/40	0.94	0.11	61,70,82,89	0
25	BCR	c	515	40/40	0.94	0.15	75,86,94,95	0
32	LHG	d	407	49/49	0.94	0.27	48,66,80,86	0
32	LHG	d	408	49/49	0.94	0.15	43,54,73,84	0
32	LHG	d	409	49/49	0.94	0.22	60,69,125,134	0
25	BCR	d	405	40/40	0.94	0.13	58,69,91,104	0
27	SQD	a	409	54/54	0.94	0.20	71,87,124,125	0
36	CA	v	201	1/1	0.94	0.28	117,117,117,117	0
39	MG	J	102	1/1	0.94	0.11	61,61,61,61	0
32	LHG	D	409	49/49	0.95	0.15	44,53,73,86	0
32	LHG	D	410	49/49	0.95	0.18	50,64,123,134	0
25	BCR	T	101	40/40	0.95	0.14	43,54,64,64	0
23	CLA	b	614	65/65	0.95	0.15	40,48,112,114	0
25	BCR	b	618	40/40	0.95	0.22	39,55,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	502	65/65	0.95	0.14	53,60,73,81	0
23	CLA	c	502	65/65	0.95	0.13	57,66,80,84	0
23	CLA	C	504	65/65	0.95	0.14	55,63,74,79	0
23	CLA	B	601	65/65	0.95	0.24	57,78,119,129	0
23	CLA	B	611	65/65	0.95	0.17	40,45,64,75	0
29	PL9	D	408	55/55	0.95	0.18	39,49,61,70	0
23	CLA	c	506	65/65	0.95	0.14	50,62,85,89	0
26	GOL	B	623	6/6	0.95	0.14	73,86,93,97	0
23	CLA	B	603	65/65	0.95	0.14	44,52,68,73	0
23	CLA	c	509	65/65	0.95	0.25	53,63,127,129	0
35	DGD	c	517	62/66	0.95	0.21	51,65,96,104	0
23	CLA	c	512	65/65	0.95	0.13	60,72,86,94	0
23	CLA	b	604	65/65	0.95	0.24	40,48,108,117	0
23	CLA	b	607	65/65	0.95	0.18	38,45,78,87	0
23	CLA	C	511	65/65	0.95	0.22	53,62,85,92	0
23	CLA	b	610	65/65	0.95	0.16	50,56,70,78	0
25	BCR	C	516	40/40	0.95	0.14	54,64,79,83	0
36	CA	o	301	1/1	0.95	0.13	104,104,104,104	0
23	CLA	C	512	65/65	0.95	0.13	58,68,84,91	0
25	BCR	K	101	40/40	0.95	0.14	63,74,77,80	0
39	MG	j	102	1/1	0.95	0.07	68,68,68,68	0
23	CLA	b	606	65/65	0.96	0.12	46,55,120,127	0
23	CLA	A	408	65/65	0.96	0.12	44,51,115,124	0
23	CLA	c	510	65/65	0.96	0.19	60,66,87,92	0
25	BCR	t	102	40/40	0.96	0.15	42,59,74,75	0
23	CLA	c	511	65/65	0.96	0.32	58,66,75,79	0
23	CLA	C	503	65/65	0.96	0.18	50,59,82,93	0
23	CLA	B	610	65/65	0.96	0.15	47,53,67,83	0
23	CLA	b	611	65/65	0.96	0.22	43,50,70,82	0
26	GOL	C	523	6/6	0.96	0.15	60,63,69,69	0
23	CLA	B	606	65/65	0.96	0.12	44,53,102,110	0
24	PHO	A	407	64/64	0.96	0.15	38,43,53,62	0
24	PHO	D	402	64/64	0.96	0.26	41,51,56,57	0
25	BCR	A	409	40/40	0.96	0.12	40,50,59,61	0
25	BCR	B	618	40/40	0.96	0.16	43,54,71,76	0
25	BCR	B	619	40/40	0.96	0.10	48,59,76,80	0
23	CLA	B	607	65/65	0.96	0.17	37,46,67,75	0
23	CLA	b	615	65/65	0.96	0.12	47,56,78,82	0
25	BCR	D	407	40/40	0.96	0.17	52,63,101,108	0
23	CLA	a	407	65/65	0.96	0.16	46,55,130,131	0
23	CLA	B	616	65/65	0.96	0.17	47,58,137,141	0
23	CLA	C	509	65/65	0.96	0.19	50,58,123,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	603	65/65	0.96	0.17	47,54,76,85	0
25	BCR	b	617	40/40	0.96	0.16	41,48,59,64	0
23	CLA	C	510	65/65	0.96	0.13	56,64,85,88	0
25	BCR	b	619	40/40	0.96	0.11	49,59,85,92	0
23	CLA	b	605	65/65	0.96	0.16	42,49,69,75	0
23	CLA	c	507	65/65	0.96	0.12	61,74,127,135	0
23	CLA	b	608	65/65	0.97	0.21	50,57,73,78	0
24	PHO	a	416	64/64	0.97	0.19	45,52,58,65	0
25	BCR	c	516	40/40	0.97	0.10	57,69,76,79	0
23	CLA	C	506	65/65	0.97	0.15	50,57,90,94	0
23	CLA	a	405	65/65	0.97	0.21	45,53,124,126	0
23	CLA	B	613	65/65	0.97	0.22	39,47,87,92	0
23	CLA	A	406	65/65	0.97	0.22	40,48,104,113	0
23	CLA	b	613	65/65	0.97	0.28	40,48,81,86	0
23	CLA	B	615	65/65	0.97	0.12	46,52,78,89	0
23	CLA	B	608	65/65	0.97	0.19	45,53,70,73	0
23	CLA	B	604	65/65	0.97	0.19	38,45,105,110	0
23	CLA	B	605	65/65	0.97	0.12	40,46,61,72	0
23	CLA	d	402	65/65	0.97	0.16	40,46,62,68	0
25	BCR	a	408	40/40	0.97	0.10	42,50,58,61	0
38	HEM	f	101	43/43	0.97	0.20	70,83,119,127	0
23	CLA	A	404	65/65	0.97	0.23	39,42,67,72	0
23	CLA	B	612	65/65	0.97	0.16	42,50,61,66	0
40	HEC	v	203	43/43	0.97	0.11	59,65,70,75	0
25	BCR	B	617	40/40	0.98	0.13	40,50,60,62	0
23	CLA	D	405	65/65	0.98	0.26	38,44,62,70	0
23	CLA	A	405	65/65	0.98	0.18	38,44,54,56	0
37	BCT	D	401	4/4	0.98	0.07	59,64,65,66	0
37	BCT	d	401	4/4	0.98	0.09	57,58,64,67	0
38	HEM	E	103	43/43	0.98	0.12	62,71,86,98	0
24	PHO	a	406	64/64	0.98	0.15	40,47,52,55	0
36	CA	C	524	1/1	0.98	0.21	72,72,72,72	0
23	CLA	d	403	65/65	0.98	0.24	42,47,71,80	0
40	HEC	V	201	43/43	0.98	0.09	50,53,58,62	0
23	CLA	a	404	65/65	0.98	0.20	43,46,67,80	0
36	CA	c	523	1/1	0.99	0.10	81,81,81,81	0
21	FE2	A	401	1/1	0.99	0.03	61,61,61,61	0
21	FE2	a	401	1/1	0.99	0.02	61,61,61,61	0
22	CL	A	403	1/1	0.99	0.13	45,45,45,45	0
22	CL	a	403	1/1	0.99	0.13	49,49,49,49	0
28	OEX	A	412	10/10	0.99	0.11	44,49,53,56	0
28	OEX	a	413	10/10	1.00	0.11	45,54,55,56	0

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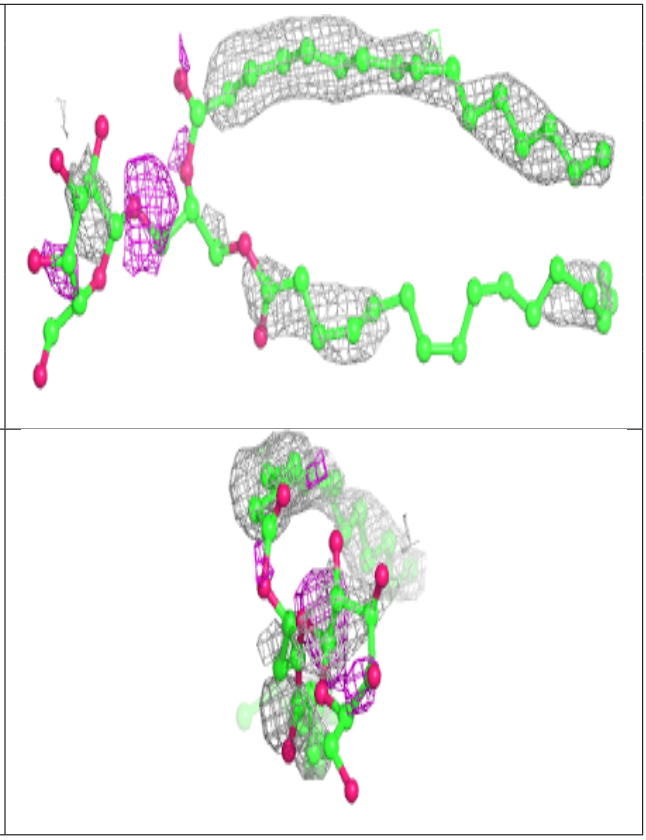
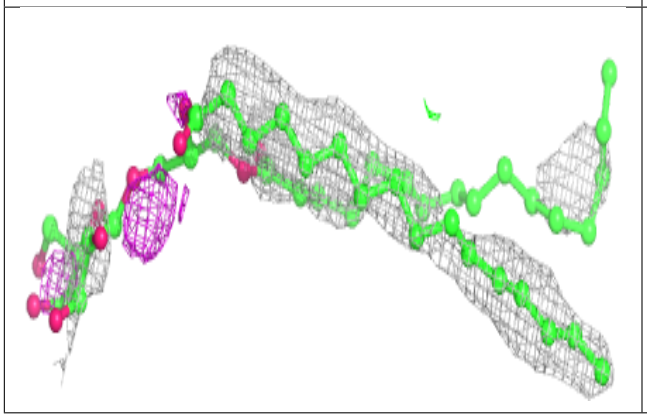
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CL	A	402	1/1	1.00	0.06	40,40,40,40	0
22	CL	a	402	1/1	1.00	0.10	48,48,48,48	0

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

Electron density around LMG C 521:

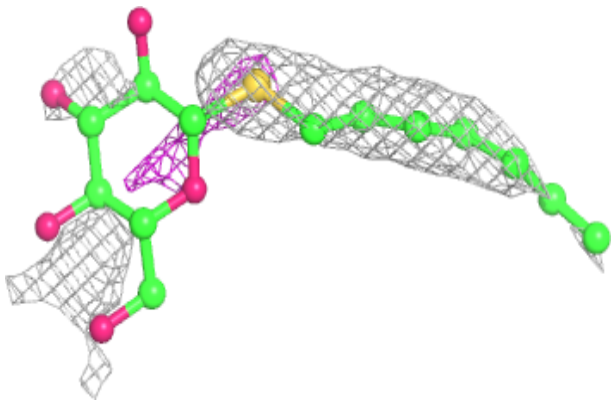
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

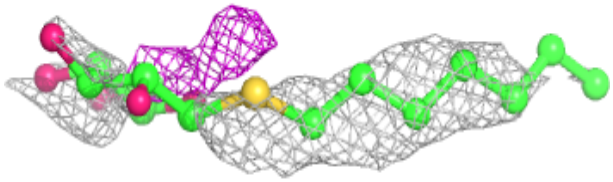


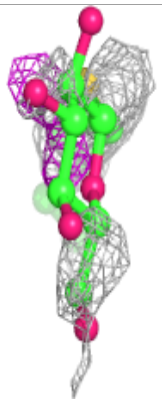


Electron density around HTG b 622:

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

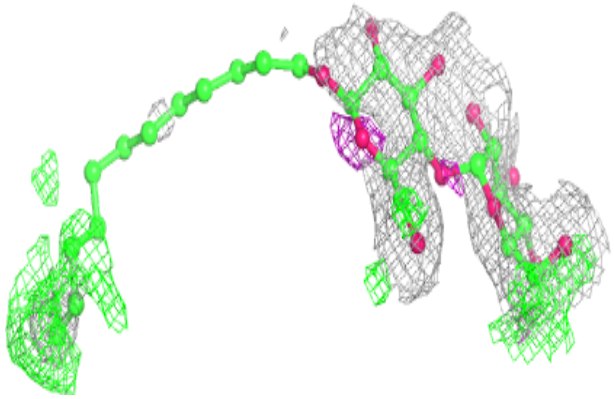


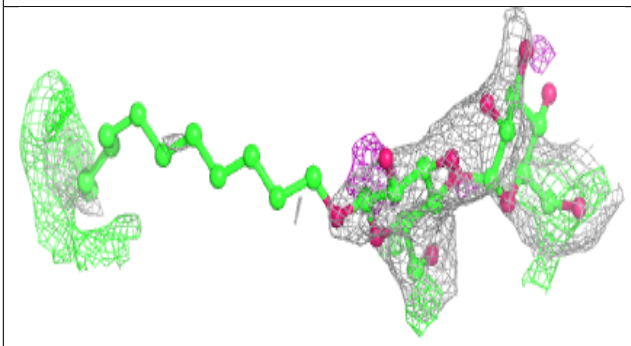


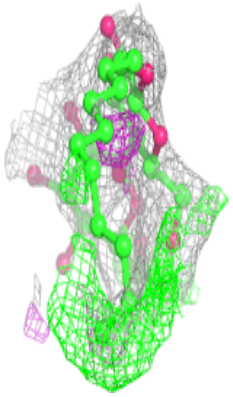


Electron density around LMT E 102:

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

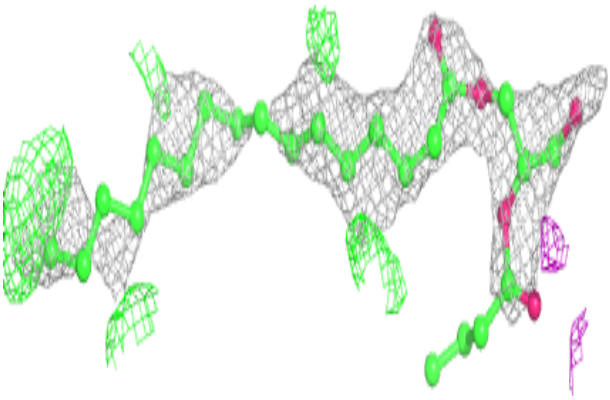


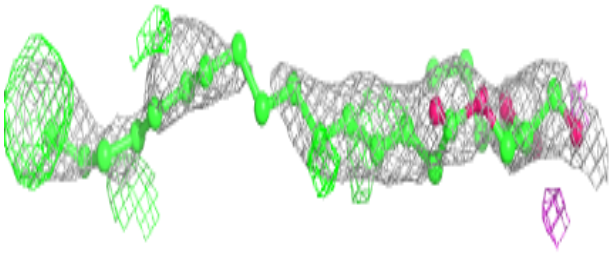


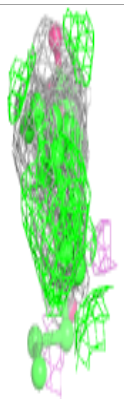


Electron density around UNL A 414:

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

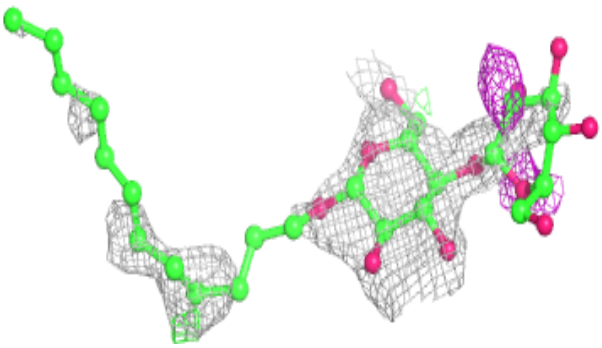


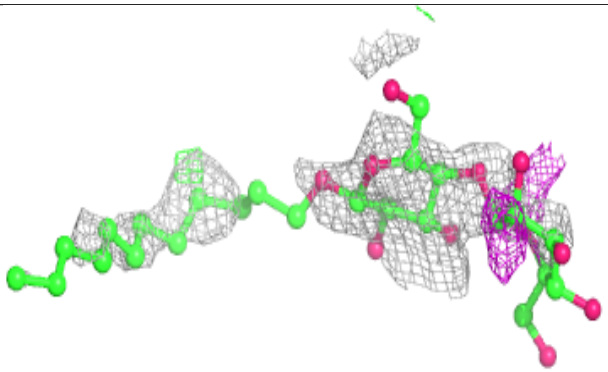


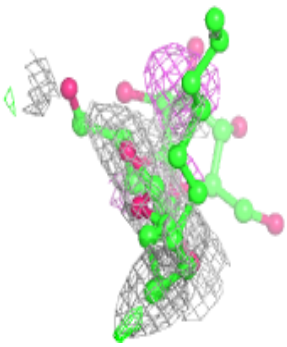


Electron density around LMT C 525:

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

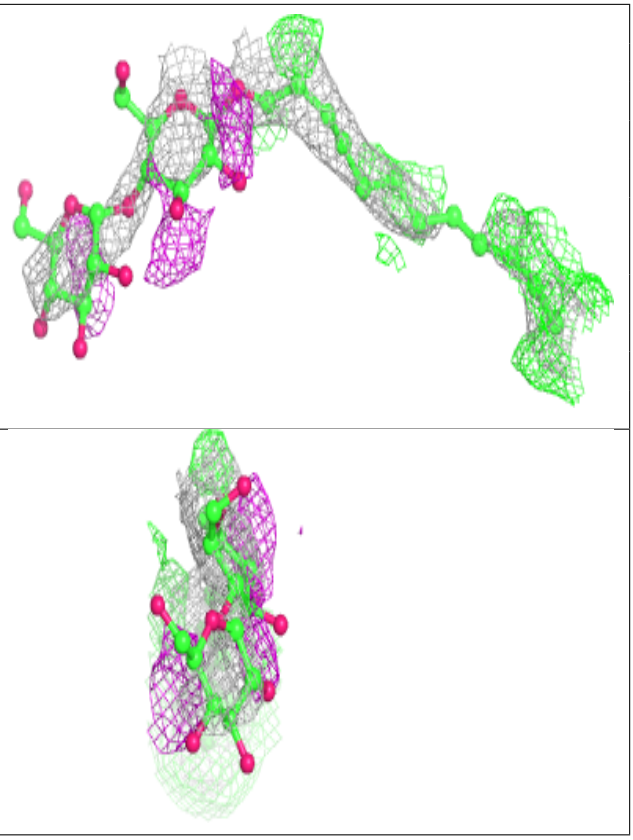


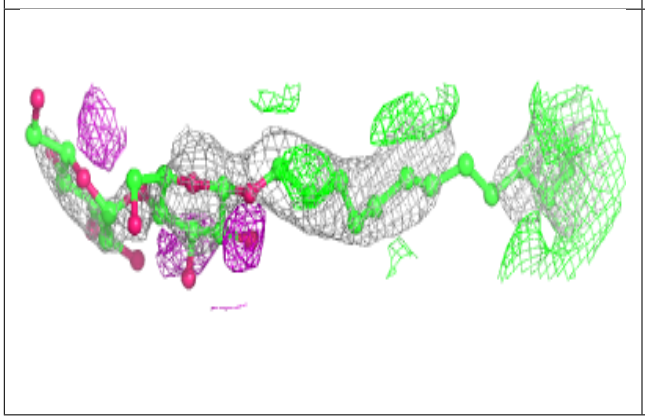




Electron density around LMT a 412:

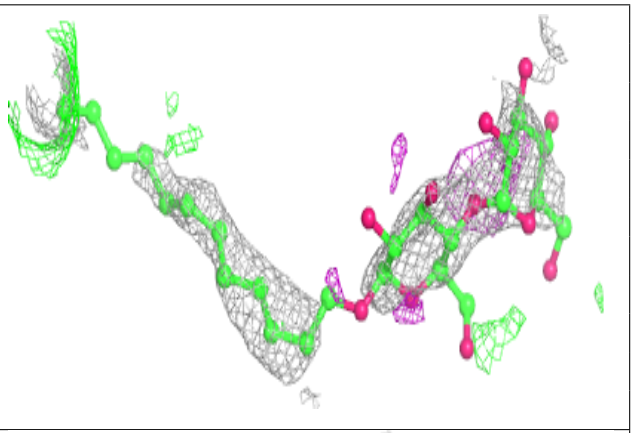
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

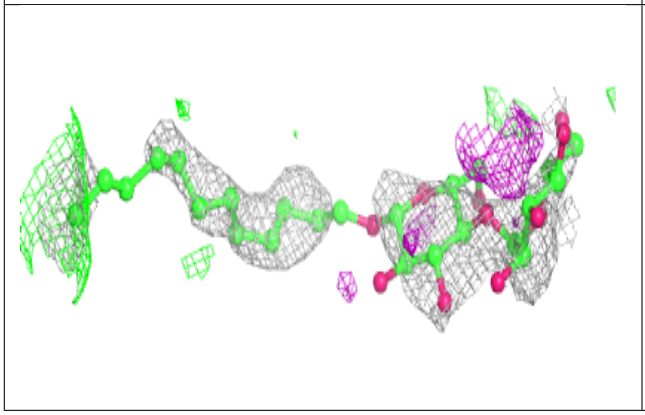


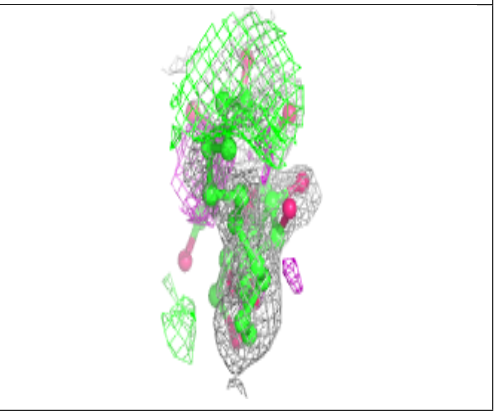


Electron density around LMT D 403:

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

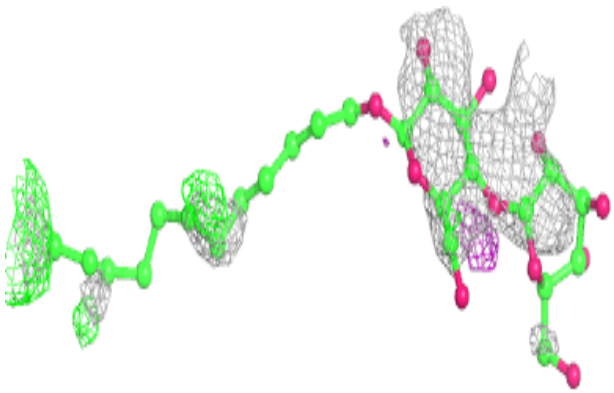


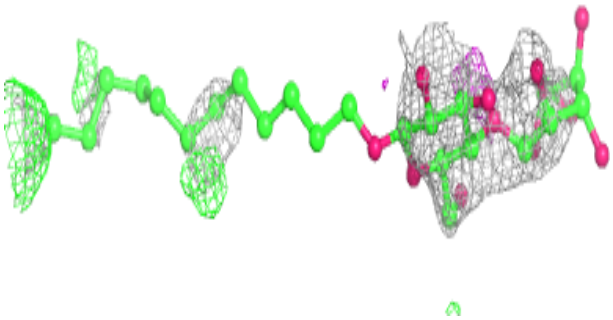


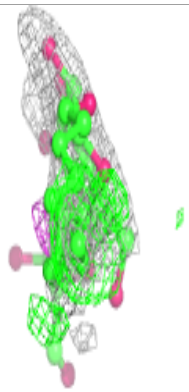


Electron density around LMT e 101:

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

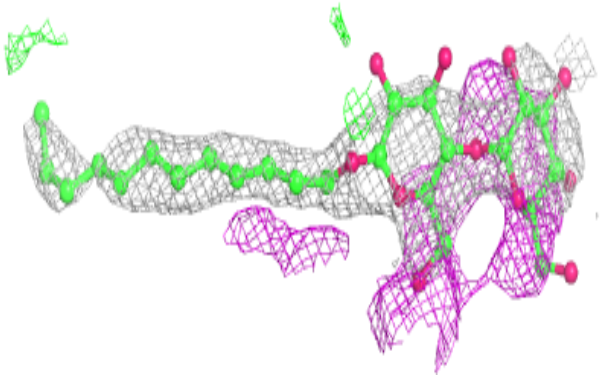


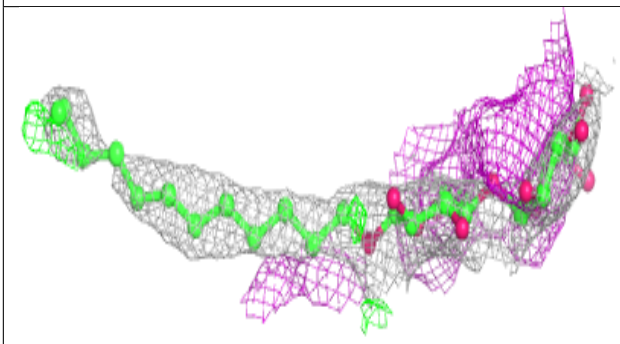


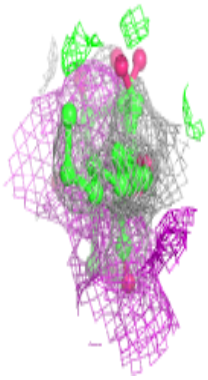


Electron density around LMT m 103:

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

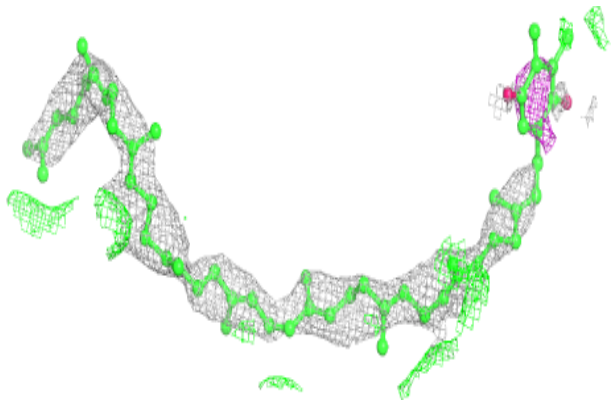


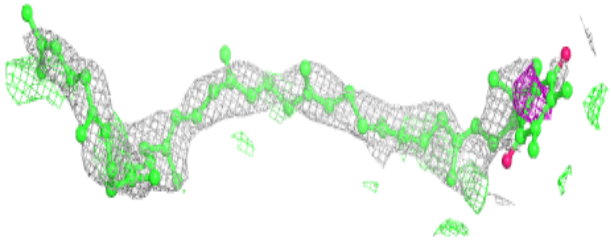


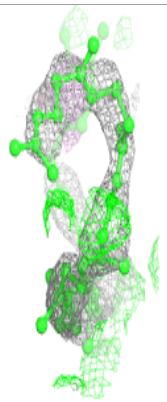


Electron density around PL9 A 413:

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

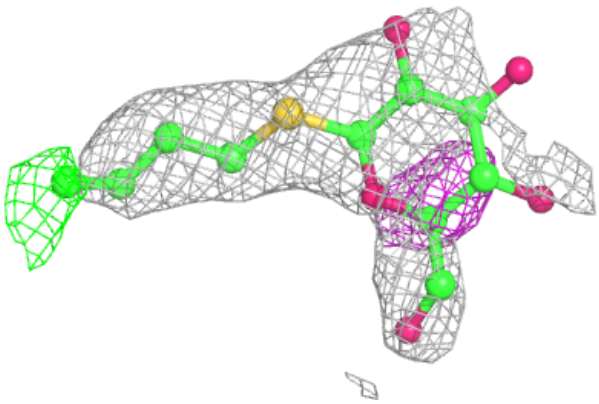


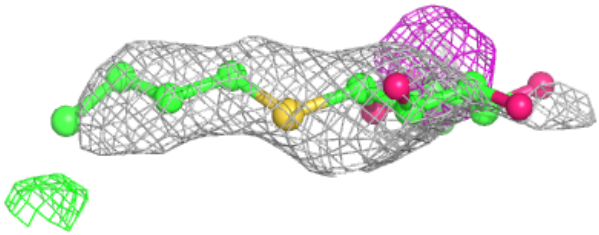


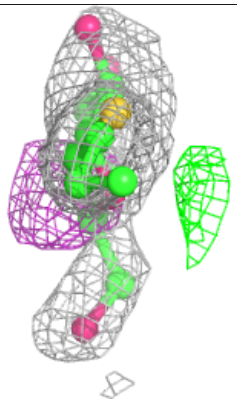


Electron density around HTG D 413:

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

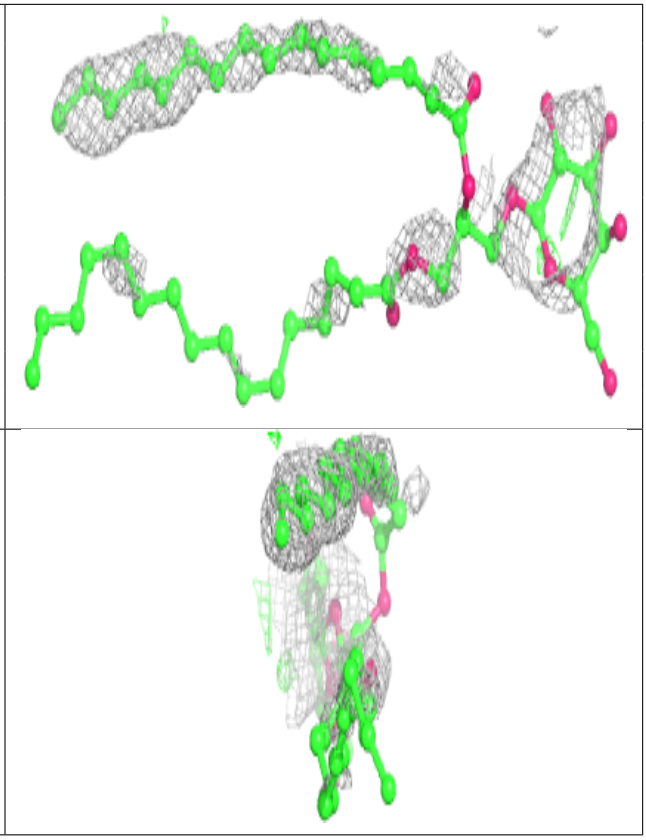






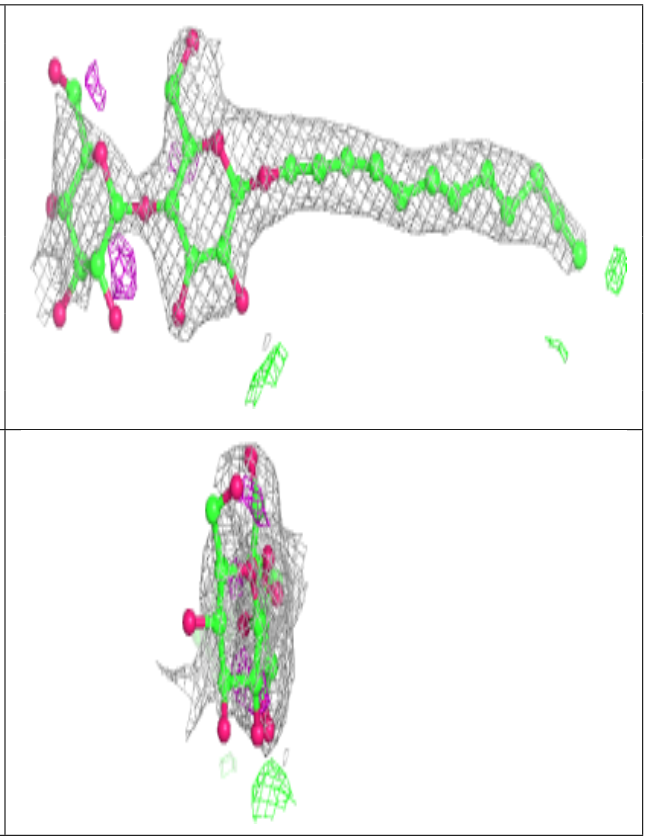
Electron density around LMG c 521:

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



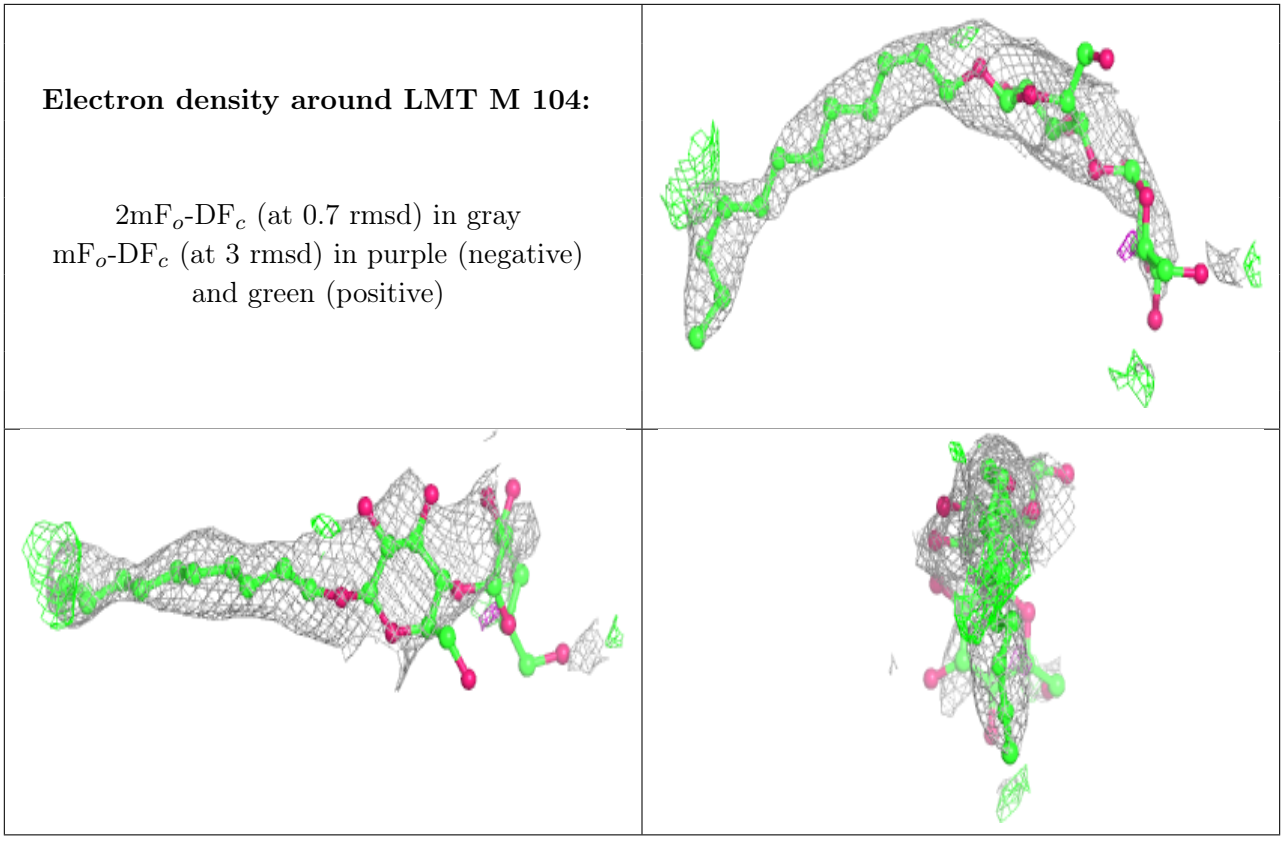
Electron density around LMT M 102:

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



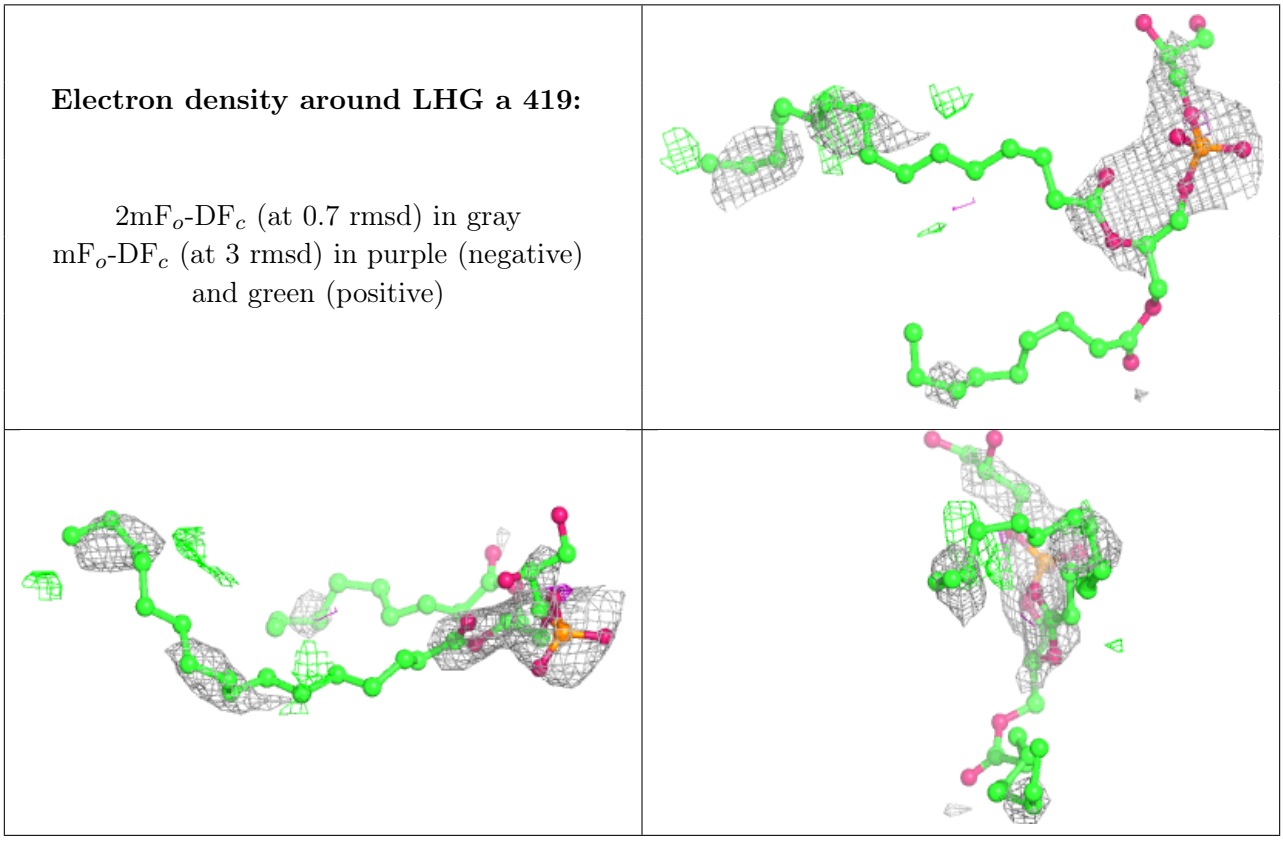
Electron density around LMT M 104:

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



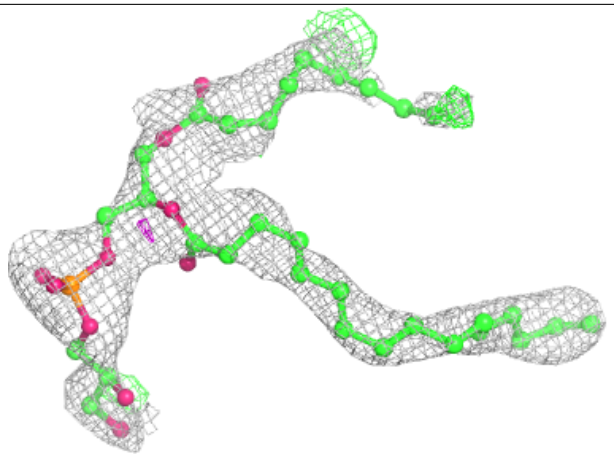
Electron density around LHG a 419:

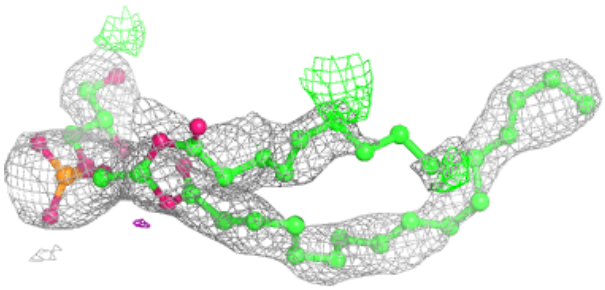
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

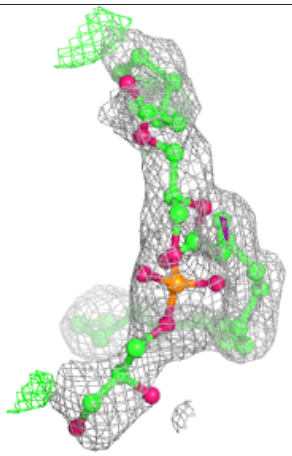


Electron density around LHG E 101:

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

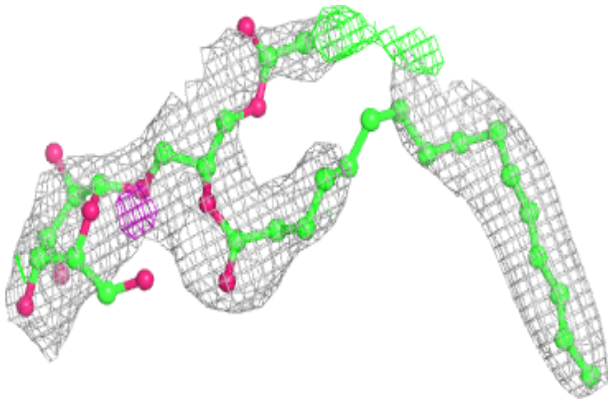


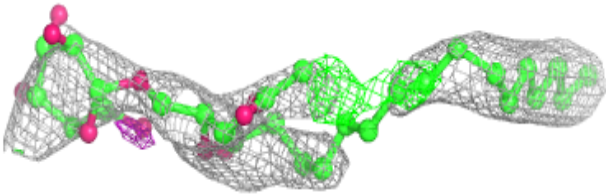


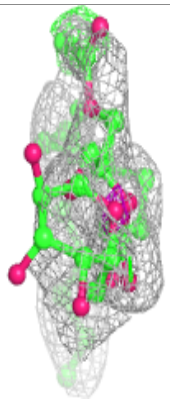


Electron density around LMG Z 101:

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

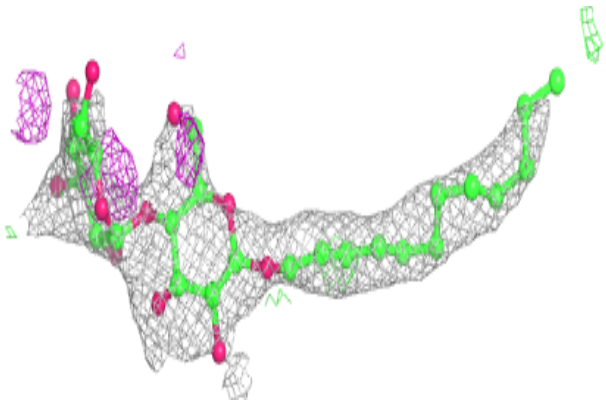


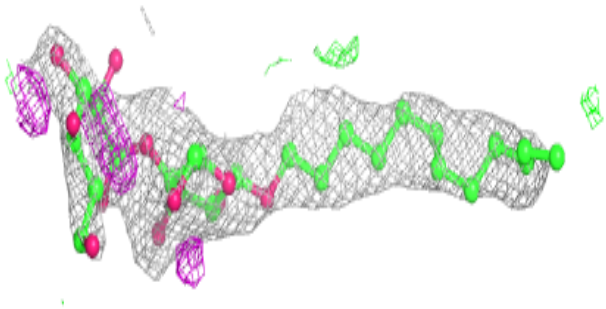




Electron density around LMT D 404:

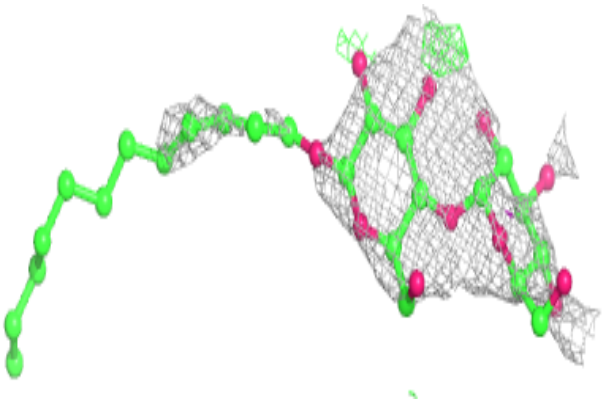
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

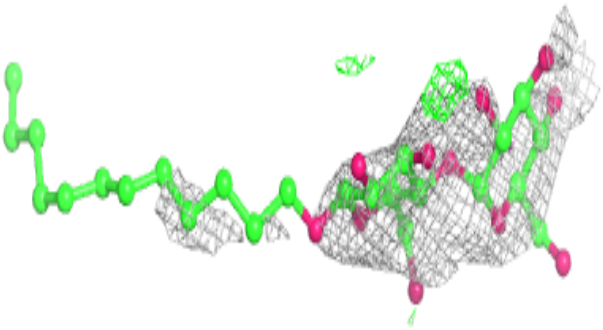


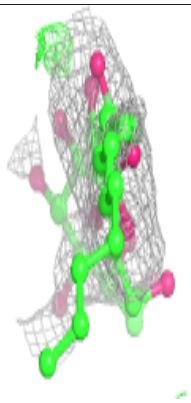


Electron density around LMT a 418:

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

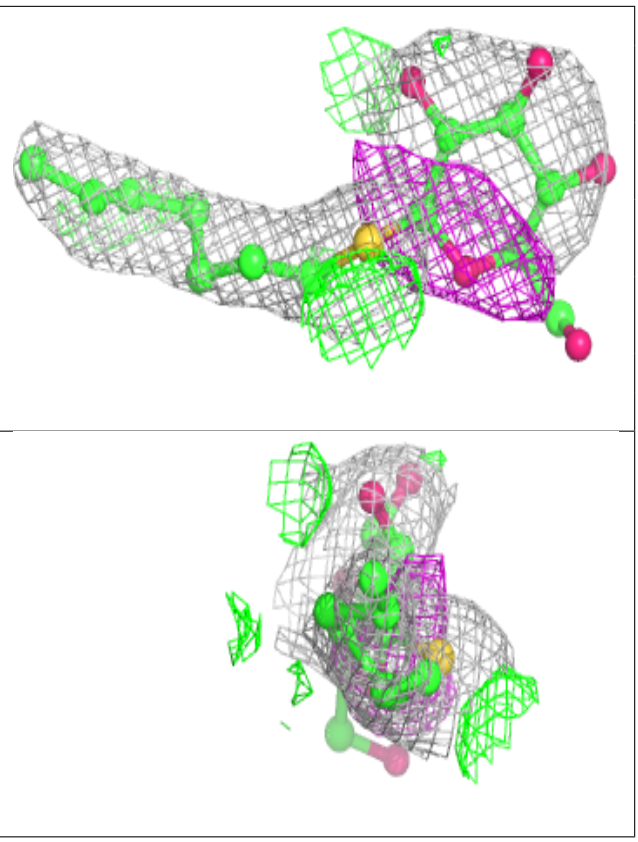






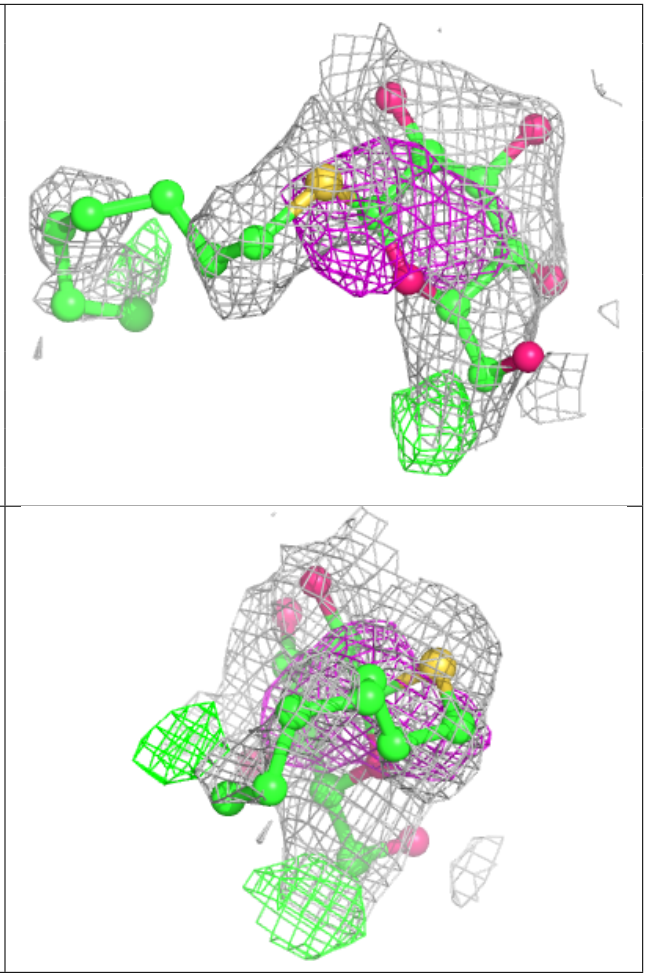
Electron density around HTG B 621:

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



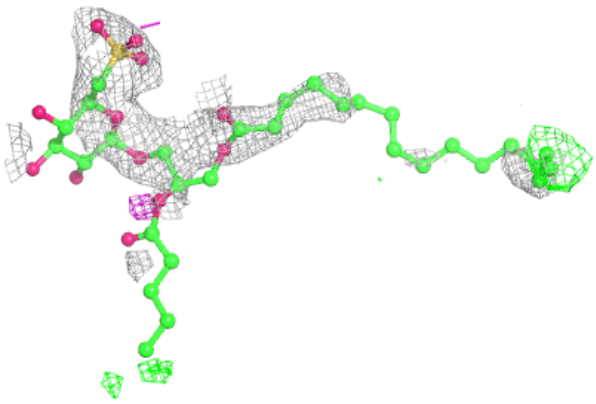
Electron density around HTG B 622:

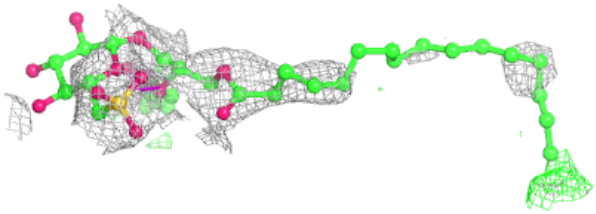
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

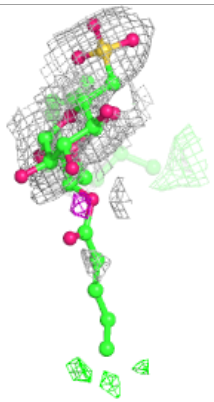


Electron density around SQD f 102:

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

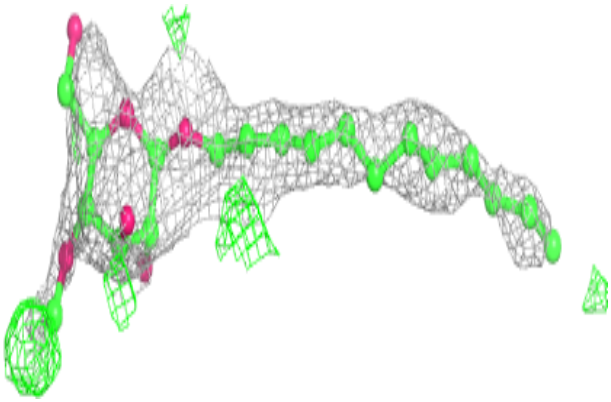


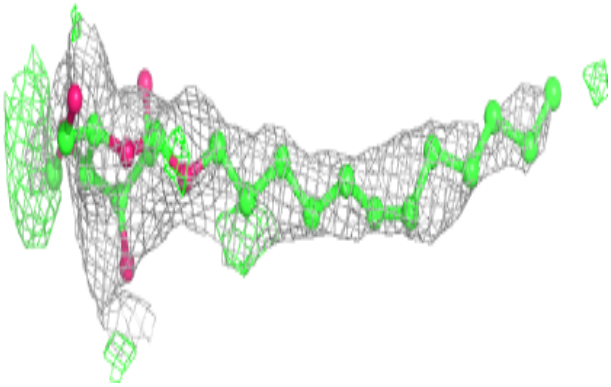


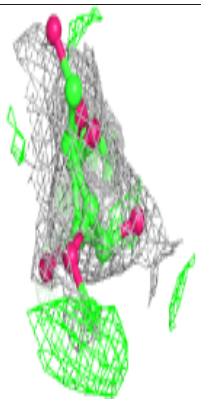


Electron density around LMT b 620:

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

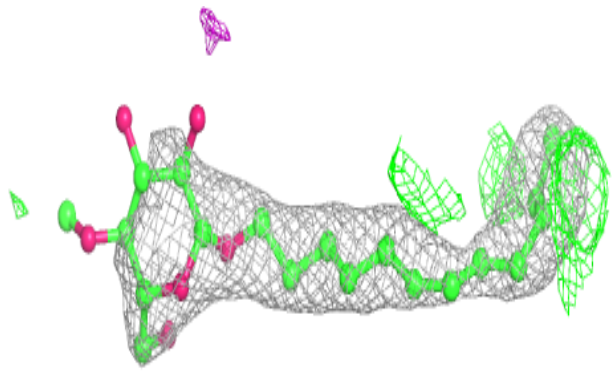


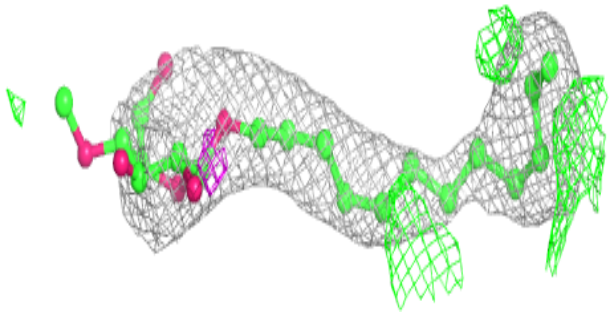


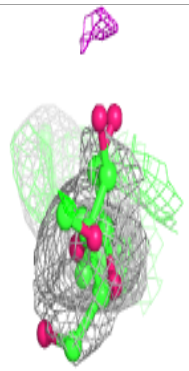


Electron density around LMT b 626:

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

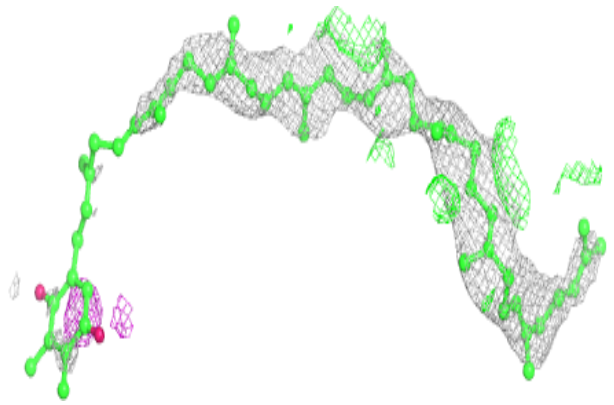


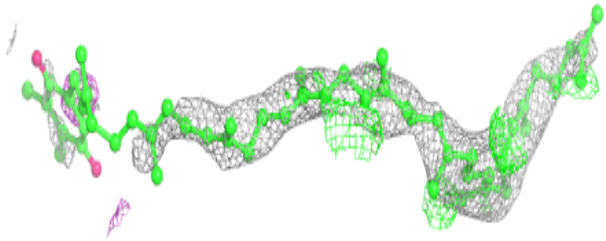


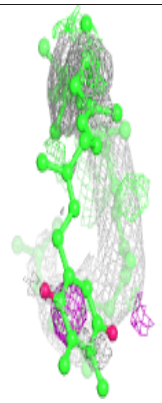


Electron density around PL9 a 414:

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

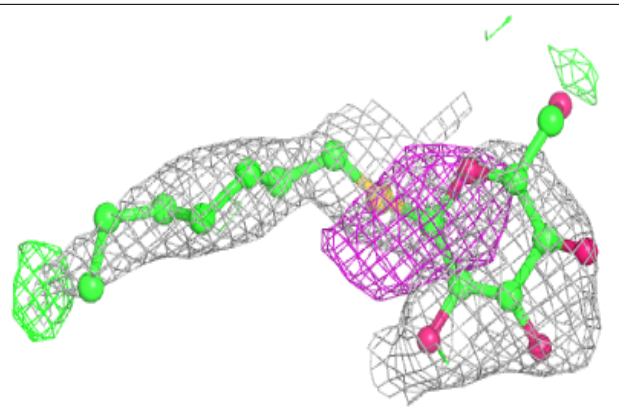


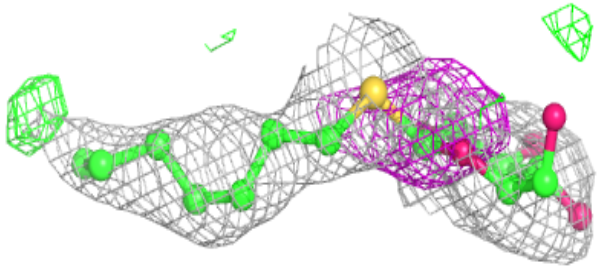


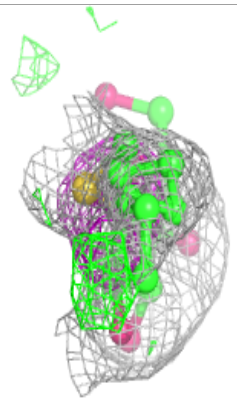


Electron density around HTG b 621:

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

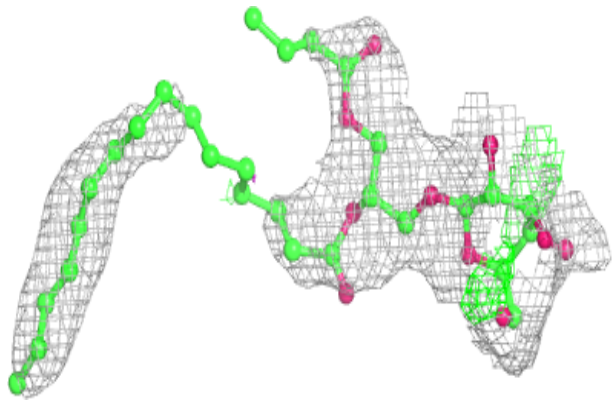


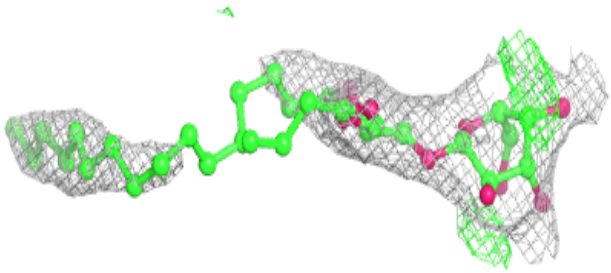


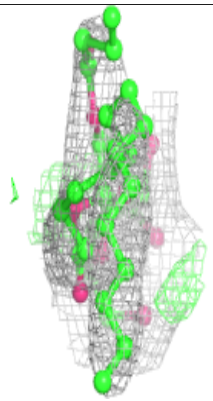


Electron density around LMG z 101:

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

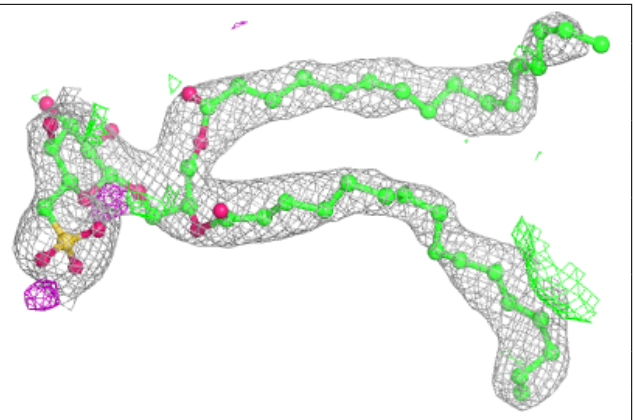


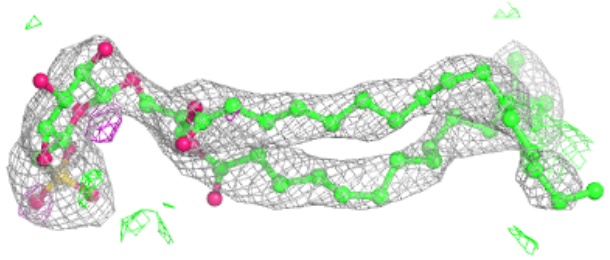


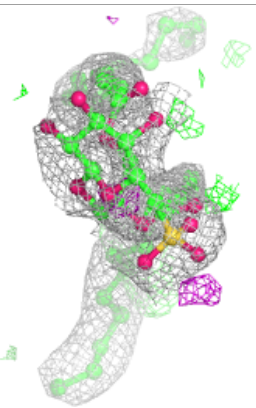


Electron density around SQD L 102:

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

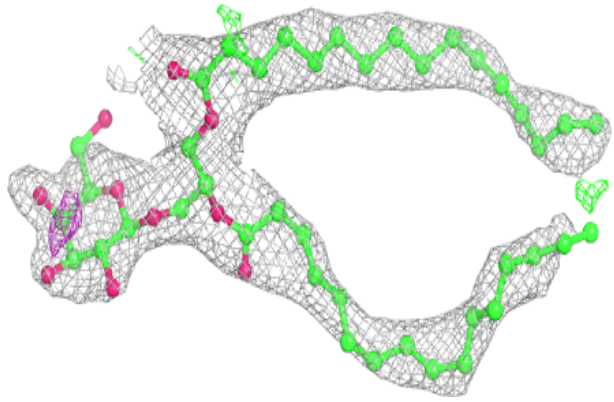


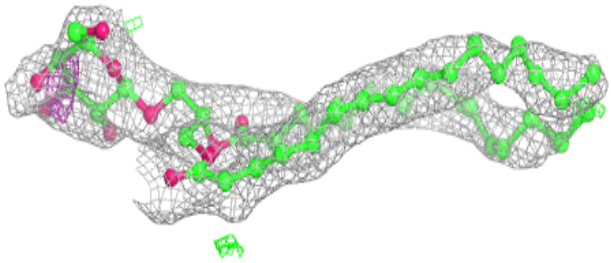


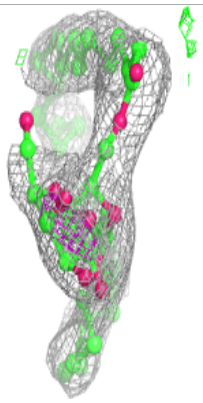


Electron density around LMG a 417:

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

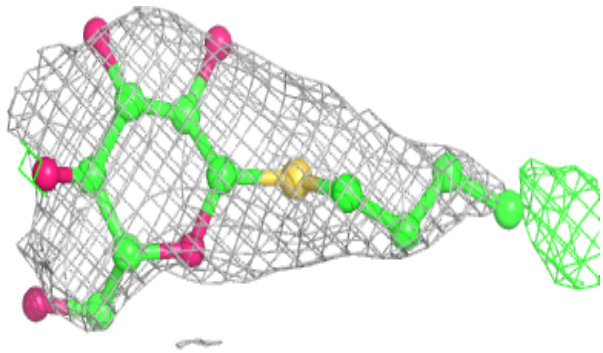


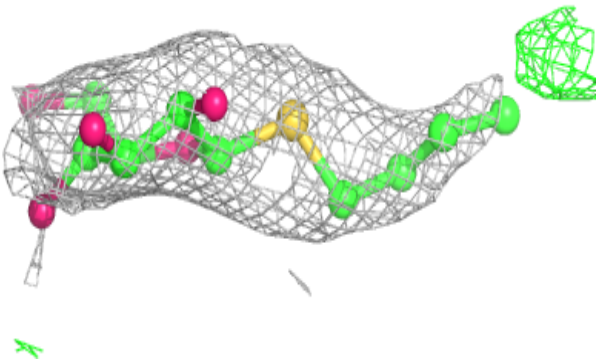


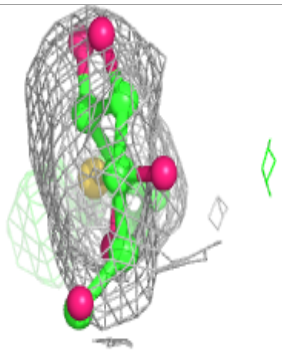


Electron density around HTG h 101:

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

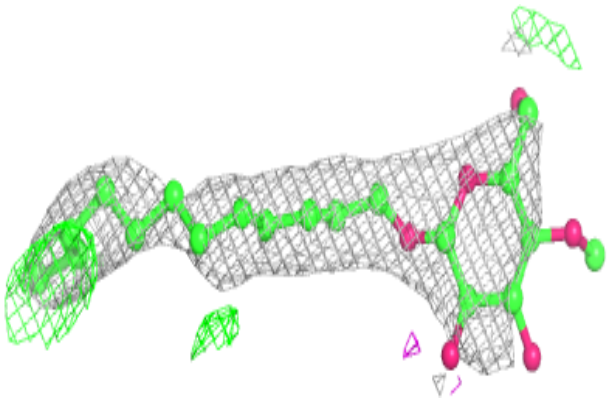


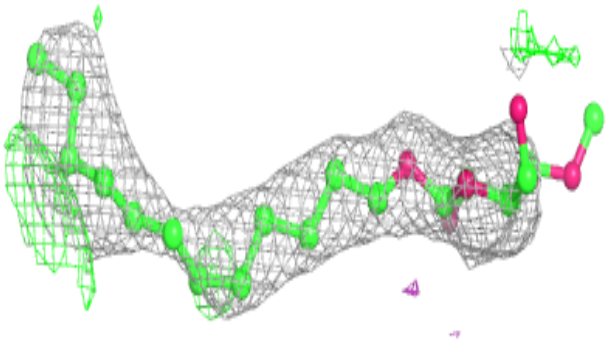


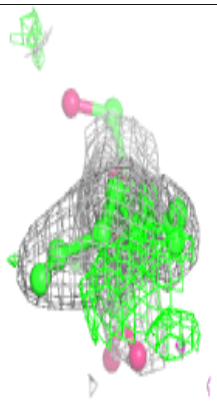


Electron density around LMT B 628:

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

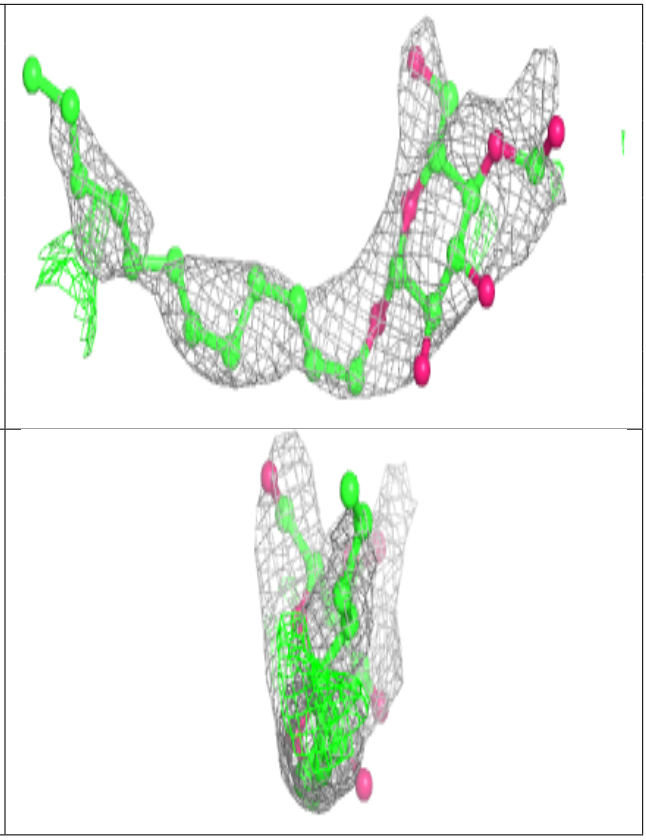






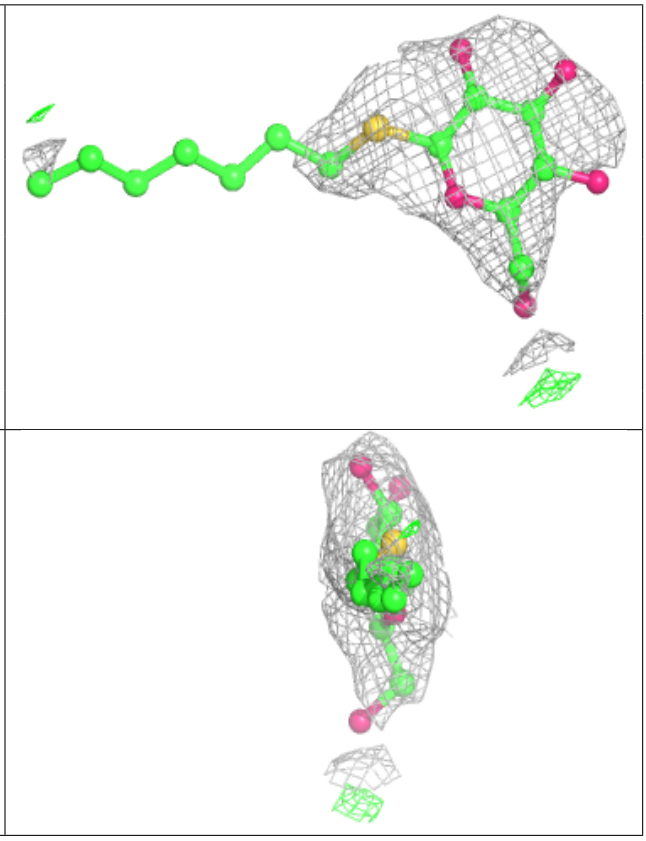
Electron density around LMT t 101:

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



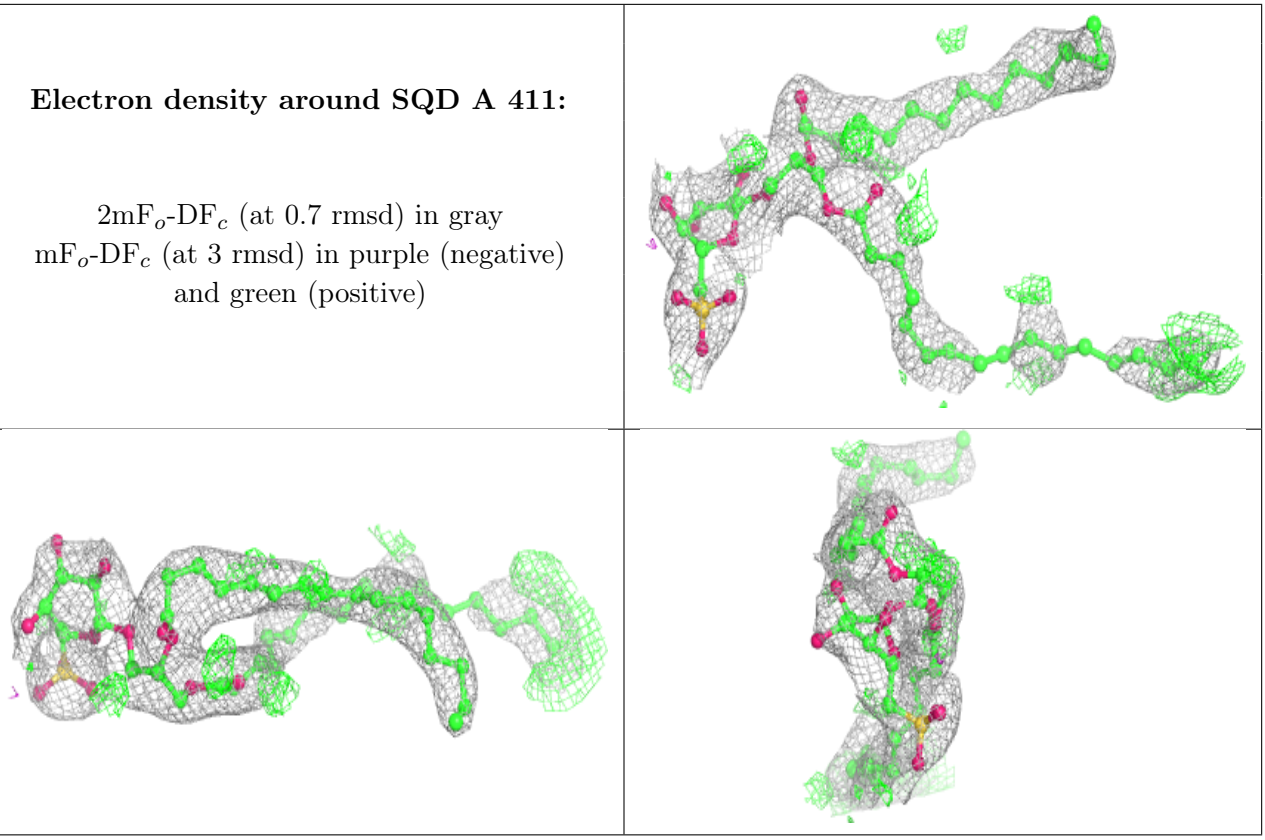
Electron density around HTG c 522:

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



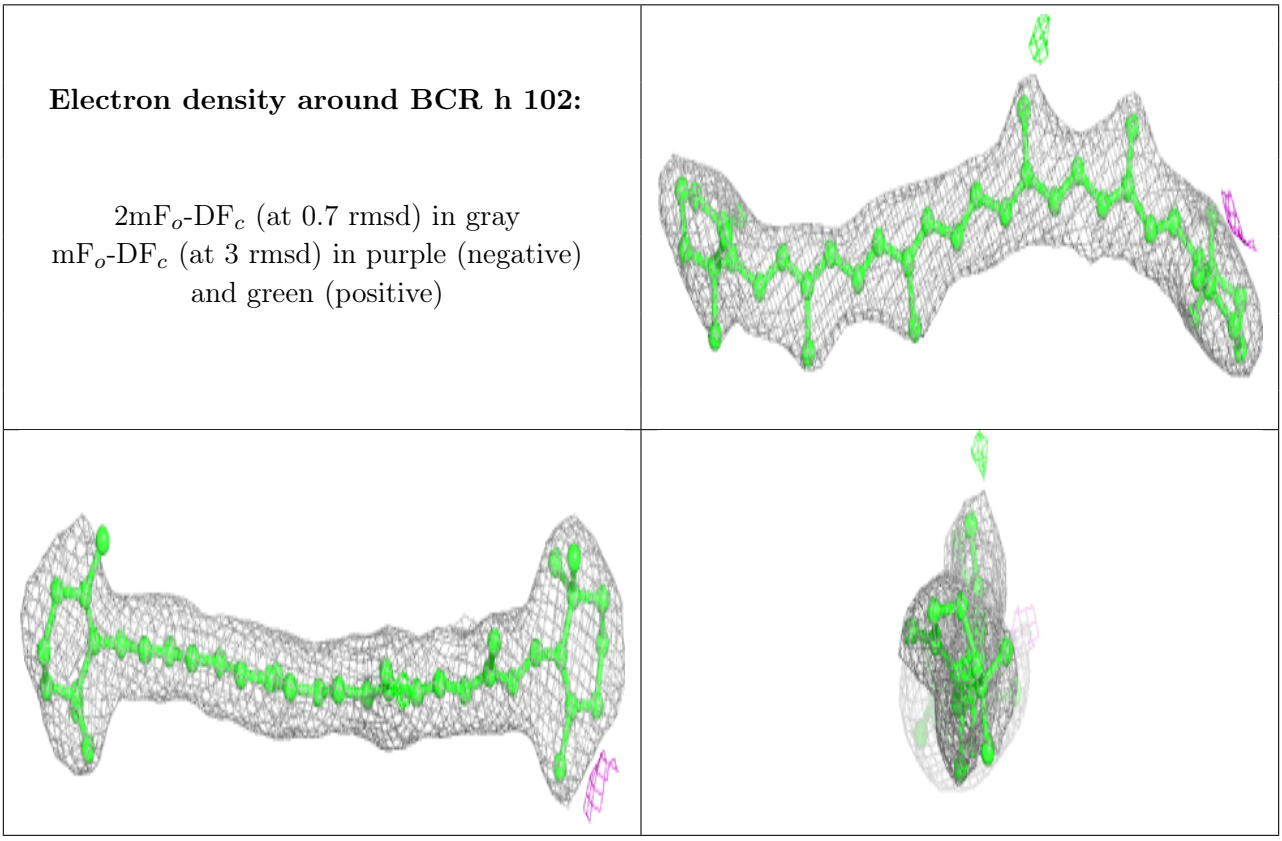
Electron density around SQD A 411:

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



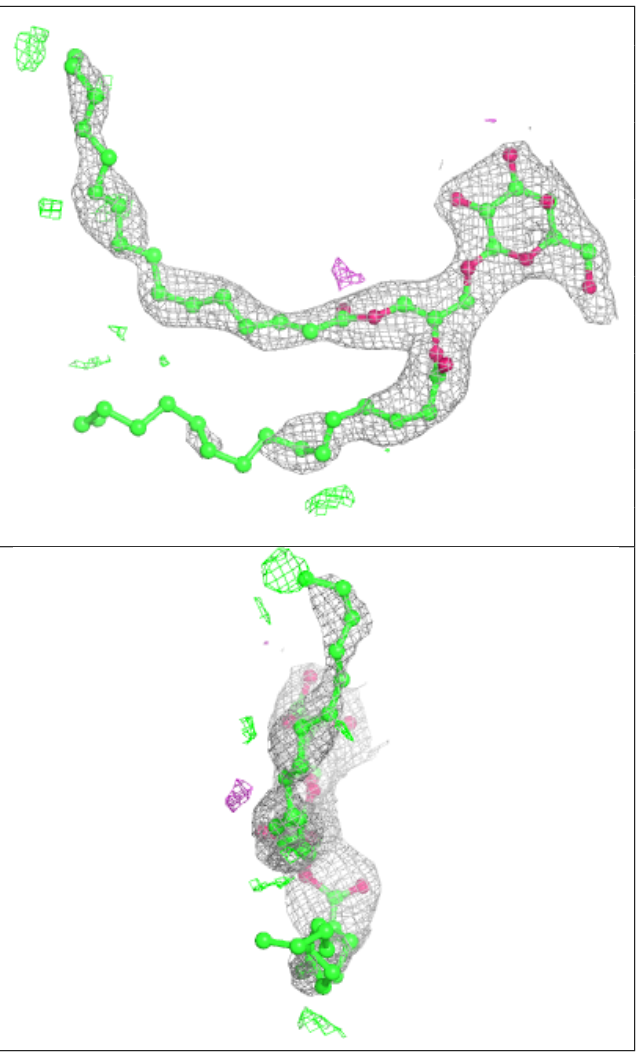
Electron density around BCR h 102:

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



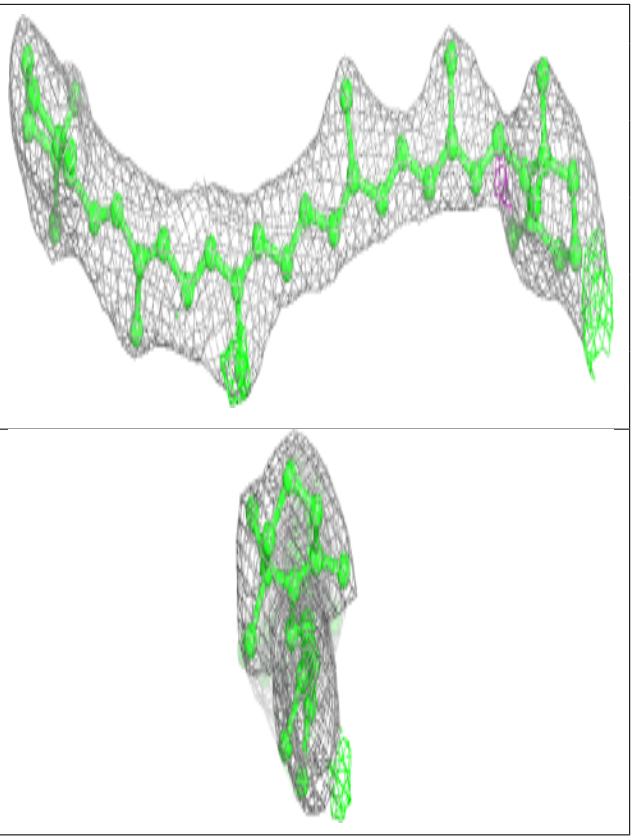
Electron density around LMG C 520:

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



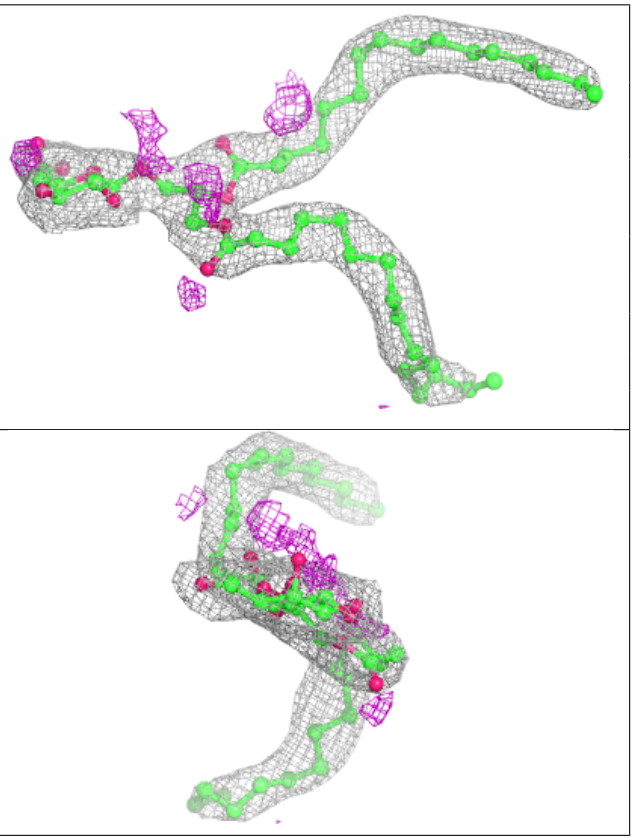
Electron density around BCR H 101:

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



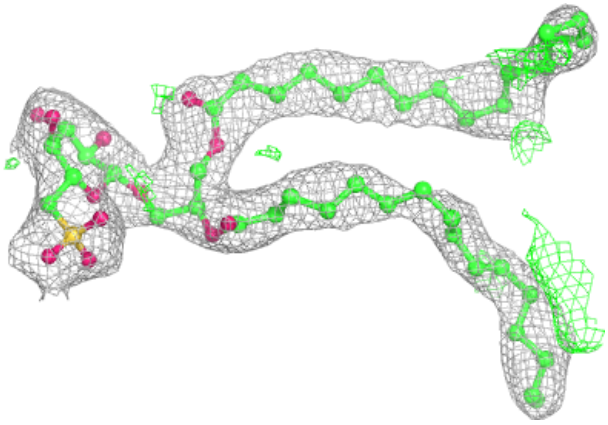
Electron density around LMG m 101:

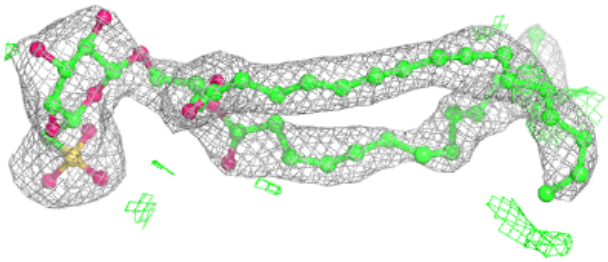
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

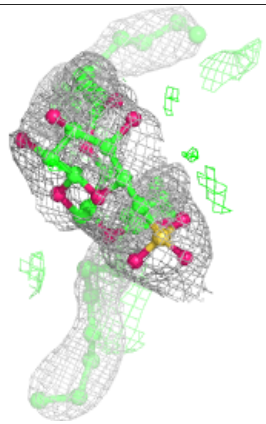


Electron density around SQD B 620:

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

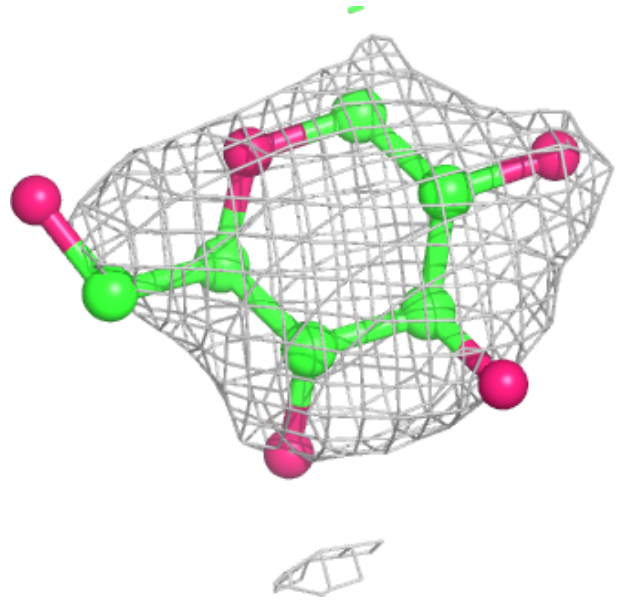


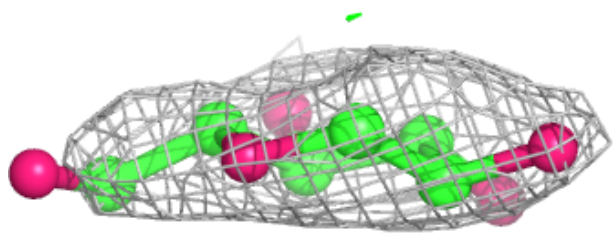


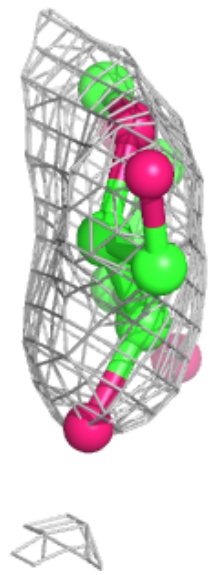


Electron density around HTG V 202:

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

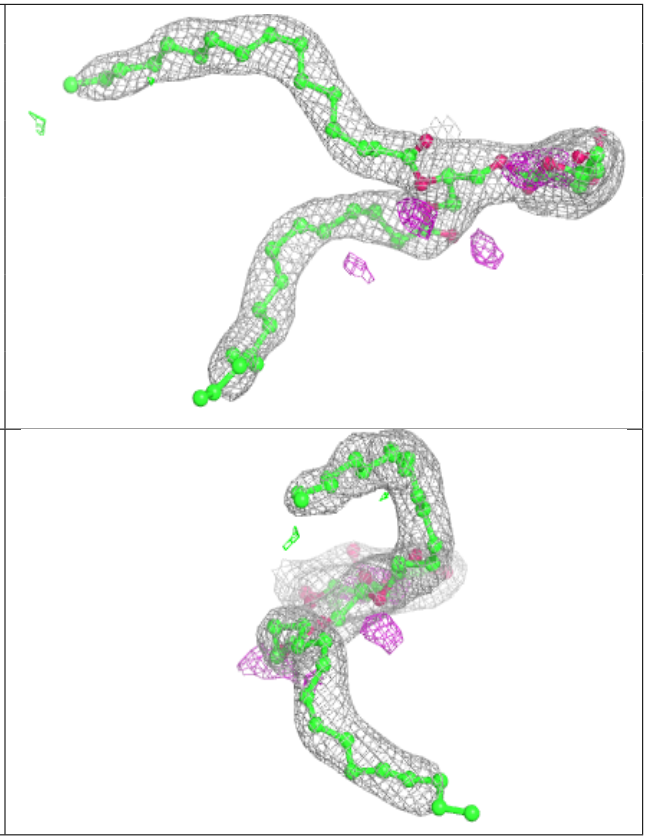


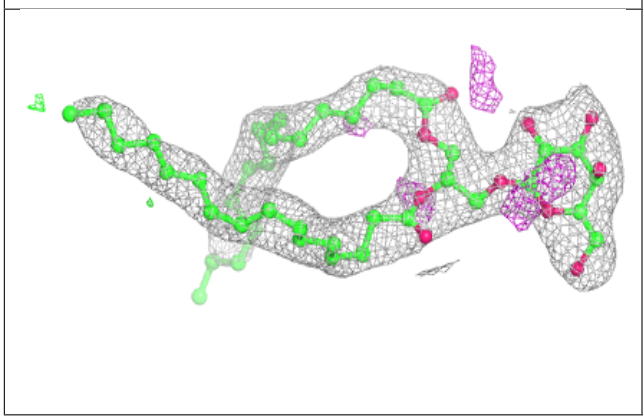




Electron density around LMG M 101:

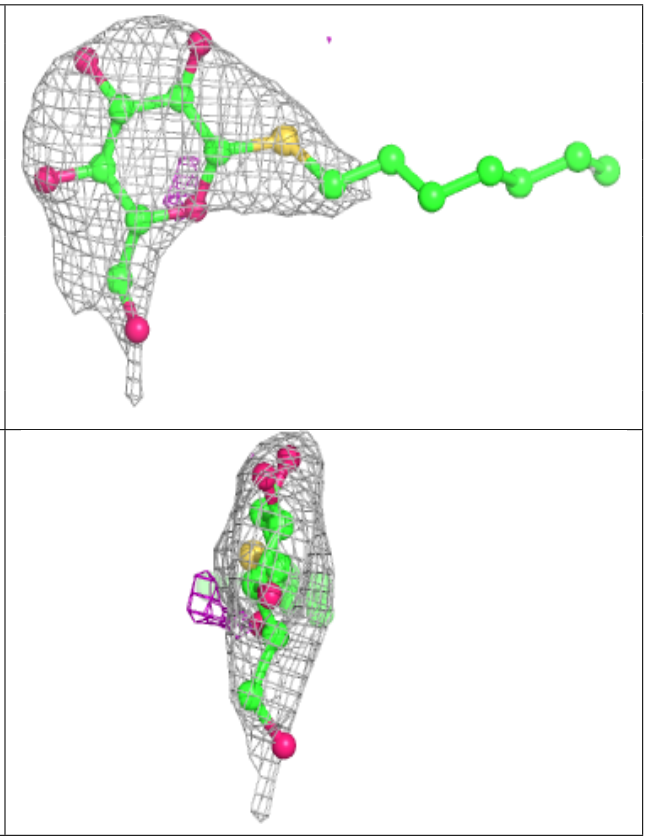
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

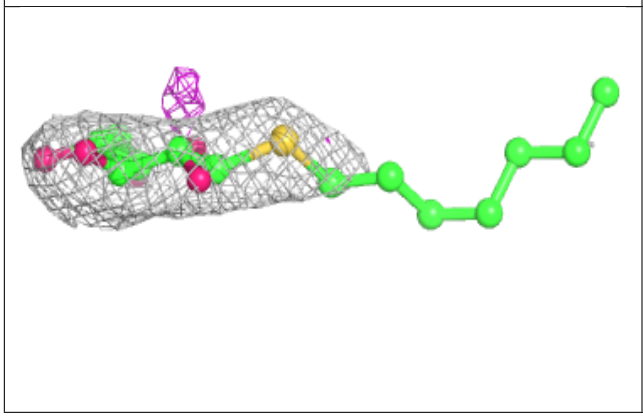




Electron density around HTG C 522:

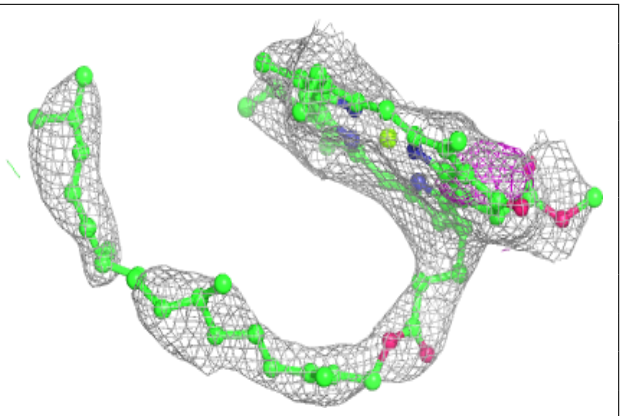
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

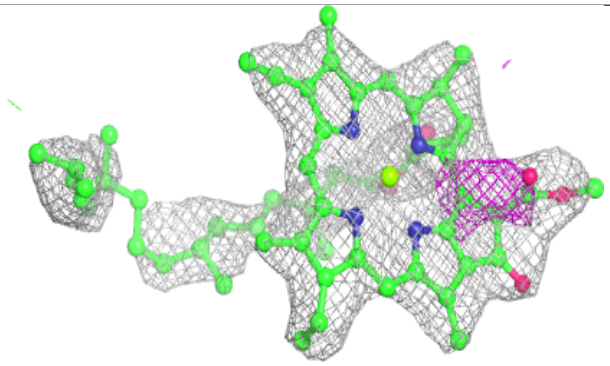


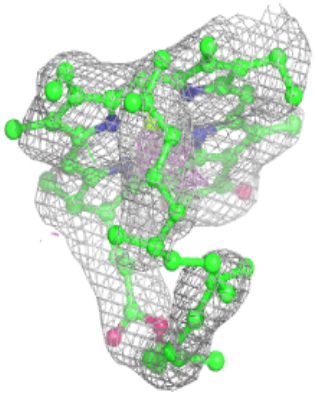


Electron density around CLA C 514:

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

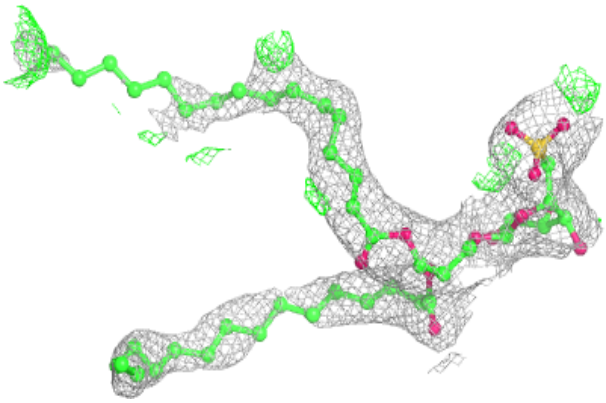


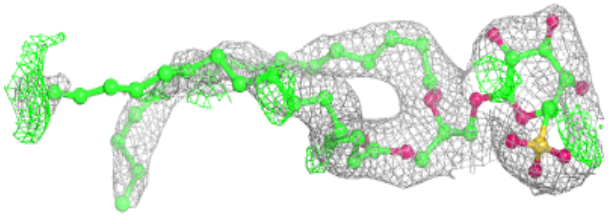


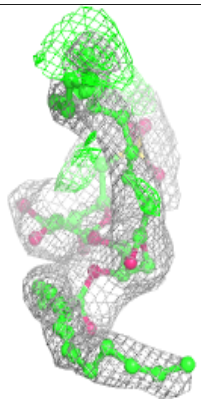


Electron density around SQD a 411:

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

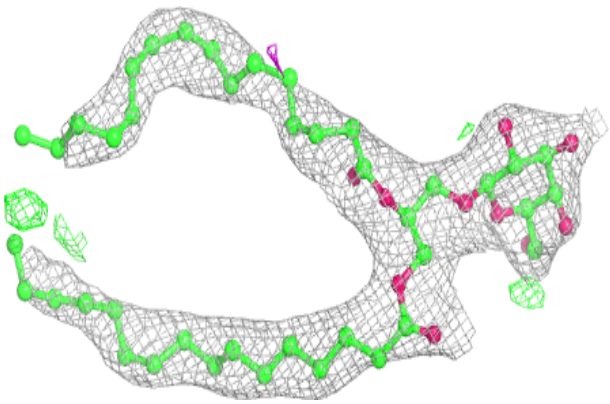


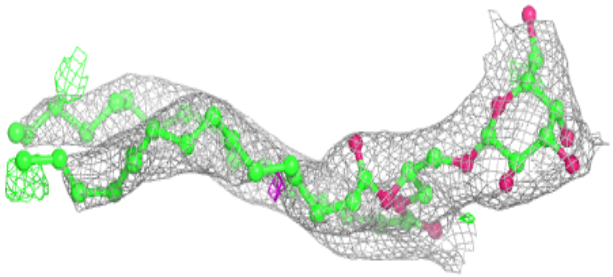


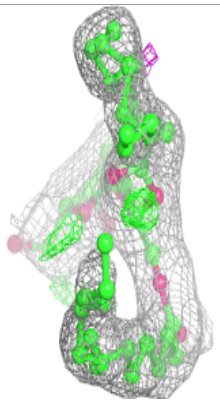


Electron density around LMG A 415:

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

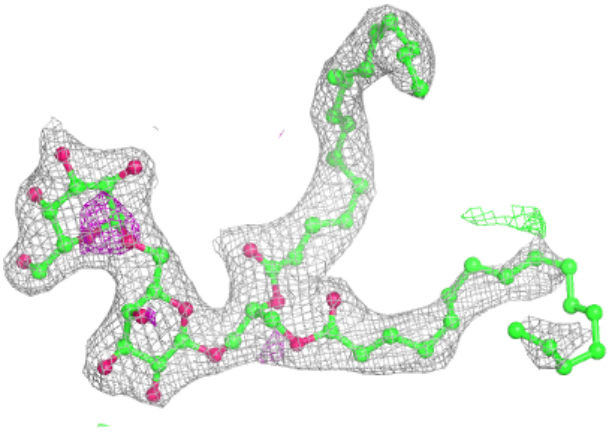


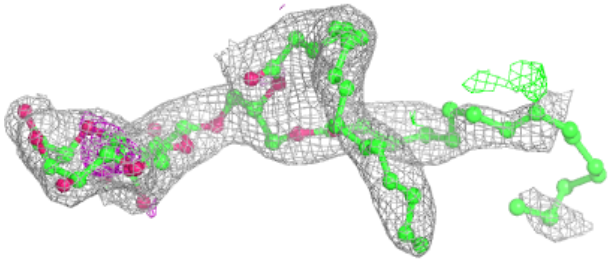


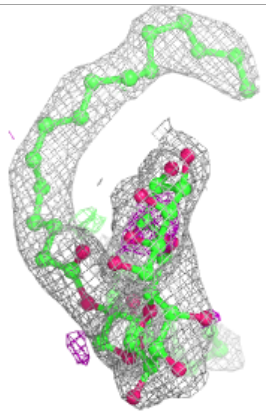


Electron density around DGD C 518:

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

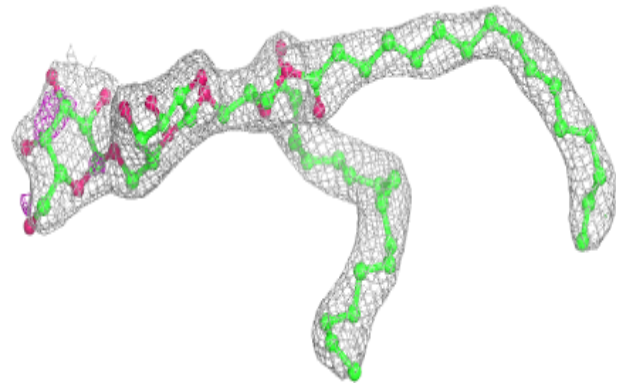


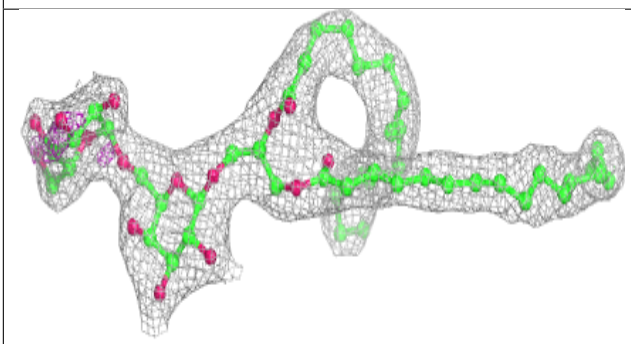


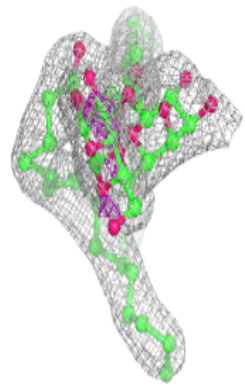


Electron density around DGD h 103:

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

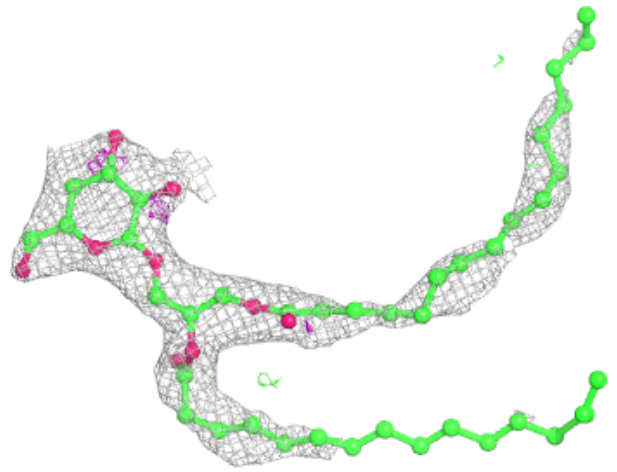


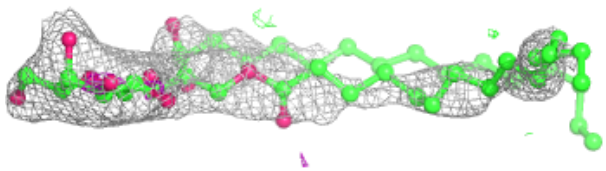


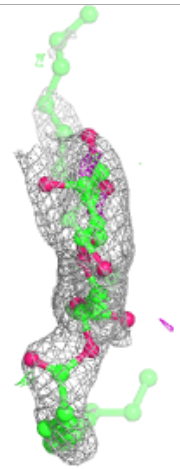


Electron density around LMG c 520:

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

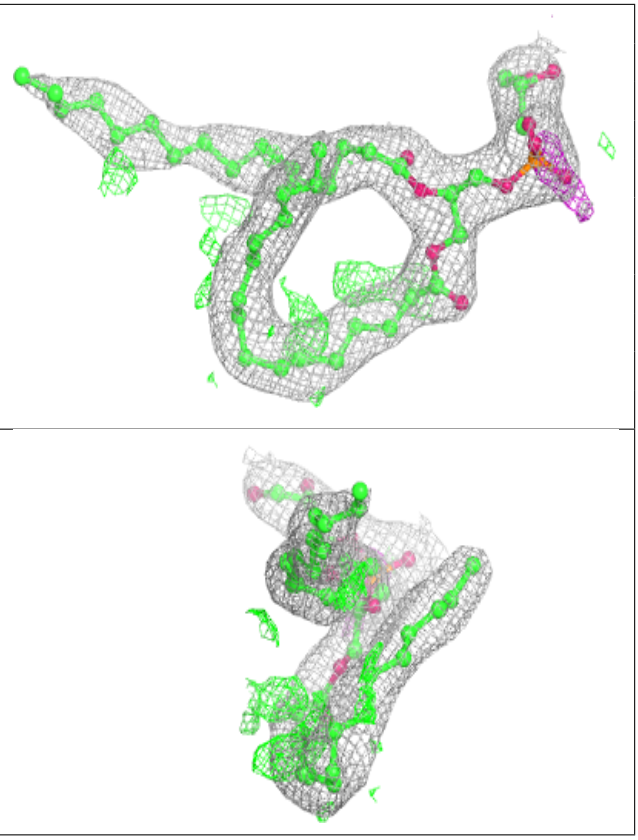






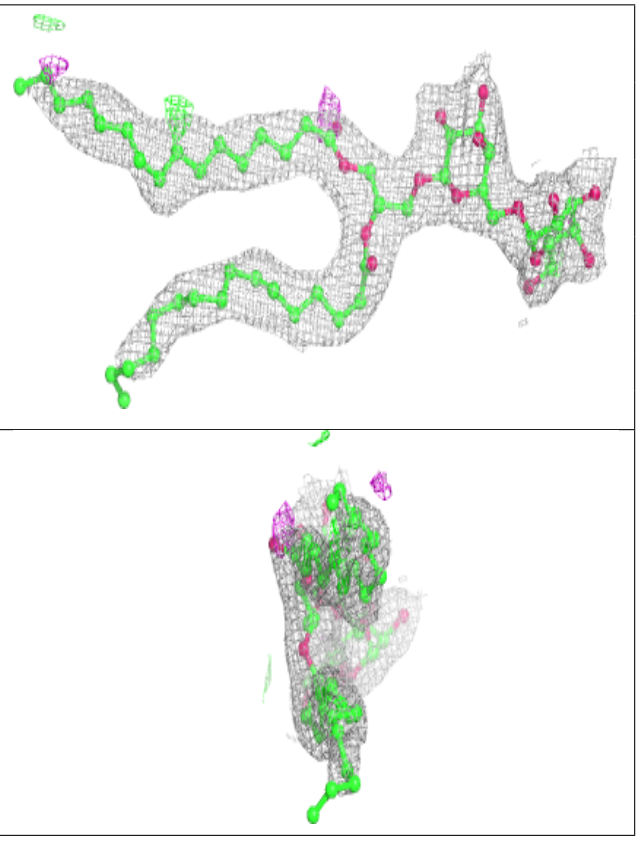
Electron density around LHG A 416:

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



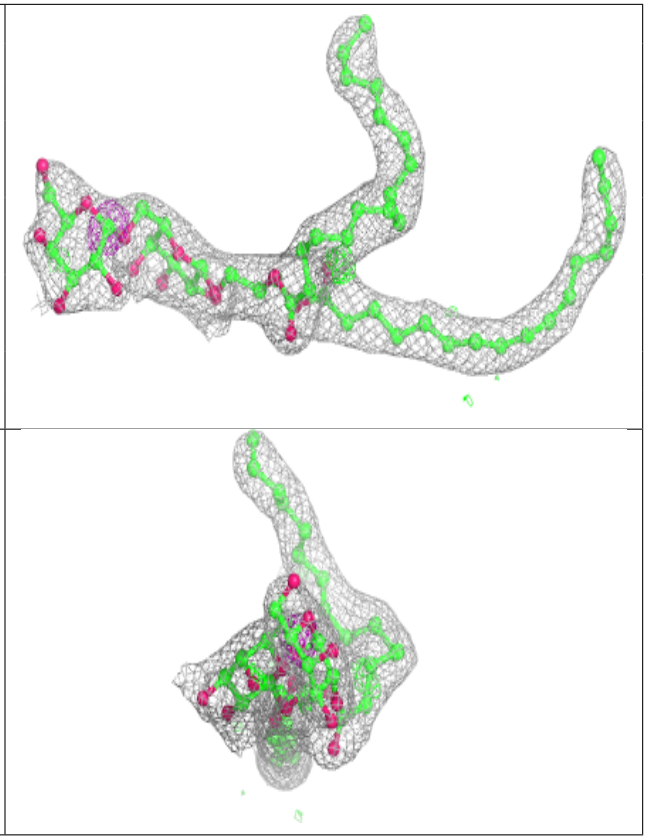
Electron density around DGD C 519:

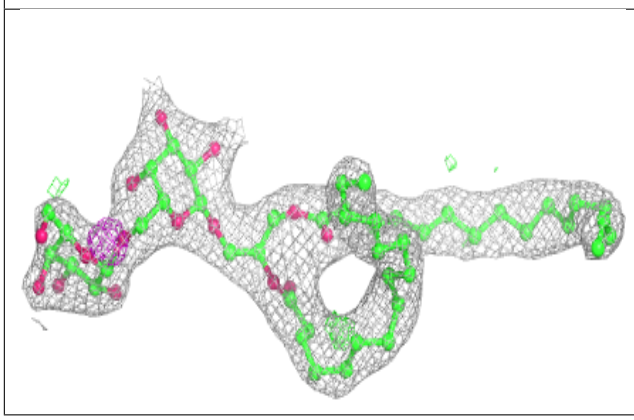
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DGD H 102:

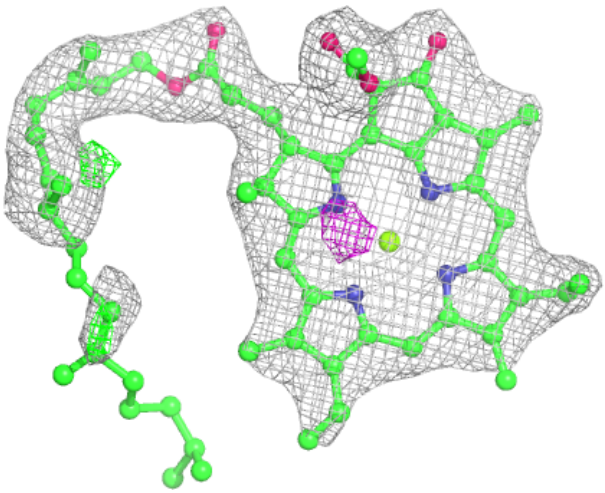
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

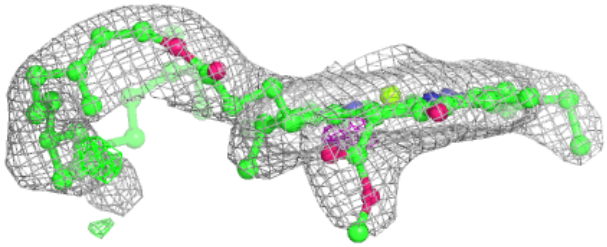


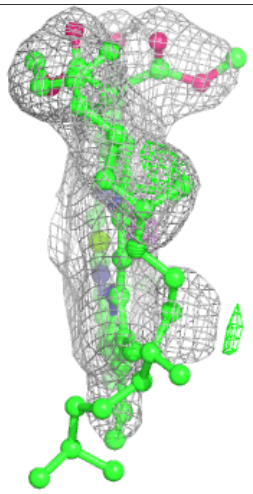


Electron density around CLA C 513:

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

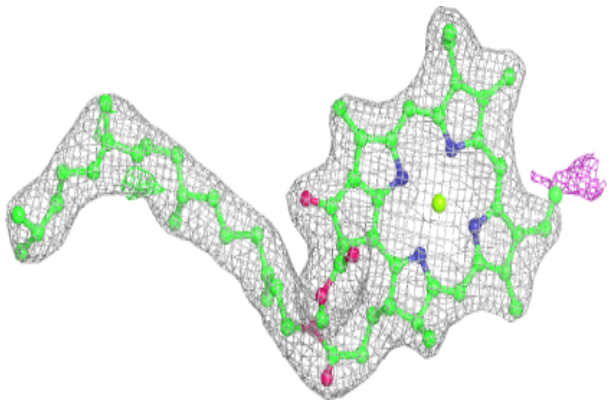


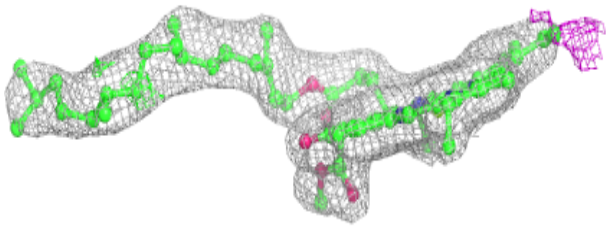


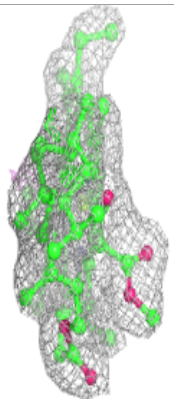


Electron density around CLA B 602:

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

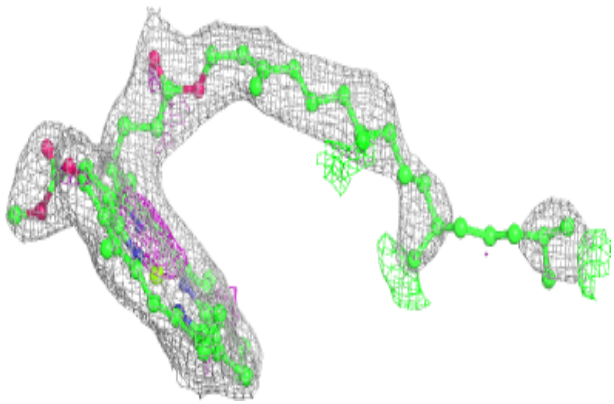


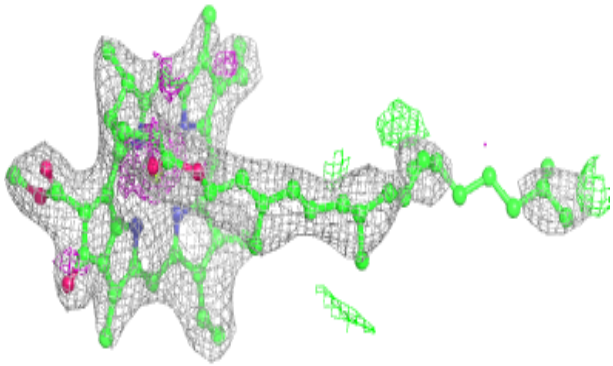


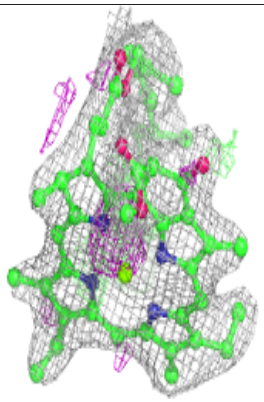


Electron density around CLA C 505:

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

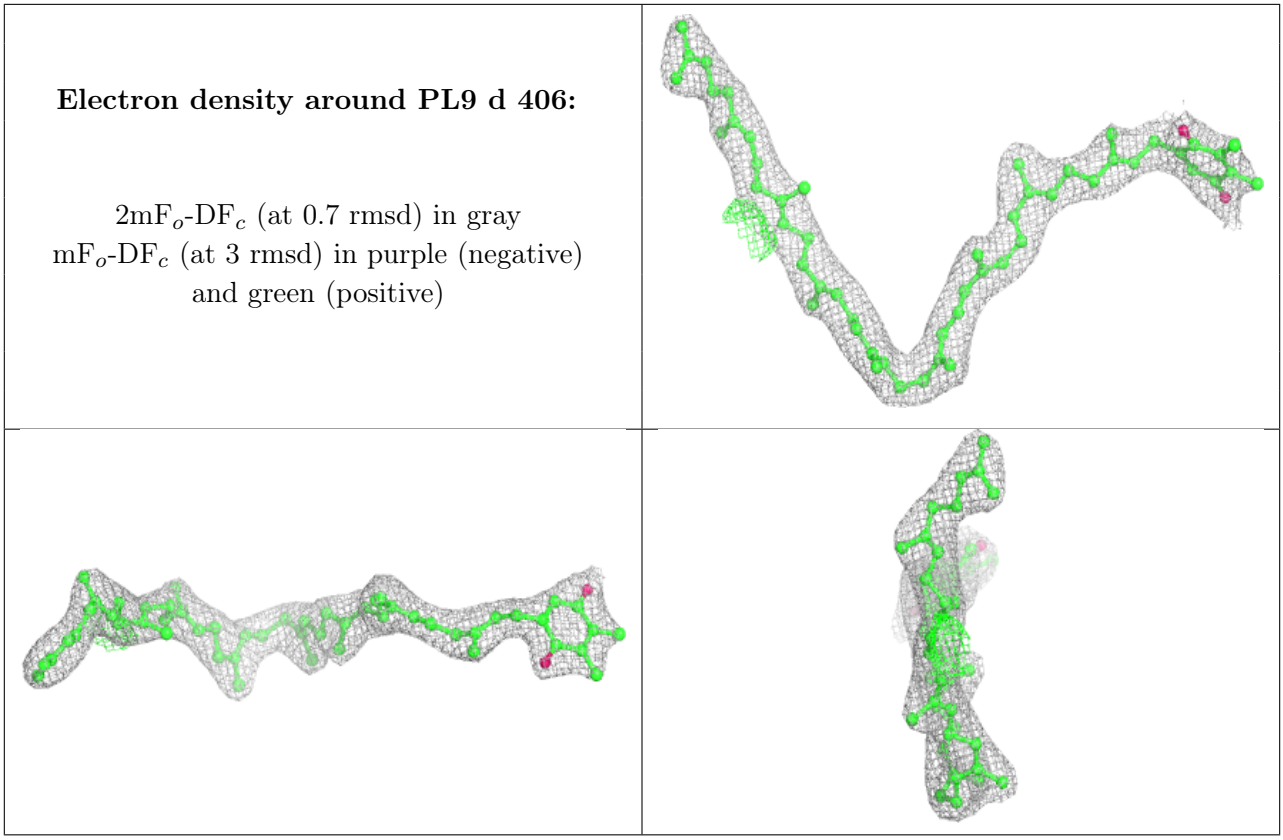






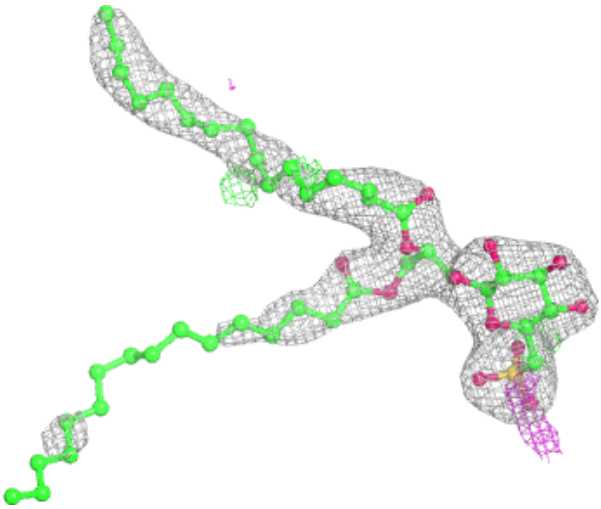
Electron density around PL9 d 406:

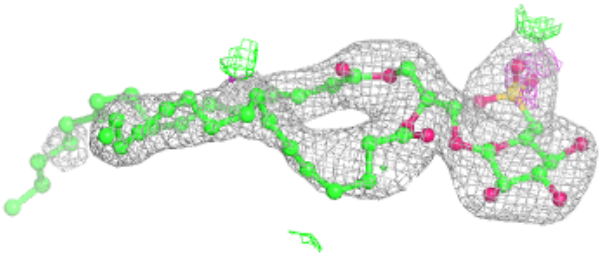
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

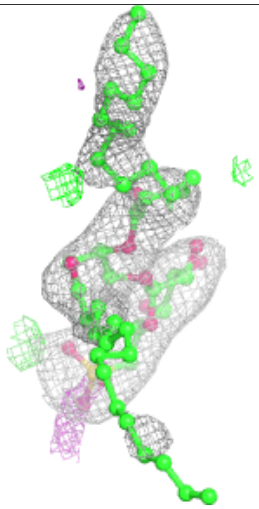


Electron density around SQD C 501:

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

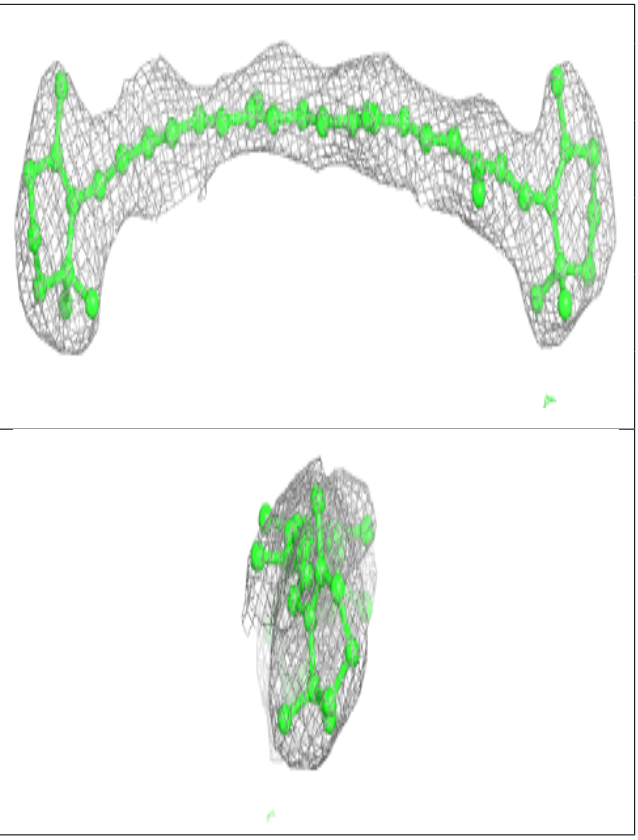






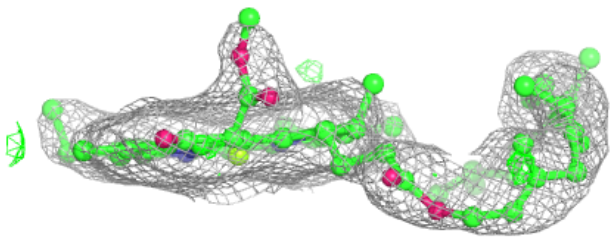
Electron density around BCR k 101:

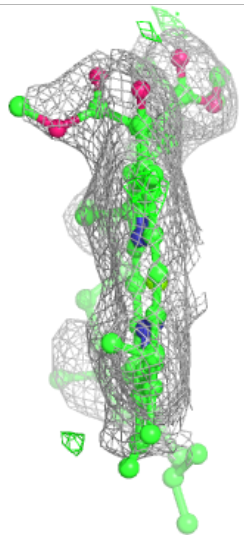
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA c 513:

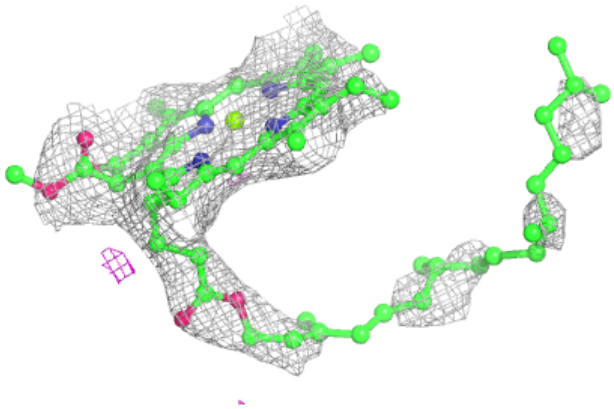
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

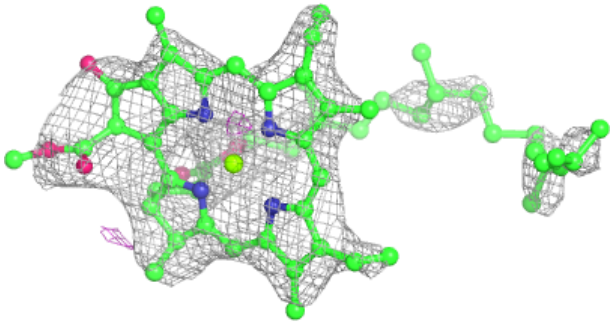


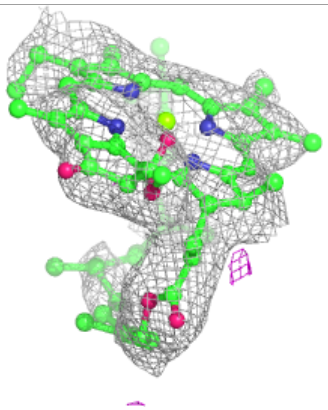


Electron density around CLA c 514:

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

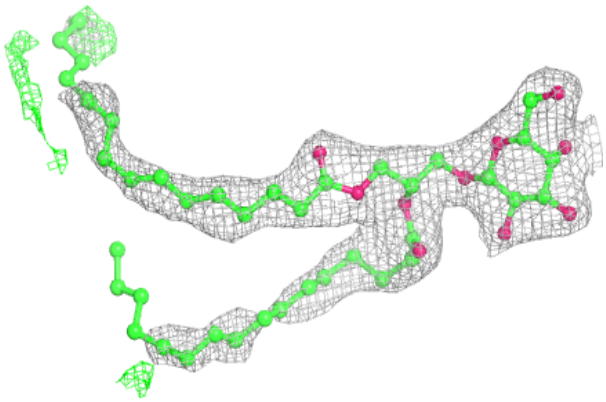


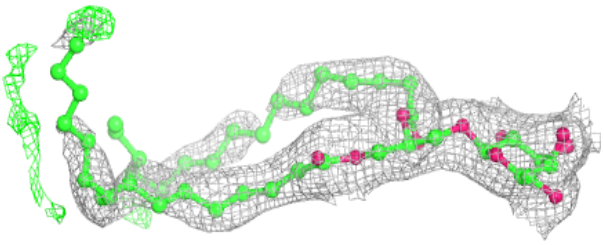


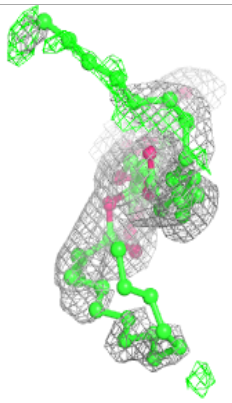


Electron density around LMG D 414:

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

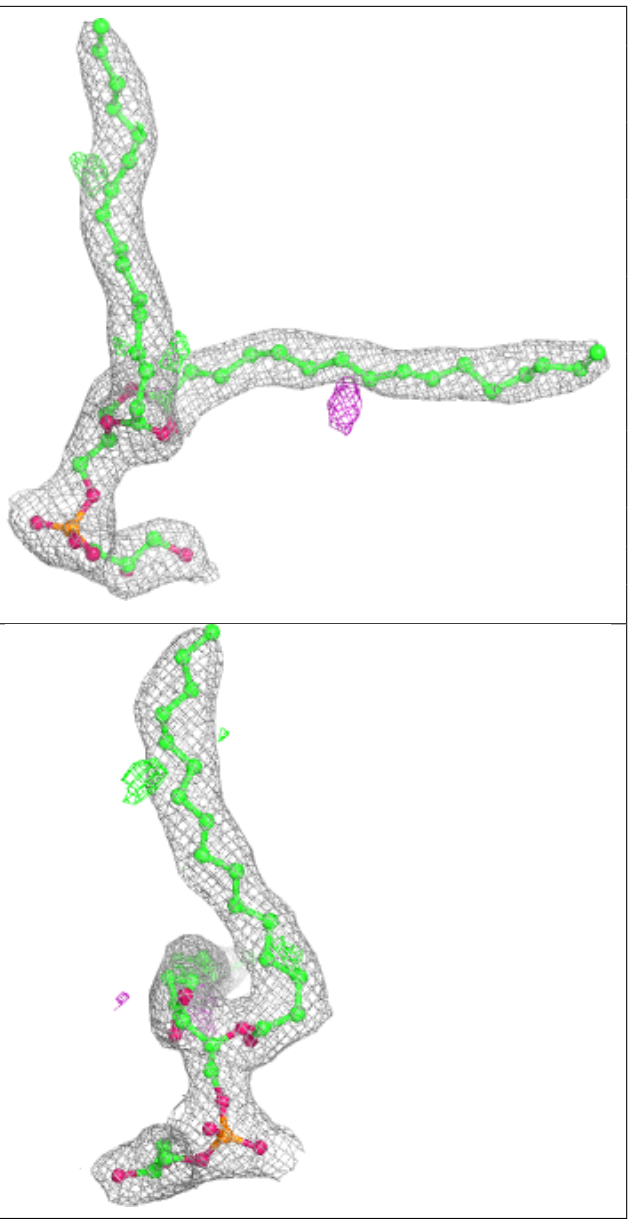






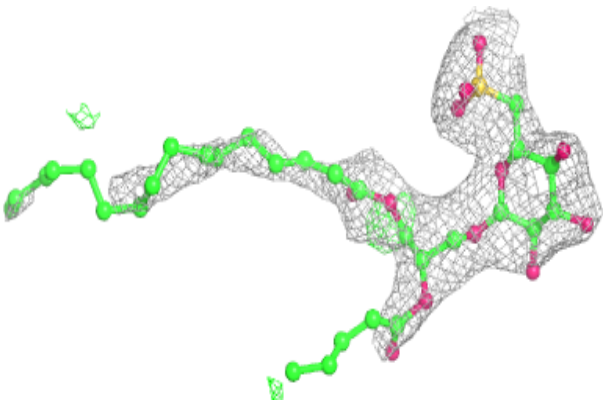
Electron density around LHG b 628:

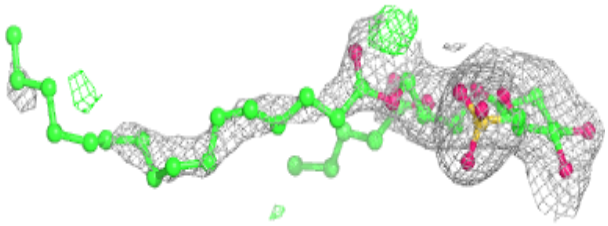
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

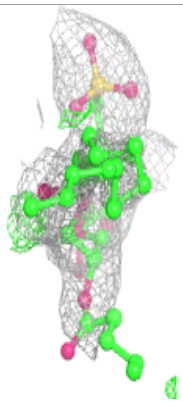


Electron density around SQD D 415:

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

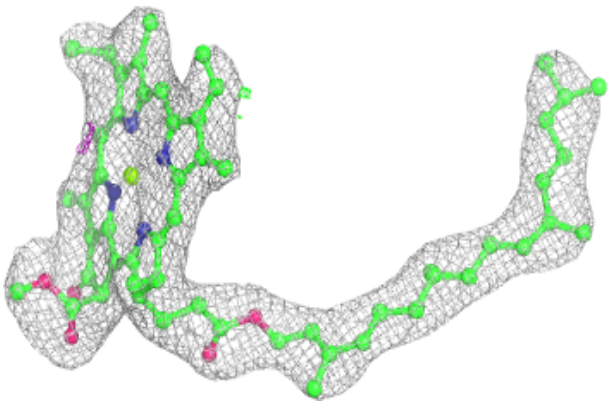


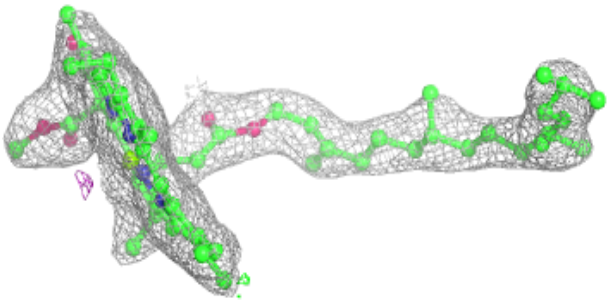


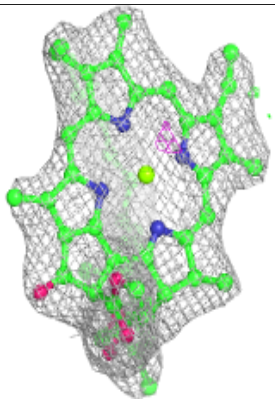


Electron density around CLA B 609:

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

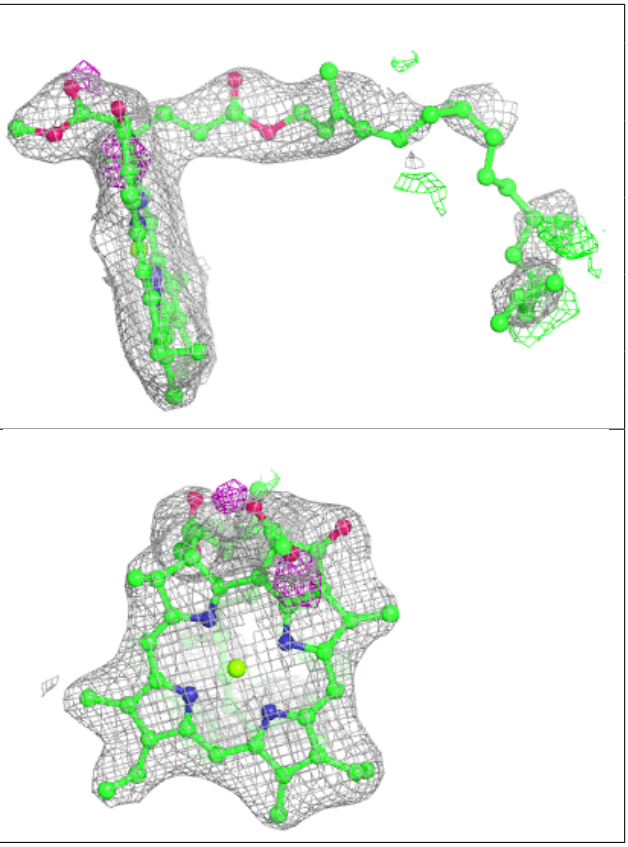


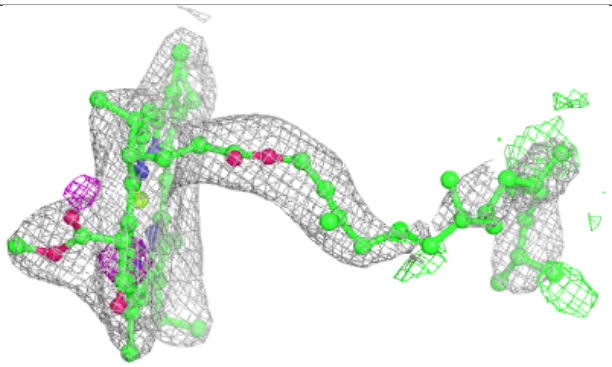




Electron density around CLA C 507:

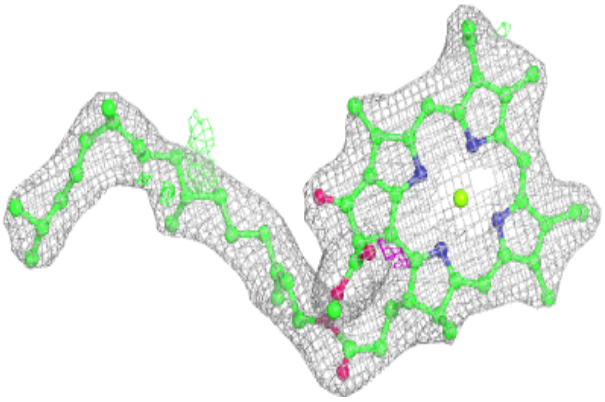
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

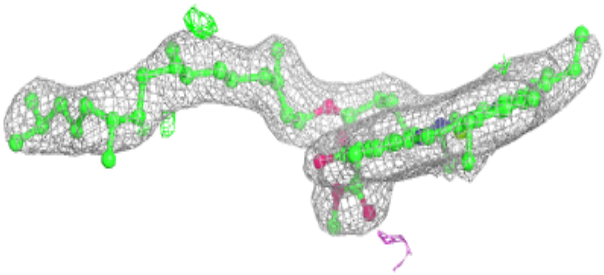


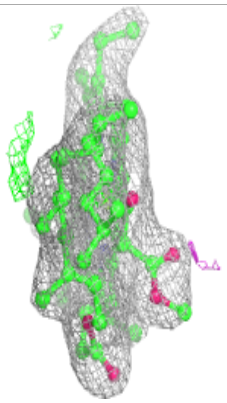


Electron density around CLA b 602:

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

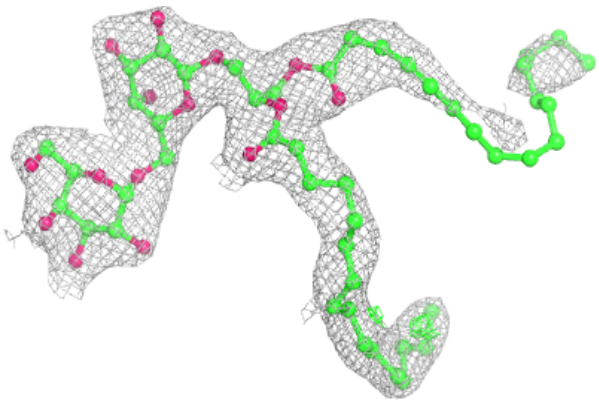


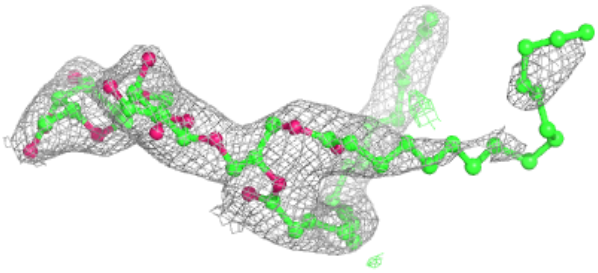


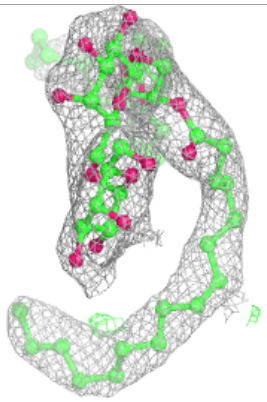


Electron density around DGD c 518:

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

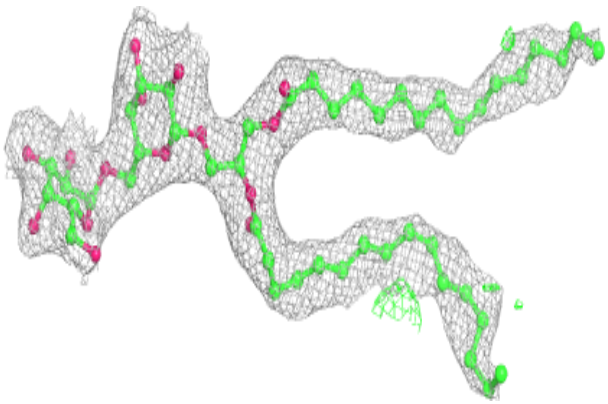


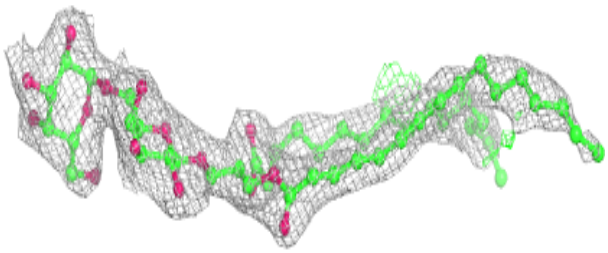


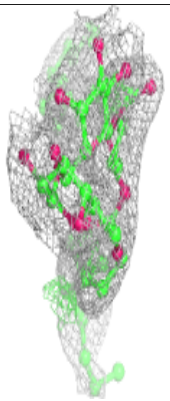


Electron density around DGD c 519:

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

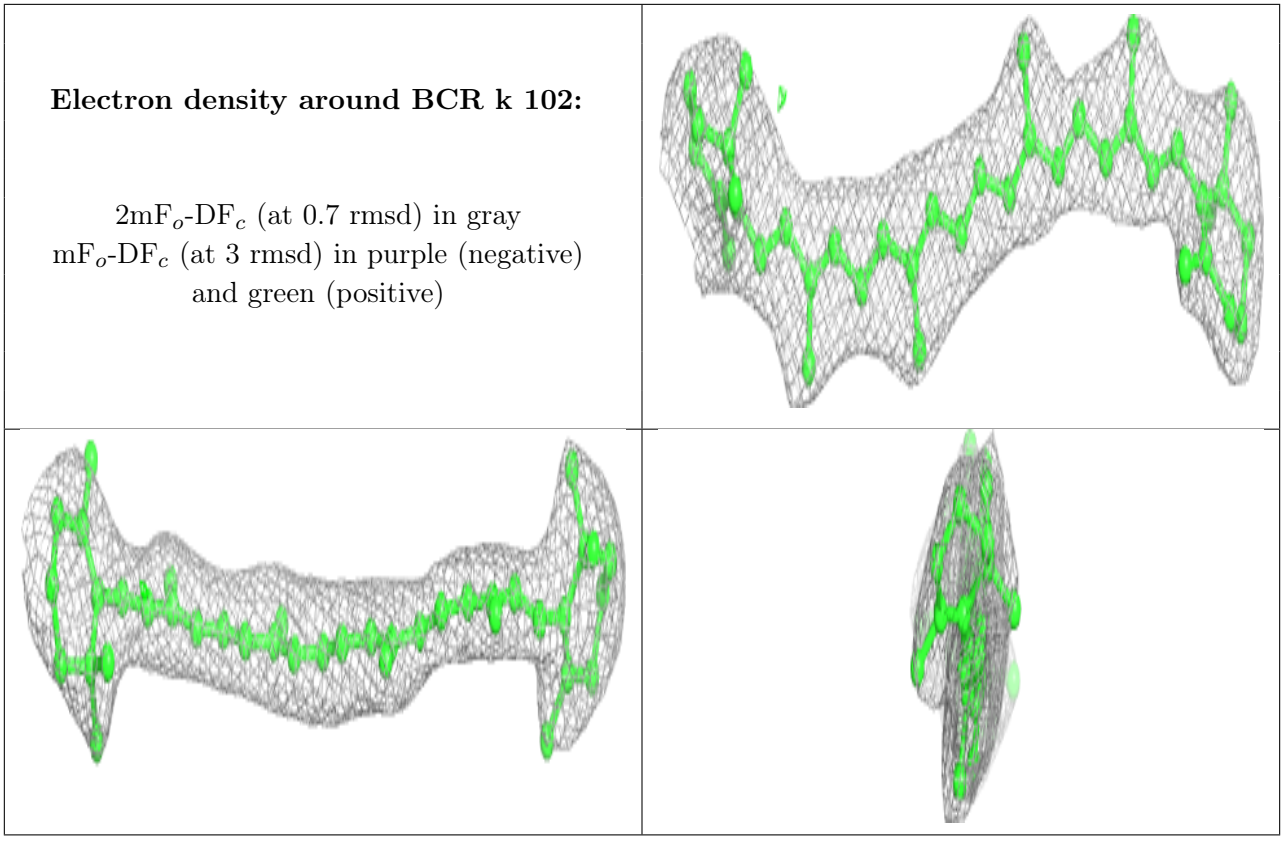






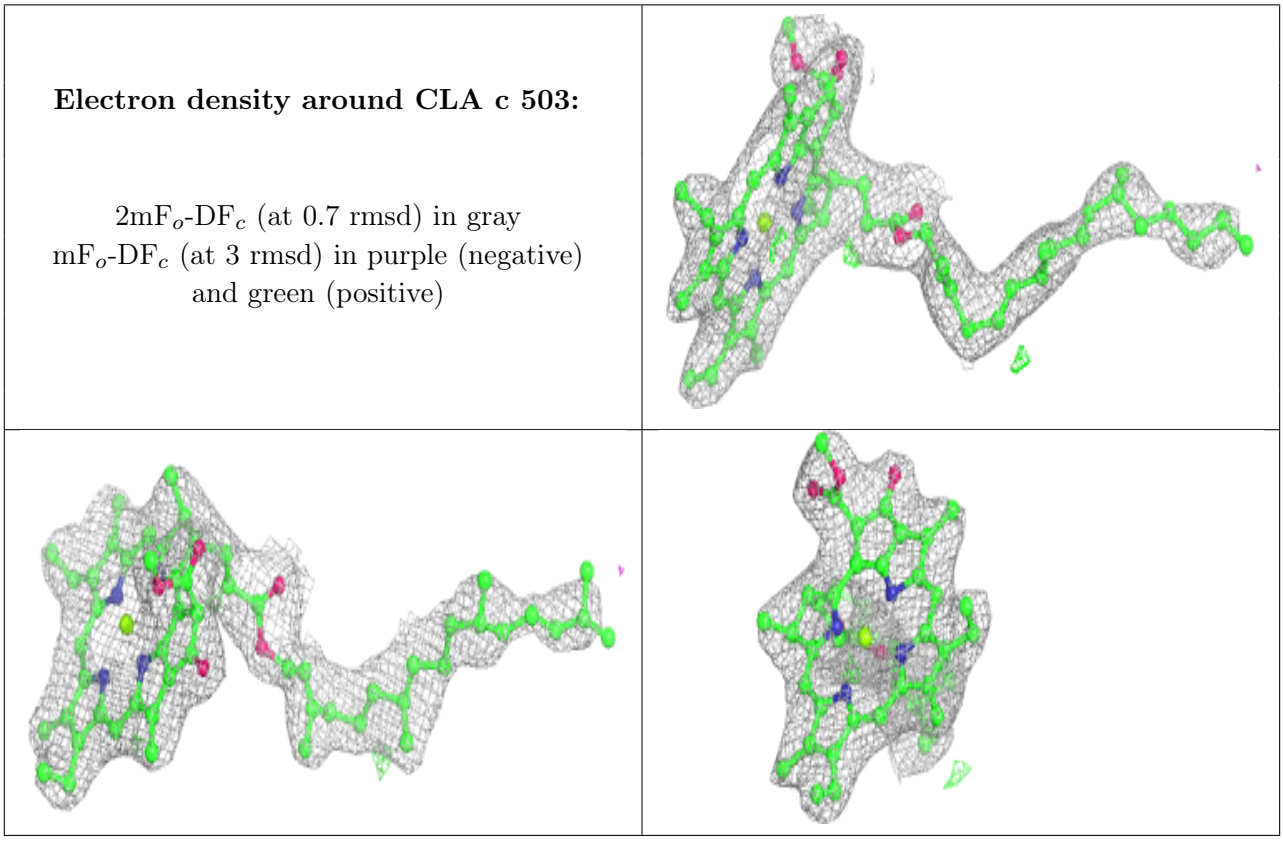
Electron density around BCR k 102:

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



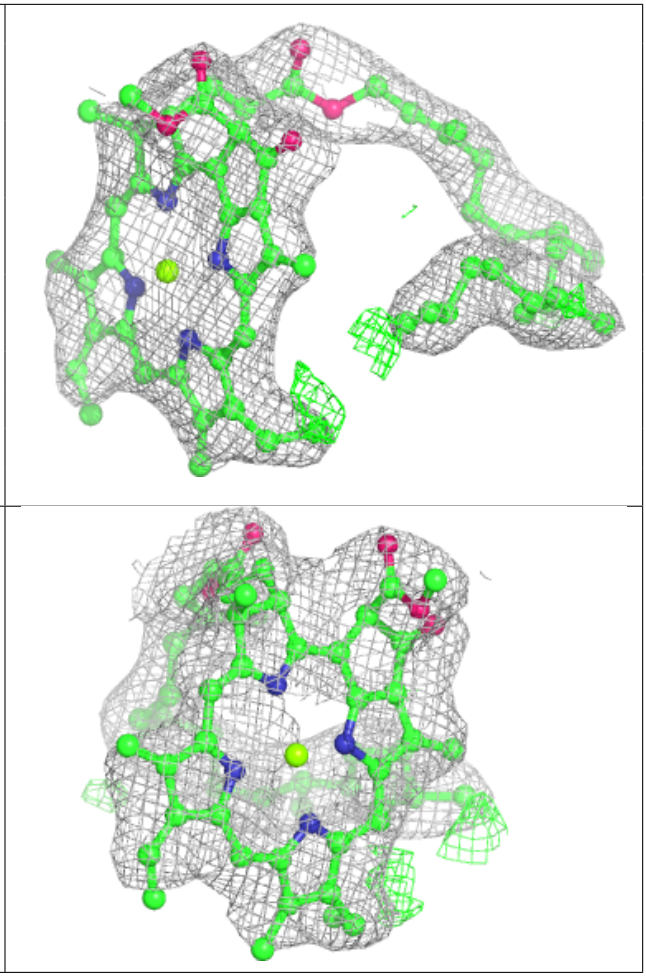
Electron density around CLA c 503:

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



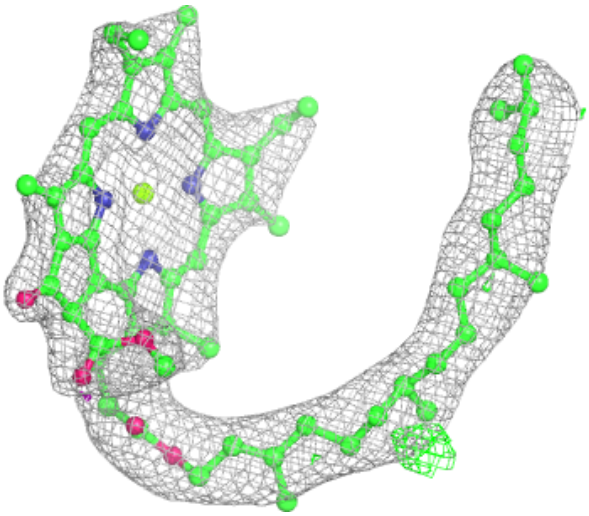
Electron density around CLA c 504:

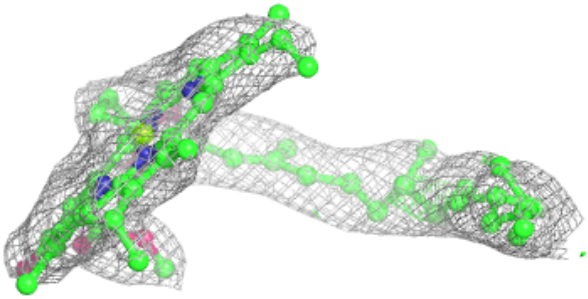
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

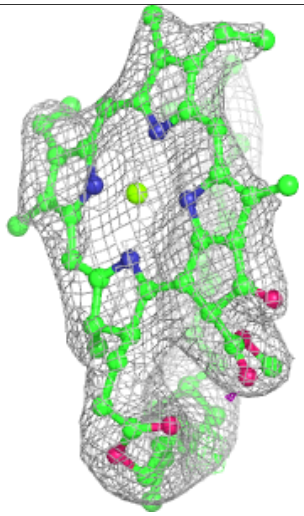


Electron density around CLA c 508:

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

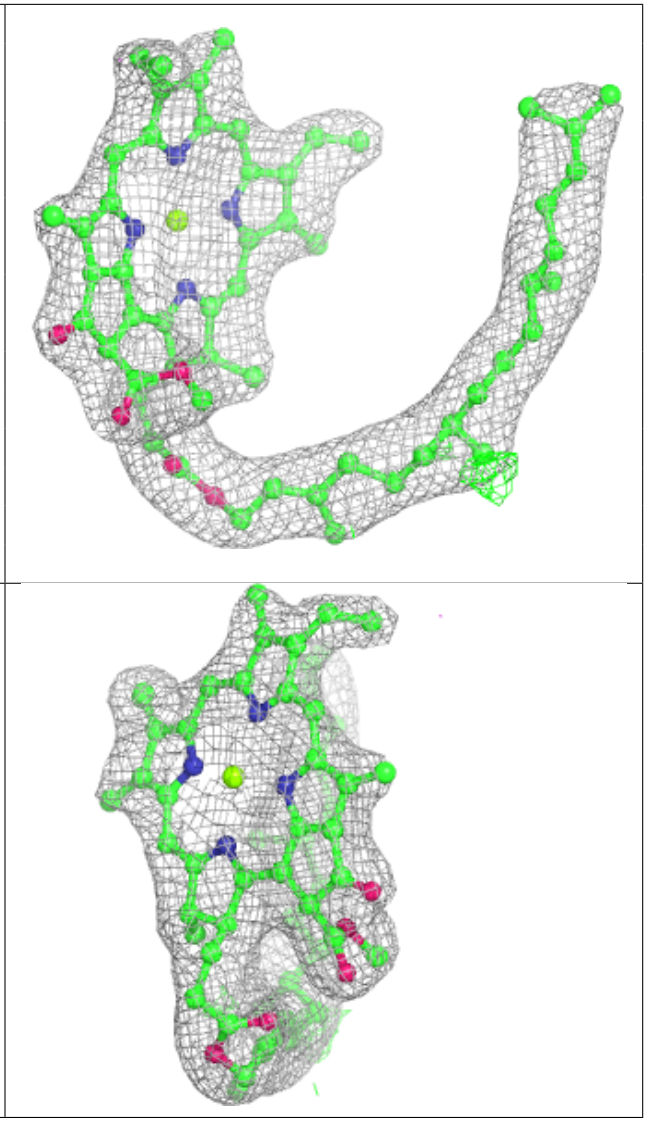






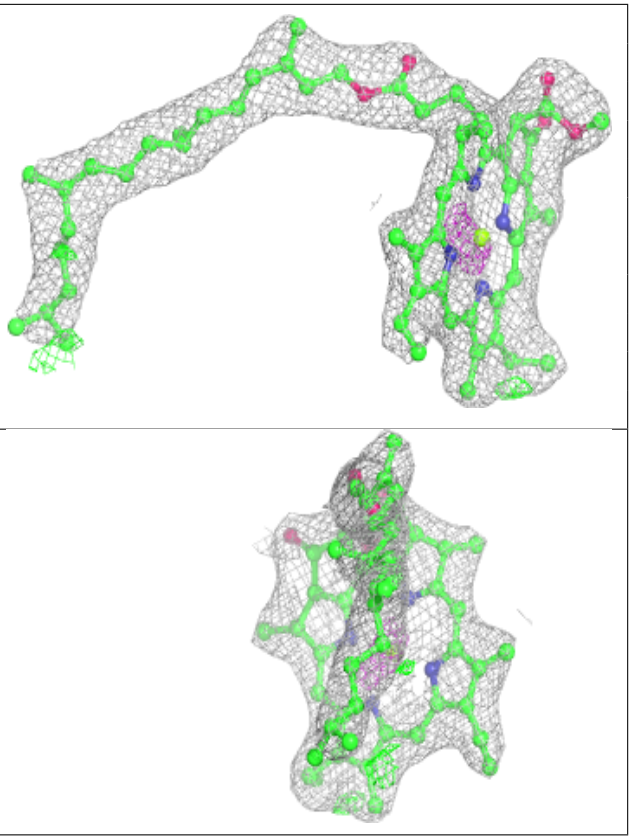
Electron density around CLA C 508:

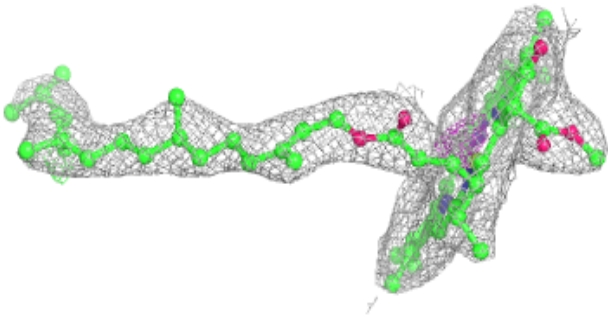
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA b 609:

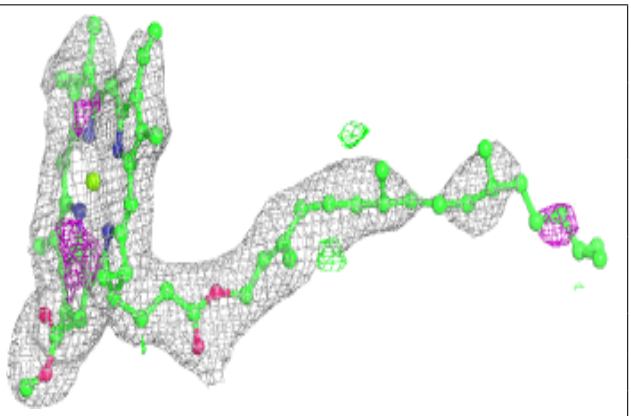
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

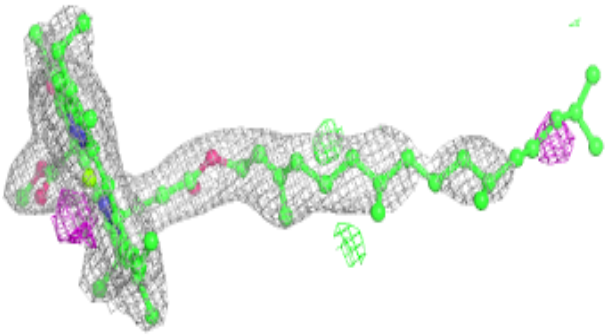


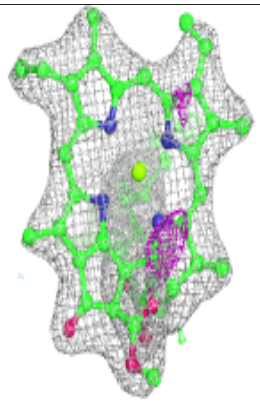


Electron density around CLA d 404:

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

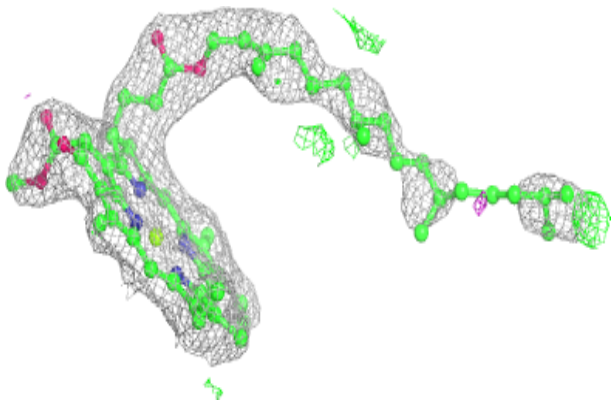


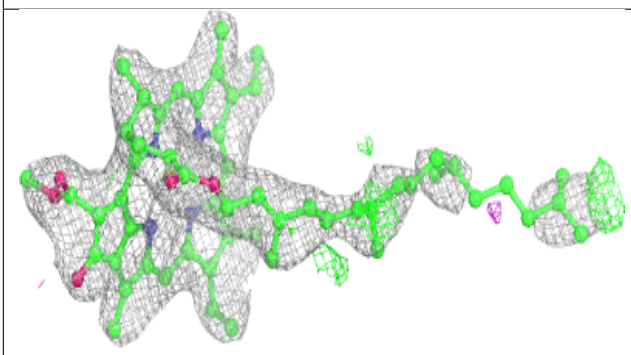


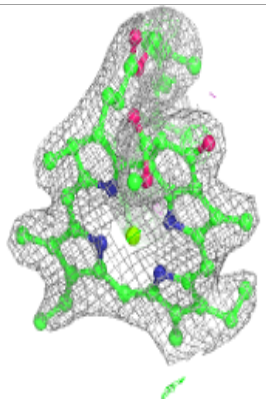


Electron density around CLA c 505:

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

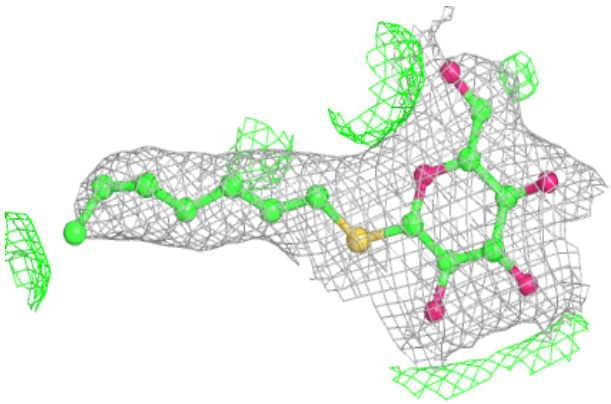


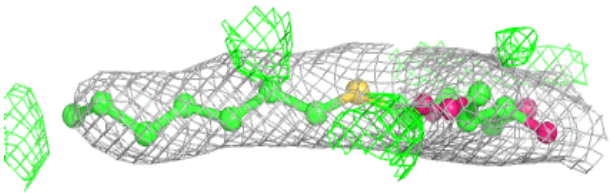


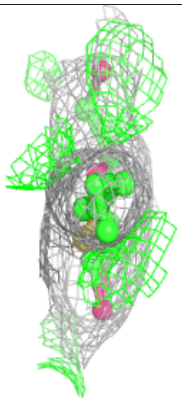


Electron density around HTG b 624:

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

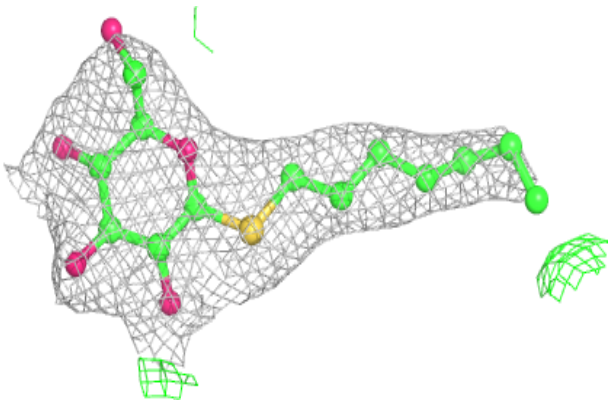


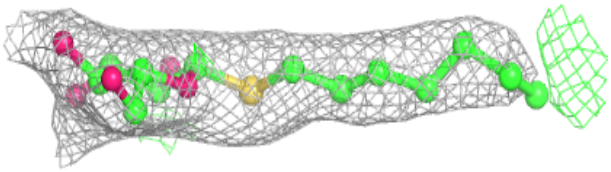


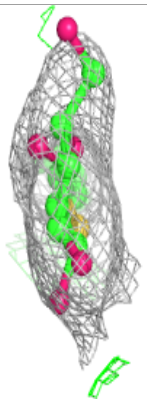


Electron density around HTG B 624:

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

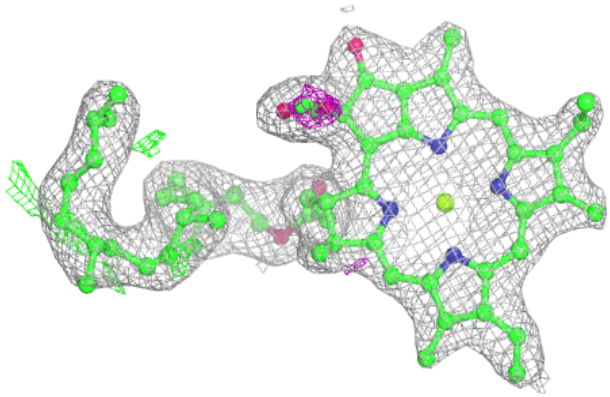


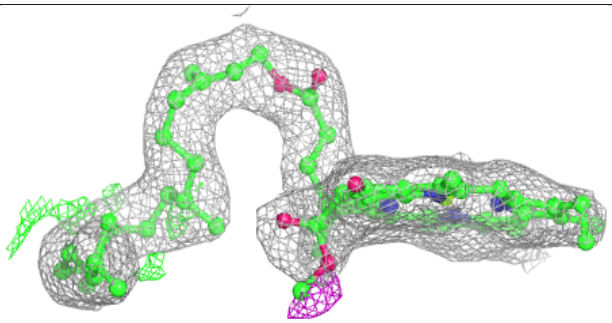


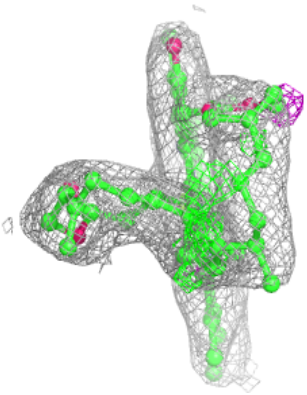


Electron density around CLA b 612:

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

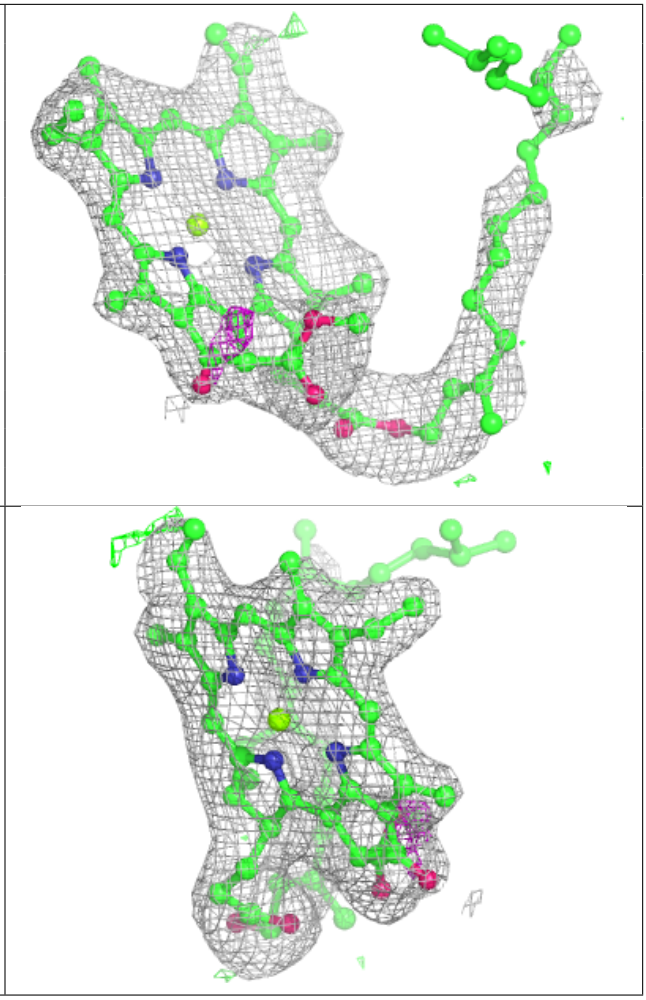






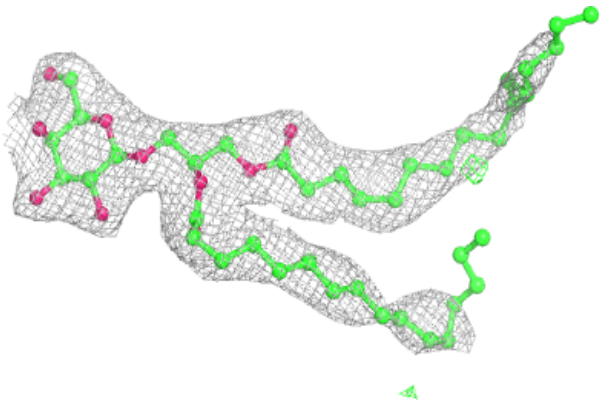
Electron density around CLA b 616:

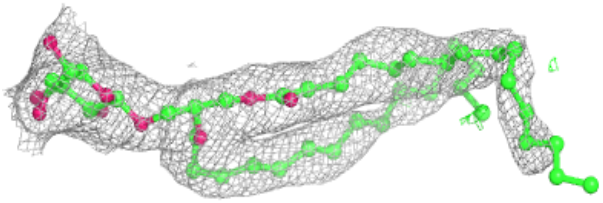
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

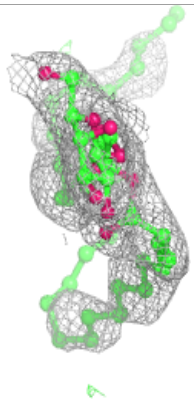


Electron density around LMG d 412:

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

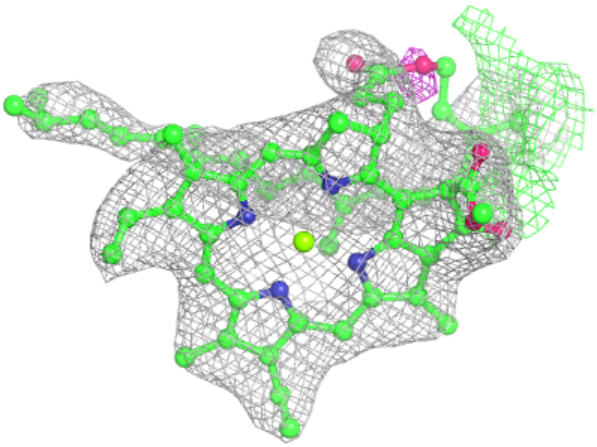


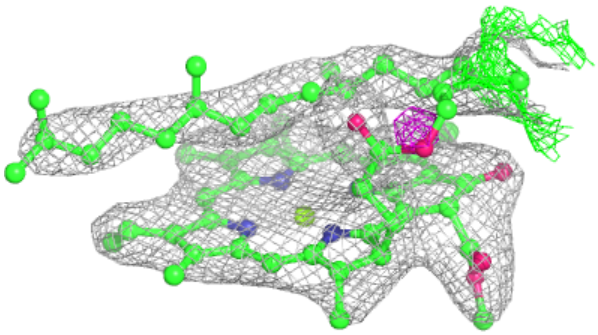


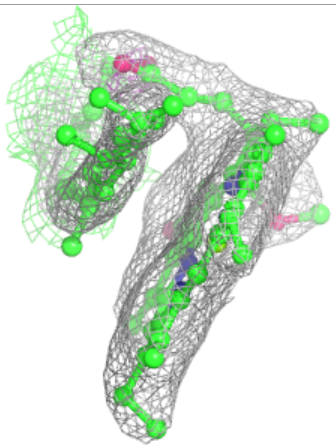


Electron density around CLA b 601:

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

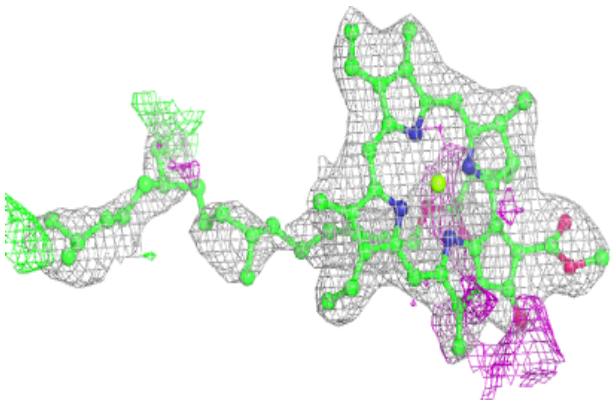


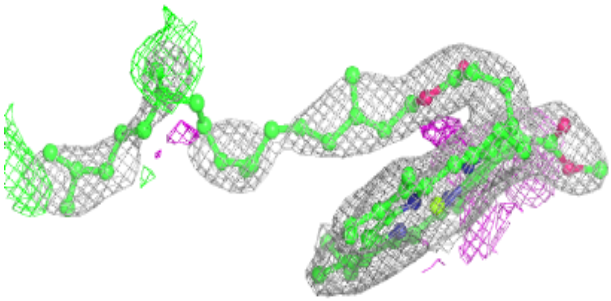


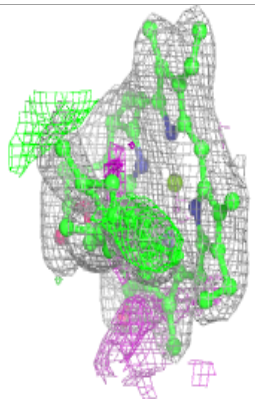


Electron density around CLA B 614:

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

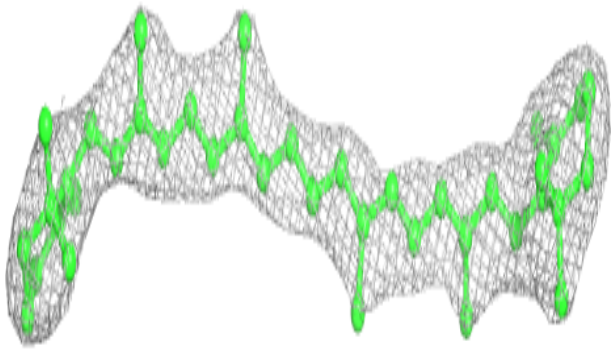


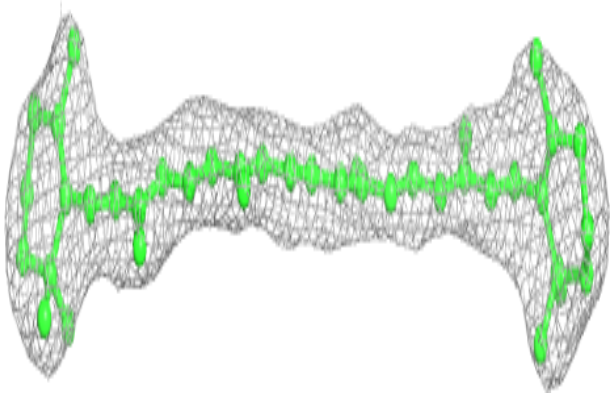


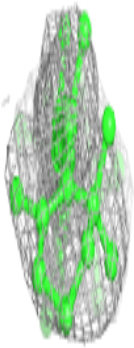


Electron density around BCR C 515:

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

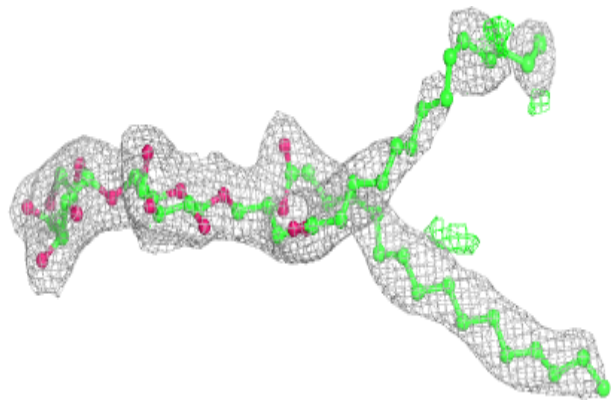


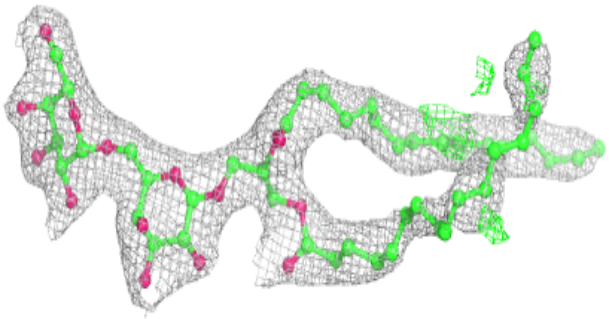


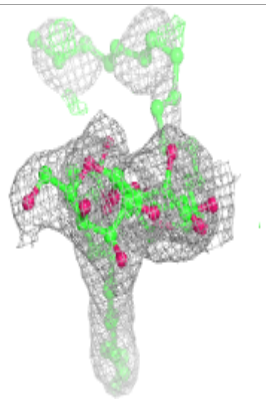


Electron density around DGD C 517:

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

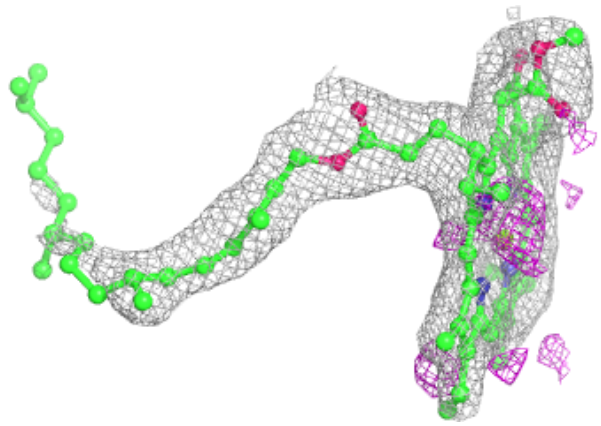


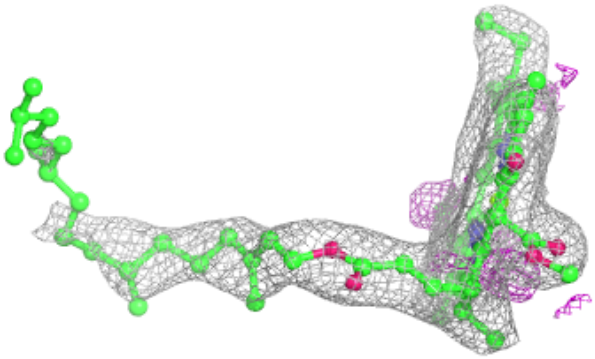


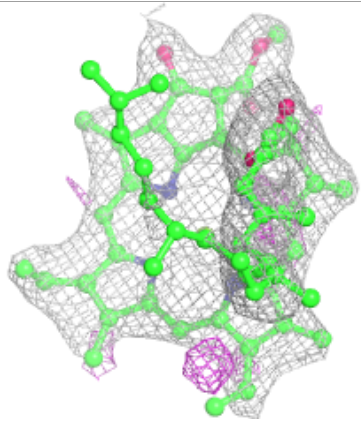


Electron density around CLA D 406:

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

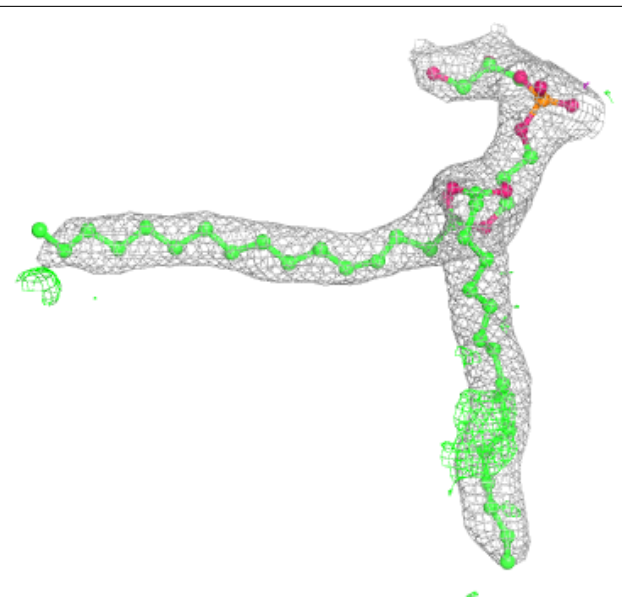


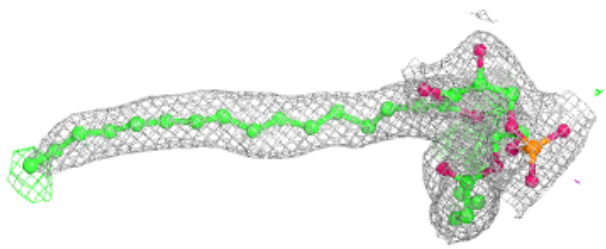


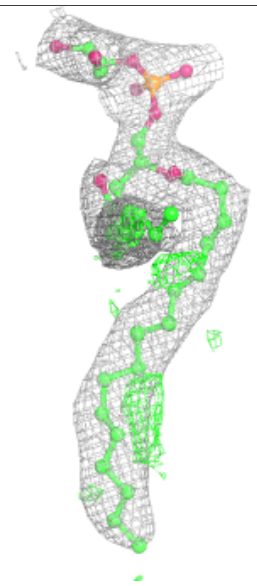


Electron density around LHG L 101:

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

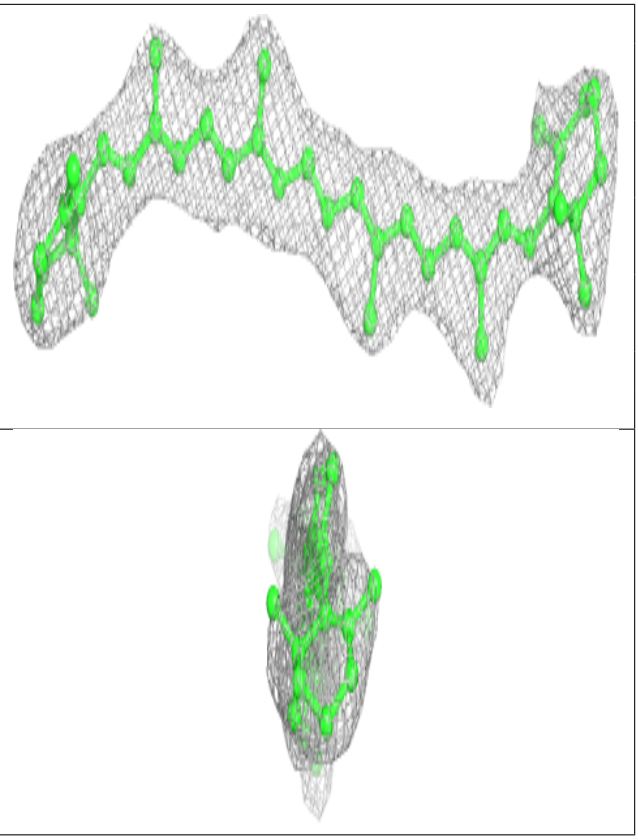






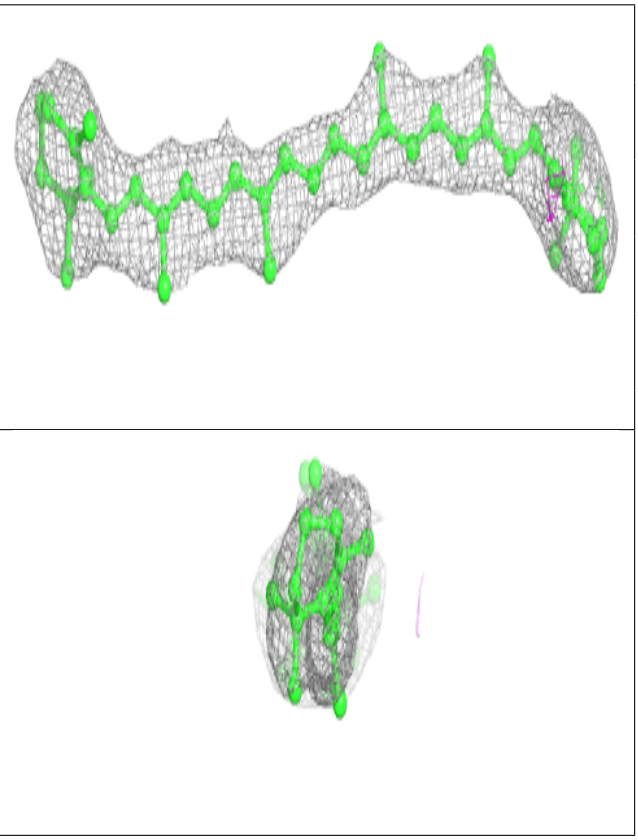
Electron density around BCR Y 101:

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



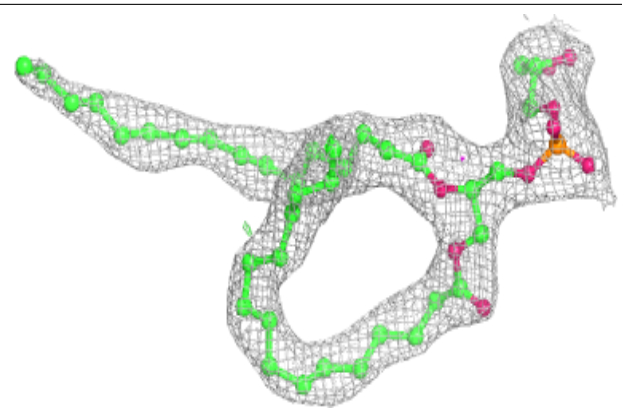
Electron density around BCR c 515:

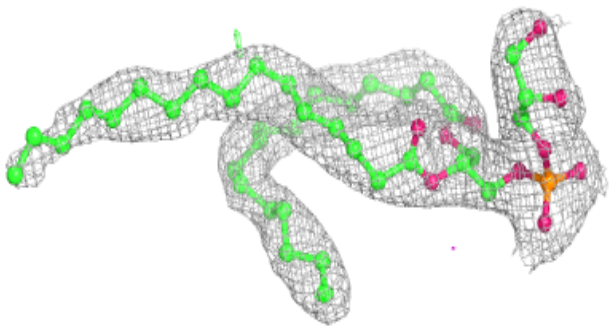
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

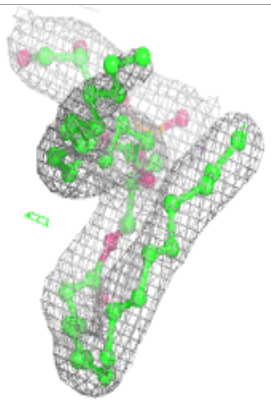


Electron density around LHG d 407:

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

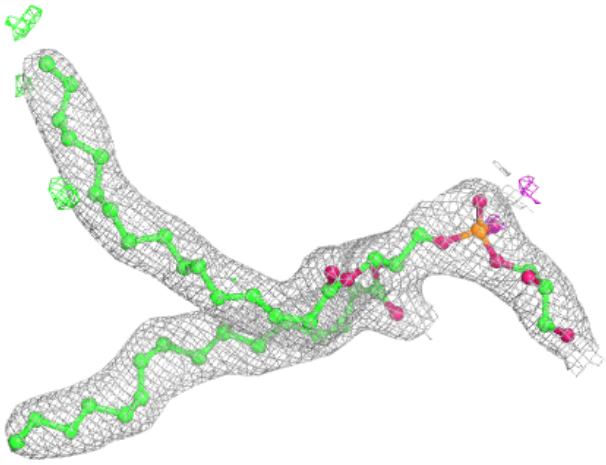


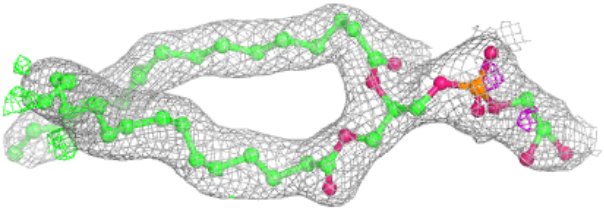


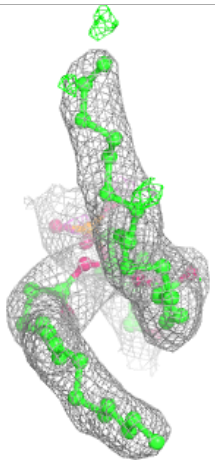


Electron density around LHG d 408:

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

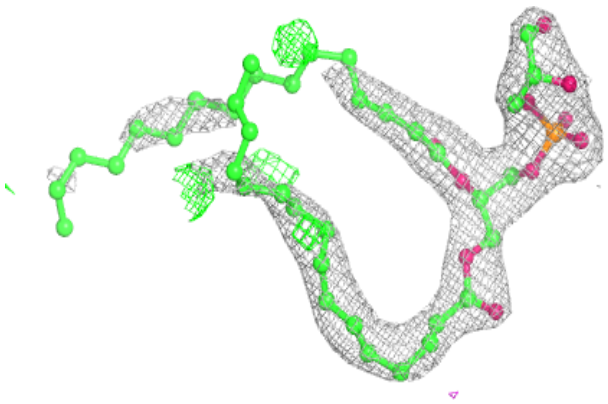


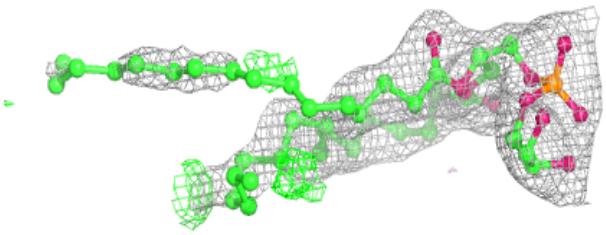


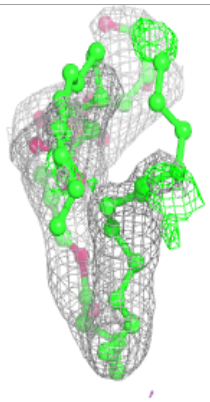


Electron density around LHG d 409:

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

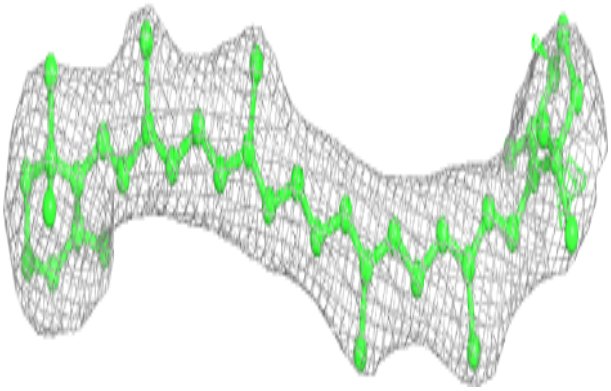


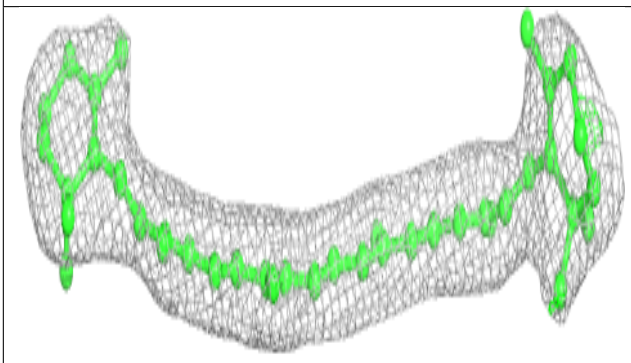


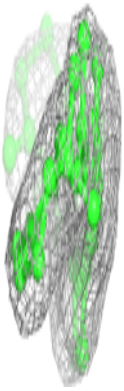


Electron density around BCR d 405:

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

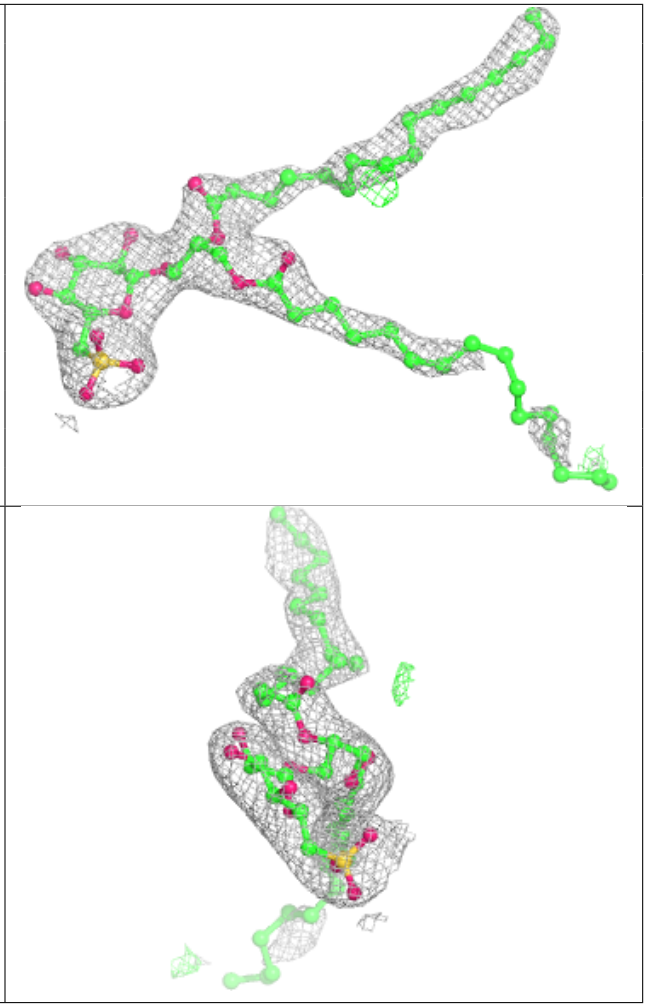






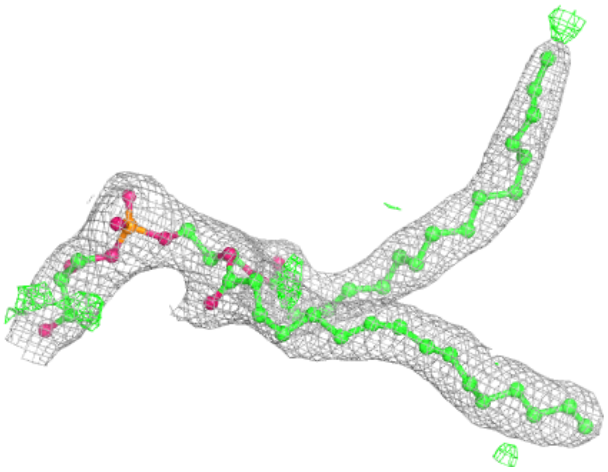
Electron density around SQD a 409:

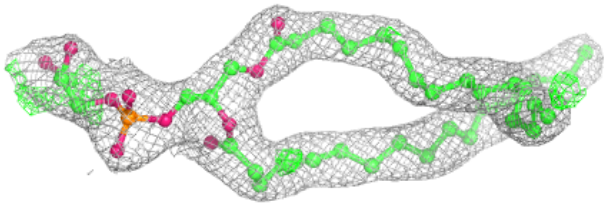
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

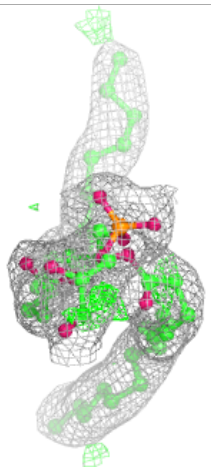


Electron density around LHG D 409:

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

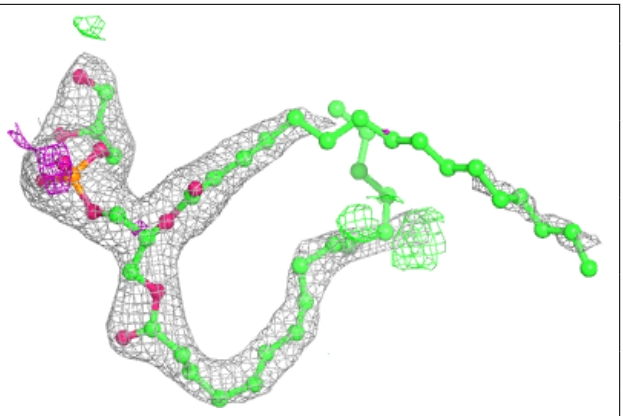


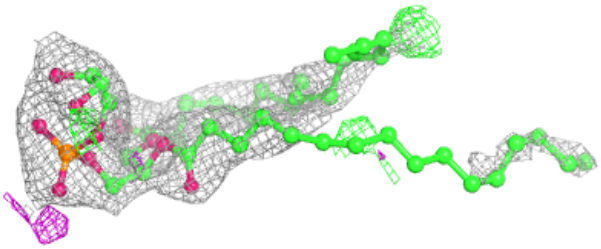


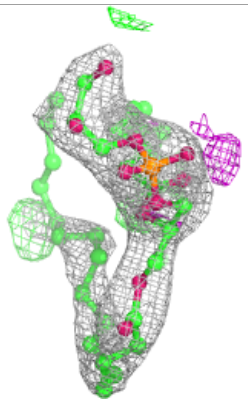


Electron density around LHG D 410:

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

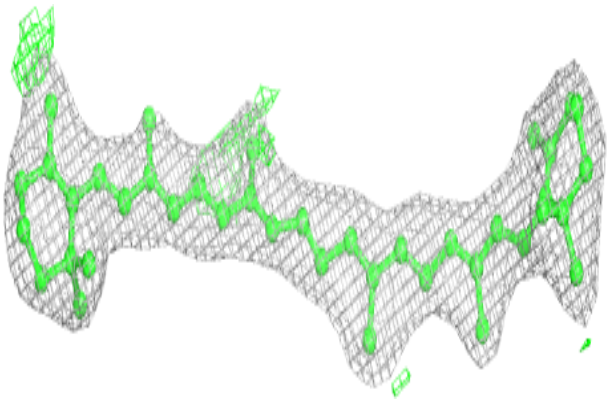


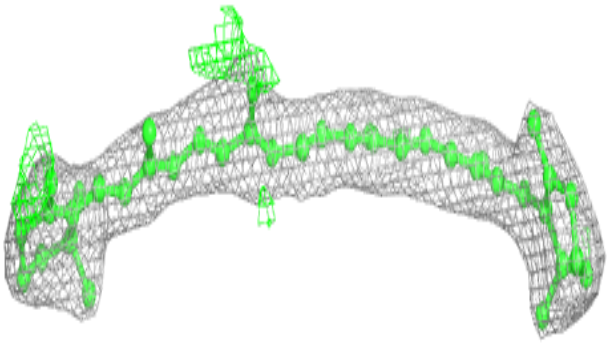


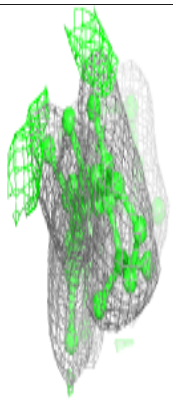


Electron density around BCR T 101:

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

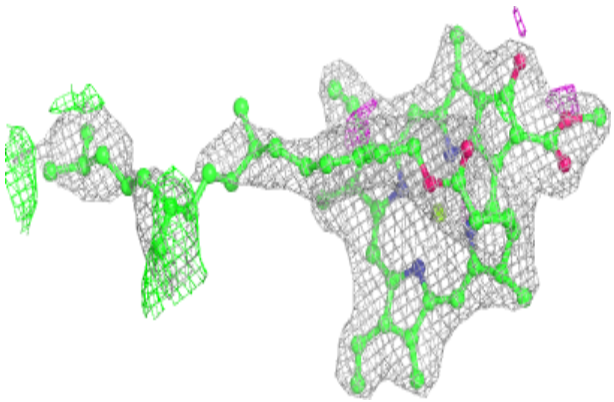


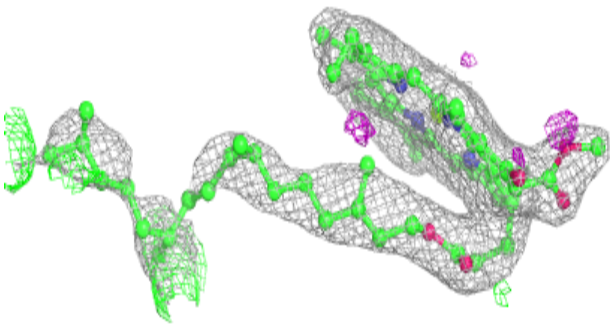


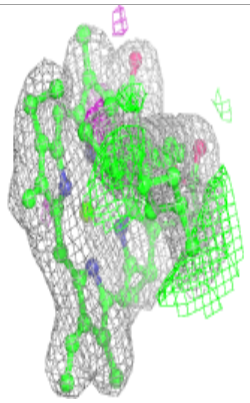


Electron density around CLA b 614:

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

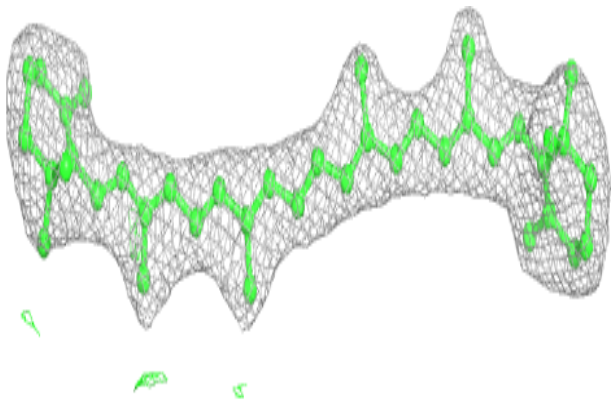


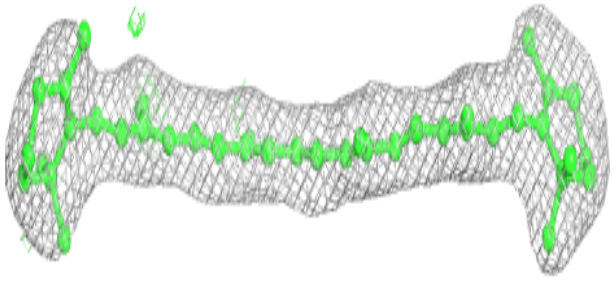


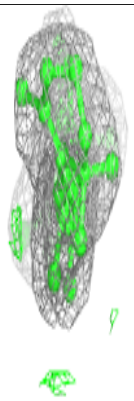


Electron density around BCR b 618:

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

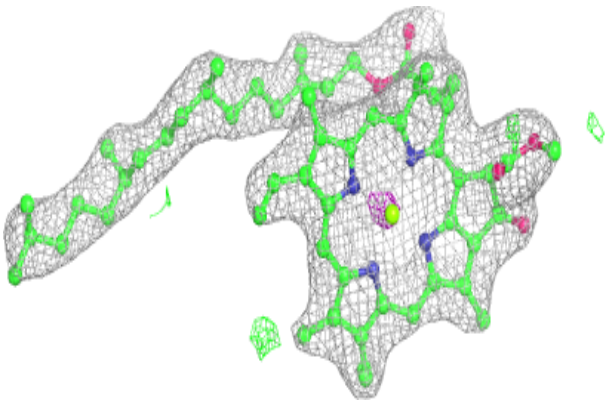


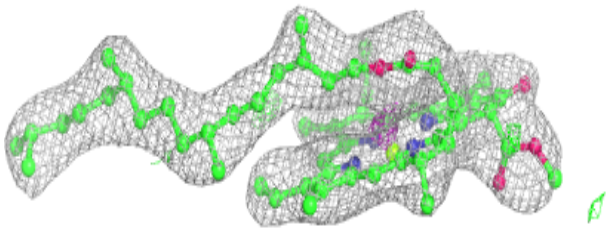


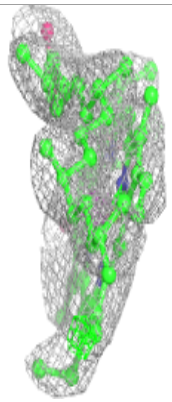


Electron density around CLA C 502:

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

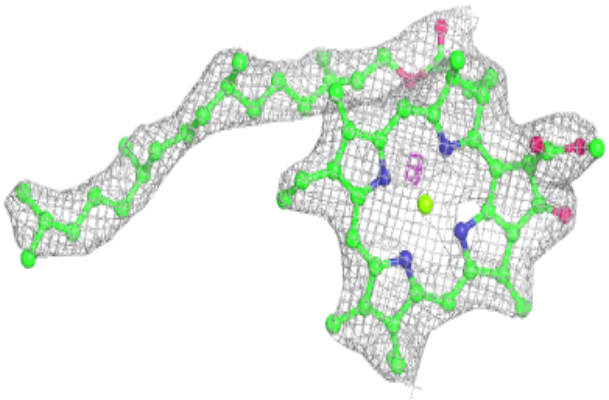


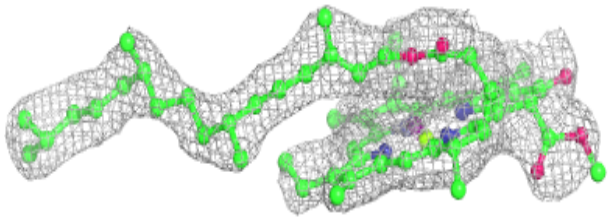


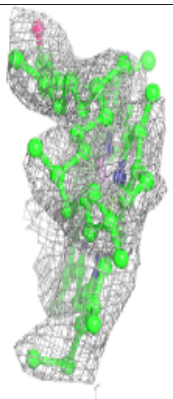


Electron density around CLA c 502:

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

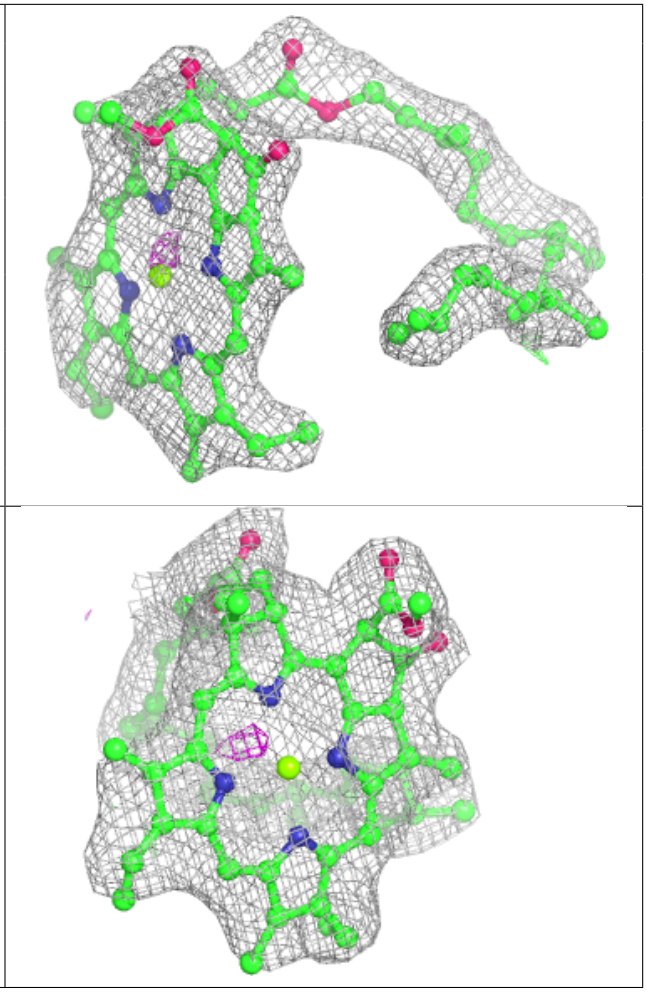






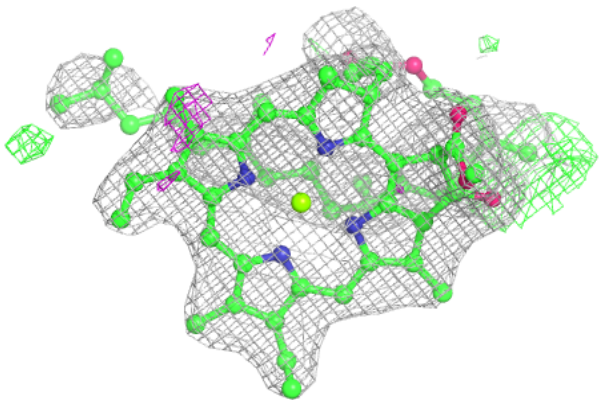
Electron density around CLA C 504:

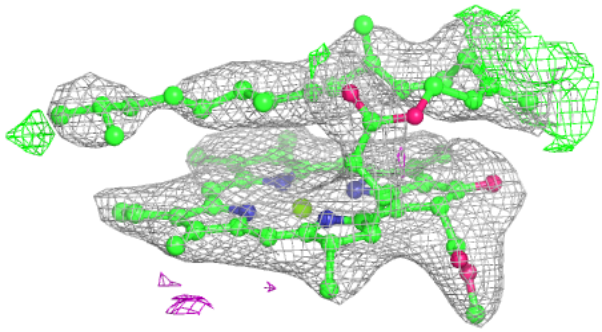
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

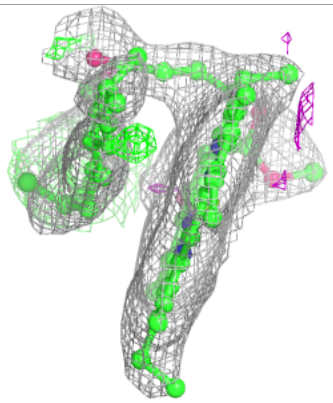


Electron density around CLA B 601:

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

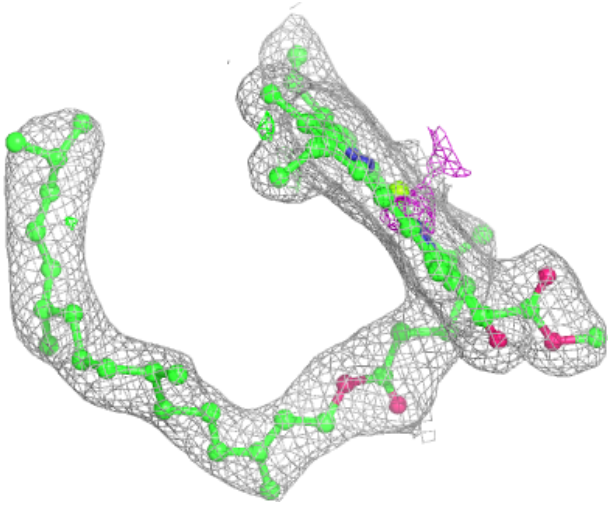


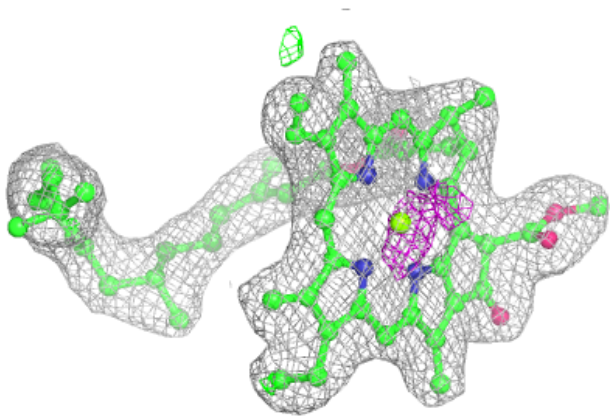


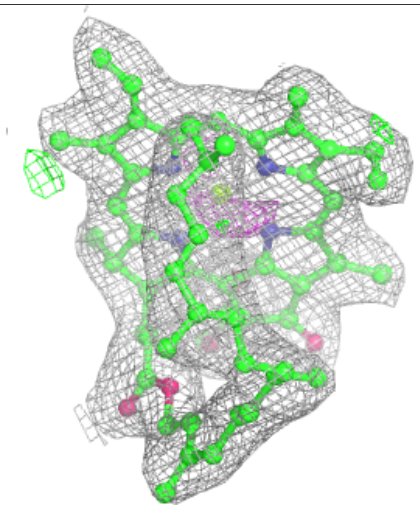


Electron density around CLA B 611:

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

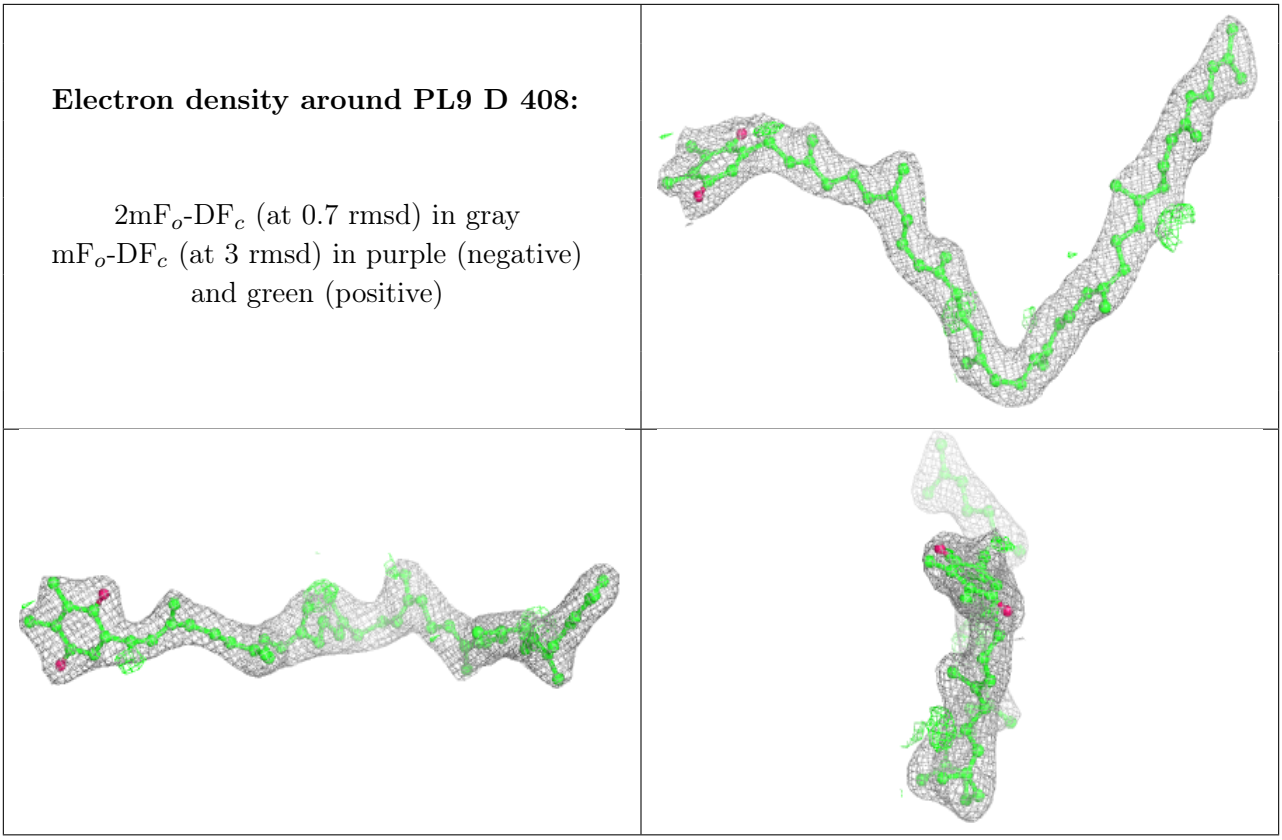






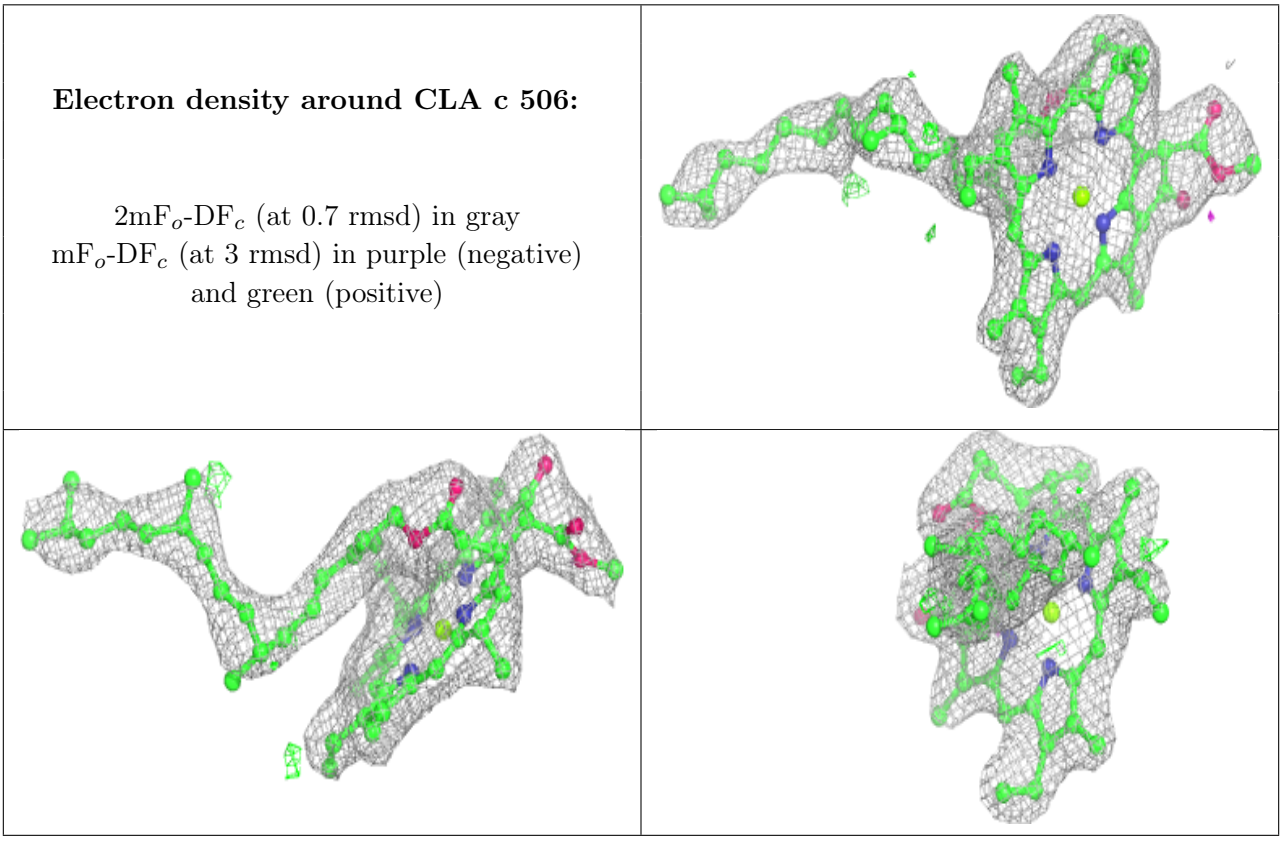
Electron density around PL9 D 408:

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



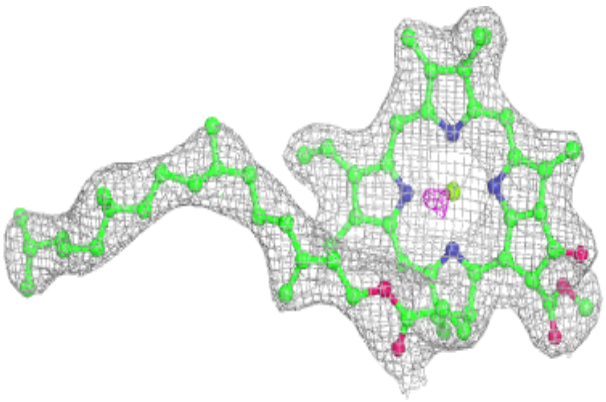
Electron density around CLA c 506:

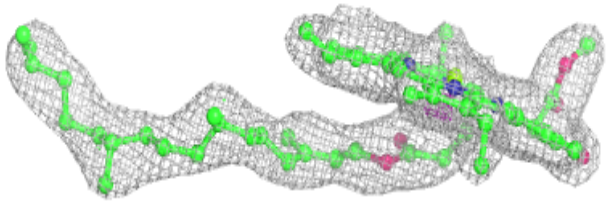
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

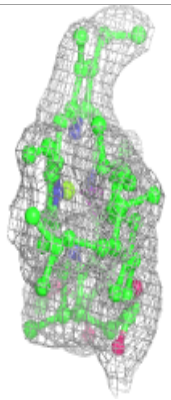


Electron density around CLA B 603:

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

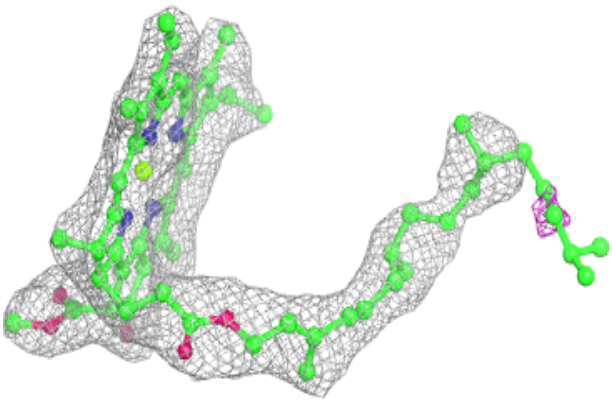


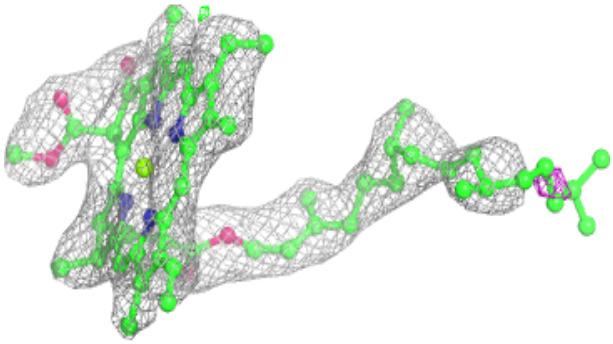


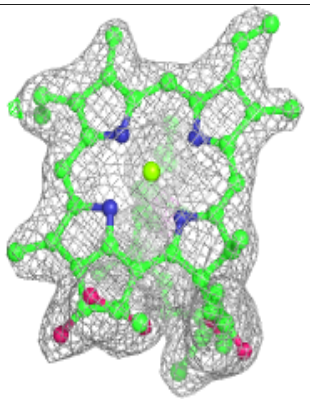


Electron density around CLA c 509:

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

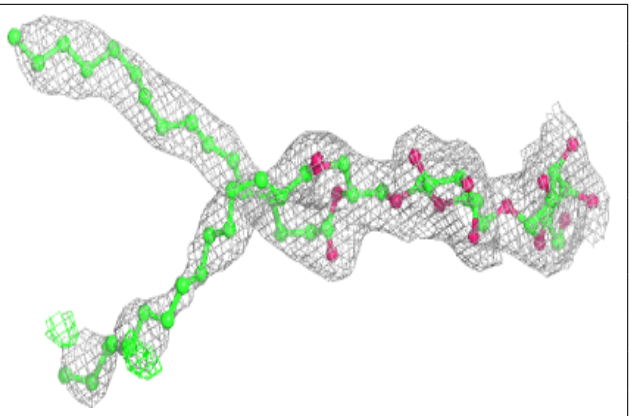


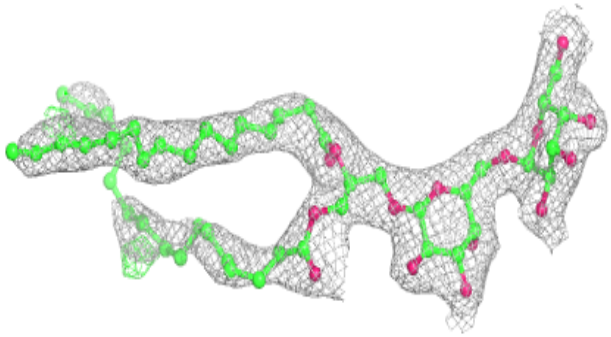


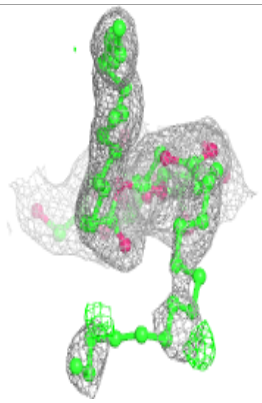


Electron density around DGD c 517:

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

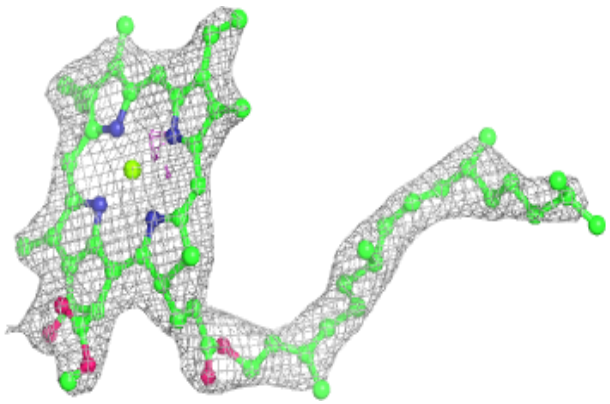


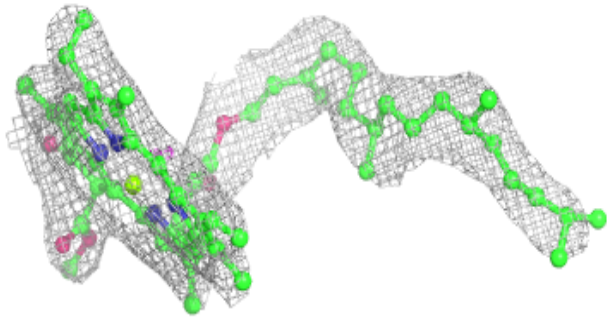


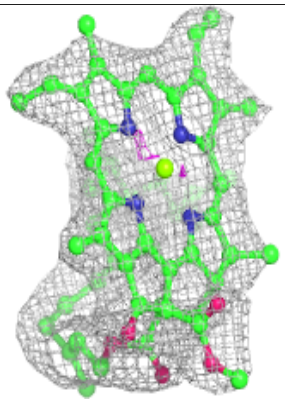


Electron density around CLA c 512:

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

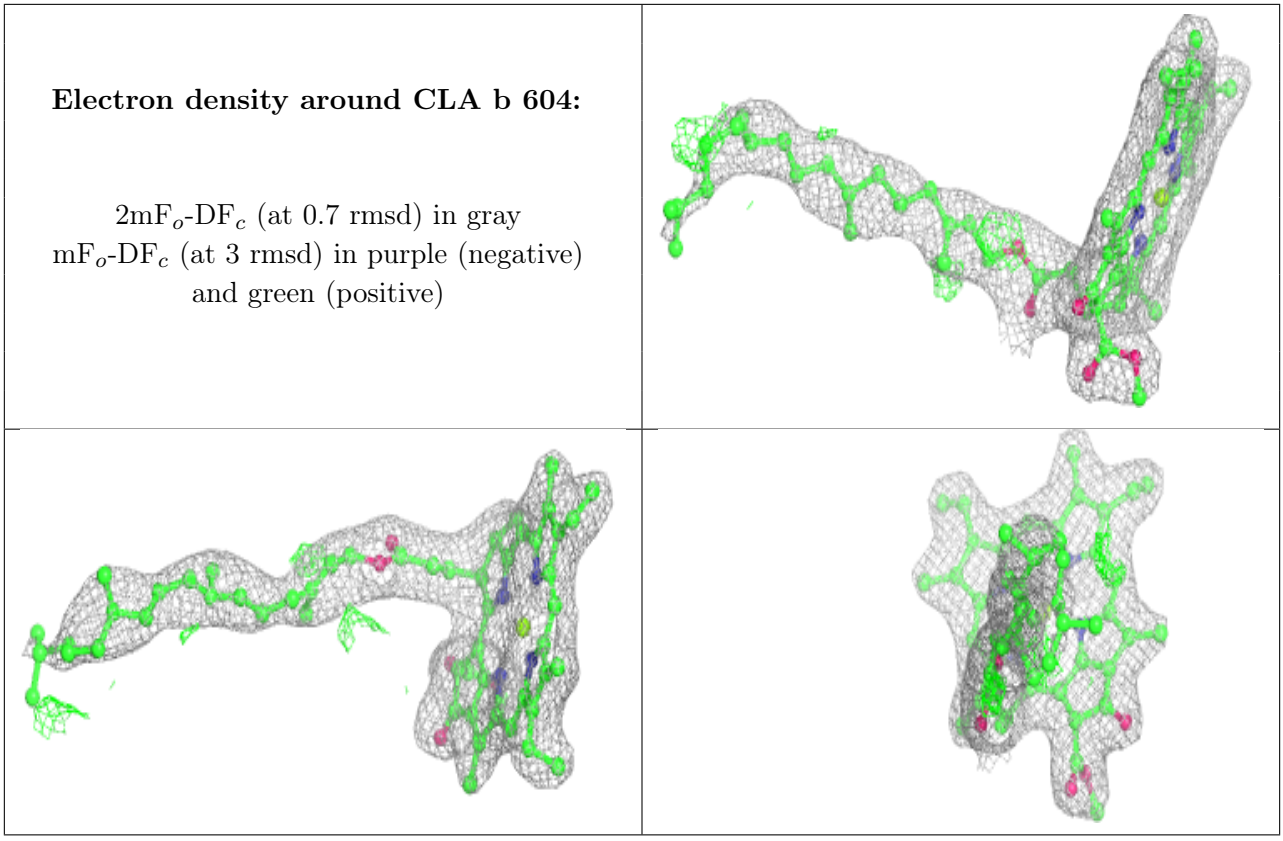






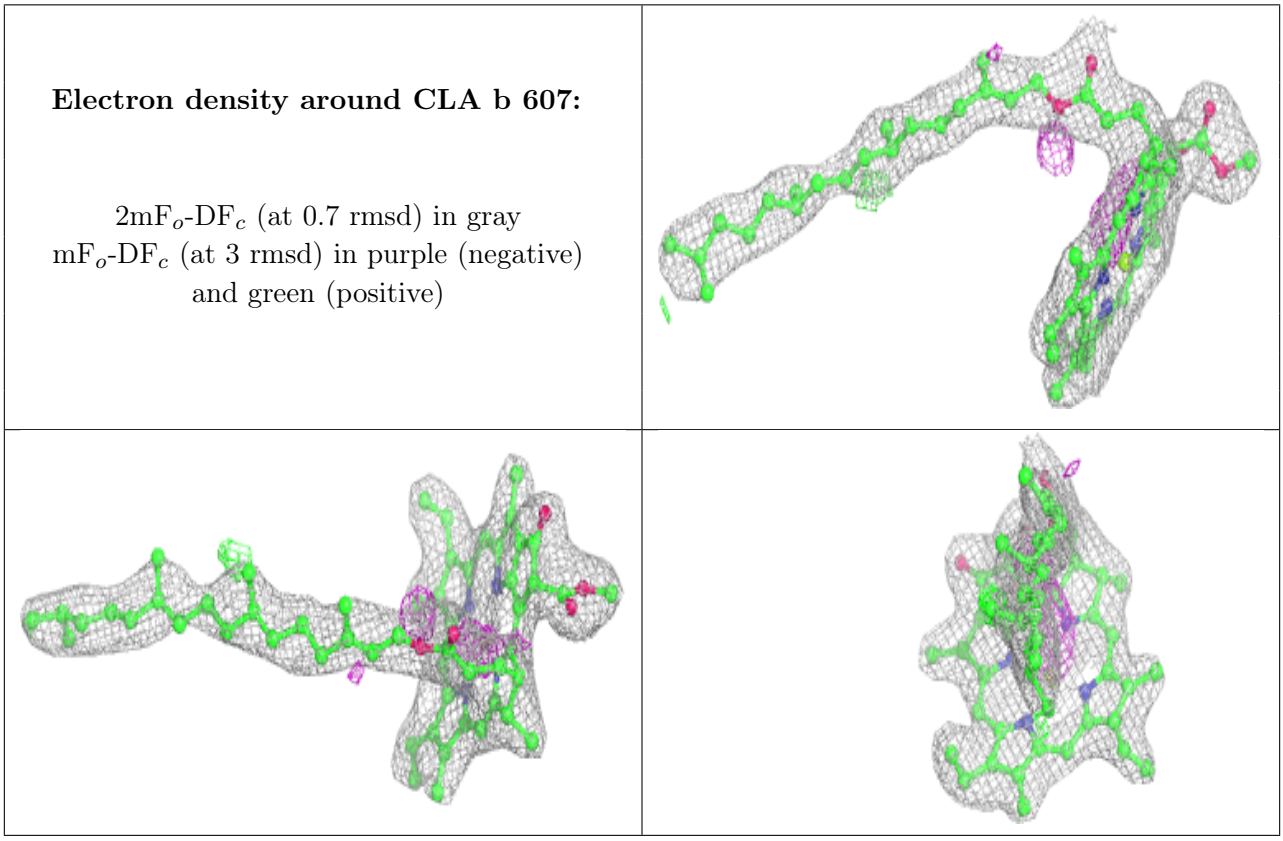
Electron density around CLA b 604:

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



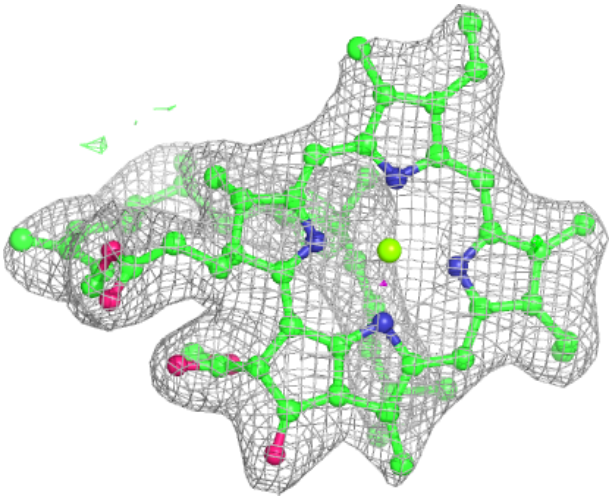
Electron density around CLA b 607:

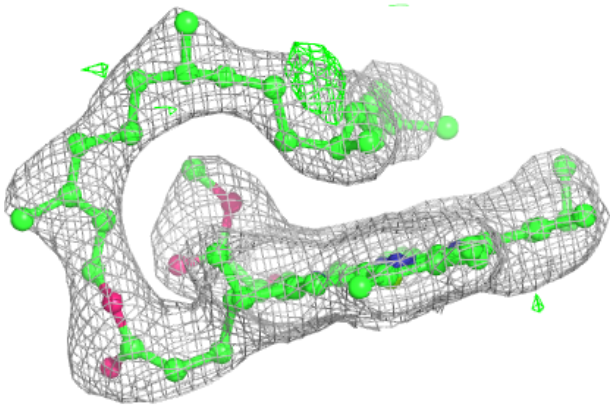
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

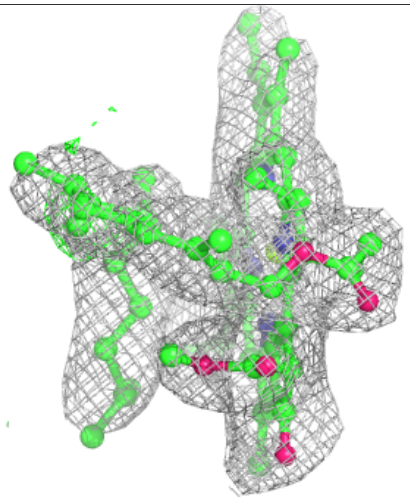


Electron density around CLA C 511:

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

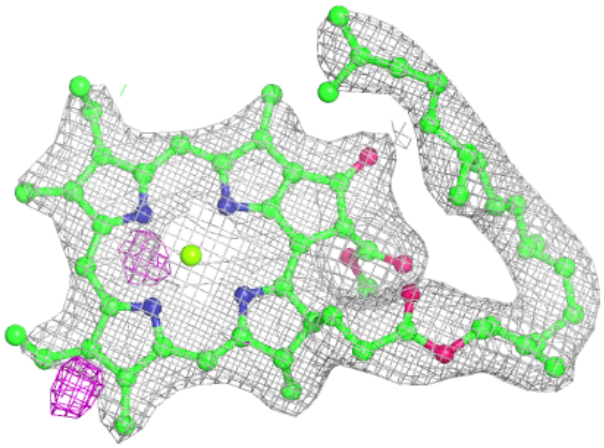


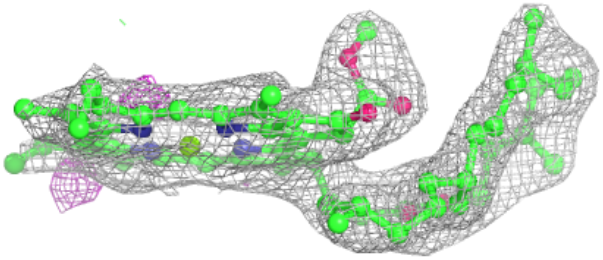


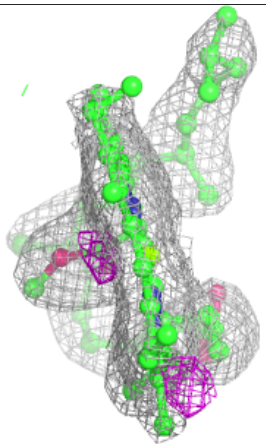


Electron density around CLA b 610:

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

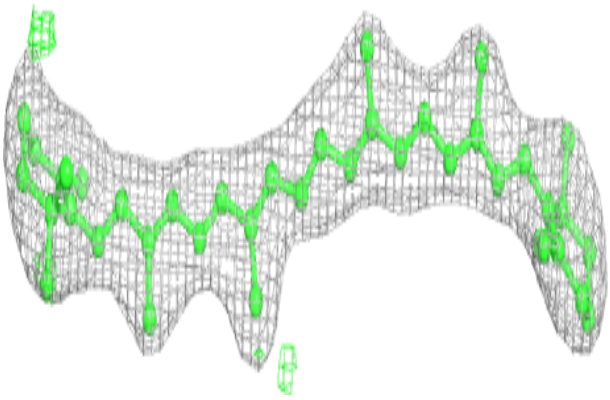


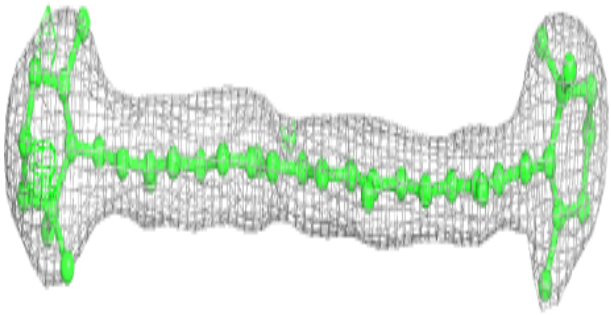


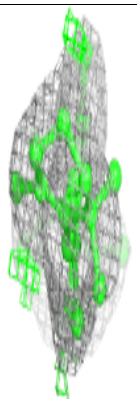


Electron density around BCR C 516:

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

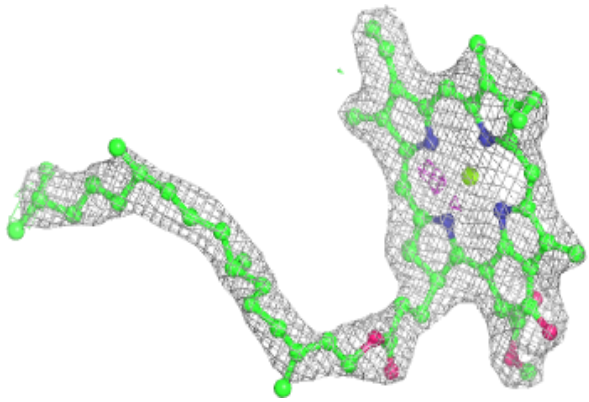


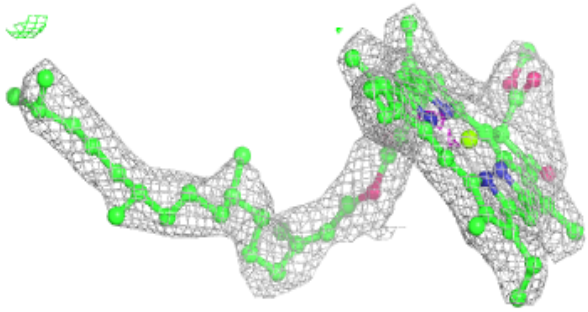


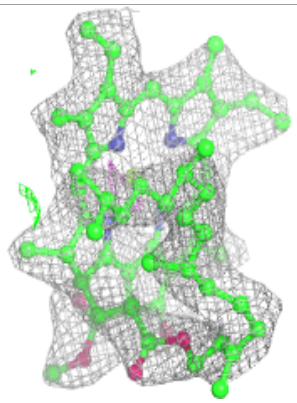


Electron density around CLA C 512:

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

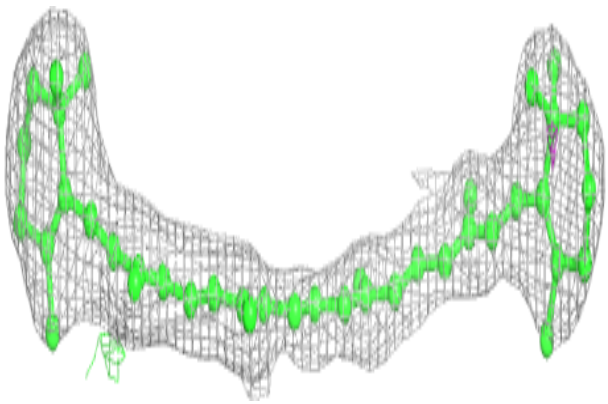


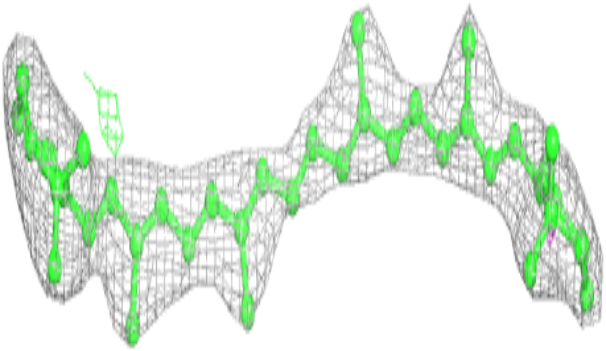


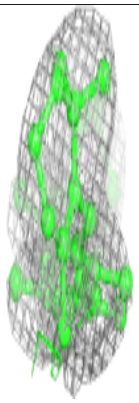


Electron density around BCR K 101:

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

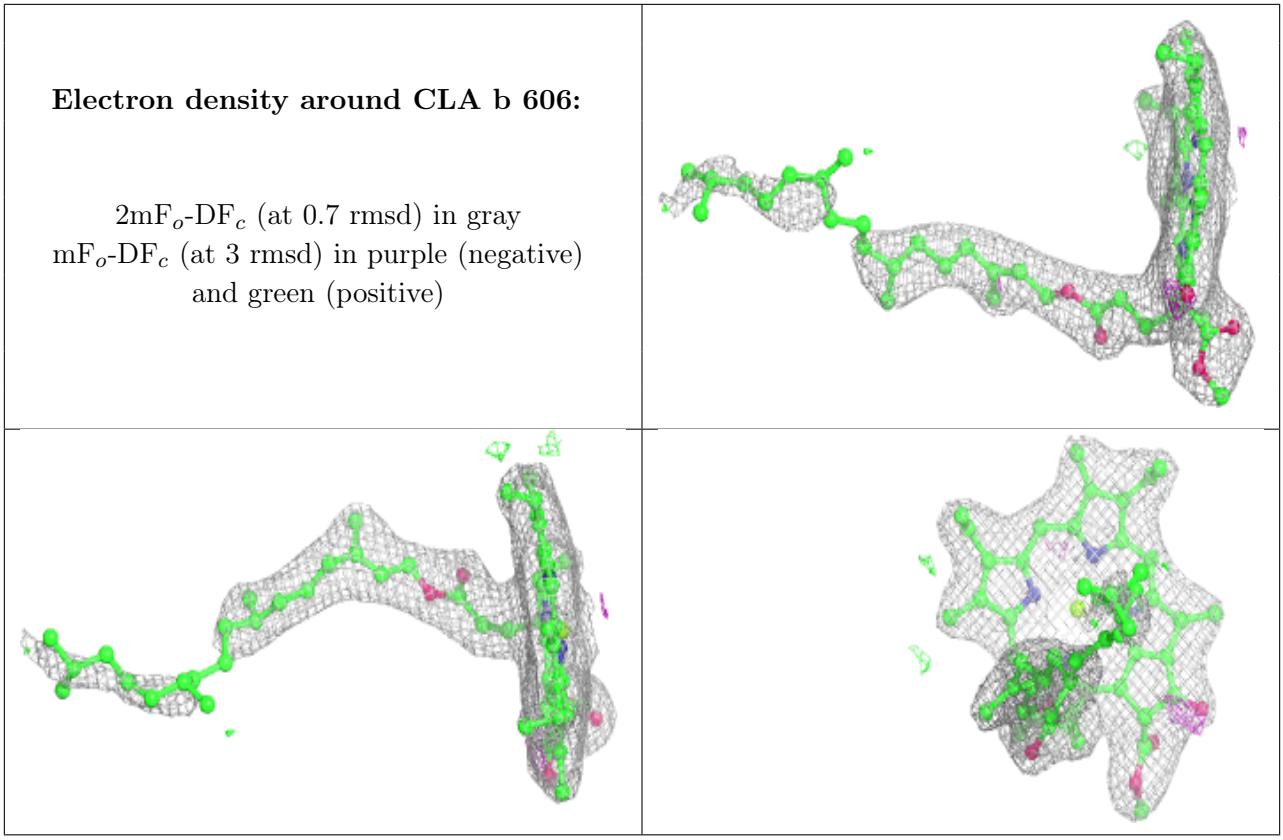






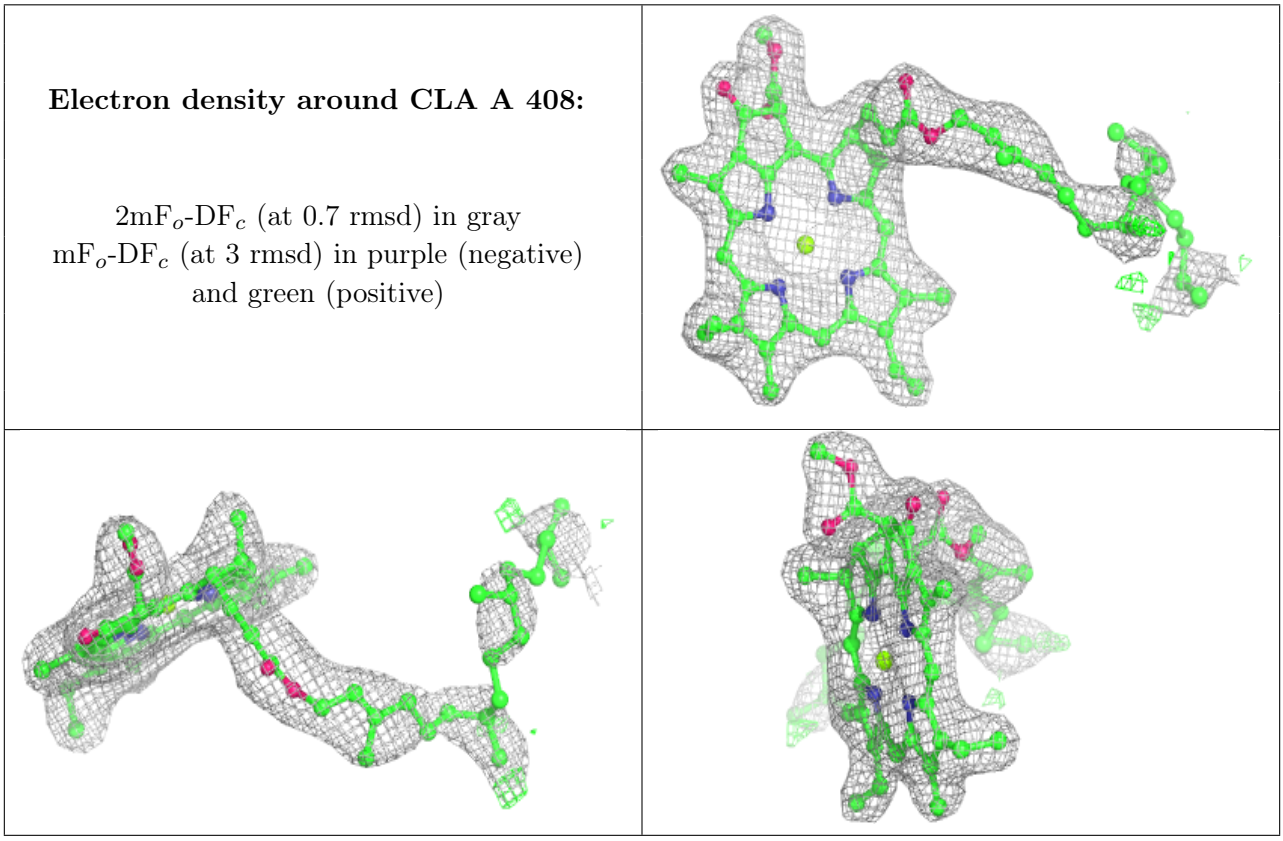
Electron density around CLA b 606:

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



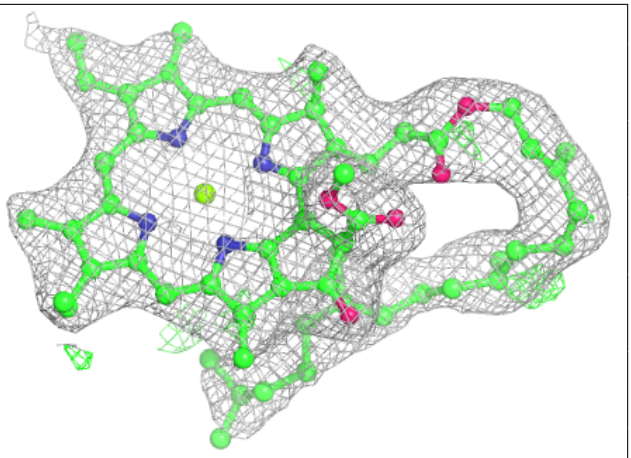
Electron density around CLA A 408:

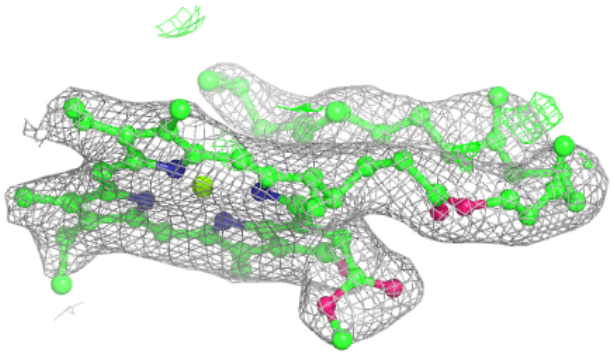
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

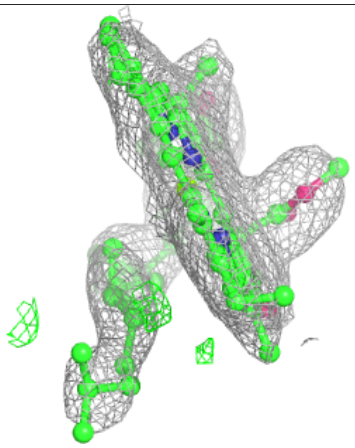


Electron density around CLA c 510:

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

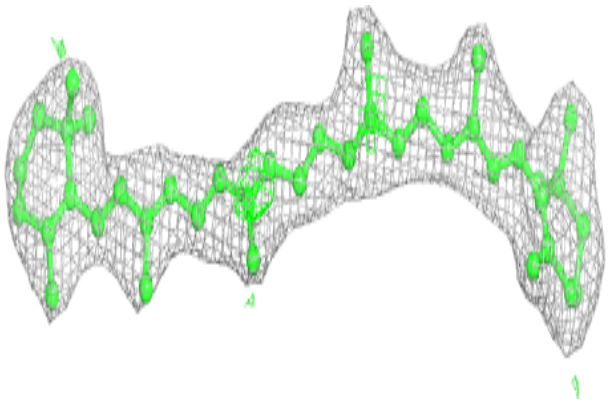


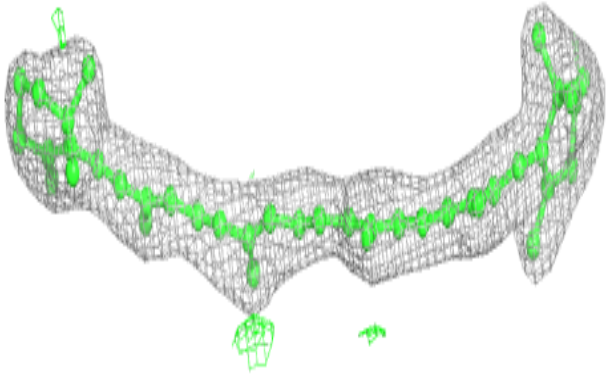


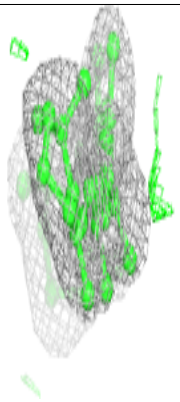


Electron density around BCR t 102:

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

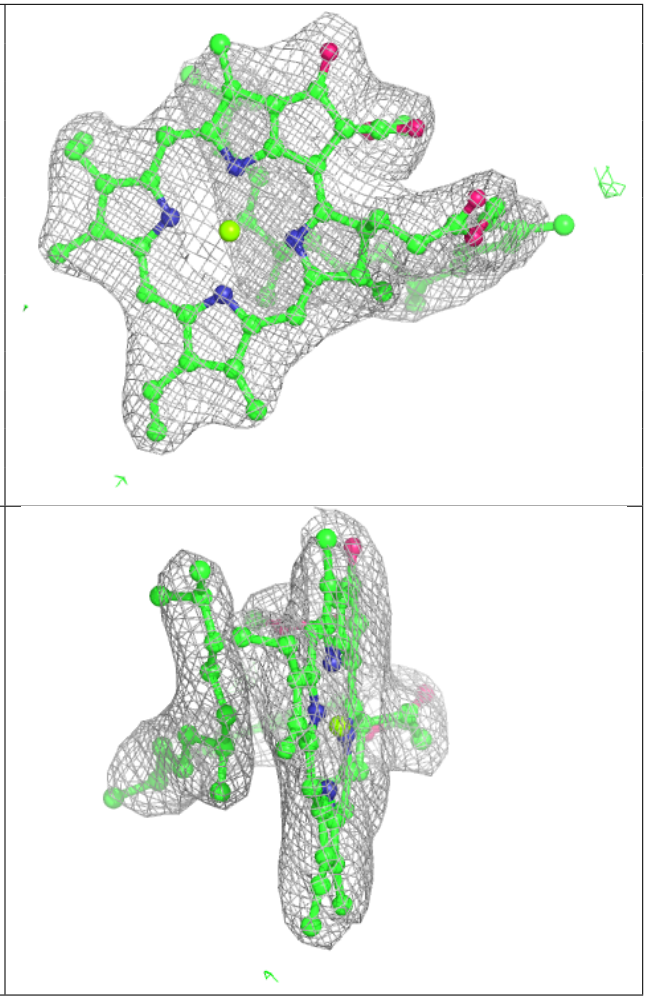






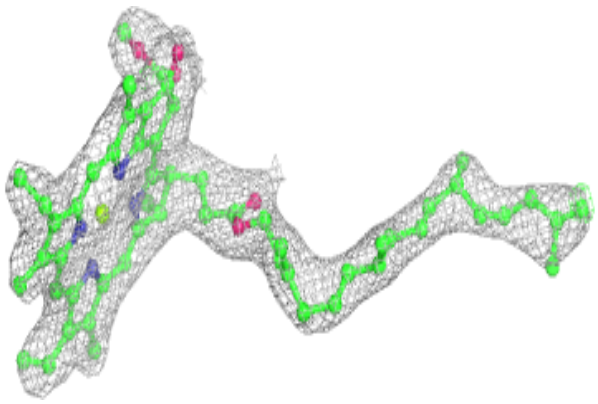
Electron density around CLA c 511:

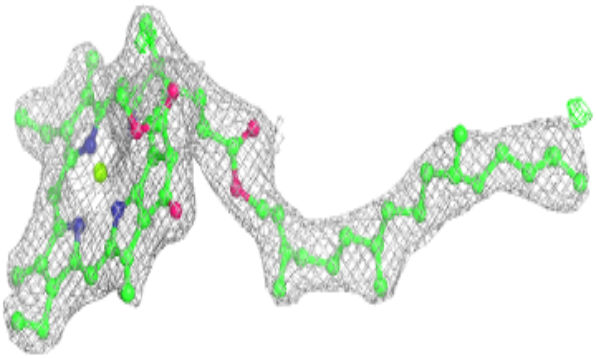
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

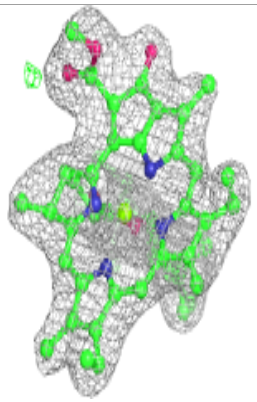


Electron density around CLA C 503:

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

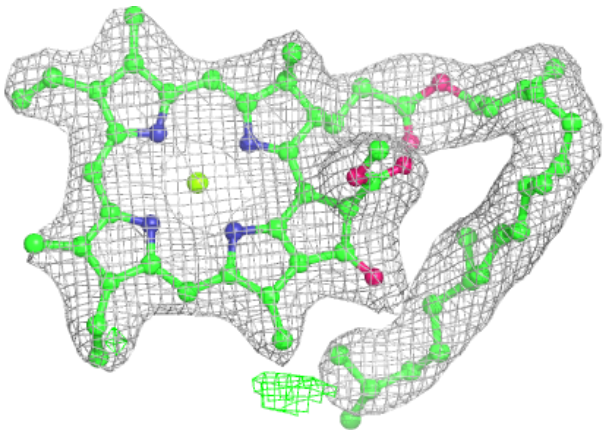


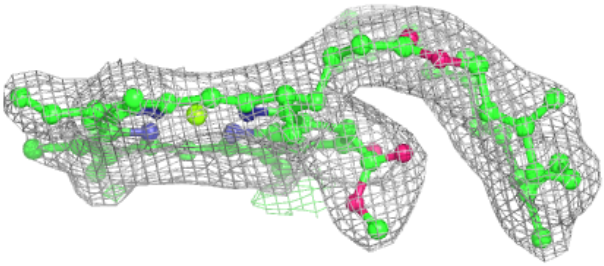


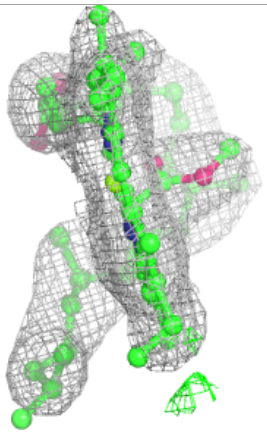


Electron density around CLA B 610:

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

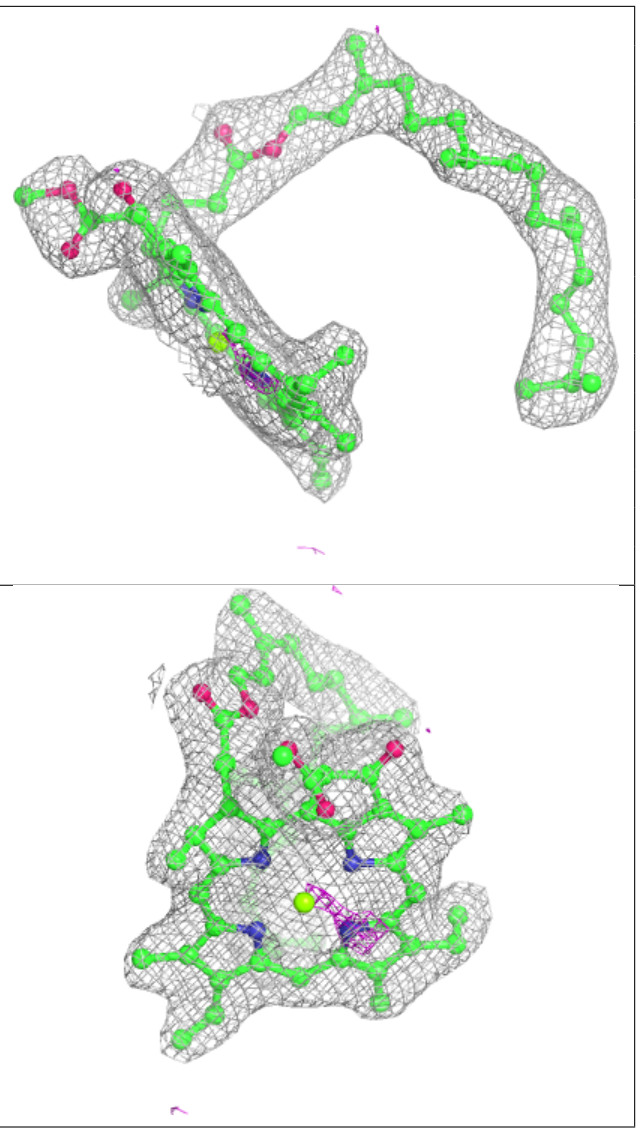






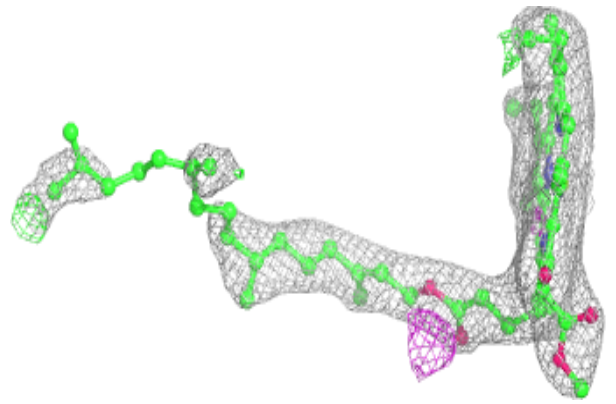
Electron density around CLA b 611:

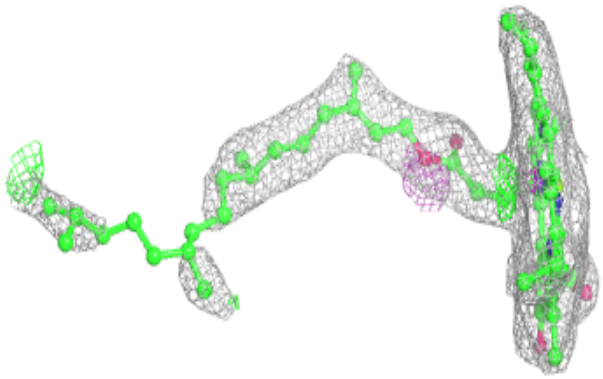
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

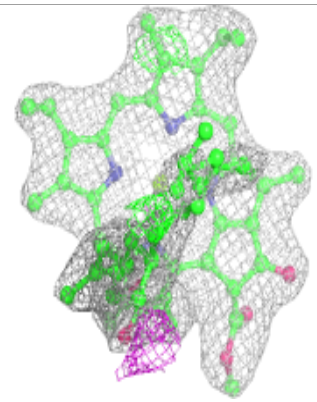


Electron density around CLA B 606:

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

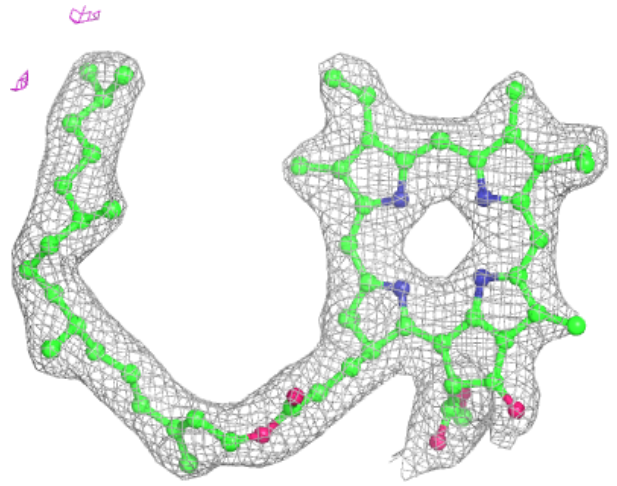


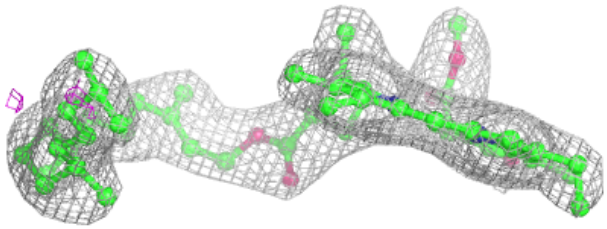


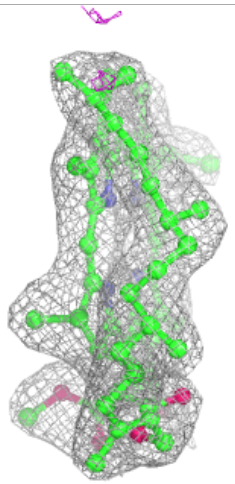


Electron density around PHO A 407:

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

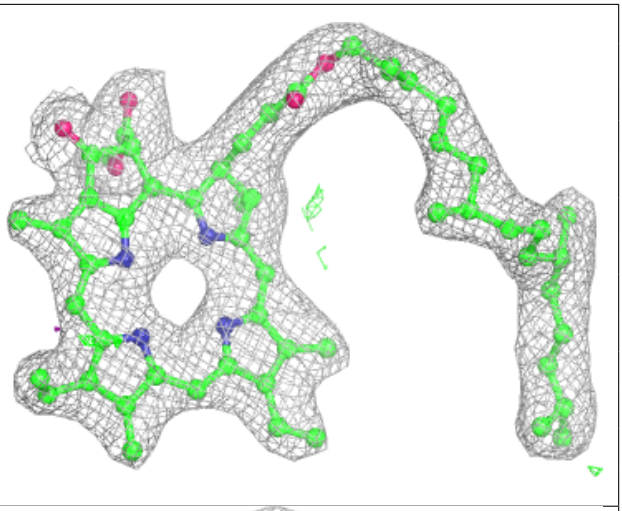


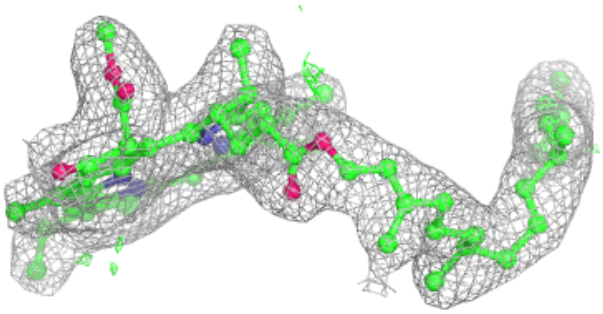


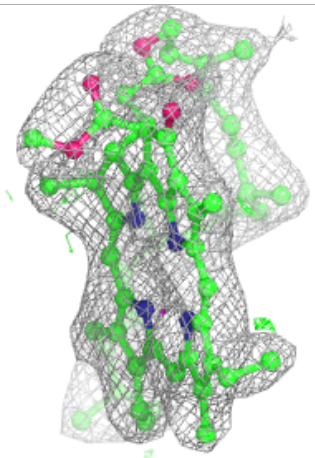


Electron density around PHO D 402:

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

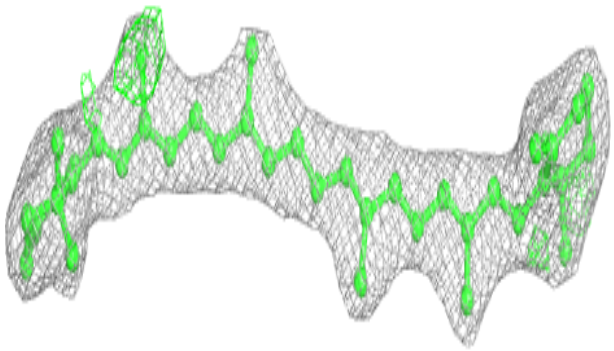


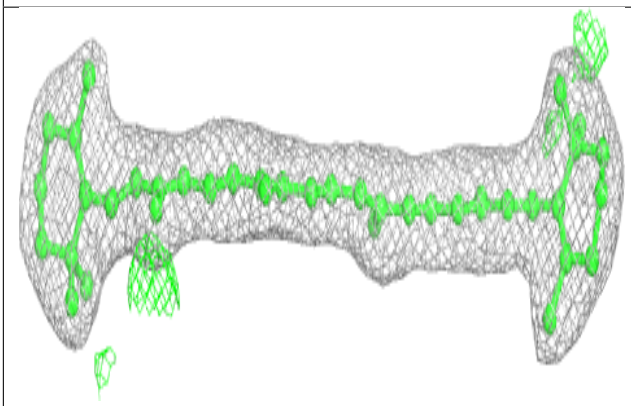


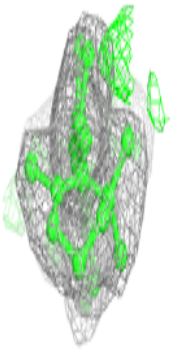


Electron density around BCR A 409:

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

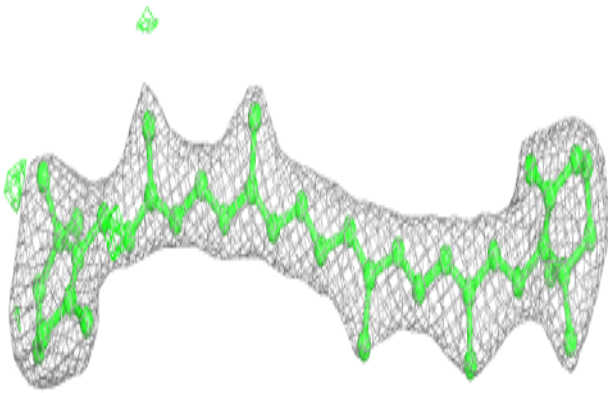


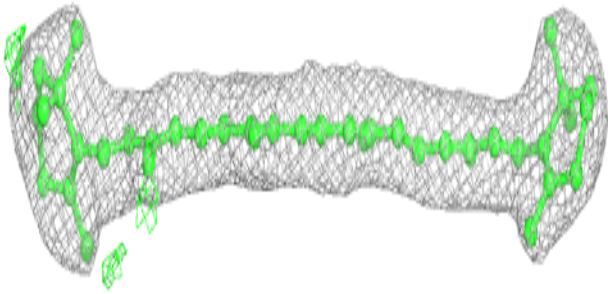


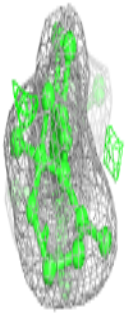


Electron density around BCR B 618:

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

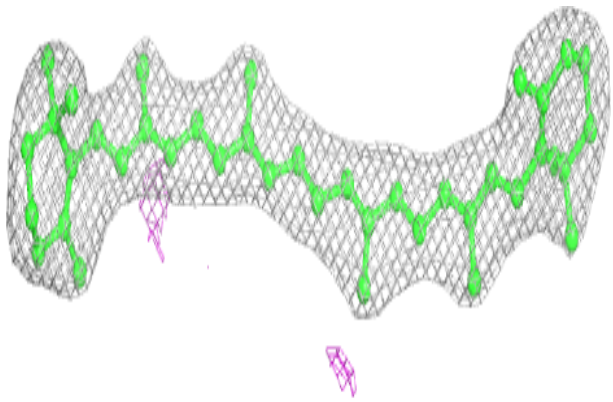


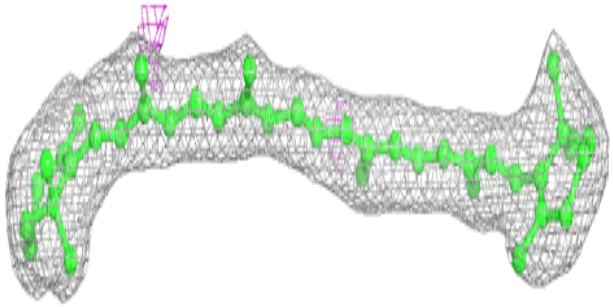


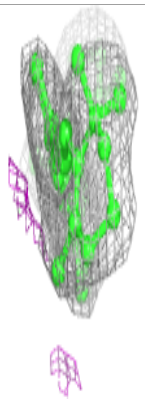


Electron density around BCR B 619:

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

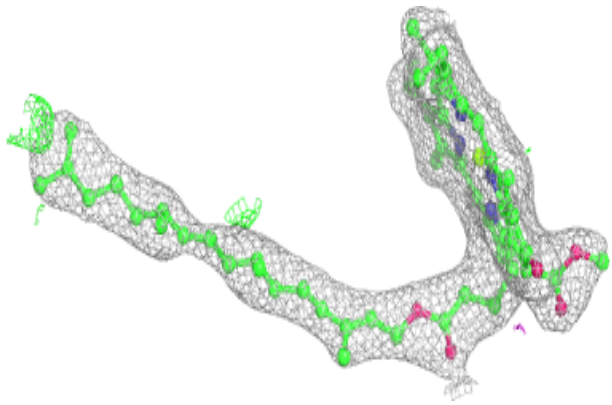


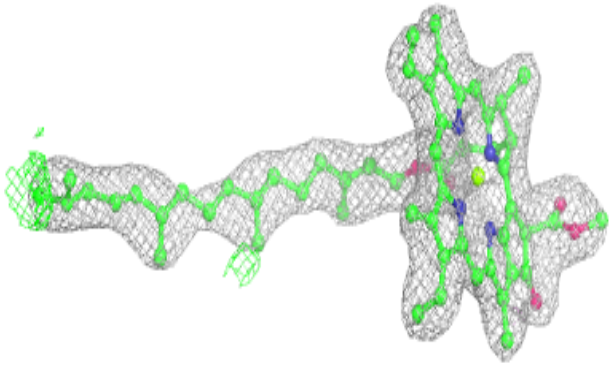


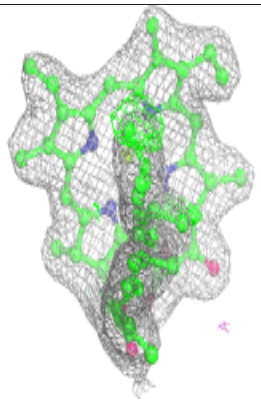


Electron density around CLA B 607:

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

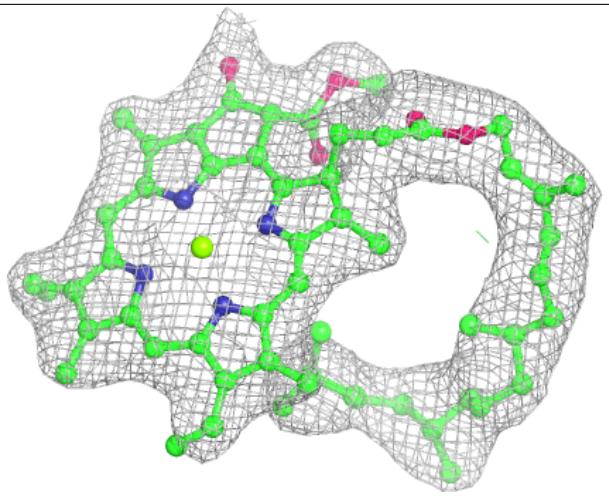


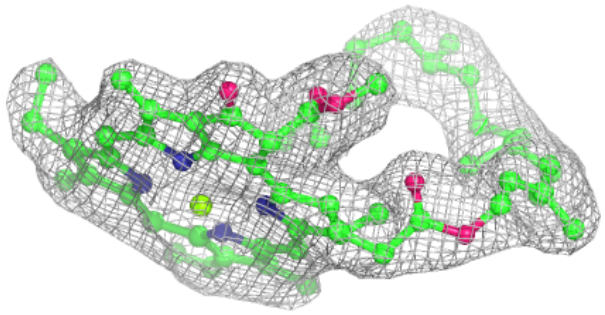


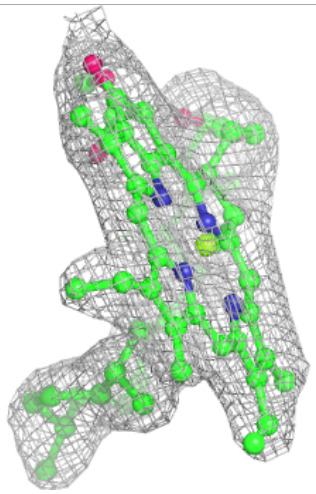


Electron density around CLA b 615:

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

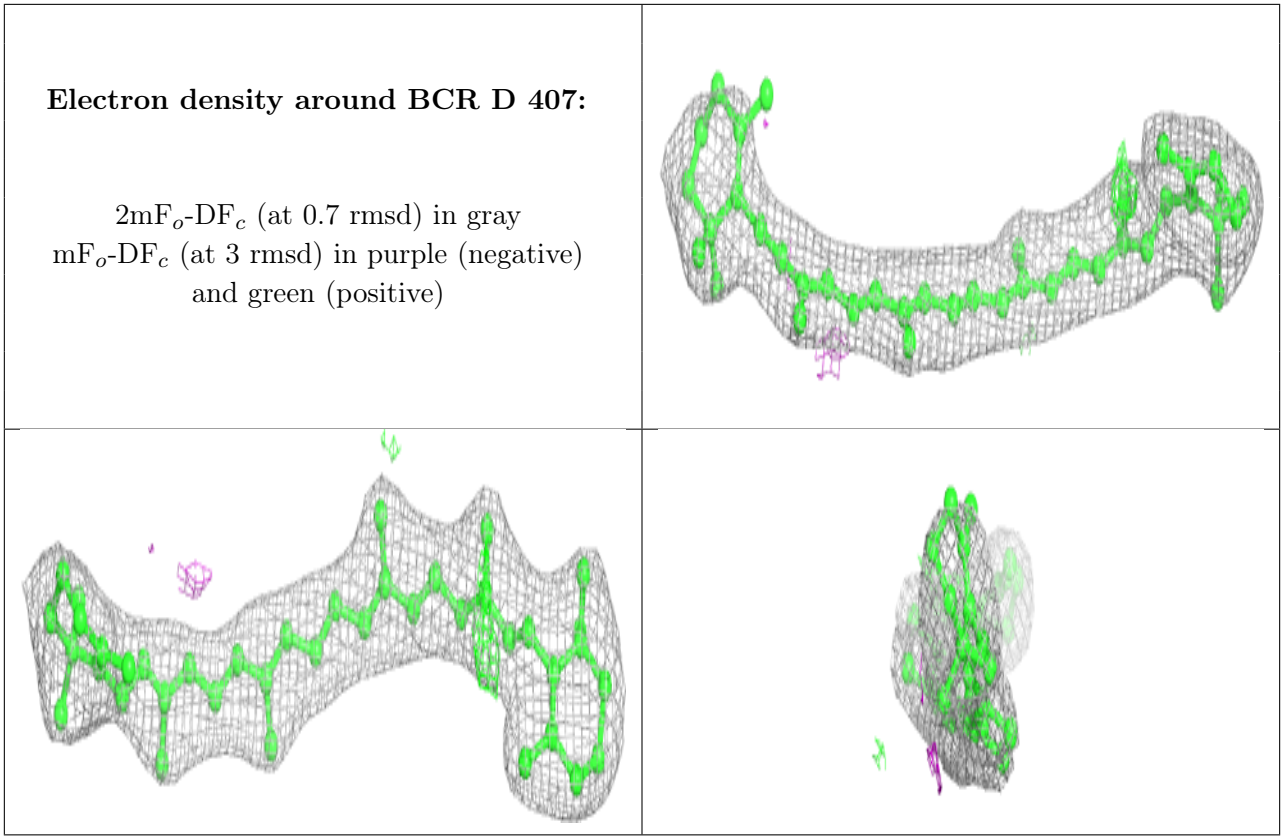






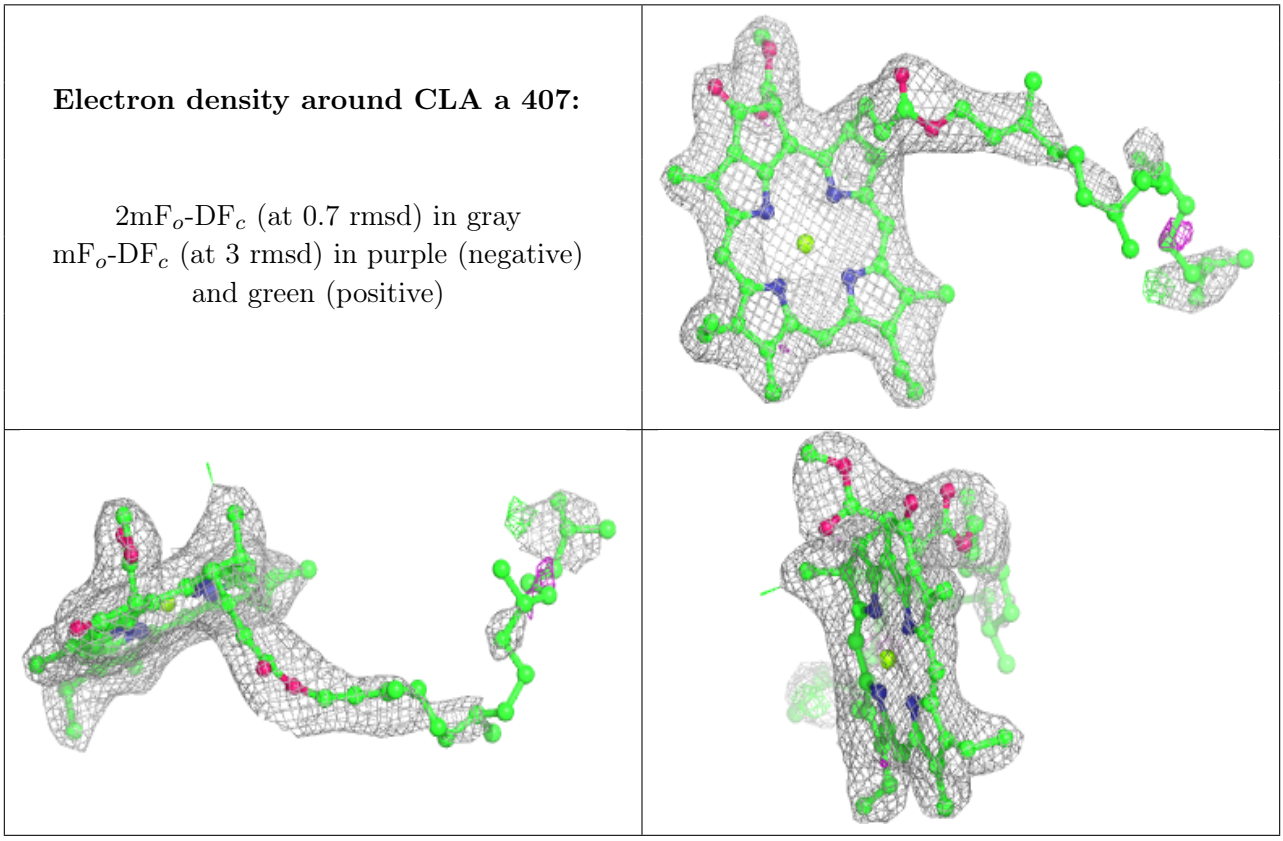
Electron density around BCR D 407:

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



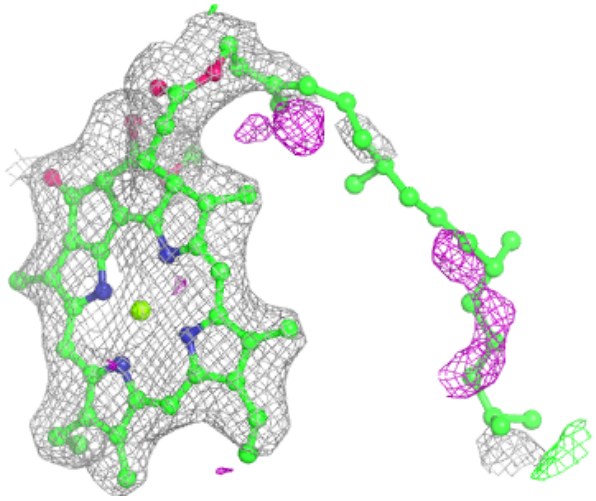
Electron density around CLA a 407:

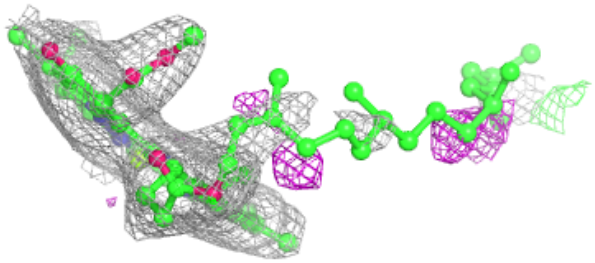
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

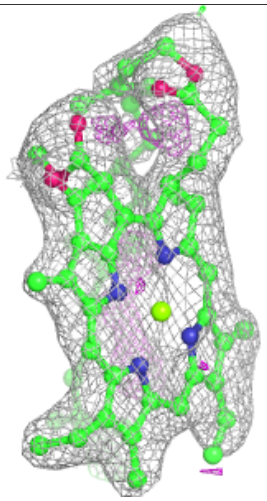


Electron density around CLA B 616:

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

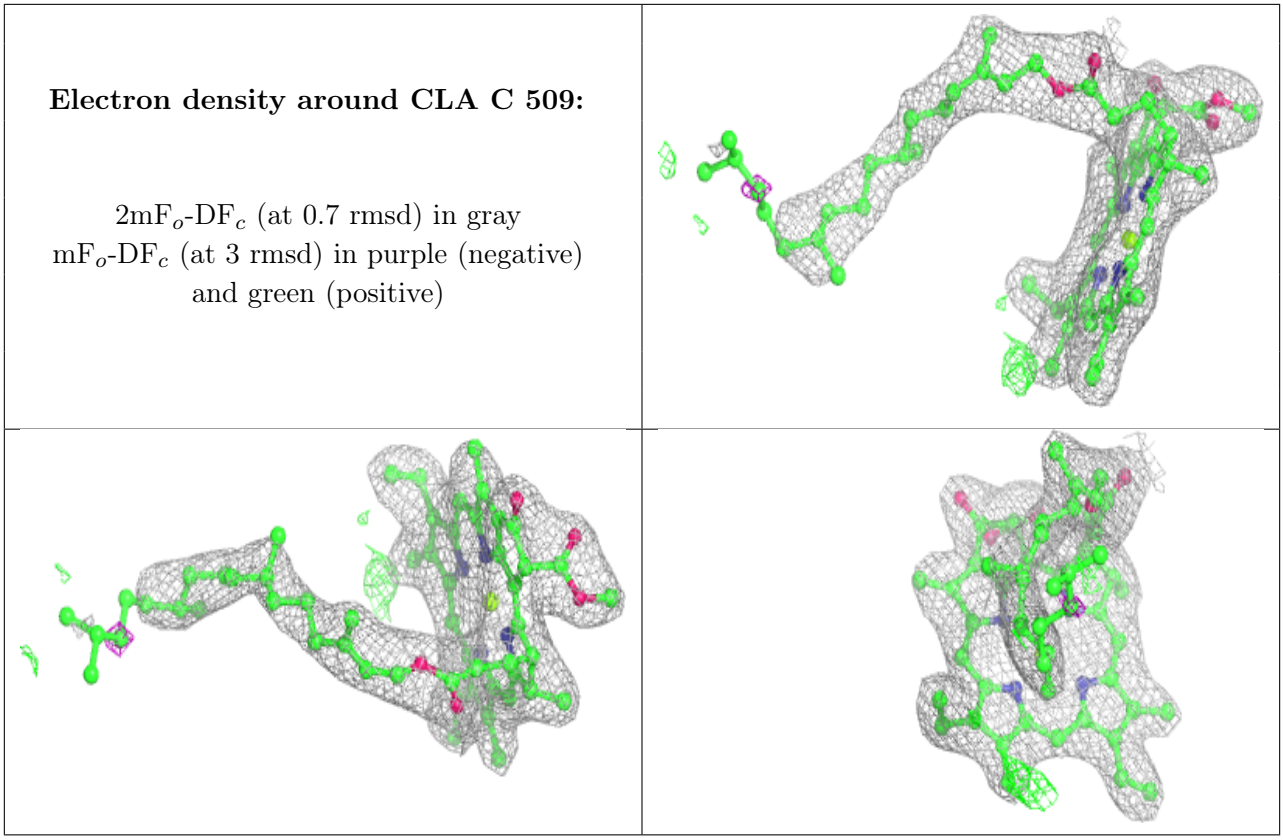






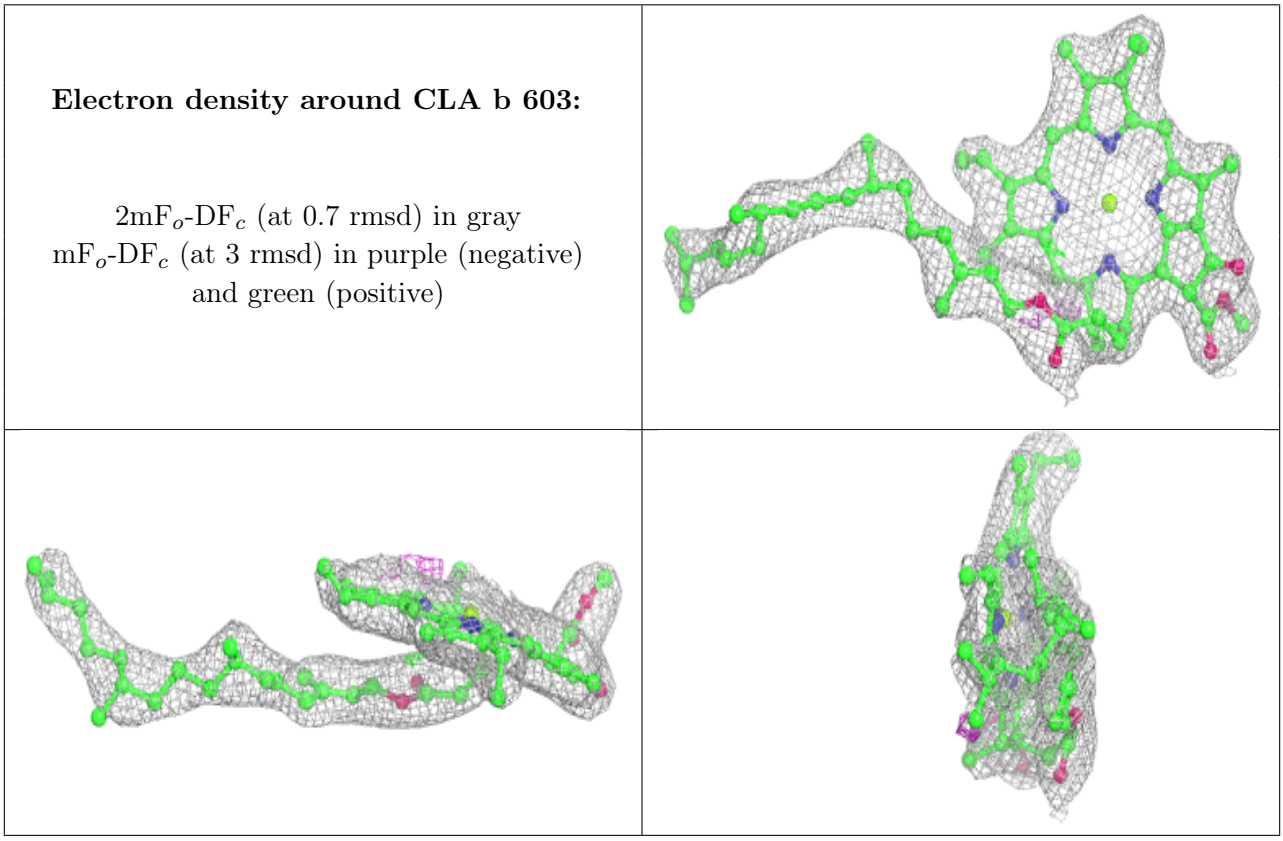
Electron density around CLA C 509:

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



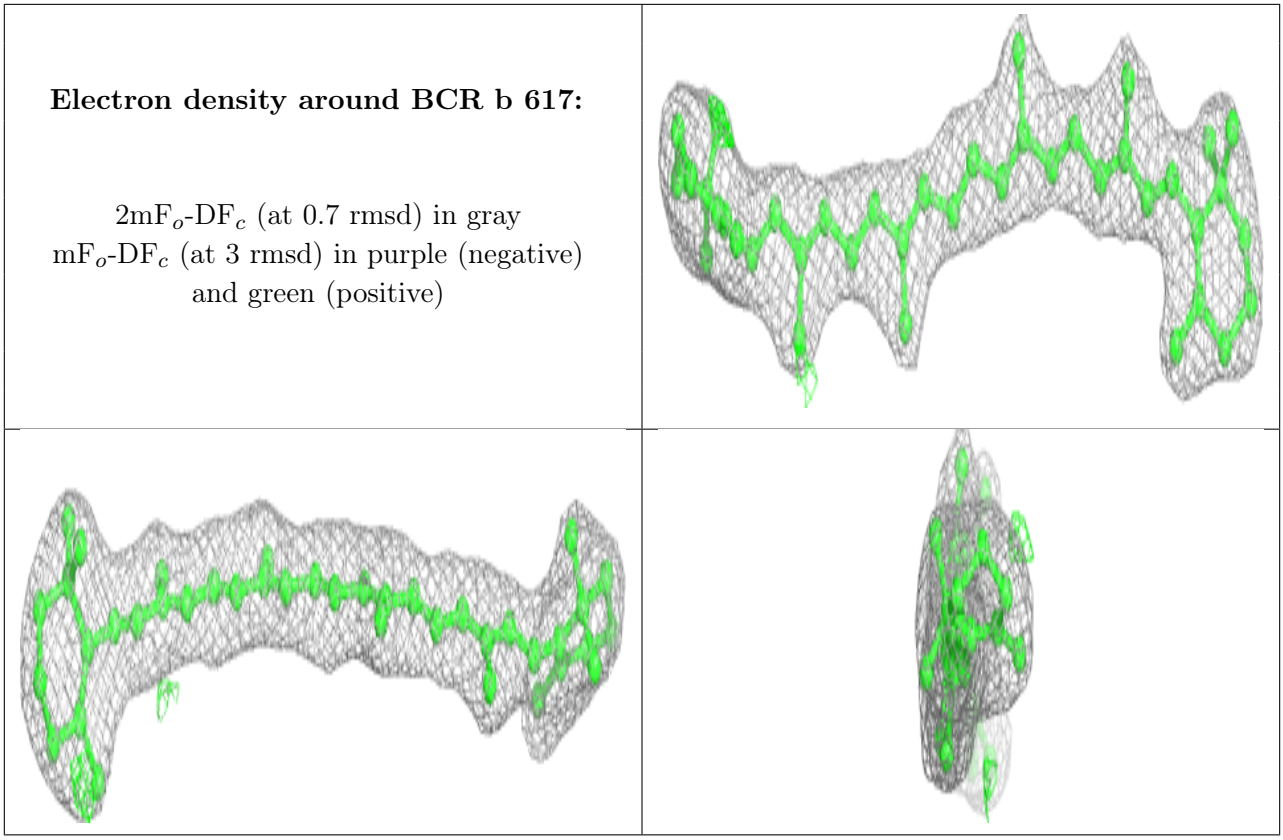
Electron density around CLA b 603:

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



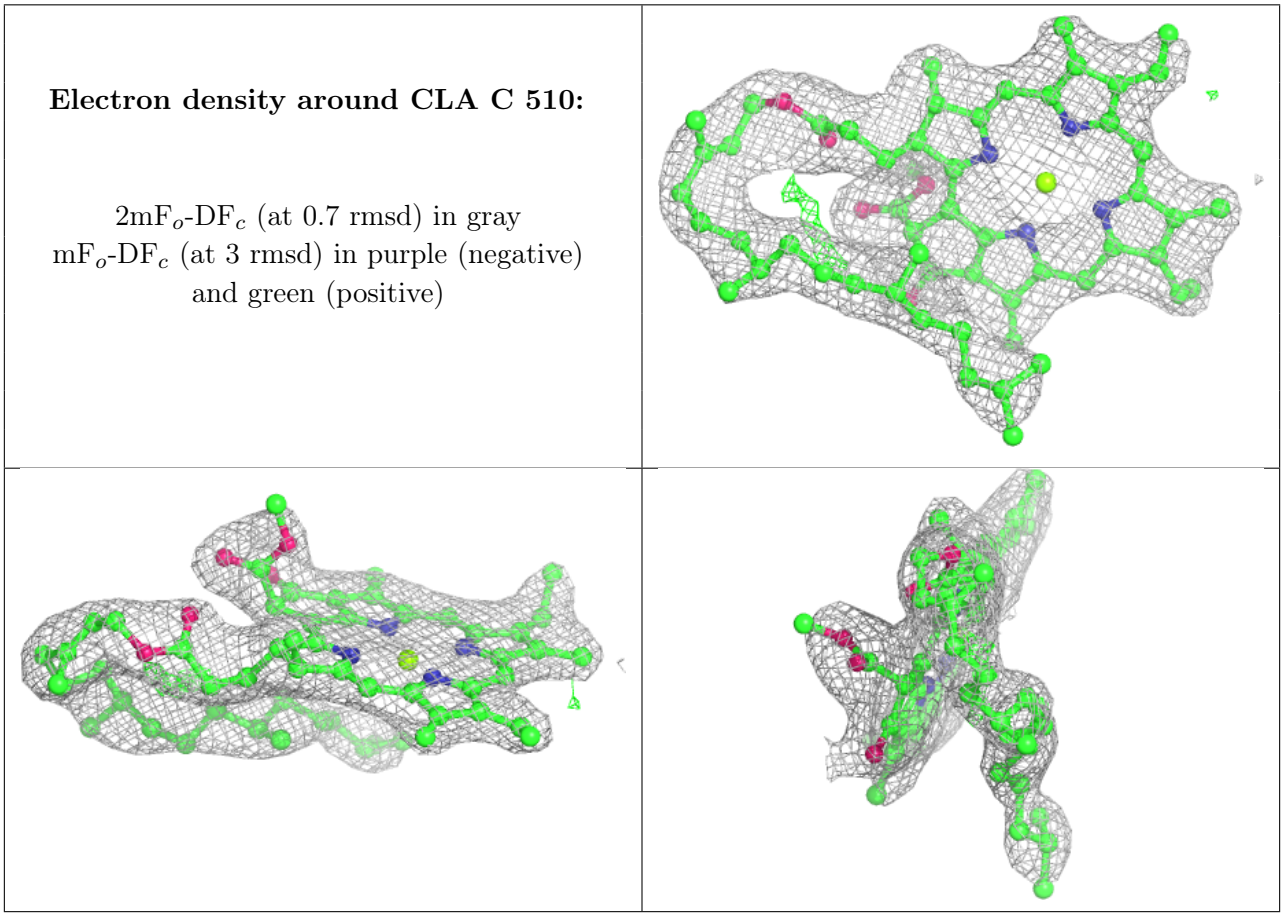
Electron density around BCR b 617:

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



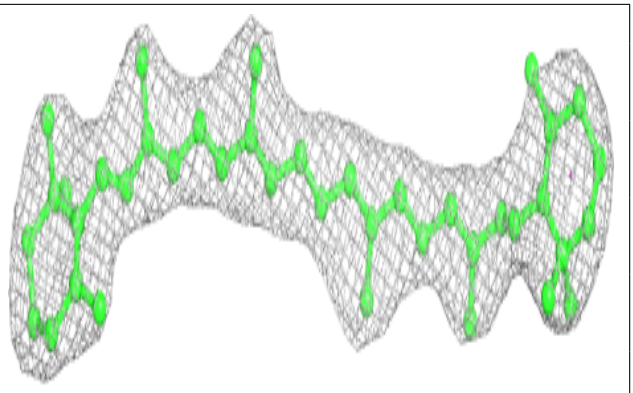
Electron density around CLA C 510:

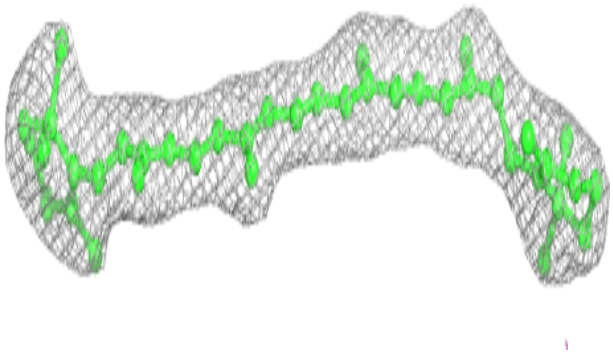
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

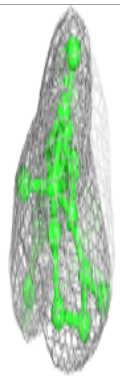


Electron density around BCR b 619:

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

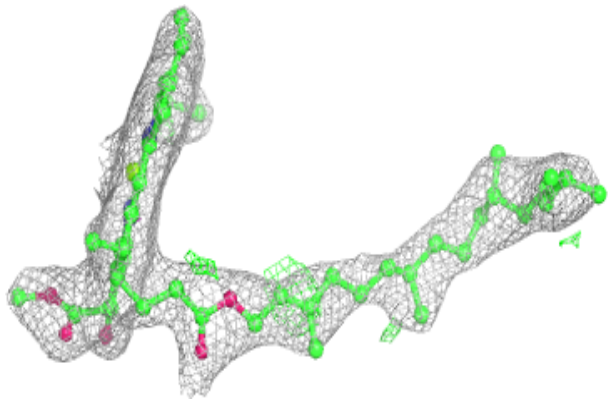


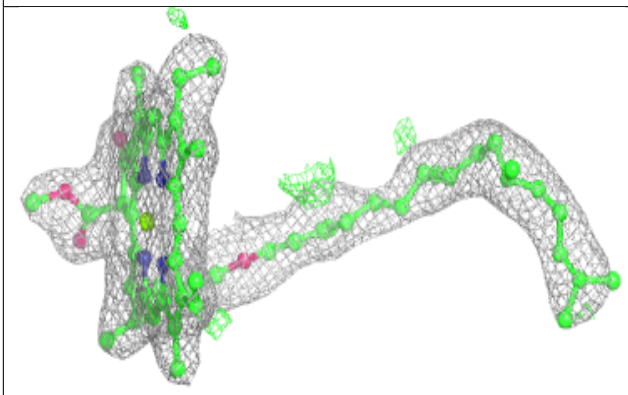


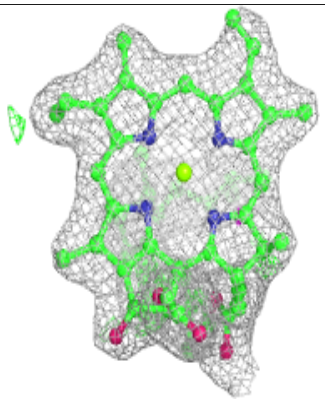


Electron density around CLA b 605:

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

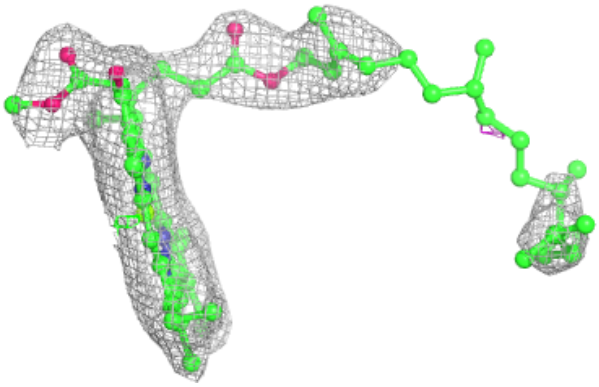


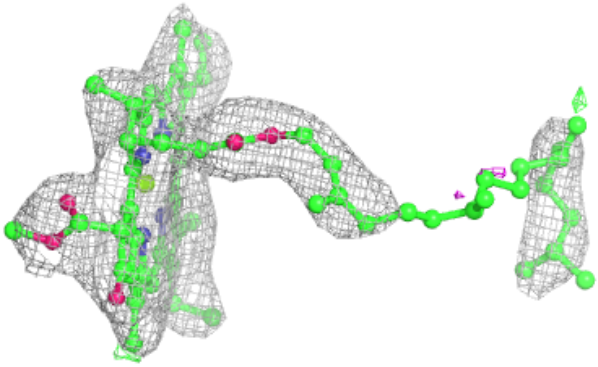


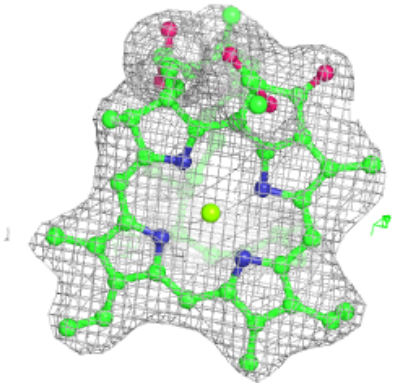


Electron density around CLA c 507:

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

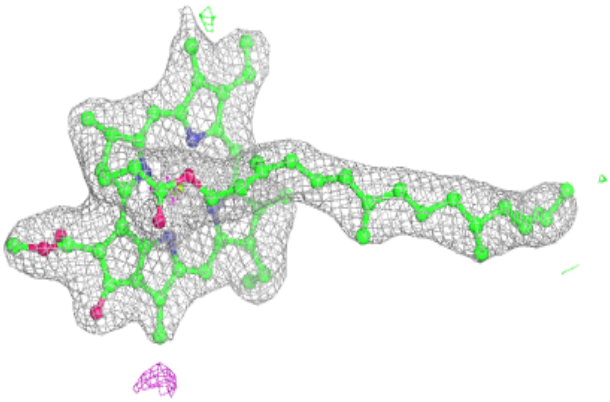


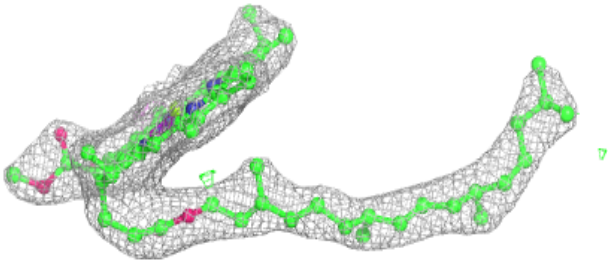


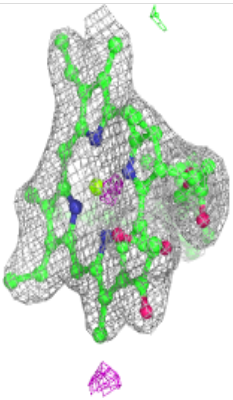


Electron density around CLA b 608:

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

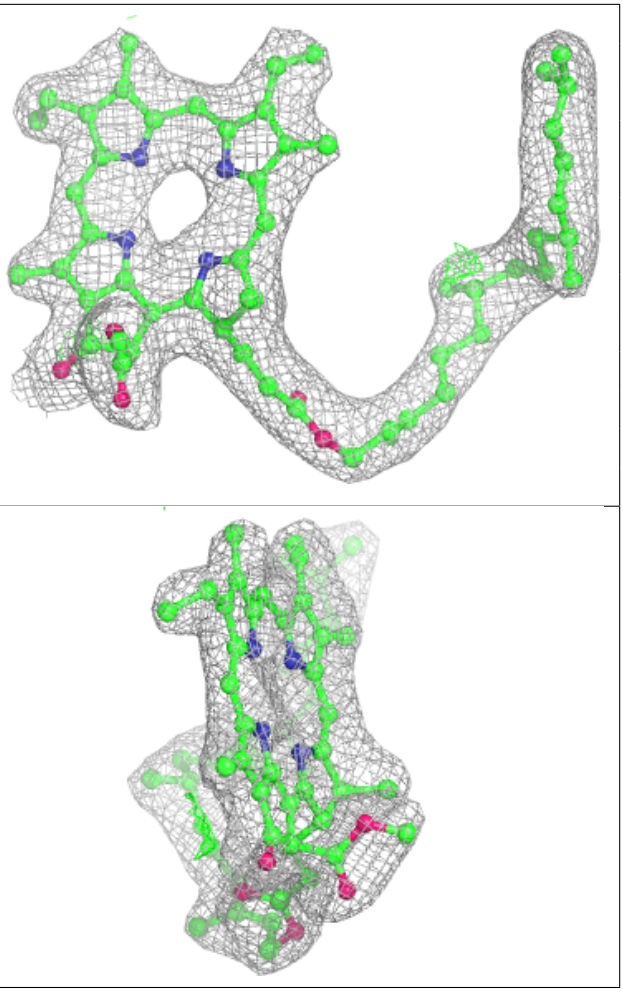






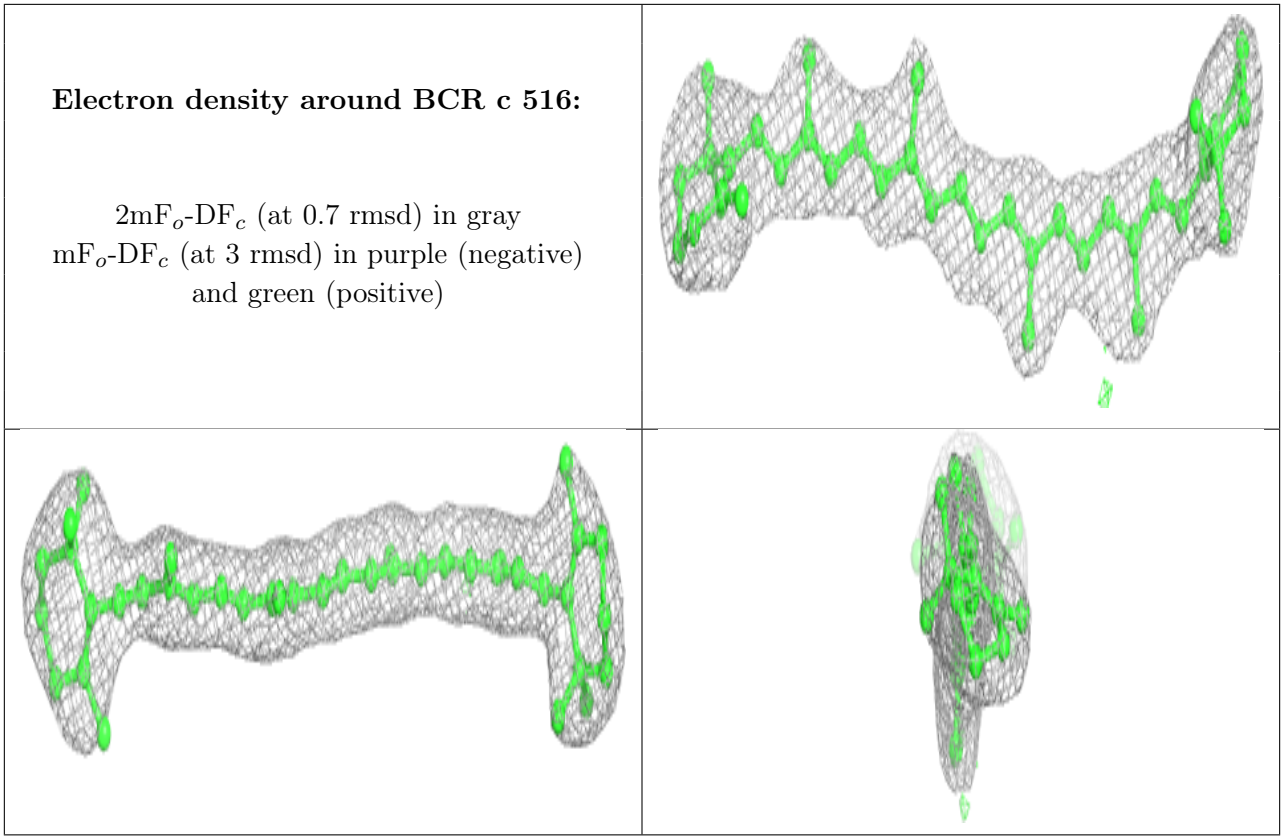
Electron density around PHO a 416:

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



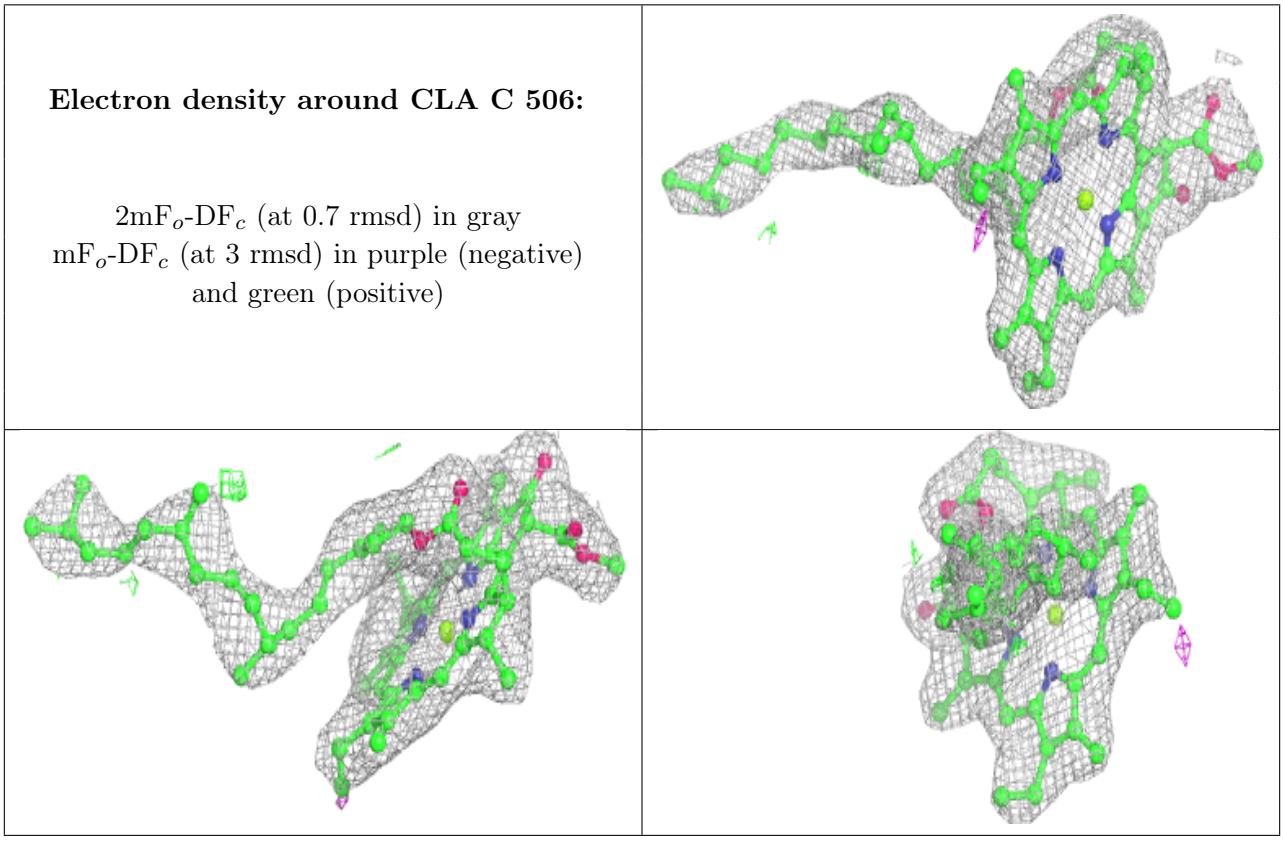
Electron density around BCR c 516:

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



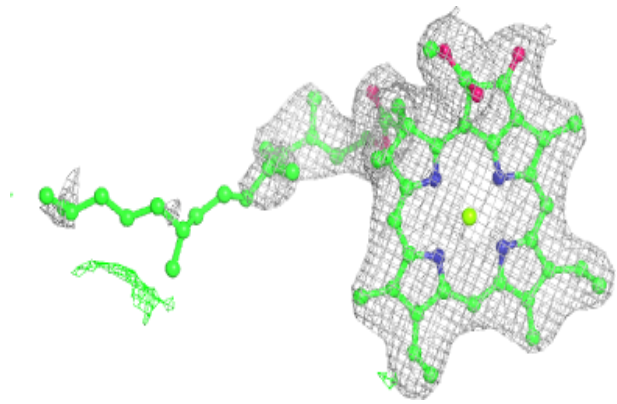
Electron density around CLA C 506:

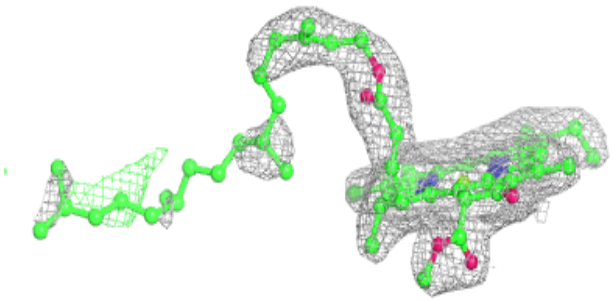
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

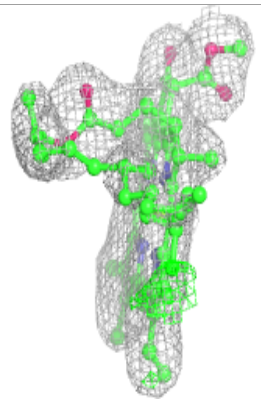


Electron density around CLA a 405:

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

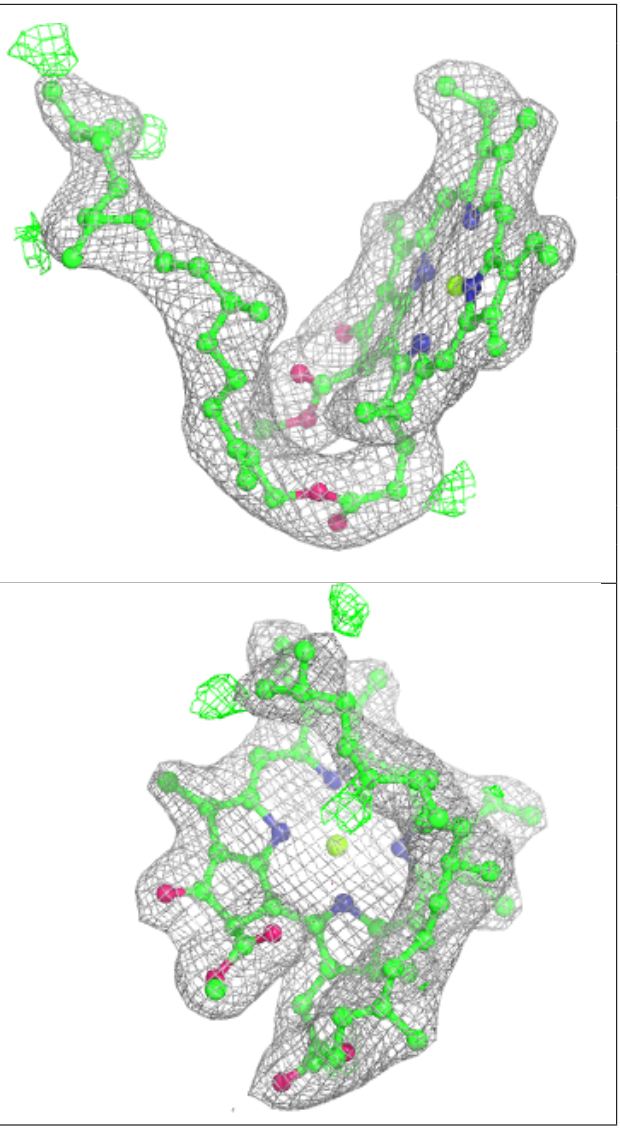






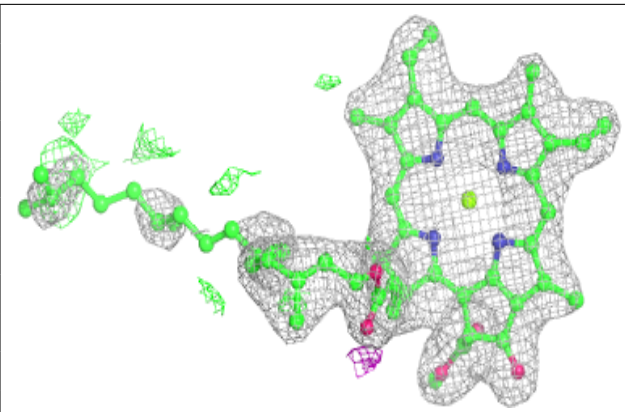
Electron density around CLA B 613:

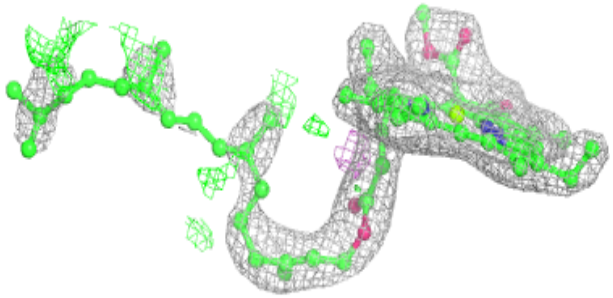
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

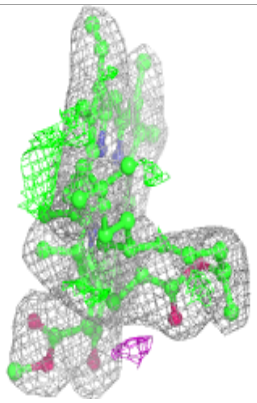


Electron density around CLA A 406:

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

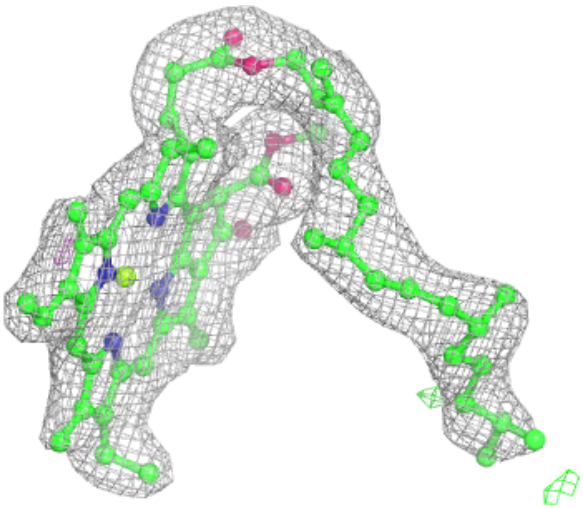


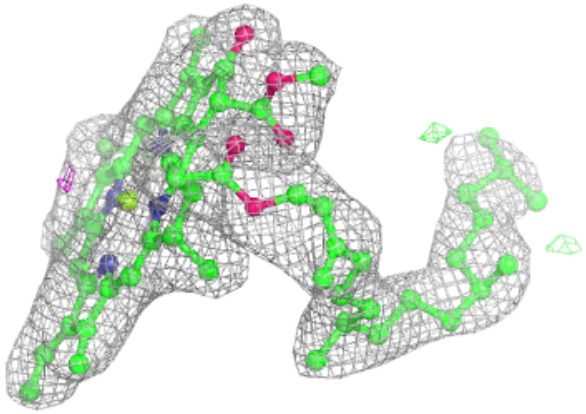


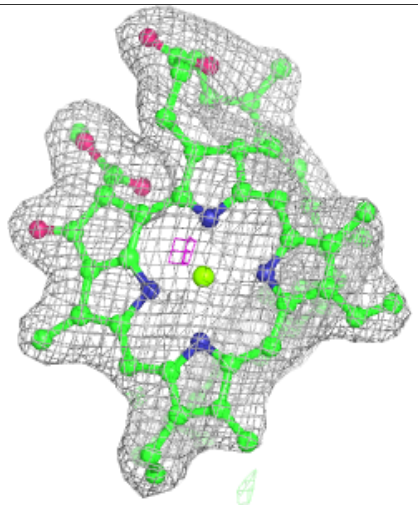


Electron density around CLA b 613:

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

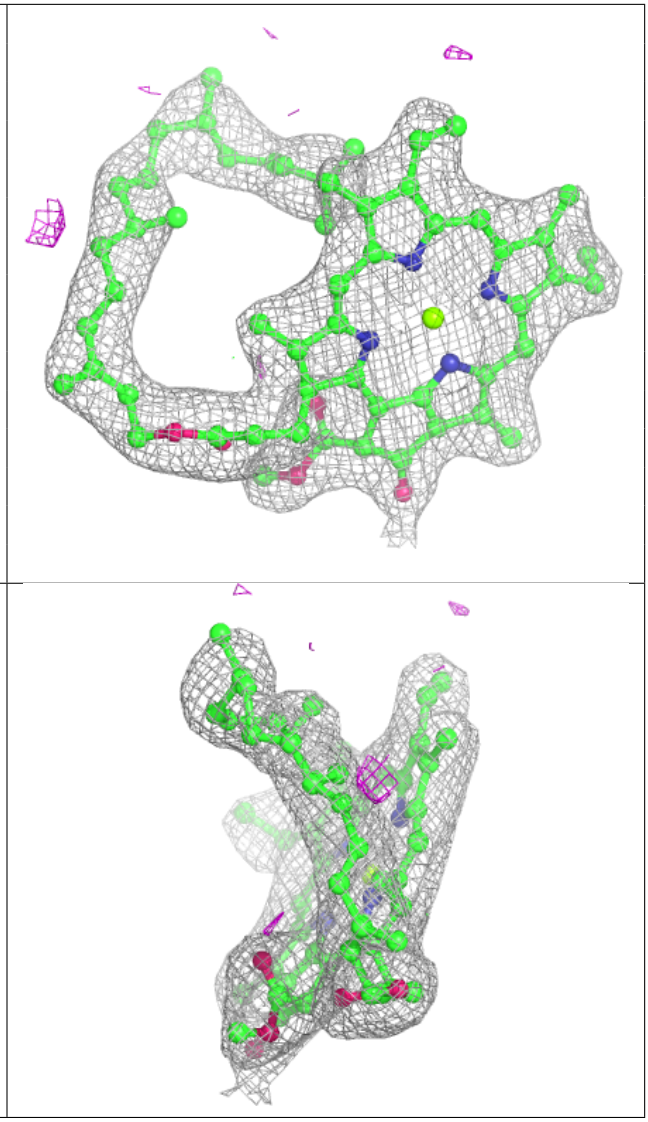






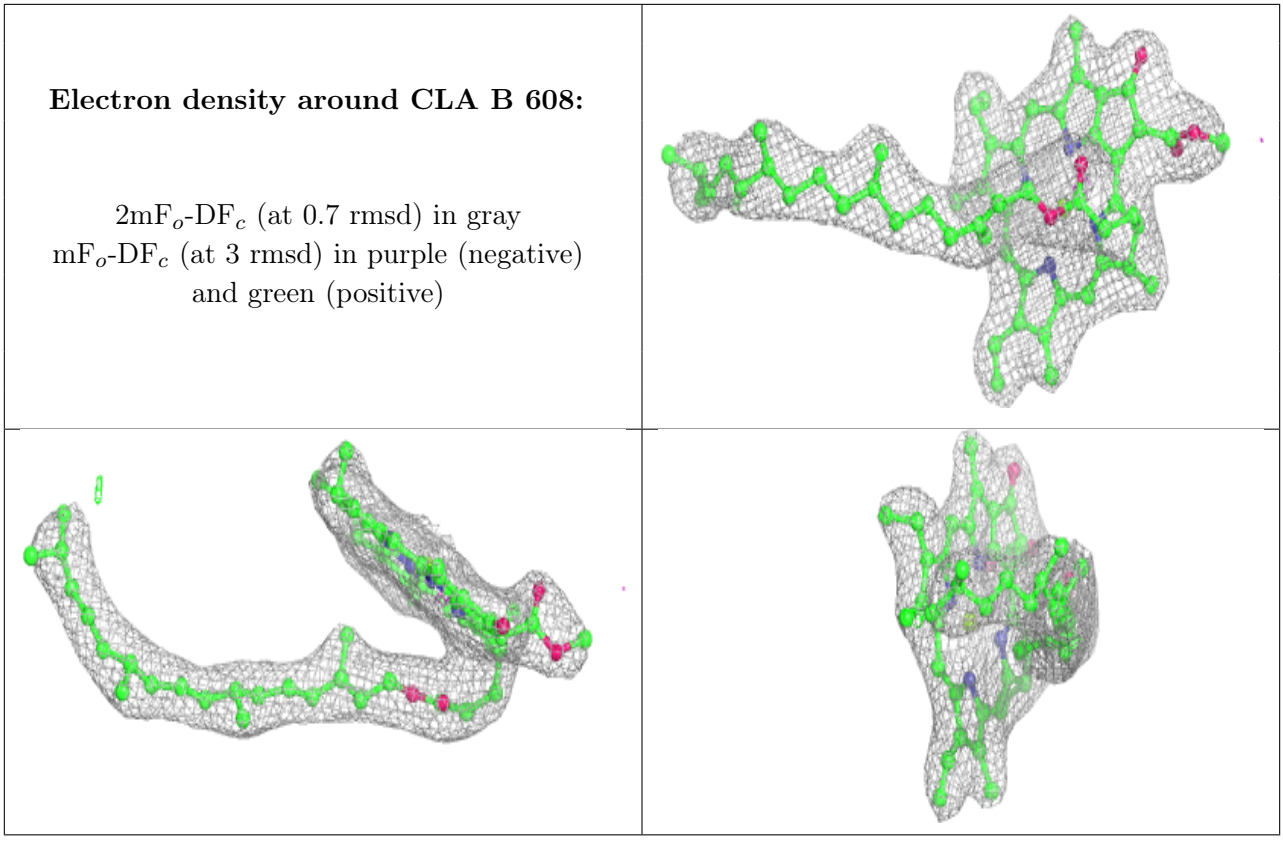
Electron density around CLA B 615:

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



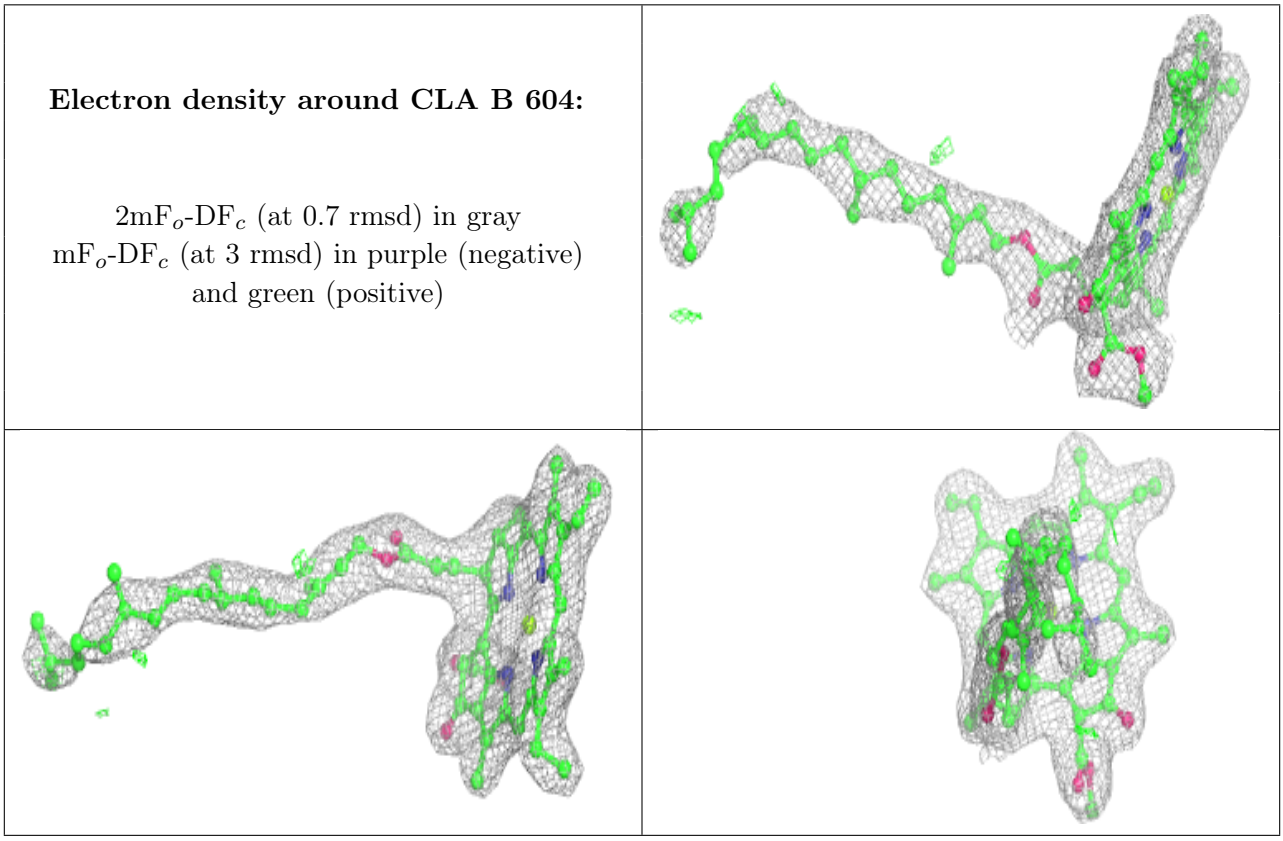
Electron density around CLA B 608:

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



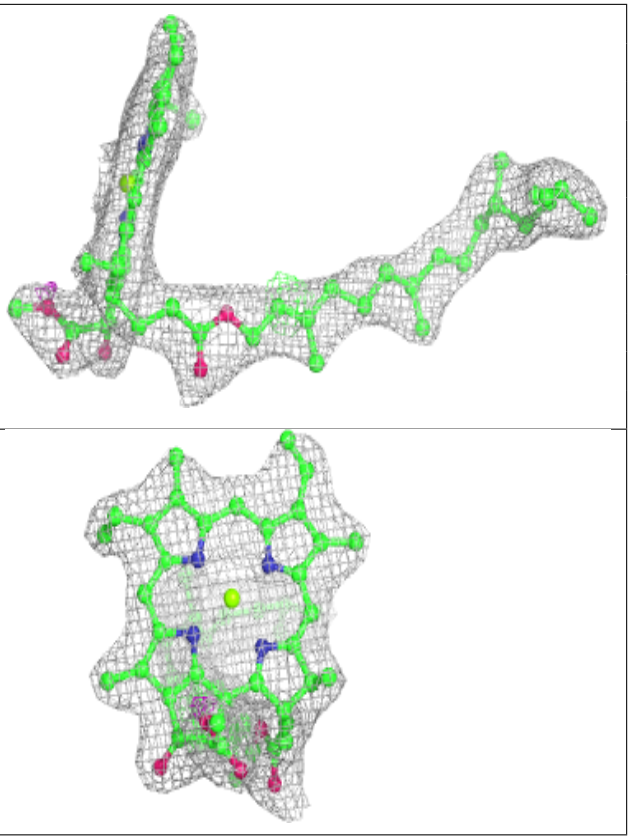
Electron density around CLA B 604:

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



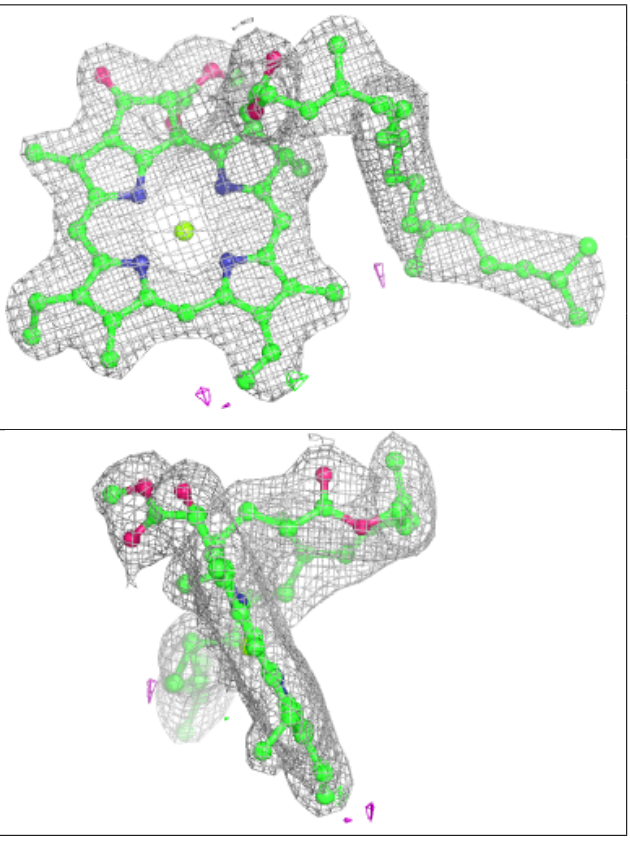
Electron density around CLA B 605:

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



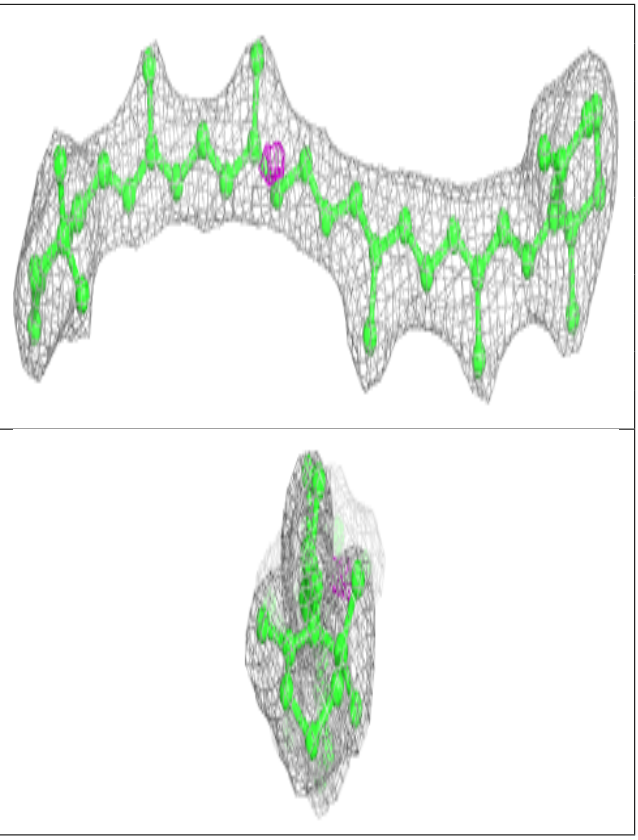
Electron density around CLA d 402:

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



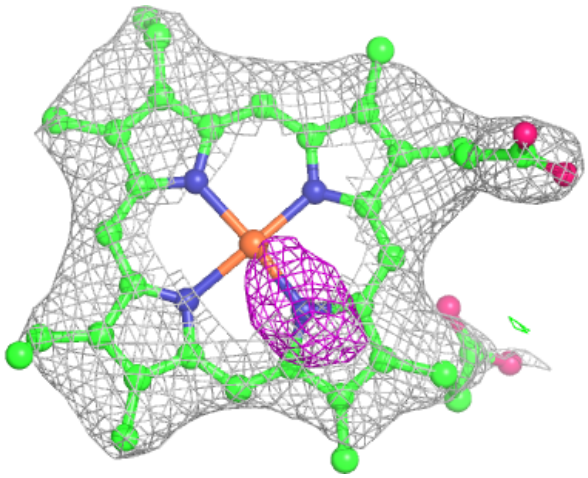
Electron density around BCR a 408:

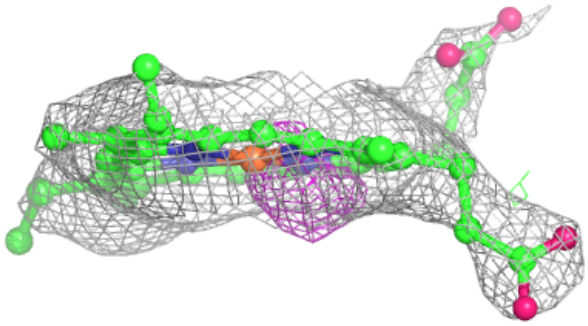
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

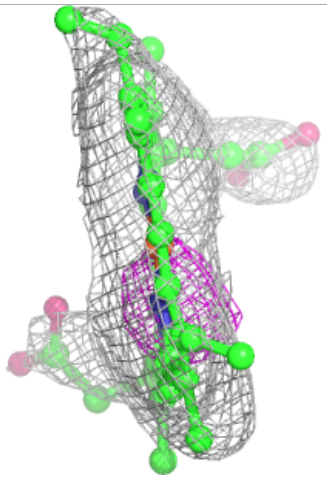


Electron density around HEM f 101:

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

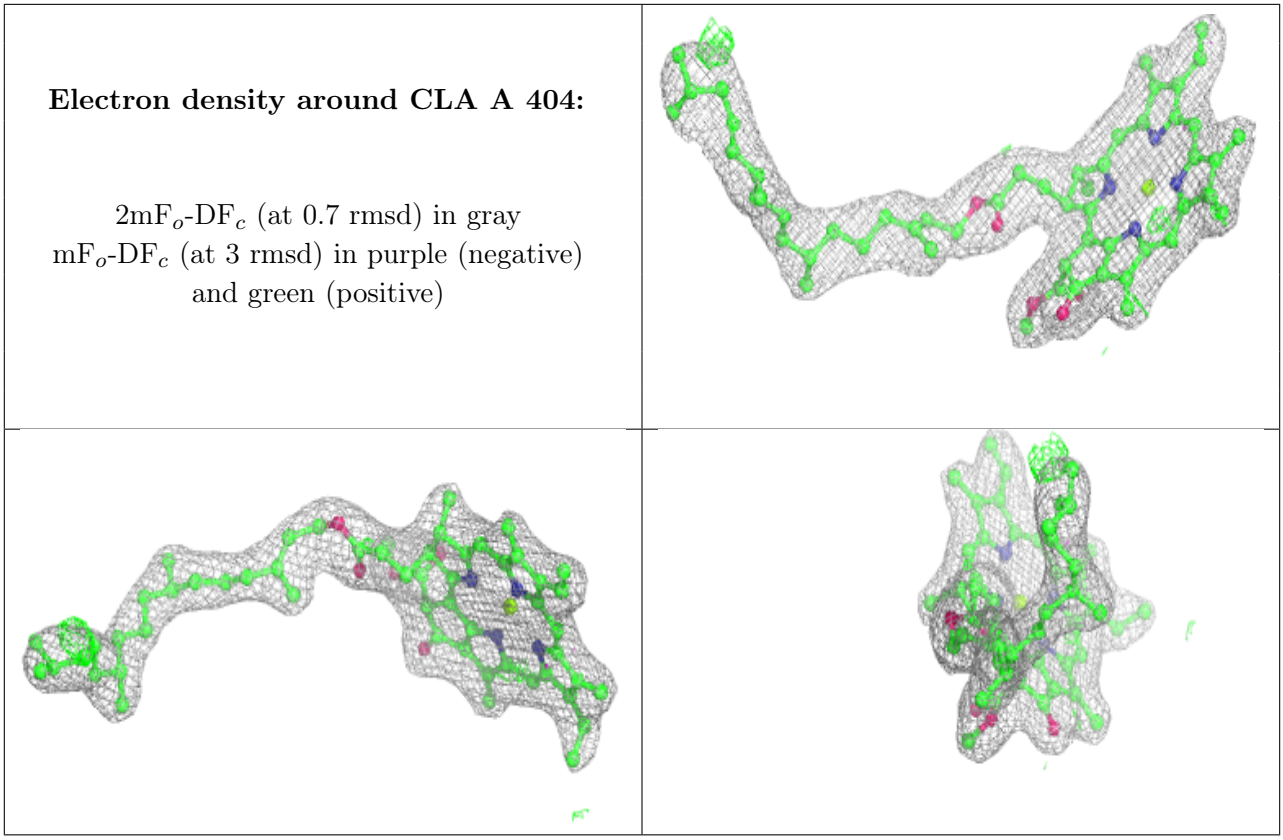






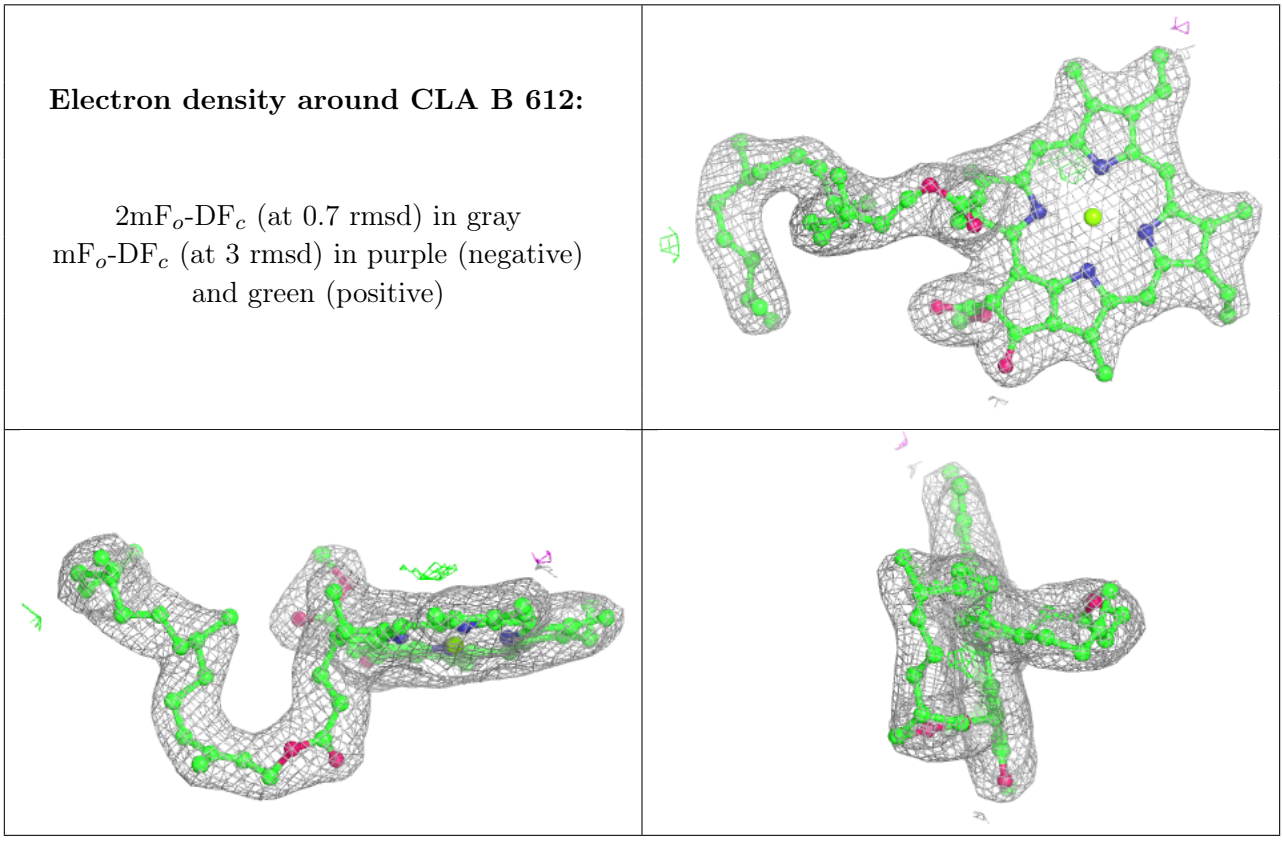
Electron density around CLA A 404:

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



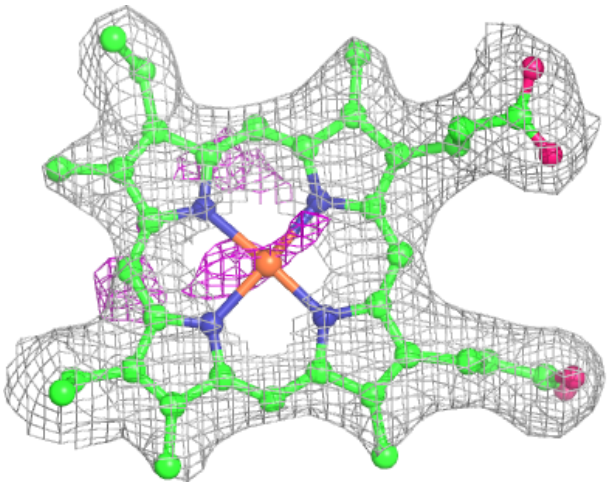
Electron density around CLA B 612:

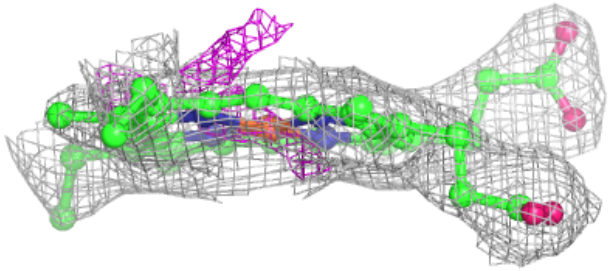
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

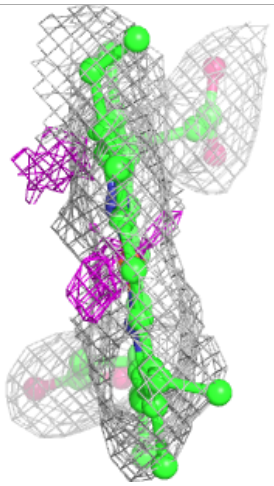


Electron density around HEC v 203:

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

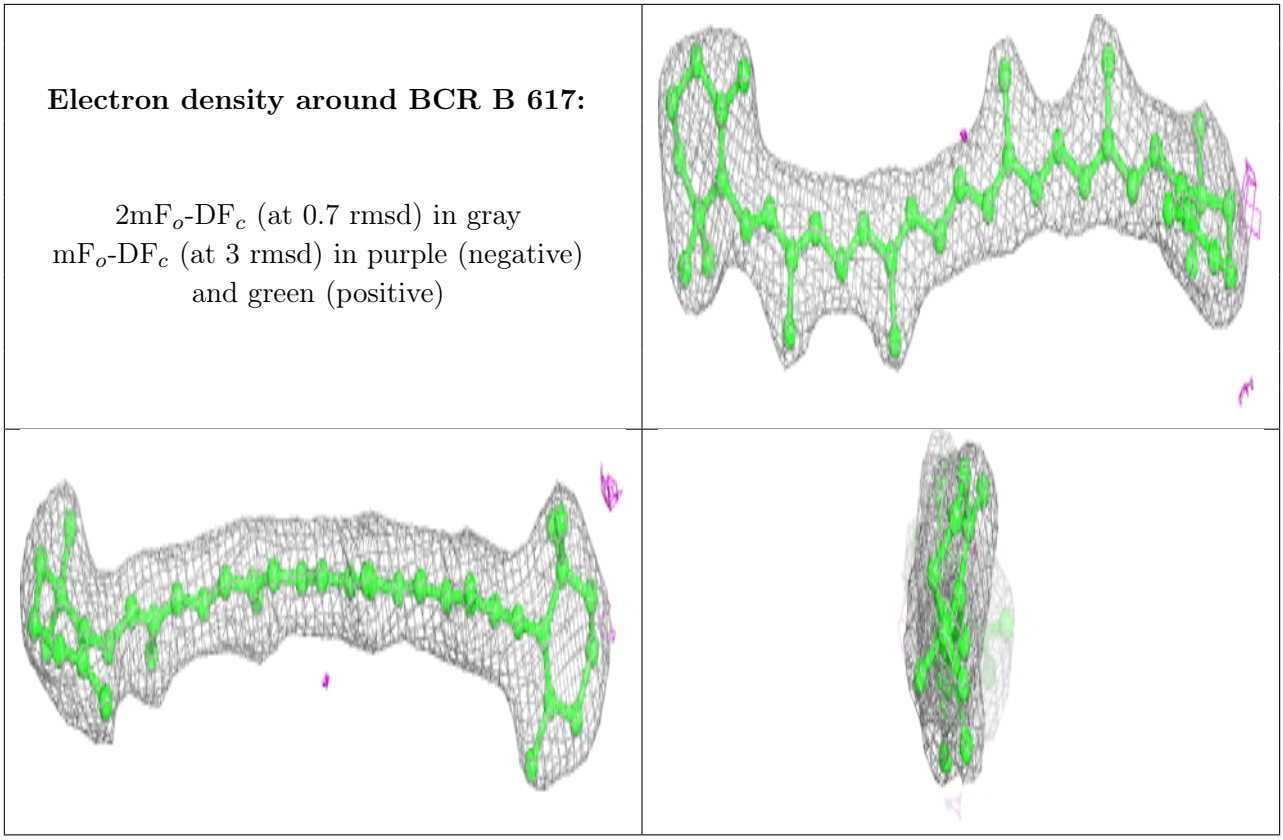






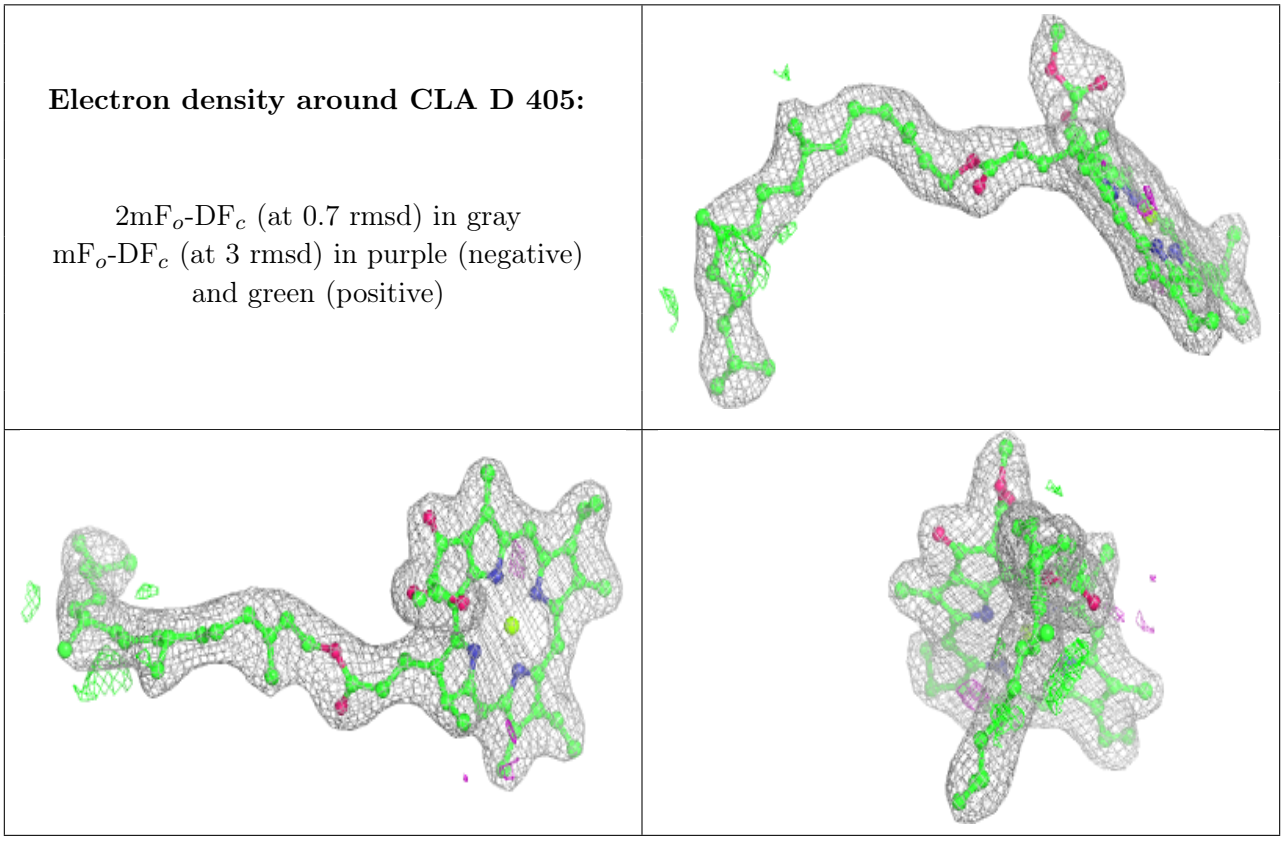
Electron density around BCR B 617:

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



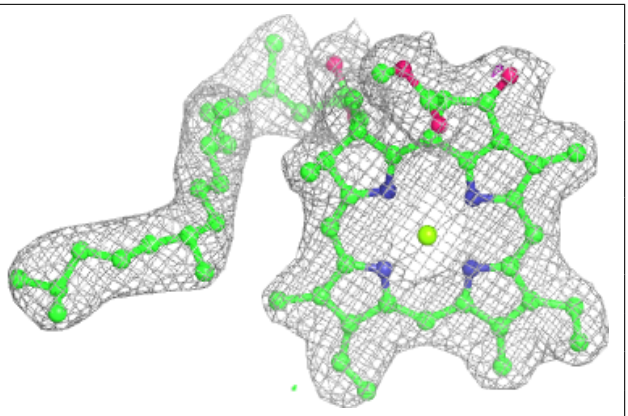
Electron density around CLA D 405:

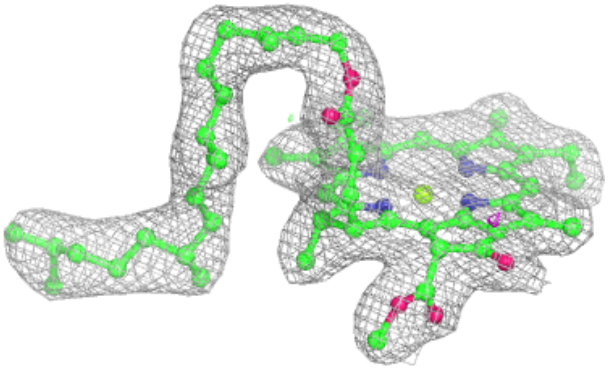
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

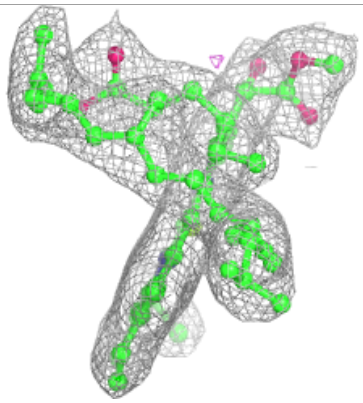


Electron density around CLA A 405:

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

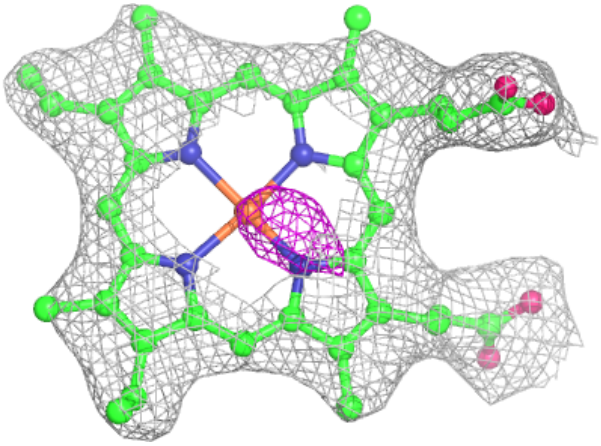


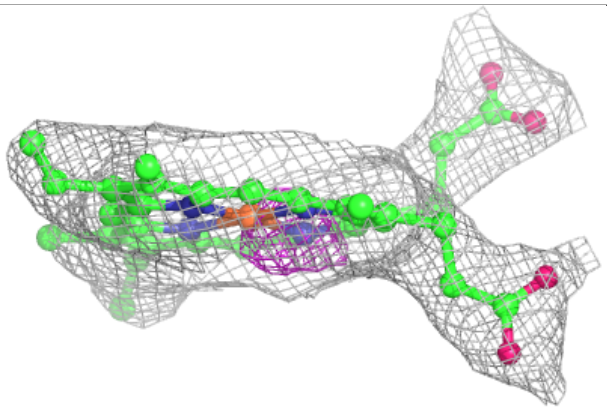


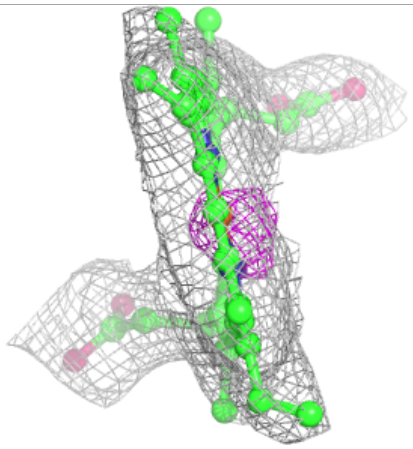


Electron density around HEM E 103:

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

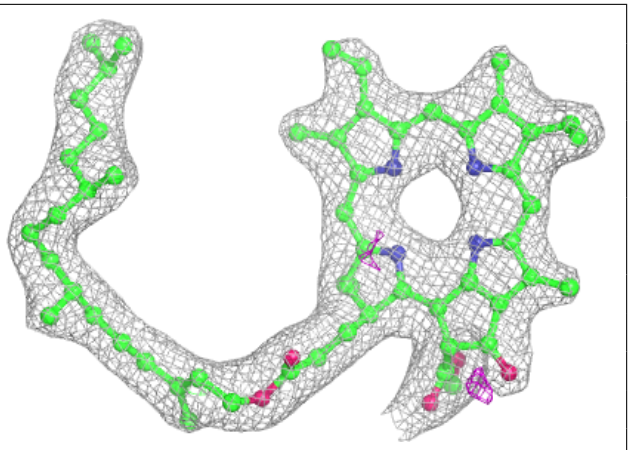


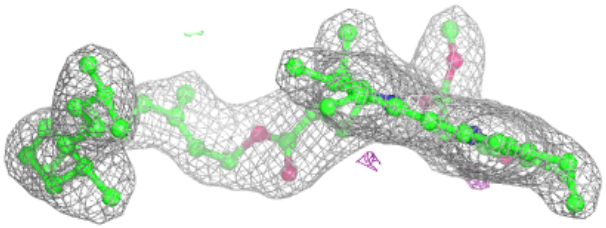


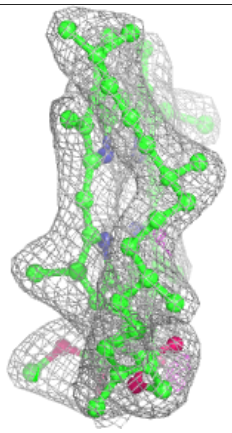


Electron density around PHO a 406:

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

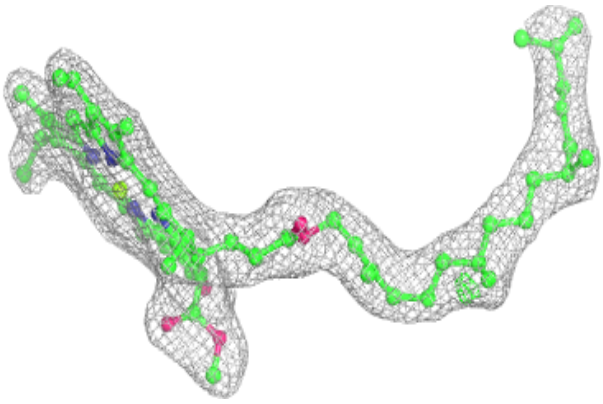


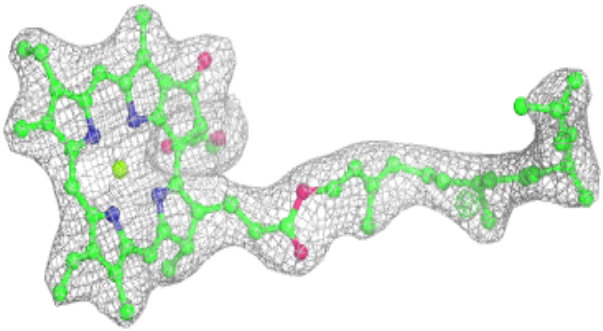


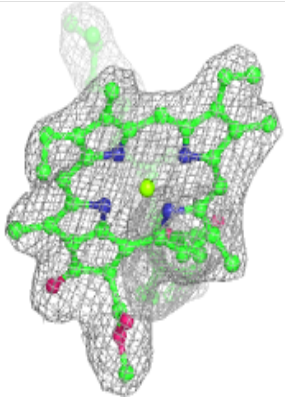


Electron density around CLA d 403:

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

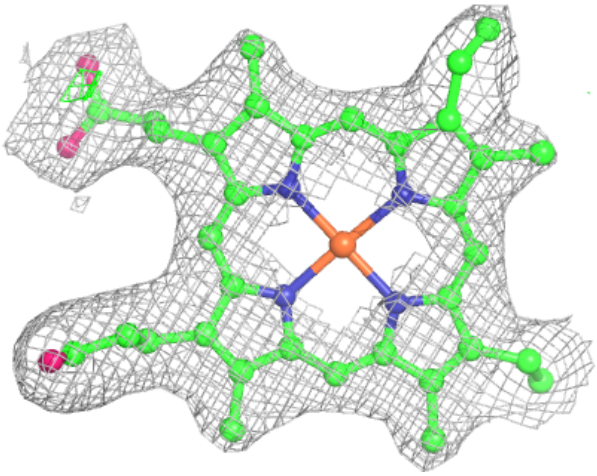


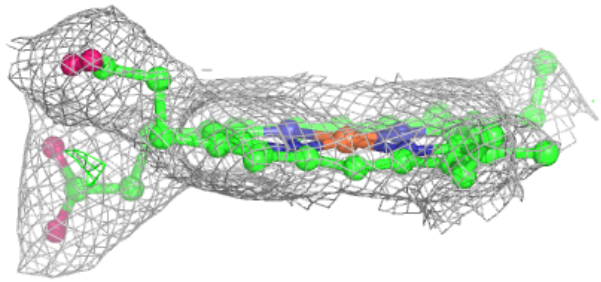


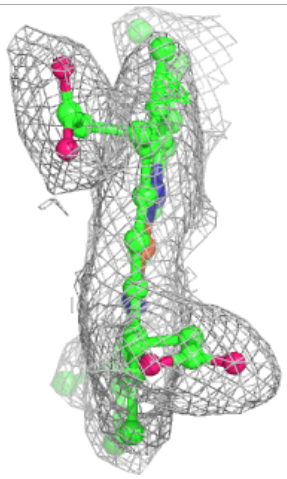


Electron density around HEC V 201:

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

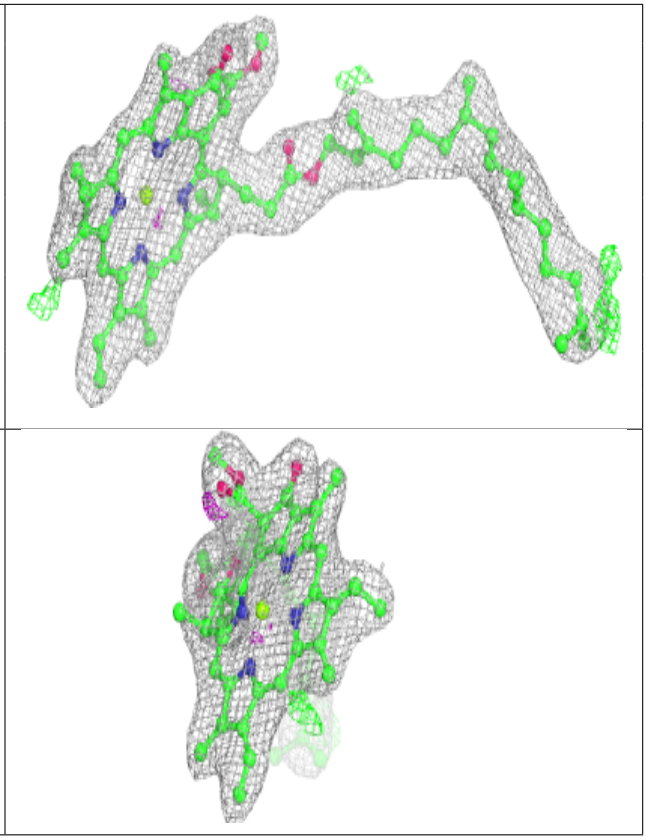






Electron density around CLA a 404:

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



6.5 Other polymers (i)

There are no such residues in this entry.