Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 09:27 PM EDT

PDB ID	:	6W1P
Title	:	RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.26 Angstrom resolution
Authors	:	Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovski, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on	:	2020-03-04
Resolution	:	2.26 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:

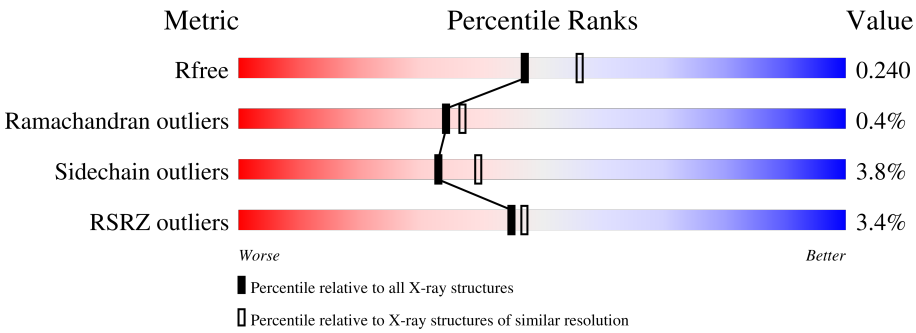
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

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 2.26 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	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	334	% 99% .
1	a	334	96% .
2	B	506	% 98% .

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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)	:	2.35.1

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Mol	Chain	Length	Quality of chain
2	b	506	3% 98%
3	C	461	.% 94%
3	c	461	.% 95%
4	D	352	96%
4	d	352	.% 93%
5	E	84	2% 94%
5	e	84	6% 93% 5%
6	F	45	2% 73% 24%
6	f	45	2% 71% 24%
7	H	66	2% 92% 6%
7	h	66	6% 88% 8% 5%
8	I	38	5% 89% 5% 5%
8	i	38	8% 89% 5% 5%
9	J	40	10% 88% 10%
9	j	40	10% 88% 10%
10	K	46	4% 74% 7% 20%
10	k	46	74% 7% 20%
11	L	37	100%
11	l	37	8% 86% 11%
12	M	36	3% 89% 8%
12	m	36	81% 8% 11%
13	O	272	4% 85% 5% 10%
13	o	272	5% 86% 10%
14	R	40	28% 70% 15% 15%
14	r	40	58% 60% 18% 22%

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Mol	Chain	Length	Quality of chain
15	T	30	3% 97%
15	t	30	10% 93% 7%
16	U	134	2% 69% 28%
16	u	134	70% 28%
17	V	163	79% 16%
17	v	163	2% 82% 16%
18	X	41	7% 90% 7%
18	x	41	12% 90% 5% 5%
19	Y	46	20% 54% 41%
19	y	46	9% 59% 7% 35%
20	Z	62	18% 89% 11%
20	z	62	18% 87% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	d	403	X	-	-	-

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 103385 atoms, of which 51555 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 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	334	5130	1717	2508	431	459	15	0	0	0
1	a	334	5118	1714	2499	431	459	15	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	505	7864	2631	3859	666	695	13	0	5	0
2	b	505	7800	2610	3822	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	442	6768	2249	3342	571	593	13	0	2	0
3	c	451	6913	2290	3413	587	610	13	0	2	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	341	5330	1800	2613	444	461	12	0	0	0
4	d	341	5342	1804	2619	444	463	12	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	82	1316	436	650	107	123	0	1	0
5	e	82	1311	434	647	108	122	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	34	556	187	281	45	42	1	0	0	0
6	f	34	556	187	281	45	42	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	H	N	O	S			
7	H	65	1042	341	532	82	85	2	0	0	0
7	h	63	1016	333	518	80	83	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	H	N	O	S			
8	I	36	607	200	311	46	49	1	0	0	0
8	i	36	607	200	311	46	49	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
9	J	36	525	174	268	40	42	1	0	0	0
9	j	36	525	174	268	40	42	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	H	N	O			
10	K	37	598	204	305	43	46	0	0	0
10	k	37	598	204	305	43	46	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
11	L	37	620	202	316	48	53	1	0	0	0
11	l	36	600	197	304	47	52		0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
12	M	33	525	171	269	37	47	1	0	0	0
12	m	32	518	168	267	36	46	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
13	O	244	3698	1168	1828	313	385	4	0	1	0
13	o	244	3718	1170	1844	317	383	4	0	0	0

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
14	R	34	569	184	298	47	40	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
14	r	31	493	162	253	42	36	0	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
15	T	30	519	181	261	36	39	2	0	0	0
			Total	C	H	N	O	S			
15	t	30	512	180	256	36	38	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
16	U	97	1546	491	772	129	154	0	0	0
			Total	C	H	N	O			
16	u	97	1546	491	772	129	154	0	0	0

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
17	V	137	2132	675	1068	177	208	4	0	0	0
			Total	C	H	N	O	S			
17	v	137	2132	675	1068	177	208	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
18	X	38	593	188	312	45	48	0	0	0
			Total	C	H	N	O			
18	x	39	602	191	316	46	49	0	0	0

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
19	Y	27	413	128	217	35	30	3	0	0	0
19	y	30	459	144	241	35	36	3	0	0	0

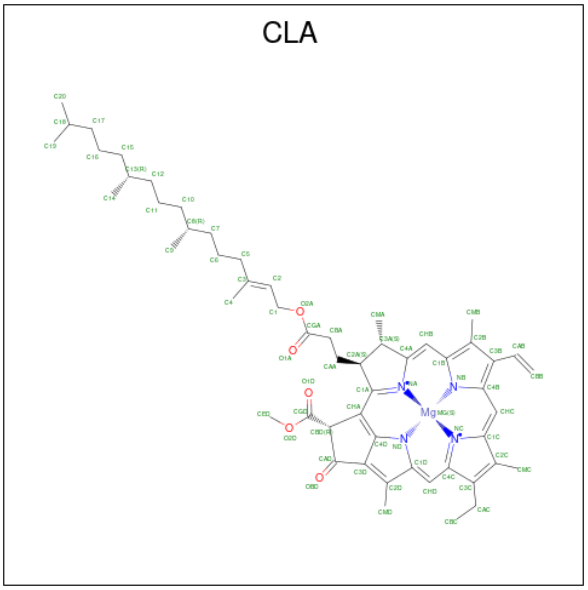
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
20	Z	62	995	328	516	72	77	2	0	0	0
20	z	62	986	326	509	72	77	2	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 CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
22	A	1	137	55	72	1	4	5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
22	A	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	A	1	102	44	48	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	B	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
22	C	1	117	49	58	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	C	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	D	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	D	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	D	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	a	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	b	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	119	50	59	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	132	54	68	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0

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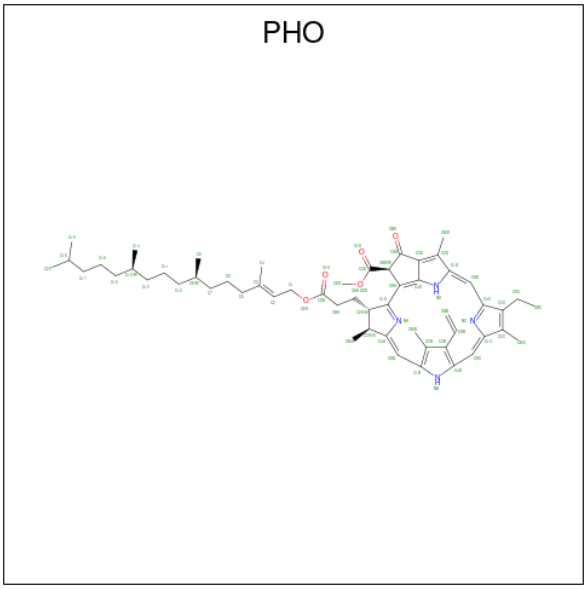
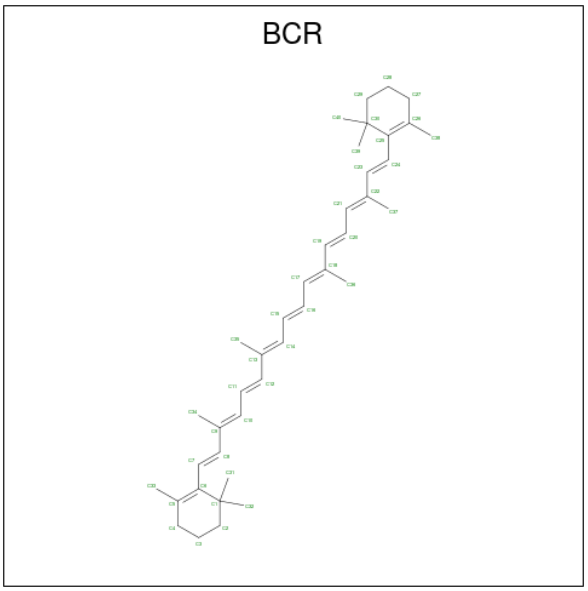
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	c	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	d	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	d	1	137	55	72	1	4	5	0	0
			Total	C	H	Mg	N	O		
22	d	1	137	55	72	1	4	5	0	0

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
23	A	1	138	55	74	4	5	0	0
			Total	C	H	N	O		
23	D	1	138	55	74	4	5	0	0
			Total	C	H	N	O		
23	a	1	138	55	74	4	5	0	0
			Total	C	H	N	O		
23	d	1	138	55	74	4	5	0	0

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
24	A	1	96	40	56	0	0
24	B	1	96	40	56	0	0
24	B	1	96	40	56	0	0
24	B	1	96	40	56	0	0
24	C	1	96	40	56	0	0
24	C	1	96	40	56	0	0
24	D	1	96	40	56	0	0
24	H	1	96	40	56	0	0
24	K	1	96	40	56	0	0
24	T	1	96	40	56	0	0
24	Z	1	96	40	56	0	0
24	a	1	96	40	56	0	0
24	b	1	96	40	56	0	0
24	b	1	96	40	56	0	0

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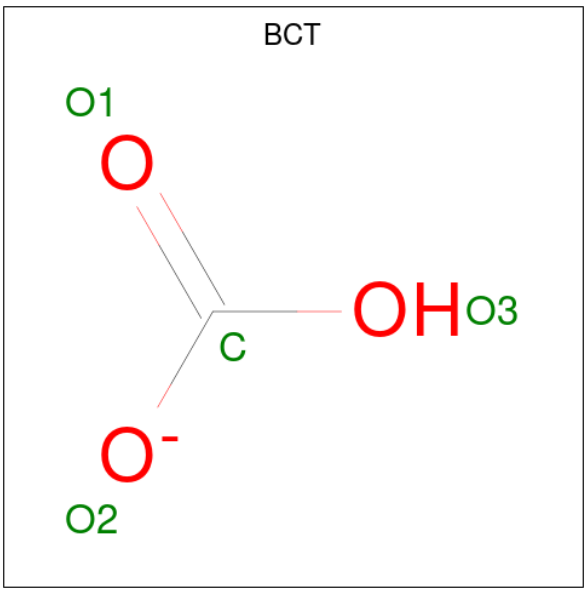
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
24	b	1	96	40	56	0	0
24	c	1	96	40	56	0	0
24	c	1	96	40	56	0	0
24	d	1	96	40	56	0	0
24	k	1	96	40	56	0	0
24	k	1	96	40	56	0	0
24	t	1	96	40	56	0	0
24	x	1	96	40	56	0	0

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

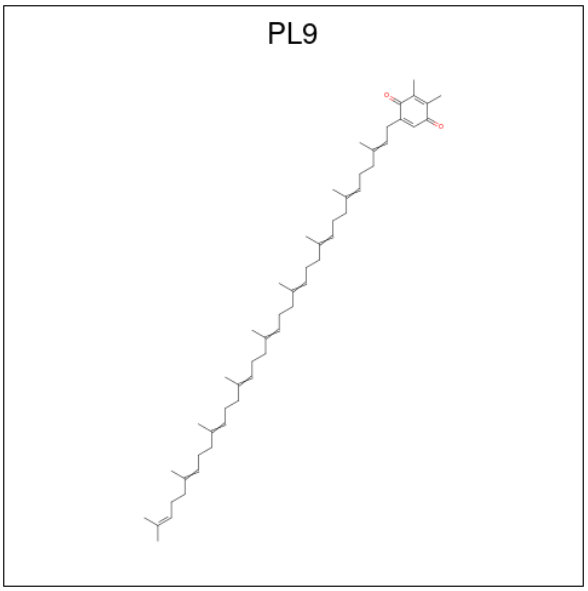
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
25	A	2	2	2	0	0
25	a	2	2	2	0	0

- Molecule 26 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



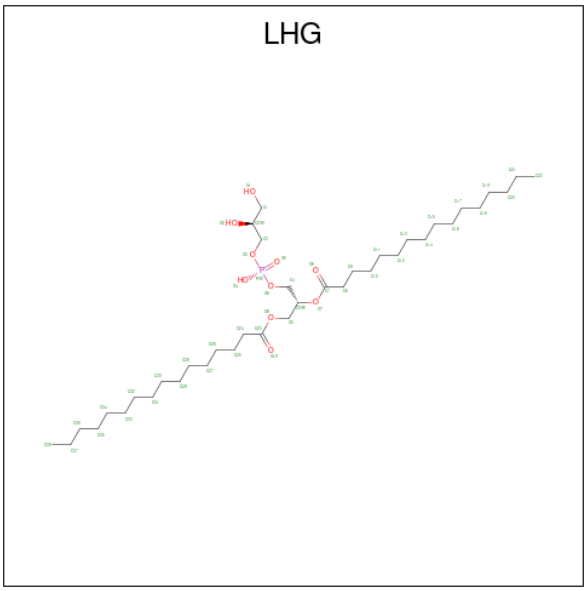
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
26	A	1	5	1	1	3	0	0
26	a	1	5	1	1	3	0	0

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



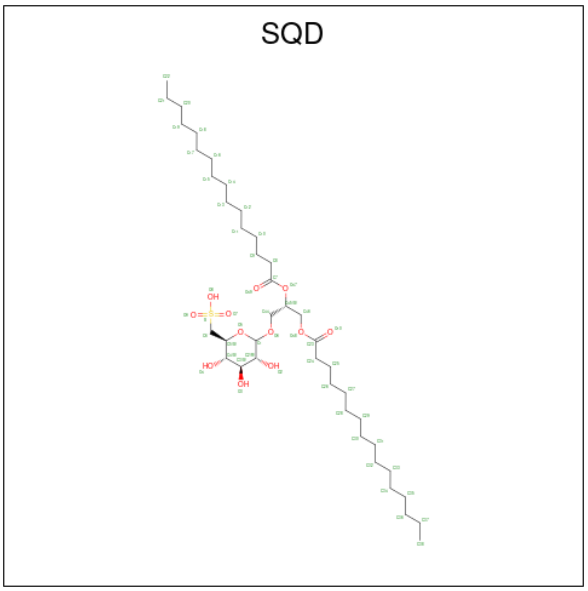
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
27	A	1	135	53	80	2	0	0
27	D	1	135	53	80	2	0	0
27	a	1	135	53	80	2	0	0
27	d	1	135	53	80	2	0	0

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			113	36	66	10	1		
28	A	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	B	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

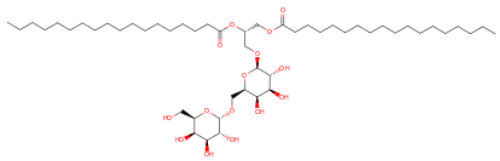
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C H O S 121 39 69 12 1	0	0
29	A	1	Total C H O 104 35 65 4	0	0
29	B	1	Total C H O S 132 41 78 12 1	0	0
29	F	1	Total C H O S 81 25 45 10 1	0	0
29	L	1	Total C H O S 113 36 64 12 1	0	0
29	a	1	Total C H O S 131 41 77 12 1	0	0
29	a	1	Total C H O 92 31 56 5	0	0
29	f	1	Total C H O S 89 28 48 12 1	0	0

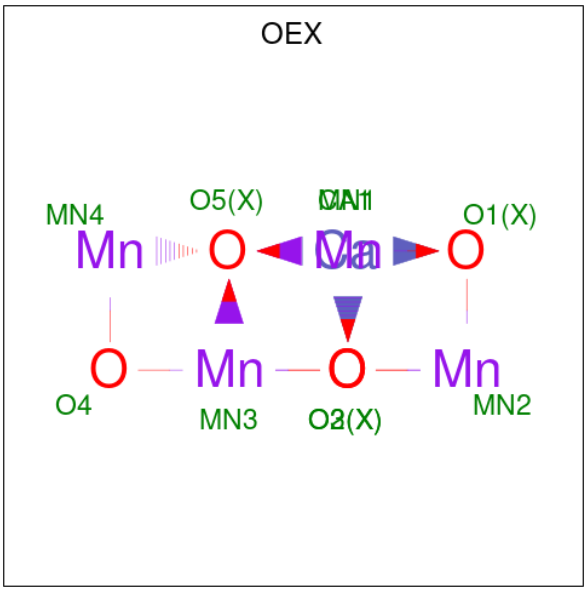
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

DGD



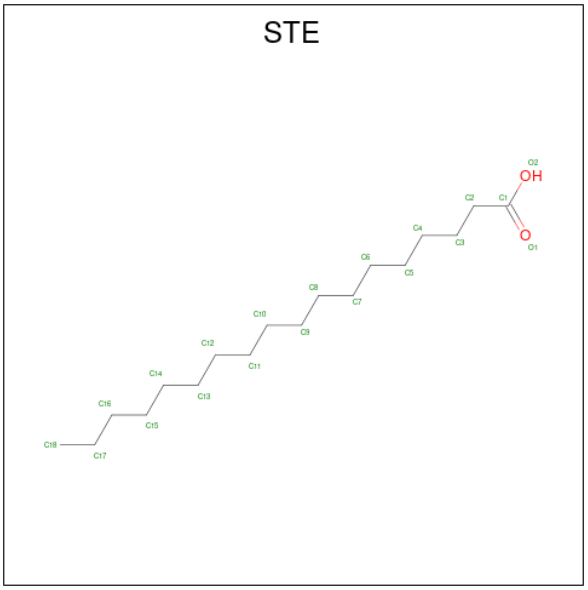
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
30	A	1	161	51	95	15	0	0
			Total	C	H	O		
30	C	1	141	47	79	15	0	0
			Total	C	H	O		
30	C	1	141	47	79	15	0	0
			Total	C	H	O		
30	C	1	141	47	79	15	0	0
			Total	C	H	O		
30	H	1	141	47	79	15	0	0
			Total	C	H	O		
30	c	1	141	47	79	15	0	0
			Total	C	H	O		
30	c	1	139	47	77	15	0	0
			Total	C	H	O		
30	c	1	139	47	77	15	0	0
			Total	C	H	O		
30	h	1	140	47	78	15	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
32	B	1	28	10	16	2	0	0
			Total	C	H	O		
32	B	1	43	15	26	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 28 10 16 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H 41 15 26	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	L	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	T	1	Total C H 44 15 29	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0

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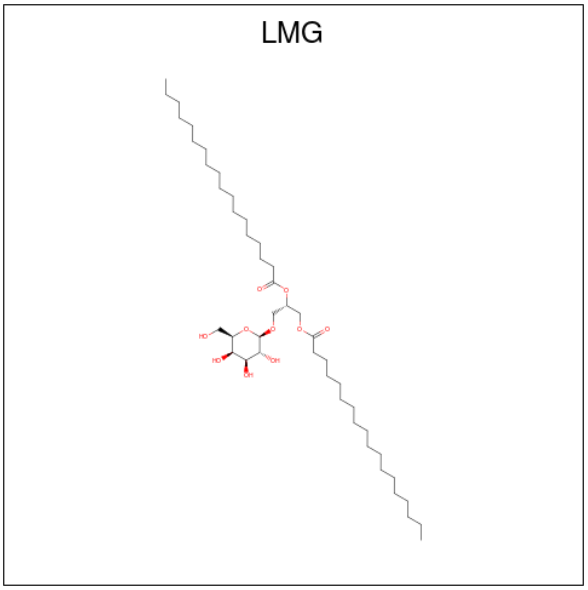
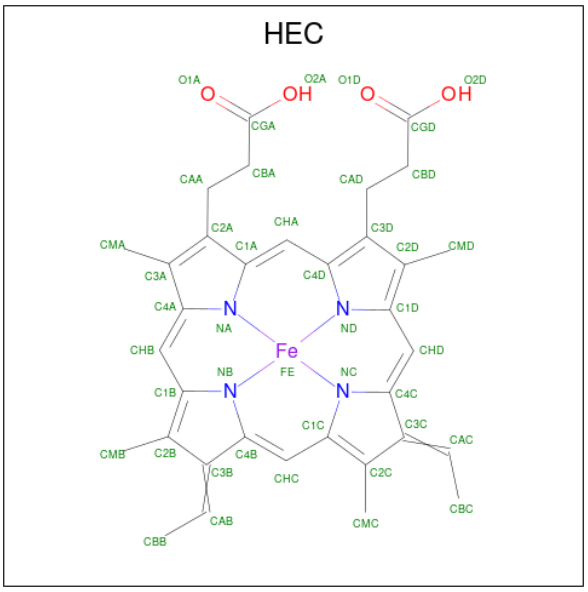
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	h	1	Total C H 41 14 27	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	k	1	Total C H O 28 10 16 2	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	t	1	Total C H 26 10 16	0	0
32	t	1	Total C H O 46 16 28 2	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 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	H	O		
33	B	1	141	45	86	10	0	0
			Total	C	H	O		
33	C	1	112	38	64	10	0	0
			Total	C	H	O		
33	D	1	122	41	71	10	0	0
			Total	C	H	O		
33	D	1	78	27	45	6	0	0
			Total	C	H	O		
33	D	1	68	24	40	4	0	0
			Total	C	H	O		
33	M	1	122	41	71	10	0	0
			Total	C	H	O		
33	Y	1	114	38	66	10	0	0
			Total	C	H	O		
33	b	1	140	45	85	10	0	0
			Total	C	H	O		
33	c	1	80	27	43	10	0	0
			Total	C	H	O		
33	c	1	117	38	69	10	0	0
			Total	C	H	O		
33	c	1	116	39	67	10	0	0
			Total	C	H	O		
33	d	1	100	34	56	10	0	0
			Total	C	H	O		
33	m	1	122	41	71	10	0	0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
34	E	1	75	34	1	32	4	4	0	0
34	V	1	73	34	1	30	4	4	0	0
34	e	1	75	34	1	32	4	4	0	0
34	v	1	73	34	1	30	4	4	0	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
35	A	132	132	132	0	0
35	B	174	174	174	0	0
35	C	139	139	139	0	0
35	D	116	116	116	0	0
35	E	26	26	26	0	0
35	F	4	4	4	0	0
35	H	16	16	16	0	0
35	I	14	14	14	0	0
35	J	9	9	9	0	0
35	K	7	7	7	0	0
35	L	9	9	9	0	0
35	M	5	5	5	0	0
35	O	78	78	78	0	0
35	R	1	1	1	0	0
35	T	9	9	9	0	0
35	U	34	34	34	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	V	53	Total O 53 53	0	0
35	X	12	Total O 12 12	0	0
35	Y	6	Total O 6 6	0	0
35	Z	1	Total O 1 1	0	0
35	a	109	Total O 109 109	0	0
35	b	134	Total O 134 134	0	0
35	c	130	Total O 130 130	0	0
35	d	91	Total O 91 91	0	0
35	e	15	Total O 15 15	0	0
35	f	8	Total O 8 8	0	0
35	h	26	Total O 26 26	0	0
35	i	7	Total O 7 7	0	0
35	j	9	Total O 9 9	0	0
35	k	6	Total O 6 6	0	0
35	l	10	Total O 10 10	0	0
35	m	3	Total O 3 3	0	0
35	o	81	Total O 81 81	0	0
35	r	7	Total O 7 7	0	0
35	t	11	Total O 11 11	0	0
35	u	43	Total O 43 43	0	0
35	v	37	Total O 37 37	0	0

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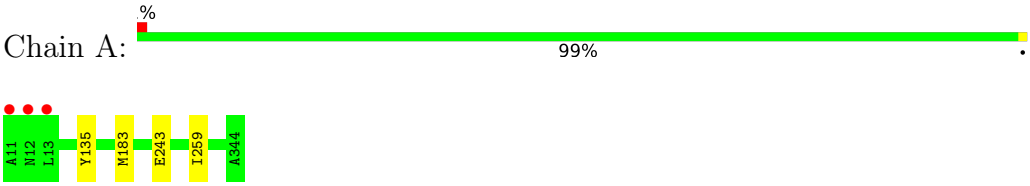
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
35	x	4	4	4	0	0
			Total	O		
35	y	2	2	2	0	0
			Total	O		
35	z	4	4	4	0	0

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.

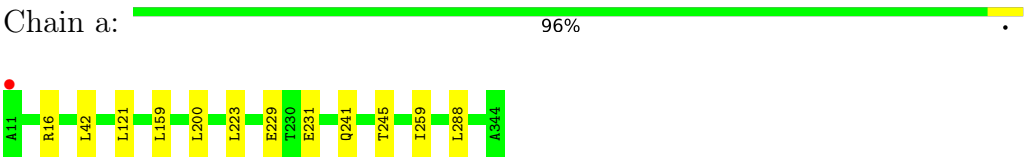
• Molecule 1: Photosystem II protein D1 1

Chain A:



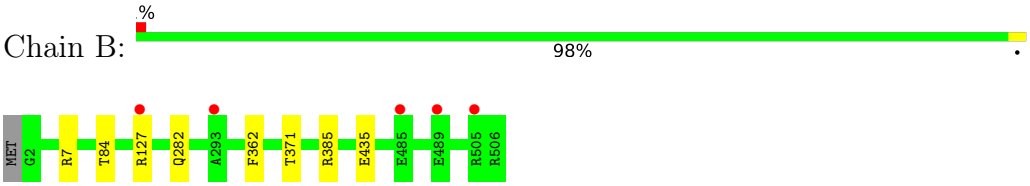
• Molecule 1: Photosystem II protein D1 1

Chain a:



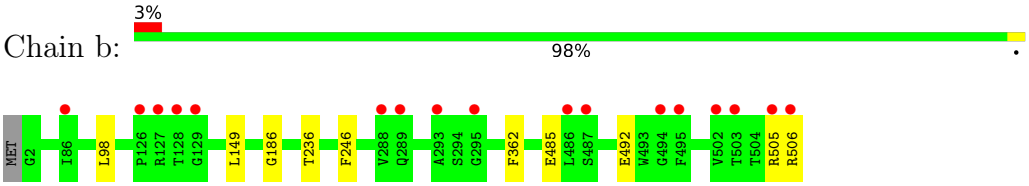
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



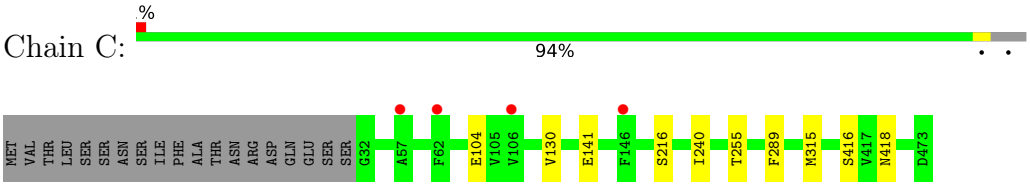
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



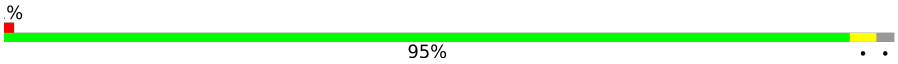
• Molecule 3: Photosystem II CP43 reaction center protein

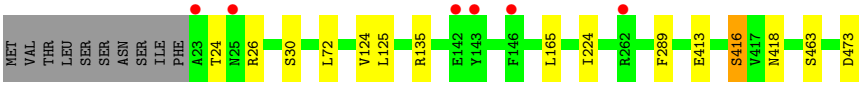
Chain C:



• Molecule 3: Photosystem II CP43 reaction center protein

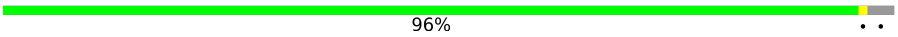
Chain c:

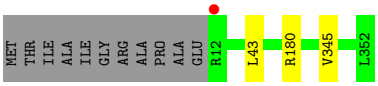




• Molecule 4: Photosystem II D2 protein

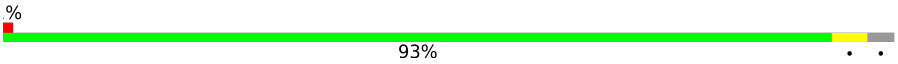
Chain D:

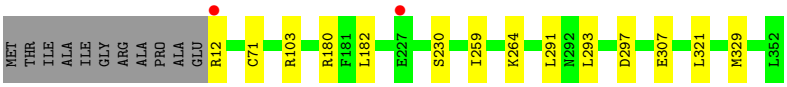




• Molecule 4: Photosystem II D2 protein

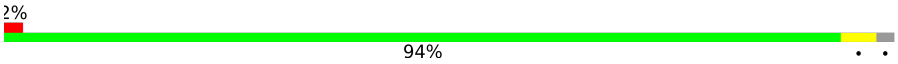
Chain d:

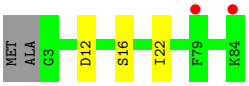




• Molecule 5: Cytochrome b559 subunit alpha

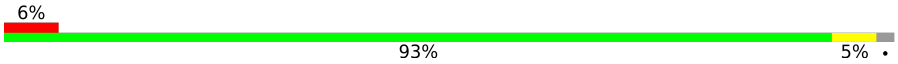
Chain E:

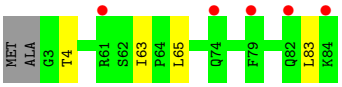




• Molecule 5: Cytochrome b559 subunit alpha

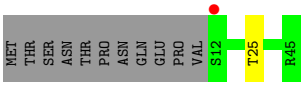
Chain e:





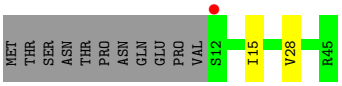
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



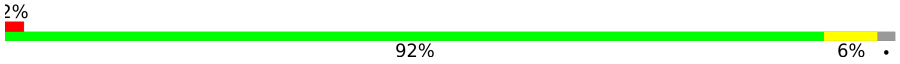
• Molecule 6: Cytochrome b559 subunit beta

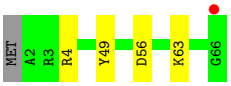
Chain f:



• Molecule 7: Photosystem II reaction center protein H

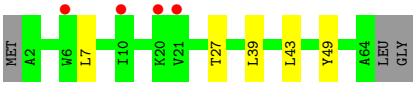
Chain H:





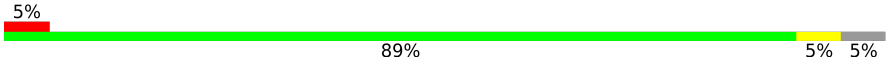
• Molecule 7: Photosystem II reaction center protein H

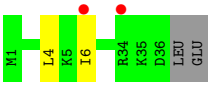
Chain h:



• Molecule 8: Photosystem II reaction center protein I

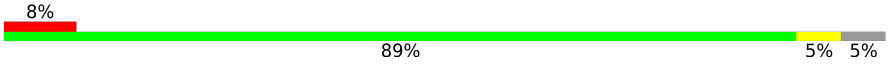
Chain I:

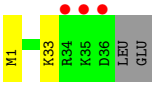




• Molecule 8: Photosystem II reaction center protein I

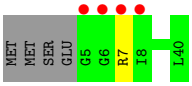
Chain i:





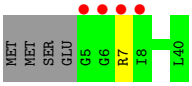
• Molecule 9: Photosystem II reaction center protein J

Chain J:



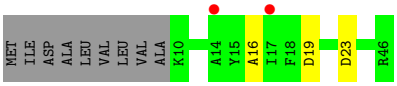
• Molecule 9: Photosystem II reaction center protein J

Chain j:



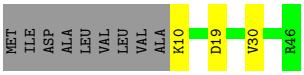
• Molecule 10: Photosystem II reaction center protein K

Chain K:



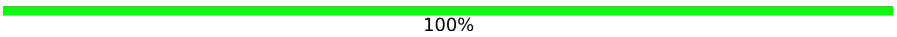
• Molecule 10: Photosystem II reaction center protein K

Chain k:



• Molecule 11: Photosystem II reaction center protein L

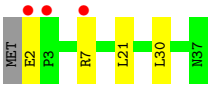
Chain L:



There are no outlier residues recorded for this chain.

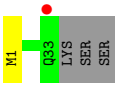
• Molecule 11: Photosystem II reaction center protein L

Chain l:



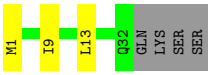
• Molecule 12: Photosystem II reaction center protein M

Chain M:



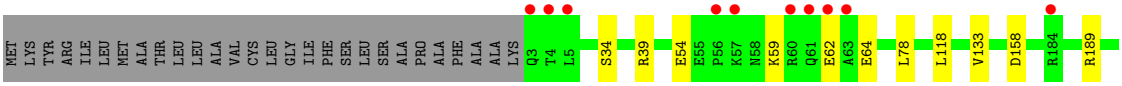
• Molecule 12: Photosystem II reaction center protein M

Chain m:



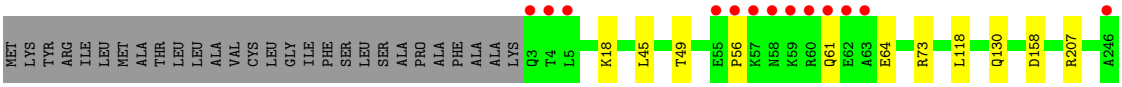
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



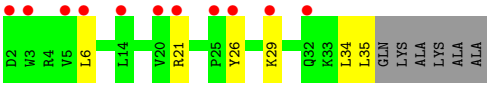
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



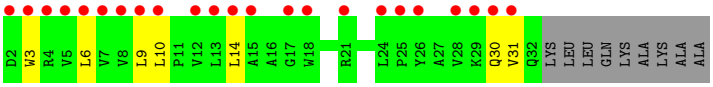
• Molecule 14: Photosystem II protein Y

Chain R:



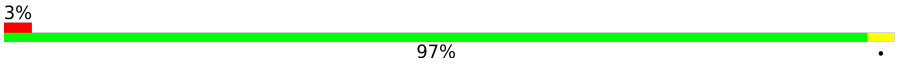
• Molecule 14: Photosystem II protein Y

Chain r:



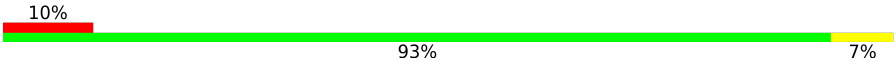
• Molecule 15: Photosystem II reaction center protein T

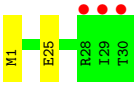
Chain T:



• Molecule 15: Photosystem II reaction center protein T

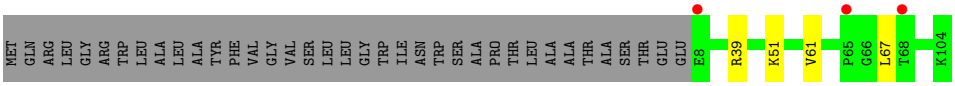
Chain t:





• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:

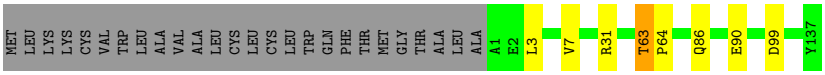


• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:

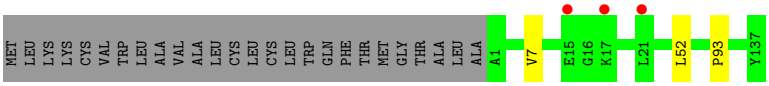
• Molecule 17: Cytochrome c-550

Chain V:



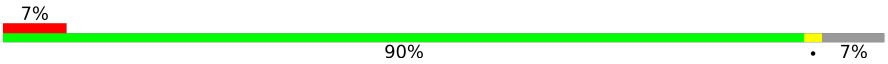
• Molecule 17: Cytochrome c-550

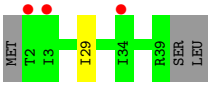
Chain v:



• Molecule 18: Photosystem II reaction center X protein

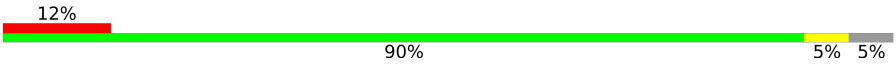
Chain X:

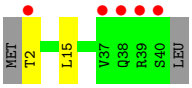




• Molecule 18: Photosystem II reaction center X protein

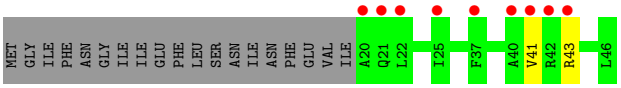
Chain x:





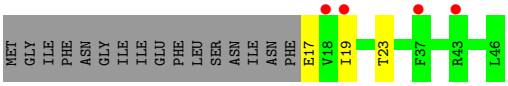
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



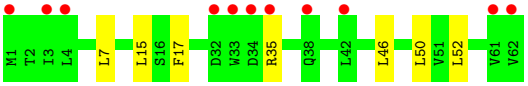
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:



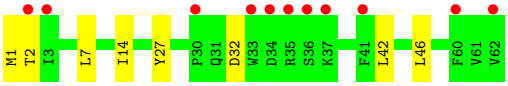
• Molecule 20: Photosystem II reaction center protein Z

Chain Z:



• Molecule 20: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.96Å 221.64Å 307.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.26 33.54 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.54-2.26) 86.8 (33.54-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.83 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.173 , 0.241 0.173 , 0.240	Depositor DCC
R_{free} test set	3302 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	103385	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: CL, PL9, OEX, DGD, CLA, FME, SQD, LMG, HEC, STE, PHO, BCT, BCR, FE2, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.70	1/2707 (0.0%)	0.72	1/3692 (0.0%)
1	a	0.67	0/2704	0.70	0/3688
2	B	0.68	0/4161	0.71	2/5669 (0.0%)
2	b	0.65	0/4118	0.69	0/5611
3	C	0.64	0/3547	0.68	0/4830
3	c	0.61	0/3619	0.69	1/4926 (0.0%)
4	D	0.67	0/2812	0.70	0/3832
4	d	0.66	1/2821 (0.0%)	0.72	1/3844 (0.0%)
5	E	0.56	0/688	0.65	0/940
5	e	0.59	0/683	0.65	0/932
6	F	0.54	0/284	0.58	0/387
6	f	0.62	0/284	0.62	0/387
7	H	0.74	0/523	0.72	0/713
7	h	0.61	0/511	0.75	0/697
8	I	0.66	0/293	0.68	0/396
8	i	0.69	0/293	0.68	0/396
9	J	0.59	0/263	0.66	0/356
9	j	0.57	0/263	0.65	0/356
10	K	0.52	0/303	0.70	1/416 (0.2%)
10	k	0.55	0/303	0.65	0/416
11	L	0.70	0/311	0.68	0/422
11	l	0.66	0/303	0.76	0/412
12	M	0.72	0/249	0.74	0/341
12	m	0.71	0/244	0.75	0/334
13	O	0.63	0/1904	0.76	2/2585 (0.1%)
13	o	0.63	0/1905	0.76	1/2583 (0.0%)
14	R	0.51	0/277	0.61	0/380
14	r	0.44	0/246	0.59	0/339
15	T	0.69	0/257	0.67	0/349
15	t	0.68	0/255	0.66	0/346
16	U	0.60	0/785	0.69	0/1064
16	u	0.64	0/785	0.76	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	V	0.62	0/1085	0.72	1/1473 (0.1%)
17	v	0.60	0/1085	0.68	0/1473
18	X	0.52	0/284	0.63	0/384
18	x	0.47	0/289	0.61	0/391
19	Y	0.51	0/197	0.61	0/264
19	y	0.43	0/219	0.52	0/294
20	Z	0.54	0/490	0.60	0/669
20	z	0.48	0/488	0.59	0/666
All	All	0.64	2/42838 (0.0%)	0.70	10/58317 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
17	V	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	71	CYS	CB-SG	-5.34	1.73	1.81
1	A	135	TYR	CD1-CE1	-5.24	1.31	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	63	THR	C-N-CD	-7.40	104.32	120.60
4	d	297	ASP	CB-CG-OD1	6.41	124.06	118.30
1	A	183	MET	CA-CB-CG	6.01	123.52	113.30
2	B	385	ARG	NE-CZ-NH2	-5.96	117.32	120.30
13	o	158	ASP	CB-CG-OD1	5.91	123.62	118.30
13	O	158	ASP	CB-CG-OD1	5.43	123.19	118.30
10	K	23	ASP	CB-CG-OD1	5.29	123.06	118.30
3	c	473	ASP	CB-CG-OD1	5.24	123.02	118.30
2	B	7	ARG	NE-CZ-NH2	-5.08	117.76	120.30
13	O	223	ASP	CB-CG-OD1	5.07	122.87	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
2	b	186	GLY	Peptide

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	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	41	46
1	a	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	41	46
2	B	508/506 (100%)	497 (98%)	11 (2%)	0	100	100
2	b	503/506 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	442/461 (96%)	428 (97%)	13 (3%)	1 (0%)	47	55
3	c	451/461 (98%)	435 (96%)	15 (3%)	1 (0%)	47	55
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	29 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	34/40 (85%)	32 (94%)	1 (3%)	1 (3%)	4	2
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	4	2
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	12 (5%)	3 (1%)	13	9
13	o	242/272 (89%)	231 (96%)	9 (4%)	2 (1%)	19	17
14	R	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	1
14	r	29/40 (72%)	26 (90%)	1 (3%)	2 (7%)	1	0
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	91 (96%)	2 (2%)	2 (2%)	7	3
17	V	135/163 (83%)	130 (96%)	4 (3%)	1 (1%)	22	21
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
20	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
All	All	5240/5666 (92%)	5062 (97%)	159 (3%)	19 (0%)	34	37

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER

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Mol	Chain	Res	Type
14	r	30	GLN
14	R	34	LEU
19	Y	43	ARG
13	o	73	ARG
20	z	2	THR
10	K	16	ALA
13	o	56	PRO
14	r	31	VAL
9	J	7	ARG
1	a	259	ILE
16	u	53	ALA
13	O	133	VAL
16	u	52	ASN
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	270/270 (100%)	269 (100%)	1 (0%)	91	94
1	a	269/270 (100%)	258 (96%)	11 (4%)	30	36
2	B	408/404 (101%)	402 (98%)	6 (2%)	65	75
2	b	402/404 (100%)	393 (98%)	9 (2%)	52	61
3	C	346/362 (96%)	337 (97%)	9 (3%)	46	55
3	c	354/362 (98%)	339 (96%)	15 (4%)	30	34
4	D	276/283 (98%)	273 (99%)	3 (1%)	73	82
4	d	277/283 (98%)	265 (96%)	12 (4%)	29	33
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	21
5	e	71/73 (97%)	67 (94%)	4 (6%)	21	21
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	42
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	13
7	H	54/55 (98%)	50 (93%)	4 (7%)	13	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	6
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	17
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	49
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	34
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	46
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	13
13	O	206/228 (90%)	197 (96%)	9 (4%)	28	32
13	o	207/228 (91%)	199 (96%)	8 (4%)	32	38
14	R	28/32 (88%)	23 (82%)	5 (18%)	2	0
14	r	23/32 (72%)	18 (78%)	5 (22%)	1	0
15	T	26/26 (100%)	25 (96%)	1 (4%)	33	39
15	t	25/26 (96%)	24 (96%)	1 (4%)	31	37
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	28
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	58
17	V	117/138 (85%)	111 (95%)	6 (5%)	24	25
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	55
18	X	31/34 (91%)	30 (97%)	1 (3%)	39	47
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	16
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	23
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	2
All	All	4328/4622 (94%)	4163 (96%)	165 (4%)	33	39

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	GLU

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Mol	Chain	Res	Type
2	B	84	THR
2	B	127	ARG
2	B	282	GLN
2	B	362	PHE
2	B	371	THR
2	B	435	GLU
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	216	SER
3	C	240	ILE
3	C	255	THR
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
4	D	43	LEU
4	D	180	ARG
4	D	345	VAL
5	E	12	ASP
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	4	ARG
7	H	49	TYR
7	H	56	ASP
7	H	63	LYS
8	I	4	LEU
8	I	6	ILE
10	K	19	ASP
13	O	34	SER
13	O	39	ARG
13	O	54	GLU
13	O	64	GLU
13	O	78	LEU
13	O	118	LEU
13	O	189	ARG
13	O	196	GLN
13	O	214	THR
14	R	6	LEU
14	R	21	ARG
14	R	26	TYR

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Mol	Chain	Res	Type
14	R	29	LYS
14	R	35	LEU
15	T	25	GLU
16	U	39	ARG
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	31	ARG
17	V	86	GLN
17	V	90	GLU
17	V	99	ASP
18	X	29	ILE
19	Y	41	VAL
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
20	Z	52	LEU
1	a	16	ARG
1	a	42	LEU
1	a	121	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	231	GLU
1	a	241	GLN
1	a	245	THR
1	a	288	LEU
2	b	98	LEU
2	b	149	LEU
2	b	236	THR
2	b	246	PHE
2	b	362	PHE
2	b	485	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG

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Mol	Chain	Res	Type
3	c	24	THR
3	c	26	ARG
3	c	30	SER
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	165	LEU
3	c	224	ILE
3	c	289	PHE
3	c	413[A]	GLU
3	c	413[B]	GLU
3	c	416	SER
3	c	418	ASN
3	c	463	SER
4	d	12	ARG
4	d	103	ARG
4	d	180	ARG
4	d	182	LEU
4	d	230	SER
4	d	259	ILE
4	d	264	LYS
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	4	THR
5	e	63	ILE
5	e	65	LEU
5	e	83	LEU
6	f	15	ILE
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
7	h	39	LEU
7	h	43	LEU
7	h	49	TYR
8	i	33	LYS
9	j	7	ARG
10	k	10	LYS
10	k	19	ASP

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Mol	Chain	Res	Type
10	k	30	VAL
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	9	ILE
12	m	13	LEU
13	o	18	LYS
13	o	45	LEU
13	o	49	THR
13	o	61	GLN
13	o	64	GLU
13	o	118	LEU
13	o	130	GLN
13	o	207	ARG
14	r	3	TRP
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
14	r	14	LEU
15	t	25	GLU
16	u	51	LYS
16	u	52	ASN
17	v	7	VAL
17	v	52	LEU
17	v	93	PRO
18	x	2	THR
18	x	15	LEU
19	y	17	GLU
19	y	19	ILE
19	y	23	THR
20	z	1	MET
20	z	7	LEU
20	z	14	ILE
20	z	27	TYR
20	z	32	ASP
20	z	42	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	181	ASN
1	A	338	ASN
2	B	409	GLN
3	C	418	ASN
13	O	36	GLN
13	O	88	ASN
14	R	22	ASN
17	V	86	GLN
18	X	38	GLN
1	a	19	ASN
5	e	60	GLN
7	h	59	ASN
13	o	61	GLN
14	r	30	GLN
16	u	52	ASN
16	u	78	ASN
20	z	31	GLN
20	z	38	GLN

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	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.87	0	7,9,11	1.19	1 (14%)
12	FME	M	1	12	8,9,10	1.03	0	7,9,11	1.16	1 (14%)
8	FME	I	1	8	8,9,10	1.12	0	7,9,11	0.78	0
15	FME	T	1	15	8,9,10	0.88	0	7,9,11	1.09	0
15	FME	t	1	15	8,9,10	1.20	1 (12%)	7,9,11	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	0.99	1 (12%)	7,9,11	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
15	FME	T	1	15	-	3/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.58	1.42	1.46
12	m	1	FME	CA-N	-2.03	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	CA-N-CN	-2.37	119.17	122.82
12	M	1	FME	C-CA-N	-2.07	105.99	109.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
12	M	1	FME	CA-CB-CG-SD
15	T	1	FME	C-CA-CB-CG
8	i	1	FME	C-CA-CB-CG

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 189 ligands modelled in this entry, 6 are monoatomic - 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	$\#\|Z\| > 2$
29	SQD	B	623	-	53,54,54	0.96	2 (3%)	62,65,65	1.89	11 (17%)
32	STE	B	626	-	14,14,19	0.55	0	13,13,19	0.40	0
33	LMG	M	101	-	51,51,55	0.98	4 (7%)	59,59,63	1.42	8 (13%)
22	CLA	C	513	-	65,73,73	1.59	7 (10%)	76,113,113	1.57	13 (17%)
32	STE	D	411	-	19,19,19	0.76	1 (5%)	19,19,19	1.27	3 (15%)
22	CLA	b	605	-	65,73,73	1.36	10 (15%)	76,113,113	1.54	14 (18%)
34	HEC	v	201	17	32,50,50	2.42	4 (12%)	24,82,82	1.65	4 (16%)
22	CLA	A	402	-	65,73,73	1.42	9 (13%)	76,113,113	1.30	9 (11%)
22	CLA	B	612	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	10 (13%)
22	CLA	c	512	-	65,73,73	1.61	9 (13%)	76,113,113	1.52	13 (17%)
30	DGD	A	415	-	67,67,67	1.32	8 (11%)	81,81,81	1.40	14 (17%)
32	STE	b	625	-	9,9,19	0.52	0	8,8,19	0.50	0
24	BCR	c	514	-	41,41,41	0.99	2 (4%)	56,56,56	1.37	9 (16%)
33	LMG	D	409	-	31,31,55	1.05	3 (9%)	33,33,63	1.07	0
32	STE	d	411	-	16,16,19	0.78	0	16,16,19	1.00	1 (6%)
27	PL9	a	410	-	55,55,55	0.92	3 (5%)	68,69,69	1.60	10 (14%)
29	SQD	f	101	-	40,41,54	1.12	4 (10%)	49,52,65	1.92	12 (24%)
31	OEX	a	415	1,35,3	0,15,15	-	-	-		
32	STE	B	621	-	16,16,19	0.79	1 (6%)	16,16,19	0.91	1 (6%)
27	PL9	d	406	-	55,55,55	1.60	9 (16%)	68,69,69	1.85	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	B	610	-	65,73,73	1.52	10 (15%)	76,113,113	1.39	11 (14%)
32	STE	M	104	-	17,17,19	0.42	0	16,16,19	0.84	0
29	SQD	a	413	-	35,35,54	1.18	2 (5%)	37,37,65	1.38	7 (18%)
22	CLA	B	613	-	65,73,73	1.30	6 (9%)	76,113,113	1.50	12 (15%)
22	CLA	b	604	-	65,73,73	1.51	7 (10%)	76,113,113	1.65	15 (19%)
32	STE	B	624	-	11,11,19	1.00	1 (9%)	11,11,19	0.87	0
22	CLA	B	603	-	65,73,73	1.63	9 (13%)	76,113,113	1.43	11 (14%)
22	CLA	c	510	-	65,73,73	1.66	12 (18%)	76,113,113	1.45	9 (11%)
32	STE	k	101	-	11,11,19	0.82	0	11,11,19	0.87	0
32	STE	L	103	-	11,11,19	0.79	0	11,11,19	1.25	1 (9%)
22	CLA	b	601	35	65,73,73	1.82	12 (18%)	76,113,113	1.40	10 (13%)
22	CLA	a	403	35	65,73,73	1.63	7 (10%)	76,113,113	1.58	14 (18%)
24	BCR	b	619	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	10 (17%)
23	PHO	a	404	-	51,69,69	1.10	3 (5%)	47,99,99	1.40	8 (17%)
24	BCR	b	618	-	41,41,41	1.26	3 (7%)	56,56,56	1.33	10 (17%)
32	STE	M	103	-	9,9,19	0.44	0	8,8,19	0.73	0
33	LMG	m	101	-	51,51,55	1.17	6 (11%)	59,59,63	1.49	8 (13%)
22	CLA	b	615	-	65,73,73	1.82	12 (18%)	76,113,113	1.34	6 (7%)
32	STE	h	102	-	13,13,19	0.49	0	12,12,19	0.53	0
22	CLA	C	510	-	65,73,73	1.34	8 (12%)	76,113,113	1.48	9 (11%)
22	CLA	c	506	-	65,73,73	1.52	10 (15%)	76,113,113	1.34	11 (14%)
24	BCR	C	515	-	41,41,41	1.22	5 (12%)	56,56,56	1.34	6 (10%)
30	DGD	C	517	-	63,63,67	1.39	9 (14%)	77,77,81	1.37	8 (10%)
32	STE	a	414	-	11,11,19	0.92	0	11,11,19	1.04	0
24	BCR	b	617	-	41,41,41	1.13	3 (7%)	56,56,56	1.45	9 (16%)
22	CLA	B	609	-	65,73,73	1.72	10 (15%)	76,113,113	1.49	12 (15%)
22	CLA	B	617	-	60,68,73	1.65	11 (18%)	70,107,113	1.77	12 (17%)
28	LHG	d	407	-	48,48,48	1.04	3 (6%)	51,54,54	1.30	5 (9%)
22	CLA	a	405	-	65,73,73	1.62	11 (16%)	76,113,113	1.52	9 (11%)
22	CLA	B	607	-	65,73,73	1.75	8 (12%)	76,113,113	1.62	11 (14%)
31	OEX	A	416	1,35,3	0,15,15	-	-	-		
30	DGD	c	516	-	63,63,67	1.15	6 (9%)	77,77,81	1.40	9 (11%)
26	BCT	A	409	21	2,3,3	1.22	0	2,3,3	2.65	1 (50%)
22	CLA	d	404	-	65,73,73	1.58	11 (16%)	76,113,113	1.47	10 (13%)
32	STE	c	520	-	19,19,19	0.75	0	19,19,19	1.02	1 (5%)
28	LHG	D	408	-	48,48,48	0.77	1 (2%)	51,54,54	1.34	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	BCR	x	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
24	BCR	T	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	4 (7%)
22	CLA	C	514	-	65,73,73	1.54	11 (16%)	76,113,113	1.56	14 (18%)
24	BCR	C	501	-	41,41,41	1.01	3 (7%)	56,56,56	1.26	7 (12%)
32	STE	I	101	-	14,14,19	0.60	0	13,13,19	0.45	0
24	BCR	D	405	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
32	STE	b	621	-	19,19,19	0.77	1 (5%)	19,19,19	1.06	2 (10%)
22	CLA	C	503	-	65,73,73	1.52	13 (20%)	76,113,113	1.55	12 (15%)
27	PL9	D	406	-	55,55,55	1.85	7 (12%)	68,69,69	1.80	18 (26%)
22	CLA	A	403	35	65,73,73	1.65	9 (13%)	76,113,113	1.32	7 (9%)
22	CLA	B	611	35	65,73,73	1.80	10 (15%)	76,113,113	1.33	9 (11%)
22	CLA	b	614	-	65,73,73	1.74	11 (16%)	76,113,113	1.41	14 (18%)
22	CLA	c	511	3	65,73,73	1.93	11 (16%)	76,113,113	1.45	10 (13%)
22	CLA	b	603	-	65,73,73	1.52	10 (15%)	76,113,113	1.55	14 (18%)
24	BCR	d	405	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
34	HEC	E	101	5,6	32,50,50	2.39	4 (12%)	24,82,82	2.04	5 (20%)
30	DGD	c	517	-	63,63,67	1.20	7 (11%)	77,77,81	1.38	9 (11%)
28	LHG	A	411	-	46,46,48	1.05	3 (6%)	49,52,54	1.19	3 (6%)
30	DGD	H	102	-	63,63,67	1.48	13 (20%)	77,77,81	1.42	11 (14%)
32	STE	C	520	-	11,11,19	0.77	0	11,11,19	1.37	2 (18%)
32	STE	T	102	-	14,14,19	0.43	0	13,13,19	0.78	0
23	PHO	D	401	-	51,69,69	1.26	9 (17%)	47,99,99	1.26	7 (14%)
26	BCT	a	409	21	2,3,3	1.29	0	2,3,3	4.06	2 (100%)
22	CLA	b	606	-	65,73,73	1.74	8 (12%)	76,113,113	1.60	9 (11%)
24	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	8 (14%)
22	CLA	c	503	-	65,73,73	1.63	11 (16%)	76,113,113	1.55	11 (14%)
22	CLA	b	608	-	65,73,73	1.53	9 (13%)	76,113,113	1.20	6 (7%)
22	CLA	c	513	-	65,73,73	1.58	9 (13%)	76,113,113	1.37	8 (10%)
28	LHG	a	412	-	41,41,48	1.06	4 (9%)	44,47,54	1.29	3 (6%)
32	STE	J	101	-	11,11,19	0.67	0	11,11,19	1.33	2 (18%)
22	CLA	c	501	-	65,73,73	1.38	9 (13%)	76,113,113	1.54	9 (11%)
32	STE	b	624	-	19,19,19	0.90	0	19,19,19	0.82	1 (5%)
24	BCR	A	406	-	41,41,41	1.02	3 (7%)	56,56,56	1.49	11 (19%)
32	STE	H	103	-	17,17,19	0.54	0	16,16,19	0.53	0
32	STE	C	522	-	11,11,19	0.84	0	11,11,19	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	STE	j	101	-	11,11,19	1.05	0	11,11,19	0.80	1 (9%)
22	CLA	D	402	-	65,73,73	1.55	8 (12%)	76,113,113	1.53	9 (11%)
33	LMG	Y	101	-	48,48,55	1.04	4 (8%)	56,56,63	1.37	8 (14%)
28	LHG	l	101	-	48,48,48	0.77	0	51,54,54	1.26	4 (7%)
33	LMG	D	410	-	26,26,55	1.03	1 (3%)	26,26,63	1.14	2 (7%)
24	BCR	t	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	5 (8%)
22	CLA	c	508	-	64,72,73	1.56	9 (14%)	74,111,113	1.52	10 (13%)
22	CLA	B	604	-	65,73,73	1.68	8 (12%)	76,113,113	1.53	13 (17%)
22	CLA	B	614	-	65,73,73	1.67	6 (9%)	76,113,113	1.50	11 (14%)
32	STE	t	104	-	17,17,19	0.73	0	17,17,19	1.16	1 (5%)
28	LHG	d	408	-	48,48,48	0.72	1 (2%)	51,54,54	1.18	4 (7%)
33	LMG	d	410	-	44,44,55	1.01	3 (6%)	52,52,63	1.46	7 (13%)
33	LMG	c	519	-	37,37,55	1.18	4 (10%)	45,45,63	1.31	6 (13%)
33	LMG	b	622	-	55,55,55	1.42	7 (12%)	63,63,63	1.51	8 (12%)
22	CLA	b	616	-	60,68,73	1.41	9 (15%)	70,107,113	1.57	8 (11%)
22	CLA	B	616	-	65,73,73	1.53	6 (9%)	76,113,113	1.41	10 (13%)
22	CLA	C	508	35	65,73,73	1.36	7 (10%)	76,113,113	1.37	7 (9%)
32	STE	B	601	-	11,11,19	0.79	0	11,11,19	1.31	1 (9%)
28	LHG	d	409	-	38,38,48	0.92	1 (2%)	41,44,54	1.26	3 (7%)
32	STE	C	521	-	15,15,19	0.66	0	14,14,19	0.39	0
29	SQD	F	101	-	35,36,54	1.04	2 (5%)	42,45,65	1.82	9 (21%)
22	CLA	B	615	-	65,73,73	1.91	13 (20%)	76,113,113	1.42	9 (11%)
22	CLA	b	610	35	65,73,73	1.54	10 (15%)	76,113,113	1.39	11 (14%)
32	STE	Z	102	-	7,7,19	0.50	0	6,6,19	0.56	0
22	CLA	B	606	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	11 (14%)
24	BCR	c	515	-	41,41,41	1.08	4 (9%)	56,56,56	1.42	6 (10%)
32	STE	t	102	-	13,13,19	0.66	0	13,13,19	1.30	1 (7%)
32	STE	b	620	-	15,15,19	0.60	0	14,14,19	0.62	0
22	CLA	c	504	35	60,68,73	1.59	9 (15%)	70,107,113	1.50	9 (12%)
23	PHO	d	401	-	51,69,69	1.09	5 (9%)	47,99,99	1.42	9 (19%)
32	STE	t	103	-	9,9,19	0.51	0	8,8,19	0.45	0
29	SQD	a	411	-	53,54,54	0.96	5 (9%)	62,65,65	1.89	13 (20%)
32	STE	M	102	-	14,14,19	0.78	0	14,14,19	0.95	0
22	CLA	B	605	-	65,73,73	1.37	7 (10%)	76,113,113	1.83	13 (17%)
29	SQD	L	101	-	48,49,54	0.98	2 (4%)	57,60,65	2.29	15 (26%)
22	CLA	b	612	-	65,73,73	1.34	5 (7%)	76,113,113	1.40	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	LMG	c	521	-	48,48,55	1.16	5 (10%)	56,56,63	1.25	6 (10%)
22	CLA	B	602	35	65,73,73	1.89	11 (16%)	76,113,113	1.32	6 (7%)
22	CLA	D	404	-	65,73,73	1.46	8 (12%)	76,113,113	1.60	13 (17%)
32	STE	b	626	-	19,19,19	0.73	0	19,19,19	1.12	1 (5%)
22	CLA	a	402	-	65,73,73	1.59	9 (13%)	76,113,113	1.36	10 (13%)
24	BCR	a	406	-	41,41,41	1.02	2 (4%)	56,56,56	1.15	5 (8%)
22	CLA	b	613	-	65,73,73	1.48	11 (16%)	76,113,113	1.58	14 (18%)
22	CLA	C	509	-	65,73,73	1.68	7 (10%)	76,113,113	1.45	12 (15%)
24	BCR	Z	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.46	10 (17%)
22	CLA	b	611	-	65,73,73	1.49	8 (12%)	76,113,113	1.59	12 (15%)
22	CLA	C	504	-	65,73,73	1.65	11 (16%)	76,113,113	1.82	9 (11%)
29	SQD	A	414	-	38,38,54	1.16	3 (7%)	40,40,65	1.39	4 (10%)
22	CLA	b	607	35	65,73,73	1.54	8 (12%)	76,113,113	1.46	9 (11%)
24	BCR	K	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.26	4 (7%)
28	LHG	B	622	-	48,48,48	1.01	3 (6%)	51,54,54	1.33	6 (11%)
22	CLA	A	405	-	54,62,73	1.76	9 (16%)	62,99,113	1.61	12 (19%)
22	CLA	c	509	-	65,73,73	1.60	7 (10%)	76,113,113	1.50	9 (11%)
22	CLA	c	502	-	65,73,73	1.39	6 (9%)	76,113,113	1.39	9 (11%)
32	STE	b	623	-	15,15,19	0.76	0	15,15,19	0.86	0
33	LMG	c	522	-	49,49,55	0.98	3 (6%)	57,57,63	1.36	5 (8%)
33	LMG	D	407	-	51,51,55	1.14	4 (7%)	59,59,63	1.31	6 (10%)
22	CLA	d	403	35	65,73,73	1.51	10 (15%)	76,113,113	1.61	12 (15%)
22	CLA	c	505	-	65,73,73	1.43	7 (10%)	76,113,113	1.33	7 (9%)
24	BCR	k	102	-	41,41,41	1.08	4 (9%)	56,56,56	1.20	6 (10%)
22	CLA	C	505	35	59,67,73	1.59	10 (16%)	68,105,113	1.49	10 (14%)
30	DGD	h	101	-	63,63,67	1.22	9 (14%)	77,77,81	1.50	14 (18%)
22	CLA	c	507	35	65,73,73	1.51	12 (18%)	76,113,113	1.43	8 (10%)
28	LHG	A	413	-	48,48,48	1.09	5 (10%)	51,54,54	1.24	6 (11%)
22	CLA	b	609	-	65,73,73	1.87	11 (16%)	76,113,113	1.51	12 (15%)
23	PHO	A	404	-	51,69,69	1.24	6 (11%)	47,99,99	1.36	9 (19%)
22	CLA	C	512	3	65,73,73	1.63	10 (15%)	76,113,113	1.40	8 (10%)
22	CLA	B	608	35	65,73,73	1.47	12 (18%)	76,113,113	1.65	10 (13%)
22	CLA	D	403	35	65,73,73	1.30	7 (10%)	76,113,113	1.32	10 (13%)
22	CLA	C	506	-	65,73,73	1.54	8 (12%)	76,113,113	1.41	7 (9%)
22	CLA	C	507	-	65,73,73	1.49	4 (6%)	76,113,113	1.16	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	C	502	-	65,73,73	1.72	10 (15%)	76,113,113	1.39	14 (18%)
24	BCR	B	620	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	7 (12%)
33	LMG	B	627	-	55,55,55	1.48	7 (12%)	63,63,63	1.61	9 (14%)
30	DGD	C	519	-	63,63,67	1.14	7 (11%)	77,77,81	1.35	9 (11%)
32	STE	E	102	-	11,11,19	0.94	0	11,11,19	1.05	0
32	STE	x	102	-	19,19,19	0.70	0	19,19,19	0.81	1 (5%)
28	LHG	L	102	-	48,48,48	0.87	2 (4%)	51,54,54	1.23	3 (5%)
24	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.48	9 (16%)
30	DGD	c	518	-	63,63,67	1.22	6 (9%)	77,77,81	1.40	9 (11%)
33	LMG	C	516	-	48,48,55	0.95	2 (4%)	56,56,63	1.26	6 (10%)
22	CLA	b	602	-	65,73,73	1.66	10 (15%)	76,113,113	1.59	11 (14%)
22	CLA	d	402	-	65,73,73	1.65	7 (10%)	76,113,113	1.49	11 (14%)
34	HEC	e	101	5,6	32,50,50	2.40	5 (15%)	24,82,82	2.10	3 (12%)
32	STE	B	625	-	15,15,19	0.56	0	14,14,19	0.48	0
22	CLA	C	511	-	65,73,73	1.68	10 (15%)	76,113,113	1.43	8 (10%)
27	PL9	A	410	-	55,55,55	1.20	3 (5%)	68,69,69	1.49	13 (19%)
34	HEC	V	201	17	32,50,50	1.93	3 (9%)	24,82,82	2.26	7 (29%)
24	BCR	k	103	-	41,41,41	0.99	2 (4%)	56,56,56	1.30	7 (12%)
29	SQD	A	412	-	51,52,54	1.08	5 (9%)	60,63,65	1.99	13 (21%)
30	DGD	C	518	-	63,63,67	1.38	8 (12%)	77,77,81	1.45	10 (12%)
24	BCR	B	618	-	41,41,41	1.25	3 (7%)	56,56,56	1.30	8 (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
29	SQD	B	623	-	-	20/49/69/69	0/1/1/1
32	STE	B	626	-	-	11/12/12/17	-
33	LMG	M	101	-	-	23/46/66/70	0/1/1/1
22	CLA	C	513	-	1/1/20/20	20/37/115/115	-
32	STE	D	411	-	-	11/17/17/17	-
22	CLA	b	605	-	1/1/20/20	11/37/115/115	-
34	HEC	v	201	17	-	2/10/54/54	-
22	CLA	A	402	-	1/1/20/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	612	-	1/1/20/20	7/37/115/115	-
22	CLA	c	512	-	1/1/20/20	22/37/115/115	-
30	DGD	A	415	-	-	27/55/95/95	0/2/2/2
32	STE	b	625	-	-	3/7/7/17	-
24	BCR	c	514	-	-	16/29/63/63	0/2/2/2
33	LMG	D	409	-	-	16/33/33/70	-
32	STE	d	411	-	-	8/14/14/17	-
27	PL9	a	410	-	-	25/53/73/73	0/1/1/1
29	SQD	f	101	-	-	12/36/56/69	0/1/1/1
32	STE	B	621	-	-	6/14/14/17	-
27	PL9	d	406	-	-	17/53/73/73	0/1/1/1
22	CLA	B	610	-	-	4/37/115/115	-
32	STE	M	104	-	-	8/15/15/17	-
29	SQD	a	413	-	-	12/37/37/69	-
22	CLA	B	613	-	1/1/20/20	6/37/115/115	-
22	CLA	b	604	-	1/1/20/20	5/37/115/115	-
32	STE	B	624	-	-	5/9/9/17	-
22	CLA	B	603	-	1/1/20/20	13/37/115/115	-
22	CLA	c	510	-	1/1/20/20	13/37/115/115	-
32	STE	k	101	-	-	3/9/9/17	-
32	STE	L	103	-	-	5/9/9/17	-
22	CLA	b	601	35	1/1/20/20	17/37/115/115	-
22	CLA	a	403	35	-	16/37/115/115	-
24	BCR	b	619	-	-	11/29/63/63	0/2/2/2
23	PHO	a	404	-	-	8/37/103/103	0/5/6/6
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
32	STE	M	103	-	-	3/7/7/17	-
33	LMG	m	101	-	-	21/46/66/70	0/1/1/1
22	CLA	b	615	-	1/1/20/20	8/37/115/115	-
32	STE	h	102	-	-	7/11/11/17	-
22	CLA	C	510	-	1/1/20/20	18/37/115/115	-
22	CLA	c	506	-	1/1/20/20	19/37/115/115	-
24	BCR	C	515	-	-	8/29/63/63	0/2/2/2
30	DGD	C	517	-	-	21/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	a	414	-	-	3/9/9/17	-
24	BCR	b	617	-	-	6/29/63/63	0/2/2/2
22	CLA	B	609	-	-	5/37/115/115	-
22	CLA	B	617	-	1/1/19/20	9/31/109/115	-
28	LHG	d	407	-	-	18/53/53/53	-
22	CLA	a	405	-	1/1/20/20	11/37/115/115	-
22	CLA	B	607	-	1/1/20/20	8/37/115/115	-
30	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	d	404	-	-	5/37/115/115	-
32	STE	c	520	-	-	7/17/17/17	-
28	LHG	D	408	-	-	16/53/53/53	-
24	BCR	x	101	-	-	3/29/63/63	0/2/2/2
24	BCR	T	101	-	-	9/29/63/63	0/2/2/2
22	CLA	C	514	-	-	14/37/115/115	-
24	BCR	C	501	-	-	7/29/63/63	0/2/2/2
32	STE	I	101	-	-	6/12/12/17	-
24	BCR	D	405	-	-	5/29/63/63	0/2/2/2
32	STE	b	621	-	-	7/17/17/17	-
22	CLA	C	503	-	1/1/20/20	8/37/115/115	-
27	PL9	D	406	-	-	9/53/73/73	0/1/1/1
22	CLA	A	403	35	1/1/20/20	3/37/115/115	-
22	CLA	B	611	35	1/1/20/20	3/37/115/115	-
22	CLA	b	614	-	1/1/20/20	20/37/115/115	-
22	CLA	c	511	3	1/1/20/20	14/37/115/115	-
22	CLA	b	603	-	1/1/20/20	11/37/115/115	-
24	BCR	d	405	-	-	6/29/63/63	0/2/2/2
34	HEC	E	101	5,6	-	2/10/54/54	-
30	DGD	c	517	-	-	18/51/91/95	0/2/2/2
28	LHG	A	411	-	-	24/51/51/53	-
30	DGD	H	102	-	-	18/51/91/95	0/2/2/2
32	STE	C	520	-	-	4/9/9/17	-
32	STE	T	102	-	-	8/12/12/17	-
23	PHO	D	401	-	-	4/37/103/103	0/5/6/6
22	CLA	b	606	-	1/1/20/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	619	-	-	9/29/63/63	0/2/2/2
22	CLA	c	503	-	1/1/20/20	9/37/115/115	-
22	CLA	b	608	-	-	4/37/115/115	-
22	CLA	c	513	-	1/1/20/20	10/37/115/115	-
28	LHG	a	412	-	-	25/46/46/53	-
32	STE	J	101	-	-	8/9/9/17	-
22	CLA	c	501	-	1/1/20/20	3/37/115/115	-
32	STE	b	624	-	-	7/17/17/17	-
24	BCR	A	406	-	-	11/29/63/63	0/2/2/2
32	STE	H	103	-	-	10/15/15/17	-
32	STE	C	522	-	-	3/9/9/17	-
32	STE	j	101	-	-	1/9/9/17	-
22	CLA	D	402	-	1/1/20/20	5/37/115/115	-
33	LMG	Y	101	-	-	20/43/63/70	0/1/1/1
28	LHG	l	101	-	-	20/53/53/53	-
33	LMG	D	410	-	-	8/22/22/70	-
24	BCR	t	101	-	-	8/29/63/63	0/2/2/2
22	CLA	c	508	-	1/1/19/20	18/36/114/115	-
22	CLA	B	604	-	1/1/20/20	13/37/115/115	-
22	CLA	B	614	-	1/1/20/20	16/37/115/115	-
32	STE	t	104	-	-	8/15/15/17	-
28	LHG	d	408	-	-	20/53/53/53	-
33	LMG	d	410	-	-	14/39/59/70	0/1/1/1
33	LMG	c	519	-	-	7/31/51/70	0/1/1/1
33	LMG	b	622	-	-	28/50/70/70	0/1/1/1
22	CLA	b	616	-	1/1/19/20	7/31/109/115	-
22	CLA	B	616	-	1/1/20/20	9/37/115/115	-
22	CLA	C	508	35	1/1/20/20	7/37/115/115	-
32	STE	B	601	-	-	2/9/9/17	-
28	LHG	d	409	-	-	12/43/43/53	-
32	STE	C	521	-	-	5/13/13/17	-
29	SQD	F	101	-	-	10/28/48/69	0/1/1/1
22	CLA	B	615	-	1/1/20/20	12/37/115/115	-
22	CLA	b	610	35	1/1/20/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	Z	102	-	-	3/5/5/17	-
22	CLA	B	606	-	1/1/20/20	11/37/115/115	-
24	BCR	c	515	-	-	5/29/63/63	0/2/2/2
32	STE	t	102	-	-	5/11/11/17	-
32	STE	b	620	-	-	6/13/13/17	-
22	CLA	c	504	35	1/1/19/20	10/31/109/115	-
23	PHO	d	401	-	-	5/37/103/103	0/5/6/6
32	STE	t	103	-	-	5/7/7/17	-
29	SQD	a	411	-	-	21/49/69/69	0/1/1/1
32	STE	M	102	-	-	5/12/12/17	-
22	CLA	B	605	-	1/1/20/20	10/37/115/115	-
29	SQD	L	101	-	-	21/44/64/69	0/1/1/1
22	CLA	b	612	-	1/1/20/20	10/37/115/115	-
33	LMG	c	521	-	-	23/43/63/70	0/1/1/1
22	CLA	B	602	35	1/1/20/20	22/37/115/115	-
22	CLA	D	404	-	1/1/20/20	10/37/115/115	-
32	STE	b	626	-	-	8/17/17/17	-
22	CLA	a	402	-	1/1/20/20	4/37/115/115	-
24	BCR	a	406	-	-	5/29/63/63	0/2/2/2
22	CLA	b	613	-	1/1/20/20	7/37/115/115	-
22	CLA	C	509	-	1/1/20/20	6/37/115/115	-
24	BCR	Z	101	-	-	8/29/63/63	0/2/2/2
22	CLA	b	611	-	1/1/20/20	8/37/115/115	-
22	CLA	C	504	-	1/1/20/20	4/37/115/115	-
29	SQD	A	414	-	-	14/39/39/69	-
22	CLA	b	607	35	1/1/20/20	13/37/115/115	-
24	BCR	K	101	-	-	13/29/63/63	0/2/2/2
28	LHG	B	622	-	-	20/53/53/53	-
22	CLA	A	405	-	1/1/17/20	4/24/102/115	-
22	CLA	c	509	-	1/1/20/20	15/37/115/115	-
22	CLA	c	502	-	1/1/20/20	7/37/115/115	-
32	STE	b	623	-	-	5/13/13/17	-
33	LMG	c	522	-	-	16/44/64/70	0/1/1/1
33	LMG	D	407	-	-	15/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	403	35	1/1/20/20	11/37/115/115	-
22	CLA	c	505	-	1/1/20/20	13/37/115/115	-
24	BCR	k	102	-	-	10/29/63/63	0/2/2/2
22	CLA	C	505	35	1/1/18/20	8/30/108/115	-
30	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	c	507	35	1/1/20/20	12/37/115/115	-
28	LHG	A	413	-	-	29/53/53/53	-
22	CLA	b	609	-	1/1/20/20	6/37/115/115	-
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
22	CLA	C	512	3	1/1/20/20	6/37/115/115	-
22	CLA	B	608	35	1/1/20/20	8/37/115/115	-
22	CLA	D	403	35	1/1/20/20	7/37/115/115	-
22	CLA	C	506	-	1/1/20/20	8/37/115/115	-
22	CLA	C	507	-	1/1/20/20	12/37/115/115	-
22	CLA	C	502	-	1/1/20/20	4/37/115/115	-
24	BCR	B	620	-	-	4/29/63/63	0/2/2/2
33	LMG	B	627	-	-	28/50/70/70	0/1/1/1
30	DGD	C	519	-	-	12/51/91/95	0/2/2/2
32	STE	E	102	-	-	5/9/9/17	-
32	STE	x	102	-	-	14/17/17/17	-
28	LHG	L	102	-	-	21/53/53/53	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
33	LMG	C	516	-	-	23/43/63/70	0/1/1/1
22	CLA	b	602	-	1/1/20/20	11/37/115/115	-
22	CLA	d	402	-	-	6/37/115/115	-
34	HEC	e	101	5,6	-	2/10/54/54	-
32	STE	B	625	-	-	6/13/13/17	-
22	CLA	C	511	-	1/1/20/20	11/37/115/115	-
27	PL9	A	410	-	-	24/53/73/73	0/1/1/1
34	HEC	V	201	17	-	2/10/54/54	-
24	BCR	k	103	-	-	6/29/63/63	0/2/2/2
29	SQD	A	412	-	-	18/47/67/69	0/1/1/1
30	DGD	C	518	-	-	20/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2

All (929) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	406	PL9	C7-C3	-10.03	1.41	1.51
22	b	609	CLA	C4B-NB	8.97	1.43	1.35
22	B	607	CLA	MG-NA	8.88	2.27	2.06
22	B	604	CLA	MG-ND	8.83	2.23	2.05
22	B	611	CLA	C4B-NB	8.83	1.43	1.35
34	e	101	HEC	C2B-C3B	-8.64	1.31	1.40
22	B	602	CLA	C4B-NB	8.57	1.42	1.35
34	v	201	HEC	C2B-C3B	-8.29	1.32	1.40
22	b	604	CLA	C4B-NB	8.09	1.42	1.35
22	a	403	CLA	C4B-NB	8.04	1.42	1.35
22	c	504	CLA	C4B-NB	8.01	1.42	1.35
22	b	606	CLA	MG-NA	7.97	2.25	2.06
22	c	511	CLA	C4B-NB	7.94	1.42	1.35
22	A	403	CLA	C4B-NB	7.93	1.42	1.35
22	B	602	CLA	MG-NA	7.78	2.24	2.06
22	b	601	CLA	C4B-NB	7.66	1.42	1.35
22	b	602	CLA	C4B-NB	7.61	1.42	1.35
22	C	509	CLA	C4B-NB	7.61	1.42	1.35
34	E	101	HEC	C2B-C3B	-7.59	1.32	1.40
22	c	509	CLA	C4B-NB	7.58	1.42	1.35
22	C	502	CLA	C4B-NB	7.57	1.42	1.35
22	b	601	CLA	MG-NA	7.54	2.24	2.06
22	c	512	CLA	C4B-NB	7.53	1.41	1.35
22	B	603	CLA	C4B-NB	7.51	1.41	1.35
34	v	201	HEC	C3C-C2C	-7.46	1.33	1.40
34	E	101	HEC	C3C-C2C	-7.46	1.33	1.40
22	b	615	CLA	MG-NA	7.45	2.24	2.06
22	d	404	CLA	C4B-NB	7.40	1.41	1.35
22	B	615	CLA	C4B-NB	7.40	1.41	1.35
22	C	507	CLA	C4B-NB	7.34	1.41	1.35
22	B	615	CLA	MG-ND	-7.28	1.91	2.05
22	B	616	CLA	C4B-NB	7.24	1.41	1.35
22	C	505	CLA	C4B-NB	7.18	1.41	1.35
22	A	405	CLA	C4B-NB	7.12	1.41	1.35
22	b	608	CLA	C4B-NB	7.10	1.41	1.35
22	c	505	CLA	C4B-NB	7.09	1.41	1.35
22	B	614	CLA	C4B-NB	7.04	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	611	CLA	C4B-NB	7.02	1.41	1.35
22	C	512	CLA	C4B-NB	7.02	1.41	1.35
22	c	503	CLA	C4B-NB	6.97	1.41	1.35
22	d	402	CLA	C4B-NB	6.96	1.41	1.35
22	C	506	CLA	C4B-NB	6.95	1.41	1.35
22	B	610	CLA	C4B-NB	6.91	1.41	1.35
27	d	406	PL9	C6-C1	-6.88	1.36	1.48
22	C	508	CLA	C4B-NB	6.85	1.41	1.35
22	B	614	CLA	MG-ND	-6.84	1.92	2.05
22	C	511	CLA	C4B-NB	6.77	1.41	1.35
22	a	402	CLA	C4B-NB	6.74	1.41	1.35
22	b	607	CLA	C4B-NB	6.71	1.41	1.35
34	V	201	HEC	C2B-C3B	-6.69	1.33	1.40
22	c	506	CLA	C4B-NB	6.68	1.41	1.35
22	c	513	CLA	C4B-NB	6.67	1.41	1.35
22	b	614	CLA	C4B-NB	6.61	1.41	1.35
22	b	603	CLA	C4B-NB	6.55	1.41	1.35
22	c	511	CLA	MG-NA	6.46	2.21	2.06
22	C	504	CLA	C4B-NB	6.38	1.40	1.35
22	c	508	CLA	C4B-NB	6.36	1.40	1.35
22	C	513	CLA	C4B-NB	6.35	1.40	1.35
34	e	101	HEC	C3C-C2C	-6.33	1.34	1.40
22	c	511	CLA	MG-ND	6.32	2.18	2.05
22	B	617	CLA	C4B-NB	6.28	1.40	1.35
22	B	606	CLA	C4B-NB	6.23	1.40	1.35
22	d	403	CLA	C4B-NB	6.21	1.40	1.35
22	B	609	CLA	C4B-NB	6.20	1.40	1.35
22	b	612	CLA	C4B-NB	6.15	1.40	1.35
22	B	612	CLA	C4B-NB	6.12	1.40	1.35
22	C	510	CLA	C4B-NB	6.11	1.40	1.35
22	C	504	CLA	MG-NA	6.10	2.20	2.06
22	C	511	CLA	MG-NC	6.10	2.20	2.06
22	C	514	CLA	C4B-NB	6.05	1.40	1.35
22	C	509	CLA	MG-NA	5.94	2.20	2.06
22	B	609	CLA	MG-NA	5.83	2.20	2.06
22	b	615	CLA	C4B-NB	5.82	1.40	1.35
22	C	513	CLA	MG-NA	5.81	2.20	2.06
22	a	405	CLA	MG-NC	-5.77	1.92	2.06
22	c	502	CLA	C4B-NB	5.76	1.40	1.35
22	D	404	CLA	C4B-NB	5.72	1.40	1.35
22	C	503	CLA	C4B-NB	5.71	1.40	1.35
33	B	627	LMG	C4-C5	5.63	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C4B-NB	5.62	1.40	1.35
22	D	402	CLA	C4B-NB	5.53	1.40	1.35
22	c	510	CLA	MG-ND	-5.43	1.95	2.05
22	a	405	CLA	C4B-NB	5.41	1.40	1.35
22	b	606	CLA	C4B-NB	5.40	1.40	1.35
22	b	610	CLA	C4B-NB	5.32	1.40	1.35
22	B	605	CLA	MG-NA	5.31	2.18	2.06
22	B	613	CLA	C4B-NB	5.24	1.39	1.35
22	A	402	CLA	C4B-NB	5.21	1.39	1.35
22	b	614	CLA	C1D-ND	5.19	1.44	1.37
22	c	501	CLA	C4B-NB	5.13	1.39	1.35
22	D	404	CLA	MG-NC	5.10	2.18	2.06
22	B	607	CLA	C4B-NB	5.09	1.39	1.35
22	C	506	CLA	MG-NC	5.03	2.18	2.06
22	c	513	CLA	MG-ND	-5.01	1.95	2.05
22	b	613	CLA	C4B-NB	4.97	1.39	1.35
22	b	615	CLA	MG-NC	-4.90	1.94	2.06
22	c	509	CLA	MG-ND	4.89	2.15	2.05
22	B	609	CLA	MG-ND	-4.89	1.96	2.05
22	C	512	CLA	MG-NA	4.88	2.17	2.06
22	b	605	CLA	C4B-NB	4.88	1.39	1.35
22	c	510	CLA	MG-NA	4.81	2.17	2.06
22	B	603	CLA	MG-ND	-4.71	1.96	2.05
34	e	101	HEC	C3D-C2D	4.71	1.51	1.37
22	b	609	CLA	MG-NC	4.68	2.17	2.06
22	A	405	CLA	C4D-ND	-4.66	1.31	1.37
22	d	402	CLA	C4D-ND	-4.64	1.31	1.37
22	b	614	CLA	MG-ND	-4.64	1.96	2.05
34	V	201	HEC	C3C-C2C	-4.64	1.35	1.40
22	D	402	CLA	MG-NA	4.63	2.17	2.06
29	a	413	SQD	O47-C7	4.63	1.47	1.34
22	b	602	CLA	C4D-ND	-4.62	1.31	1.37
22	b	603	CLA	MG-NA	4.61	2.17	2.06
34	E	101	HEC	C3D-C2D	4.60	1.51	1.37
22	D	403	CLA	C4B-NB	4.58	1.39	1.35
22	b	613	CLA	MG-NC	-4.58	1.95	2.06
22	b	609	CLA	MG-ND	-4.57	1.96	2.05
22	c	503	CLA	MG-NC	4.57	2.17	2.06
22	C	513	CLA	C4D-ND	-4.56	1.31	1.37
34	v	201	HEC	C3D-C2D	4.55	1.51	1.37
22	c	510	CLA	C4B-NB	4.54	1.39	1.35
22	b	610	CLA	MG-ND	-4.52	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	C4B-NB	4.51	1.39	1.35
22	A	402	CLA	C4D-ND	-4.49	1.31	1.37
22	c	507	CLA	MG-NA	4.49	2.16	2.06
24	H	101	BCR	C30-C25	-4.49	1.47	1.53
22	C	502	CLA	MG-NA	4.45	2.16	2.06
30	C	519	DGD	O2G-C2G	-4.45	1.35	1.46
22	b	602	CLA	MG-NA	4.43	2.16	2.06
22	B	606	CLA	C4D-ND	-4.42	1.31	1.37
22	D	402	CLA	CMB-C2B	-4.37	1.42	1.51
22	c	508	CLA	C4D-ND	-4.36	1.31	1.37
22	b	612	CLA	C4D-ND	-4.35	1.31	1.37
22	c	505	CLA	C4D-ND	-4.33	1.31	1.37
22	c	510	CLA	C1D-ND	4.30	1.43	1.37
22	B	617	CLA	MG-ND	4.29	2.14	2.05
22	a	402	CLA	MG-NA	4.28	2.16	2.06
33	D	407	LMG	C4-C5	4.27	1.62	1.53
24	b	618	BCR	C30-C25	-4.27	1.47	1.53
22	B	608	CLA	MG-NC	4.25	2.16	2.06
22	b	616	CLA	C4B-NB	4.24	1.39	1.35
24	B	618	BCR	C30-C25	-4.21	1.48	1.53
33	m	101	LMG	C4-C3	4.20	1.63	1.52
24	d	405	BCR	C1-C6	-4.20	1.48	1.53
22	b	606	CLA	C1D-ND	4.18	1.42	1.37
24	C	515	BCR	C1-C6	-4.17	1.48	1.53
22	A	405	CLA	C1D-ND	4.14	1.42	1.37
22	b	610	CLA	C1D-ND	4.14	1.42	1.37
34	V	201	HEC	C3D-C2D	4.14	1.49	1.37
24	b	619	BCR	C30-C25	-4.12	1.48	1.53
22	B	611	CLA	CMB-C2B	-4.11	1.43	1.51
24	B	618	BCR	C1-C6	-4.10	1.48	1.53
22	B	616	CLA	C1D-ND	4.09	1.42	1.37
22	B	615	CLA	MG-NA	4.09	2.16	2.06
22	a	403	CLA	C4D-ND	-4.08	1.32	1.37
33	b	622	LMG	O6-C1	4.07	1.52	1.41
22	a	403	CLA	CHC-C1C	4.07	1.45	1.35
22	c	512	CLA	C4D-ND	-4.06	1.32	1.37
22	B	604	CLA	C4B-NB	4.05	1.38	1.35
30	C	518	DGD	C4D-C3D	4.04	1.62	1.52
22	C	514	CLA	MG-NA	4.03	2.15	2.06
22	D	402	CLA	MG-NC	-4.01	1.96	2.06
22	a	402	CLA	C1D-ND	4.00	1.42	1.37
22	b	615	CLA	C4D-ND	-4.00	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C1D-ND	3.98	1.42	1.37
22	b	605	CLA	C4D-ND	-3.97	1.32	1.37
22	B	609	CLA	C1D-ND	3.96	1.42	1.37
27	D	406	PL9	C11-C9	-3.96	1.43	1.51
22	b	611	CLA	MG-NA	3.96	2.15	2.06
22	c	502	CLA	C4D-ND	-3.92	1.32	1.37
28	d	407	LHG	O7-C5	-3.91	1.36	1.46
30	c	517	DGD	O2E-C2E	-3.91	1.33	1.43
22	B	605	CLA	C4B-NB	3.90	1.38	1.35
24	x	101	BCR	C30-C25	-3.87	1.48	1.53
22	C	506	CLA	CHC-C1C	3.86	1.44	1.35
22	c	507	CLA	C4D-ND	-3.86	1.32	1.37
22	b	613	CLA	MG-NA	3.86	2.15	2.06
22	C	507	CLA	C4D-ND	-3.85	1.32	1.37
22	B	606	CLA	C1D-ND	3.85	1.42	1.37
22	B	614	CLA	C4D-ND	-3.84	1.32	1.37
22	d	402	CLA	MG-NA	3.84	2.15	2.06
24	B	620	BCR	C1-C6	-3.84	1.48	1.53
22	C	511	CLA	C1D-ND	3.84	1.42	1.37
22	B	617	CLA	MG-NA	3.83	2.15	2.06
22	b	610	CLA	C4D-ND	-3.83	1.32	1.37
22	b	602	CLA	C1D-ND	3.82	1.42	1.37
22	d	403	CLA	C1D-ND	3.81	1.42	1.37
24	B	620	BCR	C30-C25	-3.81	1.48	1.53
22	a	405	CLA	C1D-ND	3.80	1.42	1.37
30	C	517	DGD	C6E-C5E	3.79	1.64	1.51
22	c	503	CLA	C1D-ND	3.79	1.42	1.37
22	C	502	CLA	MG-ND	3.78	2.13	2.05
28	A	411	LHG	P-O6	3.78	1.74	1.59
22	B	613	CLA	C4D-ND	-3.77	1.32	1.37
22	B	611	CLA	C1D-ND	3.76	1.42	1.37
22	d	403	CLA	C4D-ND	-3.75	1.32	1.37
22	b	607	CLA	MG-ND	-3.74	1.98	2.05
22	B	603	CLA	C4D-ND	-3.74	1.32	1.37
24	b	617	BCR	C1-C6	-3.72	1.48	1.53
22	a	405	CLA	MG-ND	-3.72	1.98	2.05
22	D	404	CLA	C1D-ND	3.71	1.42	1.37
22	B	602	CLA	C1D-ND	3.71	1.42	1.37
22	c	511	CLA	C1D-ND	3.70	1.42	1.37
22	b	614	CLA	CHC-C1C	3.69	1.44	1.35
30	C	517	DGD	O2G-C2G	-3.69	1.37	1.46
33	b	622	LMG	C7-C8	3.69	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	403	CLA	C1D-ND	3.69	1.42	1.37
22	a	403	CLA	MG-NC	3.69	2.15	2.06
22	b	616	CLA	C4D-ND	-3.68	1.32	1.37
22	b	616	CLA	C1D-ND	3.67	1.42	1.37
22	C	503	CLA	MG-NA	3.67	2.15	2.06
30	H	102	DGD	O5D-C1E	3.67	1.46	1.40
22	b	601	CLA	C1D-ND	3.66	1.42	1.37
22	b	606	CLA	C1B-NB	3.66	1.38	1.35
30	H	102	DGD	O2G-C2G	-3.66	1.37	1.46
22	c	506	CLA	C1D-ND	3.66	1.42	1.37
22	b	609	CLA	CMB-C2B	-3.65	1.44	1.51
28	B	622	LHG	O7-C5	-3.65	1.37	1.46
29	B	623	SQD	O47-C7	3.64	1.44	1.34
22	b	614	CLA	C4D-ND	-3.63	1.32	1.37
22	C	514	CLA	C1D-ND	3.63	1.42	1.37
22	C	502	CLA	C4D-ND	-3.63	1.32	1.37
29	A	414	SQD	O48-C23	3.62	1.43	1.33
22	d	402	CLA	C1D-ND	3.62	1.42	1.37
22	D	402	CLA	C4D-ND	-3.62	1.32	1.37
22	B	615	CLA	C4D-ND	-3.61	1.32	1.37
22	c	511	CLA	CHC-C1C	3.61	1.44	1.35
22	C	502	CLA	C3B-C2B	-3.60	1.35	1.40
29	L	101	SQD	O48-C23	3.60	1.43	1.33
22	C	504	CLA	MG-NC	3.60	2.14	2.06
22	b	609	CLA	C1D-ND	3.58	1.42	1.37
22	d	404	CLA	C1D-ND	3.57	1.42	1.37
22	C	505	CLA	C1D-ND	3.57	1.42	1.37
22	C	509	CLA	MG-ND	-3.56	1.98	2.05
22	B	612	CLA	C4D-ND	-3.55	1.32	1.37
22	C	511	CLA	CHC-C1C	3.55	1.44	1.35
29	F	101	SQD	O48-C23	3.55	1.43	1.33
22	B	611	CLA	MG-NA	3.54	2.14	2.06
24	t	101	BCR	C1-C6	-3.54	1.48	1.53
29	A	414	SQD	O47-C45	-3.50	1.41	1.47
22	c	501	CLA	MG-NA	3.50	2.14	2.06
22	B	611	CLA	C3B-C2B	-3.50	1.35	1.40
22	d	403	CLA	MG-NA	3.49	2.14	2.06
24	D	405	BCR	C1-C6	-3.49	1.49	1.53
22	A	403	CLA	C4D-ND	-3.49	1.32	1.37
22	B	610	CLA	CMD-C2D	-3.49	1.43	1.50
29	A	414	SQD	O47-C7	3.49	1.44	1.34
30	c	518	DGD	O5D-C1E	3.48	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	MG-NA	3.48	2.14	2.06
33	b	622	LMG	O1-C1	3.47	1.46	1.40
22	c	513	CLA	C1D-ND	3.47	1.42	1.37
22	B	611	CLA	C4D-ND	-3.47	1.32	1.37
30	C	518	DGD	O2D-C2D	-3.46	1.34	1.43
29	f	101	SQD	O47-C7	3.46	1.44	1.34
22	a	402	CLA	CHC-C1C	3.46	1.43	1.35
22	b	611	CLA	C4D-ND	-3.45	1.32	1.37
30	A	415	DGD	C3E-C2E	3.44	1.61	1.52
33	b	622	LMG	C3-C2	3.44	1.61	1.52
30	H	102	DGD	C4E-C5E	3.43	1.60	1.53
24	T	101	BCR	C30-C25	-3.43	1.49	1.53
22	c	501	CLA	C4D-ND	-3.43	1.33	1.37
30	A	415	DGD	C3G-C2G	3.42	1.61	1.50
22	B	608	CLA	C1D-ND	3.41	1.42	1.37
22	b	606	CLA	C4D-ND	-3.41	1.33	1.37
24	t	101	BCR	C30-C25	-3.41	1.49	1.53
22	A	402	CLA	CHC-C1C	3.40	1.43	1.35
24	Z	101	BCR	C30-C25	-3.40	1.49	1.53
30	h	101	DGD	C4E-C5E	3.40	1.60	1.53
33	M	101	LMG	C9-C8	3.40	1.61	1.50
22	D	403	CLA	C4D-ND	-3.40	1.33	1.37
22	B	607	CLA	CHC-C1C	3.39	1.43	1.35
22	C	512	CLA	C1D-ND	3.38	1.41	1.37
22	B	611	CLA	MG-ND	-3.38	1.99	2.05
22	d	402	CLA	CMB-C2B	-3.37	1.44	1.51
22	C	509	CLA	CHC-C1C	3.37	1.43	1.35
22	b	607	CLA	CMB-C2B	-3.37	1.44	1.51
22	a	403	CLA	C1D-ND	3.37	1.41	1.37
23	D	401	PHO	C3B-C2B	-3.36	1.35	1.40
22	D	403	CLA	C1D-ND	3.35	1.41	1.37
22	c	512	CLA	C1D-ND	3.35	1.41	1.37
22	b	614	CLA	MG-NA	3.35	2.14	2.06
22	c	506	CLA	C4D-ND	-3.35	1.33	1.37
33	d	410	LMG	C4-C5	3.34	1.60	1.53
22	a	402	CLA	MG-ND	-3.34	1.99	2.05
24	C	515	BCR	C30-C25	-3.34	1.49	1.53
27	d	406	PL9	C7-C3	3.34	1.54	1.51
22	b	610	CLA	C3B-C2B	-3.34	1.35	1.40
22	b	613	CLA	C4D-ND	-3.34	1.33	1.37
22	c	508	CLA	C1D-ND	3.33	1.41	1.37
22	C	514	CLA	MG-ND	3.31	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	CHC-C1C	3.31	1.43	1.35
28	d	409	LHG	P-O6	3.30	1.72	1.59
22	B	612	CLA	C1D-ND	3.30	1.41	1.37
24	b	617	BCR	C30-C25	-3.30	1.49	1.53
27	d	406	PL9	C31-C29	-3.30	1.44	1.51
29	f	101	SQD	O48-C23	3.30	1.43	1.33
22	B	611	CLA	CHC-C1C	3.30	1.43	1.35
22	A	403	CLA	CMD-C2D	-3.29	1.43	1.50
22	c	503	CLA	C4D-ND	-3.29	1.33	1.37
22	C	513	CLA	MG-ND	-3.27	1.99	2.05
22	C	509	CLA	C1D-ND	3.27	1.41	1.37
22	c	509	CLA	C4D-ND	-3.27	1.33	1.37
22	B	605	CLA	C4D-ND	-3.26	1.33	1.37
22	c	510	CLA	CMB-C2B	-3.26	1.44	1.51
22	a	402	CLA	CMB-C2B	-3.26	1.44	1.51
29	a	411	SQD	O48-C23	3.26	1.42	1.33
22	a	405	CLA	C4D-ND	-3.26	1.33	1.37
22	B	615	CLA	MG-NC	3.25	2.14	2.06
22	B	613	CLA	C1D-ND	3.25	1.41	1.37
23	a	404	PHO	CAC-C3C	-3.24	1.46	1.52
27	d	406	PL9	C53-C6	-3.24	1.43	1.50
22	b	601	CLA	CHC-C1C	3.24	1.43	1.35
22	B	604	CLA	C4D-ND	-3.24	1.33	1.37
22	c	512	CLA	C3B-C2B	-3.24	1.35	1.40
22	b	603	CLA	CHC-C1C	3.24	1.43	1.35
22	B	617	CLA	C4D-ND	-3.22	1.33	1.37
22	C	503	CLA	C4D-ND	-3.22	1.33	1.37
22	C	511	CLA	MG-ND	-3.22	1.99	2.05
33	m	101	LMG	C4-C5	3.21	1.59	1.53
22	d	402	CLA	CHC-C1C	3.20	1.43	1.35
22	c	512	CLA	CHC-C1C	3.20	1.43	1.35
33	b	622	LMG	C1-C2	3.19	1.61	1.52
22	B	608	CLA	C4D-ND	-3.19	1.33	1.37
22	b	607	CLA	C4D-ND	-3.19	1.33	1.37
22	b	615	CLA	CMB-C2B	-3.19	1.45	1.51
22	C	502	CLA	CHC-C1C	3.18	1.43	1.35
22	c	513	CLA	C4D-ND	-3.18	1.33	1.37
27	A	410	PL9	C7-C3	-3.18	1.48	1.51
22	B	616	CLA	C4D-ND	-3.17	1.33	1.37
22	B	607	CLA	C3B-C2B	-3.17	1.36	1.40
22	C	504	CLA	C4D-ND	-3.16	1.33	1.37
22	B	616	CLA	CMB-C2B	-3.16	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	CHC-C1C	3.14	1.43	1.35
22	c	510	CLA	C4D-ND	-3.14	1.33	1.37
33	D	407	LMG	O2-C2	-3.14	1.35	1.43
30	c	516	DGD	O5D-C1E	3.14	1.45	1.40
22	C	511	CLA	C4D-ND	-3.13	1.33	1.37
22	b	608	CLA	C4D-ND	-3.13	1.33	1.37
24	c	514	BCR	C30-C25	-3.13	1.49	1.53
24	B	619	BCR	C30-C25	-3.13	1.49	1.53
22	c	506	CLA	MG-ND	-3.13	1.99	2.05
24	c	515	BCR	C30-C25	-3.13	1.49	1.53
24	k	102	BCR	C1-C6	-3.12	1.49	1.53
29	L	101	SQD	O47-C7	3.12	1.43	1.34
22	A	405	CLA	MG-NA	-3.12	1.98	2.06
22	B	616	CLA	CHC-C1C	3.12	1.43	1.35
22	C	512	CLA	C4D-ND	-3.11	1.33	1.37
24	B	619	BCR	C1-C6	-3.11	1.49	1.53
22	b	603	CLA	C4D-ND	-3.10	1.33	1.37
22	C	503	CLA	C3B-C2B	-3.10	1.36	1.40
22	B	607	CLA	C1D-ND	3.10	1.41	1.37
22	C	507	CLA	CHC-C1C	3.10	1.42	1.35
22	C	506	CLA	C1D-ND	3.08	1.41	1.37
22	d	403	CLA	CHC-C1C	3.08	1.42	1.35
24	K	101	BCR	C30-C25	-3.08	1.49	1.53
33	c	521	LMG	C7-C8	3.08	1.60	1.50
28	A	413	LHG	C24-C23	3.07	1.59	1.50
30	C	518	DGD	O3D-C3D	-3.07	1.35	1.43
22	c	513	CLA	CHC-C1C	3.07	1.42	1.35
22	C	510	CLA	C4D-ND	-3.06	1.33	1.37
24	D	405	BCR	C30-C25	-3.06	1.49	1.53
22	A	403	CLA	MG-ND	-3.06	1.99	2.05
28	A	413	LHG	O8-C23	3.06	1.42	1.33
24	a	406	BCR	C38-C26	-3.06	1.45	1.50
22	c	510	CLA	C3B-C2B	-3.06	1.36	1.40
22	c	507	CLA	C3B-C2B	-3.05	1.36	1.40
22	c	502	CLA	CHC-C1C	3.05	1.42	1.35
22	B	610	CLA	C4D-ND	-3.04	1.33	1.37
22	B	602	CLA	CHC-C1C	3.04	1.42	1.35
29	A	412	SQD	O47-C7	3.04	1.42	1.34
30	A	415	DGD	C4D-C3D	3.04	1.60	1.52
22	c	508	CLA	CHC-C1C	3.03	1.42	1.35
30	C	517	DGD	C4D-C3D	3.03	1.60	1.52
22	B	614	CLA	CHC-C1C	3.03	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	CHC-C1C	3.02	1.42	1.35
24	k	102	BCR	C30-C25	-3.02	1.49	1.53
22	C	505	CLA	C4D-ND	-3.02	1.33	1.37
22	c	512	CLA	CMB-C2B	-3.02	1.45	1.51
30	C	518	DGD	C6D-C5D	3.02	1.61	1.51
22	B	607	CLA	C4D-ND	-3.01	1.33	1.37
23	A	404	PHO	C3B-C2B	-3.01	1.36	1.40
33	D	409	LMG	C7-C8	3.01	1.58	1.51
22	C	505	CLA	CHC-C1C	3.00	1.42	1.35
33	Y	101	LMG	C4-C5	3.00	1.59	1.53
22	B	604	CLA	C1D-ND	2.99	1.41	1.37
22	A	402	CLA	MG-ND	-2.99	1.99	2.05
22	B	610	CLA	MG-NA	2.99	2.13	2.06
22	c	504	CLA	CHC-C1C	2.99	1.42	1.35
22	a	405	CLA	CMC-C2C	-2.98	1.44	1.50
22	b	615	CLA	CHC-C1C	2.98	1.42	1.35
22	B	603	CLA	CHC-C1C	2.98	1.42	1.35
22	a	405	CLA	CMB-C2B	-2.97	1.45	1.51
24	b	619	BCR	C1-C6	-2.97	1.49	1.53
33	B	627	LMG	C3-C2	2.97	1.59	1.52
22	B	612	CLA	CMD-C2D	-2.97	1.44	1.50
22	C	510	CLA	C1D-ND	2.96	1.41	1.37
22	C	512	CLA	MG-NC	2.95	2.13	2.06
22	b	607	CLA	C3B-C2B	-2.95	1.36	1.40
22	B	607	CLA	C3B-CAB	-2.95	1.41	1.47
22	b	608	CLA	CHC-C1C	2.94	1.42	1.35
22	B	609	CLA	CHC-C1C	2.94	1.42	1.35
22	c	509	CLA	CMB-C2B	-2.94	1.45	1.51
22	b	604	CLA	C4D-ND	-2.94	1.33	1.37
33	Y	101	LMG	C1-C2	2.94	1.61	1.52
22	d	404	CLA	CHC-C1C	2.93	1.42	1.35
22	B	612	CLA	CHC-C1C	2.93	1.42	1.35
22	B	617	CLA	C1D-ND	2.93	1.41	1.37
22	c	505	CLA	CMB-C2B	-2.93	1.45	1.51
24	d	405	BCR	C30-C25	-2.93	1.49	1.53
29	A	412	SQD	O48-C23	2.93	1.41	1.33
24	C	501	BCR	C30-C25	-2.93	1.49	1.53
22	c	501	CLA	C3B-C2B	-2.93	1.36	1.40
22	C	513	CLA	CHC-C1C	2.93	1.42	1.35
22	b	605	CLA	C1D-ND	2.92	1.41	1.37
22	c	502	CLA	CMD-C2D	-2.92	1.44	1.50
22	b	616	CLA	MG-NA	2.92	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	CLA	CMC-C2C	-2.92	1.44	1.50
22	b	605	CLA	MG-ND	-2.91	2.00	2.05
29	a	413	SQD	O48-C23	2.91	1.41	1.33
22	b	601	CLA	MG-ND	2.90	2.11	2.05
22	C	514	CLA	C4D-ND	-2.90	1.33	1.37
22	C	503	CLA	MG-ND	-2.90	2.00	2.05
30	H	102	DGD	C1E-C2E	2.90	1.60	1.52
27	D	406	PL9	C52-C5	-2.90	1.44	1.50
24	T	101	BCR	C1-C6	-2.89	1.49	1.53
22	B	614	CLA	C3B-CAB	-2.89	1.42	1.47
22	b	609	CLA	CHC-C1C	2.89	1.42	1.35
22	C	512	CLA	CMB-C2B	-2.89	1.45	1.51
22	C	507	CLA	C3B-C2B	-2.88	1.36	1.40
23	A	404	PHO	CMA-C3A	-2.88	1.48	1.53
22	A	403	CLA	CMB-C2B	-2.88	1.45	1.51
22	c	503	CLA	CHC-C1C	2.88	1.42	1.35
22	B	615	CLA	CMB-C2B	-2.88	1.45	1.51
22	B	603	CLA	CMB-C2B	-2.87	1.45	1.51
24	Z	101	BCR	C1-C6	-2.87	1.49	1.53
29	B	623	SQD	O48-C23	2.87	1.41	1.33
22	B	610	CLA	C1D-ND	2.86	1.41	1.37
22	c	512	CLA	C3B-CAB	-2.86	1.42	1.47
28	D	408	LHG	O7-C5	-2.85	1.39	1.46
22	b	607	CLA	CHC-C1C	2.85	1.42	1.35
33	B	627	LMG	O7-C10	2.85	1.42	1.34
33	B	627	LMG	C4-C3	2.84	1.59	1.52
24	K	101	BCR	C1-C6	-2.84	1.49	1.53
22	B	602	CLA	C3B-C2B	-2.83	1.36	1.40
22	B	613	CLA	CHC-C1C	2.83	1.42	1.35
22	c	505	CLA	CHC-C1C	2.83	1.42	1.35
33	D	410	LMG	O8-C28	2.83	1.40	1.30
22	C	508	CLA	CHC-C1C	2.83	1.42	1.35
30	A	415	DGD	C4E-C5E	2.83	1.59	1.53
22	c	508	CLA	MG-NC	2.82	2.13	2.06
22	b	612	CLA	CHC-C1C	2.82	1.42	1.35
22	c	504	CLA	C4D-ND	-2.82	1.33	1.37
22	b	602	CLA	CMD-C2D	-2.81	1.44	1.50
22	b	609	CLA	C4D-ND	-2.81	1.33	1.37
33	M	101	LMG	O7-C8	-2.81	1.39	1.46
22	C	502	CLA	C1D-ND	2.80	1.41	1.37
22	b	605	CLA	CHC-C1C	2.80	1.42	1.35
22	C	502	CLA	CMD-C2D	-2.79	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	CMB-C2B	-2.79	1.45	1.51
33	c	521	LMG	O1-C1	2.79	1.45	1.40
22	d	404	CLA	C4D-ND	-2.79	1.33	1.37
33	b	622	LMG	C9-C8	2.78	1.59	1.50
33	d	410	LMG	O7-C8	-2.78	1.39	1.46
28	a	412	LHG	P-O6	2.78	1.70	1.59
30	C	518	DGD	O2G-C2G	-2.78	1.39	1.46
33	c	521	LMG	C3-C2	2.78	1.59	1.52
27	d	406	PL9	C46-C44	-2.77	1.45	1.51
27	D	406	PL9	C26-C24	-2.77	1.45	1.51
29	A	412	SQD	O2-C2	-2.76	1.36	1.43
30	H	102	DGD	O3G-C1D	2.76	1.44	1.40
22	c	503	CLA	CMB-C2B	-2.76	1.45	1.51
28	A	411	LHG	O3-C3	-2.76	1.34	1.44
24	a	406	BCR	C1-C6	-2.75	1.50	1.53
22	c	503	CLA	MG-NA	2.75	2.12	2.06
22	c	509	CLA	C1D-ND	2.75	1.41	1.37
22	b	615	CLA	CMD-C2D	-2.75	1.45	1.50
22	B	617	CLA	C3B-CAB	-2.74	1.42	1.47
30	H	102	DGD	O4D-C4D	-2.74	1.36	1.43
22	b	613	CLA	C1D-ND	2.74	1.41	1.37
22	c	501	CLA	C4B-CHC	-2.74	1.33	1.41
22	b	611	CLA	C1D-ND	2.74	1.41	1.37
22	b	608	CLA	MG-NA	2.74	2.12	2.06
22	B	608	CLA	CMB-C2B	-2.73	1.46	1.51
30	H	102	DGD	C6E-C5E	2.73	1.61	1.51
22	b	608	CLA	MG-NC	-2.73	1.99	2.06
28	a	412	LHG	O8-C23	2.73	1.41	1.33
24	c	515	BCR	C1-C6	-2.72	1.50	1.53
22	c	503	CLA	C3B-C2B	-2.72	1.36	1.40
22	c	504	CLA	C1D-ND	2.72	1.41	1.37
22	B	617	CLA	CHC-C1C	2.71	1.41	1.35
22	c	513	CLA	CMB-C2B	-2.71	1.46	1.51
22	c	506	CLA	MG-NC	2.71	2.12	2.06
30	H	102	DGD	C4D-C3D	2.70	1.59	1.52
22	C	510	CLA	CHC-C1C	2.70	1.41	1.35
24	k	103	BCR	C30-C25	-2.70	1.50	1.53
24	x	101	BCR	C1-C6	-2.69	1.50	1.53
22	b	613	CLA	CMB-C2B	-2.69	1.46	1.51
30	C	517	DGD	C6D-C5D	2.69	1.60	1.51
22	B	604	CLA	C3B-C2B	-2.69	1.36	1.40
22	D	402	CLA	CMD-C2D	-2.69	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	406	PL9	C35-C34	-2.68	1.43	1.50
22	C	514	CLA	CHC-C1C	2.68	1.41	1.35
28	A	413	LHG	P-O6	2.68	1.70	1.59
22	b	616	CLA	CMD-C2D	-2.68	1.45	1.50
33	M	101	LMG	C1-C2	2.68	1.60	1.52
22	D	403	CLA	CHC-C1C	2.68	1.41	1.35
22	c	506	CLA	CHC-C1C	2.68	1.41	1.35
33	C	516	LMG	C4-C5	2.67	1.58	1.53
22	b	604	CLA	CHC-C1C	2.67	1.41	1.35
22	C	514	CLA	CMB-C2B	-2.66	1.46	1.51
23	D	401	PHO	CMB-C2B	-2.66	1.45	1.51
22	B	612	CLA	CMB-C2B	-2.66	1.46	1.51
22	c	505	CLA	C3B-C2B	-2.65	1.36	1.40
22	b	604	CLA	C1D-ND	2.65	1.41	1.37
23	A	404	PHO	CMD-C2D	-2.65	1.45	1.51
30	h	101	DGD	C1E-C2E	2.64	1.60	1.52
30	C	517	DGD	C3G-C2G	2.64	1.58	1.50
30	h	101	DGD	C3G-C2G	2.64	1.58	1.50
22	C	508	CLA	C4D-ND	-2.64	1.34	1.37
22	B	615	CLA	C3B-CAB	-2.64	1.42	1.47
22	b	613	CLA	CMD-C2D	-2.64	1.45	1.50
22	c	504	CLA	CMB-C2B	-2.64	1.46	1.51
30	c	516	DGD	O2G-C2G	-2.63	1.40	1.46
23	d	401	PHO	CMC-C2C	-2.63	1.45	1.51
22	C	504	CLA	CMB-C2B	-2.63	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.63	1.46	1.51
22	d	404	CLA	CMB-C2B	-2.63	1.46	1.51
22	c	504	CLA	MG-NA	2.62	2.12	2.06
22	b	611	CLA	CMB-C2B	-2.62	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.62	1.46	1.51
22	c	507	CLA	CHC-C1C	2.62	1.41	1.35
22	b	612	CLA	CMB-C2B	-2.62	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.62	1.46	1.51
24	T	101	BCR	C38-C26	-2.61	1.46	1.50
22	A	405	CLA	MG-ND	2.61	2.11	2.05
33	C	516	LMG	C4-C3	2.60	1.59	1.52
22	c	502	CLA	C1D-ND	2.60	1.41	1.37
27	d	406	PL9	C25-C24	-2.59	1.44	1.50
28	L	102	LHG	O8-C23	2.59	1.40	1.33
22	B	610	CLA	O2D-CGD	2.59	1.39	1.33
22	A	403	CLA	CHC-C1C	2.59	1.41	1.35
23	d	401	PHO	CAC-C3C	-2.59	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	CMC-C2C	-2.59	1.45	1.50
30	C	517	DGD	C2A-C1A	-2.58	1.43	1.50
33	m	101	LMG	O7-C8	-2.58	1.40	1.46
22	b	606	CLA	CHC-C1C	2.57	1.41	1.35
22	c	503	CLA	CMC-C2C	-2.57	1.45	1.50
22	c	510	CLA	CHC-C1C	2.56	1.41	1.35
30	c	518	DGD	C3E-C2E	2.56	1.58	1.52
22	d	404	CLA	MG-ND	-2.56	2.00	2.05
22	d	403	CLA	CMB-C2B	-2.56	1.46	1.51
33	B	627	LMG	O1-C1	2.56	1.44	1.40
30	A	415	DGD	O3G-C1D	2.55	1.44	1.40
22	C	503	CLA	CHC-C1C	2.55	1.41	1.35
27	D	406	PL9	C3-C4	-2.54	1.45	1.49
33	m	101	LMG	C6-C5	2.54	1.60	1.51
33	m	101	LMG	O6-C1	2.54	1.48	1.41
22	a	402	CLA	CMC-C2C	-2.53	1.45	1.50
22	C	503	CLA	CMD-C2D	-2.53	1.45	1.50
22	c	511	CLA	C4D-ND	-2.53	1.34	1.37
23	D	401	PHO	C3B-CAB	-2.53	1.42	1.47
22	c	503	CLA	C3B-CAB	-2.53	1.42	1.47
24	c	514	BCR	C1-C6	-2.53	1.50	1.53
22	C	510	CLA	CMB-C2B	-2.53	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.53	1.45	1.50
24	A	406	BCR	C1-C6	-2.52	1.50	1.53
22	B	605	CLA	CHC-C1C	2.52	1.41	1.35
22	C	505	CLA	MG-NC	2.52	2.12	2.06
22	D	403	CLA	CMD-C2D	-2.52	1.45	1.50
22	b	613	CLA	C4B-CHC	-2.52	1.34	1.41
27	A	410	PL9	C3-C4	-2.52	1.45	1.49
22	b	603	CLA	C3B-CAB	-2.52	1.42	1.47
22	b	611	CLA	CMD-C2D	-2.51	1.45	1.50
23	D	401	PHO	O2D-CGD	2.51	1.39	1.33
22	C	514	CLA	C4B-CHC	-2.51	1.34	1.41
30	A	415	DGD	C1E-C2E	2.51	1.59	1.52
22	b	609	CLA	CMD-C2D	-2.51	1.45	1.50
30	c	516	DGD	O3E-C3E	-2.50	1.37	1.43
22	c	511	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	603	CLA	CMD-C2D	-2.50	1.45	1.50
22	b	603	CLA	CMD-C2D	-2.50	1.45	1.50
22	b	610	CLA	CMD-C2D	-2.50	1.45	1.50
22	b	614	CLA	CMB-C2B	-2.49	1.46	1.51
33	c	519	LMG	C6-C5	2.49	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	CHC-C1C	2.49	1.41	1.35
22	c	511	CLA	MG-NC	2.49	2.12	2.06
22	c	508	CLA	CMB-C2B	-2.49	1.46	1.51
22	D	404	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	503	CLA	CMC-C2C	-2.49	1.45	1.50
22	C	505	CLA	O2D-CGD	2.48	1.39	1.33
22	b	611	CLA	CHC-C1C	2.48	1.41	1.35
22	B	604	CLA	CMC-C2C	-2.48	1.45	1.50
22	B	605	CLA	C1D-ND	2.48	1.40	1.37
33	D	407	LMG	C1-C2	2.47	1.59	1.52
22	B	610	CLA	C4B-CHC	-2.47	1.34	1.41
22	B	617	CLA	C4B-CHC	-2.47	1.34	1.41
22	B	617	CLA	CMD-C2D	-2.47	1.45	1.50
22	B	602	CLA	MG-NC	-2.47	2.00	2.06
22	d	404	CLA	C4B-CHC	-2.46	1.34	1.41
22	a	405	CLA	C4B-CHC	-2.46	1.34	1.41
22	B	609	CLA	C4D-ND	-2.45	1.34	1.37
24	A	406	BCR	C38-C26	-2.45	1.46	1.50
30	c	517	DGD	C6E-C5E	2.45	1.60	1.51
22	C	503	CLA	MG-NC	2.45	2.12	2.06
22	C	509	CLA	CMD-C2D	-2.45	1.45	1.50
22	b	601	CLA	C4D-ND	-2.44	1.34	1.37
22	d	404	CLA	CMC-C2C	-2.44	1.45	1.50
22	A	405	CLA	C4B-CHC	-2.44	1.34	1.41
30	h	101	DGD	O2D-C2D	-2.44	1.37	1.43
23	D	401	PHO	CAC-C3C	-2.44	1.48	1.52
22	b	615	CLA	CMC-C2C	-2.44	1.45	1.50
22	b	603	CLA	C1D-ND	2.43	1.40	1.37
22	b	602	CLA	CAC-C3C	-2.43	1.44	1.51
22	C	506	CLA	MG-ND	2.43	2.10	2.05
22	b	610	CLA	C3D-C4D	2.43	1.49	1.44
22	b	606	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	606	CLA	C4B-CHC	-2.43	1.34	1.41
30	c	517	DGD	C4D-C5D	2.42	1.58	1.53
23	D	401	PHO	CMD-C2D	-2.42	1.45	1.51
22	c	501	CLA	CMB-C2B	-2.42	1.46	1.51
22	c	501	CLA	CAC-C3C	-2.42	1.44	1.51
30	h	101	DGD	O1G-C1G	-2.41	1.39	1.45
22	d	403	CLA	CHD-C4C	2.41	1.44	1.39
33	c	522	LMG	C4-C3	2.41	1.58	1.52
22	c	506	CLA	C4B-CHC	-2.41	1.34	1.41
30	c	518	DGD	O4D-C4D	-2.40	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	404	CLA	MG-NC	-2.40	2.00	2.06
22	C	505	CLA	C4B-CHC	-2.40	1.34	1.41
22	b	601	CLA	O2A-CGA	2.40	1.40	1.33
33	Y	101	LMG	O8-C9	-2.39	1.39	1.45
22	c	507	CLA	CMB-C2B	-2.39	1.46	1.51
28	d	407	LHG	O8-C23	2.39	1.40	1.33
24	B	618	BCR	C38-C26	-2.39	1.47	1.50
22	B	602	CLA	C4D-ND	-2.39	1.34	1.37
22	A	403	CLA	C3B-C2B	-2.39	1.37	1.40
24	C	501	BCR	C1-C6	-2.39	1.50	1.53
22	d	403	CLA	CMA-C3A	-2.38	1.48	1.53
22	b	608	CLA	CMA-C3A	-2.38	1.48	1.53
22	C	508	CLA	CMB-C2B	-2.38	1.46	1.51
22	B	615	CLA	C3B-C2B	-2.38	1.37	1.40
30	H	102	DGD	O2D-C2D	-2.38	1.37	1.43
22	C	506	CLA	C4D-ND	-2.37	1.34	1.37
22	d	404	CLA	CMD-C2D	-2.37	1.45	1.50
22	c	508	CLA	MG-NA	2.37	2.11	2.06
30	C	519	DGD	C1G-C2G	2.37	1.58	1.50
33	m	101	LMG	O1-C7	-2.37	1.39	1.43
22	B	606	CLA	C1C-NC	-2.37	1.34	1.37
22	B	608	CLA	CMC-C2C	-2.37	1.45	1.50
27	d	406	PL9	C11-C9	-2.37	1.46	1.51
22	c	507	CLA	CMC-C2C	-2.37	1.45	1.50
22	A	405	CLA	CAC-C3C	-2.36	1.45	1.51
22	B	606	CLA	CMB-C2B	-2.36	1.46	1.51
22	b	614	CLA	CMD-C2D	-2.36	1.45	1.50
23	A	404	PHO	CAC-C3C	-2.36	1.48	1.52
22	B	604	CLA	MG-NA	2.35	2.11	2.06
22	c	502	CLA	CMC-C2C	-2.35	1.45	1.50
22	b	602	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	608	CLA	C1D-C2D	2.35	1.50	1.45
30	c	516	DGD	C3G-C2G	2.35	1.57	1.50
22	c	513	CLA	C4B-CHC	-2.35	1.34	1.41
22	c	512	CLA	CMC-C2C	-2.34	1.45	1.50
23	A	404	PHO	CMC-C2C	-2.34	1.46	1.51
28	A	413	LHG	O7-C5	-2.34	1.40	1.46
22	B	608	CLA	CHC-C1C	2.34	1.41	1.35
22	a	403	CLA	CMB-C2B	-2.34	1.46	1.51
34	E	101	HEC	C1C-CHC	-2.34	1.34	1.41
22	c	510	CLA	CMC-C2C	-2.33	1.45	1.50
22	C	503	CLA	C1D-ND	2.33	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	402	CLA	C1D-ND	2.33	1.40	1.37
22	b	609	CLA	CMC-C2C	-2.33	1.45	1.50
24	C	515	BCR	C36-C18	-2.33	1.46	1.50
30	h	101	DGD	O3E-C3E	-2.33	1.37	1.43
33	M	101	LMG	C3-C2	2.33	1.58	1.52
32	D	411	STE	C2-C1	2.32	1.56	1.50
22	c	506	CLA	CMD-C2D	-2.32	1.45	1.50
30	H	102	DGD	O1G-C1G	-2.32	1.39	1.45
22	B	608	CLA	CMD-C2D	-2.32	1.45	1.50
22	b	614	CLA	C3B-C2B	-2.32	1.37	1.40
22	B	605	CLA	O2D-CGD	2.32	1.38	1.33
23	d	401	PHO	CMD-C2D	-2.32	1.46	1.51
29	a	411	SQD	O47-C7	2.31	1.40	1.34
22	b	616	CLA	C3D-C4D	2.31	1.49	1.44
30	C	519	DGD	O6D-C5D	-2.31	1.38	1.44
30	H	102	DGD	O6D-C5D	-2.30	1.38	1.44
22	B	608	CLA	C3B-C2B	-2.30	1.37	1.40
28	a	412	LHG	C6-C5	2.30	1.57	1.50
22	b	614	CLA	CAC-C3C	-2.30	1.45	1.51
22	b	608	CLA	CMB-C2B	-2.30	1.46	1.51
22	b	610	CLA	CMC-C2C	-2.30	1.45	1.50
30	H	102	DGD	O5D-C6D	-2.30	1.39	1.43
22	b	608	CLA	C3B-CAB	-2.30	1.43	1.47
22	C	502	CLA	CMC-C2C	-2.30	1.45	1.50
22	C	504	CLA	C3B-CAB	-2.29	1.43	1.47
29	a	411	SQD	O3-C3	-2.29	1.37	1.43
22	A	403	CLA	MG-NC	2.29	2.11	2.06
30	A	415	DGD	O2G-C1B	2.29	1.40	1.34
22	C	511	CLA	CMC-C2C	-2.28	1.46	1.50
22	A	402	CLA	CMC-C2C	-2.28	1.46	1.50
29	F	101	SQD	O3-C3	-2.28	1.37	1.43
22	c	505	CLA	CMD-C2D	-2.28	1.46	1.50
22	b	602	CLA	CHC-C1C	2.28	1.40	1.35
30	C	518	DGD	C4E-C3E	2.28	1.58	1.52
22	C	508	CLA	C3B-CAB	-2.28	1.43	1.47
30	c	517	DGD	O4D-C4D	-2.27	1.37	1.43
22	c	503	CLA	CMD-C2D	-2.27	1.46	1.50
22	A	402	CLA	CMB-C2B	-2.27	1.46	1.51
22	C	512	CLA	C3B-C2B	-2.27	1.37	1.40
22	B	610	CLA	C3B-C2B	-2.26	1.37	1.40
22	c	504	CLA	O2D-CGD	2.26	1.38	1.33
22	b	610	CLA	C3B-CAB	-2.26	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	BCR	C38-C26	-2.26	1.47	1.50
22	B	615	CLA	C1B-NB	2.26	1.37	1.35
22	D	403	CLA	C3B-CAB	-2.26	1.43	1.47
22	B	603	CLA	C3B-C2B	-2.26	1.37	1.40
33	B	627	LMG	O8-C28	2.25	1.39	1.33
33	D	409	LMG	C9-C8	2.25	1.57	1.50
30	h	101	DGD	O3G-C3G	-2.25	1.39	1.43
24	C	515	BCR	C33-C5	-2.25	1.47	1.50
22	b	607	CLA	CMD-C2D	-2.25	1.46	1.50
22	A	402	CLA	C1D-ND	2.25	1.40	1.37
22	B	615	CLA	CHC-C1C	2.25	1.40	1.35
29	f	101	SQD	O4-C4	-2.24	1.37	1.43
22	B	607	CLA	CMB-C2B	-2.24	1.47	1.51
30	c	516	DGD	O1G-C1A	2.24	1.39	1.33
30	C	518	DGD	C1E-C2E	2.24	1.58	1.52
30	c	518	DGD	O4E-C4E	-2.24	1.37	1.43
22	B	615	CLA	C1A-CHA	-2.24	1.33	1.43
22	B	603	CLA	C1D-ND	2.24	1.40	1.37
22	b	615	CLA	C3B-CAB	-2.23	1.43	1.47
22	b	605	CLA	C4B-CHC	-2.23	1.34	1.41
22	b	610	CLA	C4B-CHC	-2.23	1.34	1.41
30	A	415	DGD	C3D-C2D	2.23	1.58	1.52
22	C	513	CLA	C1D-ND	2.23	1.40	1.37
23	d	401	PHO	C3B-CAB	-2.23	1.43	1.47
32	b	621	STE	C2-C1	2.23	1.55	1.50
22	b	616	CLA	C3B-C2B	-2.22	1.37	1.40
22	b	615	CLA	C3B-C2B	-2.22	1.37	1.40
22	c	510	CLA	C4B-CHC	-2.22	1.34	1.41
22	d	402	CLA	MG-ND	2.22	2.10	2.05
30	C	519	DGD	O5D-C1E	2.22	1.44	1.40
30	c	516	DGD	C6D-C5D	2.22	1.58	1.51
33	c	519	LMG	C4-C5	2.22	1.57	1.53
22	B	606	CLA	CHC-C1C	2.22	1.40	1.35
22	c	507	CLA	MG-ND	2.21	2.10	2.05
22	B	610	CLA	CHD-C1D	-2.21	1.34	1.38
22	a	405	CLA	CMD-C2D	-2.21	1.46	1.50
22	b	603	CLA	C1A-CHA	-2.21	1.33	1.43
30	c	517	DGD	O3D-C3D	-2.21	1.37	1.43
30	C	517	DGD	O1A-C1A	2.21	1.29	1.22
24	k	102	BCR	C38-C26	-2.20	1.47	1.50
34	v	201	HEC	C1D-ND	2.20	1.40	1.36
22	b	602	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	e	101	HEC	C4B-C3B	2.20	1.47	1.43
22	B	608	CLA	CMA-C3A	-2.20	1.48	1.53
22	c	507	CLA	C1D-ND	2.20	1.40	1.37
22	B	616	CLA	C3B-C2B	-2.20	1.37	1.40
22	B	617	CLA	CMB-C2B	-2.19	1.47	1.51
23	a	404	PHO	O2D-CGD	2.19	1.38	1.33
30	c	518	DGD	O2E-C2E	-2.19	1.37	1.43
22	B	608	CLA	CAC-C3C	-2.19	1.45	1.51
22	B	608	CLA	C3B-CAB	-2.19	1.43	1.47
29	A	412	SQD	O3-C3	-2.19	1.37	1.43
22	b	607	CLA	CMC-C2C	-2.19	1.46	1.50
22	c	507	CLA	C3B-CAB	-2.19	1.43	1.47
22	d	404	CLA	C3B-CAB	-2.19	1.43	1.47
22	b	613	CLA	CHC-C1C	2.19	1.40	1.35
23	d	401	PHO	O2A-C1	-2.18	1.40	1.46
22	B	605	CLA	C4C-C3C	2.18	1.48	1.45
24	b	618	BCR	C38-C26	-2.18	1.47	1.50
24	k	103	BCR	C1-C6	-2.18	1.50	1.53
22	B	611	CLA	C1B-NB	2.18	1.37	1.35
30	h	101	DGD	O2E-C2E	-2.18	1.37	1.43
32	B	624	STE	O1-C1	2.18	1.29	1.22
22	b	604	CLA	CMB-C2B	-2.18	1.47	1.51
33	c	521	LMG	C1-C2	2.18	1.58	1.52
22	b	616	CLA	CMB-C2B	-2.17	1.47	1.51
22	C	510	CLA	O2D-CGD	2.17	1.38	1.33
24	A	406	BCR	C33-C5	-2.17	1.47	1.50
22	c	504	CLA	MG-NC	-2.17	2.01	2.06
22	c	513	CLA	CMC-C2C	-2.17	1.46	1.50
33	c	522	LMG	O8-C9	-2.17	1.40	1.45
24	k	102	BCR	C33-C5	-2.16	1.47	1.50
22	B	609	CLA	C3B-CAB	-2.16	1.43	1.47
27	d	406	PL9	C3-C4	-2.16	1.46	1.49
22	b	613	CLA	C5-C3	-2.16	1.46	1.51
22	c	501	CLA	CMD-C2D	-2.16	1.46	1.50
30	c	517	DGD	O3E-C3E	-2.16	1.37	1.43
30	C	519	DGD	O1G-C1G	-2.15	1.40	1.45
24	c	515	BCR	C38-C26	-2.15	1.47	1.50
22	c	506	CLA	CAC-C3C	-2.15	1.45	1.51
28	B	622	LHG	C24-C23	2.15	1.57	1.50
22	D	404	CLA	CMC-C2C	-2.15	1.46	1.50
22	a	405	CLA	CAC-C3C	-2.15	1.45	1.51
33	Y	101	LMG	C3-C2	2.15	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	CMC-C2C	-2.15	1.46	1.50
22	b	609	CLA	C3B-CAB	-2.15	1.43	1.47
30	c	517	DGD	O3G-C3G	-2.15	1.39	1.43
22	c	507	CLA	C3D-C4D	2.15	1.49	1.44
22	c	506	CLA	CMB-C2B	-2.15	1.47	1.51
22	C	508	CLA	C3B-C2B	-2.14	1.37	1.40
22	B	603	CLA	MG-NA	-2.14	2.01	2.06
30	C	517	DGD	O1G-C1A	2.14	1.39	1.33
22	A	402	CLA	MG-NA	-2.14	2.01	2.06
22	b	605	CLA	CMC-C2C	-2.14	1.46	1.50
23	D	401	PHO	CMA-C3A	-2.14	1.49	1.53
27	a	410	PL9	C53-C6	-2.14	1.46	1.50
22	b	601	CLA	C3D-C4D	2.14	1.49	1.44
27	d	406	PL9	C10-C9	-2.14	1.45	1.50
22	C	506	CLA	C3B-CAB	-2.14	1.43	1.47
27	a	410	PL9	C40-C39	-2.13	1.45	1.50
22	A	405	CLA	CMC-C2C	-2.13	1.46	1.50
24	b	618	BCR	C36-C18	-2.13	1.46	1.50
22	C	502	CLA	CMB-C2B	-2.13	1.47	1.51
22	b	605	CLA	CMD-C2D	-2.13	1.46	1.50
22	b	611	CLA	CAA-C2A	-2.13	1.50	1.54
22	a	402	CLA	C4D-ND	-2.13	1.34	1.37
33	c	519	LMG	C1-C2	2.13	1.58	1.52
28	d	407	LHG	C24-C23	2.13	1.56	1.50
33	c	519	LMG	O1-C1	2.13	1.43	1.40
22	C	503	CLA	C1B-NB	2.13	1.37	1.35
33	B	627	LMG	C14-C13	2.13	1.63	1.51
22	C	514	CLA	C3B-CAB	-2.13	1.43	1.47
22	B	609	CLA	C1B-NB	2.12	1.37	1.35
30	h	101	DGD	O5D-C1E	2.12	1.43	1.40
22	b	601	CLA	CMB-C2B	-2.12	1.47	1.51
22	c	512	CLA	CMD-C2D	-2.12	1.46	1.50
33	b	622	LMG	O1-C7	2.12	1.47	1.43
22	b	615	CLA	C4B-CHC	-2.12	1.35	1.41
22	C	504	CLA	C3B-C2B	-2.12	1.37	1.40
22	b	601	CLA	C1B-NB	2.12	1.37	1.35
22	c	510	CLA	CAA-C2A	-2.12	1.50	1.54
30	C	518	DGD	C1G-C2G	2.12	1.57	1.50
24	b	617	BCR	C33-C5	-2.12	1.47	1.50
27	A	410	PL9	C41-C39	2.11	1.55	1.51
22	b	602	CLA	MG-NC	-2.11	2.01	2.06
28	L	102	LHG	O7-C5	-2.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	522	LMG	C3-C2	2.11	1.57	1.52
22	A	405	CLA	C3B-CAB	-2.11	1.43	1.47
22	B	602	CLA	C3B-CAB	-2.11	1.43	1.47
22	C	509	CLA	O2A-CGA	2.11	1.39	1.33
22	B	611	CLA	C3B-CAB	-2.10	1.43	1.47
22	D	403	CLA	CMB-C2B	-2.10	1.47	1.51
22	D	404	CLA	C3B-C2B	-2.10	1.37	1.40
22	c	510	CLA	C3D-C4D	2.10	1.48	1.44
22	C	513	CLA	CMB-C2B	-2.10	1.47	1.51
23	A	404	PHO	C4-C3	-2.10	1.45	1.50
29	a	411	SQD	O2-C2	-2.10	1.38	1.43
22	C	511	CLA	CMB-C2B	-2.10	1.47	1.51
30	C	519	DGD	O5D-C6D	2.10	1.47	1.43
33	d	410	LMG	O8-C28	2.10	1.39	1.33
22	c	507	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	616	CLA	CHC-C1C	2.09	1.40	1.35
24	c	515	BCR	C33-C5	-2.09	1.47	1.50
22	c	509	CLA	CMD-C2D	-2.09	1.46	1.50
22	a	402	CLA	C1D-C2D	2.09	1.49	1.45
22	c	511	CLA	C3B-CAB	-2.09	1.43	1.47
29	a	411	SQD	O5-C5	-2.09	1.39	1.44
22	b	605	CLA	C3B-C2B	-2.09	1.37	1.40
28	a	412	LHG	C24-C23	2.09	1.56	1.50
30	H	102	DGD	C6D-C5D	2.08	1.58	1.51
22	C	504	CLA	CMD-C2D	-2.08	1.46	1.50
22	b	603	CLA	CMC-C2C	-2.08	1.46	1.50
22	C	512	CLA	C1B-NB	2.08	1.37	1.35
32	B	621	STE	C2-C1	2.08	1.55	1.50
22	B	602	CLA	CMC-C2C	-2.08	1.46	1.50
22	B	606	CLA	C4B-CHC	-2.08	1.35	1.41
22	b	612	CLA	CHD-C1D	-2.08	1.34	1.38
22	C	504	CLA	C1D-ND	2.08	1.40	1.37
30	c	518	DGD	C4D-C3D	2.08	1.57	1.52
22	B	609	CLA	CMD-C2D	-2.07	1.46	1.50
27	D	406	PL9	C16-C14	2.07	1.55	1.51
22	b	601	CLA	CMD-C2D	-2.07	1.46	1.50
22	C	503	CLA	C4B-CHC	-2.07	1.35	1.41
22	C	504	CLA	C3D-C4D	2.07	1.48	1.44
22	C	514	CLA	CMD-C2D	-2.07	1.46	1.50
22	D	404	CLA	C1B-NB	2.06	1.37	1.35
34	e	101	HEC	C4D-CHA	-2.06	1.35	1.41
22	c	511	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	C1D-C2D	2.06	1.49	1.45
29	A	412	SQD	O4-C4	-2.06	1.38	1.43
22	b	609	CLA	C3D-C4D	2.06	1.48	1.44
28	d	408	LHG	O7-C7	2.05	1.40	1.34
29	f	101	SQD	O2-C2	-2.05	1.38	1.43
28	A	413	LHG	P-O3	2.05	1.67	1.59
33	D	409	LMG	O8-C28	2.05	1.39	1.33
22	b	613	CLA	O2A-CGA	2.05	1.39	1.33
22	B	613	CLA	C1A-CHA	-2.05	1.34	1.43
28	A	411	LHG	O8-C23	2.05	1.39	1.33
23	a	404	PHO	C1A-C2A	2.04	1.54	1.51
27	a	410	PL9	C52-C5	-2.04	1.46	1.50
22	d	403	CLA	MG-NC	-2.04	2.01	2.06
22	C	505	CLA	C3B-C2B	-2.04	1.37	1.40
22	c	508	CLA	O2A-CGA	2.04	1.39	1.33
22	c	511	CLA	C3C-C2C	2.04	1.41	1.36
22	C	506	CLA	CMC-C2C	-2.04	1.46	1.50
22	C	511	CLA	CMD-C2D	-2.04	1.46	1.50
22	a	403	CLA	C3B-CAB	-2.04	1.43	1.47
22	d	403	CLA	C4B-CHC	-2.04	1.35	1.41
22	b	604	CLA	MG-NA	2.03	2.11	2.06
33	c	521	LMG	C9-C8	2.03	1.56	1.50
22	c	513	CLA	MG-NA	-2.03	2.01	2.06
30	C	517	DGD	C3D-C2D	2.03	1.57	1.52
22	b	615	CLA	C1D-ND	2.03	1.40	1.37
22	C	514	CLA	C3B-C2B	-2.03	1.37	1.40
22	C	512	CLA	CMD-C2D	-2.03	1.46	1.50
24	C	515	BCR	C38-C26	-2.03	1.47	1.50
22	B	609	CLA	C4B-CHC	-2.03	1.35	1.41
33	D	407	LMG	O7-C10	2.03	1.40	1.34
22	a	405	CLA	MG-NA	2.03	2.11	2.06
22	C	510	CLA	C1D-C2D	2.03	1.49	1.45
23	D	401	PHO	CAA-C2A	-2.02	1.49	1.54
23	D	401	PHO	CMC-C2C	-2.02	1.46	1.51
22	C	511	CLA	C3D-C4D	2.02	1.48	1.44
28	B	622	LHG	C3-C2	2.02	1.58	1.51
22	c	501	CLA	C1D-ND	2.02	1.40	1.37
22	b	605	CLA	CMB-C2B	-2.02	1.47	1.51
22	B	610	CLA	CHC-C1C	2.02	1.40	1.35
22	C	510	CLA	C4B-CHC	-2.02	1.35	1.41
22	B	613	CLA	MG-NA	2.02	2.11	2.06
22	b	601	CLA	C3B-CAB	-2.01	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	402	CLA	CHC-C1C	2.01	1.40	1.35
22	D	404	CLA	CHC-C1C	2.01	1.40	1.35
22	B	615	CLA	OBD-CAD	-2.01	1.19	1.22
22	c	505	CLA	CAA-C2A	-2.01	1.50	1.54
22	A	402	CLA	CAA-C2A	-2.01	1.50	1.54
30	C	519	DGD	C4E-C3E	2.01	1.57	1.52
22	c	508	CLA	C3C-C2C	2.01	1.41	1.36
22	b	603	CLA	C3B-C2B	-2.01	1.37	1.40
22	C	508	CLA	CMD-C2D	-2.01	1.46	1.50
22	c	504	CLA	CMC-C2C	-2.00	1.46	1.50

All (1317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	C4A-NA-C1A	10.83	111.58	106.71
22	B	617	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	L	101	SQD	O6-C1-C2	9.35	122.90	108.30
29	A	412	SQD	O6-C1-C2	8.82	122.07	108.30
22	B	607	CLA	C4A-NA-C1A	8.69	110.61	106.71
22	B	605	CLA	C4A-NA-C1A	8.65	110.60	106.71
29	a	411	SQD	O6-C1-C2	8.21	121.12	108.30
34	e	101	HEC	CBD-CAD-C3D	-8.01	98.95	112.62
34	E	101	HEC	CBD-CAD-C3D	-8.00	98.97	112.62
22	c	503	CLA	C4A-NA-C1A	7.80	110.21	106.71
22	c	507	CLA	C4A-NA-C1A	7.67	110.15	106.71
27	d	406	PL9	C7-C3-C4	7.45	122.94	116.88
22	C	503	CLA	C4A-NA-C1A	7.42	110.04	106.71
22	B	608	CLA	C4A-NA-C1A	7.24	109.96	106.71
22	b	604	CLA	C4A-NA-C1A	7.14	109.92	106.71
22	d	402	CLA	C4A-NA-C1A	7.13	109.91	106.71
22	b	606	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	c	511	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	C	512	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	b	607	CLA	C4A-NA-C1A	6.85	109.78	106.71
29	B	623	SQD	O6-C1-C2	6.64	118.67	108.30
22	c	509	CLA	C4A-NA-C1A	6.52	109.64	106.71
27	D	406	PL9	C7-C3-C4	6.49	122.16	116.88
22	c	501	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	c	508	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	C	510	CLA	C4A-NA-C1A	6.38	109.57	106.71
27	a	410	PL9	C7-C3-C4	6.31	122.01	116.88
22	b	616	CLA	C4A-NA-C1A	6.28	109.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	511	CLA	C4A-NA-C1A	6.27	109.53	106.71
22	C	508	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	B	612	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	D	402	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	c	510	CLA	C4A-NA-C1A	6.23	109.50	106.71
22	b	601	CLA	C4A-NA-C1A	6.19	109.49	106.71
22	B	602	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	b	609	CLA	C4A-NA-C1A	5.93	109.37	106.71
29	f	101	SQD	O6-C1-C2	5.92	117.55	108.30
22	C	513	CLA	C4A-NA-C1A	5.87	109.34	106.71
22	b	614	CLA	C4A-NA-C1A	5.77	109.30	106.71
22	b	602	CLA	C4A-NA-C1A	5.55	109.20	106.71
22	a	405	CLA	C4A-NA-C1A	5.55	109.20	106.71
22	C	514	CLA	C4A-NA-C1A	5.51	109.18	106.71
22	B	613	CLA	C4A-NA-C1A	5.35	109.11	106.71
22	D	404	CLA	CMB-C2B-C1B	-5.32	120.29	128.46
29	L	101	SQD	O9-S-C6	5.30	113.23	106.94
22	b	616	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
22	B	606	CLA	C4A-NA-C1A	5.29	109.08	106.71
29	F	101	SQD	O6-C1-C2	5.28	116.55	108.30
29	A	412	SQD	O7-S-C6	5.25	113.17	106.94
34	V	201	HEC	CMB-C2B-C1B	-5.24	120.41	128.46
22	d	404	CLA	CMB-C2B-C1B	-5.16	120.54	128.46
22	B	615	CLA	O2D-CGD-O1D	-5.14	113.79	123.84
29	L	101	SQD	O7-S-C6	5.14	113.05	106.94
22	b	615	CLA	C4A-NA-C1A	5.12	109.01	106.71
22	c	504	CLA	CMB-C2B-C1B	-5.11	120.60	128.46
29	B	623	SQD	O7-S-C6	5.08	112.97	106.94
22	D	402	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
33	b	622	LMG	C1-O6-C5	-5.03	103.81	113.69
22	b	606	CLA	O2D-CGD-O1D	-4.98	114.11	123.84
34	V	201	HEC	CMC-C2C-C1C	-4.97	120.83	128.46
22	B	610	CLA	C4A-NA-C1A	4.97	108.94	106.71
29	L	101	SQD	O47-C7-C8	4.95	122.17	111.50
22	d	403	CLA	CHD-C1D-ND	-4.94	119.91	124.45
29	a	413	SQD	O47-C7-C8	4.94	122.16	111.50
22	b	602	CLA	O2D-CGD-O1D	-4.91	114.24	123.84
22	B	616	CLA	C4A-NA-C1A	4.90	108.91	106.71
22	D	403	CLA	C4A-NA-C1A	4.90	108.91	106.71
22	c	505	CLA	C4A-NA-C1A	4.89	108.91	106.71
22	a	403	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
22	b	609	CLA	CMB-C2B-C1B	-4.89	120.95	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C4A-NA-C1A	4.82	108.87	106.71
22	B	605	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
22	a	403	CLA	C4A-NA-C1A	4.78	108.85	106.71
22	b	611	CLA	O2D-CGD-O1D	-4.76	114.53	123.84
26	a	409	BCT	O2-C-O1	4.72	131.80	119.55
29	A	414	SQD	C45-O47-C7	4.72	123.94	117.88
22	B	608	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
22	d	404	CLA	CMB-C2B-C3B	4.64	133.37	124.68
22	b	605	CLA	C4A-NA-C1A	4.63	108.79	106.71
29	B	623	SQD	O47-C7-C8	4.63	121.47	111.50
29	f	101	SQD	O7-S-C6	4.63	112.44	106.94
22	A	402	CLA	CHB-C4A-NA	4.62	130.90	124.51
22	a	402	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
22	c	502	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
22	b	616	CLA	CMB-C2B-C3B	4.58	133.25	124.68
22	b	603	CLA	CMB-C2B-C3B	4.58	133.24	124.68
22	C	514	CLA	O2D-CGD-O1D	-4.55	114.94	123.84
22	d	403	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
22	b	603	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
34	V	201	HEC	CMB-C2B-C3B	4.53	131.14	125.82
30	C	517	DGD	O3G-C3G-C2G	-4.52	99.99	110.90
22	C	510	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
22	D	404	CLA	CMB-C2B-C3B	4.50	133.11	124.68
22	C	509	CLA	O2D-CGD-O1D	-4.48	115.07	123.84
22	b	604	CLA	C1-C2-C3	-4.47	118.32	126.04
22	C	505	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
22	B	604	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
22	c	502	CLA	CMB-C2B-C3B	4.43	132.97	124.68
29	f	101	SQD	O9-S-C6	4.42	112.19	106.94
22	c	508	CLA	CHD-C1D-ND	-4.41	120.40	124.45
29	A	412	SQD	C1-C2-C3	-4.36	100.93	110.00
22	B	604	CLA	CMB-C2B-C3B	4.34	132.80	124.68
22	d	402	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
22	B	608	CLA	CMB-C2B-C3B	4.30	132.73	124.68
22	b	611	CLA	C4A-NA-C1A	4.30	108.64	106.71
30	C	518	DGD	O3G-C3G-C2G	-4.29	100.54	110.90
22	d	404	CLA	CHD-C1D-ND	-4.29	120.51	124.45
22	b	612	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
33	B	627	LMG	C1-O6-C5	-4.29	105.27	113.69
28	d	409	LHG	O8-C23-O10	-4.26	112.83	123.59
22	B	603	CLA	CMB-C2B-C1B	-4.25	121.92	128.46
22	c	513	CLA	C4A-NA-C1A	4.25	108.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
22	B	615	CLA	C4A-NA-C1A	4.24	108.61	106.71
28	a	412	LHG	O4-P-O5	4.23	133.16	112.24
22	b	615	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
22	B	605	CLA	CMB-C2B-C3B	4.22	132.58	124.68
28	l	101	LHG	O4-P-O5	4.22	133.11	112.24
22	B	614	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
33	b	622	LMG	O6-C5-C6	4.19	116.86	106.44
28	L	102	LHG	O4-P-O5	4.18	132.89	112.24
22	b	610	CLA	C4A-NA-C1A	4.16	108.58	106.71
29	a	411	SQD	O8-S-C6	4.16	112.36	105.74
24	b	617	BCR	C2-C1-C6	4.16	116.88	110.48
33	m	101	LMG	O3-C3-C2	-4.12	100.81	110.35
28	D	408	LHG	O4-P-O5	4.11	132.56	112.24
28	B	622	LHG	O4-P-O5	4.10	132.52	112.24
33	B	627	LMG	O6-C1-C2	-4.10	101.68	110.35
29	F	101	SQD	O8-S-C6	4.10	112.27	105.74
22	C	509	CLA	C4A-NA-C1A	4.09	108.55	106.71
22	B	616	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
29	A	412	SQD	O8-S-C6	4.08	112.25	105.74
22	B	604	CLA	C4A-NA-C1A	4.08	108.54	106.71
22	C	513	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
30	H	102	DGD	O3G-C3G-C2G	-4.05	101.13	110.90
28	d	408	LHG	O4-P-O5	4.04	132.23	112.24
22	B	614	CLA	C4-C3-C5	4.02	122.03	115.27
22	b	613	CLA	C1-C2-C3	-4.02	119.09	126.04
22	c	512	CLA	O2D-CGD-O1D	-4.02	115.99	123.84
22	C	509	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
22	A	403	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
22	C	506	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
24	B	620	BCR	C2-C1-C6	3.99	116.63	110.48
22	b	603	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
22	b	613	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
22	c	501	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
29	f	101	SQD	O9-S-O7	-3.97	100.22	113.95
22	b	606	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
22	C	513	CLA	CHB-C4A-NA	3.94	129.96	124.51
22	d	403	CLA	CHB-C4A-NA	3.94	129.96	124.51
27	D	406	PL9	C7-C3-C2	-3.94	118.12	123.30
33	m	101	LMG	O1-C1-C2	-3.93	102.16	108.30
22	c	509	CLA	O2A-CGA-O1A	-3.92	113.69	123.59
22	C	506	CLA	CAC-C3C-C4C	3.91	129.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	511	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
29	F	101	SQD	O9-S-C6	3.90	111.58	106.94
22	a	403	CLA	CMB-C2B-C3B	3.90	131.97	124.68
27	a	410	PL9	C7-C3-C2	-3.89	118.18	123.30
30	C	517	DGD	O1G-C1A-C2A	-3.89	99.70	111.91
33	B	627	LMG	C1-C2-C3	-3.89	101.90	110.00
22	C	511	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
22	D	404	CLA	C4A-NA-C1A	3.88	108.45	106.71
28	A	413	LHG	O4-P-O5	3.88	131.42	112.24
29	a	411	SQD	O7-S-C6	3.87	111.53	106.94
22	a	405	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
22	D	404	CLA	C1B-CHB-C4A	-3.86	122.46	130.12
22	b	613	CLA	CED-O2D-CGD	3.86	124.66	115.94
22	D	404	CLA	O2D-CGD-O1D	-3.86	116.30	123.84
29	F	101	SQD	C1-O5-C5	-3.86	106.12	113.69
22	A	405	CLA	C1B-CHB-C4A	-3.85	122.48	130.12
22	c	506	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
29	B	623	SQD	C1-C2-C3	-3.85	101.98	110.00
24	k	103	BCR	C37-C22-C21	-3.83	117.55	122.92
22	c	508	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
28	d	407	LHG	O4-P-O5	3.82	131.13	112.24
22	c	512	CLA	CHB-C4A-NA	3.82	129.79	124.51
34	V	201	HEC	CBD-CAD-C3D	-3.80	106.14	112.62
22	B	613	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
24	c	515	BCR	C35-C13-C14	-3.79	117.62	122.92
27	A	410	PL9	C36-C34-C33	-3.79	113.46	121.12
22	A	405	CLA	CMB-C2B-C3B	3.79	131.76	124.68
22	B	615	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
28	d	409	LHG	O4-P-O5	3.78	130.92	112.24
29	B	623	SQD	C1-O5-C5	-3.77	106.29	113.69
22	B	603	CLA	CHB-C4A-NA	3.77	129.72	124.51
22	b	611	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
29	B	623	SQD	O9-S-O7	-3.76	100.92	113.95
22	B	602	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
22	C	506	CLA	CMB-C2B-C3B	3.76	131.71	124.68
33	B	627	LMG	C7-O1-C1	3.76	121.08	113.74
28	A	411	LHG	O4-P-O5	3.75	130.80	112.24
29	A	414	SQD	O47-C7-C8	3.74	119.55	111.50
22	b	606	CLA	O2D-CGD-CBD	3.73	117.90	111.27
23	A	404	PHO	C5-C3-C2	3.73	128.66	121.12
29	L	101	SQD	C1-C2-C3	-3.72	102.25	110.00
22	b	613	CLA	CHB-C4A-NA	3.71	129.65	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	518	DGD	O3G-C3G-C2G	-3.71	101.95	110.90
24	H	101	BCR	C36-C18-C17	-3.71	117.73	122.92
33	d	410	LMG	O2-C2-C1	-3.70	101.05	110.05
22	d	403	CLA	C4A-NA-C1A	3.70	108.37	106.71
22	c	512	CLA	C1-C2-C3	-3.69	119.66	126.04
24	c	514	BCR	C2-C1-C6	3.69	116.16	110.48
34	v	201	HEC	CBD-CAD-C3D	-3.69	106.33	112.62
22	c	504	CLA	CMB-C2B-C3B	3.69	131.57	124.68
27	d	406	PL9	C35-C34-C36	3.68	121.47	115.27
22	C	508	CLA	CHB-C4A-NA	3.68	129.60	124.51
22	b	605	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
29	F	101	SQD	C1-C2-C3	-3.67	102.35	110.00
22	B	609	CLA	C6-C7-C8	-3.67	104.05	115.92
22	c	504	CLA	C4A-NA-C1A	3.66	108.35	106.71
22	c	505	CLA	CHB-C4A-NA	3.65	129.56	124.51
22	B	611	CLA	C4A-NA-C1A	3.65	108.35	106.71
22	c	504	CLA	CHD-C1D-ND	-3.65	121.10	124.45
22	b	607	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
22	a	405	CLA	O2D-CGD-O1D	-3.63	116.73	123.84
22	c	510	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
22	A	402	CLA	C7-C6-C5	-3.61	103.55	113.36
22	b	601	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
24	Z	101	BCR	C15-C16-C17	-3.61	116.08	123.47
29	L	101	SQD	O2-C2-C1	3.61	118.81	110.05
24	C	515	BCR	C2-C1-C6	3.61	116.03	110.48
29	B	623	SQD	O8-S-C6	3.61	111.49	105.74
22	b	610	CLA	CHB-C4A-NA	3.61	129.50	124.51
22	C	510	CLA	CMB-C2B-C3B	3.60	131.41	124.68
22	B	603	CLA	CHD-C1D-ND	-3.60	121.15	124.45
22	B	609	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
24	A	406	BCR	C27-C26-C25	3.59	127.94	122.73
22	B	603	CLA	CMB-C2B-C3B	3.59	131.39	124.68
22	B	609	CLA	O2D-CGD-CBD	3.58	117.64	111.27
28	a	412	LHG	O8-C23-C24	3.58	123.15	111.91
22	B	606	CLA	O1D-CGD-CBD	3.58	131.81	124.48
22	a	403	CLA	CHD-C1D-ND	-3.58	121.17	124.45
24	H	101	BCR	C27-C26-C25	3.57	127.92	122.73
22	b	605	CLA	C4-C3-C5	3.57	121.28	115.27
22	c	509	CLA	CHD-C1D-ND	-3.57	121.17	124.45
24	H	101	BCR	C29-C30-C25	3.57	115.98	110.48
24	B	620	BCR	C29-C30-C25	3.57	115.97	110.48
22	C	502	CLA	C4A-NA-C1A	3.56	108.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	C4A-NA-C1A	3.55	108.30	106.71
33	b	622	LMG	C3-C4-C5	-3.55	103.91	110.24
22	D	402	CLA	CMB-C2B-C3B	3.54	131.30	124.68
22	B	611	CLA	C1B-CHB-C4A	-3.54	123.12	130.12
22	B	613	CLA	O2A-CGA-O1A	-3.53	114.67	123.59
30	C	518	DGD	O2D-C2D-C1D	-3.53	101.47	110.05
22	c	502	CLA	CHD-C1D-ND	-3.53	121.21	124.45
22	c	513	CLA	CHB-C4A-NA	3.53	129.39	124.51
22	b	608	CLA	CHB-C4A-NA	3.52	129.38	124.51
33	B	627	LMG	O7-C10-C11	3.52	119.09	111.50
30	C	519	DGD	O3E-C3E-C2E	-3.52	102.21	110.35
22	B	614	CLA	C1-C2-C3	-3.52	119.96	126.04
22	B	613	CLA	CMB-C2B-C3B	3.51	131.24	124.68
22	C	514	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
22	b	608	CLA	CHD-C1D-ND	-3.50	121.23	124.45
33	d	410	LMG	O1-C1-C2	-3.50	102.84	108.30
22	C	507	CLA	C4A-NA-C1A	3.50	108.28	106.71
22	B	611	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
22	c	501	CLA	CHD-C1D-ND	-3.48	121.25	124.45
27	D	406	PL9	C20-C19-C21	3.48	121.13	115.27
22	A	405	CLA	O2D-CGD-CBD	3.48	117.45	111.27
24	T	101	BCR	C7-C8-C9	-3.47	120.99	126.23
29	a	411	SQD	O47-C7-O49	-3.47	115.32	123.70
22	b	611	CLA	O2D-CGD-CBD	3.47	117.43	111.27
24	c	515	BCR	C2-C1-C6	3.47	115.82	110.48
22	B	614	CLA	C4A-NA-C1A	3.46	108.26	106.71
34	v	201	HEC	C1D-C2D-C3D	-3.46	104.59	107.00
22	B	614	CLA	CMB-C2B-C3B	3.46	131.14	124.68
22	B	616	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
29	a	411	SQD	C1-C2-C3	-3.44	102.83	110.00
26	A	409	BCT	O2-C-O1	3.44	128.47	119.55
22	A	405	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
33	M	101	LMG	O6-C1-O1	-3.44	101.84	109.97
22	C	509	CLA	O2D-CGD-CBD	3.43	117.36	111.27
22	B	604	CLA	CHD-C1D-ND	-3.43	121.30	124.45
24	b	617	BCR	C38-C26-C25	-3.42	120.68	124.53
22	B	605	CLA	C2C-C1C-NC	3.42	113.18	109.97
22	C	504	CLA	C7-C6-C5	-3.42	104.07	113.36
30	h	101	DGD	O3G-C3G-C2G	-3.42	102.65	110.90
22	B	605	CLA	O2D-CGD-CBD	3.42	117.34	111.27
22	c	513	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
33	B	627	LMG	C9-C8-C7	-3.40	103.73	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	PL9	C37-C38-C39	-3.40	119.46	127.66
22	C	503	CLA	C2D-C1D-ND	-3.40	107.60	110.10
22	b	603	CLA	CHD-C1D-ND	-3.40	121.33	124.45
27	A	410	PL9	C40-C39-C41	3.39	120.98	115.27
30	h	101	DGD	O6E-C5E-C4E	3.39	115.86	109.69
22	d	403	CLA	CMB-C2B-C3B	3.39	131.02	124.68
22	C	504	CLA	O2A-C1-C2	-3.39	99.73	108.64
22	C	513	CLA	CMB-C2B-C3B	3.39	131.01	124.68
22	C	505	CLA	O2A-CGA-O1A	-3.39	115.05	123.59
33	c	522	LMG	C1-O6-C5	-3.38	107.05	113.69
29	A	412	SQD	C1-O5-C5	-3.38	107.06	113.69
22	c	512	CLA	C4A-NA-C1A	3.38	108.22	106.71
22	a	403	CLA	CHB-C4A-NA	3.38	129.18	124.51
29	a	411	SQD	C1-O5-C5	-3.37	107.06	113.69
33	Y	101	LMG	O6-C1-O1	-3.37	102.00	109.97
22	b	613	CLA	C4A-NA-C1A	3.37	108.22	106.71
24	H	101	BCR	C38-C26-C25	-3.36	120.75	124.53
22	C	505	CLA	CED-O2D-CGD	3.36	123.54	115.94
29	A	412	SQD	O47-C7-C8	3.36	118.75	111.50
22	b	602	CLA	O2D-CGD-CBD	3.36	117.24	111.27
22	c	506	CLA	CMB-C2B-C3B	3.36	130.96	124.68
22	B	608	CLA	CHB-C4A-NA	3.36	129.15	124.51
22	B	617	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
22	A	403	CLA	O2D-CGD-CBD	3.35	117.21	111.27
22	C	502	CLA	O2A-CGA-O1A	-3.34	115.16	123.59
22	c	506	CLA	C4A-NA-C1A	3.34	108.21	106.71
22	B	605	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
34	v	201	HEC	CMC-C2C-C1C	-3.33	123.35	128.46
22	a	405	CLA	O2D-CGD-CBD	3.33	117.18	111.27
34	e	101	HEC	CBA-CAA-C2A	-3.33	107.00	112.60
29	a	411	SQD	O47-C7-C8	3.33	118.67	111.50
30	c	518	DGD	O5D-C1E-C2E	3.32	113.48	108.30
22	b	601	CLA	CHB-C4A-NA	3.32	129.10	124.51
22	b	609	CLA	CMB-C2B-C3B	3.32	130.88	124.68
23	d	401	PHO	CBA-CAA-C2A	-3.31	104.13	113.81
22	c	511	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
22	a	402	CLA	CMB-C2B-C3B	3.31	130.87	124.68
22	b	612	CLA	CMB-C2B-C3B	3.30	130.86	124.68
22	A	402	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
24	t	101	BCR	C7-C8-C9	-3.29	121.27	126.23
22	C	514	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	b	613	CLA	C1B-CHB-C4A	-3.28	123.62	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	O1D-CGD-CBD	3.28	131.19	124.48
30	C	519	DGD	O3G-C3G-C2G	-3.27	103.00	110.90
22	b	613	CLA	CMB-C2B-C3B	3.27	130.80	124.68
23	a	404	PHO	C1-C2-C3	-3.27	120.39	126.04
22	C	505	CLA	CMB-C2B-C3B	3.26	130.78	124.68
22	B	604	CLA	C16-C15-C13	-3.26	105.38	115.92
29	L	101	SQD	O9-S-O7	-3.26	102.67	113.95
27	d	406	PL9	C40-C39-C41	3.26	120.75	115.27
22	B	611	CLA	O2A-CGA-O1A	-3.25	115.38	123.59
22	c	501	CLA	CED-O2D-CGD	-3.25	108.58	115.94
22	B	609	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
26	a	409	BCT	O3-C-O1	-3.25	111.11	119.55
22	A	403	CLA	CMB-C2B-C3B	3.25	130.76	124.68
22	d	403	CLA	O2D-CGD-CBD	3.25	117.04	111.27
22	B	610	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
22	C	505	CLA	C4-C3-C5	3.25	120.73	115.27
22	C	511	CLA	CMB-C2B-C3B	3.25	130.75	124.68
24	c	514	BCR	C11-C10-C9	-3.25	122.68	127.31
30	C	518	DGD	O5D-C6D-C5D	-3.25	103.04	109.05
22	b	603	CLA	O2D-CGD-CBD	3.24	117.03	111.27
22	C	513	CLA	C1-C2-C3	-3.23	120.45	126.04
22	d	402	CLA	CMB-C2B-C3B	3.23	130.72	124.68
22	C	504	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
33	m	101	LMG	C1-O6-C5	-3.22	107.37	113.69
22	a	402	CLA	C4A-NA-C1A	3.22	108.15	106.71
27	d	406	PL9	C31-C32-C33	-3.21	101.33	111.88
22	c	513	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	b	616	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
22	C	512	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
22	b	611	CLA	C2D-C1D-ND	-3.20	107.75	110.10
28	A	413	LHG	O8-C23-C24	3.20	121.94	111.91
24	c	515	BCR	C27-C26-C25	3.20	127.37	122.73
24	C	501	BCR	C27-C26-C25	3.19	127.36	122.73
22	b	616	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
29	A	412	SQD	O9-S-O7	-3.19	102.92	113.95
24	b	617	BCR	C11-C10-C9	-3.19	122.76	127.31
22	c	505	CLA	CHD-C1D-ND	-3.19	121.53	124.45
22	B	613	CLA	C11-C12-C13	-3.18	105.63	115.92
22	D	403	CLA	CMB-C2B-C3B	3.18	130.62	124.68
22	B	616	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
22	d	404	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
22	B	610	CLA	C2C-C1C-NC	3.17	112.94	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	DGD	O2E-C2E-C1E	-3.16	102.37	110.05
29	L	101	SQD	C3-C4-C5	3.16	115.88	110.24
23	d	401	PHO	CMC-C2C-C3C	3.16	130.89	124.94
22	b	604	CLA	CHB-C4A-NA	3.16	128.88	124.51
24	b	618	BCR	C36-C18-C17	-3.16	118.50	122.92
22	b	605	CLA	CMB-C2B-C3B	3.15	130.58	124.68
23	a	404	PHO	O2D-CGD-CBD	3.15	114.99	111.00
22	c	502	CLA	C4A-NA-C1A	3.15	108.12	106.71
29	L	101	SQD	O48-C23-C24	3.15	121.79	111.91
33	c	519	LMG	O3-C3-C2	-3.14	103.08	110.35
23	A	404	PHO	OBD-CAD-CBD	-3.13	121.23	125.82
24	A	406	BCR	C38-C26-C27	-3.13	107.60	113.62
24	k	103	BCR	C29-C30-C25	3.13	115.30	110.48
23	D	401	PHO	O1D-CGD-CBD	3.12	129.94	124.74
23	a	404	PHO	CMB-C2B-C3B	3.12	130.52	124.68
22	b	613	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
22	b	602	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
22	B	603	CLA	O2D-CGD-CBD	3.12	116.81	111.27
22	a	402	CLA	O2A-CGA-O1A	-3.12	115.72	123.59
22	B	612	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
22	D	402	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
30	c	516	DGD	O6D-C1D-O3G	-3.11	102.61	109.97
30	C	518	DGD	O3G-C1D-C2D	-3.10	103.46	108.30
33	Y	101	LMG	O1-C7-C8	-3.10	103.42	110.90
22	C	509	CLA	CMB-C2B-C3B	3.10	130.48	124.68
22	b	606	CLA	CMB-C2B-C3B	3.10	130.48	124.68
28	L	102	LHG	C20-C19-C18	-3.10	98.69	114.42
22	B	612	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	a	405	CLA	CHB-C4A-NA	3.08	128.78	124.51
30	h	101	DGD	C3G-C2G-C1G	-3.08	104.50	111.79
24	c	515	BCR	C36-C18-C17	-3.08	118.61	122.92
22	c	513	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
24	B	619	BCR	C35-C13-C14	-3.07	118.62	122.92
22	b	605	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
22	B	616	CLA	CHB-C4A-NA	3.07	128.76	124.51
33	m	101	LMG	O1-C7-C8	-3.06	103.50	110.90
22	c	503	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
22	B	605	CLA	CHD-C1D-ND	-3.06	121.64	124.45
22	b	608	CLA	O2D-CGD-CBD	3.06	116.70	111.27
27	d	406	PL9	C36-C34-C33	-3.06	114.93	121.12
24	C	501	BCR	C40-C30-C25	3.05	115.25	110.30
30	C	517	DGD	O5D-C6D-C5D	-3.05	103.40	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	503	CLA	C4-C3-C5	3.05	120.40	115.27
30	C	518	DGD	O3E-C3E-C2E	-3.05	103.30	110.35
22	c	507	CLA	CHD-C1D-ND	-3.04	121.66	124.45
22	C	502	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
24	d	405	BCR	C24-C23-C22	-3.04	121.65	126.23
27	A	410	PL9	C7-C3-C4	3.04	119.34	116.88
22	d	402	CLA	O1D-CGD-CBD	3.03	130.69	124.48
22	B	607	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
22	c	509	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
24	H	101	BCR	C2-C1-C6	3.03	115.14	110.48
22	B	616	CLA	CMB-C2B-C3B	3.03	130.34	124.68
28	D	408	LHG	O8-C23-O10	-3.03	115.95	123.59
22	c	505	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	C	507	CLA	O1D-CGD-CBD	3.03	130.67	124.48
24	C	515	BCR	C15-C16-C17	-3.03	117.28	123.47
30	c	518	DGD	O6E-C5E-C4E	3.02	115.18	109.69
28	D	408	LHG	O8-C23-C24	3.01	121.36	111.91
22	b	611	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	C	513	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
22	b	604	CLA	CAA-CBA-CGA	-3.01	104.47	113.25
24	B	618	BCR	C2-C1-C6	3.01	115.11	110.48
23	a	404	PHO	O2D-CGD-O1D	-3.00	117.97	123.84
29	L	101	SQD	O5-C5-C4	3.00	115.14	109.69
27	a	410	PL9	C27-C28-C29	-3.00	120.43	127.66
24	A	406	BCR	C16-C15-C14	-3.00	117.33	123.47
22	c	508	CLA	CMB-C2B-C3B	3.00	130.29	124.68
23	D	401	PHO	C1-C2-C3	-3.00	120.86	126.04
30	A	415	DGD	C1E-O6E-C5E	3.00	119.57	113.69
24	Z	101	BCR	C11-C10-C9	-2.99	123.04	127.31
22	B	612	CLA	O2D-CGD-CBD	2.99	116.59	111.27
22	B	606	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
27	d	406	PL9	C37-C38-C39	-2.99	120.45	127.66
22	a	402	CLA	O1D-CGD-CBD	2.99	130.60	124.48
24	b	619	BCR	C29-C30-C25	2.99	115.08	110.48
22	B	609	CLA	CMB-C2B-C3B	2.99	130.26	124.68
22	C	512	CLA	C1-C2-C3	-2.98	120.88	126.04
33	c	522	LMG	O6-C1-O1	-2.98	102.92	109.97
22	b	601	CLA	O2D-CGD-CBD	2.97	116.55	111.27
22	c	504	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
22	B	609	CLA	CHD-C1D-ND	-2.97	121.72	124.45
22	c	512	CLA	CHD-C1D-ND	-2.97	121.72	124.45
22	B	608	CLA	C1B-CHB-C4A	-2.97	124.24	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	613	CLA	C1-C2-C3	-2.97	120.91	126.04
22	b	603	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
22	b	610	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
22	b	601	CLA	CHD-C1D-ND	-2.96	121.73	124.45
30	c	516	DGD	O3G-C3G-C2G	-2.96	103.75	110.90
32	C	520	STE	O2-C1-C2	2.96	123.54	114.03
24	t	101	BCR	C34-C9-C10	-2.96	118.78	122.92
22	c	512	CLA	O2A-CGA-O1A	-2.96	116.13	123.59
22	c	513	CLA	CMB-C2B-C3B	2.96	130.21	124.68
22	c	504	CLA	O2D-CGD-CBD	2.95	116.51	111.27
23	d	401	PHO	O1D-CGD-CBD	2.95	129.65	124.74
28	l	101	LHG	O8-C23-O10	-2.95	116.15	123.59
22	b	609	CLA	O1D-CGD-CBD	2.95	130.51	124.48
24	T	101	BCR	C27-C26-C25	2.94	127.00	122.73
22	c	513	CLA	C1-C2-C3	-2.94	120.97	126.04
27	D	406	PL9	C7-C8-C9	-2.94	121.91	126.79
22	B	613	CLA	CHD-C1D-ND	-2.93	121.76	124.45
27	a	410	PL9	C21-C19-C18	-2.93	115.18	121.12
29	A	412	SQD	O5-C1-C2	-2.93	104.15	110.35
22	D	403	CLA	CHB-C4A-NA	2.93	128.56	124.51
22	B	613	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	A	403	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
34	V	201	HEC	C1D-C2D-C3D	-2.92	104.96	107.00
22	d	403	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	a	403	CLA	O2D-CGD-CBD	2.92	116.45	111.27
33	m	101	LMG	O7-C10-O9	-2.91	116.66	123.70
24	Z	101	BCR	C7-C8-C9	-2.91	121.84	126.23
30	A	415	DGD	C4E-C3E-C2E	-2.91	105.74	110.82
22	a	405	CLA	CMB-C2B-C3B	2.91	130.12	124.68
27	D	406	PL9	C40-C39-C41	2.91	120.17	115.27
22	C	503	CLA	C1D-ND-C4D	2.91	108.40	106.33
30	c	517	DGD	O6D-C1D-O3G	-2.91	103.09	109.97
24	k	102	BCR	C38-C26-C25	-2.90	121.27	124.53
22	B	615	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
22	C	510	CLA	CHB-C4A-NA	2.90	128.53	124.51
33	d	410	LMG	O6-C1-O1	-2.90	103.10	109.97
27	d	406	PL9	C7-C3-C2	-2.90	119.49	123.30
30	C	517	DGD	O3E-C3E-C2E	-2.90	103.65	110.35
22	B	603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
30	c	518	DGD	O5E-C6E-C5E	-2.90	101.35	111.29
22	a	403	CLA	C1D-ND-C4D	2.89	108.39	106.33
30	A	415	DGD	O3G-C3G-C2G	-2.89	103.92	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	514	CLA	CMB-C2B-C3B	2.89	130.09	124.68
23	d	401	PHO	CMB-C2B-C3B	2.89	130.08	124.68
22	b	610	CLA	C2C-C1C-NC	2.89	112.68	109.97
24	b	619	BCR	C36-C18-C17	-2.89	118.88	122.92
22	b	605	CLA	CHD-C1D-ND	-2.88	121.80	124.45
24	K	101	BCR	C15-C16-C17	-2.88	117.56	123.47
30	c	517	DGD	O3D-C3D-C4D	-2.88	103.68	110.35
22	b	602	CLA	CHB-C4A-NA	2.88	128.50	124.51
30	H	102	DGD	C1D-C2D-C3D	-2.88	103.99	110.00
24	b	617	BCR	C29-C30-C25	2.88	114.91	110.48
22	b	614	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
29	a	411	SQD	O48-C23-C24	2.88	120.94	111.91
22	b	616	CLA	CHD-C1D-ND	-2.88	121.81	124.45
22	b	602	CLA	C1-C2-C3	-2.87	121.07	126.04
22	B	609	CLA	C4A-NA-C1A	2.87	108.00	106.71
24	k	102	BCR	C27-C26-C25	2.87	126.90	122.73
30	A	415	DGD	O1G-C1A-O1A	-2.87	116.34	123.59
30	A	415	DGD	O5E-C6E-C5E	-2.87	101.45	111.29
30	c	518	DGD	C3D-C4D-C5D	-2.87	105.13	110.24
27	A	410	PL9	C22-C23-C24	-2.86	120.77	127.66
23	d	401	PHO	C1-C2-C3	-2.86	121.09	126.04
22	c	509	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	a	403	CLA	C2D-C1D-ND	-2.85	108.00	110.10
22	A	402	CLA	CAC-C3C-C4C	2.85	128.51	124.81
22	B	610	CLA	O2A-CGA-O1A	-2.85	116.40	123.59
27	d	406	PL9	C22-C23-C24	-2.85	120.80	127.66
24	C	501	BCR	C2-C1-C6	2.85	114.87	110.48
22	b	615	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	b	602	CLA	CMB-C2B-C3B	2.85	130.00	124.68
22	B	607	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
28	D	408	LHG	O7-C7-C8	-2.85	105.37	111.50
33	B	627	LMG	O7-C10-O9	-2.84	116.83	123.70
30	C	519	DGD	C8B-C7B-C6B	-2.84	100.00	114.42
27	D	406	PL9	C30-C29-C31	-2.84	110.49	115.27
22	B	615	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	b	604	CLA	CMA-C3A-C4A	2.84	119.40	111.77
22	C	513	CLA	CHD-C1D-ND	-2.83	121.85	124.45
30	A	415	DGD	O6E-C5E-C4E	2.83	114.84	109.69
22	B	609	CLA	C1D-ND-C4D	-2.83	104.32	106.33
22	b	610	CLA	CAA-CBA-CGA	-2.83	104.98	113.25
22	b	612	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	B	622	LHG	C11-C10-C9	-2.82	100.11	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	613	CLA	O1D-CGD-CBD	2.82	130.25	124.48
22	A	402	CLA	CMB-C2B-C3B	2.82	129.94	124.68
22	D	403	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
22	D	404	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
24	C	515	BCR	C27-C26-C25	2.81	126.81	122.73
24	D	405	BCR	C24-C23-C22	-2.81	121.99	126.23
22	b	604	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
22	C	504	CLA	O1D-CGD-CBD	2.81	130.22	124.48
22	b	604	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
32	B	601	STE	O2-C1-C2	2.80	123.03	114.03
22	b	616	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	c	517	DGD	C6D-O5D-C1E	2.80	119.21	113.74
22	d	404	CLA	CED-O2D-CGD	2.80	122.26	115.94
22	B	606	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
33	d	410	LMG	O6-C5-C4	2.79	114.76	109.69
24	T	101	BCR	C31-C1-C6	2.79	114.82	110.30
22	c	512	CLA	O1D-CGD-CBD	2.79	130.19	124.48
22	C	502	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
33	D	407	LMG	C3-C4-C5	-2.78	105.28	110.24
29	A	412	SQD	O4-C4-C3	-2.78	103.93	110.35
22	B	610	CLA	CMB-C2B-C3B	2.77	129.87	124.68
24	B	618	BCR	C27-C26-C25	2.77	126.76	122.73
22	b	602	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	A	402	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	b	610	CLA	C2D-C1D-ND	2.77	112.14	110.10
30	h	101	DGD	C1E-O6E-C5E	2.77	119.12	113.69
24	Z	101	BCR	C36-C18-C17	-2.76	119.06	122.92
32	t	104	STE	C3-C2-C1	-2.76	107.53	114.47
33	b	622	LMG	O2-C2-C1	-2.75	103.36	110.05
33	M	101	LMG	O7-C10-O9	-2.75	117.06	123.70
22	b	607	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	c	508	CLA	CHB-C4A-NA	2.75	128.31	124.51
30	H	102	DGD	O6D-C1D-O3G	-2.74	103.49	109.97
29	a	413	SQD	C46-C45-C44	-2.74	105.39	111.80
22	C	502	CLA	CHD-C1D-ND	-2.74	121.94	124.45
22	D	403	CLA	C7-C6-C5	-2.74	105.93	113.36
24	t	101	BCR	C1-C6-C5	-2.73	118.76	122.61
34	E	101	HEC	C1D-C2D-C3D	-2.73	105.09	107.00
24	A	406	BCR	C30-C25-C26	-2.73	118.77	122.61
22	C	502	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	b	605	CLA	O1D-CGD-CBD	2.73	130.06	124.48
28	d	407	LHG	O8-C23-C24	2.73	120.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	519	DGD	CAB-C9B-C8B	-2.73	100.59	114.42
30	h	101	DGD	O6D-C1D-O3G	-2.73	103.52	109.97
22	B	605	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	B	603	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
22	d	402	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
28	d	407	LHG	O8-C23-O10	-2.71	116.75	123.59
24	b	619	BCR	C11-C10-C9	-2.71	123.44	127.31
24	c	514	BCR	C15-C16-C17	-2.71	117.92	123.47
22	b	605	CLA	C1-C2-C3	-2.70	121.37	126.04
22	B	608	CLA	C2A-C1A-CHA	2.70	128.59	123.86
30	C	517	DGD	C6D-O5D-C1E	2.70	119.01	113.74
27	a	410	PL9	C20-C19-C21	2.70	119.81	115.27
24	b	617	BCR	C27-C26-C25	2.69	126.64	122.73
33	Y	101	LMG	O7-C10-O9	-2.69	117.19	123.70
22	b	613	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
30	h	101	DGD	O3E-C3E-C2E	-2.69	104.13	110.35
22	B	604	CLA	CHB-C4A-NA	2.69	128.23	124.51
29	a	413	SQD	O49-C7-C8	-2.69	113.25	123.73
29	f	101	SQD	C1-C2-C3	-2.68	104.41	110.00
22	C	513	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	b	602	CLA	C4-C3-C5	2.68	119.78	115.27
22	b	612	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
22	b	612	CLA	CAC-C3C-C4C	2.68	128.28	124.81
22	d	403	CLA	CHD-C1D-C2D	2.68	131.09	125.48
27	d	406	PL9	C30-C29-C31	-2.67	110.77	115.27
22	b	614	CLA	CHB-C4A-NA	2.67	128.21	124.51
27	D	406	PL9	C36-C34-C33	-2.67	115.71	121.12
29	a	413	SQD	O48-C23-O10	-2.67	116.85	123.59
22	C	508	CLA	CAA-CBA-CGA	-2.67	105.45	113.25
22	B	611	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	B	608	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
22	d	402	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
22	B	603	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
28	B	622	LHG	O8-C23-C24	2.67	120.27	111.91
27	A	410	PL9	C36-C37-C38	-2.67	103.12	111.88
23	D	401	PHO	CMB-C2B-C3B	2.66	129.66	124.68
24	B	620	BCR	C1-C6-C5	-2.66	118.87	122.61
29	L	101	SQD	C45-O47-C7	2.66	124.33	117.79
30	H	102	DGD	C1E-O6E-C5E	2.66	118.90	113.69
30	h	101	DGD	C4E-C3E-C2E	-2.65	106.19	110.82
22	C	510	CLA	CHD-C1D-ND	-2.65	122.02	124.45
30	c	517	DGD	O3G-C3G-C2G	-2.65	104.50	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	402	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
22	c	501	CLA	O2D-CGD-CBD	2.65	115.97	111.27
30	C	517	DGD	O6D-C1D-O3G	-2.65	103.70	109.97
24	Z	101	BCR	C33-C5-C6	-2.65	121.56	124.53
22	C	509	CLA	CHD-C1D-ND	-2.65	122.02	124.45
22	B	604	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
22	b	610	CLA	C1D-ND-C4D	-2.65	104.46	106.33
22	b	612	CLA	CHB-C4A-NA	2.64	128.17	124.51
22	c	501	CLA	C2C-C1C-NC	2.64	112.45	109.97
33	c	519	LMG	O8-C28-O10	-2.64	116.92	123.59
24	B	618	BCR	C23-C22-C21	-2.64	114.89	118.94
22	C	503	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
24	B	619	BCR	C15-C14-C13	-2.64	123.54	127.31
22	c	501	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
29	L	101	SQD	O5-C1-C2	-2.64	104.77	110.35
29	B	623	SQD	C46-C45-C44	-2.64	105.56	111.79
24	A	406	BCR	C2-C1-C6	2.63	114.54	110.48
22	b	603	CLA	C4A-NA-C1A	2.63	107.89	106.71
22	b	611	CLA	CMB-C2B-C3B	2.63	129.60	124.68
30	C	518	DGD	CDB-CCB-CBB	-2.63	101.06	114.42
24	x	101	BCR	C27-C26-C25	2.63	126.55	122.73
32	C	520	STE	O2-C1-O1	-2.63	116.75	123.30
22	c	509	CLA	CHB-C4A-NA	2.62	128.14	124.51
29	B	623	SQD	O9-S-C6	2.62	110.05	106.94
24	Z	101	BCR	C2-C1-C6	2.62	114.51	110.48
22	b	602	CLA	CAC-C3C-C4C	2.62	128.21	124.81
22	B	617	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
22	b	607	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
30	C	519	DGD	O6D-C1D-O3G	-2.62	103.78	109.97
22	A	403	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
28	d	407	LHG	C11-C10-C9	-2.62	101.14	114.42
24	A	406	BCR	C40-C30-C25	2.61	114.54	110.30
27	d	406	PL9	C50-C49-C48	-2.61	115.10	122.65
22	A	405	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	C	505	CLA	C2D-C1D-ND	-2.61	108.18	110.10
23	d	401	PHO	O2D-CGD-O1D	-2.61	118.74	123.84
22	b	609	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
29	f	101	SQD	C44-O6-C1	2.61	118.83	113.74
22	B	617	CLA	CHD-C1D-ND	-2.61	122.06	124.45
22	B	604	CLA	C2D-C1D-ND	-2.61	108.18	110.10
24	Z	101	BCR	C29-C30-C25	2.60	114.49	110.48
29	B	623	SQD	C3-C4-C5	2.60	114.88	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	507	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
29	a	411	SQD	O9-S-O7	-2.60	104.94	113.95
30	A	415	DGD	C3E-C4E-C5E	-2.60	105.60	110.24
23	A	404	PHO	CMB-C2B-C3B	2.60	129.54	124.68
33	c	521	LMG	C6-C5-C4	-2.60	106.92	113.00
22	b	610	CLA	CHA-C1A-NA	-2.60	120.45	126.40
24	B	619	BCR	C2-C1-C6	2.60	114.48	110.48
22	B	609	CLA	CHA-C1A-NA	-2.60	120.45	126.40
22	B	603	CLA	C16-C15-C13	-2.59	107.53	115.92
22	B	612	CLA	CHB-C4A-NA	2.59	128.10	124.51
28	A	411	LHG	O8-C23-C24	2.59	120.05	111.91
29	f	101	SQD	O5-C1-C2	-2.59	104.86	110.35
27	A	410	PL9	O2-C1-C2	-2.59	115.84	121.78
22	C	514	CLA	C2D-C1D-ND	-2.59	108.19	110.10
29	A	412	SQD	O47-C7-O49	-2.59	117.44	123.70
22	c	512	CLA	C2D-C1D-ND	-2.59	108.20	110.10
22	C	502	CLA	O2D-CGD-CBD	2.59	115.86	111.27
22	B	607	CLA	CMB-C2B-C3B	2.59	129.51	124.68
22	b	614	CLA	CHD-C1D-ND	-2.58	122.08	124.45
22	a	405	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
22	b	613	CLA	C2C-C1C-NC	2.58	112.39	109.97
22	C	514	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
22	A	405	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
33	d	410	LMG	O7-C10-O9	-2.58	117.47	123.70
24	x	101	BCR	C16-C15-C14	-2.57	118.20	123.47
22	b	614	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
34	v	201	HEC	CMB-C2B-C1B	-2.57	124.51	128.46
24	B	620	BCR	C33-C5-C6	-2.57	121.64	124.53
27	A	410	PL9	O1-C4-C3	-2.57	117.89	120.72
24	c	514	BCR	C35-C13-C14	-2.57	119.33	122.92
22	B	617	CLA	O2D-CGD-CBD	2.57	115.83	111.27
33	c	521	LMG	O1-C1-C2	-2.57	104.30	108.30
22	D	402	CLA	CED-O2D-CGD	2.56	121.74	115.94
22	B	610	CLA	CHA-C1A-NA	-2.56	120.53	126.40
33	c	522	LMG	O8-C28-O10	-2.56	117.12	123.59
22	c	512	CLA	CHC-C1C-NC	2.56	128.09	124.20
30	C	518	DGD	C1D-O6D-C5D	-2.56	108.66	113.69
29	f	101	SQD	O47-C7-C8	2.56	117.94	110.80
22	c	509	CLA	CMB-C2B-C3B	2.56	129.46	124.68
22	b	605	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	c	509	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
24	d	405	BCR	C27-C26-C25	2.55	126.44	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	x	101	BCR	C37-C22-C21	-2.55	119.35	122.92
22	B	604	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
24	A	406	BCR	C15-C16-C17	-2.55	118.25	123.47
28	B	622	LHG	O8-C23-O10	-2.55	117.16	123.59
22	a	403	CLA	CHD-C1D-C2D	2.55	130.83	125.48
22	a	403	CLA	C2A-C1A-CHA	2.55	128.31	123.86
22	d	403	CLA	C1D-ND-C4D	2.55	108.14	106.33
30	h	101	DGD	C3D-C4D-C5D	-2.55	105.70	110.24
27	A	410	PL9	O2-C1-C6	2.54	125.00	120.59
24	C	501	BCR	C38-C26-C27	-2.54	108.73	113.62
24	Z	101	BCR	C38-C26-C25	-2.54	121.67	124.53
24	K	101	BCR	C27-C26-C25	2.54	126.42	122.73
24	b	617	BCR	C29-C28-C27	2.54	117.06	111.38
22	C	506	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	c	502	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
33	M	101	LMG	C38-C37-C36	-2.54	101.53	114.42
23	d	401	PHO	C1B-NB-C4B	2.54	112.31	107.09
22	C	514	CLA	O1D-CGD-CBD	2.54	129.68	124.48
27	D	406	PL9	O2-C1-C2	-2.54	115.96	121.78
33	C	516	LMG	O6-C1-O1	-2.54	103.97	109.97
22	b	604	CLA	CHD-C1D-ND	-2.53	122.13	124.45
24	Z	101	BCR	C36-C18-C19	2.53	122.06	118.08
30	c	516	DGD	CCB-CBB-CAB	-2.53	101.59	114.42
30	A	415	DGD	CDB-CCB-CBB	-2.53	101.60	114.42
22	D	404	CLA	CED-O2D-CGD	2.53	121.65	115.94
22	B	614	CLA	CHA-C1A-NA	-2.53	120.61	126.40
22	b	612	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
22	c	503	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
24	D	405	BCR	C2-C1-C6	2.52	114.36	110.48
22	B	607	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
24	H	101	BCR	C30-C25-C26	-2.52	119.07	122.61
22	B	617	CLA	CAA-CBA-CGA	-2.52	105.90	113.25
33	D	407	LMG	O2-C2-C1	-2.51	103.94	110.05
22	b	604	CLA	CMB-C2B-C3B	2.51	129.38	124.68
24	k	103	BCR	C11-C10-C9	-2.51	123.73	127.31
28	d	408	LHG	C5-O7-C7	-2.51	111.62	117.79
30	c	516	DGD	O1G-C1A-C2A	-2.50	104.05	111.91
28	d	407	LHG	O7-C7-C8	-2.50	106.11	111.50
28	a	412	LHG	C11-C10-C9	-2.50	101.74	114.42
22	d	404	CLA	O2A-C1-C2	-2.50	102.07	108.64
22	c	510	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
23	A	404	PHO	C4-C3-C2	-2.50	117.27	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c	521	LMG	O2-C2-C1	-2.50	103.98	110.05
22	B	612	CLA	C1-C2-C3	-2.49	121.73	126.04
22	B	611	CLA	C1-C2-C3	-2.49	121.73	126.04
27	a	410	PL9	C22-C23-C24	-2.49	121.66	127.66
30	C	519	DGD	C4D-C3D-C2D	-2.49	106.47	110.82
33	Y	101	LMG	C7-O1-C1	2.49	118.61	113.74
22	c	503	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	A	405	CLA	C1D-CHD-C4C	-2.49	120.69	126.06
24	C	515	BCR	C34-C9-C10	-2.49	119.44	122.92
22	C	503	CLA	C2A-C1A-CHA	2.49	128.21	123.86
27	A	410	PL9	C40-C39-C38	-2.48	117.30	123.68
30	C	518	DGD	C6D-O5D-C1E	2.48	118.59	113.74
27	a	410	PL9	O2-C1-C2	-2.48	116.09	121.78
24	C	515	BCR	C33-C5-C6	-2.48	121.74	124.53
22	B	607	CLA	O2D-CGD-CBD	2.48	115.68	111.27
22	A	402	CLA	CHC-C1C-NC	2.48	127.97	124.20
30	C	519	DGD	O2E-C2E-C3E	-2.48	104.61	110.35
22	C	508	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
24	d	405	BCR	C33-C5-C6	-2.48	121.75	124.53
32	b	621	STE	O2-C1-O1	-2.48	117.12	123.30
22	C	503	CLA	CMA-C3A-C4A	2.48	118.43	111.77
27	D	406	PL9	O2-C1-C6	2.48	124.88	120.59
22	C	503	CLA	CAC-C3C-C4C	2.47	128.02	124.81
22	c	510	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
22	b	610	CLA	C2A-C1A-CHA	2.47	128.18	123.86
22	c	512	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
22	B	604	CLA	CHD-C4C-NC	2.47	128.09	124.20
22	C	503	CLA	CHA-C1A-NA	-2.47	120.75	126.40
23	a	404	PHO	C5-C3-C2	2.47	126.11	121.12
30	c	517	DGD	C3E-C4E-C5E	-2.47	105.84	110.24
22	B	617	CLA	CMB-C2B-C3B	2.47	129.29	124.68
22	b	611	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
32	D	411	STE	O2-C1-O1	-2.46	117.16	123.30
27	d	406	PL9	C41-C39-C38	-2.46	116.13	121.12
33	B	627	LMG	O5-C6-C5	-2.46	102.85	111.29
24	k	103	BCR	C27-C26-C25	2.46	126.30	122.73
22	B	607	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	D	402	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
29	F	101	SQD	O48-C23-O10	-2.46	117.39	123.59
30	c	518	DGD	O6D-C1D-O3G	-2.46	104.16	109.97
22	a	403	CLA	C3C-C4C-NC	-2.45	107.82	110.57
29	a	411	SQD	O8-S-O9	-2.45	105.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	408	LHG	C18-C17-C16	-2.45	101.97	114.42
30	c	517	DGD	CDB-CCB-CBB	-2.45	101.99	114.42
22	B	612	CLA	CHD-C4C-NC	2.45	128.06	124.20
22	C	514	CLA	O2A-C1-C2	-2.45	102.21	108.64
22	B	617	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	C	506	CLA	O1D-CGD-CBD	2.44	129.49	124.48
22	D	403	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	B	606	CLA	CAA-CBA-CGA	-2.44	106.12	113.25
22	B	613	CLA	CHB-C4A-NA	2.44	127.88	124.51
27	a	410	PL9	C35-C34-C36	2.44	119.37	115.27
24	B	618	BCR	C30-C25-C26	-2.44	119.18	122.61
22	b	605	CLA	CHC-C1C-NC	2.43	127.90	124.20
22	B	612	CLA	C5-C3-C2	2.43	126.04	121.12
22	C	507	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
23	d	401	PHO	C4A-C3A-C2A	-2.43	100.52	102.84
27	D	406	PL9	C40-C39-C38	-2.43	117.44	123.68
22	b	613	CLA	C7-C6-C5	-2.43	106.76	113.36
24	c	514	BCR	C3-C4-C5	-2.43	109.74	114.08
30	c	516	DGD	O4D-C4D-C5D	-2.43	103.27	109.30
22	B	610	CLA	O2D-CGD-CBD	2.42	115.58	111.27
22	b	611	CLA	CHD-C1D-C2D	2.42	130.56	125.48
22	b	610	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
27	D	406	PL9	C31-C32-C33	-2.42	103.91	111.88
22	b	604	CLA	CHC-C1C-NC	2.42	127.88	124.20
32	c	520	STE	C3-C2-C1	-2.42	108.37	114.47
30	H	102	DGD	C6B-C5B-C4B	-2.42	102.14	114.42
22	c	506	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
22	A	405	CLA	C2C-C1C-NC	2.42	112.24	109.97
23	D	401	PHO	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	604	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
22	B	608	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	a	402	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	b	614	CLA	O1D-CGD-CBD	2.41	129.41	124.48
22	c	508	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
22	c	504	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	D	404	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	C	507	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	A	404	PHO	O2A-CGA-O1A	-2.41	117.52	123.59
28	l	101	LHG	C27-C26-C25	-2.41	102.21	114.42
30	c	516	DGD	C4A-C3A-C2A	-2.40	104.56	113.19
22	C	505	CLA	O2D-CGD-CBD	2.40	115.54	111.27
22	B	610	CLA	C7-C6-C5	-2.40	106.84	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	f	101	SQD	O5-C5-C4	2.40	114.06	109.69
23	D	401	PHO	CMC-C2C-C3C	2.40	129.47	124.94
22	c	506	CLA	O1D-CGD-CBD	2.40	129.39	124.48
24	k	103	BCR	C2-C1-C6	2.40	114.17	110.48
22	B	602	CLA	CHD-C1D-ND	-2.40	122.25	124.45
22	c	510	CLA	O1D-CGD-CBD	2.39	129.38	124.48
29	a	411	SQD	O9-S-C6	2.39	109.78	106.94
22	D	402	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	D	406	PL9	C11-C12-C13	-2.39	104.02	111.88
22	B	607	CLA	C3B-C4B-NB	-2.39	106.12	109.21
29	F	101	SQD	O2-C2-C3	2.39	115.88	110.35
22	B	617	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	x	101	BCR	C36-C18-C17	-2.39	119.58	122.92
24	H	101	BCR	C16-C15-C14	-2.39	118.59	123.47
22	C	507	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	b	614	CLA	CBC-CAC-C3C	-2.39	105.86	112.43
22	c	511	CLA	CHD-C1D-ND	-2.39	122.26	124.45
22	B	607	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
32	L	103	STE	O2-C1-C2	2.38	121.68	114.03
22	c	507	CLA	CHD-C4C-NC	2.38	127.95	124.20
22	B	604	CLA	CHD-C1D-C2D	2.38	130.47	125.48
33	m	101	LMG	C38-C37-C36	-2.38	102.35	114.42
22	B	614	CLA	CAC-C3C-C4C	2.38	127.89	124.81
22	c	508	CLA	O2A-CGA-O1A	-2.38	117.60	123.59
22	c	512	CLA	C3C-C4C-NC	-2.37	107.91	110.57
22	b	609	CLA	C5-C3-C2	2.37	125.92	121.12
30	c	517	DGD	C1E-O6E-C5E	2.37	118.34	113.69
22	c	507	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	b	618	BCR	C37-C22-C21	-2.37	119.60	122.92
22	B	616	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
22	C	504	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	A	406	BCR	C36-C18-C17	-2.37	119.61	122.92
22	b	609	CLA	CED-O2D-CGD	2.37	121.29	115.94
29	f	101	SQD	C45-O47-C7	2.37	123.62	117.79
22	b	611	CLA	C3C-C4C-NC	-2.37	107.92	110.57
22	B	614	CLA	CHD-C1D-ND	-2.36	122.28	124.45
22	B	605	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
27	D	406	PL9	C22-C23-C24	-2.36	121.98	127.66
22	a	405	CLA	CMD-C2D-C3D	2.36	133.04	127.61
29	L	101	SQD	O47-C7-O49	-2.36	118.00	123.70
27	d	406	PL9	C26-C27-C28	-2.36	104.13	111.88
27	d	406	PL9	C8-C7-C3	2.36	118.64	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406	BCR	C2-C1-C6	2.36	114.11	110.48
22	b	611	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
22	A	403	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	b	618	BCR	C30-C25-C26	-2.36	119.30	122.61
24	T	101	BCR	C1-C6-C5	-2.35	119.30	122.61
33	Y	101	LMG	O8-C28-O10	-2.35	117.65	123.59
24	D	405	BCR	C8-C7-C6	-2.35	120.59	127.20
22	B	612	CLA	CMB-C2B-C3B	2.35	129.08	124.68
22	C	502	CLA	C2D-C1D-ND	-2.35	108.37	110.10
23	D	401	PHO	CMD-C2D-C3D	2.35	129.07	124.68
33	m	101	LMG	O8-C28-O10	-2.35	117.67	123.59
22	c	506	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
24	B	620	BCR	C30-C25-C26	-2.35	119.31	122.61
30	A	415	DGD	CBB-CAB-C9B	-2.34	102.53	114.42
32	t	102	STE	O2-C1-C2	2.34	121.54	114.03
30	A	415	DGD	O2D-C2D-C1D	-2.34	104.37	110.05
22	B	606	CLA	C14-C13-C15	-2.34	102.83	111.29
33	Y	101	LMG	O2-C2-C1	-2.33	104.38	110.05
22	B	610	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
22	c	513	CLA	O1D-CGD-CBD	2.33	129.25	124.48
29	a	413	SQD	O48-C23-C24	2.33	119.22	111.91
22	B	614	CLA	O2A-C1-C2	-2.33	102.52	108.64
29	f	101	SQD	C3-C4-C5	2.33	114.39	110.24
24	b	618	BCR	C11-C10-C9	-2.33	123.99	127.31
24	a	406	BCR	C35-C13-C14	-2.33	119.67	122.92
22	b	613	CLA	CHD-C1D-ND	-2.33	122.32	124.45
22	b	606	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
22	B	616	CLA	CHD-C1D-ND	-2.32	122.32	124.45
32	D	411	STE	O2-C1-C2	2.32	121.49	114.03
22	a	403	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	b	616	CLA	O1D-CGD-CBD	2.32	129.23	124.48
22	a	402	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	B	616	CLA	O1D-CGD-CBD	2.32	129.22	124.48
22	C	505	CLA	CHA-C1A-NA	-2.32	121.09	126.40
33	Y	101	LMG	C38-C37-C36	-2.31	102.68	114.42
33	b	622	LMG	O8-C28-O10	-2.31	117.76	123.59
22	B	606	CLA	C2C-C1C-NC	2.31	112.14	109.97
28	D	408	LHG	C20-C19-C18	-2.31	102.69	114.42
22	C	514	CLA	O2D-CGD-CBD	2.31	115.37	111.27
32	d	411	STE	O2-C1-C2	2.31	121.45	114.03
22	c	511	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
24	b	617	BCR	C8-C7-C6	-2.30	120.73	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	BCR	C24-C23-C22	-2.30	122.75	126.23
22	C	508	CLA	CHD-C1D-ND	-2.30	122.34	124.45
24	t	101	BCR	C27-C26-C25	2.30	126.07	122.73
22	c	507	CLA	CAA-CBA-CGA	-2.30	106.54	113.25
30	c	517	DGD	CBB-CAB-C9B	-2.30	102.76	114.42
22	d	402	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
24	D	405	BCR	C27-C26-C25	2.30	126.06	122.73
22	B	609	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	b	606	CLA	CHD-C1D-ND	-2.30	122.34	124.45
30	h	101	DGD	CDB-CCB-CBB	-2.30	102.77	114.42
28	A	411	LHG	O3-P-O5	-2.29	100.10	109.07
30	c	518	DGD	CDB-CCB-CBB	-2.29	102.78	114.42
24	A	406	BCR	C8-C7-C6	-2.29	120.76	127.20
27	D	406	PL9	C35-C34-C36	2.29	119.13	115.27
29	a	413	SQD	O47-C45-C44	2.29	116.58	108.36
29	F	101	SQD	O5-C5-C4	2.29	113.86	109.69
22	C	512	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
24	B	618	BCR	C33-C5-C6	-2.29	121.96	124.53
22	B	610	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
27	a	410	PL9	O2-C1-C6	2.29	124.56	120.59
22	b	601	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
24	B	618	BCR	C3-C4-C5	-2.29	109.99	114.08
22	c	508	CLA	O2D-CGD-CBD	2.29	115.33	111.27
22	b	606	CLA	CHD-C4C-NC	2.29	127.81	124.20
30	h	101	DGD	C7B-C6B-C5B	-2.28	102.83	114.42
33	b	622	LMG	O1-C1-C2	-2.28	104.74	108.30
22	c	511	CLA	C3C-C4C-NC	-2.28	108.01	110.57
24	k	102	BCR	C30-C25-C26	-2.28	119.40	122.61
22	B	605	CLA	O2A-C1-C2	2.28	114.62	108.64
22	b	608	CLA	C1-O2A-CGA	2.28	122.42	116.44
24	B	619	BCR	C15-C16-C17	-2.28	118.81	123.47
34	E	101	HEC	CMC-C2C-C1C	-2.27	124.97	128.46
24	B	620	BCR	C8-C9-C10	-2.27	115.45	118.94
22	b	603	CLA	C3B-C4B-NB	-2.27	106.27	109.21
22	b	603	CLA	C2D-C1D-ND	-2.27	108.43	110.10
29	A	412	SQD	O2-C2-C1	2.27	115.56	110.05
22	C	512	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
24	B	620	BCR	C32-C1-C6	-2.27	106.62	110.30
24	b	617	BCR	C36-C18-C17	-2.27	119.74	122.92
29	f	101	SQD	O48-C23-C24	2.27	119.03	111.91
33	D	407	LMG	O4-C4-C5	2.27	114.93	109.30
22	b	614	CLA	CMB-C2B-C3B	2.27	128.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C15-C14-C13	-2.27	124.08	127.31
32	D	411	STE	C3-C2-C1	-2.27	108.76	114.47
29	B	623	SQD	O48-C23-O10	-2.27	117.87	123.59
22	C	506	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
22	d	403	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	d	402	CLA	C4-C3-C5	2.26	119.08	115.27
28	B	622	LHG	C18-C17-C16	-2.26	102.95	114.42
22	b	604	CLA	C11-C12-C13	-2.26	108.61	115.92
22	b	603	CLA	CHD-C1D-C2D	2.26	130.22	125.48
22	C	504	CLA	C3A-C2A-C1A	2.26	104.72	101.34
22	b	605	CLA	O1A-CGA-CBA	2.26	132.53	123.73
22	C	513	CLA	O2D-CGD-CBD	2.26	115.28	111.27
22	B	603	CLA	C11-C12-C13	-2.26	108.63	115.92
22	C	509	CLA	CHB-C4A-NA	2.25	127.63	124.51
33	c	521	LMG	C9-C8-C7	-2.25	106.46	111.79
22	B	607	CLA	CED-O2D-CGD	2.25	121.03	115.94
22	c	503	CLA	C6-C5-C3	2.25	119.36	113.45
22	c	502	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
22	b	612	CLA	C4A-NA-C1A	2.25	107.72	106.71
32	x	102	STE	C3-C2-C1	-2.25	108.80	114.47
28	B	622	LHG	O3-P-O5	-2.25	100.28	109.07
22	c	505	CLA	C11-C10-C8	-2.25	108.65	115.92
33	C	516	LMG	C9-C8-C7	-2.25	106.47	111.79
30	h	101	DGD	CBB-CAB-C9B	-2.25	103.02	114.42
22	c	501	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	B	612	CLA	C2D-C1D-ND	-2.24	108.45	110.10
30	C	518	DGD	O6D-C1D-O3G	-2.24	104.66	109.97
24	d	405	BCR	C2-C1-C6	2.24	113.94	110.48
22	C	503	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
23	A	404	PHO	CMC-C2C-C3C	2.24	129.17	124.94
30	c	518	DGD	C1D-C2D-C3D	-2.24	105.33	110.00
22	C	504	CLA	CMD-C2D-C3D	2.24	132.77	127.61
32	B	621	STE	O2-C1-C2	2.24	121.23	114.03
24	c	514	BCR	C38-C26-C25	-2.24	122.01	124.53
23	a	404	PHO	C6-C5-C3	2.24	119.32	113.45
22	b	612	CLA	C9-C8-C10	-2.24	103.19	111.29
22	b	607	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
22	B	617	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
22	b	609	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
30	A	415	DGD	C3G-C2G-C1G	-2.23	106.50	111.79
24	d	405	BCR	C8-C7-C6	-2.23	120.93	127.20
22	B	608	CLA	CAC-C3C-C4C	2.23	127.71	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	M	101	LMG	C4-C3-C2	-2.23	106.93	110.82
22	a	402	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
22	C	512	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	b	619	BCR	C16-C15-C14	-2.23	118.91	123.47
24	d	405	BCR	C16-C15-C14	-2.23	118.91	123.47
24	c	514	BCR	C27-C26-C25	2.23	125.97	122.73
22	b	609	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	A	403	CLA	CAC-C3C-C4C	2.23	127.70	124.81
30	h	101	DGD	O2E-C2E-C3E	-2.23	105.20	110.35
22	b	614	CLA	CAA-C2A-C3A	2.23	118.88	112.78
28	l	101	LHG	O8-C23-C24	2.23	118.90	111.91
22	c	506	CLA	CHB-C4A-NA	2.23	127.59	124.51
22	C	503	CLA	CMB-C2B-C3B	2.23	128.84	124.68
30	H	102	DGD	C3E-C4E-C5E	-2.23	106.27	110.24
27	d	406	PL9	C12-C13-C14	-2.22	122.30	127.66
22	a	403	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
22	D	404	CLA	CGD-CBD-CAD	-2.22	103.54	110.73
22	B	605	CLA	C1-O2A-CGA	-2.22	110.62	116.44
30	c	516	DGD	O6E-C5E-C4E	2.22	113.73	109.69
24	t	101	BCR	C38-C26-C27	-2.22	109.35	113.62
22	d	402	CLA	CMD-C2D-C1D	2.22	128.62	124.71
22	c	505	CLA	CHD-C4C-NC	2.22	127.70	124.20
29	F	101	SQD	C44-O6-C1	2.22	117.52	113.84
27	A	410	PL9	C11-C12-C13	-2.21	104.60	111.88
22	b	614	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
22	b	603	CLA	C3C-C4C-NC	-2.21	108.09	110.57
22	d	403	CLA	CAC-C3C-C4C	2.21	127.68	124.81
22	b	614	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	A	406	BCR	C34-C9-C8	-2.21	114.59	118.08
24	A	406	BCR	C33-C5-C6	-2.21	122.05	124.53
33	d	410	LMG	C3-C4-C5	-2.21	106.30	110.24
22	B	614	CLA	C11-C10-C8	-2.21	108.78	115.92
24	k	103	BCR	C8-C7-C6	-2.21	121.00	127.20
22	b	615	CLA	C1-O2A-CGA	2.21	122.23	116.44
22	C	511	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
22	D	403	CLA	C2C-C1C-NC	2.20	112.03	109.97
22	C	512	CLA	O2D-CGD-CBD	2.20	115.18	111.27
30	H	102	DGD	C8B-C7B-C6B	-2.20	103.25	114.42
30	h	101	DGD	C1D-C2D-C3D	-2.20	105.42	110.00
22	A	402	CLA	CED-O2D-CGD	2.20	120.91	115.94
24	b	619	BCR	C38-C26-C25	-2.20	122.06	124.53
29	a	411	SQD	C3-C4-C5	2.20	114.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	602	CLA	C14-C13-C15	-2.20	103.33	111.29
33	c	519	LMG	C9-C8-C7	-2.20	106.59	111.79
22	b	604	CLA	CMD-C2D-C3D	2.20	132.67	127.61
33	M	101	LMG	C3-C4-C5	-2.20	106.32	110.24
22	B	610	CLA	C1D-ND-C4D	-2.19	104.78	106.33
24	x	101	BCR	C33-C5-C6	-2.19	122.06	124.53
33	M	101	LMG	O5-C6-C5	-2.19	103.76	111.29
22	c	512	CLA	CHD-C1D-C2D	2.19	130.08	125.48
30	C	517	DGD	O2D-C2D-C1D	-2.19	104.73	110.05
29	A	412	SQD	O5-C5-C4	2.19	113.67	109.69
33	D	407	LMG	O8-C28-O10	-2.19	118.07	123.59
22	C	502	CLA	OBD-CAD-C3D	2.19	133.78	128.52
23	d	401	PHO	CAA-CBA-CGA	-2.18	106.87	113.25
22	d	404	CLA	CHA-C1A-NA	-2.18	121.39	126.40
30	c	516	DGD	O6E-C1E-O5D	-2.18	104.80	109.97
29	a	413	SQD	C45-O47-C7	2.18	123.17	117.79
24	k	102	BCR	C33-C5-C6	-2.18	122.08	124.53
33	M	101	LMG	C31-C30-C29	-2.18	105.35	113.19
24	b	617	BCR	C3-C4-C5	-2.18	110.18	114.08
22	c	511	CLA	CMB-C2B-C3B	2.18	128.76	124.68
24	C	515	BCR	C38-C26-C25	-2.18	122.08	124.53
22	C	508	CLA	CMB-C2B-C3B	2.18	128.76	124.68
22	b	607	CLA	CHD-C1D-ND	-2.18	122.45	124.45
22	C	511	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	C	503	CLA	C4D-CHA-C1A	2.18	123.90	121.25
33	b	622	LMG	O5-C6-C5	-2.18	103.82	111.29
22	C	513	CLA	C6-C5-C3	-2.18	107.75	113.45
22	b	613	CLA	CAA-CBA-CGA	2.17	119.61	113.25
22	C	508	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
23	A	404	PHO	C1-C2-C3	-2.17	122.29	126.04
24	B	619	BCR	C32-C1-C6	-2.17	106.78	110.30
22	C	502	CLA	CMB-C2B-C3B	2.17	128.74	124.68
30	C	518	DGD	C4E-C3E-C2E	-2.17	107.03	110.82
27	A	410	PL9	C31-C29-C28	2.17	125.51	121.12
34	E	101	HEC	O2D-CGD-CBD	2.17	121.00	114.03
24	B	618	BCR	C15-C16-C17	-2.17	119.03	123.47
27	D	406	PL9	C42-C43-C44	-2.17	122.44	127.66
22	c	503	CLA	CHD-C1D-ND	-2.17	122.46	124.45
24	d	405	BCR	C38-C26-C25	-2.16	122.10	124.53
22	b	607	CLA	O1A-CGA-CBA	2.16	132.18	123.73
22	c	502	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
22	C	505	CLA	CHA-C4D-ND	2.16	137.02	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	609	CLA	C1D-ND-C4D	-2.16	104.80	106.33
30	H	102	DGD	O2D-C2D-C1D	-2.16	104.80	110.05
24	Z	101	BCR	C3-C4-C5	-2.16	110.22	114.08
30	A	415	DGD	CGB-CFB-CEB	-2.16	103.48	114.42
24	a	406	BCR	C28-C27-C26	-2.16	110.23	114.08
30	H	102	DGD	O5D-C1E-C2E	2.16	111.67	108.30
22	C	512	CLA	C4-C3-C5	2.15	118.89	115.27
28	A	413	LHG	O8-C23-O10	-2.15	118.16	123.59
33	c	522	LMG	O6-C1-C2	-2.15	105.79	110.35
22	D	402	CLA	C6-C5-C3	2.15	119.10	113.45
22	c	504	CLA	C1-O2A-CGA	2.15	122.09	116.44
22	c	511	CLA	CHD-C4C-NC	2.15	127.59	124.20
29	a	411	SQD	C18-C17-C16	-2.15	103.52	114.42
22	C	502	CLA	C4-C3-C5	2.15	118.88	115.27
22	C	513	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	C	511	CLA	O2D-CGD-CBD	2.15	115.08	111.27
24	a	406	BCR	C27-C26-C25	2.15	125.85	122.73
24	b	619	BCR	C24-C23-C22	-2.15	122.99	126.23
23	a	404	PHO	OBD-CAD-CBD	-2.15	122.68	125.82
30	h	101	DGD	O6E-C1E-O5D	-2.15	104.89	109.97
27	A	410	PL9	C12-C13-C14	-2.14	122.50	127.66
29	A	414	SQD	O48-C23-O10	-2.14	118.18	123.59
22	C	513	CLA	C2A-C3A-C4A	2.14	105.33	101.87
22	B	603	CLA	CHC-C1C-NC	2.14	127.45	124.20
22	b	613	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
33	c	522	LMG	O5-C6-C5	-2.14	103.94	111.29
27	D	406	PL9	C32-C33-C34	-2.14	122.50	127.66
30	c	516	DGD	C3E-C4E-C5E	-2.14	106.42	110.24
22	c	502	CLA	C1-O2A-CGA	2.14	122.06	116.44
22	b	612	CLA	CMD-C2D-C3D	2.14	132.54	127.61
27	A	410	PL9	C27-C28-C29	-2.14	122.51	127.66
22	d	403	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
22	D	404	CLA	CAC-C3C-C4C	2.14	127.58	124.81
27	d	406	PL9	C7-C8-C9	-2.14	123.23	126.79
22	C	502	CLA	CHD-C4C-NC	2.14	127.57	124.20
22	b	603	CLA	CHD-C4C-NC	2.13	127.57	124.20
33	C	516	LMG	O8-C28-O10	-2.13	118.20	123.59
22	c	508	CLA	CHD-C4C-NC	2.13	127.56	124.20
22	c	503	CLA	CAC-C3C-C4C	2.13	127.58	124.81
22	b	605	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
33	D	407	LMG	O1-C7-C8	-2.13	105.76	110.90
22	A	402	CLA	CHD-C1D-ND	-2.13	122.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	BCR	C8-C7-C6	-2.13	121.22	127.20
22	b	615	CLA	CHD-C4C-C3C	-2.13	121.71	124.84
22	B	606	CLA	CMB-C2B-C3B	2.13	128.66	124.68
22	b	608	CLA	CHA-C1A-NA	-2.13	121.53	126.40
32	b	621	STE	O2-C1-C2	2.13	120.86	114.03
33	d	410	LMG	C40-C39-C38	-2.13	103.63	114.42
22	c	502	CLA	CHD-C1D-C2D	2.12	129.94	125.48
34	E	101	HEC	O1D-CGD-CBD	-2.12	116.26	123.08
28	A	413	LHG	C20-C19-C18	-2.12	103.65	114.42
24	b	618	BCR	C36-C18-C19	2.12	121.42	118.08
22	b	605	CLA	CHA-C1A-NA	-2.12	121.54	126.40
28	D	408	LHG	C17-C16-C15	-2.12	103.66	114.42
22	c	503	CLA	C3B-C4B-NB	-2.12	106.47	109.21
22	C	505	CLA	CHD-C1D-ND	-2.12	122.51	124.45
28	A	413	LHG	C11-C10-C9	-2.12	103.69	114.42
22	C	509	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	c	510	CLA	O2A-C1-C2	-2.11	103.08	108.64
30	H	102	DGD	CEB-CDB-CCB	-2.11	103.70	114.42
33	D	407	LMG	C1-C2-C3	-2.11	105.60	110.00
22	C	509	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
24	B	618	BCR	C38-C26-C25	-2.11	122.16	124.53
33	C	516	LMG	C1-C2-C3	-2.11	105.60	110.00
22	D	404	CLA	C1-O2A-CGA	-2.11	110.91	116.44
22	C	514	CLA	C3C-C4C-NC	-2.11	108.20	110.57
22	b	601	CLA	CMB-C2B-C3B	2.11	128.62	124.68
22	b	608	CLA	CHD-C1D-C2D	2.11	129.90	125.48
30	A	415	DGD	O2E-C2E-C1E	-2.11	104.93	110.05
22	b	601	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
22	C	509	CLA	CHA-C4D-ND	2.11	136.90	132.50
22	b	611	CLA	CGD-CBD-CAD	-2.11	103.92	110.73
30	A	415	DGD	O4D-C4D-C5D	-2.10	104.07	109.30
22	B	611	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	a	403	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	b	604	CLA	CED-O2D-CGD	2.10	120.70	115.94
22	B	602	CLA	C4-C3-C5	2.10	118.81	115.27
22	c	507	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
22	B	609	CLA	CHD-C4C-NC	2.10	127.52	124.20
22	B	611	CLA	C2A-C1A-CHA	2.10	127.53	123.86
22	B	616	CLA	CHA-C4D-ND	2.10	136.90	132.50
33	C	516	LMG	C38-C37-C36	-2.10	103.76	114.42
22	b	614	CLA	C7-C6-C5	-2.10	107.65	113.36
24	b	618	BCR	C15-C16-C17	-2.10	119.17	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	C2A-C3A-C4A	2.10	105.26	101.87
22	c	509	CLA	O2D-CGD-CBD	2.10	115.00	111.27
33	b	622	LMG	C6-C5-C4	-2.10	108.08	113.00
22	b	607	CLA	O2A-C1-C2	-2.10	103.12	108.64
22	c	510	CLA	C16-C15-C13	-2.10	109.14	115.92
22	b	614	CLA	CHA-C4D-ND	2.10	136.89	132.50
22	B	606	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
24	C	501	BCR	C15-C16-C17	-2.10	119.18	123.47
24	b	618	BCR	C27-C26-C25	2.10	125.77	122.73
33	B	627	LMG	O6-C5-C4	2.10	113.50	109.69
28	d	409	LHG	O8-C6-C5	-2.10	102.33	108.43
24	b	619	BCR	C15-C16-C17	-2.10	119.18	123.47
22	D	403	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	c	511	CLA	C11-C12-C13	-2.09	109.16	115.92
24	H	101	BCR	C35-C13-C14	-2.09	120.00	122.92
28	d	408	LHG	O8-C23-C24	2.09	118.46	111.91
24	x	101	BCR	C2-C1-C6	2.09	113.69	110.48
22	b	606	CLA	C2C-C1C-NC	2.09	111.93	109.97
22	B	615	CLA	O2D-CGD-CBD	2.09	114.98	111.27
32	J	101	STE	O2-C1-C2	2.09	120.73	114.03
22	b	615	CLA	CHA-C1A-NA	-2.09	121.62	126.40
30	H	102	DGD	C4E-C3E-C2E	-2.09	107.18	110.82
22	C	504	CLA	C6-C7-C8	-2.08	109.18	115.92
22	b	603	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	d	402	CLA	CHD-C1D-ND	-2.08	122.54	124.45
33	c	519	LMG	O2-C2-C3	-2.08	105.53	110.35
32	b	624	STE	O2-C1-O1	-2.08	118.11	123.30
24	B	619	BCR	C27-C26-C25	2.08	125.75	122.73
22	B	617	CLA	C1-O2A-CGA	2.08	121.90	116.44
33	c	519	LMG	C38-C37-C36	-2.08	103.87	114.42
33	m	101	LMG	O2-C2-C1	-2.08	105.00	110.05
22	b	610	CLA	C4-C3-C5	2.08	118.77	115.27
24	b	619	BCR	C27-C26-C25	2.08	125.75	122.73
32	J	101	STE	C3-C2-C1	-2.08	109.24	114.47
22	d	402	CLA	CHA-C4D-ND	2.08	136.84	132.50
22	b	603	CLA	C9-C8-C10	-2.07	103.78	111.29
22	C	514	CLA	C4-C3-C5	2.07	118.76	115.27
22	D	403	CLA	C3B-C4B-NB	-2.07	106.53	109.21
24	K	101	BCR	C38-C26-C25	-2.07	122.20	124.53
29	A	412	SQD	O5-C1-O6	2.07	114.89	109.97
22	B	606	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	D	404	CLA	O1D-CGD-CBD	2.07	128.72	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	512	CLA	C4-C3-C5	2.07	118.76	115.27
22	C	510	CLA	CAC-C3C-C4C	2.07	127.50	124.81
22	c	506	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
22	c	511	CLA	C2D-C1D-ND	-2.07	108.58	110.10
33	D	410	LMG	O9-C10-C11	2.07	129.72	123.08
22	B	617	CLA	C5-C3-C2	2.07	125.30	121.12
33	c	521	LMG	O7-C10-O9	-2.07	118.71	123.70
24	x	101	BCR	C11-C10-C9	-2.07	124.36	127.31
22	C	511	CLA	O1D-CGD-CBD	2.06	128.71	124.48
30	c	518	DGD	CBB-CAB-C9B	-2.06	103.94	114.42
22	c	507	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
24	b	619	BCR	C36-C18-C19	2.06	121.33	118.08
22	C	514	CLA	C4D-CHA-C1A	-2.06	118.74	121.25
23	a	404	PHO	CMC-C2C-C3C	2.06	128.83	124.94
24	k	103	BCR	C36-C18-C17	-2.06	120.04	122.92
28	L	102	LHG	C9-C8-C7	-2.06	106.14	113.62
24	K	101	BCR	C36-C18-C17	-2.06	120.04	122.92
22	B	605	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	b	618	BCR	C34-C9-C10	-2.05	120.05	122.92
23	A	404	PHO	CMA-C3A-C2A	-2.05	105.72	113.99
22	D	403	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
30	C	517	DGD	C4A-C3A-C2A	-2.05	105.81	113.19
22	c	507	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
22	B	605	CLA	C11-C10-C8	-2.05	109.29	115.92
22	c	503	CLA	C2D-C1D-ND	-2.05	108.59	110.10
22	B	602	CLA	O1D-CGD-CBD	2.05	128.68	124.48
22	b	604	CLA	C3A-C2A-C1A	2.05	104.40	101.34
22	B	606	CLA	CHB-C4A-NA	2.05	127.34	124.51
22	A	405	CLA	CHC-C1C-C2C	-2.04	121.07	126.72
22	B	604	CLA	O1D-CGD-CBD	2.04	128.66	124.48
27	d	406	PL9	C15-C14-C13	-2.04	118.44	123.68
24	b	618	BCR	C39-C30-C25	-2.04	106.99	110.30
24	a	406	BCR	C33-C5-C6	-2.04	122.24	124.53
22	D	402	CLA	C4-C3-C5	2.04	118.70	115.27
33	Y	101	LMG	C31-C30-C29	-2.04	105.86	113.19
34	e	101	HEC	C1D-C2D-C3D	-2.04	105.58	107.00
24	B	619	BCR	C33-C5-C6	-2.04	122.24	124.53
24	c	515	BCR	C35-C13-C12	2.04	121.29	118.08
22	B	615	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
22	D	404	CLA	CHA-C1A-NA	-2.04	121.73	126.40
33	c	519	LMG	C40-C39-C38	-2.04	104.08	114.42
24	c	515	BCR	C15-C14-C13	-2.04	124.40	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	614	CLA	C3C-C4C-NC	-2.04	108.29	110.57
33	C	516	LMG	C35-C34-C33	-2.04	104.09	114.42
22	c	506	CLA	C4-C3-C2	-2.04	118.46	123.68
24	k	102	BCR	C1-C6-C5	-2.03	119.75	122.61
22	B	613	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
22	c	511	CLA	CMA-C3A-C4A	2.03	117.24	111.77
28	A	413	LHG	C5-O7-C7	-2.03	112.79	117.79
22	B	615	CLA	C3B-C4B-NB	-2.03	106.58	109.21
22	b	601	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
22	c	505	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
22	c	510	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	b	605	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
22	b	601	CLA	O2A-C1-C2	2.03	113.97	108.64
22	b	604	CLA	C4-C3-C5	2.03	118.69	115.27
24	B	619	BCR	C29-C30-C25	2.03	113.61	110.48
24	D	405	BCR	C7-C8-C9	-2.03	123.17	126.23
22	d	404	CLA	CHC-C1C-NC	2.03	127.28	124.20
23	D	401	PHO	OBD-CAD-CBD	-2.03	122.85	125.82
30	C	519	DGD	O6E-C5E-C4E	2.03	113.38	109.69
22	C	503	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
23	A	404	PHO	CMD-C2D-C3D	2.03	128.47	124.68
32	j	101	STE	O2-C1-O1	-2.03	118.25	123.30
22	B	613	CLA	CBC-CAC-C3C	2.03	118.02	112.43
22	C	502	CLA	C4D-CHA-C1A	2.02	123.71	121.25
24	k	102	BCR	C4-C5-C6	2.02	125.67	122.73
22	c	504	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
33	c	521	LMG	C40-C39-C38	-2.02	104.16	114.42
29	L	101	SQD	C20-C19-C18	-2.02	104.16	114.42
22	C	510	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
22	C	509	CLA	CHC-C1C-NC	2.02	127.27	124.20
22	a	402	CLA	C1-O2A-CGA	2.02	121.75	116.44
29	L	101	SQD	O47-C45-C46	2.02	115.72	108.40
22	c	503	CLA	C3A-C2A-C1A	2.02	104.36	101.34
22	C	510	CLA	C1-O2A-CGA	2.02	121.74	116.44
22	C	509	CLA	C3C-C4C-NC	-2.02	108.31	110.57
24	C	501	BCR	C37-C22-C21	-2.02	120.10	122.92
22	B	607	CLA	C7-C6-C5	-2.02	107.88	113.36
22	C	513	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
22	B	614	CLA	O2D-CGD-CBD	-2.02	107.69	111.27
22	C	514	CLA	O1A-CGA-CBA	2.01	131.59	123.73
22	d	404	CLA	C1D-ND-C4D	-2.01	104.90	106.33
29	A	414	SQD	C46-O48-C23	2.01	124.58	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	V	201	HEC	CAD-CBD-CGD	-2.01	108.11	113.76
24	b	618	BCR	C8-C7-C6	-2.01	121.55	127.20
22	c	506	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	B	608	CLA	CED-O2D-CGD	2.01	120.49	115.94
22	b	609	CLA	C4-C3-C5	-2.01	111.89	115.27
22	c	501	CLA	CHC-C1C-C2C	-2.01	121.16	126.72
33	M	101	LMG	C23-C22-C21	-2.01	104.22	114.42
24	H	101	BCR	C16-C17-C18	-2.01	124.44	127.31
22	c	506	CLA	O2A-C1-C2	-2.01	103.35	108.64
22	b	607	CLA	CHB-C4A-NA	2.01	127.29	124.51
33	D	410	LMG	C31-C30-C29	-2.01	105.97	113.19
22	B	611	CLA	O1D-CGD-CBD	2.01	128.59	124.48
22	A	405	CLA	CHD-C1D-ND	-2.01	122.61	124.45
34	V	201	HEC	O2A-CGA-CBA	2.01	120.48	114.03
24	x	101	BCR	C16-C17-C18	-2.01	124.45	127.31
22	d	404	CLA	CAA-CBA-CGA	-2.01	107.39	113.25
22	b	609	CLA	CHD-C1D-ND	-2.01	122.61	124.45
27	a	410	PL9	C11-C9-C8	-2.01	117.06	121.12
22	B	602	CLA	O2D-CGD-CBD	2.00	114.83	111.27
27	D	406	PL9	C12-C13-C14	-2.00	122.83	127.66
32	b	626	STE	O2-C1-O1	-2.00	118.31	123.30
30	C	519	DGD	O4E-C4E-C5E	-2.00	104.32	109.30
22	a	405	CLA	CHD-C1D-ND	-2.00	122.61	124.45
22	c	508	CLA	CGD-CBD-CAD	-2.00	104.25	110.73
22	b	612	CLA	C2D-C1D-ND	2.00	111.58	110.10
24	C	501	BCR	C15-C14-C13	-2.00	124.45	127.31
22	c	510	CLA	CAA-C2A-C1A	-2.00	105.42	111.97
22	C	502	CLA	CHD-C1D-C2D	2.00	129.68	125.48
22	B	609	CLA	C1B-CHB-C4A	-2.00	126.15	130.12

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	608	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	B	617	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	D	402	CLA	ND
22	D	403	CLA	ND
22	D	404	CLA	ND
22	a	402	CLA	ND
22	a	405	CLA	ND
22	b	601	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	c	501	CLA	ND
22	c	502	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	d	403	CLA	ND

All (1906) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	C	513	CLA	O2A-C1-C2-C3
22	D	403	CLA	CHA-CBD-CGD-O2D
22	b	603	CLA	C2-C3-C5-C6
22	b	603	CLA	C4-C3-C5-C6
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	C2-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CBD-CGD-O2D-CED
22	d	403	CLA	CHA-CBD-CGD-O1D
22	d	403	CLA	CHA-CBD-CGD-O2D
24	A	406	BCR	C11-C10-C9-C34
24	A	406	BCR	C11-C12-C13-C14
24	A	406	BCR	C23-C24-C25-C30
24	B	618	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C16-C17-C18-C36
24	B	618	BCR	C36-C18-C19-C20
24	B	618	BCR	C20-C21-C22-C37
24	B	619	BCR	C11-C10-C9-C8
24	B	619	BCR	C10-C11-C12-C13
24	B	619	BCR	C23-C24-C25-C30
24	B	620	BCR	C7-C8-C9-C34
24	B	620	BCR	C37-C22-C23-C24
24	C	501	BCR	C20-C21-C22-C37
24	C	515	BCR	C11-C12-C13-C14
24	C	515	BCR	C20-C21-C22-C37
24	D	405	BCR	C20-C21-C22-C37
24	D	405	BCR	C37-C22-C23-C24
24	D	405	BCR	C23-C24-C25-C26
24	H	101	BCR	C35-C13-C14-C15
24	H	101	BCR	C16-C17-C18-C36
24	H	101	BCR	C17-C18-C19-C20
24	K	101	BCR	C7-C8-C9-C34
24	K	101	BCR	C11-C12-C13-C35
24	K	101	BCR	C16-C17-C18-C36
24	K	101	BCR	C21-C22-C23-C24
24	K	101	BCR	C37-C22-C23-C24
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C37-C22-C23-C24
24	Z	101	BCR	C7-C8-C9-C34
24	Z	101	BCR	C11-C12-C13-C35
24	Z	101	BCR	C14-C15-C16-C17
24	a	406	BCR	C35-C13-C14-C15
24	b	617	BCR	C1-C6-C7-C8
24	b	617	BCR	C20-C21-C22-C37
24	b	617	BCR	C21-C22-C23-C24
24	b	619	BCR	C11-C12-C13-C14
24	b	619	BCR	C16-C17-C18-C36
24	b	619	BCR	C37-C22-C23-C24
24	c	514	BCR	C1-C6-C7-C8
24	c	514	BCR	C11-C12-C13-C14
24	c	514	BCR	C12-C13-C14-C15
24	c	514	BCR	C17-C18-C19-C20
24	c	514	BCR	C23-C24-C25-C30
24	c	515	BCR	C35-C13-C14-C15
24	c	515	BCR	C36-C18-C19-C20
24	d	405	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	d	405	BCR	C37-C22-C23-C24
24	k	102	BCR	C1-C6-C7-C8
24	k	102	BCR	C5-C6-C7-C8
24	k	102	BCR	C17-C18-C19-C20
24	k	102	BCR	C36-C18-C19-C20
24	k	103	BCR	C37-C22-C23-C24
24	t	101	BCR	C7-C8-C9-C34
24	t	101	BCR	C11-C12-C13-C14
24	t	101	BCR	C11-C12-C13-C35
24	t	101	BCR	C20-C21-C22-C37
24	x	101	BCR	C37-C22-C23-C24
27	A	410	PL9	C12-C13-C14-C16
27	A	410	PL9	C37-C38-C39-C40
27	A	410	PL9	C37-C38-C39-C41
27	A	410	PL9	C40-C39-C41-C42
27	A	410	PL9	C43-C44-C46-C47
27	A	410	PL9	C45-C44-C46-C47
27	A	410	PL9	C47-C48-C49-C51
27	D	406	PL9	C32-C33-C34-C35
27	a	410	PL9	C17-C18-C19-C20
27	a	410	PL9	C22-C23-C24-C25
27	a	410	PL9	C22-C23-C24-C26
27	a	410	PL9	C27-C28-C29-C31
27	a	410	PL9	C28-C29-C31-C32
27	a	410	PL9	C37-C38-C39-C41
27	a	410	PL9	C39-C41-C42-C43
27	d	406	PL9	C37-C38-C39-C41
27	d	406	PL9	C40-C39-C41-C42
27	d	406	PL9	C42-C43-C44-C45
27	d	406	PL9	C42-C43-C44-C46
28	A	411	LHG	O2-C2-C3-O3
28	A	411	LHG	C3-O3-P-O5
28	A	411	LHG	C3-O3-P-O6
28	A	413	LHG	O1-C1-C2-C3
28	B	622	LHG	O1-C1-C2-C3
28	D	408	LHG	O1-C1-C2-C3
28	D	408	LHG	O2-C2-C3-O3
28	D	408	LHG	C3-O3-P-O4
28	D	408	LHG	C3-O3-P-O5
28	D	408	LHG	C3-O3-P-O6
28	D	408	LHG	C4-O6-P-O4
28	L	102	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
28	a	412	LHG	O1-C1-C2-C3
28	a	412	LHG	C3-O3-P-O4
28	a	412	LHG	C3-O3-P-O5
28	a	412	LHG	C3-O3-P-O6
28	a	412	LHG	O10-C23-O8-C6
28	d	407	LHG	C3-O3-P-O4
28	d	408	LHG	C4-O6-P-O4
28	d	409	LHG	O1-C1-C2-C3
28	l	101	LHG	C4-O6-P-O3
28	l	101	LHG	C4-O6-P-O4
28	l	101	LHG	C4-O6-P-O5
29	B	623	SQD	C2-C1-O6-C44
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
29	B	623	SQD	C8-C7-O47-C45
29	L	101	SQD	C8-C7-O47-C45
29	L	101	SQD	O10-C23-O48-C46
29	a	411	SQD	O6-C44-C45-O47
29	a	413	SQD	C8-C7-O47-C45
29	f	101	SQD	O5-C1-O6-C44
30	A	415	DGD	C2B-C1B-O2G-C2G
33	C	516	LMG	O6-C1-O1-C7
33	C	516	LMG	O1-C7-C8-O7
33	C	516	LMG	O9-C10-O7-C8
33	D	409	LMG	O1-C7-C8-C9
33	D	409	LMG	O1-C7-C8-O7
33	Y	101	LMG	C11-C10-O7-C8
33	c	522	LMG	O6-C1-O1-C7
33	c	522	LMG	O10-C28-O8-C9
33	c	522	LMG	C29-C28-O8-C9
22	C	514	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED
22	C	514	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	O1D-CGD-O2D-CED
28	A	413	LHG	C24-C23-O8-C6
29	L	101	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
27	A	410	PL9	C47-C48-C49-C50
27	a	410	PL9	C47-C48-C49-C51
22	C	513	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	O1A-CGA-O2A-C1
28	A	413	LHG	O10-C23-O8-C6
29	f	101	SQD	O10-C23-O48-C46
33	M	101	LMG	O10-C28-O8-C9
22	c	510	CLA	C8-C10-C11-C12
29	L	101	SQD	O49-C7-O47-C45
29	a	413	SQD	O49-C7-O47-C45
29	f	101	SQD	O49-C7-O47-C45
30	A	415	DGD	O1B-C1B-O2G-C2G
33	D	409	LMG	O9-C10-O7-C8
33	b	622	LMG	O9-C10-O7-C8
22	d	404	CLA	C3-C5-C6-C7
28	a	412	LHG	C24-C23-O8-C6
22	B	607	CLA	C10-C11-C12-C13
33	C	516	LMG	C11-C10-O7-C8
27	d	406	PL9	C47-C48-C49-C50
22	c	511	CLA	CBD-CGD-O2D-CED
30	h	101	DGD	O6E-C5E-C6E-O5E
22	B	606	CLA	C2-C3-C5-C6
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	C3-C5-C6-C7
22	B	602	CLA	CBA-CGA-O2A-C1
33	M	101	LMG	C29-C28-O8-C9
33	Y	101	LMG	C29-C28-O8-C9
33	c	521	LMG	C29-C28-O8-C9
27	a	410	PL9	C42-C43-C44-C45
27	d	406	PL9	C32-C33-C34-C35
22	a	403	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	CBD-CGD-O2D-CED
27	A	410	PL9	C22-C23-C24-C26
27	D	406	PL9	C32-C33-C34-C36
27	a	410	PL9	C17-C18-C19-C21
27	d	406	PL9	C32-C33-C34-C36
33	c	521	LMG	O10-C28-O8-C9
24	c	514	BCR	C13-C14-C15-C16
22	B	605	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
28	B	622	LHG	O2-C2-C3-O3
29	f	101	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
22	b	610	CLA	C2C-C3C-CAC-CBC
27	a	410	PL9	C47-C48-C49-C50
22	B	614	CLA	CBD-CGD-O2D-CED
22	b	602	CLA	CBD-CGD-O2D-CED
30	H	102	DGD	C2B-C3B-C4B-C5B
32	b	624	STE	C4-C5-C6-C7
28	l	101	LHG	C7-C8-C9-C10
30	A	415	DGD	C1B-C2B-C3B-C4B
22	b	610	CLA	C4C-C3C-CAC-CBC
33	b	622	LMG	O10-C28-O8-C9
27	d	406	PL9	C47-C48-C49-C51
33	C	516	LMG	O6-C5-C6-O5
22	A	405	CLA	C4-C3-C5-C6
22	B	606	CLA	C4-C3-C5-C6
22	B	615	CLA	C4-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
27	A	410	PL9	C35-C34-C36-C37
22	A	405	CLA	C2-C3-C5-C6
22	B	615	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
27	A	410	PL9	C33-C34-C36-C37
27	d	406	PL9	C38-C39-C41-C42
32	b	620	STE	C5-C6-C7-C8
29	L	101	SQD	O5-C1-O6-C44
27	A	410	PL9	C19-C21-C22-C23
27	A	410	PL9	C44-C46-C47-C48
27	a	410	PL9	C9-C11-C12-C13
27	a	410	PL9	C34-C36-C37-C38
22	C	514	CLA	CBA-CGA-O2A-C1
33	d	410	LMG	C10-C11-C12-C13
22	c	506	CLA	O1D-CGD-O2D-CED
30	h	101	DGD	C4E-C5E-C6E-O5E
22	b	614	CLA	CBD-CGD-O2D-CED
28	A	411	LHG	C1-C2-C3-O3
28	B	622	LHG	C1-C2-C3-O3
28	D	408	LHG	C1-C2-C3-O3
22	C	514	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	CBA-CGA-O2A-C1
29	B	623	SQD	C24-C23-O48-C46
33	C	516	LMG	C4-C5-C6-O5
22	C	510	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
33	c	522	LMG	C2-C1-O1-C7
29	A	412	SQD	O6-C44-C45-O47
27	A	410	PL9	C23-C24-C26-C27
22	A	403	CLA	C14-C13-C15-C16
22	B	603	CLA	C6-C7-C8-C9
22	B	608	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C14
22	B	614	CLA	C11-C12-C13-C14
22	C	503	CLA	C14-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C9
32	C	522	STE	C4-C5-C6-C7
22	B	607	CLA	C2A-CAA-CBA-CGA
24	A	406	BCR	C11-C12-C13-C35
24	A	406	BCR	C37-C22-C23-C24
24	B	619	BCR	C7-C8-C9-C34
24	C	515	BCR	C11-C12-C13-C35
24	T	101	BCR	C11-C12-C13-C35
24	b	619	BCR	C11-C12-C13-C35
24	c	514	BCR	C7-C8-C9-C34
24	c	514	BCR	C11-C12-C13-C35
24	k	102	BCR	C7-C8-C9-C34
30	C	519	DGD	C2A-C3A-C4A-C5A
28	d	407	LHG	C7-C8-C9-C10
29	a	413	SQD	C7-C8-C9-C10
30	c	517	DGD	C1B-C2B-C3B-C4B
22	B	616	CLA	C5-C6-C7-C8
22	C	504	CLA	C5-C6-C7-C8
22	c	502	CLA	C13-C15-C16-C17
22	c	509	CLA	C13-C15-C16-C17
30	A	415	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C5-C6-C7-C8
22	C	510	CLA	C8-C10-C11-C12
22	c	511	CLA	C8-C10-C11-C12
28	B	622	LHG	C7-C8-C9-C10
33	m	101	LMG	C10-C11-C12-C13
22	C	513	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C8-C10-C11-C12
22	C	509	CLA	C15-C16-C17-C18
22	D	404	CLA	C13-C15-C16-C17
22	a	405	CLA	C5-C6-C7-C8
22	a	405	CLA	C10-C11-C12-C13
22	b	603	CLA	C5-C6-C7-C8
22	b	607	CLA	C5-C6-C7-C8
22	b	608	CLA	C8-C10-C11-C12
22	b	614	CLA	C5-C6-C7-C8
22	c	503	CLA	C5-C6-C7-C8
22	c	504	CLA	C5-C6-C7-C8
22	c	513	CLA	C5-C6-C7-C8
32	B	621	STE	C9-C10-C11-C12
28	B	622	LHG	O1-C1-C2-O2
27	A	410	PL9	C22-C23-C24-C25
27	D	406	PL9	C42-C43-C44-C45
27	a	410	PL9	C27-C28-C29-C30
27	d	406	PL9	C22-C23-C24-C25
28	a	412	LHG	C23-C24-C25-C26
28	d	407	LHG	C23-C24-C25-C26
29	L	101	SQD	C23-C24-C25-C26
30	c	517	DGD	C1A-C2A-C3A-C4A
32	L	103	STE	C1-C2-C3-C4
32	c	520	STE	C1-C2-C3-C4
33	B	627	LMG	C10-C11-C12-C13
33	Y	101	LMG	C28-C29-C30-C31
33	b	622	LMG	C28-C29-C30-C31
33	d	410	LMG	C28-C29-C30-C31
22	B	602	CLA	C10-C11-C12-C13
22	C	506	CLA	C5-C6-C7-C8
22	b	609	CLA	C15-C16-C17-C18
33	b	622	LMG	C29-C28-O8-C9
30	C	518	DGD	CCA-CDA-CEA-CFA
22	B	604	CLA	C15-C16-C17-C18
22	B	614	CLA	C8-C10-C11-C12
22	C	507	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	C	514	CLA	C15-C16-C17-C18
22	b	602	CLA	C15-C16-C17-C18
22	b	613	CLA	C15-C16-C17-C18
22	b	615	CLA	C10-C11-C12-C13
28	L	102	LHG	C7-C8-C9-C10
29	A	412	SQD	C23-C24-C25-C26
22	D	404	CLA	C10-C11-C12-C13
22	a	403	CLA	C8-C10-C11-C12
22	C	511	CLA	C6-C7-C8-C10
22	C	511	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C15
22	b	607	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C12-C13-C15
22	B	617	CLA	C3-C5-C6-C7
29	F	101	SQD	O10-C23-O48-C46
24	c	514	BCR	C15-C16-C17-C18
22	b	606	CLA	C2A-CAA-CBA-CGA
22	a	402	CLA	C15-C16-C17-C18
22	b	603	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
22	d	403	CLA	C15-C16-C17-C18
24	b	619	BCR	C22-C23-C24-C25
30	C	518	DGD	O6E-C1E-O5D-C6D
33	Y	101	LMG	O6-C1-O1-C7
27	a	410	PL9	C19-C21-C22-C23
27	a	410	PL9	C24-C26-C27-C28
24	C	501	BCR	C18-C19-C20-C21
24	C	515	BCR	C18-C19-C20-C21
24	Z	101	BCR	C10-C11-C12-C13
24	a	406	BCR	C18-C19-C20-C21
24	c	514	BCR	C10-C11-C12-C13
33	d	410	LMG	O6-C5-C6-O5
28	A	413	LHG	O2-C2-C3-O3
28	a	412	LHG	O2-C2-C3-O3
22	B	615	CLA	C13-C15-C16-C17
22	C	503	CLA	C13-C15-C16-C17
22	C	506	CLA	C10-C11-C12-C13
22	c	506	CLA	O1A-CGA-O2A-C1
33	Y	101	LMG	O10-C28-O8-C9
33	M	101	LMG	C28-C29-C30-C31
22	B	614	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C8-C10-C11-C12
22	b	611	CLA	C13-C15-C16-C17
22	b	612	CLA	C13-C15-C16-C17
22	b	615	CLA	C15-C16-C17-C18
22	c	510	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
22	a	405	CLA	O1A-CGA-O2A-C1
32	B	626	STE	C5-C6-C7-C8
22	B	607	CLA	C15-C16-C17-C18
22	B	609	CLA	C13-C15-C16-C17
22	C	511	CLA	C13-C15-C16-C17
22	b	606	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	c	511	CLA	C13-C15-C16-C17
22	c	512	CLA	C8-C10-C11-C12
22	C	513	CLA	C3-C5-C6-C7
22	C	513	CLA	C8-C10-C11-C12
22	c	508	CLA	C8-C10-C11-C12
32	B	621	STE	C1-C2-C3-C4
33	c	521	LMG	C28-C29-C30-C31
28	A	413	LHG	C1-C2-C3-O3
28	a	412	LHG	C1-C2-C3-O3
27	D	406	PL9	C30-C29-C31-C32
27	d	406	PL9	C18-C19-C21-C22
22	B	602	CLA	C15-C16-C17-C18
30	c	518	DGD	CAA-CBA-CCA-CDA
22	B	606	CLA	C16-C17-C18-C19
33	C	516	LMG	C29-C28-O8-C9
33	D	407	LMG	C10-C11-C12-C13
28	A	413	LHG	C10-C11-C12-C13
28	A	413	LHG	C29-C30-C31-C32
30	A	415	DGD	C9A-CAA-CBA-CCA
30	h	101	DGD	CBA-CCA-CDA-CEA
33	Y	101	LMG	C12-C13-C14-C15
33	m	101	LMG	C19-C20-C21-C22
22	B	617	CLA	CBD-CGD-O2D-CED
33	D	409	LMG	C11-C10-O7-C8
33	b	622	LMG	C11-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
24	A	406	BCR	C35-C13-C14-C15
24	A	406	BCR	C16-C17-C18-C36
24	C	501	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
24	C	515	BCR	C35-C13-C14-C15
24	H	101	BCR	C20-C21-C22-C37
24	a	406	BCR	C11-C10-C9-C34
24	a	406	BCR	C20-C21-C22-C37
24	b	618	BCR	C11-C10-C9-C34
28	A	413	LHG	C27-C28-C29-C30
28	B	622	LHG	C10-C11-C12-C13
28	L	102	LHG	C31-C32-C33-C34
28	d	407	LHG	C25-C26-C27-C28
28	d	408	LHG	C29-C30-C31-C32
29	B	623	SQD	C17-C18-C19-C20
30	C	517	DGD	CAB-CBB-CCB-CDB
30	C	518	DGD	C6A-C7A-C8A-C9A
30	c	516	DGD	C4B-C5B-C6B-C7B
30	c	516	DGD	C6B-C7B-C8B-C9B
32	B	626	STE	C4-C5-C6-C7
32	d	411	STE	C10-C11-C12-C13
33	B	627	LMG	C39-C40-C41-C42
33	c	521	LMG	C31-C32-C33-C34
33	m	101	LMG	C31-C32-C33-C34
30	c	518	DGD	O1A-C1A-O1G-C1G
22	B	615	CLA	C16-C17-C18-C20
33	m	101	LMG	C29-C28-O8-C9
28	a	412	LHG	C11-C12-C13-C14
28	d	407	LHG	C11-C10-C9-C8
29	B	623	SQD	C13-C14-C15-C16
29	L	101	SQD	C13-C14-C15-C16
30	A	415	DGD	CCA-CDA-CEA-CFA
30	A	415	DGD	CCB-CDB-CEB-CFB
30	h	101	DGD	C6B-C7B-C8B-C9B
32	T	102	STE	C13-C14-C15-C16
32	h	102	STE	C11-C12-C13-C14
32	x	102	STE	C2-C3-C4-C5
33	B	627	LMG	C14-C15-C16-C17
33	D	407	LMG	C12-C13-C14-C15
33	Y	101	LMG	C32-C33-C34-C35
29	L	101	SQD	C46-C45-O47-C7
23	d	401	PHO	O1D-CGD-O2D-CED
33	Y	101	LMG	O9-C10-O7-C8
22	A	403	CLA	C8-C10-C11-C12
22	c	507	CLA	C13-C15-C16-C17
22	c	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	A	414	SQD	C12-C13-C14-C15
30	A	415	DGD	C4B-C5B-C6B-C7B
30	c	516	DGD	C4A-C5A-C6A-C7A
30	c	517	DGD	C2A-C3A-C4A-C5A
32	B	601	STE	C2-C3-C4-C5
32	M	103	STE	C5-C6-C7-C8
33	C	516	LMG	C12-C13-C14-C15
28	B	622	LHG	C12-C13-C14-C15
28	B	622	LHG	C28-C29-C30-C31
28	d	408	LHG	C11-C12-C13-C14
29	F	101	SQD	C27-C28-C29-C30
30	c	518	DGD	C4B-C5B-C6B-C7B
32	B	626	STE	C12-C13-C14-C15
33	D	407	LMG	C30-C31-C32-C33
33	m	101	LMG	C30-C31-C32-C33
22	c	511	CLA	O1D-CGD-O2D-CED
28	A	411	LHG	C11-C12-C13-C14
28	d	407	LHG	C15-C16-C17-C18
30	c	518	DGD	CCA-CDA-CEA-CFA
33	c	519	LMG	C33-C34-C35-C36
33	d	410	LMG	C34-C35-C36-C37
33	M	101	LMG	O6-C5-C6-O5
24	B	618	BCR	C12-C13-C14-C15
24	B	620	BCR	C11-C10-C9-C8
24	B	620	BCR	C20-C21-C22-C23
24	C	501	BCR	C16-C17-C18-C19
24	C	515	BCR	C20-C21-C22-C23
24	H	101	BCR	C12-C13-C14-C15
24	K	101	BCR	C16-C17-C18-C19
24	a	406	BCR	C12-C13-C14-C15
24	b	619	BCR	C20-C21-C22-C23
24	c	514	BCR	C11-C10-C9-C8
24	t	101	BCR	C11-C10-C9-C8
30	C	518	DGD	C2E-C1E-O5D-C6D
33	Y	101	LMG	C2-C1-O1-C7
29	A	412	SQD	C11-C12-C13-C14
29	A	412	SQD	C26-C27-C28-C29
30	C	517	DGD	CBA-CCA-CDA-CEA
30	c	516	DGD	C7B-C8B-C9B-CAB
32	B	626	STE	C11-C10-C9-C8
32	H	103	STE	C5-C6-C7-C8
32	x	102	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	x	102	STE	C6-C7-C8-C9
33	C	516	LMG	C16-C17-C18-C19
33	M	101	LMG	C14-C15-C16-C17
33	Y	101	LMG	C39-C40-C41-C42
33	c	522	LMG	C32-C33-C34-C35
22	B	609	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
22	c	505	CLA	C16-C17-C18-C19
22	c	506	CLA	C16-C17-C18-C19
22	a	403	CLA	O1D-CGD-O2D-CED
22	b	611	CLA	C4-C3-C5-C6
28	A	413	LHG	C11-C10-C9-C8
28	d	408	LHG	C12-C13-C14-C15
30	C	517	DGD	C4B-C5B-C6B-C7B
30	C	517	DGD	CBB-CCB-CDB-CEB
30	C	518	DGD	CBB-CCB-CDB-CEB
30	c	518	DGD	C9B-CAB-CBB-CCB
30	h	101	DGD	C3B-C4B-C5B-C6B
32	J	101	STE	C5-C6-C7-C8
32	b	623	STE	C3-C4-C5-C6
32	t	103	STE	C3-C4-C5-C6
32	x	102	STE	C4-C5-C6-C7
33	B	627	LMG	C36-C37-C38-C39
33	C	516	LMG	C36-C37-C38-C39
33	D	407	LMG	C37-C38-C39-C40
33	M	101	LMG	C12-C13-C14-C15
33	M	101	LMG	C37-C38-C39-C40
33	b	622	LMG	C32-C33-C34-C35
33	c	522	LMG	C31-C32-C33-C34
22	C	507	CLA	C2-C3-C5-C6
22	B	604	CLA	C6-C7-C8-C9
22	D	402	CLA	C11-C10-C8-C9
22	a	403	CLA	C6-C7-C8-C9
22	b	602	CLA	C11-C12-C13-C14
22	b	602	CLA	C14-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C9
22	c	509	CLA	C6-C7-C8-C9
23	D	401	PHO	C14-C13-C15-C16
22	B	605	CLA	O1D-CGD-O2D-CED
32	J	101	STE	C1-C2-C3-C4
29	L	101	SQD	C18-C19-C20-C21
29	L	101	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	C6A-C7A-C8A-C9A
30	C	518	DGD	C8B-C9B-CAB-CBB
32	D	411	STE	C5-C6-C7-C8
32	D	411	STE	C11-C12-C13-C14
32	k	101	STE	C6-C7-C8-C9
32	t	102	STE	C6-C7-C8-C9
33	B	627	LMG	C17-C18-C19-C20
33	D	409	LMG	C36-C37-C38-C39
33	b	622	LMG	C19-C20-C21-C22
22	C	514	CLA	C10-C11-C12-C13
29	B	623	SQD	C34-C35-C36-C37
32	B	625	STE	C5-C6-C7-C8
33	c	521	LMG	C41-C42-C43-C44
28	d	407	LHG	O1-C1-C2-C3
28	A	413	LHG	C11-C12-C13-C14
28	A	413	LHG	C33-C34-C35-C36
28	B	622	LHG	C17-C18-C19-C20
28	L	102	LHG	C27-C28-C29-C30
30	A	415	DGD	C7B-C8B-C9B-CAB
30	C	518	DGD	CCB-CDB-CEB-CFB
32	D	411	STE	C12-C13-C14-C15
32	d	411	STE	C5-C6-C7-C8
33	C	516	LMG	C29-C30-C31-C32
33	c	521	LMG	C11-C12-C13-C14
28	A	413	LHG	C23-C24-C25-C26
29	A	412	SQD	C32-C33-C34-C35
29	L	101	SQD	C27-C28-C29-C30
29	a	411	SQD	C26-C27-C28-C29
30	A	415	DGD	C9B-CAB-CBB-CCB
30	C	517	DGD	C5B-C6B-C7B-C8B
30	C	518	DGD	C3A-C4A-C5A-C6A
30	C	519	DGD	CBA-CCA-CDA-CEA
30	H	102	DGD	CAB-CBB-CCB-CDB
30	c	517	DGD	C4A-C5A-C6A-C7A
30	c	518	DGD	CBB-CCB-CDB-CEB
32	B	625	STE	C6-C7-C8-C9
32	I	101	STE	C11-C10-C9-C8
32	T	102	STE	C14-C15-C16-C17
32	c	520	STE	C2-C3-C4-C5
33	B	627	LMG	C37-C38-C39-C40
33	b	622	LMG	C11-C12-C13-C14
33	b	622	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
33	c	521	LMG	C36-C37-C38-C39
22	B	603	CLA	C16-C17-C18-C20
22	B	615	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C20
22	c	505	CLA	C16-C17-C18-C20
30	A	415	DGD	O6D-C1D-O3G-C3G
30	c	516	DGD	O6E-C1E-O5D-C6D
28	A	411	LHG	C24-C25-C26-C27
28	d	407	LHG	C33-C34-C35-C36
29	A	412	SQD	C30-C31-C32-C33
29	A	414	SQD	C10-C11-C12-C13
32	H	103	STE	C9-C10-C11-C12
32	c	520	STE	C6-C7-C8-C9
33	D	407	LMG	C17-C18-C19-C20
33	D	410	LMG	C29-C30-C31-C32
33	M	101	LMG	C20-C21-C22-C23
33	Y	101	LMG	C37-C38-C39-C40
33	d	410	LMG	C38-C39-C40-C41
33	m	101	LMG	C39-C40-C41-C42
22	C	510	CLA	O1D-CGD-O2D-CED
28	A	411	LHG	C12-C13-C14-C15
28	A	411	LHG	C25-C26-C27-C28
28	A	413	LHG	C24-C25-C26-C27
29	A	412	SQD	C9-C10-C11-C12
30	A	415	DGD	C2A-C3A-C4A-C5A
30	C	517	DGD	C9B-CAB-CBB-CCB
30	c	518	DGD	C5B-C6B-C7B-C8B
32	h	102	STE	C13-C14-C15-C16
33	B	627	LMG	C16-C17-C18-C19
33	M	101	LMG	C33-C34-C35-C36
33	c	521	LMG	C30-C31-C32-C33
33	d	410	LMG	C36-C37-C38-C39
29	a	413	SQD	C24-C25-C26-C27
30	A	415	DGD	CEA-CFA-CGA-CHA
30	C	519	DGD	CAB-CBB-CCB-CDB
30	c	518	DGD	C7A-C8A-C9A-CAA
32	h	102	STE	C7-C8-C9-C10
33	c	519	LMG	C34-C35-C36-C37
32	t	104	STE	C12-C13-C14-C15
33	c	521	LMG	C16-C17-C18-C19
33	c	521	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C20-C21-C22-C23
22	B	614	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	C15-C16-C17-C18
29	A	412	SQD	C16-C17-C18-C19
29	A	414	SQD	C24-C25-C26-C27
29	L	101	SQD	C16-C17-C18-C19
30	H	102	DGD	C8B-C9B-CAB-CBB
32	L	103	STE	C5-C6-C7-C8
32	t	104	STE	C4-C5-C6-C7
22	b	614	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	C11-C12-C13-C14
28	A	413	LHG	C25-C26-C27-C28
28	L	102	LHG	C12-C13-C14-C15
29	A	414	SQD	C28-C29-C30-C31
29	A	414	SQD	C32-C33-C34-C35
30	A	415	DGD	C5B-C6B-C7B-C8B
30	C	518	DGD	CAA-CBA-CCA-CDA
32	T	102	STE	C6-C7-C8-C9
30	h	101	DGD	CCB-CDB-CEB-CFB
33	C	516	LMG	C38-C39-C40-C41
24	c	515	BCR	C14-C15-C16-C17
28	L	102	LHG	C23-C24-C25-C26
29	a	413	SQD	C11-C10-C9-C8
30	c	518	DGD	C6B-C7B-C8B-C9B
32	B	624	STE	C4-C5-C6-C7
33	M	101	LMG	C13-C14-C15-C16
33	c	522	LMG	C17-C18-C19-C20
22	B	617	CLA	C5-C6-C7-C8
22	c	510	CLA	C5-C6-C7-C8
22	C	511	CLA	C4-C3-C5-C6
22	c	505	CLA	C4-C3-C5-C6
23	A	404	PHO	C4-C3-C5-C6
27	d	406	PL9	C45-C44-C46-C47
22	C	511	CLA	C2-C3-C5-C6
22	b	611	CLA	C2-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
22	c	510	CLA	C2-C3-C5-C6
23	A	404	PHO	C2-C3-C5-C6
27	d	406	PL9	C43-C44-C46-C47
29	F	101	SQD	C30-C31-C32-C33
28	A	413	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	a	412	LHG	O1-C1-C2-O2
29	A	412	SQD	C14-C15-C16-C17
29	a	411	SQD	C34-C35-C36-C37
32	H	103	STE	C2-C3-C4-C5
33	b	622	LMG	C13-C14-C15-C16
33	m	101	LMG	C32-C33-C34-C35
22	B	603	CLA	C16-C17-C18-C19
22	B	606	CLA	C16-C17-C18-C20
33	Y	101	LMG	C17-C18-C19-C20
22	d	402	CLA	C2C-C3C-CAC-CBC
29	F	101	SQD	C28-C29-C30-C31
32	b	621	STE	C6-C7-C8-C9
32	b	624	STE	C11-C12-C13-C14
32	b	626	STE	C10-C11-C12-C13
22	C	513	CLA	C10-C11-C12-C13
28	d	407	LHG	C29-C30-C31-C32
28	l	101	LHG	C14-C15-C16-C17
32	Z	102	STE	C11-C12-C13-C14
22	B	617	CLA	C2-C1-O2A-CGA
30	c	516	DGD	O6D-C5D-C6D-O5D
28	a	412	LHG	C16-C17-C18-C19
29	a	413	SQD	C12-C13-C14-C15
29	a	413	SQD	C29-C30-C31-C32
30	H	102	DGD	C7A-C8A-C9A-CAA
30	c	518	DGD	C2A-C3A-C4A-C5A
33	b	622	LMG	C39-C40-C41-C42
22	B	602	CLA	C8-C10-C11-C12
22	C	507	CLA	C8-C10-C11-C12
22	C	514	CLA	C8-C10-C11-C12
22	b	613	CLA	C10-C11-C12-C13
28	A	413	LHG	C12-C13-C14-C15
28	B	622	LHG	C16-C17-C18-C19
30	h	101	DGD	C2B-C3B-C4B-C5B
32	h	102	STE	C9-C10-C11-C12
33	b	622	LMG	C16-C17-C18-C19
22	c	513	CLA	C3-C5-C6-C7
24	A	406	BCR	C23-C24-C25-C26
24	D	405	BCR	C23-C24-C25-C30
24	K	101	BCR	C1-C6-C7-C8
24	K	101	BCR	C5-C6-C7-C8
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	617	BCR	C5-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	c	514	BCR	C23-C24-C25-C26
24	d	405	BCR	C23-C24-C25-C26
28	d	408	LHG	C17-C18-C19-C20
29	A	412	SQD	C33-C34-C35-C36
29	L	101	SQD	C24-C25-C26-C27
30	A	415	DGD	CBA-CCA-CDA-CEA
30	A	415	DGD	CDA-CEA-CFA-CGA
22	B	606	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
22	b	607	CLA	C10-C11-C12-C13
22	b	611	CLA	C15-C16-C17-C18
22	c	505	CLA	C13-C15-C16-C17
22	c	508	CLA	C13-C15-C16-C17
28	A	413	LHG	C31-C32-C33-C34
29	B	623	SQD	C33-C34-C35-C36
30	C	519	DGD	C6A-C7A-C8A-C9A
30	c	518	DGD	C3A-C4A-C5A-C6A
30	h	101	DGD	CAB-CBB-CCB-CDB
32	x	102	STE	C3-C4-C5-C6
33	M	101	LMG	C15-C16-C17-C18
33	M	101	LMG	C35-C36-C37-C38
33	m	101	LMG	C11-C12-C13-C14
30	C	517	DGD	O6E-C5E-C6E-O5E
28	B	622	LHG	C23-C24-C25-C26
28	a	412	LHG	C7-C8-C9-C10
28	a	412	LHG	C27-C28-C29-C30
32	k	101	STE	C5-C6-C7-C8
22	B	608	CLA	C13-C15-C16-C17
22	B	613	CLA	C10-C11-C12-C13
22	C	507	CLA	C4-C3-C5-C6
22	B	604	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	C	509	CLA	C12-C13-C15-C16
22	b	602	CLA	C12-C13-C15-C16
22	b	603	CLA	C6-C7-C8-C10
22	b	612	CLA	C12-C13-C15-C16
22	c	506	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	511	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	C11-C12-C13-C15
23	D	401	PHO	C12-C13-C15-C16
27	a	410	PL9	C43-C44-C46-C47
22	b	602	CLA	C3-C5-C6-C7
28	D	408	LHG	C30-C31-C32-C33
28	d	407	LHG	C10-C11-C12-C13
33	D	410	LMG	C16-C17-C18-C19
33	Y	101	LMG	C33-C34-C35-C36
22	B	610	CLA	C15-C16-C17-C18
22	B	612	CLA	C8-C10-C11-C12
24	Z	101	BCR	C15-C16-C17-C18
22	B	607	CLA	CBD-CGD-O2D-CED
33	c	521	LMG	O9-C10-O7-C8
32	b	624	STE	C1-C2-C3-C4
33	D	410	LMG	C10-C11-C12-C13
33	B	627	LMG	C29-C28-O8-C9
28	d	409	LHG	C35-C36-C37-C38
29	a	411	SQD	C13-C14-C15-C16
30	H	102	DGD	C8A-C9A-CAA-CBA
32	b	620	STE	C7-C8-C9-C10
33	D	407	LMG	C21-C22-C23-C24
22	B	606	CLA	C5-C6-C7-C8
22	c	505	CLA	C5-C6-C7-C8
33	b	622	LMG	C18-C19-C20-C21
22	c	512	CLA	O1A-CGA-O2A-C1
28	B	622	LHG	C25-C26-C27-C28
28	d	408	LHG	C14-C15-C16-C17
32	d	411	STE	C3-C4-C5-C6
28	d	408	LHG	C7-C8-C9-C10
28	l	101	LHG	C15-C16-C17-C18
32	t	104	STE	C9-C10-C11-C12
33	B	627	LMG	C33-C34-C35-C36
22	b	612	CLA	C3-C5-C6-C7
29	L	101	SQD	C15-C16-C17-C18
32	b	625	STE	C2-C3-C4-C5
32	c	520	STE	C7-C8-C9-C10
33	D	407	LMG	C36-C37-C38-C39
33	b	622	LMG	C12-C13-C14-C15
24	D	405	BCR	C22-C23-C24-C25
24	Z	101	BCR	C6-C7-C8-C9
22	C	513	CLA	C5-C6-C7-C8
22	B	617	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	O1D-CGD-O2D-CED
27	A	410	PL9	C24-C26-C27-C28
28	A	411	LHG	C15-C16-C17-C18
28	D	408	LHG	C13-C14-C15-C16
32	h	102	STE	C6-C7-C8-C9
33	m	101	LMG	C17-C18-C19-C20
30	C	518	DGD	C4A-C5A-C6A-C7A
30	c	517	DGD	CAA-CBA-CCA-CDA
30	h	101	DGD	C6A-C7A-C8A-C9A
32	x	102	STE	C10-C11-C12-C13
33	B	627	LMG	C12-C13-C14-C15
33	D	409	LMG	C34-C35-C36-C37
33	Y	101	LMG	C11-C12-C13-C14
24	k	102	BCR	C14-C15-C16-C17
32	d	411	STE	C2-C3-C4-C5
33	M	101	LMG	C32-C33-C34-C35
22	B	603	CLA	C3-C5-C6-C7
28	A	413	LHG	C15-C16-C17-C18
28	D	408	LHG	C9-C10-C11-C12
28	L	102	LHG	C18-C19-C20-C21
29	F	101	SQD	C33-C34-C35-C36
32	J	101	STE	C6-C7-C8-C9
32	b	623	STE	C6-C7-C8-C9
29	f	101	SQD	C2-C1-O6-C44
29	a	411	SQD	O47-C45-C46-O48
30	A	415	DGD	C2B-C3B-C4B-C5B
30	H	102	DGD	C3B-C4B-C5B-C6B
32	t	103	STE	C6-C7-C8-C9
33	B	627	LMG	C23-C24-C25-C26
22	B	607	CLA	O1D-CGD-O2D-CED
22	D	403	CLA	C16-C17-C18-C19
22	b	615	CLA	C16-C17-C18-C19
28	D	408	LHG	C29-C30-C31-C32
29	L	101	SQD	C12-C13-C14-C15
32	b	621	STE	C14-C15-C16-C17
33	M	101	LMG	C17-C18-C19-C20
22	b	606	CLA	C8-C10-C11-C12
22	c	510	CLA	C4-C3-C5-C6
27	D	406	PL9	C38-C39-C41-C42
27	a	410	PL9	C4-C3-C7-C8
32	a	414	STE	C4-C5-C6-C7
22	B	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	C	514	CLA	C11-C10-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	612	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C12-C13-C14
22	c	507	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
30	c	516	DGD	O6E-C5E-C6E-O5E
33	b	622	LMG	O6-C5-C6-O5
28	A	413	LHG	C32-C33-C34-C35
28	D	408	LHG	C12-C13-C14-C15
22	B	614	CLA	C3-C5-C6-C7
28	A	413	LHG	C17-C18-C19-C20
28	d	408	LHG	C30-C31-C32-C33
30	C	517	DGD	C9A-CAA-CBA-CCA
32	C	520	STE	C6-C7-C8-C9
33	M	101	LMG	C38-C39-C40-C41
33	D	407	LMG	O6-C5-C6-O5
33	c	521	LMG	O6-C5-C6-O5
22	b	603	CLA	O1D-CGD-O2D-CED
28	B	622	LHG	C29-C30-C31-C32
30	c	516	DGD	C7A-C8A-C9A-CAA
30	c	516	DGD	C3B-C4B-C5B-C6B
32	B	626	STE	C6-C7-C8-C9
32	J	101	STE	C3-C4-C5-C6
32	T	102	STE	C12-C13-C14-C15
32	b	620	STE	C4-C5-C6-C7
33	D	409	LMG	C15-C16-C17-C18
33	c	519	LMG	C30-C31-C32-C33
22	B	606	CLA	O1A-CGA-O2A-C1
22	B	608	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
29	a	413	SQD	C17-C18-C19-C20
30	c	517	DGD	C8A-C9A-CAA-CBA
28	d	408	LHG	C4-O6-P-O3
28	d	409	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	D	407	LMG	C35-C36-C37-C38
33	c	522	LMG	C33-C34-C35-C36
22	D	402	CLA	C3-C5-C6-C7
32	x	102	STE	C11-C12-C13-C14
33	c	521	LMG	C40-C41-C42-C43
22	C	513	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	C11-C12-C13-C14
28	D	408	LHG	C32-C33-C34-C35
28	L	102	LHG	C16-C17-C18-C19
32	B	625	STE	C4-C5-C6-C7
33	c	521	LMG	C35-C36-C37-C38
29	a	411	SQD	C10-C11-C12-C13
30	C	519	DGD	C7A-C8A-C9A-CAA
32	C	520	STE	C3-C4-C5-C6
32	B	601	STE	C1-C2-C3-C4
22	C	512	CLA	CBA-CGA-O2A-C1
32	B	621	STE	C2-C3-C4-C5
32	D	411	STE	C3-C4-C5-C6
33	B	627	LMG	C29-C30-C31-C32
22	b	605	CLA	C15-C16-C17-C18
30	H	102	DGD	C5A-C6A-C7A-C8A
32	H	103	STE	C7-C8-C9-C10
32	t	103	STE	C4-C5-C6-C7
33	C	516	LMG	C31-C32-C33-C34
33	Y	101	LMG	C30-C31-C32-C33
33	c	522	LMG	C12-C13-C14-C15
33	m	101	LMG	C37-C38-C39-C40
28	d	407	LHG	C32-C33-C34-C35
32	j	101	STE	C3-C4-C5-C6
22	c	506	CLA	C16-C17-C18-C20
29	a	411	SQD	O6-C44-C45-C46
30	A	415	DGD	C1G-C2G-C3G-O3G
33	B	627	LMG	O1-C7-C8-C9
33	C	516	LMG	O1-C7-C8-C9
33	Y	101	LMG	O1-C7-C8-C9
33	b	622	LMG	C7-C8-C9-O8
33	c	521	LMG	C7-C8-C9-O8
33	m	101	LMG	C7-C8-C9-O8
32	M	104	STE	C13-C14-C15-C16
32	M	104	STE	C15-C16-C17-C18
33	c	519	LMG	C32-C33-C34-C35
30	C	518	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
30	C	518	DGD	C5D-C6D-O5D-C1E
30	c	517	DGD	C2G-C3G-O3G-C1D
30	c	517	DGD	C5D-C6D-O5D-C1E
33	B	627	LMG	C8-C7-O1-C1
29	A	412	SQD	C17-C18-C19-C20
30	c	518	DGD	C6A-C7A-C8A-C9A
32	B	626	STE	C2-C3-C4-C5
32	b	624	STE	C13-C14-C15-C16
32	d	411	STE	C9-C10-C11-C12
22	c	507	CLA	C10-C11-C12-C13
32	E	102	STE	C3-C4-C5-C6
27	A	410	PL9	C29-C31-C32-C33
28	l	101	LHG	C35-C36-C37-C38
30	C	519	DGD	C3B-C4B-C5B-C6B
32	B	621	STE	C6-C7-C8-C9
32	T	102	STE	C4-C5-C6-C7
28	D	408	LHG	O1-C1-C2-O2
28	d	409	LHG	O1-C1-C2-O2
30	C	517	DGD	CDA-CEA-CFA-CGA
32	M	103	STE	C1-C2-C3-C4
33	B	627	LMG	O6-C5-C6-O5
32	b	620	STE	C12-C13-C14-C15
22	b	612	CLA	C8-C10-C11-C12
24	B	619	BCR	C11-C10-C9-C34
24	k	102	BCR	C35-C13-C14-C15
24	k	103	BCR	C35-C13-C14-C15
33	c	519	LMG	O6-C5-C6-O5
30	h	101	DGD	C5B-C6B-C7B-C8B
32	H	103	STE	C1-C2-C3-C4
27	d	406	PL9	C28-C29-C31-C32
30	H	102	DGD	C1A-C2A-C3A-C4A
29	A	414	SQD	C24-C23-O48-C46
32	c	520	STE	C9-C10-C11-C12
22	C	512	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	C15-C16-C17-C18
22	c	508	CLA	C16-C17-C18-C19
28	B	622	LHG	C27-C28-C29-C30
30	H	102	DGD	CDB-CEB-CFB-CGB
32	a	414	STE	C7-C8-C9-C10
33	c	522	LMG	C11-C12-C13-C14
22	C	512	CLA	O1A-CGA-O2A-C1
22	A	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	514	CLA	C13-C15-C16-C17
30	c	518	DGD	C7B-C8B-C9B-CAB
32	C	521	STE	C3-C4-C5-C6
32	I	101	STE	C1-C2-C3-C4
28	L	102	LHG	C19-C20-C21-C22
29	f	101	SQD	C35-C36-C37-C38
30	c	516	DGD	CBA-CCA-CDA-CEA
32	C	521	STE	C6-C7-C8-C9
29	a	411	SQD	C17-C18-C19-C20
32	M	102	STE	C11-C10-C9-C8
32	t	102	STE	C2-C3-C4-C5
32	t	104	STE	C10-C11-C12-C13
33	c	522	LMG	C20-C21-C22-C23
29	A	412	SQD	C24-C23-O48-C46
28	a	412	LHG	O6-C4-C5-O7
28	d	409	LHG	C33-C34-C35-C36
28	l	101	LHG	C17-C18-C19-C20
29	F	101	SQD	C25-C26-C27-C28
32	M	104	STE	C7-C8-C9-C10
22	B	607	CLA	C13-C15-C16-C17
29	a	411	SQD	C19-C20-C21-C22
33	D	407	LMG	C19-C20-C21-C22
29	A	414	SQD	C7-C8-C9-C10
24	C	515	BCR	C11-C10-C9-C8
24	b	619	BCR	C12-C13-C14-C15
24	b	619	BCR	C16-C17-C18-C19
22	c	509	CLA	CAA-CBA-CGA-O2A
22	B	602	CLA	C5-C6-C7-C8
30	c	517	DGD	CAB-CBB-CCB-CDB
32	B	621	STE	C12-C13-C14-C15
30	c	518	DGD	C1A-C2A-C3A-C4A
27	A	410	PL9	C12-C11-C9-C10
30	c	516	DGD	C4D-C5D-C6D-O5D
22	B	603	CLA	C11-C12-C13-C15
22	B	614	CLA	C6-C7-C8-C10
22	C	506	CLA	C12-C13-C15-C16
22	C	507	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	C	514	CLA	C11-C10-C8-C7
22	a	403	CLA	C12-C13-C15-C16
22	b	603	CLA	C11-C10-C8-C7
22	b	606	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	C11-C12-C13-C15
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C10-C8-C7
22	c	506	CLA	C12-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C12-C13-C15
22	d	404	CLA	C6-C7-C8-C10
22	B	616	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	C	513	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C10-C8-C9
22	B	605	CLA	C11-C12-C13-C14
22	B	616	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C14-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C9
22	b	603	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	b	612	CLA	C6-C7-C8-C9
22	b	615	CLA	C11-C12-C13-C14
22	b	616	CLA	C6-C7-C8-C9
22	c	502	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C10-C8-C9
22	c	508	CLA	C6-C7-C8-C9
22	c	510	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C10-C8-C9
22	c	513	CLA	C11-C12-C13-C14
22	c	510	CLA	CBD-CGD-O2D-CED
24	b	619	BCR	C14-C15-C16-C17
29	A	414	SQD	C16-C17-C18-C19
30	H	102	DGD	CCA-CDA-CEA-CFA
22	B	609	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C20
32	b	620	STE	C15-C16-C17-C18
28	a	412	LHG	C8-C7-O7-C5
28	A	411	LHG	C9-C10-C11-C12
28	A	413	LHG	C35-C36-C37-C38
28	L	102	LHG	C13-C14-C15-C16
29	A	412	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	I	101	STE	C2-C3-C4-C5
33	M	101	LMG	C39-C40-C41-C42
29	a	411	SQD	C24-C23-O48-C46
29	A	412	SQD	C24-C25-C26-C27
30	C	517	DGD	C3B-C4B-C5B-C6B
33	D	409	LMG	C35-C36-C37-C38
33	c	522	LMG	C39-C40-C41-C42
22	a	402	CLA	C2C-C3C-CAC-CBC
28	l	101	LHG	C12-C13-C14-C15
28	a	412	LHG	O6-C4-C5-C6
28	d	407	LHG	C27-C28-C29-C30
29	L	101	SQD	C14-C15-C16-C17
33	b	622	LMG	C22-C23-C24-C25
32	D	411	STE	C14-C15-C16-C17
32	H	103	STE	C11-C12-C13-C14
32	x	102	STE	C12-C13-C14-C15
33	c	521	LMG	C15-C16-C17-C18
24	T	101	BCR	C18-C19-C20-C21
27	a	410	PL9	C45-C44-C46-C47
29	B	623	SQD	C35-C36-C37-C38
22	c	507	CLA	C5-C6-C7-C8
22	c	508	CLA	C5-C6-C7-C8
29	A	414	SQD	C14-C15-C16-C17
22	b	602	CLA	C13-C15-C16-C17
22	B	602	CLA	C2A-CAA-CBA-CGA
28	A	411	LHG	C11-C10-C9-C8
29	a	411	SQD	C29-C30-C31-C32
24	T	101	BCR	C13-C14-C15-C16
33	D	407	LMG	C11-C12-C13-C14
33	b	622	LMG	C15-C16-C17-C18
22	B	604	CLA	C8-C10-C11-C12
32	d	411	STE	C6-C7-C8-C9
33	c	522	LMG	C13-C14-C15-C16
28	l	101	LHG	C9-C10-C11-C12
29	A	412	SQD	O6-C44-C45-C46
29	B	623	SQD	O6-C44-C45-C46
29	a	411	SQD	C44-C45-C46-O48
30	c	516	DGD	O1G-C1G-C2G-C3G
33	b	622	LMG	O1-C7-C8-C9
33	c	521	LMG	O1-C7-C8-C9
33	m	101	LMG	O9-C10-O7-C8
28	d	407	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C14-C15-C16-C17
22	D	404	CLA	O2A-C1-C2-C3
30	c	518	DGD	O6D-C5D-C6D-O5D
30	H	102	DGD	C3A-C4A-C5A-C6A
32	a	414	STE	C6-C7-C8-C9
33	D	409	LMG	C14-C15-C16-C17
33	c	522	LMG	C19-C20-C21-C22
22	C	511	CLA	C10-C11-C12-C13
27	a	410	PL9	C18-C19-C21-C22
32	b	626	STE	C12-C13-C14-C15
33	C	516	LMG	C33-C34-C35-C36
33	c	522	LMG	C36-C37-C38-C39
28	l	101	LHG	C10-C11-C12-C13
30	c	516	DGD	C2A-C3A-C4A-C5A
32	M	104	STE	C2-C3-C4-C5
22	b	602	CLA	O1D-CGD-O2D-CED
32	B	626	STE	C3-C4-C5-C6
22	B	615	CLA	C3-C5-C6-C7
28	d	409	LHG	C29-C30-C31-C32
30	C	518	DGD	CDB-CEB-CFB-CGB
30	C	519	DGD	CCB-CDB-CEB-CFB
32	M	104	STE	C1-C2-C3-C4
32	b	624	STE	C6-C7-C8-C9
33	D	407	LMG	C39-C40-C41-C42
22	b	614	CLA	CBA-CGA-O2A-C1
28	B	622	LHG	C18-C19-C20-C21
32	t	103	STE	C7-C8-C9-C10
22	b	613	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C12-C13-C15
22	B	604	CLA	C5-C6-C7-C8
28	D	408	LHG	C25-C26-C27-C28
30	c	516	DGD	C8B-C9B-CAB-CBB
33	C	516	LMG	C19-C20-C21-C22
29	F	101	SQD	C44-C45-C46-O48
32	b	626	STE	C14-C15-C16-C17
33	D	410	LMG	C37-C38-C39-C40
28	L	102	LHG	C32-C33-C34-C35
30	A	415	DGD	O2G-C2G-C3G-O3G
33	B	627	LMG	O1-C7-C8-O7
33	b	622	LMG	O1-C7-C8-O7
33	c	521	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
29	A	414	SQD	C25-C26-C27-C28
27	d	406	PL9	C34-C36-C37-C38
28	d	407	LHG	C13-C14-C15-C16
28	d	407	LHG	C34-C35-C36-C37
22	B	602	CLA	C2-C1-O2A-CGA
22	B	614	CLA	C2-C1-O2A-CGA
22	d	402	CLA	C2-C1-O2A-CGA
28	d	409	LHG	C32-C33-C34-C35
32	b	621	STE	C3-C4-C5-C6
22	c	503	CLA	C13-C15-C16-C17
22	C	507	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C12-C13-C14
33	d	410	LMG	C14-C15-C16-C17
30	c	517	DGD	C7B-C8B-C9B-CAB
32	E	102	STE	C6-C7-C8-C9
33	D	409	LMG	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C20
22	a	403	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C19
24	B	618	BCR	C5-C6-C7-C8
24	B	619	BCR	C23-C24-C25-C26
24	K	101	BCR	C23-C24-C25-C30
24	d	405	BCR	C23-C24-C25-C30
22	B	606	CLA	C13-C15-C16-C17
22	D	403	CLA	C13-C15-C16-C17
22	D	403	CLA	C15-C16-C17-C18
32	b	626	STE	C6-C7-C8-C9
29	f	101	SQD	C33-C34-C35-C36
30	C	518	DGD	C9B-CAB-CBB-CCB
32	D	411	STE	C4-C5-C6-C7
28	d	408	LHG	C24-C23-O8-C6
24	B	619	BCR	C11-C12-C13-C14
32	b	621	STE	C15-C16-C17-C18
32	x	102	STE	C1-C2-C3-C4
30	c	516	DGD	O1B-C1B-O2G-C2G
29	a	411	SQD	C8-C7-O47-C45
22	A	405	CLA	C5-C6-C7-C8
28	B	622	LHG	C24-C25-C26-C27
33	D	407	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	D	411	STE	C6-C7-C8-C9
32	M	102	STE	C4-C5-C6-C7
32	d	411	STE	C12-C13-C14-C15
33	D	409	LMG	C37-C38-C39-C40
22	c	509	CLA	C16-C17-C18-C19
22	d	402	CLA	C3-C5-C6-C7
28	A	413	LHG	C7-C8-C9-C10
30	C	518	DGD	CBA-CCA-CDA-CEA
30	H	102	DGD	C9B-CAB-CBB-CCB
32	T	102	STE	C11-C10-C9-C8
33	C	516	LMG	C14-C15-C16-C17
30	h	101	DGD	C2A-C3A-C4A-C5A
32	B	625	STE	C11-C10-C9-C8
22	B	604	CLA	C11-C10-C8-C7
22	B	605	CLA	C11-C12-C13-C15
22	B	605	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C15
22	B	614	CLA	C12-C13-C15-C16
22	B	616	CLA	C12-C13-C15-C16
22	C	507	CLA	C6-C7-C8-C10
22	b	602	CLA	C6-C7-C8-C10
22	b	609	CLA	C12-C13-C15-C16
22	b	612	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C10-C8-C7
22	b	614	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
22	c	508	CLA	C6-C7-C8-C10
22	c	510	CLA	C6-C7-C8-C10
22	c	510	CLA	C12-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C7
22	d	403	CLA	C11-C12-C13-C15
22	b	604	CLA	C3-C5-C6-C7
29	a	411	SQD	O10-C23-O48-C46
24	A	406	BCR	C9-C10-C11-C12
24	k	102	BCR	C19-C20-C21-C22
24	k	103	BCR	C19-C20-C21-C22
22	D	404	CLA	C16-C17-C18-C19
32	B	625	STE	C11-C12-C13-C14
22	C	514	CLA	C2C-C3C-CAC-CBC
32	D	411	STE	C9-C10-C11-C12
24	B	619	BCR	C16-C17-C18-C36
24	K	101	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
24	Z	101	BCR	C11-C10-C9-C34
24	c	515	BCR	C20-C21-C22-C37
24	d	405	BCR	C11-C10-C9-C34
24	d	405	BCR	C20-C21-C22-C37
24	t	101	BCR	C35-C13-C14-C15
24	x	101	BCR	C20-C21-C22-C37
29	A	414	SQD	C23-C24-C25-C26
29	L	101	SQD	C7-C8-C9-C10
22	B	611	CLA	C16-C17-C18-C19
22	C	503	CLA	CBA-CGA-O2A-C1
22	b	601	CLA	CBA-CGA-O2A-C1
30	c	518	DGD	C2A-C1A-O1G-C1G
28	A	411	LHG	C28-C29-C30-C31
32	B	626	STE	C11-C12-C13-C14
33	M	101	LMG	C22-C23-C24-C25
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	D	404	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
22	d	404	CLA	CAD-CBD-CGD-O2D
28	d	407	LHG	O9-C7-O7-C5
32	I	101	STE	C5-C6-C7-C8
32	Z	102	STE	C13-C14-C15-C16
33	d	410	LMG	C40-C41-C42-C43
24	C	501	BCR	C6-C7-C8-C9
22	D	404	CLA	CBA-CGA-O2A-C1
22	c	513	CLA	C4-C3-C5-C6
30	c	517	DGD	O6E-C1E-O5D-C6D
22	b	615	CLA	C13-C15-C16-C17
28	a	412	LHG	C4-C5-C6-O8
28	d	408	LHG	C4-C5-C6-O8
28	d	409	LHG	C2-C3-O3-P
30	C	517	DGD	O1G-C1G-C2G-C3G
33	M	101	LMG	C7-C8-C9-O8
33	Y	101	LMG	C7-C8-C9-O8
28	d	409	LHG	O10-C23-O8-C6
28	a	412	LHG	C10-C11-C12-C13
32	t	104	STE	C13-C14-C15-C16
22	A	405	CLA	C6-C7-C8-C9
29	F	101	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	C16-C17-C18-C19
29	A	414	SQD	C9-C10-C11-C12
33	b	622	LMG	C17-C18-C19-C20
33	m	101	LMG	C13-C14-C15-C16
22	B	608	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
28	d	408	LHG	C34-C35-C36-C37
30	A	415	DGD	CBB-CCB-CDB-CEB
32	b	621	STE	C12-C13-C14-C15
33	C	516	LMG	C34-C35-C36-C37
24	H	101	BCR	C20-C21-C22-C23
24	Z	101	BCR	C16-C17-C18-C19
24	c	515	BCR	C12-C13-C14-C15
30	c	517	DGD	C2E-C1E-O5D-C6D
33	M	101	LMG	C16-C17-C18-C19
28	a	412	LHG	O7-C5-C6-O8
30	C	517	DGD	O1G-C1G-C2G-O2G
30	c	516	DGD	O1G-C1G-C2G-O2G
33	M	101	LMG	O7-C8-C9-O8
33	Y	101	LMG	O1-C7-C8-O7
30	C	517	DGD	C7A-C8A-C9A-CAA
33	B	627	LMG	O10-C28-O8-C9
28	A	413	LHG	C19-C20-C21-C22
28	d	408	LHG	C15-C16-C17-C18
22	b	616	CLA	C11-C12-C13-C15
32	b	623	STE	C7-C8-C9-C10
22	C	506	CLA	C4-C3-C5-C6
33	B	627	LMG	C35-C36-C37-C38
22	b	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	d	408	LHG	O9-C7-O7-C5
22	B	605	CLA	C14-C13-C15-C16
22	B	614	CLA	C14-C13-C15-C16
28	D	408	LHG	C11-C12-C13-C14
33	M	101	LMG	C30-C31-C32-C33
22	c	505	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	O1A-CGA-O2A-C1
32	b	623	STE	C11-C10-C9-C8
22	b	605	CLA	C10-C11-C12-C13
29	a	411	SQD	C5-C6-S-O8
28	A	411	LHG	C13-C14-C15-C16
28	A	413	LHG	C26-C27-C28-C29
24	T	101	BCR	C7-C8-C9-C34
24	b	617	BCR	C7-C8-C9-C34
24	b	617	BCR	C11-C12-C13-C35
24	k	103	BCR	C7-C8-C9-C34
33	D	409	LMG	C11-C12-C13-C14
30	h	101	DGD	C3A-C4A-C5A-C6A
30	c	517	DGD	C8B-C9B-CAB-CBB
22	C	510	CLA	C2-C1-O2A-CGA
30	C	517	DGD	C8B-C9B-CAB-CBB
32	b	620	STE	C3-C4-C5-C6
24	c	514	BCR	C9-C10-C11-C12
28	L	102	LHG	C4-O6-P-O3
30	c	516	DGD	C8A-C9A-CAA-CBA
28	A	411	LHG	C14-C15-C16-C17
22	c	513	CLA	C2-C3-C5-C6
32	H	103	STE	C4-C5-C6-C7
22	B	611	CLA	C16-C17-C18-C20
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
22	d	404	CLA	C16-C17-C18-C19
22	B	608	CLA	C15-C16-C17-C18
22	C	507	CLA	C15-C16-C17-C18
28	l	101	LHG	O6-C4-C5-C6
29	B	623	SQD	C11-C12-C13-C14
30	C	517	DGD	O1G-C1A-C2A-C3A
22	c	509	CLA	C2A-CAA-CBA-CGA
22	C	510	CLA	C3-C5-C6-C7
32	E	102	STE	C7-C8-C9-C10
22	D	404	CLA	O1D-CGD-O2D-CED
30	C	518	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
32	I	101	STE	C7-C8-C9-C10
29	F	101	SQD	C31-C32-C33-C34
33	D	409	LMG	C30-C31-C32-C33
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	513	CLA	CAD-CBD-CGD-O1D
29	a	411	SQD	C5-C6-S-O7
29	a	411	SQD	C5-C6-S-O9
33	d	410	LMG	C11-C12-C13-C14
30	C	519	DGD	CCA-CDA-CEA-CFA
32	t	103	STE	C5-C6-C7-C8
22	b	611	CLA	C10-C11-C12-C13
28	l	101	LHG	C30-C31-C32-C33
33	D	409	LMG	C10-C11-C12-C13
33	M	101	LMG	C4-C5-C6-O5
29	F	101	SQD	C24-C23-O48-C46
28	d	408	LHG	C10-C11-C12-C13
22	b	610	CLA	C16-C17-C18-C20
22	B	603	CLA	C6-C7-C8-C10
22	B	608	CLA	C12-C13-C15-C16
22	B	609	CLA	C6-C7-C8-C10
22	B	617	CLA	C6-C7-C8-C10
22	C	505	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C12-C13-C15
22	C	513	CLA	C6-C7-C8-C10
22	a	403	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C12-C13-C15
22	b	604	CLA	C6-C7-C8-C10
22	b	605	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C15
22	b	607	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	c	505	CLA	C6-C7-C8-C10
22	c	508	CLA	C12-C13-C15-C16
22	c	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	a	404	PHO	C6-C7-C8-C10
28	A	413	LHG	C16-C17-C18-C19
22	c	508	CLA	C15-C16-C17-C18
28	L	102	LHG	C29-C30-C31-C32
29	L	101	SQD	C29-C30-C31-C32
22	B	615	CLA	C2A-CAA-CBA-CGA
22	C	502	CLA	C2A-CAA-CBA-CGA
22	d	402	CLA	C4C-C3C-CAC-CBC
28	A	413	LHG	C4-C5-C6-O8
30	c	516	DGD	C2E-C1E-O5D-C6D
34	E	101	HEC	C1A-C2A-CAA-CBA
34	E	101	HEC	C3A-C2A-CAA-CBA
28	A	413	LHG	O7-C5-C6-O8
33	b	622	LMG	O7-C8-C9-O8
33	m	101	LMG	O7-C8-C9-O8
30	A	415	DGD	C6A-C7A-C8A-C9A
22	d	403	CLA	C13-C15-C16-C17
32	b	625	STE	C4-C5-C6-C7
22	C	503	CLA	O1A-CGA-O2A-C1
33	c	522	LMG	C29-C30-C31-C32
33	m	101	LMG	O6-C5-C6-O5
22	D	404	CLA	C16-C17-C18-C20
28	A	411	LHG	C2-C3-O3-P
33	C	516	LMG	C39-C40-C41-C42
22	B	610	CLA	C4-C3-C5-C6
28	B	622	LHG	C24-C23-O8-C6
30	c	517	DGD	CDA-CEA-CFA-CGA
30	c	518	DGD	C5A-C6A-C7A-C8A
22	B	617	CLA	C6-C7-C8-C9
22	C	507	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C12-C13-C14
22	C	512	CLA	C6-C7-C8-C9
22	b	614	CLA	C11-C12-C13-C14
22	b	614	CLA	C14-C13-C15-C16
22	c	506	CLA	C6-C7-C8-C9
22	c	507	CLA	C6-C7-C8-C9
24	K	101	BCR	C22-C23-C24-C25
22	D	404	CLA	O1A-CGA-O2A-C1
29	a	411	SQD	C11-C12-C13-C14
29	a	411	SQD	C24-C25-C26-C27
27	A	410	PL9	C39-C41-C42-C43
30	h	101	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
32	M	103	STE	C7-C8-C9-C10
33	m	101	LMG	C33-C34-C35-C36
24	c	514	BCR	C36-C18-C19-C20
22	b	616	CLA	C10-C11-C12-C13
28	L	102	LHG	O10-C23-O8-C6
33	M	101	LMG	C19-C20-C21-C22
22	a	402	CLA	C4C-C3C-CAC-CBC
30	C	518	DGD	C3B-C4B-C5B-C6B
30	h	101	DGD	O2G-C1B-C2B-C3B
28	l	101	LHG	C28-C29-C30-C31
30	C	519	DGD	C4B-C5B-C6B-C7B
32	x	102	STE	C9-C10-C11-C12
33	C	516	LMG	C37-C38-C39-C40
28	B	622	LHG	C19-C20-C21-C22
22	B	603	CLA	C8-C10-C11-C12
32	B	624	STE	C5-C6-C7-C8
33	D	409	LMG	C7-C8-O7-C10
33	b	622	LMG	C9-C8-O7-C10
22	b	609	CLA	O1D-CGD-O2D-CED
22	A	402	CLA	C2-C1-O2A-CGA
22	D	402	CLA	C2-C1-O2A-CGA
29	A	414	SQD	C46-C45-O47-C7
22	C	514	CLA	C4C-C3C-CAC-CBC
22	b	616	CLA	C4C-C3C-CAC-CBC
30	c	517	DGD	CCA-CDA-CEA-CFA
33	c	521	LMG	C34-C35-C36-C37
30	H	102	DGD	CDA-CEA-CFA-CGA
28	A	411	LHG	C16-C17-C18-C19
24	x	101	BCR	C9-C10-C11-C12
32	C	520	STE	C4-C5-C6-C7
22	c	506	CLA	C2C-C3C-CAC-CBC
29	a	413	SQD	C31-C32-C33-C34
22	b	605	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	C2-C3-C5-C6
29	A	412	SQD	C12-C13-C14-C15
32	B	624	STE	C3-C4-C5-C6
33	D	409	LMG	C29-C28-O8-C9
29	a	413	SQD	C14-C15-C16-C17
32	H	103	STE	C10-C11-C12-C13
22	C	507	CLA	C16-C17-C18-C20
22	C	510	CLA	C16-C17-C18-C19
30	C	518	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
32	C	521	STE	C10-C11-C12-C13
27	A	410	PL9	C34-C36-C37-C38
33	c	521	LMG	O7-C8-C9-O8
28	d	408	LHG	C3-O3-P-O6
29	a	411	SQD	C11-C10-C9-C8
33	b	622	LMG	C30-C31-C32-C33
28	B	622	LHG	C33-C34-C35-C36
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
28	d	409	LHG	C4-C5-C6-O8
22	B	602	CLA	C4-C3-C5-C6
22	B	602	CLA	C6-C7-C8-C10
22	B	605	CLA	C11-C10-C8-C7
22	C	512	CLA	C6-C7-C8-C10
22	a	403	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
22	c	509	CLA	C11-C12-C13-C15
28	l	101	LHG	C11-C12-C13-C14
33	d	410	LMG	C35-C36-C37-C38
22	C	506	CLA	C6-C7-C8-C9
22	C	509	CLA	C14-C13-C15-C16
22	a	403	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
22	c	510	CLA	C6-C7-C8-C9
23	a	404	PHO	C6-C7-C8-C9
22	B	612	CLA	C16-C17-C18-C19
22	C	510	CLA	C16-C17-C18-C20
29	L	101	SQD	C10-C11-C12-C13
30	C	517	DGD	CCA-CDA-CEA-CFA
32	C	521	STE	C13-C14-C15-C16
32	C	521	STE	C4-C5-C6-C7
32	J	101	STE	C2-C3-C4-C5
32	M	104	STE	C11-C10-C9-C8
33	D	407	LMG	C33-C34-C35-C36
33	c	521	LMG	C13-C14-C15-C16
30	C	517	DGD	C4D-C5D-C6D-O5D
22	C	511	CLA	C16-C17-C18-C19
22	c	507	CLA	C16-C17-C18-C19
28	a	412	LHG	C2-C3-O3-P
30	H	102	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
32	B	626	STE	C9-C10-C11-C12
32	h	102	STE	C12-C13-C14-C15
30	H	102	DGD	CCB-CDB-CEB-CFB
30	c	517	DGD	CDB-CEB-CFB-CGB
32	H	103	STE	C15-C16-C17-C18
33	b	622	LMG	C36-C37-C38-C39
32	M	104	STE	C4-C5-C6-C7
30	C	518	DGD	O1B-C1B-O2G-C2G
27	d	406	PL9	C15-C14-C16-C17
30	C	517	DGD	O6D-C5D-C6D-O5D
33	D	410	LMG	O9-C10-C11-C12
28	L	102	LHG	C30-C31-C32-C33
32	t	102	STE	C3-C4-C5-C6
28	d	408	LHG	C31-C32-C33-C34
29	f	101	SQD	C29-C30-C31-C32
32	C	522	STE	C6-C7-C8-C9
33	D	407	LMG	C38-C39-C40-C41
22	B	616	CLA	C10-C11-C12-C13
22	B	617	CLA	O1A-CGA-O2A-C1
22	c	507	CLA	O1A-CGA-O2A-C1
33	c	519	LMG	C29-C28-O8-C9
28	B	622	LHG	C11-C10-C9-C8
24	b	619	BCR	C9-C10-C11-C12
24	t	101	BCR	C13-C14-C15-C16
22	B	604	CLA	O1D-CGD-O2D-CED
33	B	627	LMG	C21-C22-C23-C24
22	c	506	CLA	C13-C15-C16-C17
33	B	627	LMG	C22-C23-C24-C25
32	M	102	STE	C9-C10-C11-C12
33	c	521	LMG	C39-C40-C41-C42
27	a	410	PL9	C35-C34-C36-C37
32	M	102	STE	O1-C1-C2-C3
22	B	606	CLA	C10-C11-C12-C13
27	D	406	PL9	C28-C29-C31-C32
33	C	516	LMG	O10-C28-O8-C9
32	t	104	STE	C5-C6-C7-C8
22	C	513	CLA	C2-C1-O2A-CGA
22	b	615	CLA	C2-C1-O2A-CGA
32	b	626	STE	O1-C1-C2-C3
33	Y	101	LMG	O7-C8-C9-O8
29	A	414	SQD	C30-C31-C32-C33
32	T	102	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	D	410	LMG	C12-C13-C14-C15
22	c	512	CLA	C15-C16-C17-C18
32	x	102	STE	C13-C14-C15-C16
30	H	102	DGD	O1B-C1B-C2B-C3B
28	L	102	LHG	C15-C16-C17-C18
22	C	502	CLA	CBA-CGA-O2A-C1
30	A	415	DGD	CEB-CFB-CGB-CHB
34	v	201	HEC	CAD-CBD-CGD-O1D
28	A	413	LHG	C28-C29-C30-C31
30	C	518	DGD	C5A-C6A-C7A-C8A
32	b	621	STE	C11-C10-C9-C8
33	Y	101	LMG	C38-C39-C40-C41
22	B	602	CLA	C14-C13-C15-C16
22	B	615	CLA	C6-C7-C8-C9
22	C	505	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C12-C13-C14
22	D	403	CLA	C14-C13-C15-C16
22	b	601	CLA	C14-C13-C15-C16
22	b	603	CLA	C14-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	C	508	CLA	C16-C17-C18-C20
32	b	625	STE	C5-C6-C7-C8
24	k	103	BCR	C20-C21-C22-C37
30	C	519	DGD	C4A-C5A-C6A-C7A
22	c	512	CLA	C2A-CAA-CBA-CGA
32	H	103	STE	C12-C13-C14-C15
32	M	104	STE	C10-C11-C12-C13
33	d	410	LMG	C29-C30-C31-C32
22	c	511	CLA	C16-C17-C18-C20
22	b	601	CLA	O2A-C1-C2-C3
30	A	415	DGD	C4E-C5E-C6E-O5E
28	d	408	LHG	C25-C26-C27-C28
32	J	101	STE	O1-C1-C2-C3
32	c	520	STE	O1-C1-C2-C3
22	c	510	CLA	O1D-CGD-O2D-CED
32	D	411	STE	O1-C1-C2-C3
34	V	201	HEC	CAD-CBD-CGD-O2D
29	B	623	SQD	C44-C45-O47-C7
33	B	627	LMG	C9-C8-O7-C10
22	d	403	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	CBA-CGA-O2A-C1
28	A	411	LHG	C31-C32-C33-C34
30	h	101	DGD	C7A-C8A-C9A-CAA
22	B	604	CLA	C12-C13-C15-C16
22	B	607	CLA	C12-C13-C15-C16
22	B	612	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C12-C13-C15
22	d	403	CLA	C12-C13-C15-C16
22	b	614	CLA	C13-C15-C16-C17
22	c	506	CLA	C10-C11-C12-C13
22	C	502	CLA	O1A-CGA-O2A-C1
32	B	624	STE	O1-C1-C2-C3
32	b	626	STE	O2-C1-C2-C3
22	b	610	CLA	C15-C16-C17-C18
28	A	411	LHG	C26-C27-C28-C29
28	d	407	LHG	O1-C1-C2-O2
22	b	601	CLA	C10-C11-C12-C13
22	c	512	CLA	C5-C6-C7-C8
29	L	101	SQD	C26-C27-C28-C29
28	l	101	LHG	O6-C4-C5-O7
32	B	624	STE	O2-C1-C2-C3
32	J	101	STE	O2-C1-C2-C3
27	a	410	PL9	C32-C33-C34-C35
28	a	412	LHG	C28-C29-C30-C31
22	C	508	CLA	C16-C17-C18-C19
22	c	509	CLA	C16-C17-C18-C20
22	b	601	CLA	C8-C10-C11-C12
22	C	513	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
30	A	415	DGD	CDB-CEB-CFB-CGB
22	B	610	CLA	C2-C3-C5-C6
27	a	410	PL9	C33-C34-C36-C37
32	M	102	STE	O2-C1-C2-C3
34	V	201	HEC	CAD-CBD-CGD-O1D
32	B	626	STE	C10-C11-C12-C13
28	A	411	LHG	C23-C24-C25-C26
22	c	511	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
32	b	623	STE	C2-C3-C4-C5
33	b	622	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
22	c	505	CLA	O1D-CGD-O2D-CED
33	B	627	LMG	C30-C31-C32-C33
33	B	627	LMG	C42-C43-C44-C45
24	C	501	BCR	C9-C10-C11-C12
32	c	520	STE	O2-C1-C2-C3
28	d	409	LHG	C23-C24-C25-C26
22	b	608	CLA	C16-C17-C18-C19
33	B	627	LMG	C18-C19-C20-C21
34	v	201	HEC	CAD-CBD-CGD-O2D
22	B	602	CLA	C2-C3-C5-C6
33	D	410	LMG	O7-C10-C11-C12
22	A	403	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	C	514	CLA	C6-C7-C8-C9
22	a	405	CLA	C6-C7-C8-C9
30	h	101	DGD	O1A-C1A-O1G-C1G
30	c	518	DGD	CBA-CCA-CDA-CEA
33	b	622	LMG	C14-C15-C16-C17
32	D	411	STE	O2-C1-C2-C3
28	l	101	LHG	C34-C35-C36-C37
29	f	101	SQD	C27-C28-C29-C30
30	H	102	DGD	O2G-C1B-C2B-C3B
32	B	621	STE	C7-C8-C9-C10
28	L	102	LHG	C11-C12-C13-C14
22	b	601	CLA	C16-C17-C18-C20
30	A	415	DGD	C6B-C7B-C8B-C9B
30	A	415	DGD	O1A-C1A-O1G-C1G
24	k	102	BCR	C23-C24-C25-C30
24	k	103	BCR	C23-C24-C25-C30
22	B	605	CLA	C10-C11-C12-C13
22	c	503	CLA	C15-C16-C17-C18
33	D	410	LMG	C36-C37-C38-C39
32	J	101	STE	C4-C5-C6-C7
29	B	623	SQD	C10-C11-C12-C13
24	T	101	BCR	C9-C10-C11-C12
22	c	508	CLA	C4-C3-C5-C6
27	A	410	PL9	C30-C29-C31-C32
27	a	410	PL9	C40-C39-C41-C42
24	k	102	BCR	C21-C22-C23-C24
22	c	504	CLA	C10-C11-C12-C13
33	c	519	LMG	C40-C41-C42-C43
22	c	512	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	l	101	LHG	C13-C14-C15-C16
30	c	517	DGD	C9A-CAA-CBA-CCA
27	A	410	PL9	C7-C8-C9-C11
28	A	411	LHG	C35-C36-C37-C38
29	a	413	SQD	C9-C10-C11-C12
22	B	606	CLA	C8-C10-C11-C12
22	c	504	CLA	C8-C10-C11-C12
28	A	411	LHG	O6-C4-C5-O7
32	E	102	STE	O2-C1-C2-C3
22	b	601	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	CBA-CGA-O2A-C1
33	b	622	LMG	C24-C25-C26-C27
33	B	627	LMG	C11-C12-C13-C14
22	C	513	CLA	C2-C3-C5-C6
22	D	402	CLA	C12-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C10-C8-C7
22	c	508	CLA	C2-C3-C5-C6
27	D	406	PL9	C13-C14-C16-C17
22	c	511	CLA	CBA-CGA-O2A-C1
22	B	603	CLA	C15-C16-C17-C18
32	B	626	STE	C7-C8-C9-C10
32	L	103	STE	C3-C4-C5-C6
22	B	616	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	C13-C15-C16-C17
28	l	101	LHG	O7-C7-C8-C9
32	Z	102	STE	C14-C15-C16-C17
22	B	614	CLA	C16-C17-C18-C19
32	L	103	STE	C6-C7-C8-C9
30	C	519	DGD	C2A-C1A-O1G-C1G
22	c	513	CLA	C2C-C3C-CAC-CBC
23	a	404	PHO	C4C-C3C-CAC-CBC
24	A	406	BCR	C20-C21-C22-C37
24	B	619	BCR	C35-C13-C14-C15
24	K	101	BCR	C35-C13-C14-C15
29	B	623	SQD	C24-C25-C26-C27
22	D	404	CLA	C4-C3-C5-C6
22	a	405	CLA	C4-C3-C5-C6
22	c	508	CLA	C10-C11-C12-C13
22	a	405	CLA	C2-C3-C5-C6
30	A	415	DGD	CFA-CGA-CHA-CIA

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Mol	Chain	Res	Type	Atoms
32	x	102	STE	C15-C16-C17-C18
30	c	516	DGD	O1G-C1A-C2A-C3A
22	B	609	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	b	610	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	512	CLA	C14-C13-C15-C16
23	a	404	PHO	C14-C13-C15-C16
30	c	518	DGD	CDA-CEA-CFA-CGA
32	h	102	STE	C10-C11-C12-C13
33	m	101	LMG	O8-C28-C29-C30
22	B	617	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
29	B	623	SQD	C46-C45-O47-C7
33	C	516	LMG	C7-C8-O7-C10
22	b	616	CLA	C2C-C3C-CAC-CBC
22	c	513	CLA	C2-C1-O2A-CGA
22	B	614	CLA	CAA-CBA-CGA-O2A
28	a	412	LHG	O8-C23-C24-C25
29	a	411	SQD	O47-C7-C8-C9
33	d	410	LMG	O7-C10-C11-C12
30	H	102	DGD	C9A-CAA-CBA-CCA
32	k	101	STE	C7-C8-C9-C10
27	D	406	PL9	C45-C44-C46-C47
22	c	507	CLA	C16-C17-C18-C20
32	t	104	STE	O2-C1-C2-C3
30	C	519	DGD	O6D-C5D-C6D-O5D
27	A	410	PL9	C12-C11-C9-C8
24	A	406	BCR	C17-C18-C19-C20
23	D	401	PHO	C2C-C3C-CAC-CBC
23	a	404	PHO	C2C-C3C-CAC-CBC
22	B	616	CLA	CBA-CGA-O2A-C1
22	c	509	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
32	C	522	STE	C5-C6-C7-C8
22	B	603	CLA	O2A-C1-C2-C3
22	C	514	CLA	O2A-C1-C2-C3
22	b	613	CLA	O2A-C1-C2-C3
23	A	404	PHO	O2A-C1-C2-C3
23	a	404	PHO	O2A-C1-C2-C3
29	B	623	SQD	C9-C10-C11-C12
22	B	604	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
22	C	508	CLA	C5-C6-C7-C8
22	C	507	CLA	C16-C17-C18-C19
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O1D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	D	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CHA-CBD-CGD-O1D
22	c	506	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
24	t	101	BCR	C9-C10-C11-C12
28	A	411	LHG	O6-C4-C5-C6
28	A	413	LHG	C18-C19-C20-C21
32	L	103	STE	C4-C5-C6-C7
29	A	412	SQD	O47-C7-C8-C9
28	L	102	LHG	C34-C35-C36-C37
29	A	412	SQD	O47-C45-C46-O48
28	a	412	LHG	C19-C20-C21-C22
33	B	627	LMG	C13-C14-C15-C16
32	I	101	STE	C10-C11-C12-C13
33	d	410	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
23	D	401	PHO	CHA-CBD-CGD-O2D
23	a	404	PHO	CHA-CBD-CGD-O1D
28	d	408	LHG	O1-C1-C2-O2
22	B	602	CLA	C11-C10-C8-C7
22	C	513	CLA	C12-C13-C15-C16
22	D	402	CLA	C6-C7-C8-C10
22	a	405	CLA	C12-C13-C15-C16
22	C	510	CLA	C10-C11-C12-C13
22	B	613	CLA	CAA-CBA-CGA-O2A
32	t	104	STE	O1-C1-C2-C3
22	c	511	CLA	O1A-CGA-O2A-C1
22	d	403	CLA	C4C-C3C-CAC-CBC
22	B	605	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C12-C13-C14
22	a	405	CLA	C11-C10-C8-C9
22	b	601	CLA	C6-C7-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	c	508	CLA	C14-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C9
22	d	404	CLA	C6-C7-C8-C9
27	a	410	PL9	C29-C31-C32-C33
29	L	101	SQD	C9-C10-C11-C12
24	C	501	BCR	C14-C15-C16-C17
32	T	102	STE	C5-C6-C7-C8
22	C	513	CLA	C13-C15-C16-C17
22	b	605	CLA	C8-C10-C11-C12
33	B	627	LMG	C11-C10-O7-C8
32	E	102	STE	O1-C1-C2-C3
22	b	614	CLA	C2A-CAA-CBA-CGA
27	A	410	PL9	C46-C47-C48-C49
29	f	101	SQD	C30-C31-C32-C33
30	C	517	DGD	O1B-C1B-C2B-C3B
22	B	614	CLA	C16-C17-C18-C20
22	b	612	CLA	CAA-CBA-CGA-O2A
33	m	101	LMG	C15-C16-C17-C18
28	a	412	LHG	O10-C23-C24-C25
28	d	409	LHG	O10-C23-C24-C25
24	b	619	BCR	C21-C22-C23-C24
32	d	411	STE	C11-C10-C9-C8
22	B	603	CLA	C1A-C2A-CAA-CBA
29	a	413	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
28	L	102	LHG	C9-C10-C11-C12
22	B	614	CLA	CAA-CBA-CGA-O1A
32	t	102	STE	O2-C1-C2-C3
22	c	508	CLA	CBD-CGD-O2D-CED
27	d	406	PL9	C30-C29-C31-C32
32	b	624	STE	O2-C1-C2-C3
32	B	625	STE	C14-C15-C16-C17
28	L	102	LHG	C4-O6-P-O5
28	d	408	LHG	C4-O6-P-O5
32	D	411	STE	C2-C3-C4-C5
22	B	613	CLA	CAA-CBA-CGA-O1A
22	b	613	CLA	C13-C15-C16-C17
24	K	101	BCR	C23-C24-C25-C26
32	t	102	STE	O1-C1-C2-C3
22	d	403	CLA	C16-C17-C18-C20
32	b	621	STE	C5-C6-C7-C8
24	C	515	BCR	C10-C11-C12-C13
32	x	102	STE	O2-C1-C2-C3
22	C	513	CLA	C16-C17-C18-C19
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	608	CLA	CAD-CBD-CGD-O1D
22	B	610	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O1D
22	a	403	CLA	CAD-CBD-CGD-O1D
22	b	609	CLA	CAD-CBD-CGD-O1D
22	b	611	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
29	B	623	SQD	O5-C5-C6-S
33	C	516	LMG	C9-C8-O7-C10
28	l	101	LHG	O10-C23-O8-C6
29	B	623	SQD	O10-C23-O48-C46
22	A	402	CLA	C14-C13-C15-C16
22	B	604	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C12-C13-C14
22	C	513	CLA	C11-C12-C13-C14
22	b	607	CLA	C14-C13-C15-C16
28	A	411	LHG	C29-C30-C31-C32
32	x	102	STE	C7-C8-C9-C10
28	L	102	LHG	O7-C7-C8-C9
30	C	517	DGD	O2G-C1B-C2B-C3B
32	b	624	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	b	626	STE	C9-C10-C11-C12
32	C	520	STE	C7-C8-C9-C10
33	B	627	LMG	C34-C35-C36-C37
22	B	602	CLA	CAA-CBA-CGA-O2A
30	c	517	DGD	O2G-C1B-C2B-C3B
34	e	101	HEC	CAD-CBD-CGD-O2D
22	c	502	CLA	C4C-C3C-CAC-CBC
33	d	410	LMG	C30-C31-C32-C33
23	a	404	PHO	C5-C6-C7-C8
22	B	604	CLA	C11-C12-C13-C15
22	B	614	CLA	C11-C12-C13-C15
22	B	616	CLA	C11-C12-C13-C15
22	a	402	CLA	C11-C10-C8-C7
22	a	405	CLA	C11-C10-C8-C7
22	b	601	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C12-C13-C15
22	b	605	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
23	d	401	PHO	C3A-C2A-CAA-CBA
32	b	626	STE	C15-C16-C17-C18
33	m	101	LMG	C12-C13-C14-C15
24	c	514	BCR	C21-C22-C23-C24
29	f	101	SQD	C32-C33-C34-C35
22	B	602	CLA	CAA-CBA-CGA-O1A
28	A	411	LHG	O10-C23-C24-C25
34	e	101	HEC	CAD-CBD-CGD-O1D
22	b	612	CLA	C10-C11-C12-C13
27	D	406	PL9	C46-C47-C48-C49
22	b	612	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	C8-C10-C11-C12
30	c	516	DGD	CCB-CDB-CEB-CFB
28	d	407	LHG	C18-C19-C20-C21

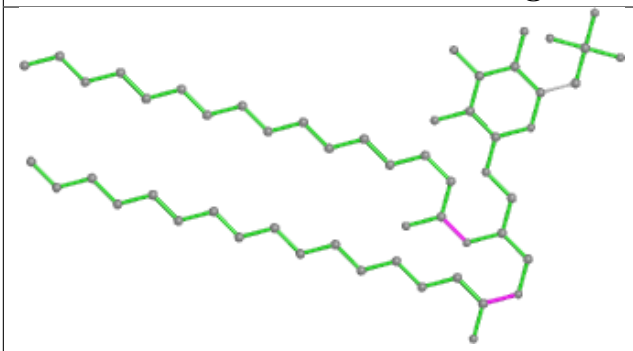
There are no ring outliers.

No monomer is involved in short contacts.

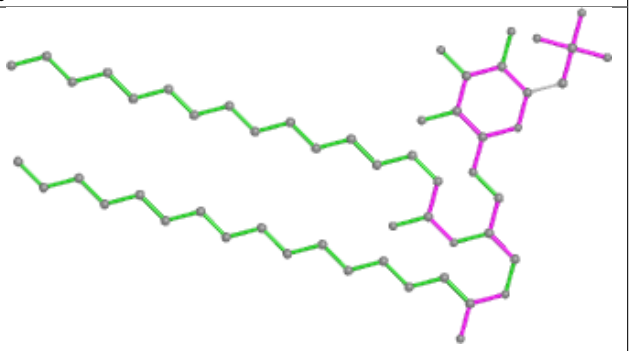
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

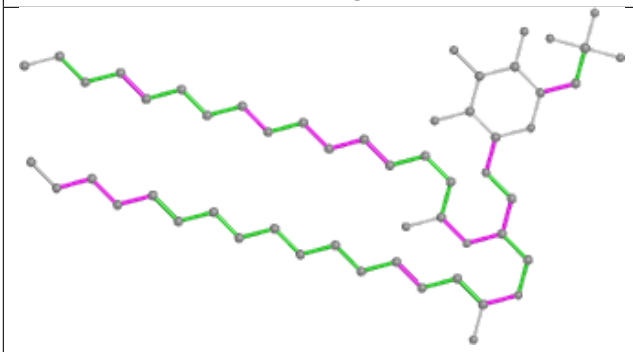
Ligand SQD B 623



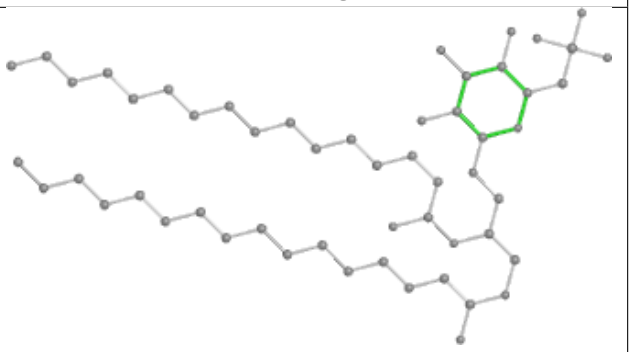
Bond lengths



Bond angles



Torsions



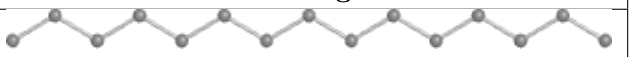
Rings

Ligand STE B 626

Bond lengths

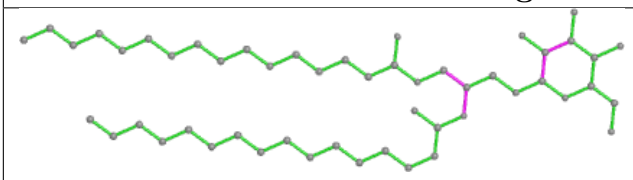
Bond angles

Torsions

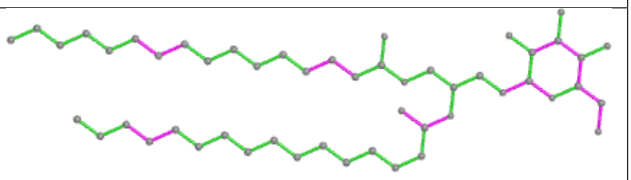


Rings

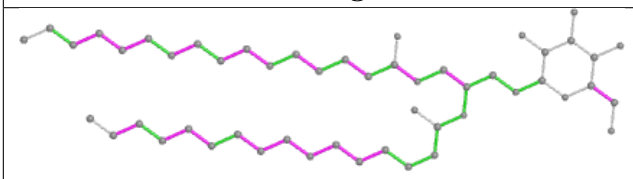
Ligand LMG M 101



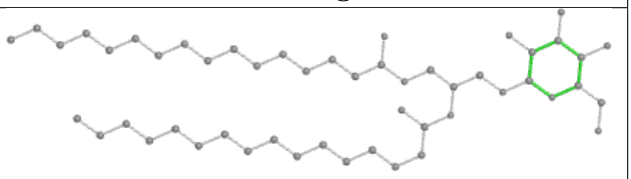
Bond lengths



Bond angles

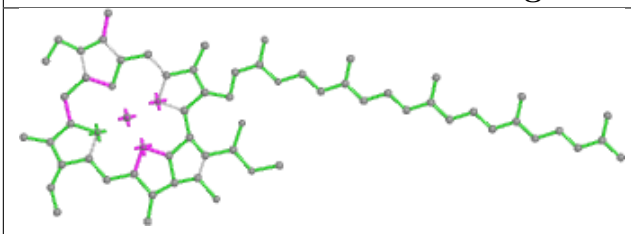


Torsions

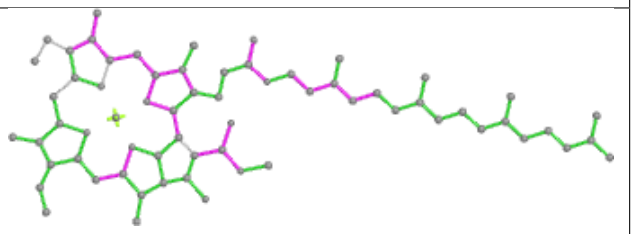


Rings

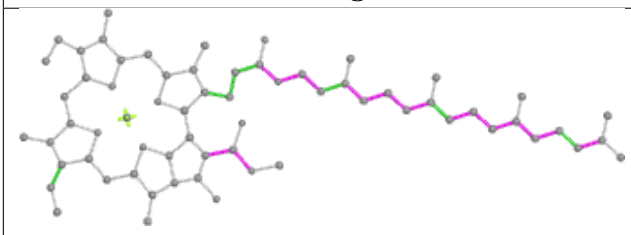
Ligand CLA C 513



Bond lengths



Bond angles



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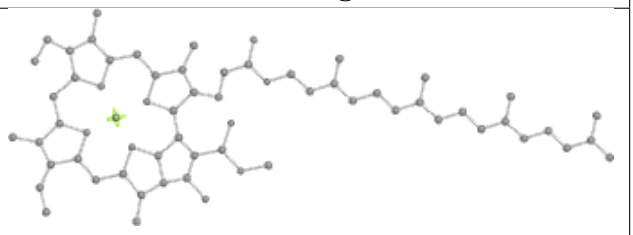
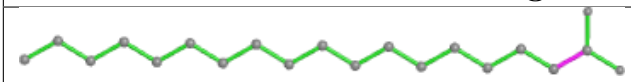
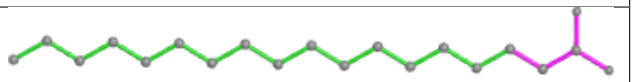


Rings

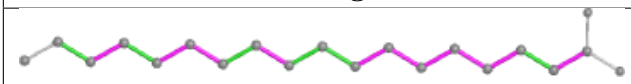
Ligand STE D 411



Bond lengths



Bond angles



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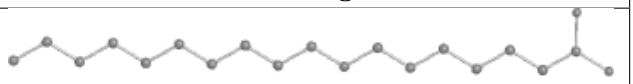
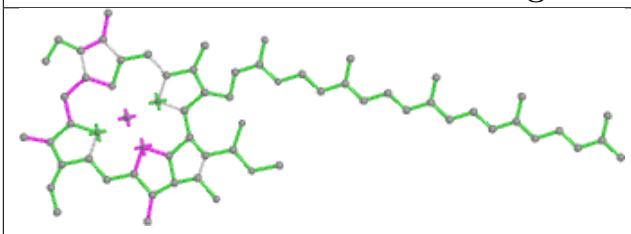
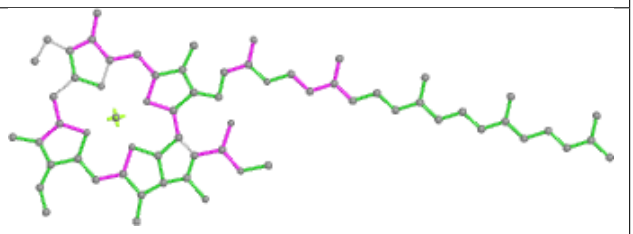


Rings

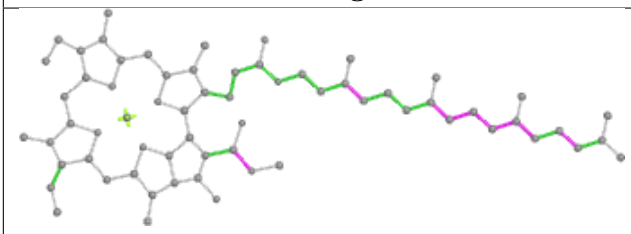
Ligand CLA b 605



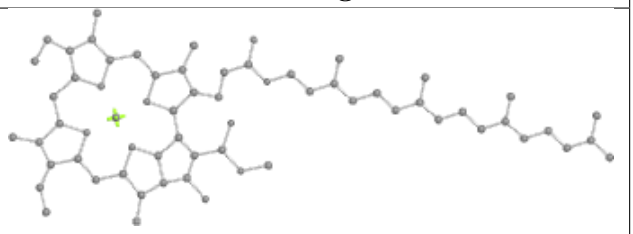
Bond lengths



Bond angles

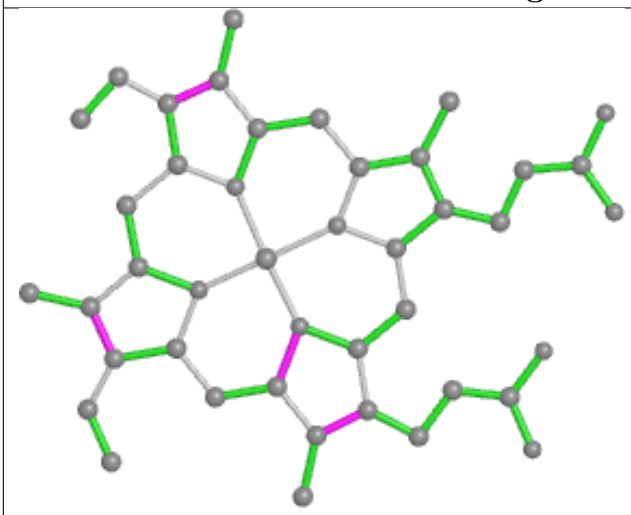


Torsions

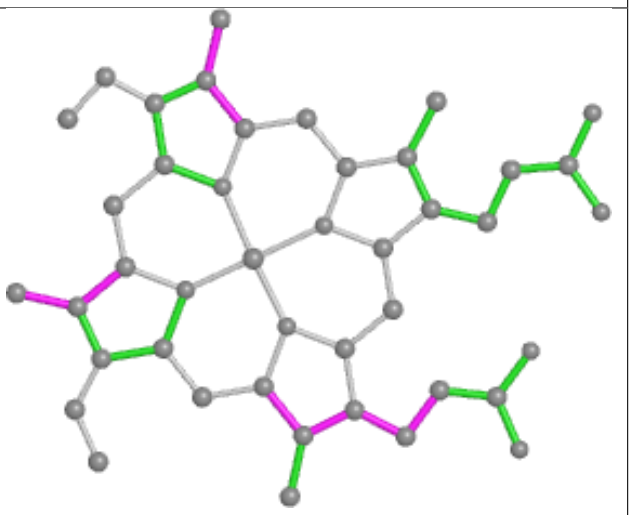


Rings

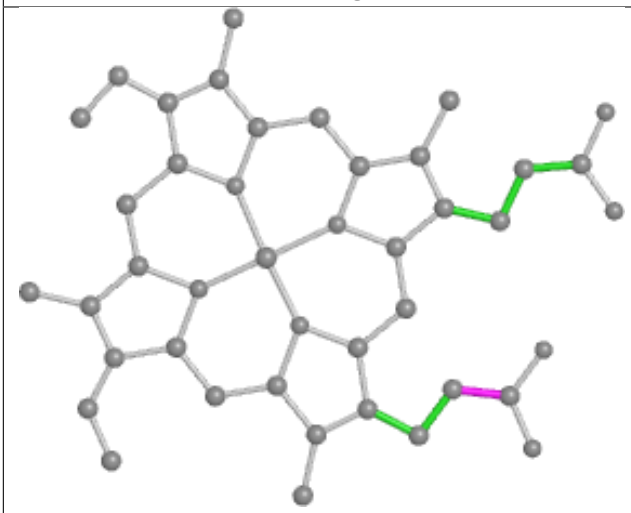
Ligand HEC v 201



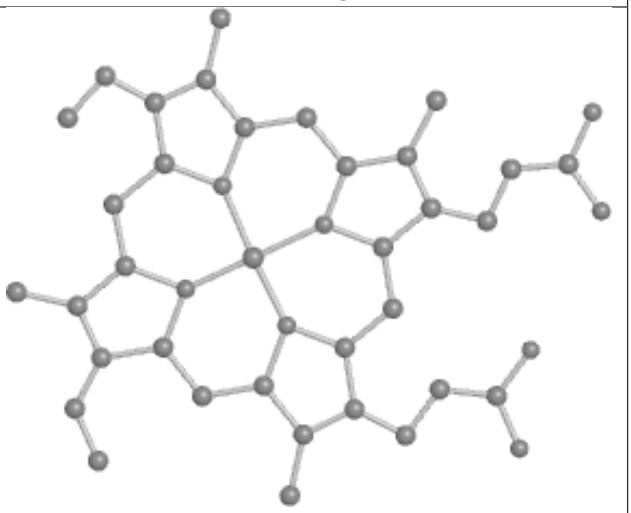
Bond lengths



Bond angles

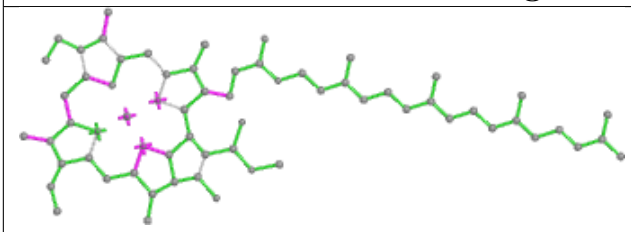


Torsions



Rings

Ligand CLA A 402



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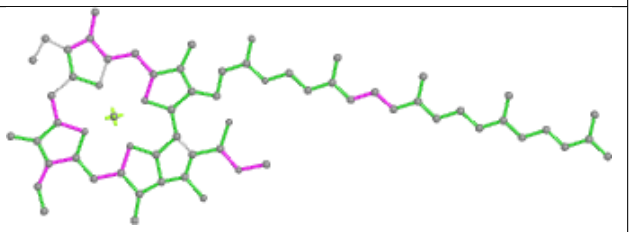

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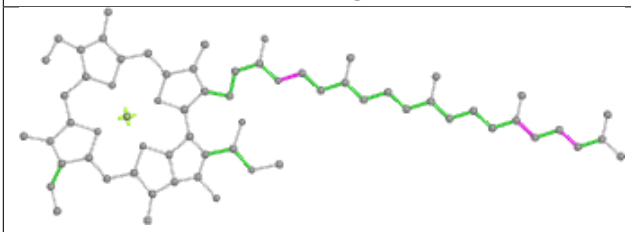

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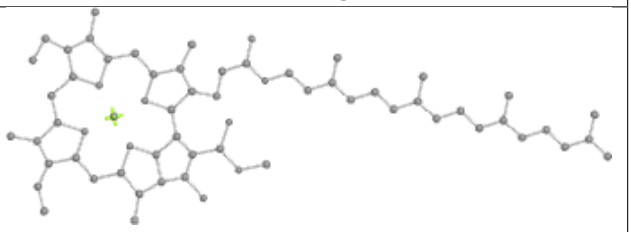
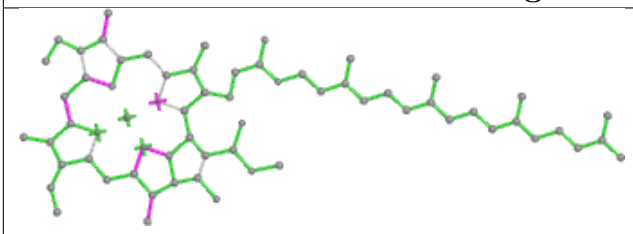


Rings

Ligand CLA B 612



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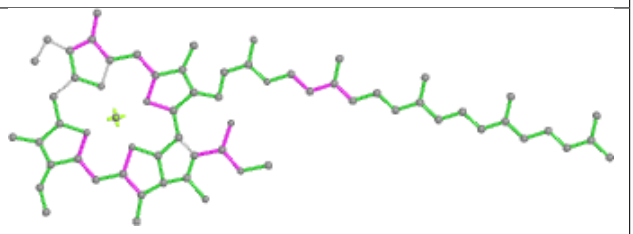

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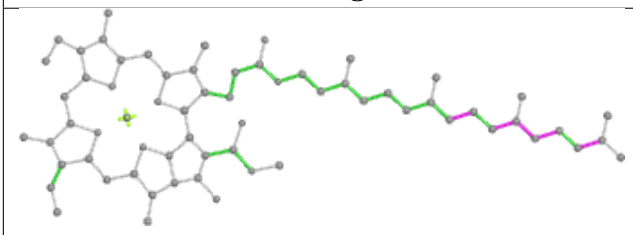

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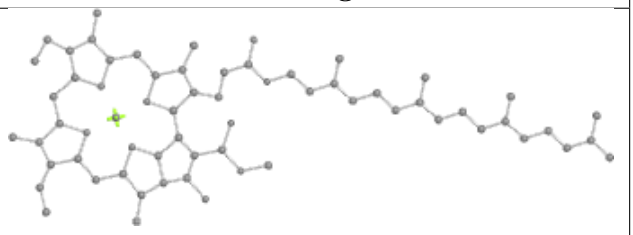
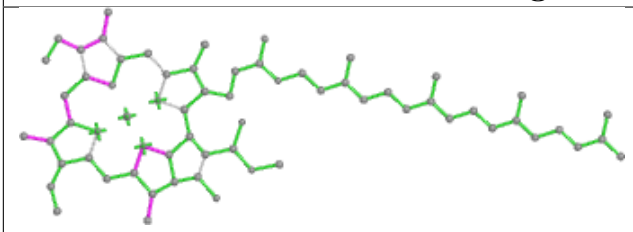


Rings

Ligand CLA c 512



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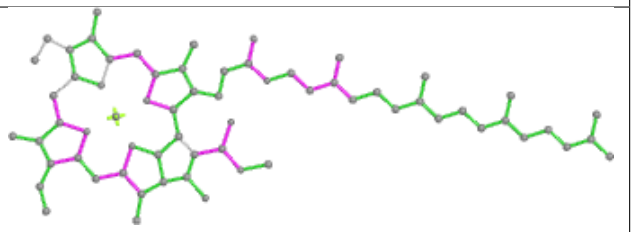
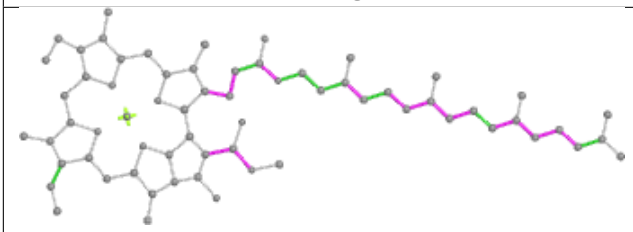


Bond angles



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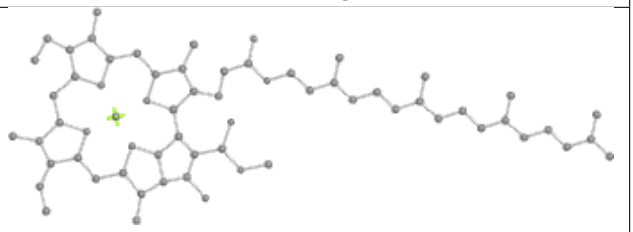
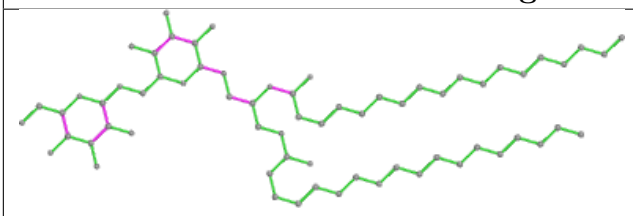


Rings

Ligand DGD A 415



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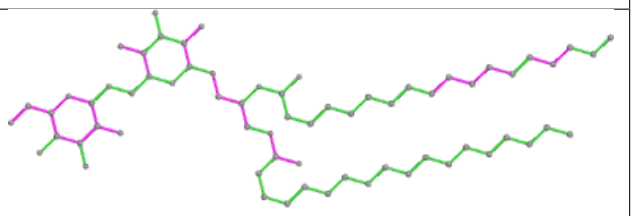
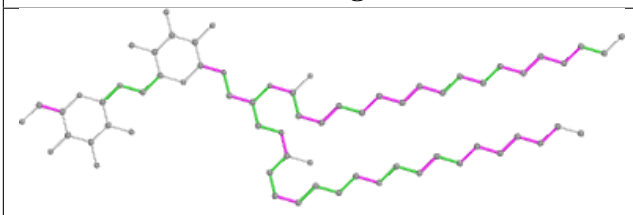


Bond angles



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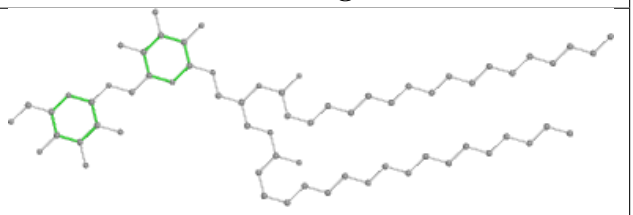
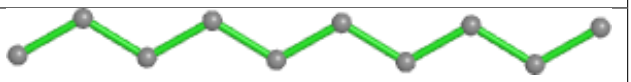


Rings

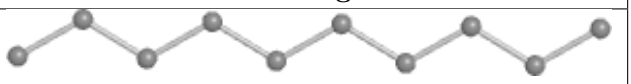
Ligand STE b 625

Bond lengths



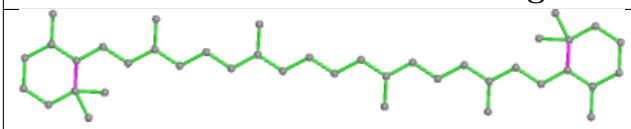
Bond angles

Torsions



Rings

Ligand BCR c 514



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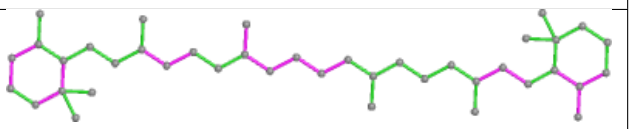
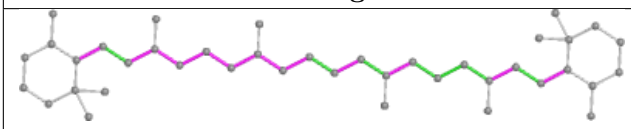


Bond angles



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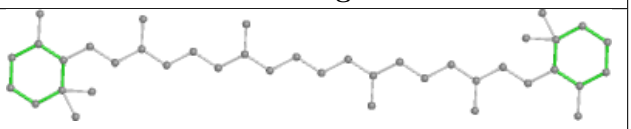
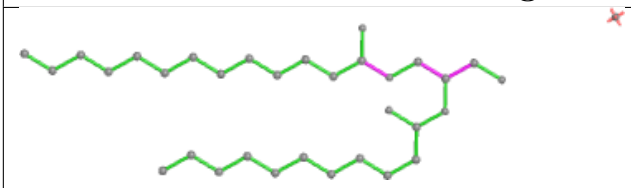


Rings

Ligand LMG D 409



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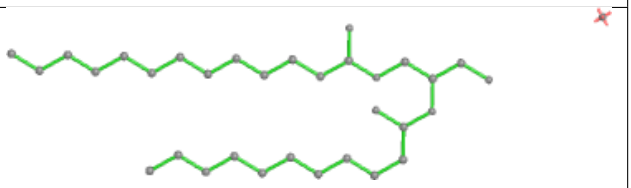
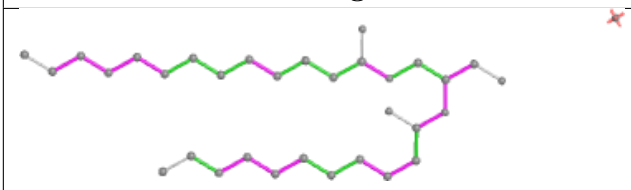


Bond angles



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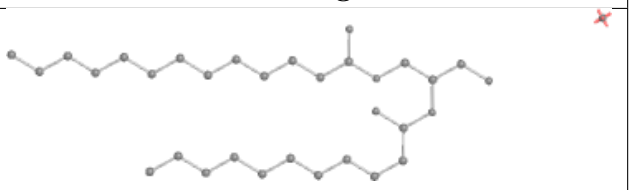
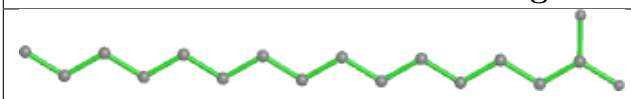


Rings

Ligand STE d 411



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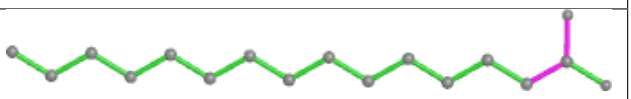
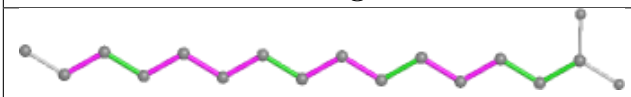
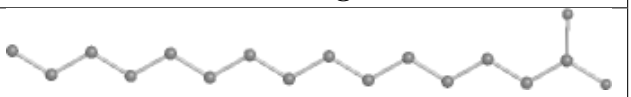


Bond angles

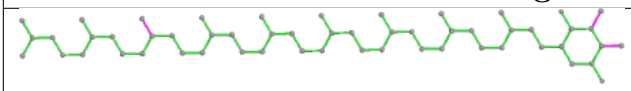


Torsions



Rings

Ligand PL9 a 410



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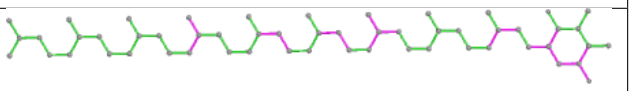
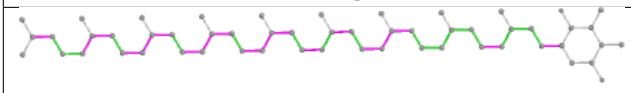


Bond angles



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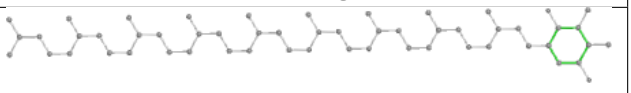
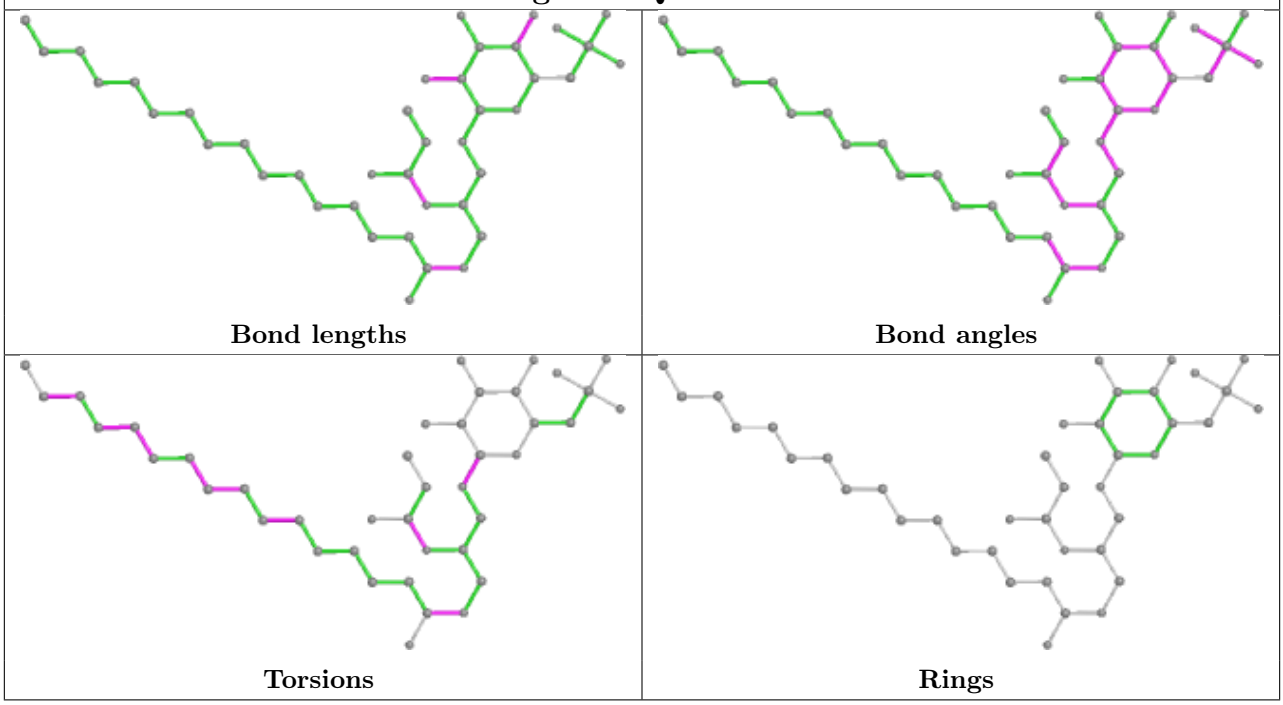
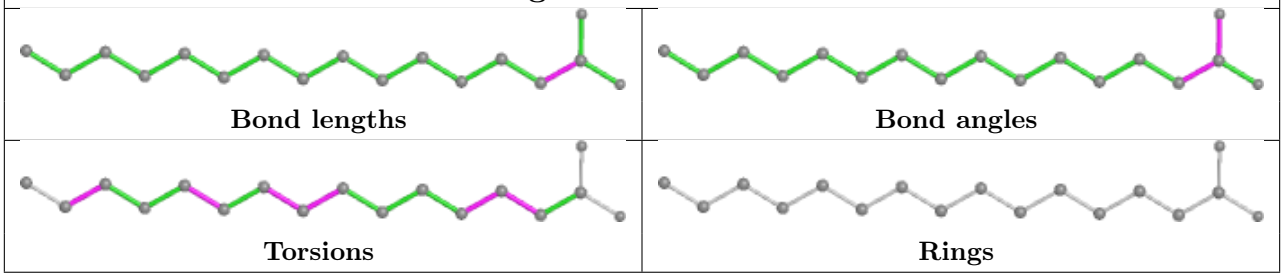


Rings

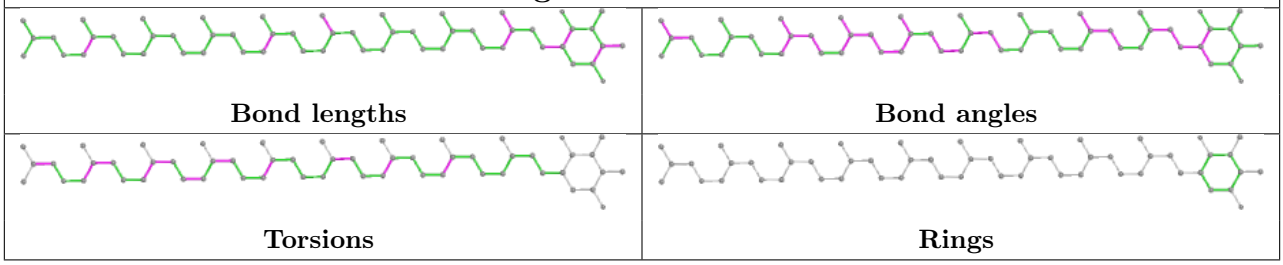
Ligand SQD f 101



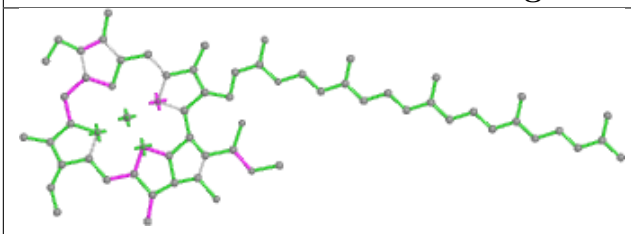
Ligand STE B 621



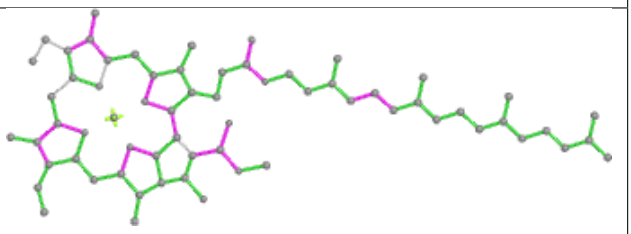
Ligand PL9 d 406



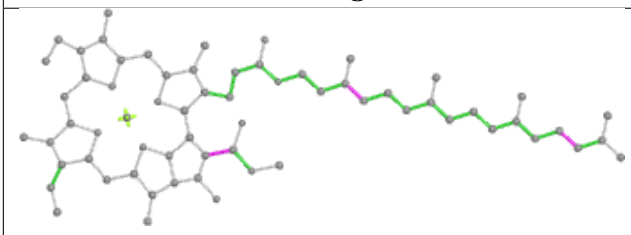
Ligand CLA B 610



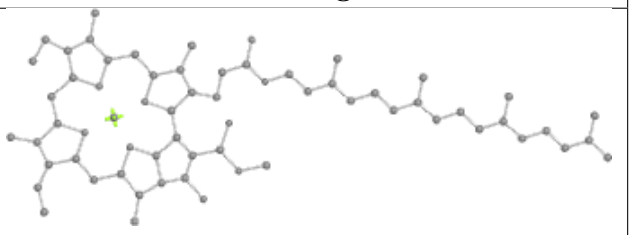
Bond lengths



Bond angles



Torsions

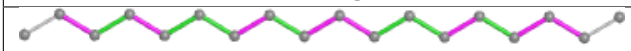


Rings

Ligand STE M 104

Bond lengths

Bond angles



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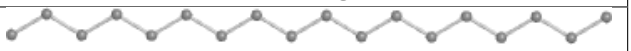
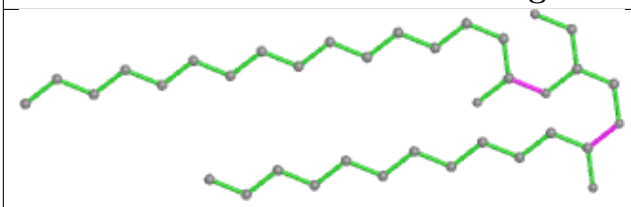
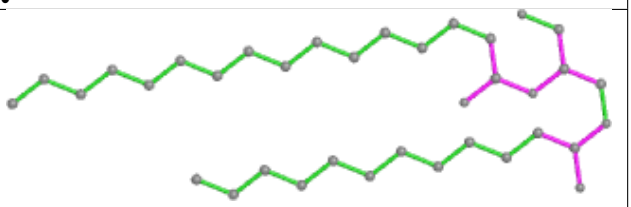


Rings

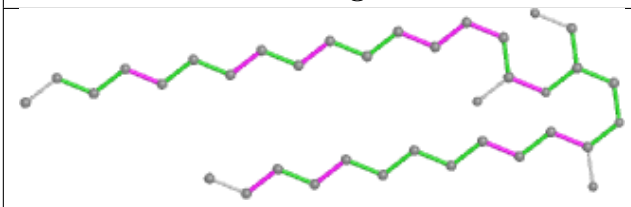
Ligand SQD a 413



Bond lengths



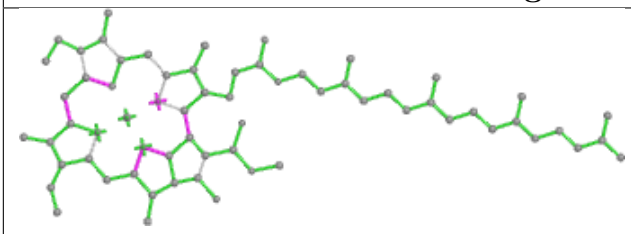
Bond angles



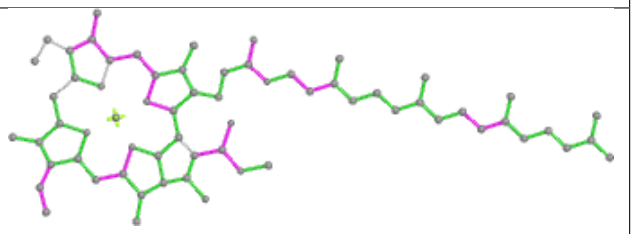
Torsions

Rings

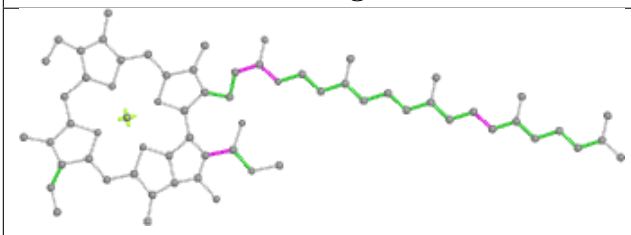
Ligand CLA B 613



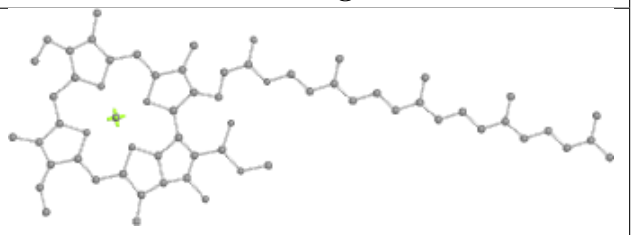
Bond lengths



Bond angles

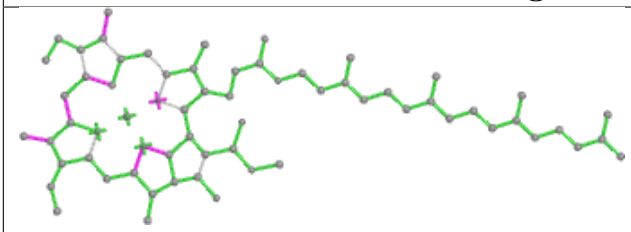


Torsions

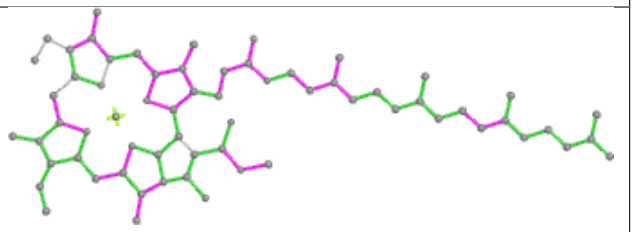


Rings

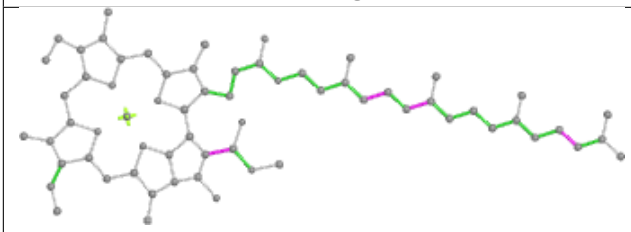
Ligand CLA b 604



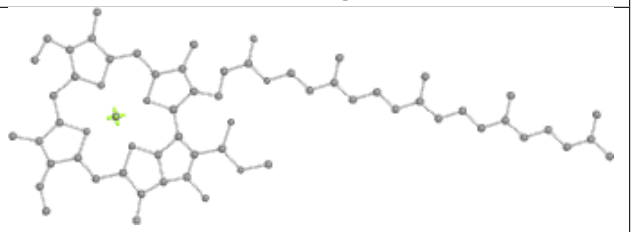
Bond lengths



Bond angles

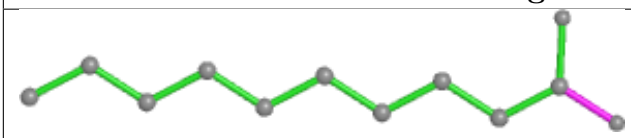


Torsions



Rings

Ligand STE B 624



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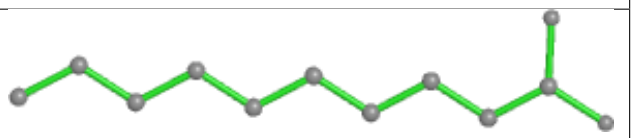
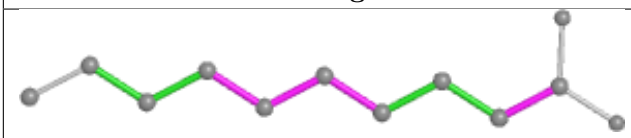


Bond angles



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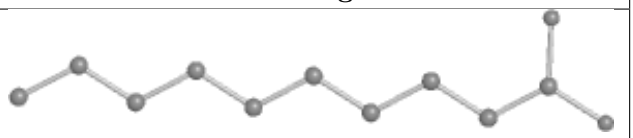
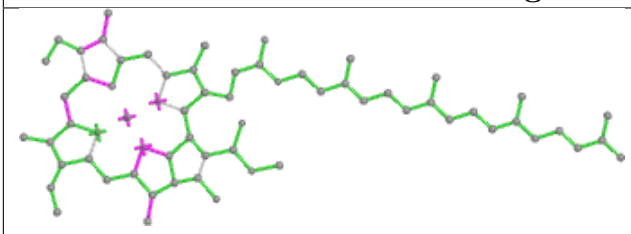


Rings

Ligand CLA B 603



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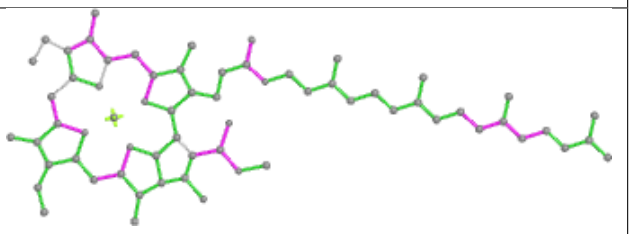
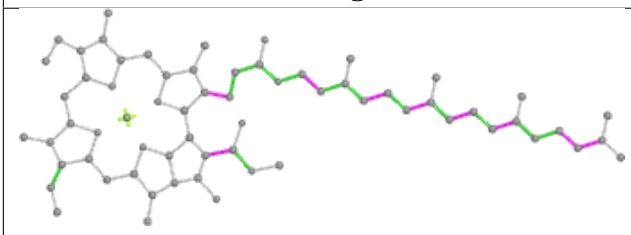


Bond angles



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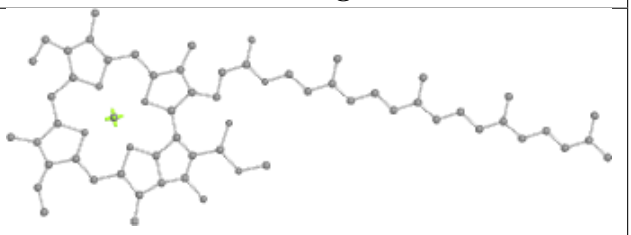
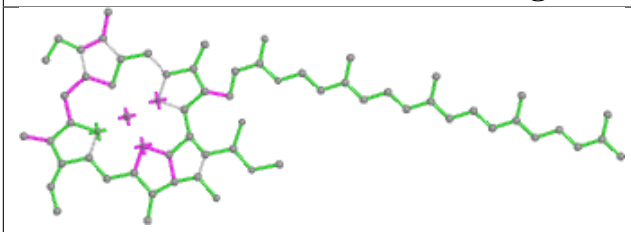


Rings

Ligand CLA c 510



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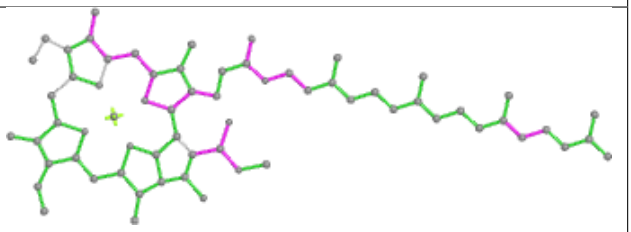

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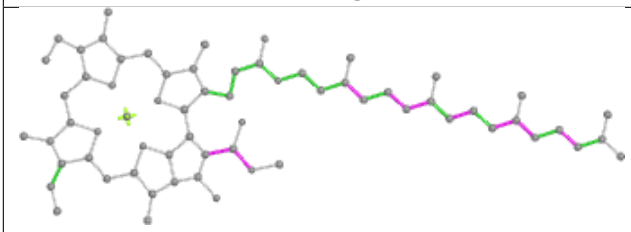

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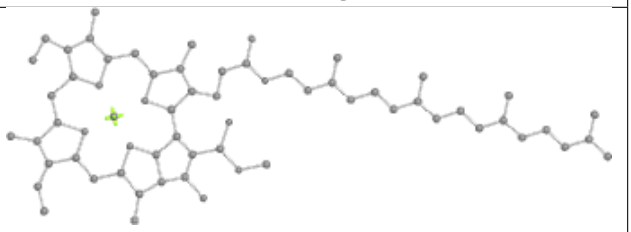
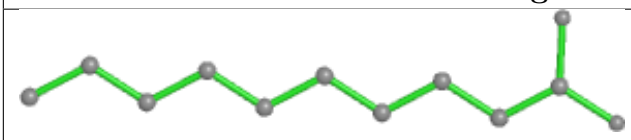


Rings

Ligand STE k 101



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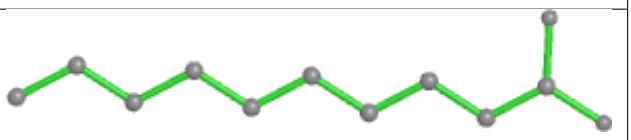
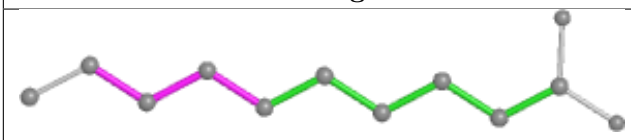


Bond angles



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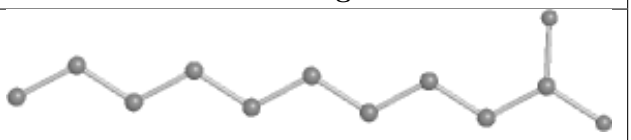
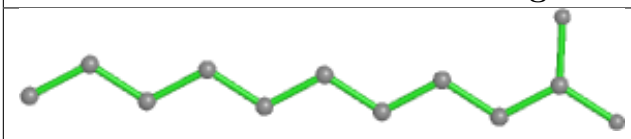


Rings

Ligand STE L 103



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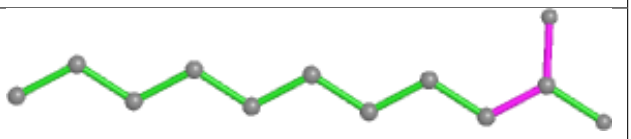
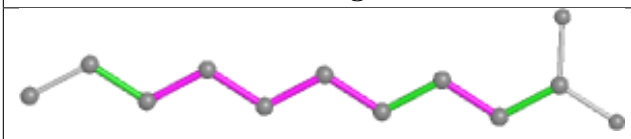


Bond angles



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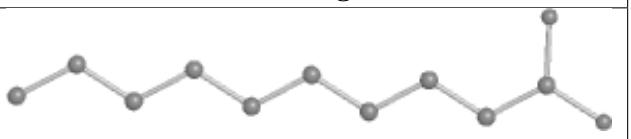
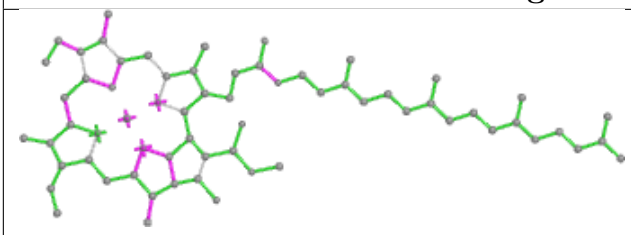


Rings

Ligand CLA b 601



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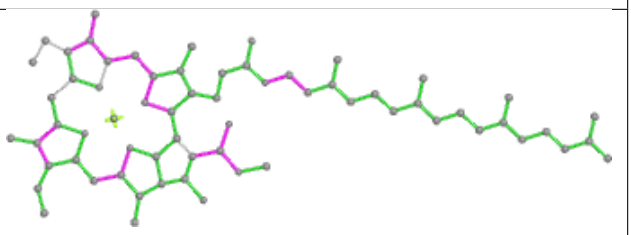
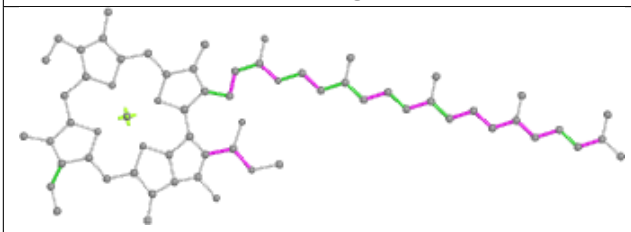


Bond angles



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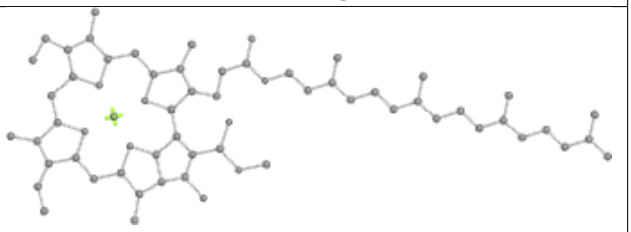
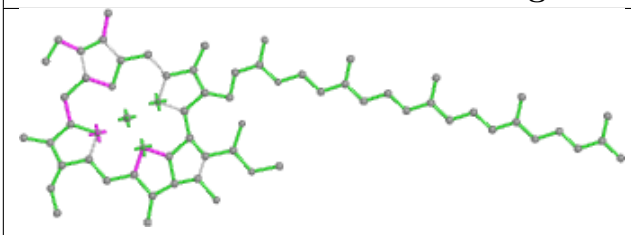


Rings

Ligand CLA a 403



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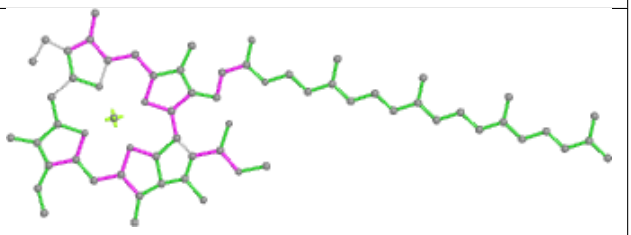
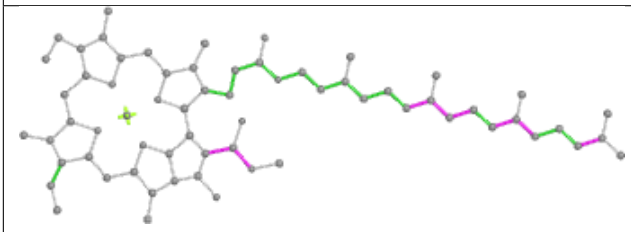
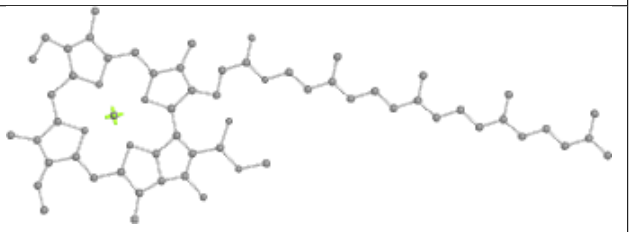


Bond angles

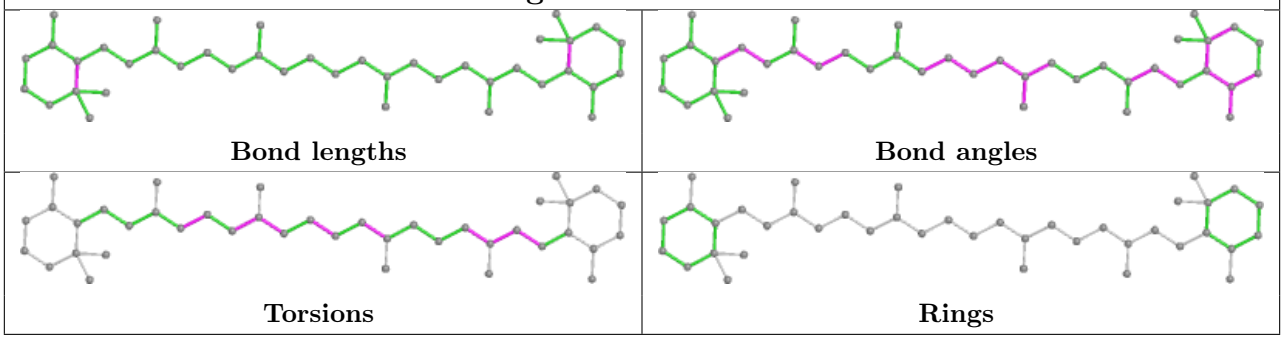


Torsions

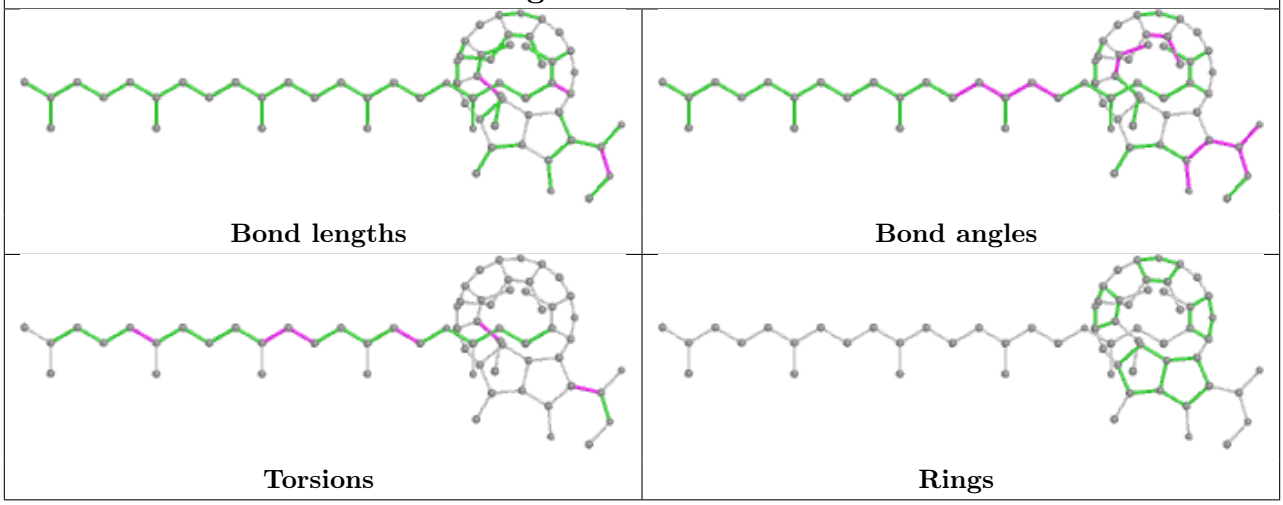


Rings

Ligand BCR b 619



Ligand PHO a 404



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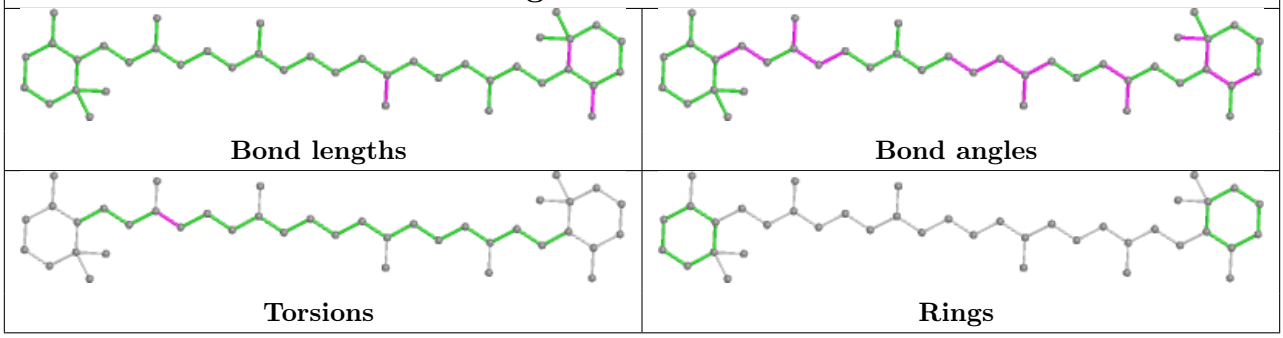
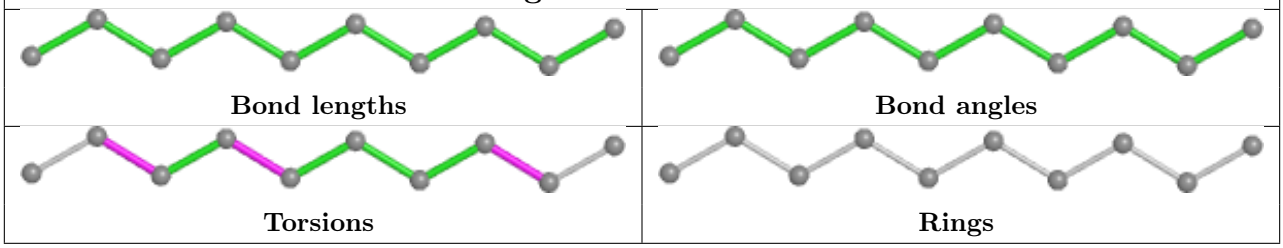


Ligand STE M 103



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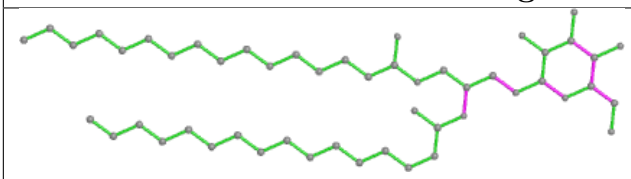
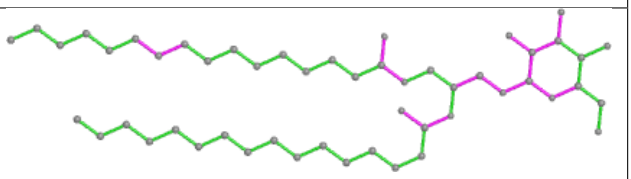
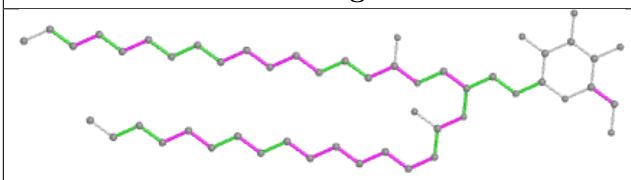


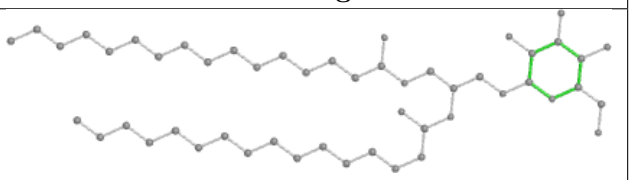
Bond lengths



Bond angles

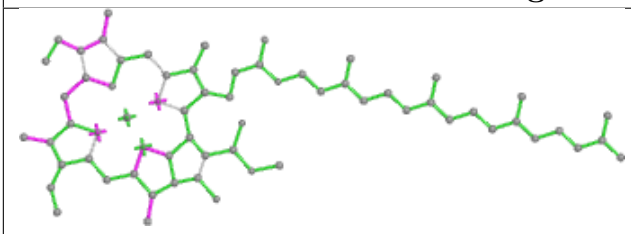


Torsions



Rings

Ligand CLA b 615



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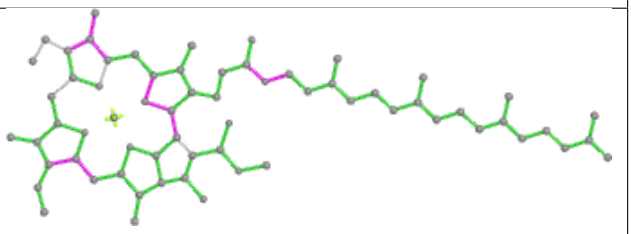
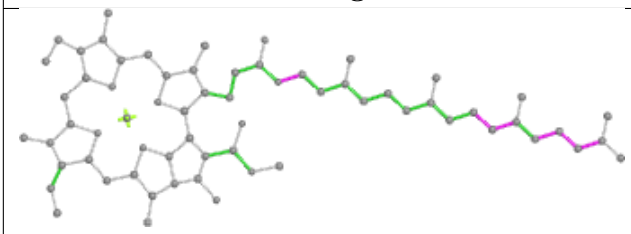


Bond angles



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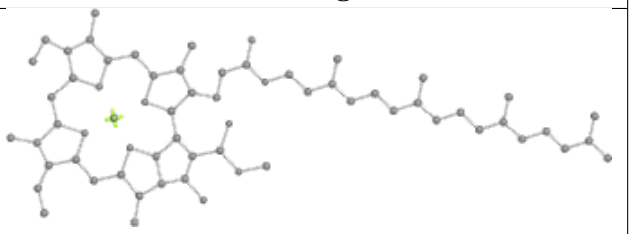
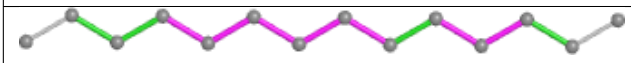


Rings

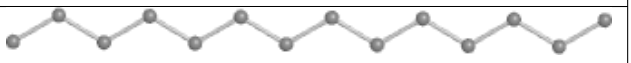
Ligand STE h 102

Bond lengths

Bond angles

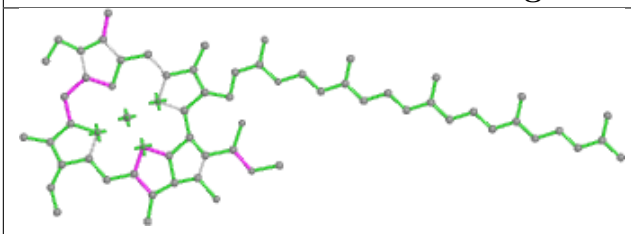


Torsions

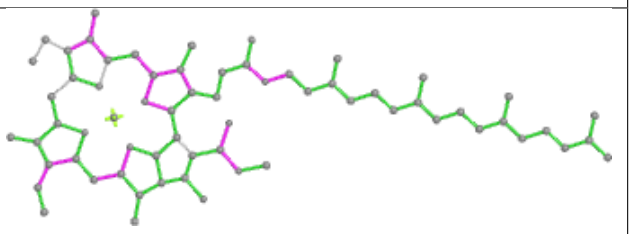


Rings

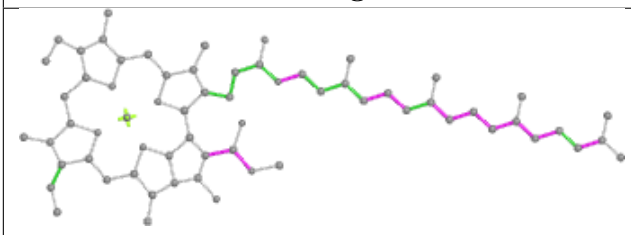
Ligand CLA C 510



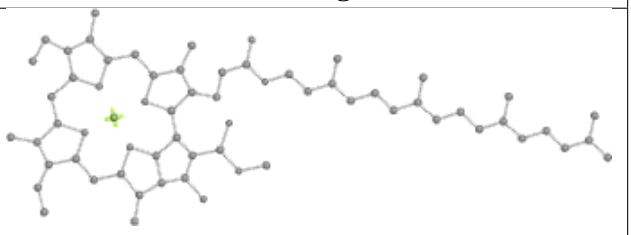
Bond lengths



Bond angles

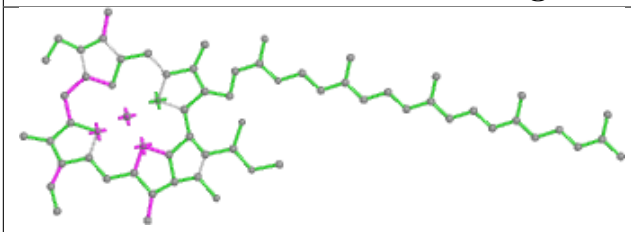


Torsions



Rings

Ligand CLA c 506



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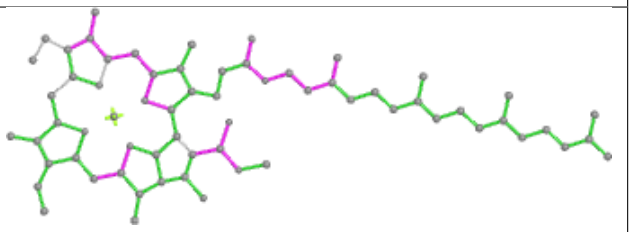
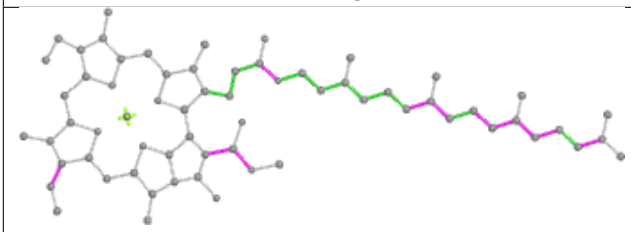
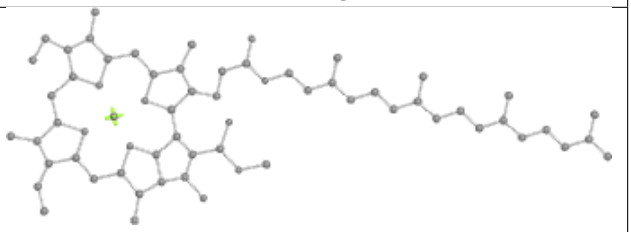


Bond angles

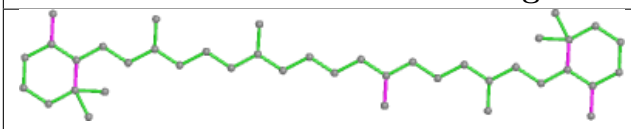


Torsions

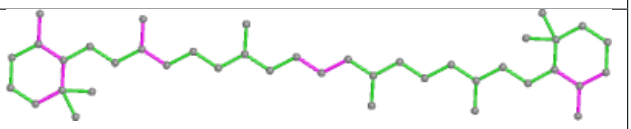


Rings

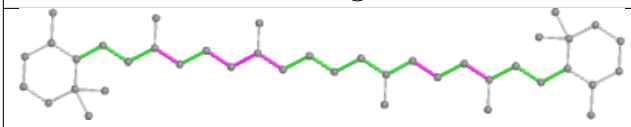
Ligand BCR C 515



Bond lengths



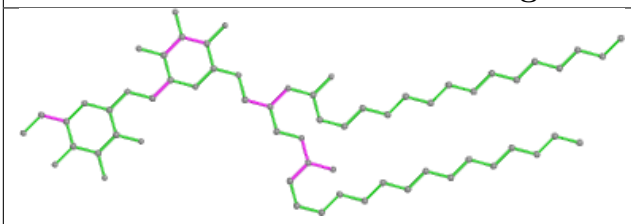
Bond angles



Torsions

Rings

Ligand DGD C 517



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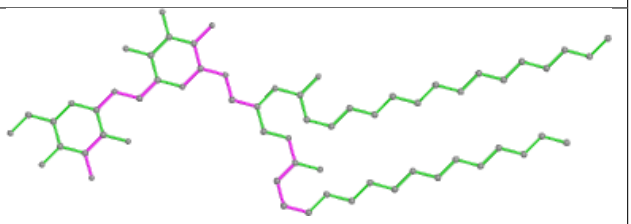
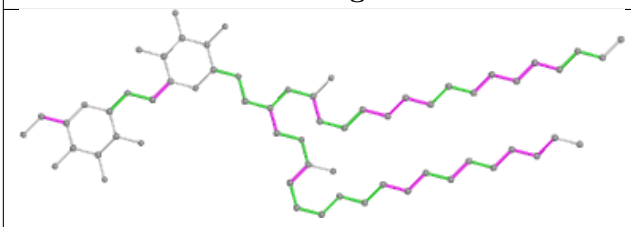
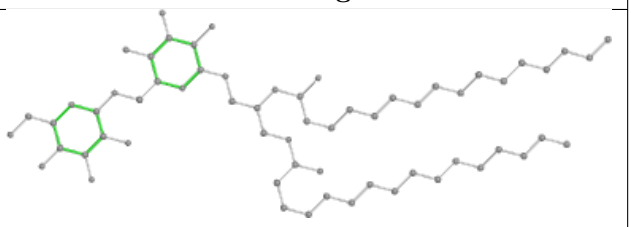


Bond angles

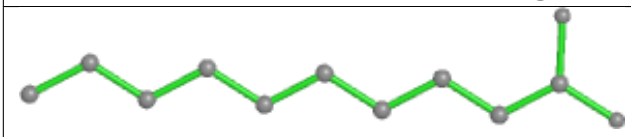


Torsions



Rings

Ligand STE a 414



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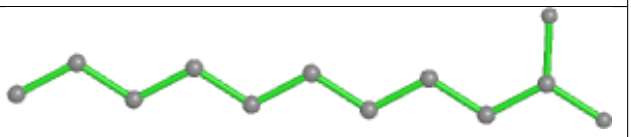
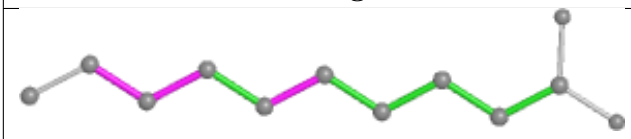
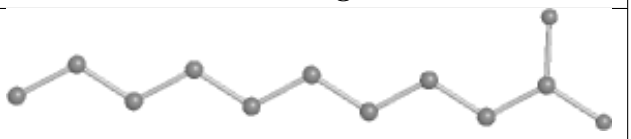


Bond angles

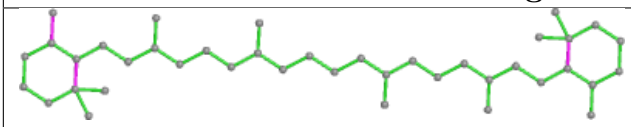


Torsions



Rings

Ligand BCR b 617



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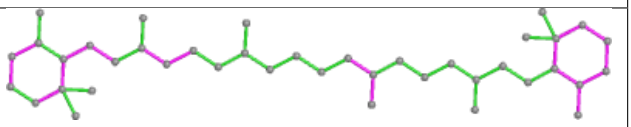
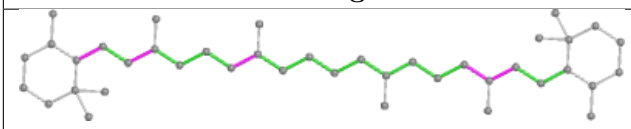
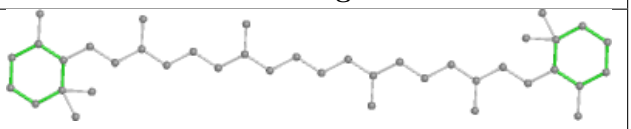


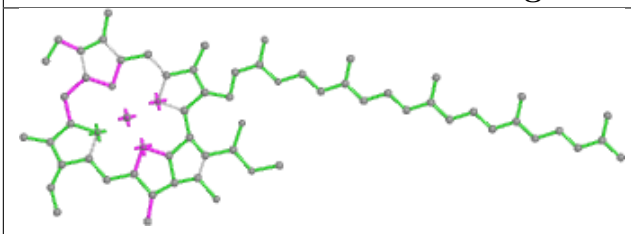
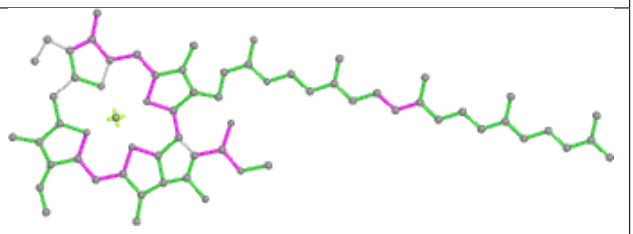
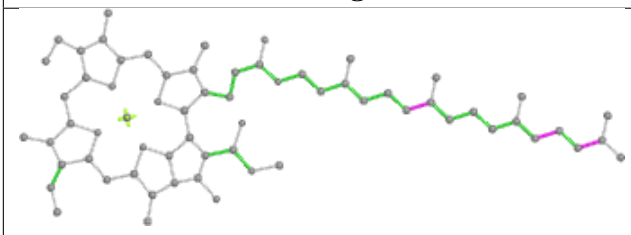
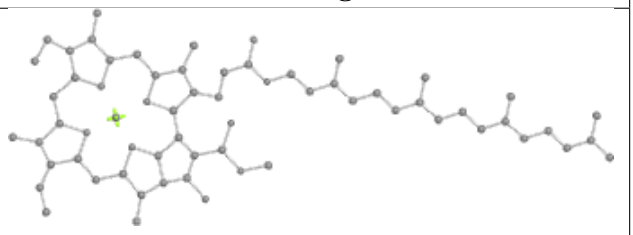
Bond angles



Torsions



Rings

Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

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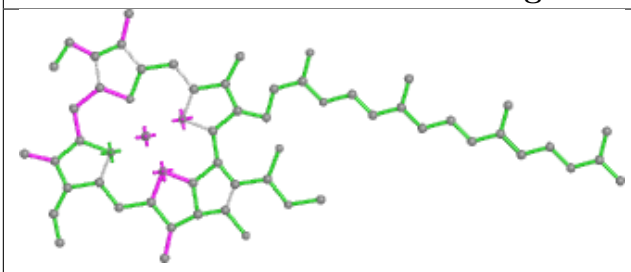
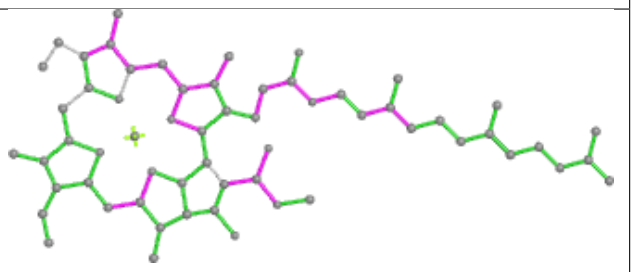
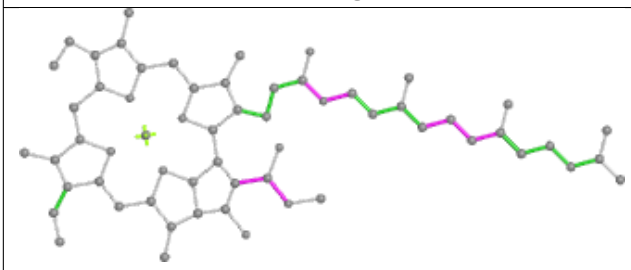
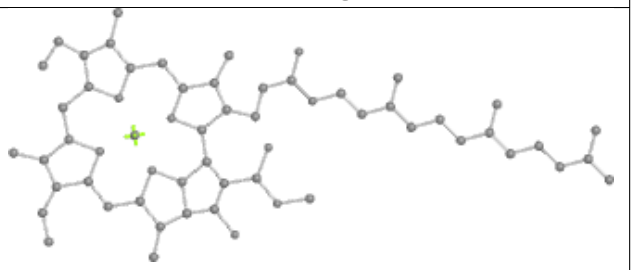
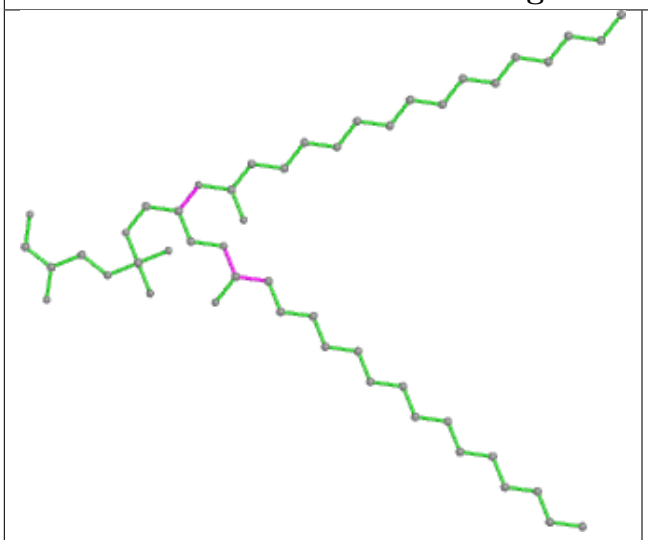
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG d 407



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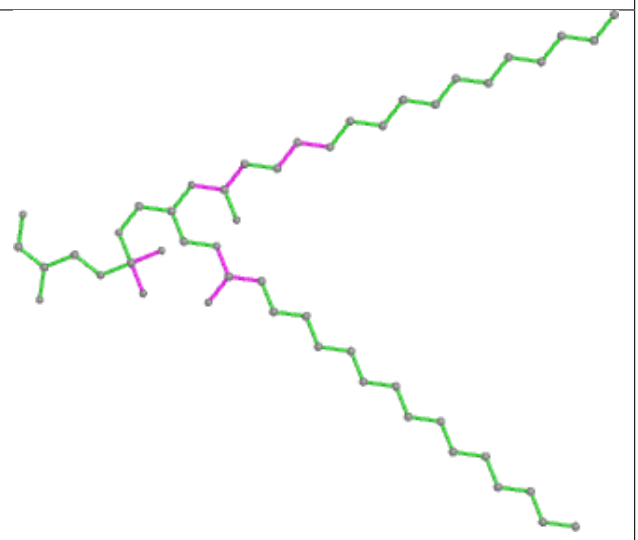
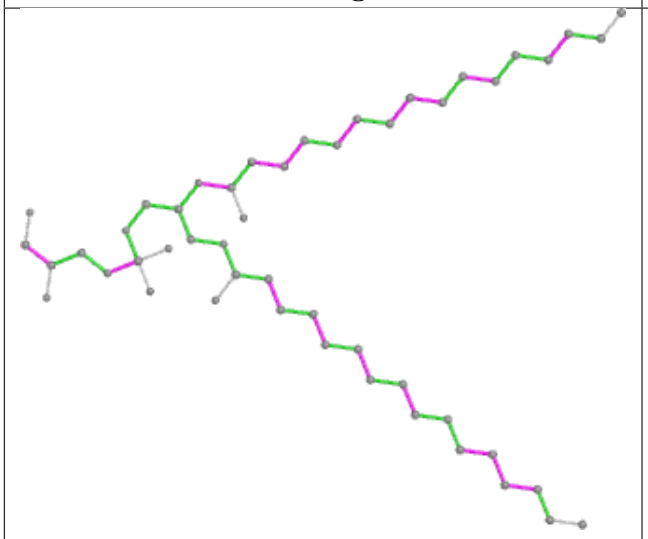


Bond angles



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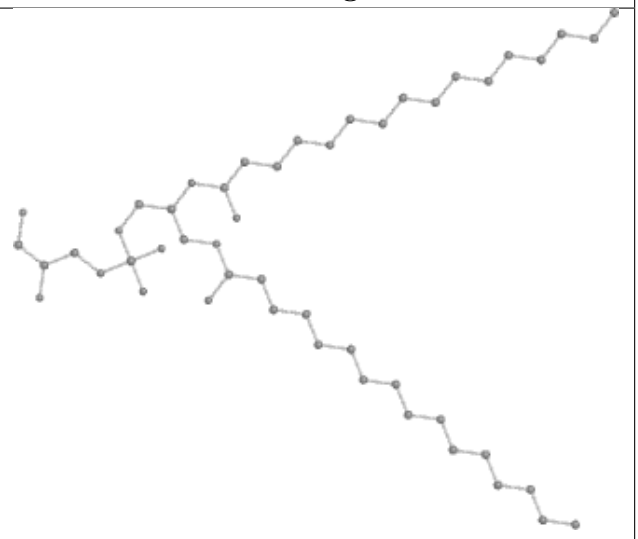
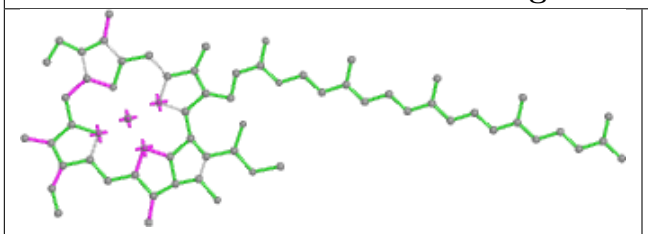


Rings

Ligand CLA a 405



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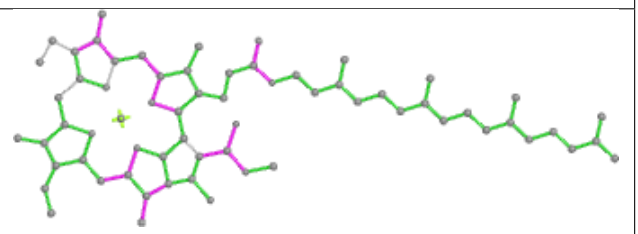
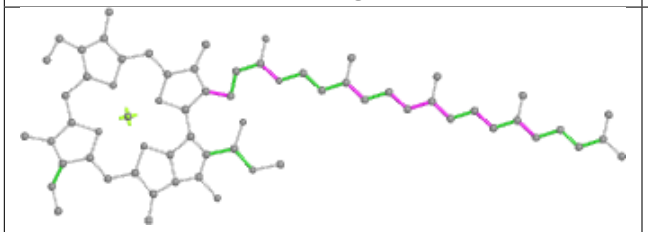


Bond angles



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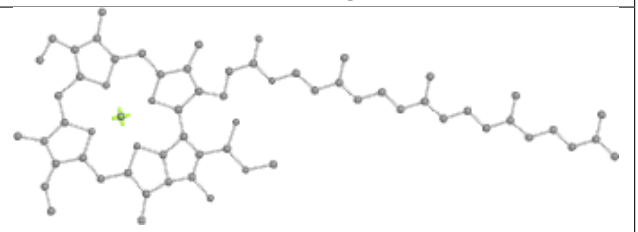
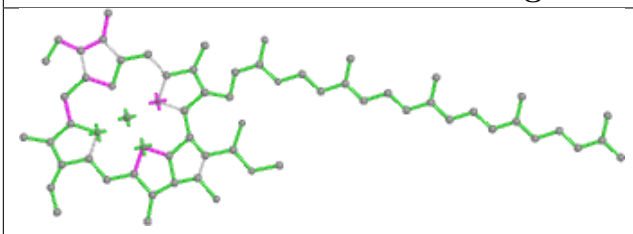


Rings

Ligand CLA B 607



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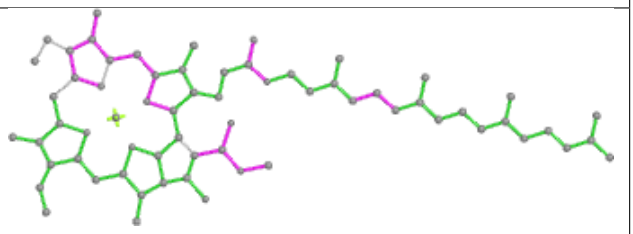
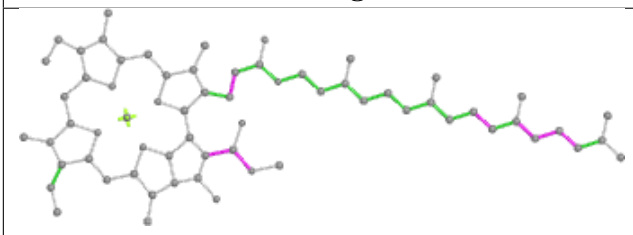
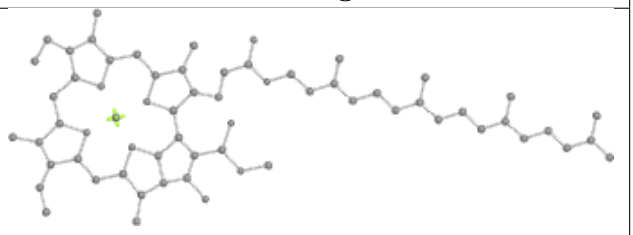


Bond angles

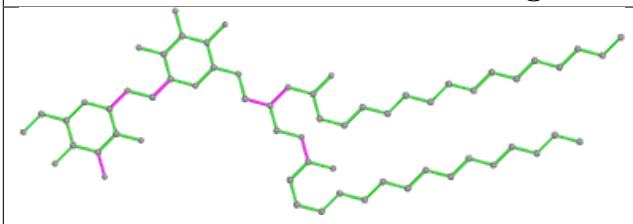


Torsions



Rings

Ligand DGD c 516



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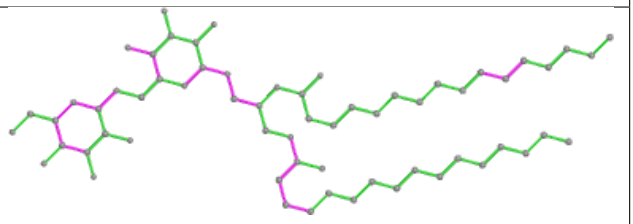

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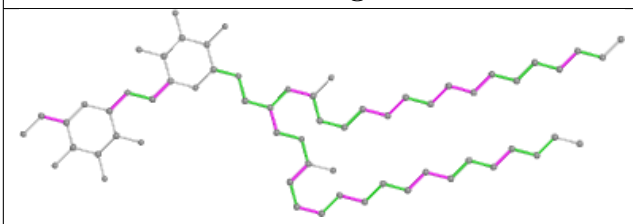

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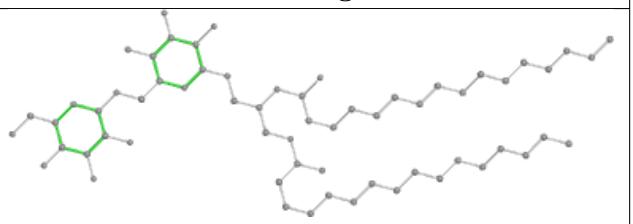
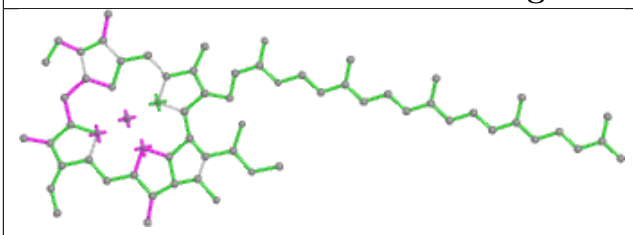


Rings

Ligand CLA d 404



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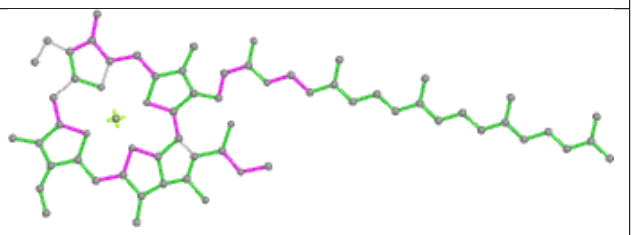
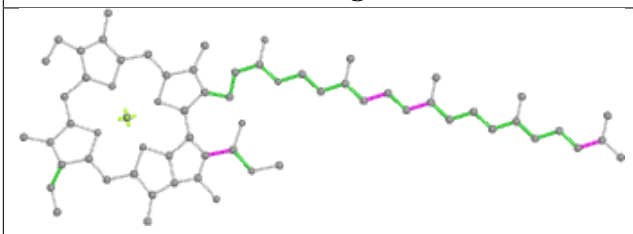


Bond angles



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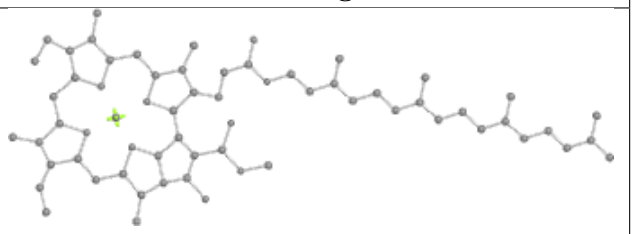
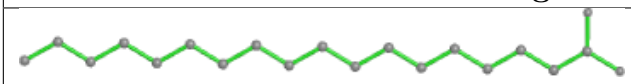


Rings

Ligand STE c 520



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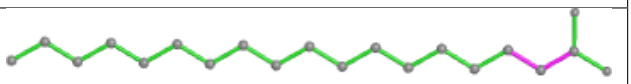
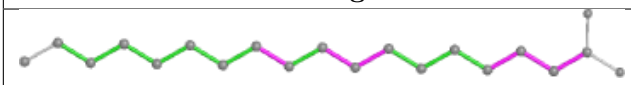


Bond angles



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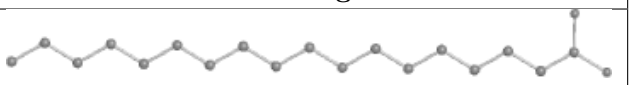
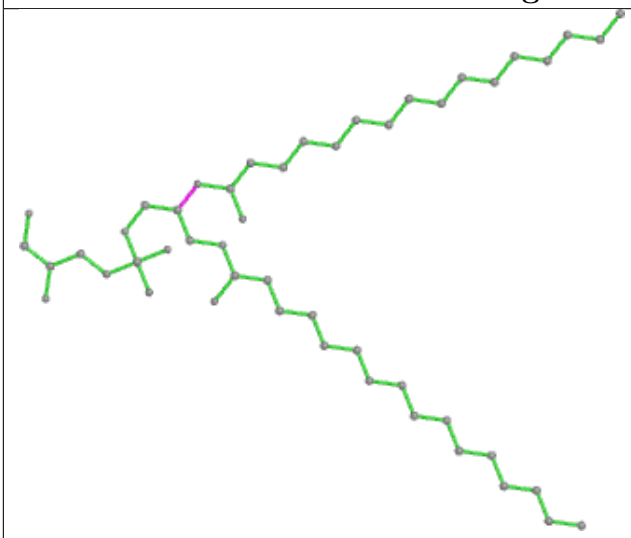


Rings

Ligand LHG D 408



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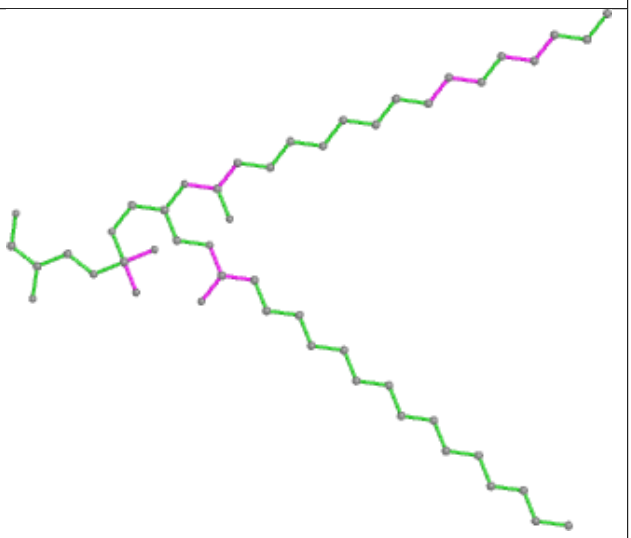
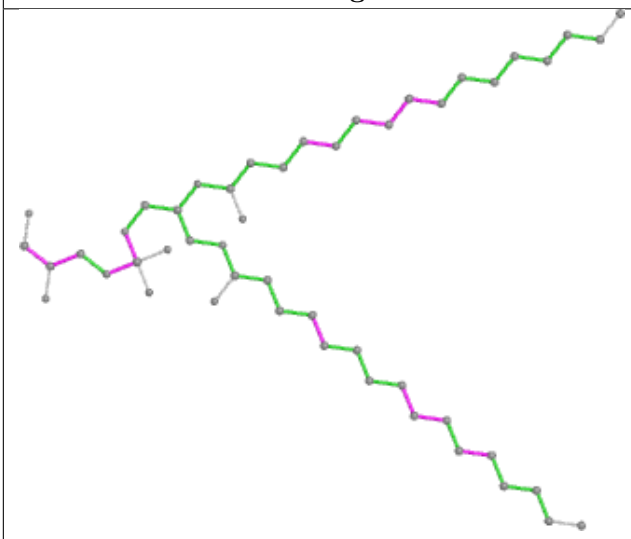


Bond angles



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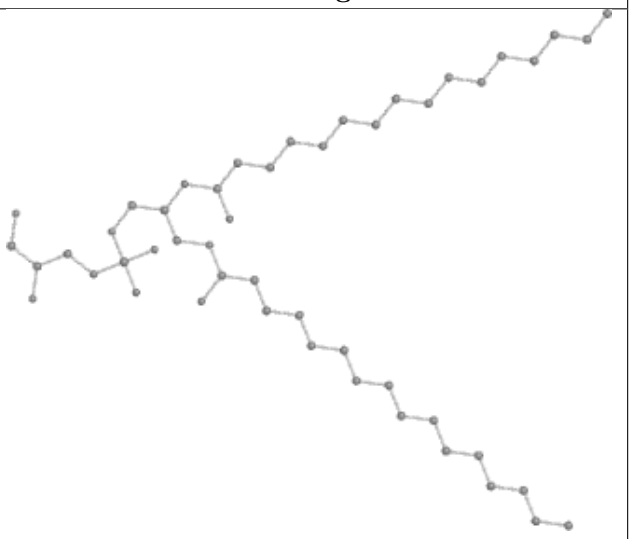
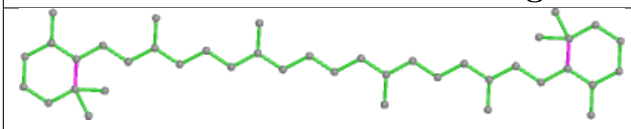


Rings

Ligand BCR x 101



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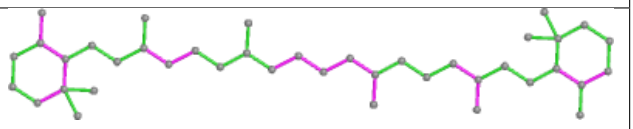
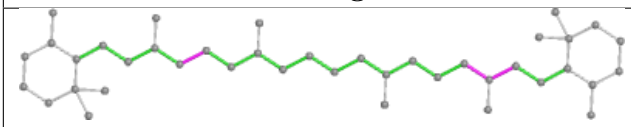
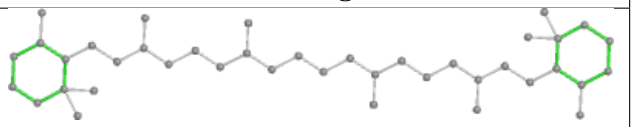


Bond angles

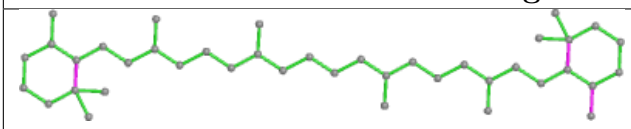


Torsions

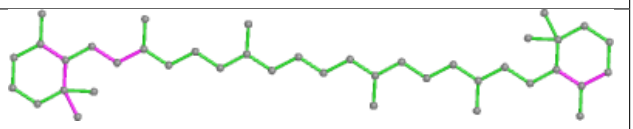


Rings

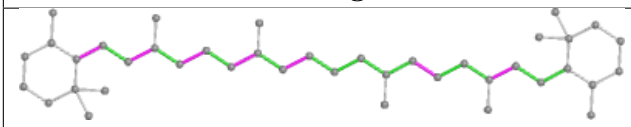
Ligand BCR T 101



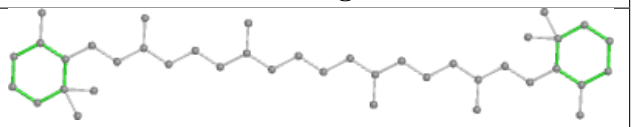
Bond lengths



Bond angles

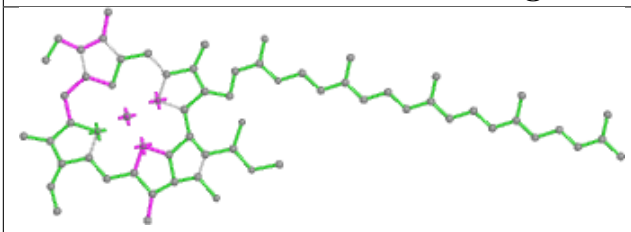


Torsions

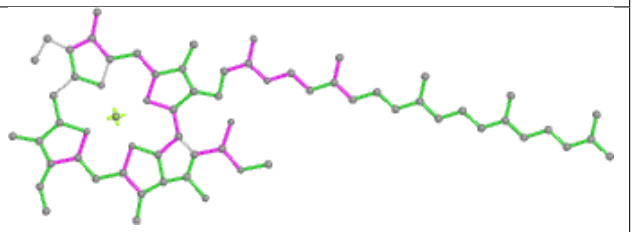


Rings

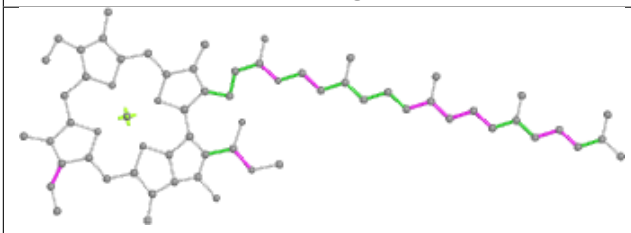
Ligand CLA C 514



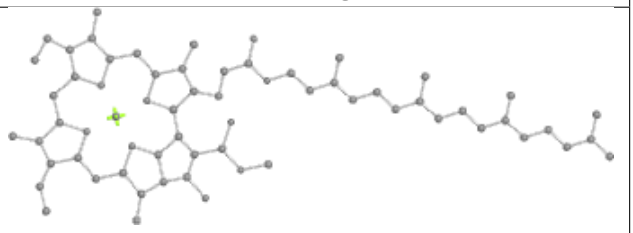
Bond lengths



Bond angles



Torsions



Rings

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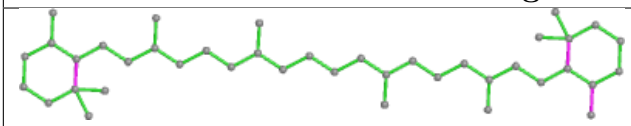
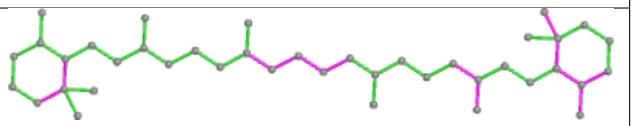
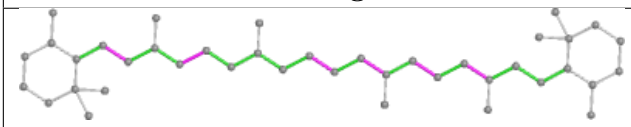


Bond lengths



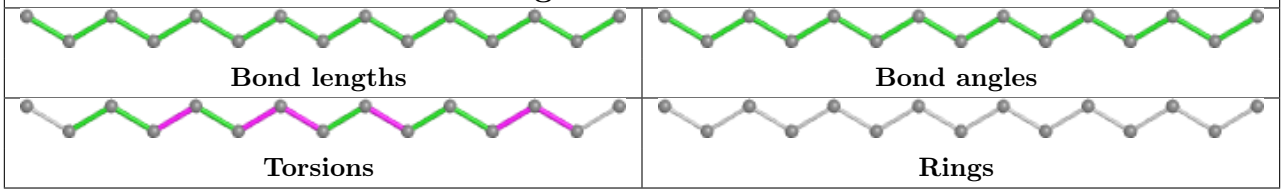
Bond angles



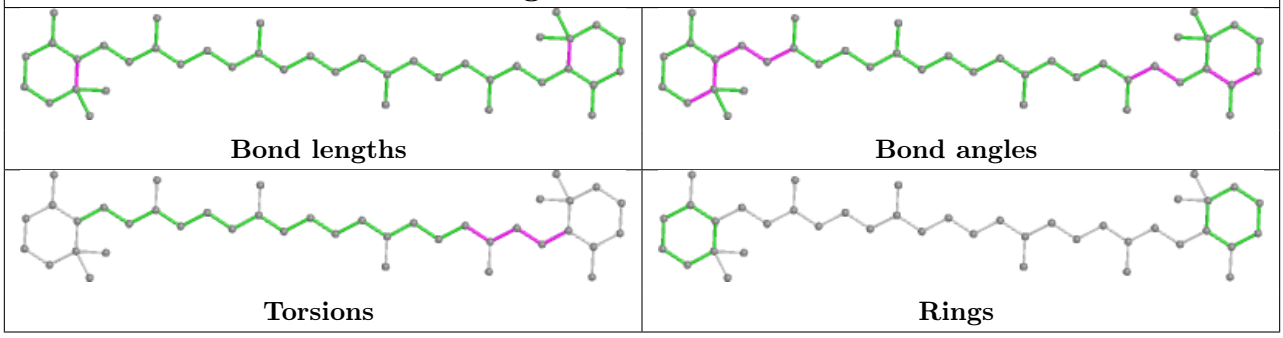
Torsions

Rings

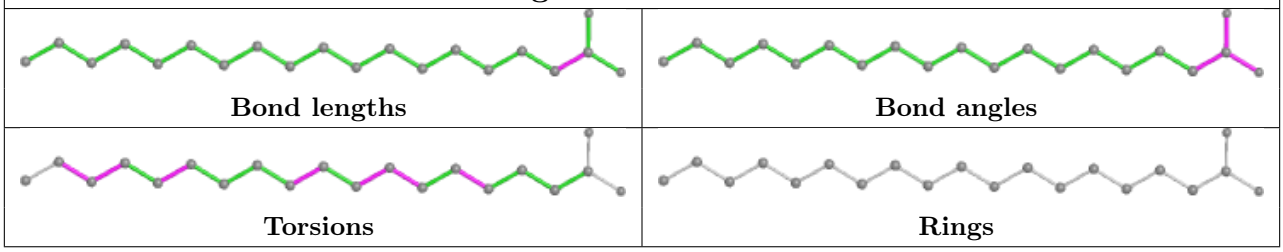
Ligand STE I 101



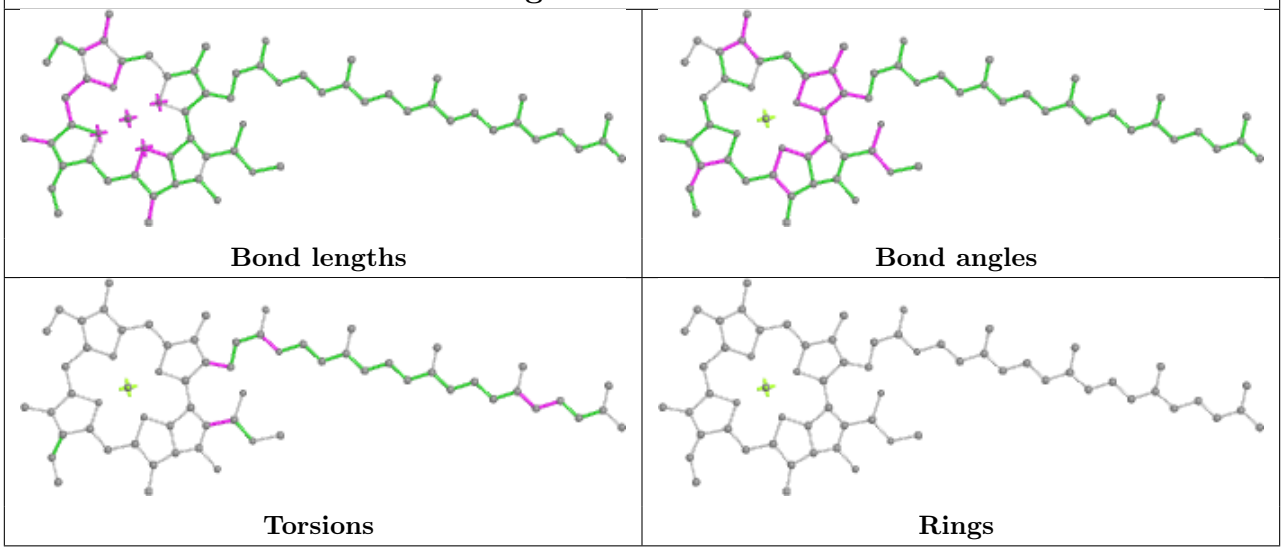
Ligand BCR D 405



Ligand STE b 621



Ligand CLA C 503



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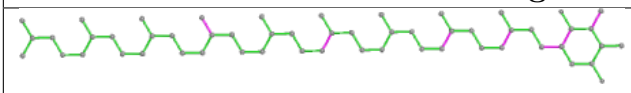
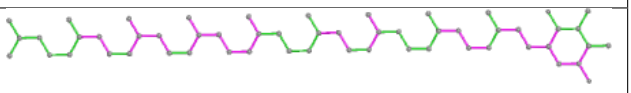
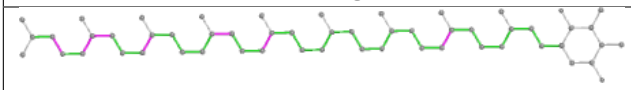


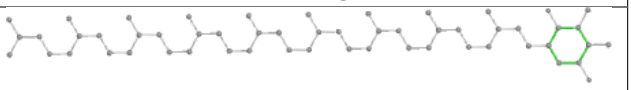
Bond lengths



Bond angles

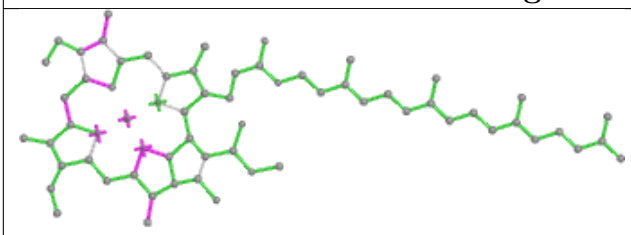


Torsions



Rings

Ligand CLA A 403



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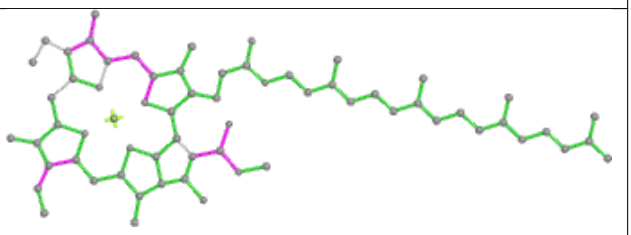
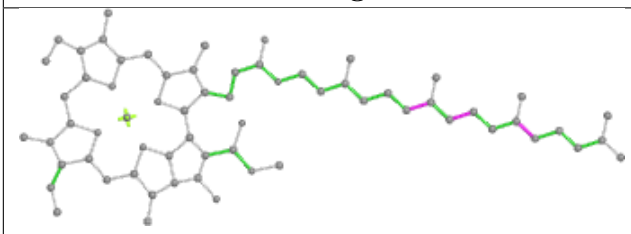


Bond angles



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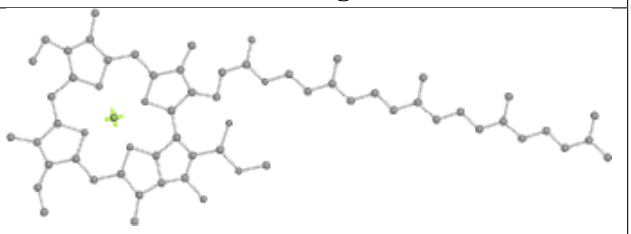
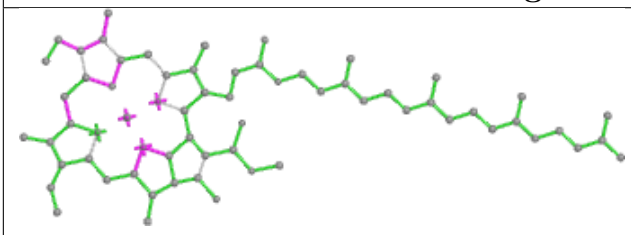


Rings

Ligand CLA B 611



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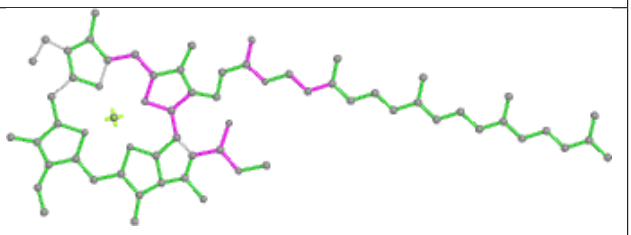
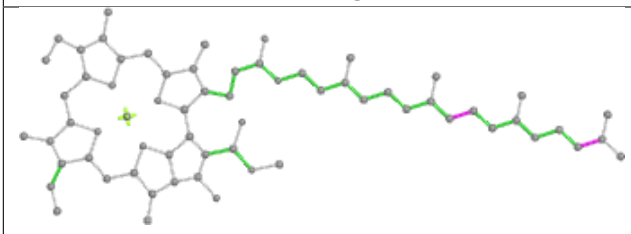


Bond angles



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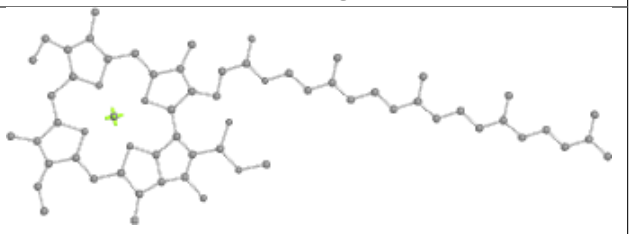

Rings

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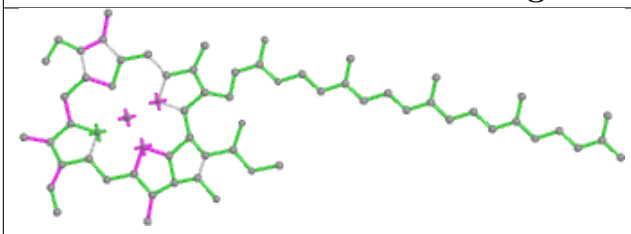

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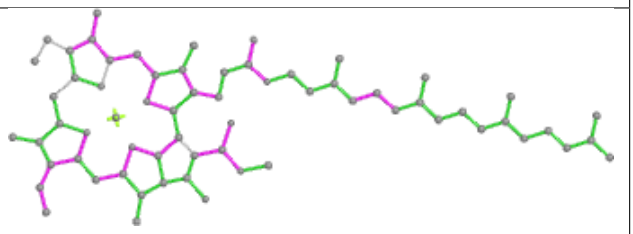
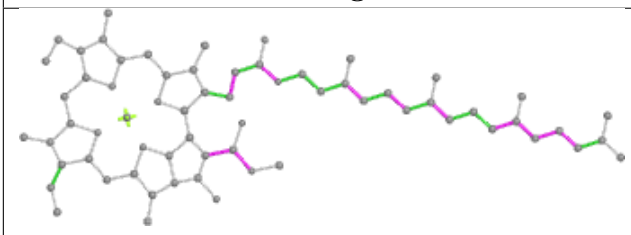


Bond angles



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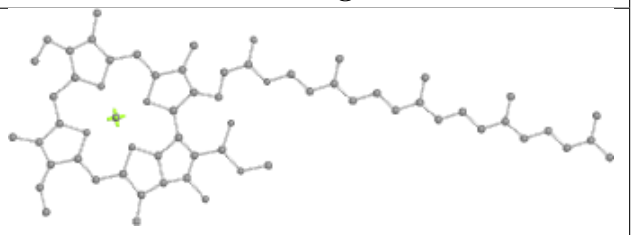
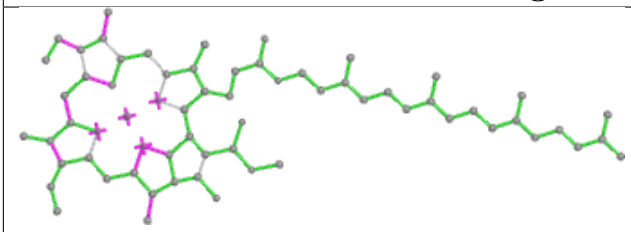


Rings

Ligand CLA c 511



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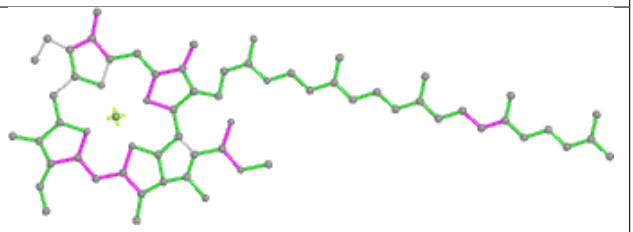

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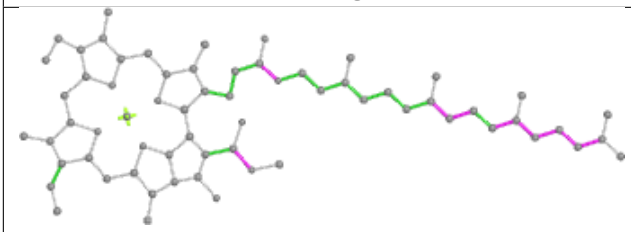

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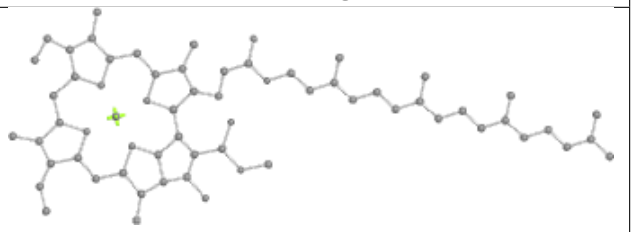

Rings

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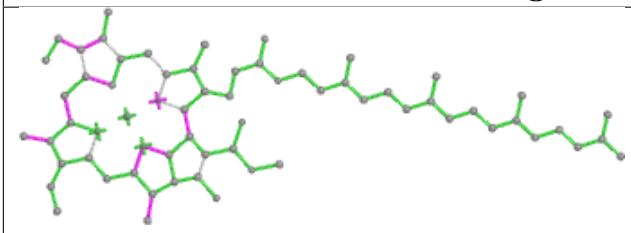

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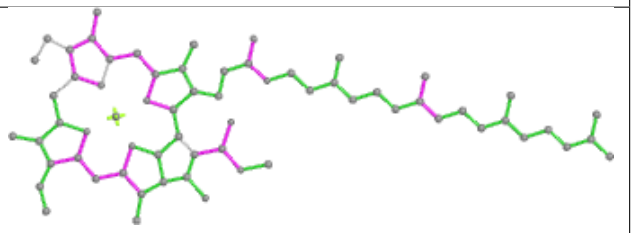
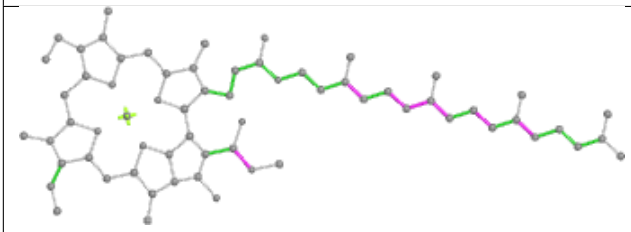


Bond angles



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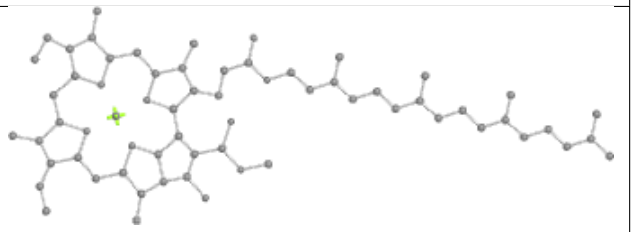
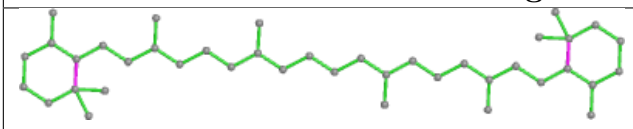


Rings

Ligand BCR d 405



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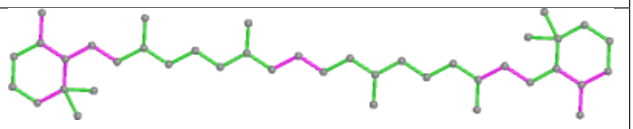
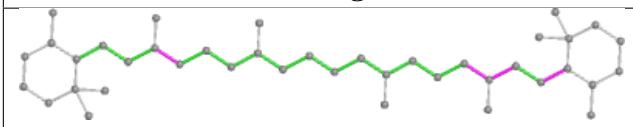


Bond angles



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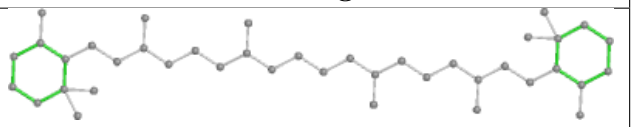
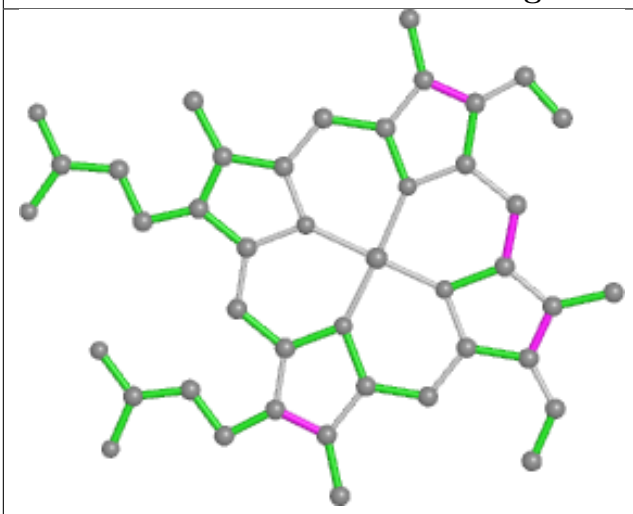


Rings

Ligand HEC E 101



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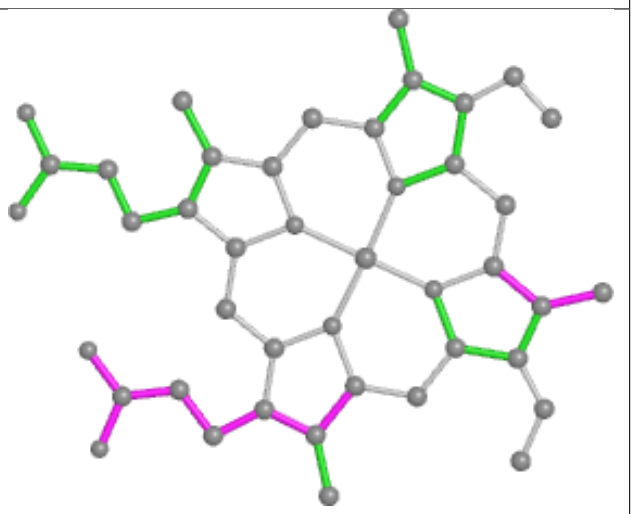
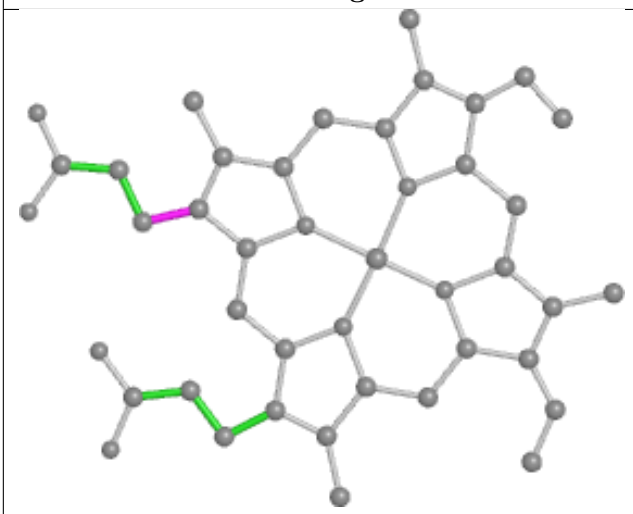


Bond angles



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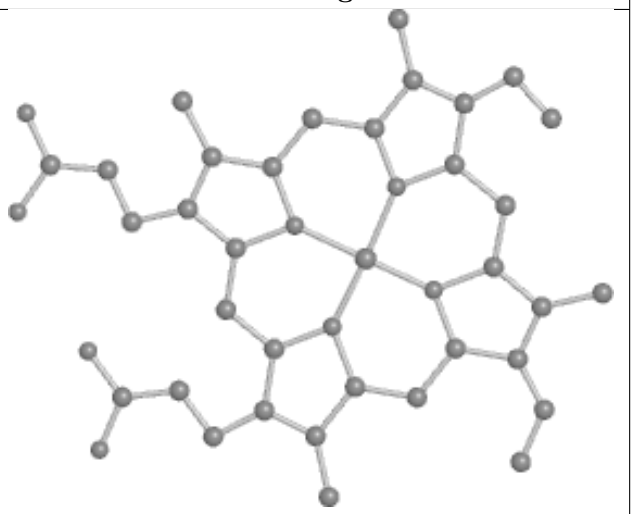
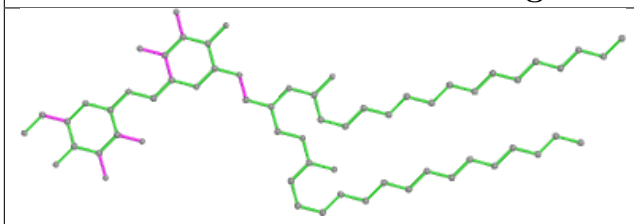
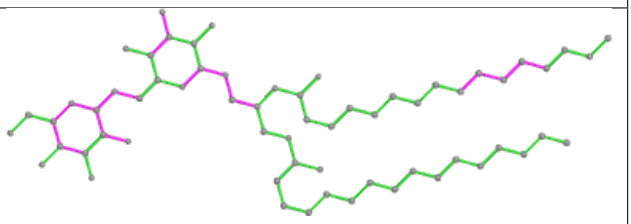


Rings

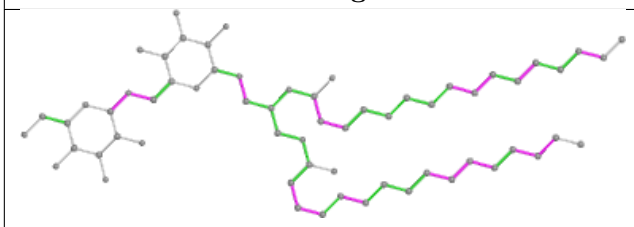
Ligand DGD c 517



Bond lengths



Bond angles



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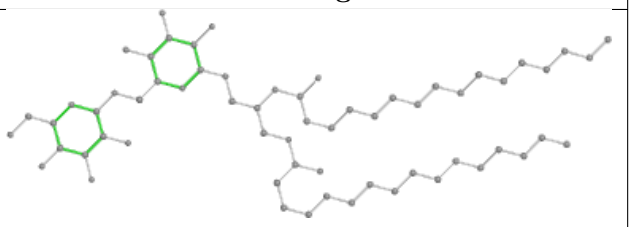
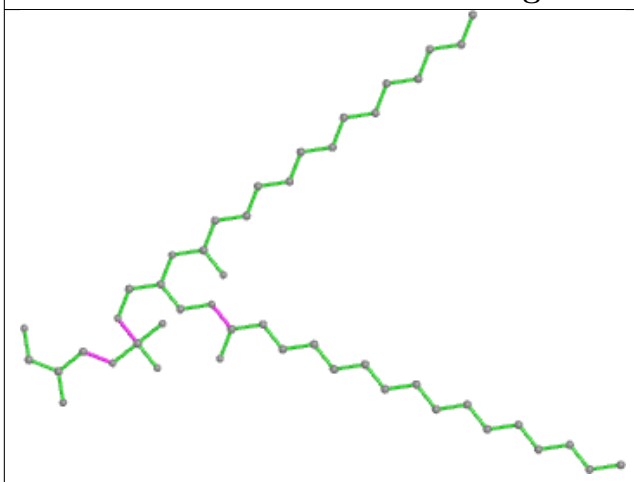
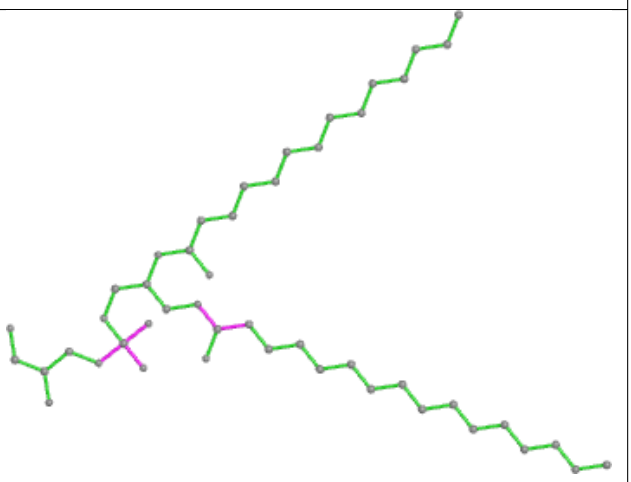


Rings

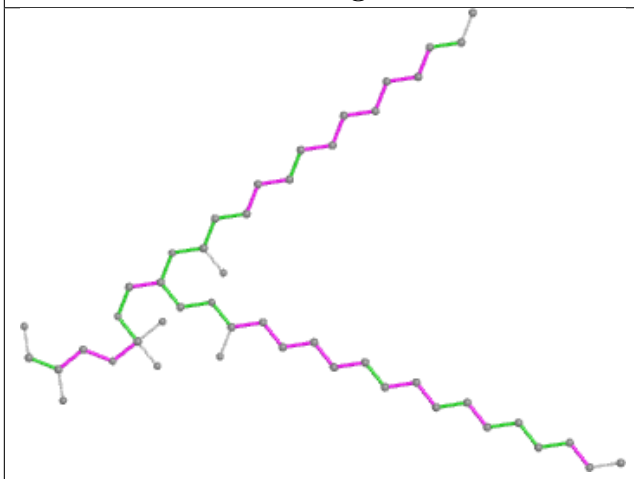
Ligand LHG A 411



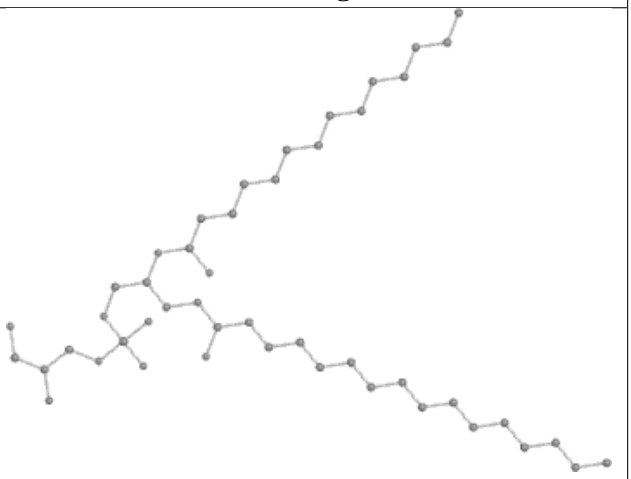
Bond lengths



Bond angles

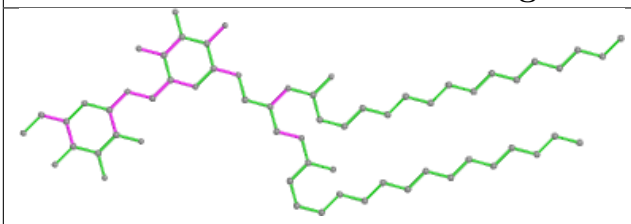


Torsions

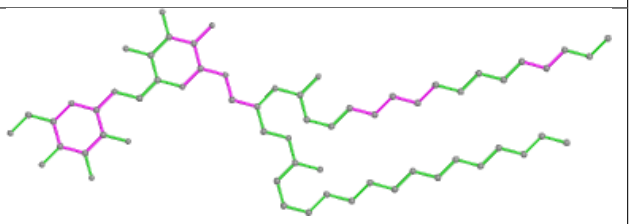


Rings

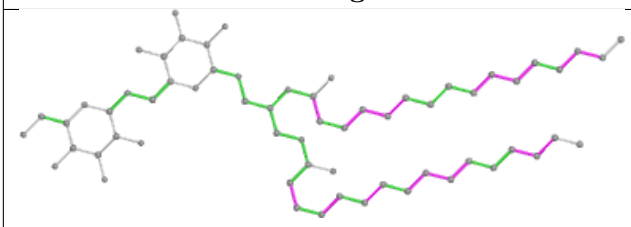
Ligand DGD H 102



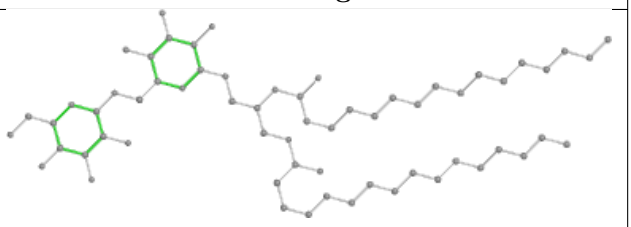
Bond lengths



Bond angles

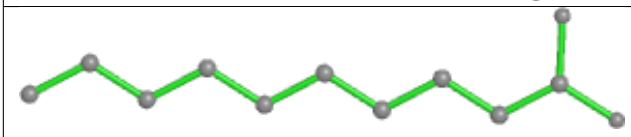


Torsions



Rings

Ligand STE C 520



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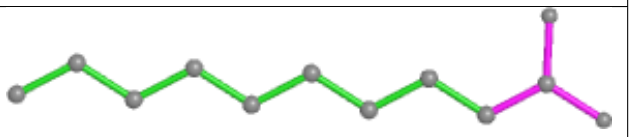

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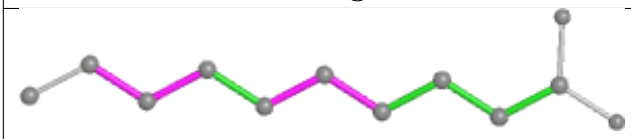

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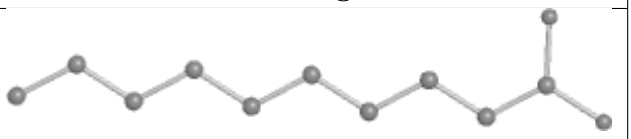
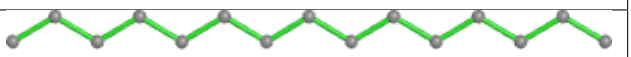


Rings

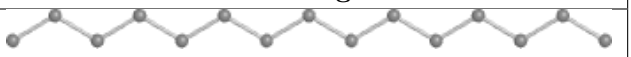
Ligand STE T 102

Bond lengths



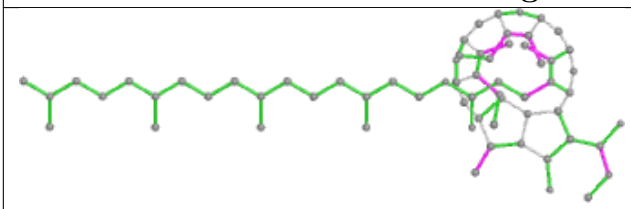
Bond angles

Torsions



Rings

Ligand PHO D 401



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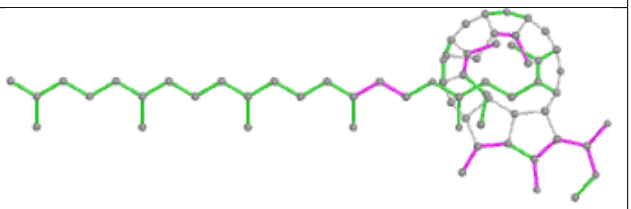
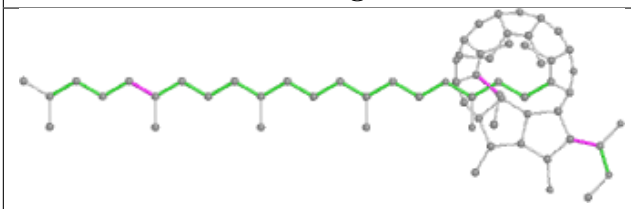


Bond angles



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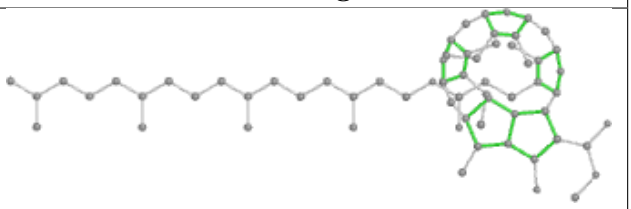
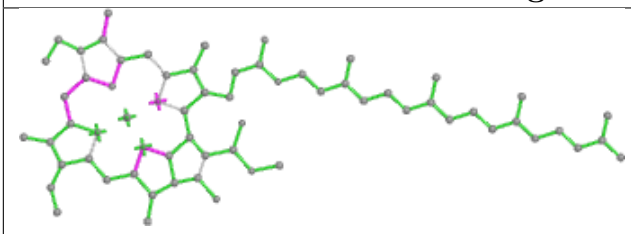


Rings

Ligand CLA b 606



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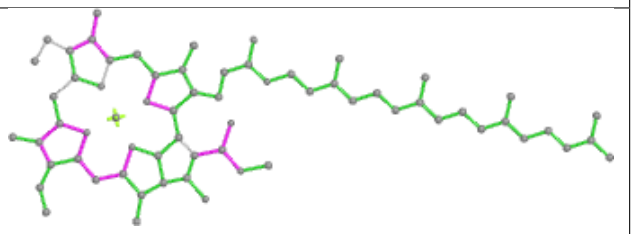
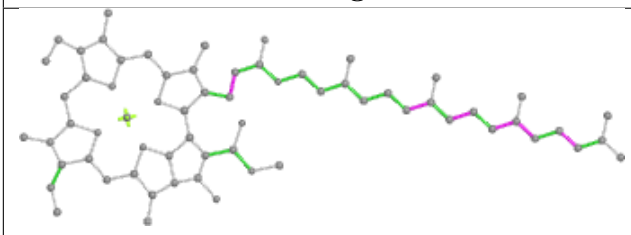


Bond angles



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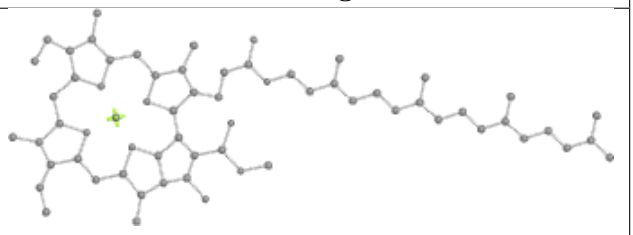
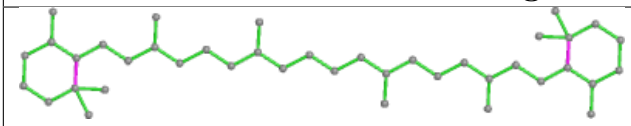


Rings

Ligand BCR B 619



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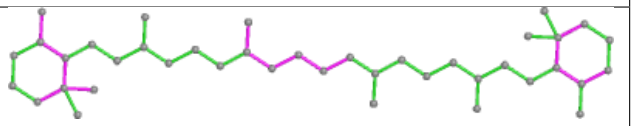
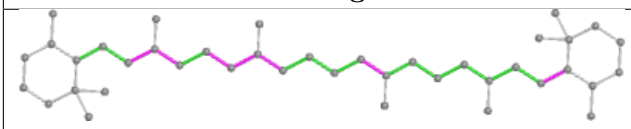


Bond angles



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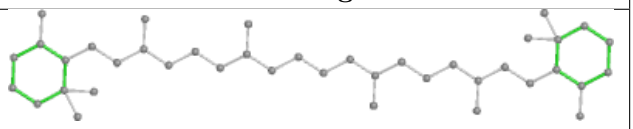
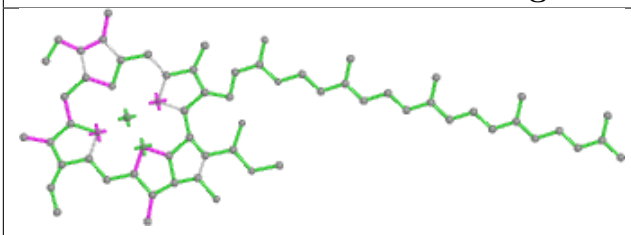
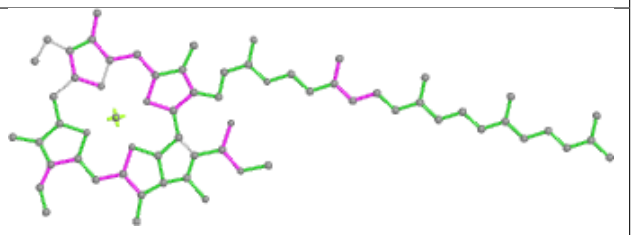


Rings

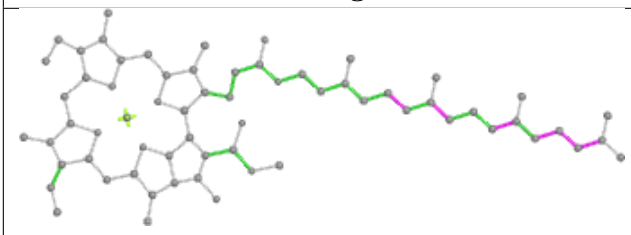
Ligand CLA c 503



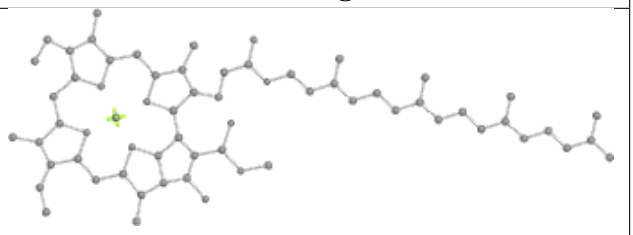
Bond lengths



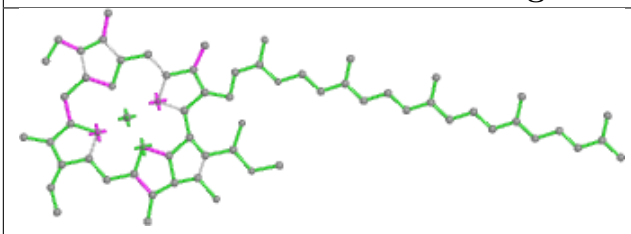
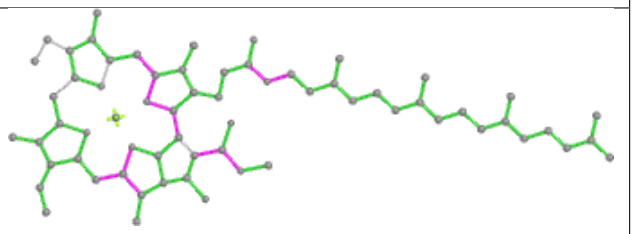
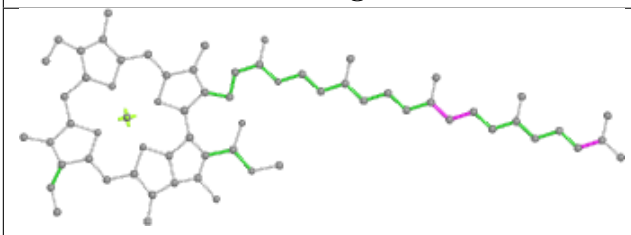
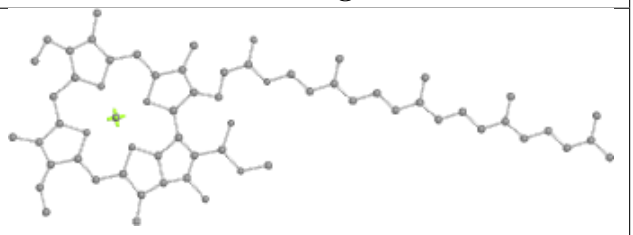
Bond angles

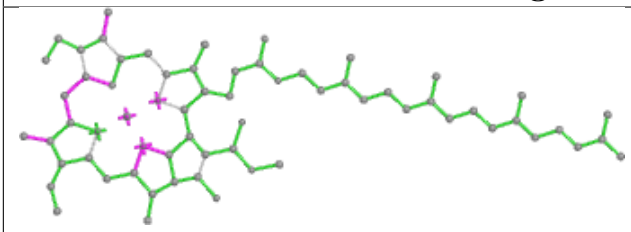
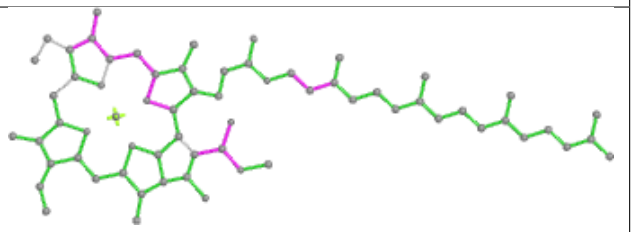
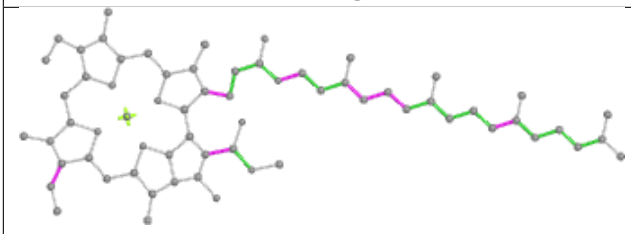
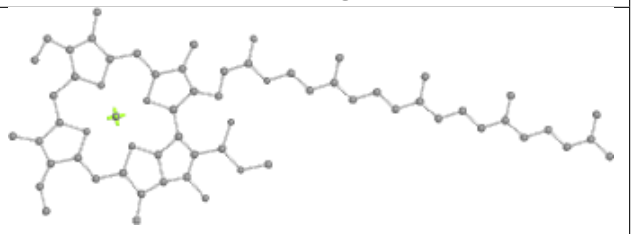


Torsions

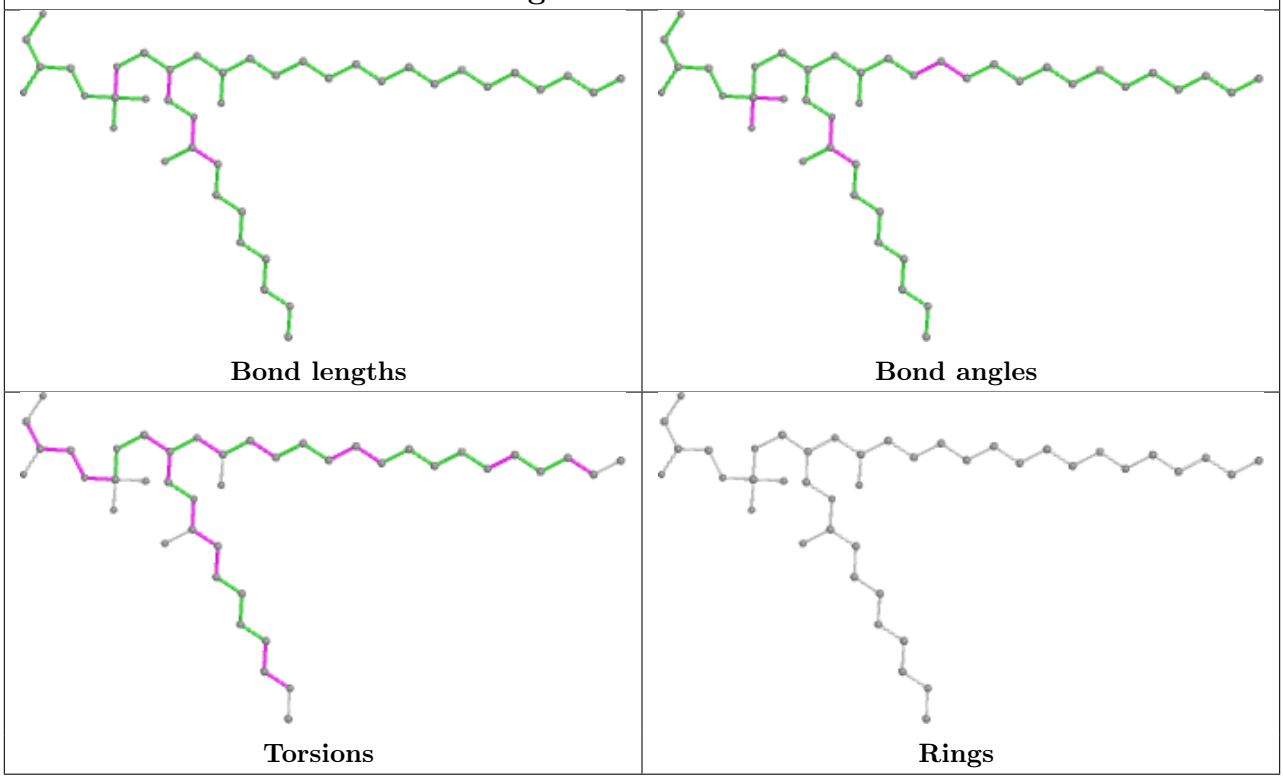


Rings

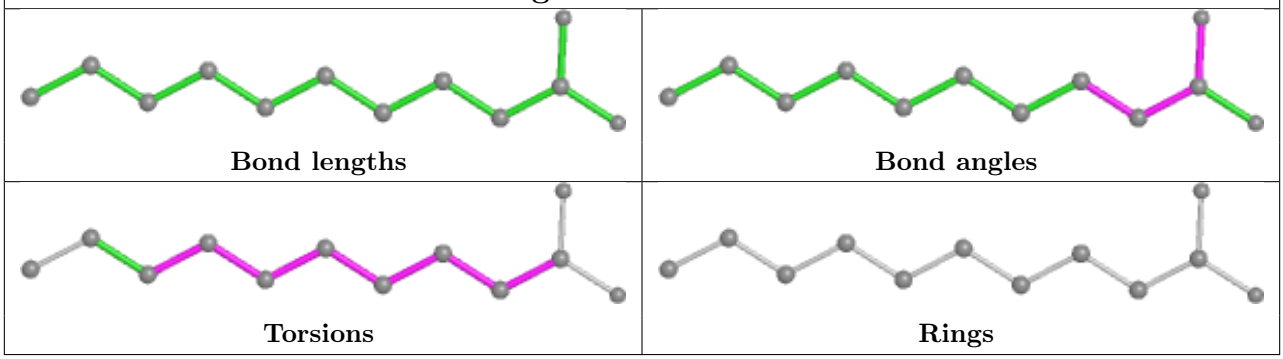
Ligand CLA b 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

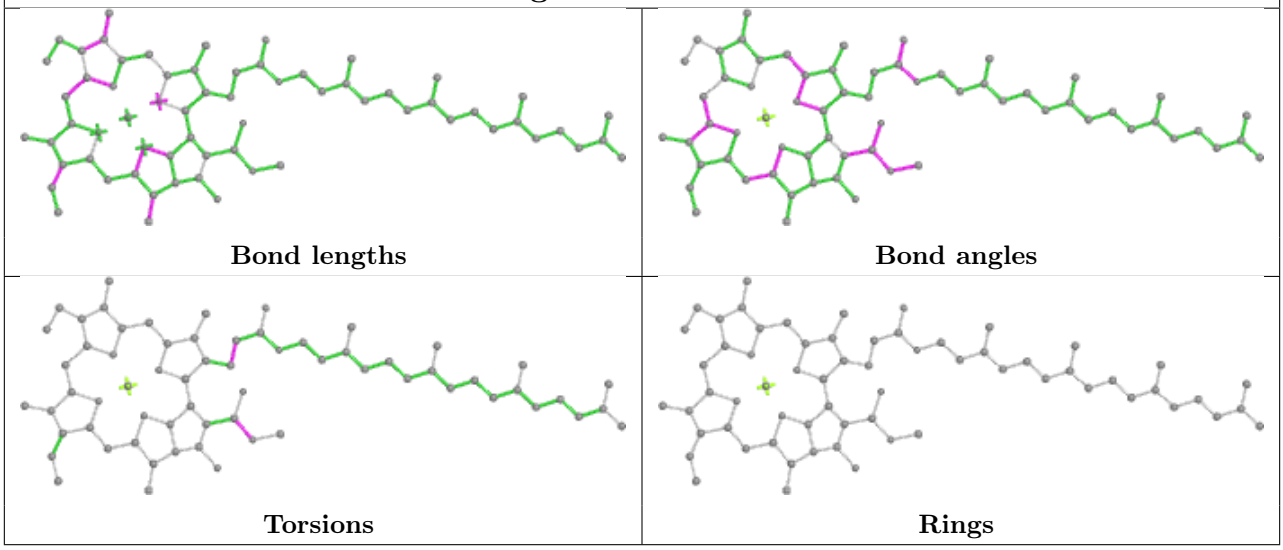
Ligand LHG a 412



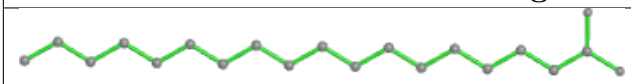
Ligand STE J 101

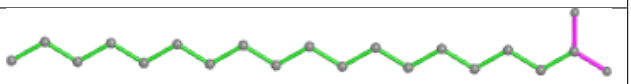


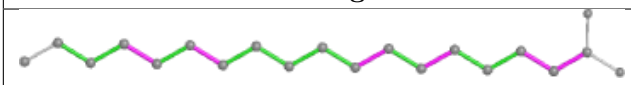
Ligand CLA c 501

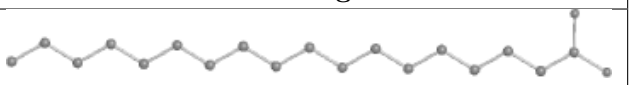


Ligand STE b 624

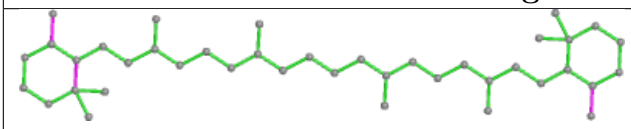

Bond lengths

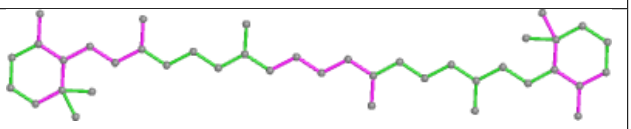

Bond angles

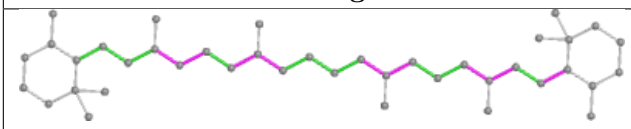

Torsions


Rings

Ligand BCR A 406


Bond lengths


Bond angles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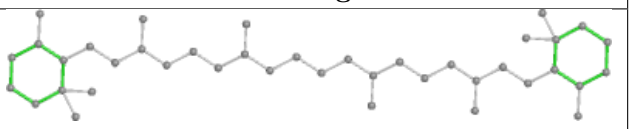
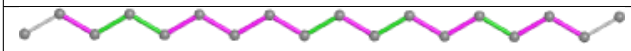
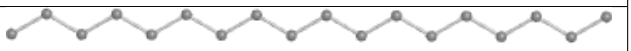

Rings

Ligand STE H 103

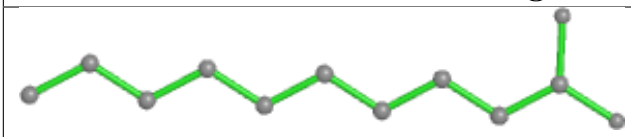
Bond lengths

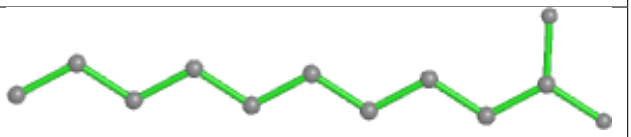
Bond angles

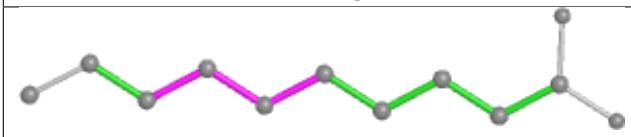

Torsions

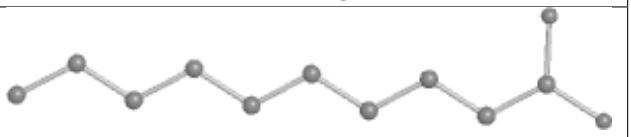

Rings

Ligand STE C 522

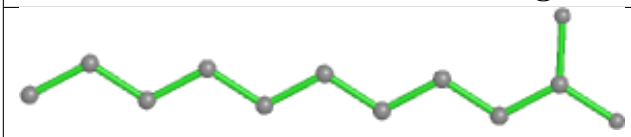

Bond lengths


Bond angles


Torsions


Rings

Ligand STE j 101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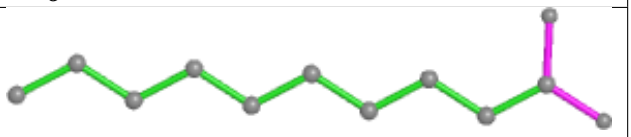
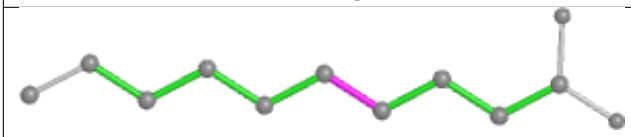

Bond angles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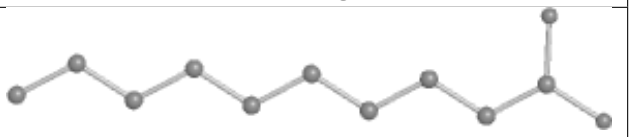
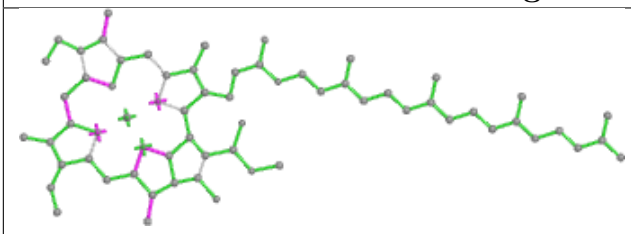
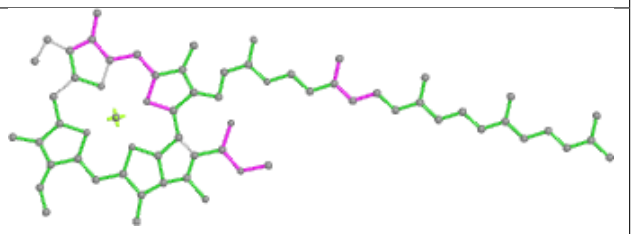
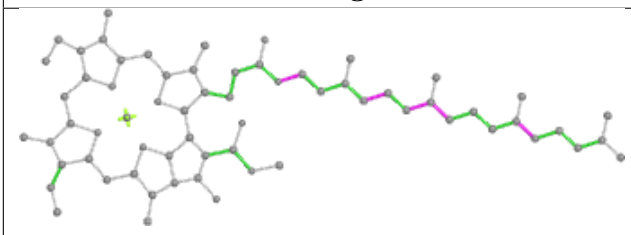
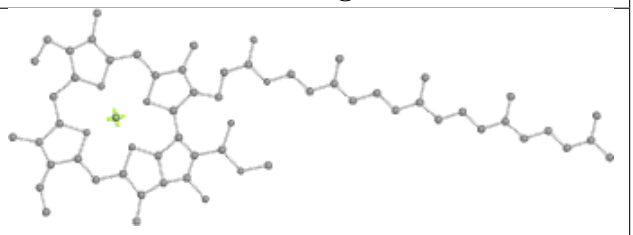

Rings

Ligand CLA D 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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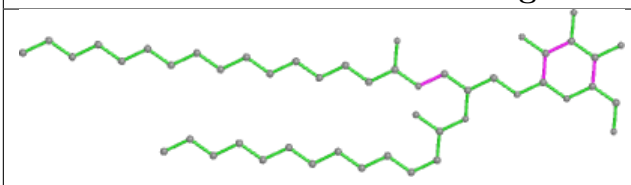
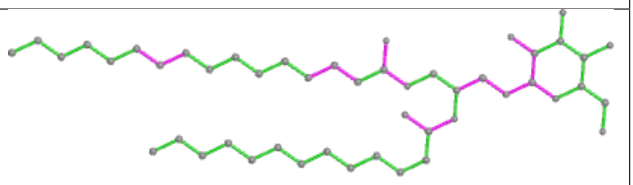
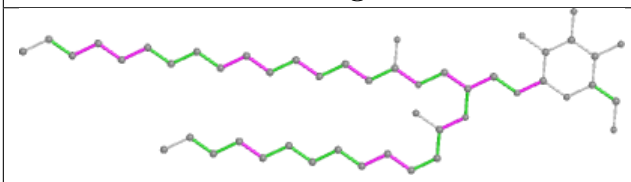
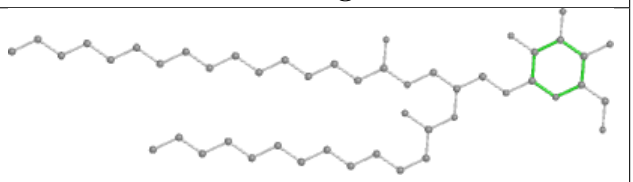
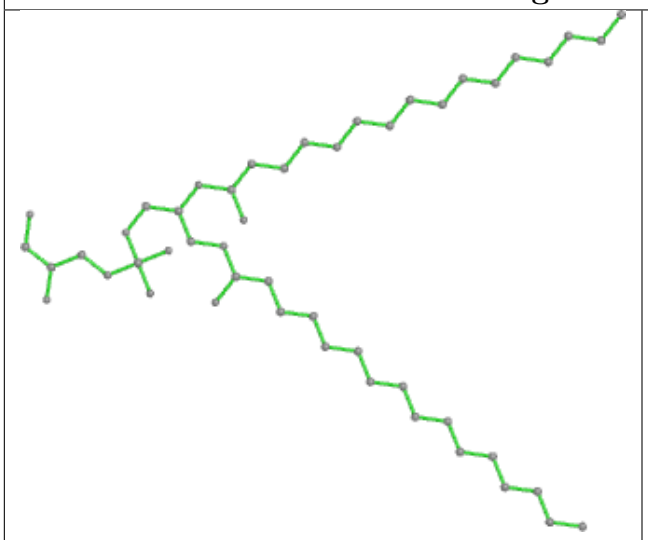
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG l 101



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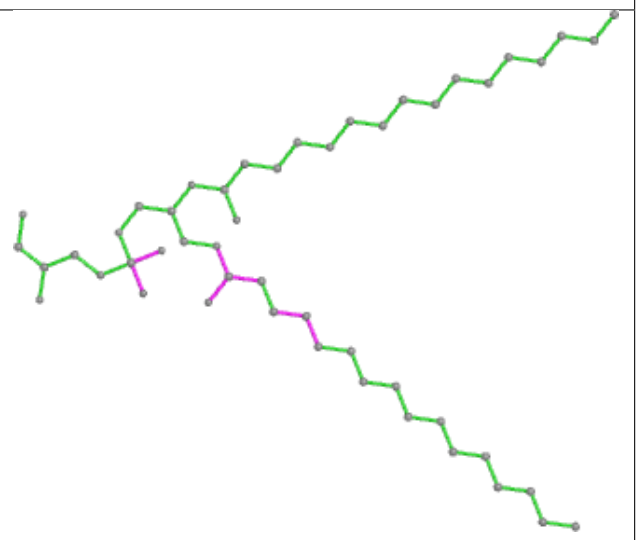

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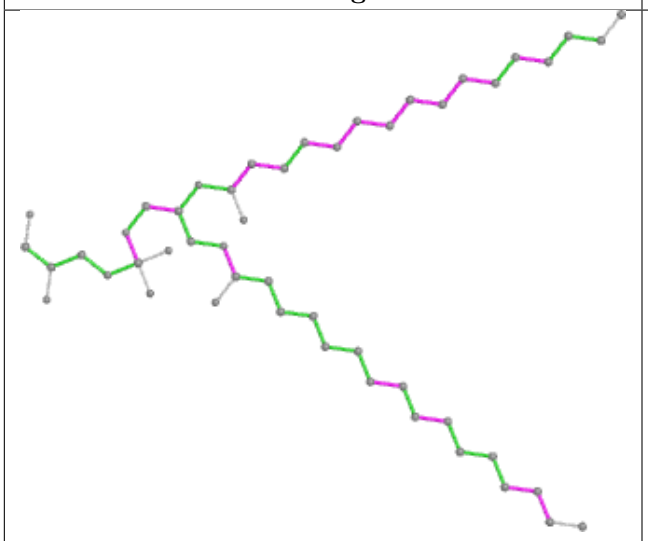

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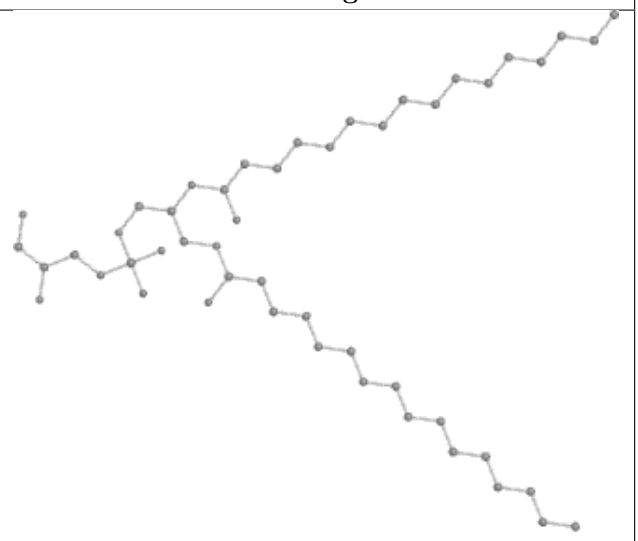
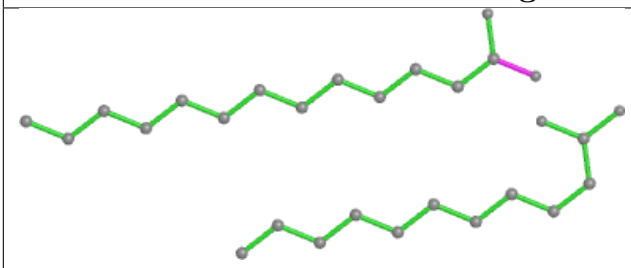


Rings

Ligand LMG D 410



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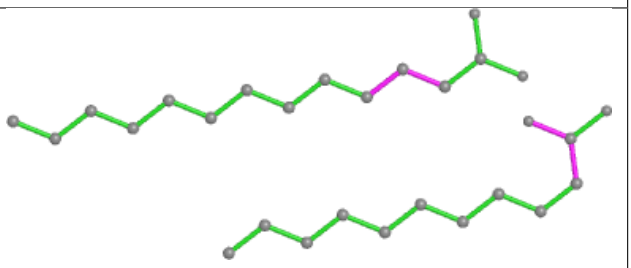

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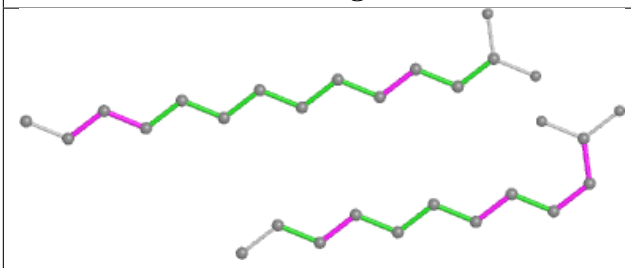

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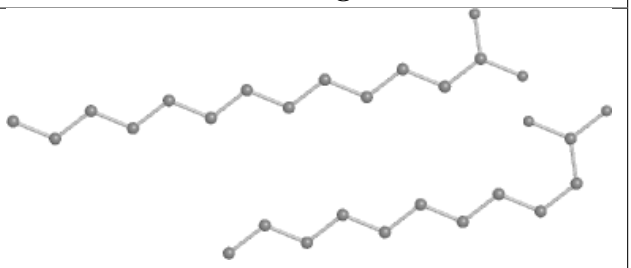
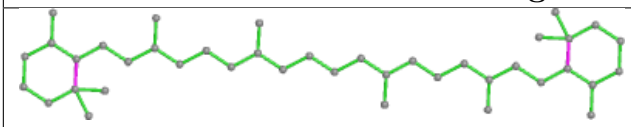


Rings

Ligand BCR t 101



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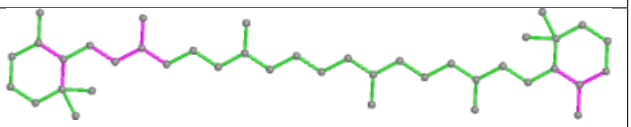

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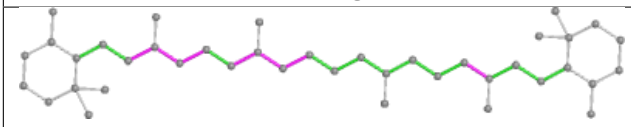
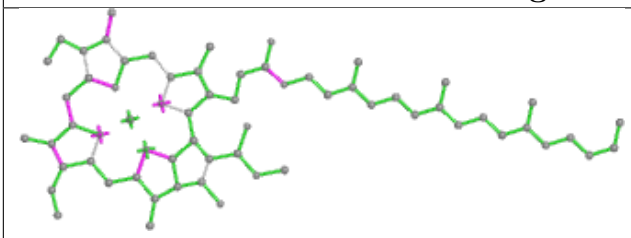


Torsions

Rings

Ligand CLA c 508



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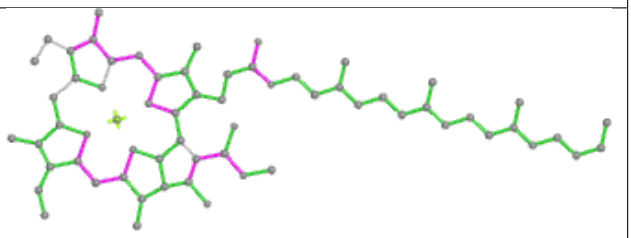

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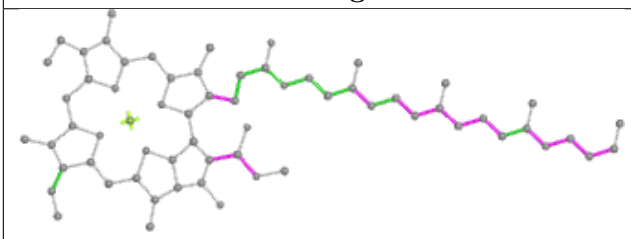

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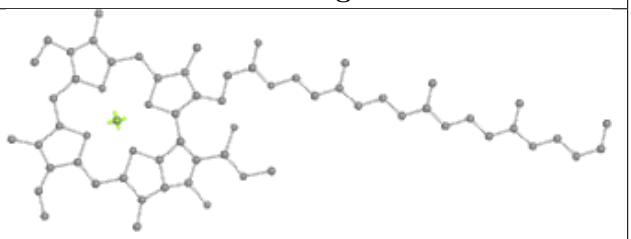

Rings

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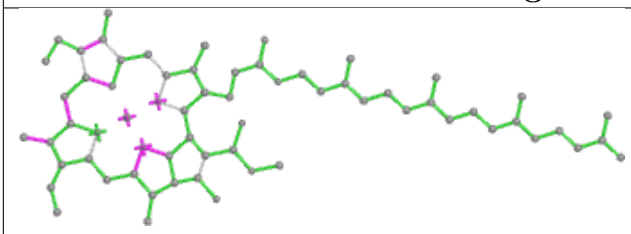

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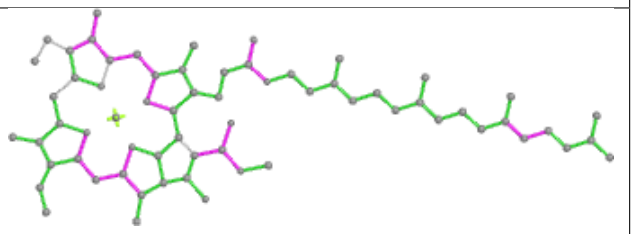

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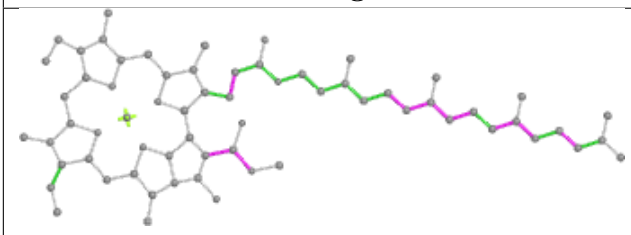

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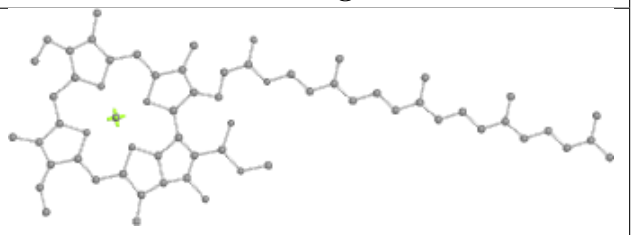

Rings

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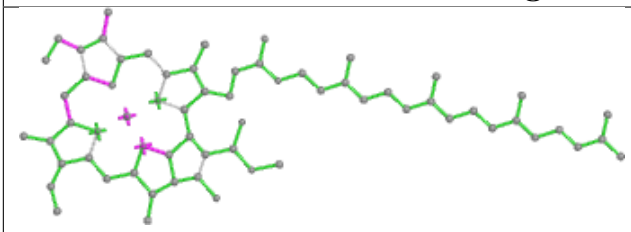

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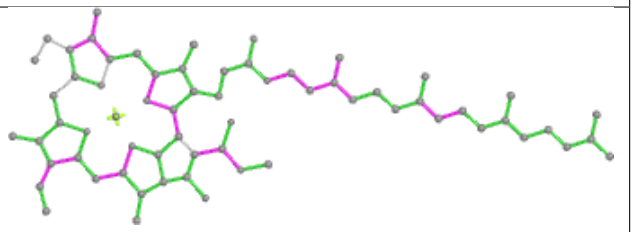

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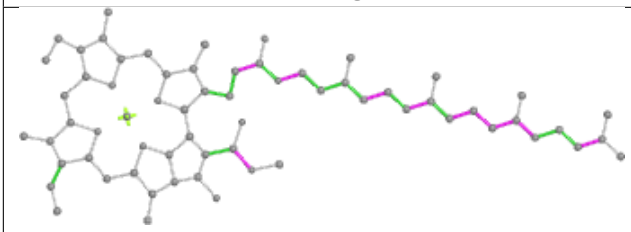

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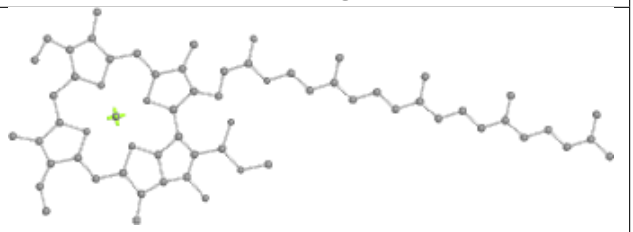
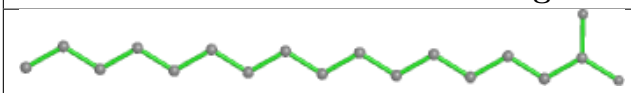


Rings

Ligand STE t 104



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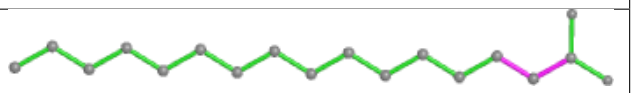

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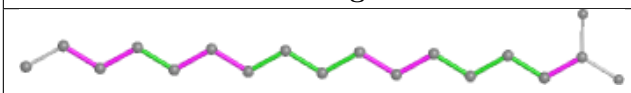

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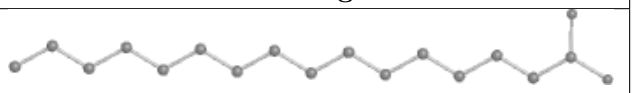
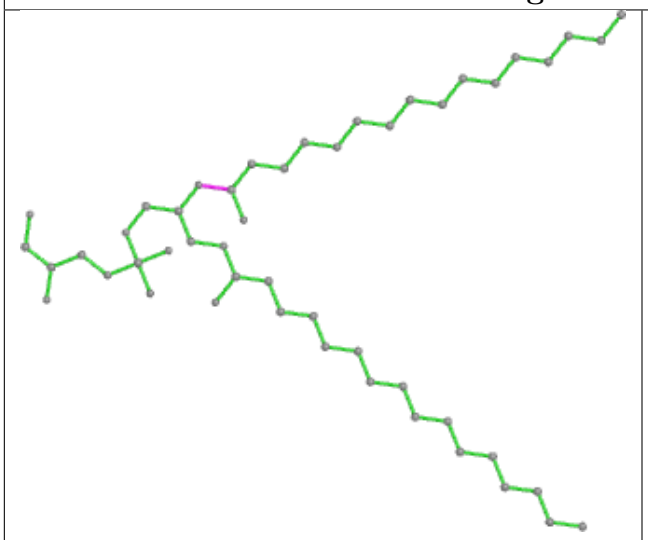


Rings

Ligand LHG d 408



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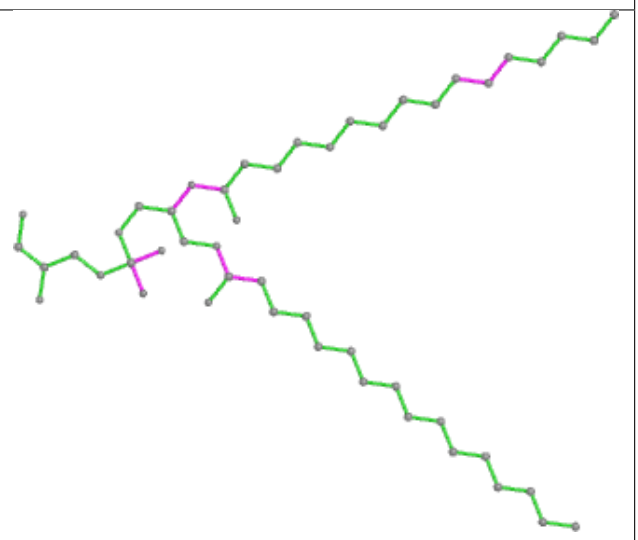

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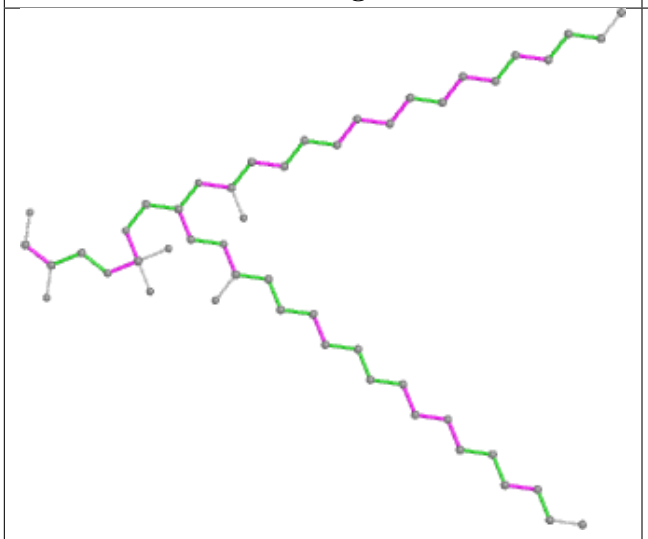

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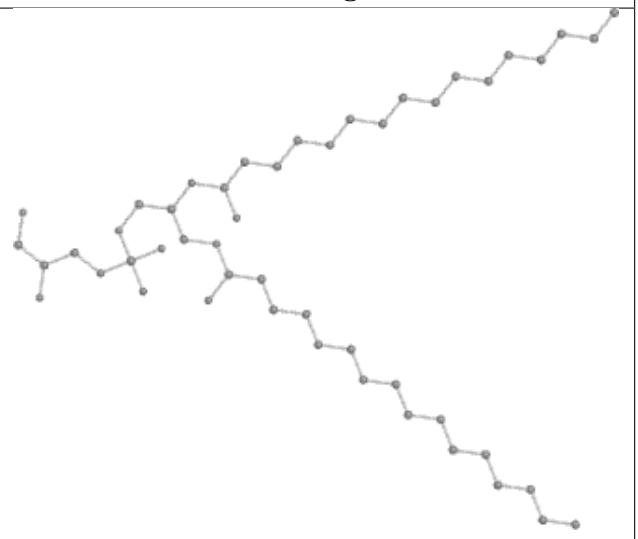
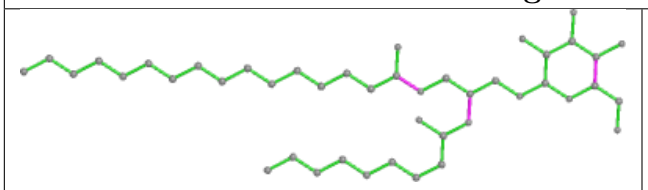


Rings

Ligand LMG d 410



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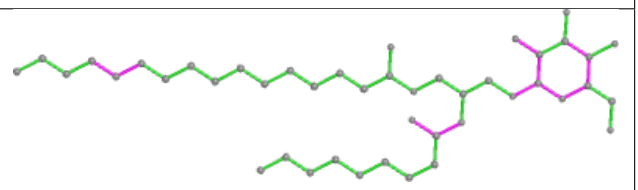
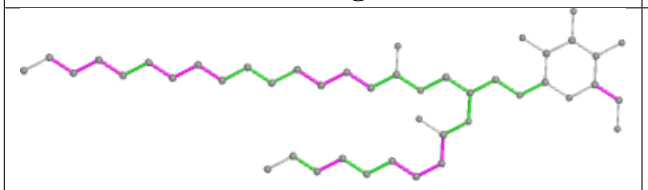


Bond angles



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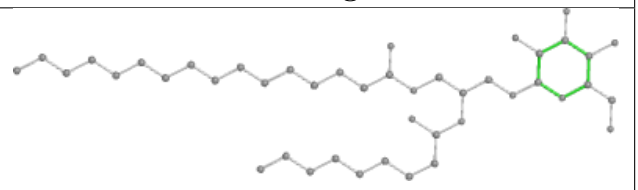
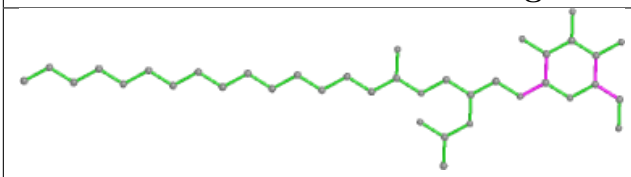


Rings

Ligand LMG c 519



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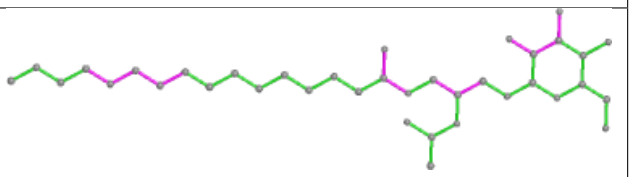
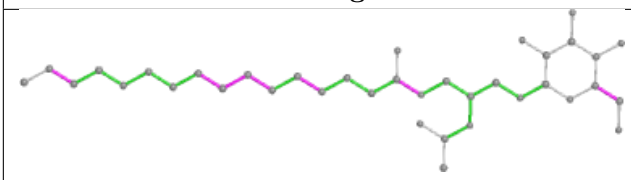


Bond angles



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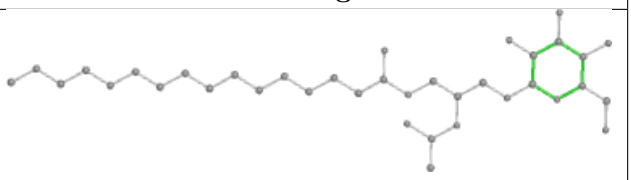
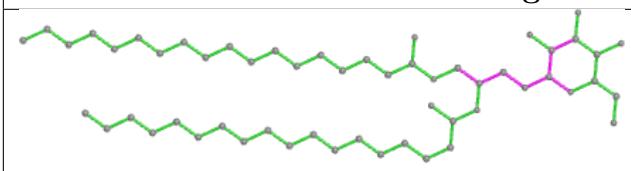
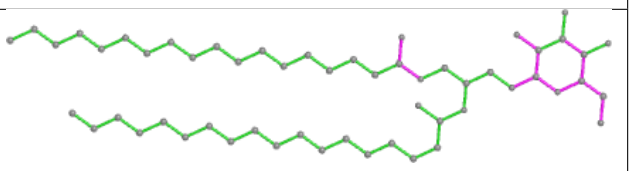


Rings

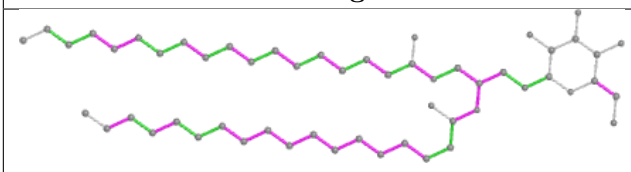
Ligand LMG b 622



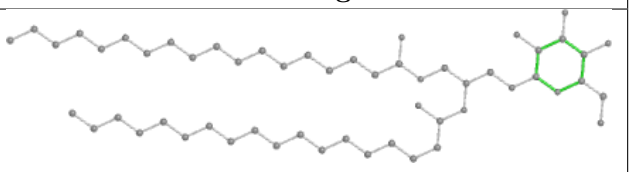
Bond lengths



Bond angles

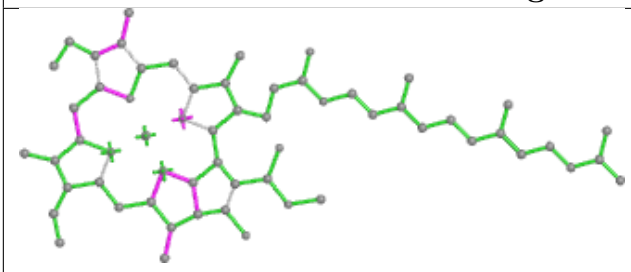


Torsions

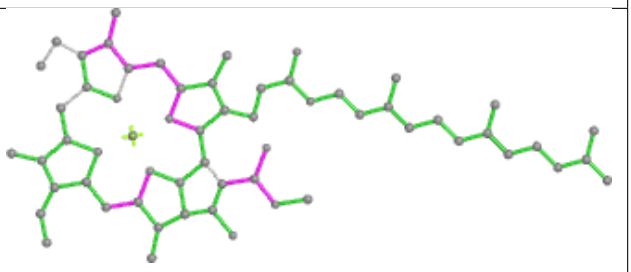


Rings

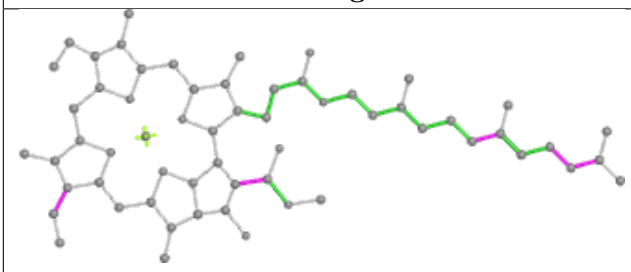
Ligand CLA b 616



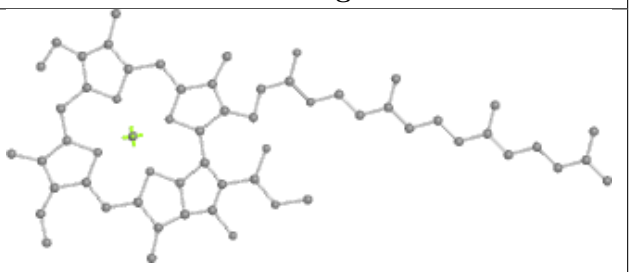
Bond lengths



Bond angles

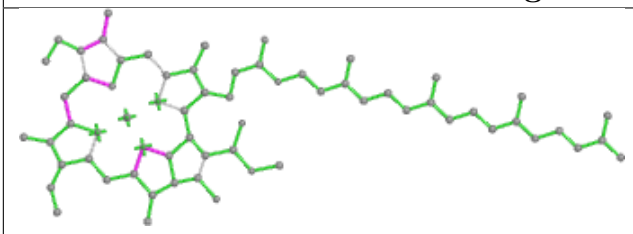


Torsions

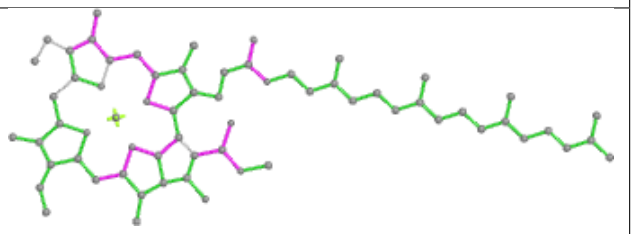


Rings

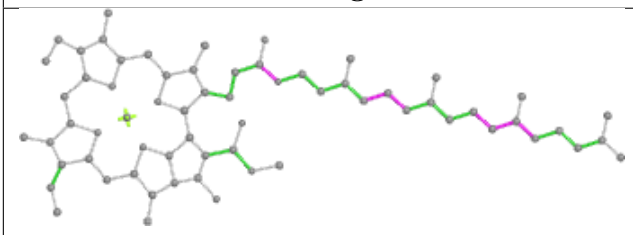
Ligand CLA B 616



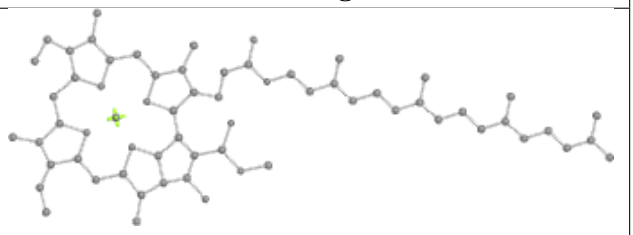
Bond lengths



Bond angles

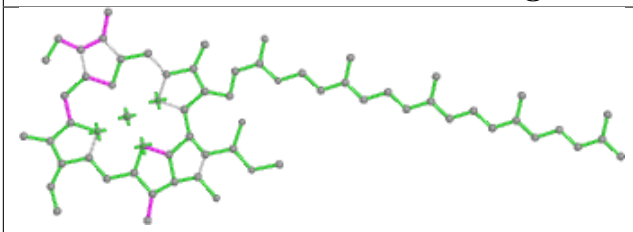


Torsions

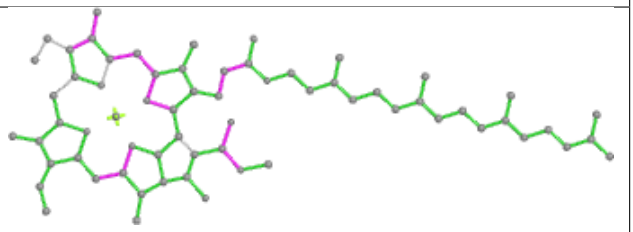


Rings

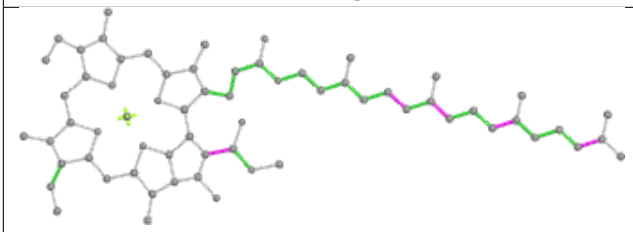
Ligand CLA C 508



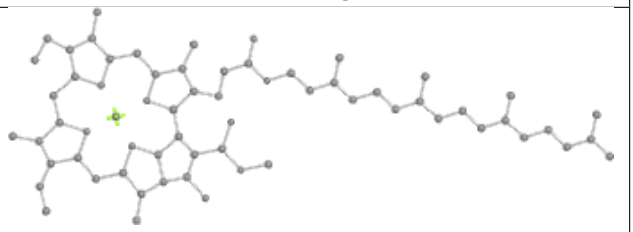
Bond lengths



Bond angles

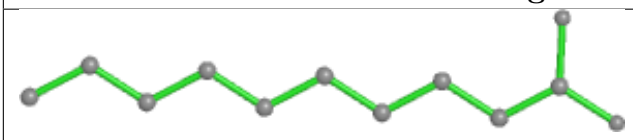


Torsions

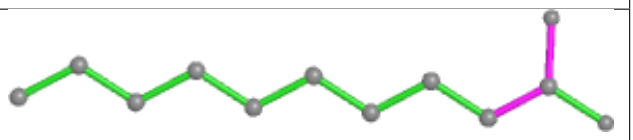


Rings

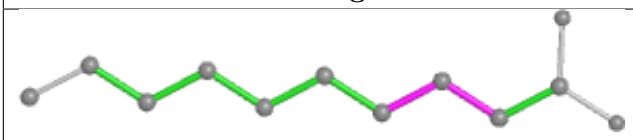
Ligand STE B 601



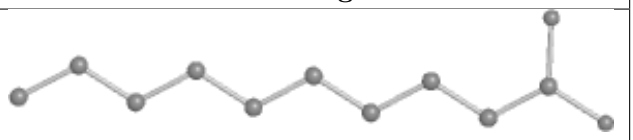
Bond lengths



Bond angles

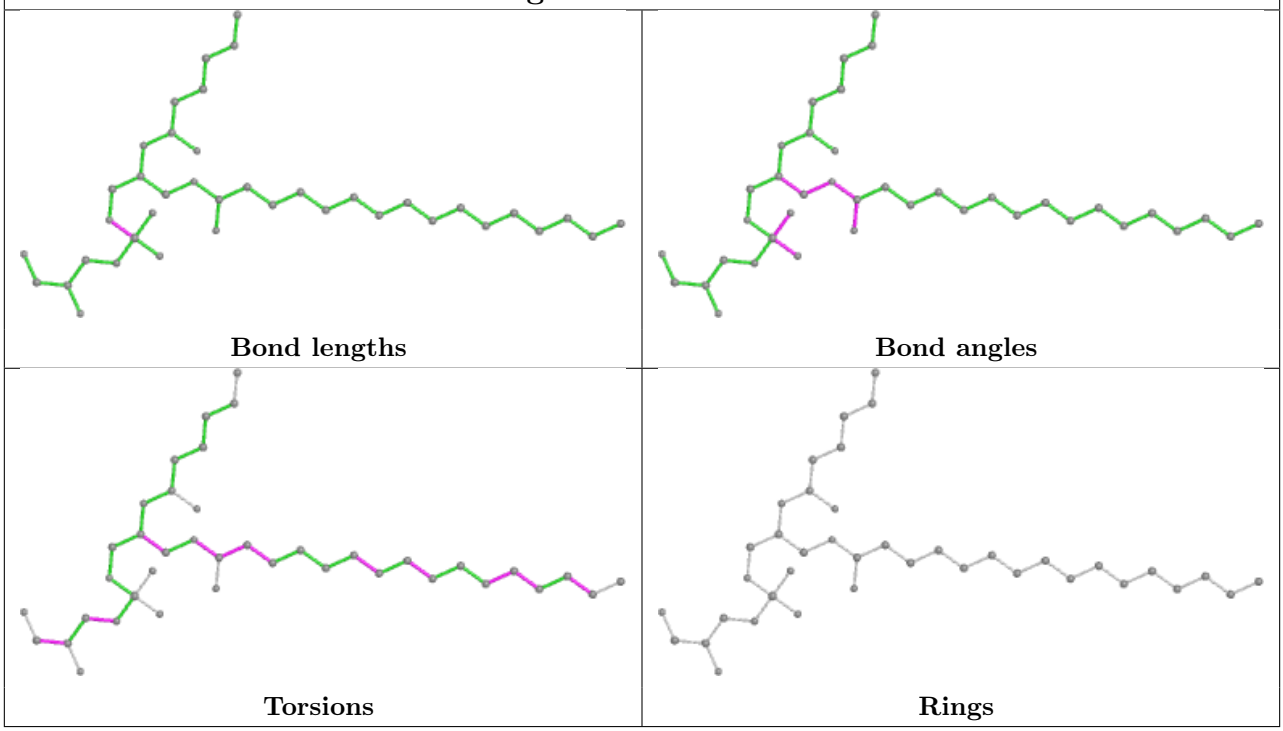


Torsions

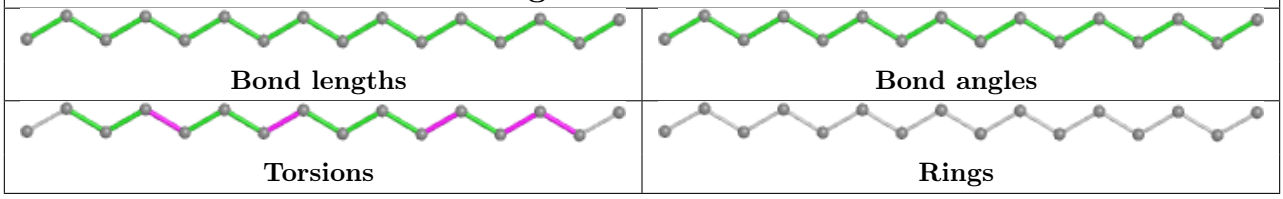


Rings

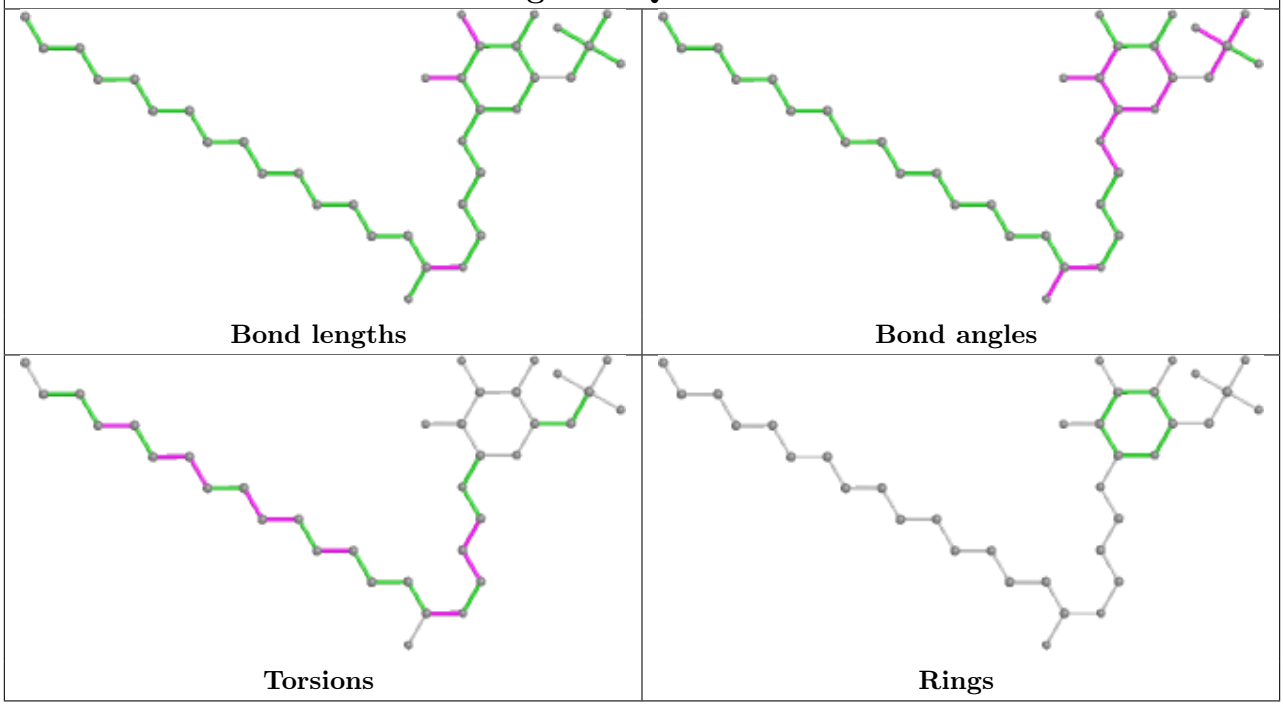
Ligand LHG d 409



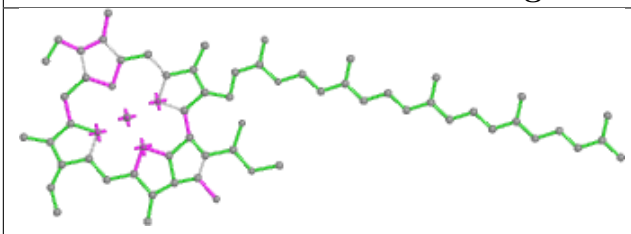
Ligand STE C 521



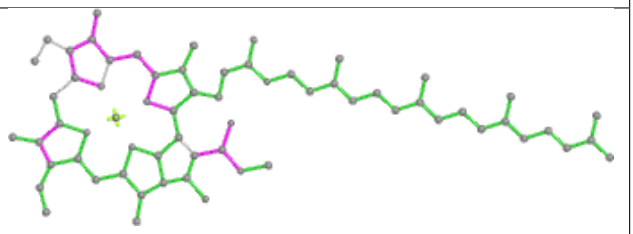
Ligand SQD F 101



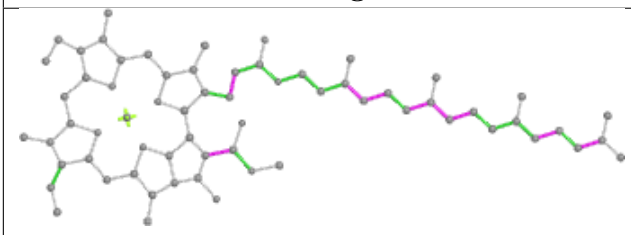
Ligand CLA B 615



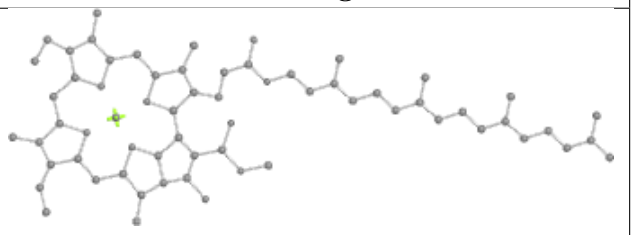
Bond lengths



Bond angles

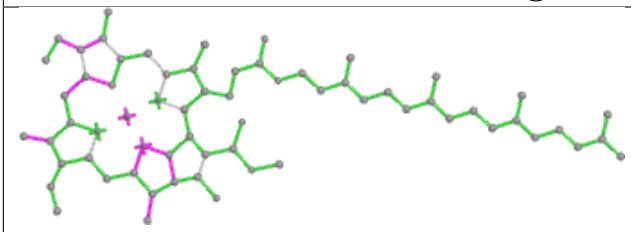


Torsions

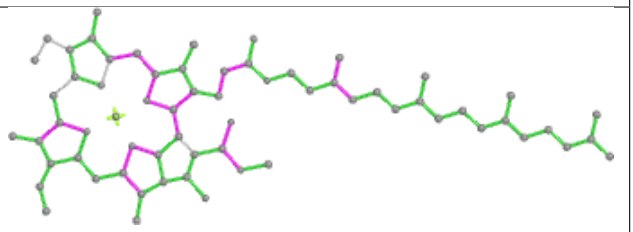


Rings

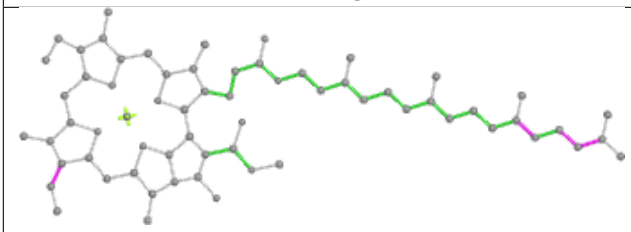
Ligand CLA b 610



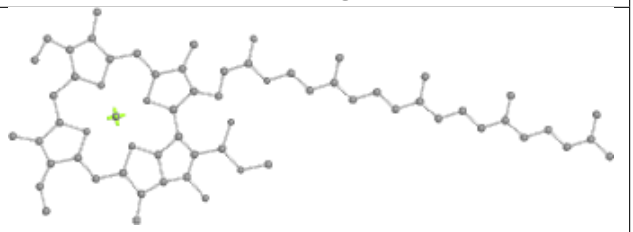
Bond lengths



Bond angles

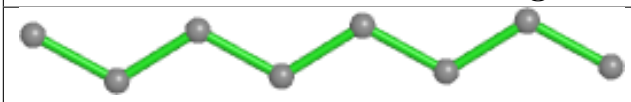


Torsions



Rings

Ligand STE Z 102



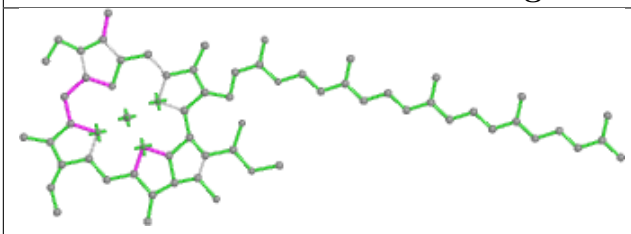
Bond lengths

Bond angles

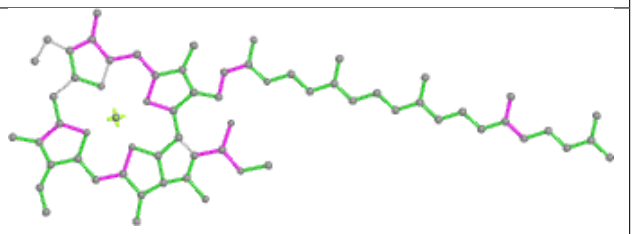
Torsions

Rings

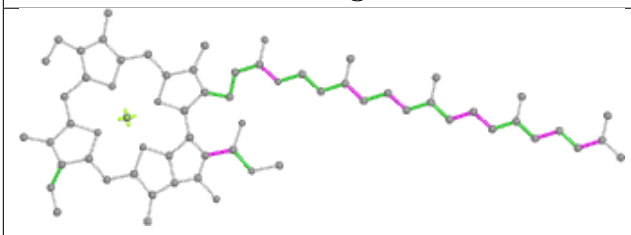
Ligand CLA B 606



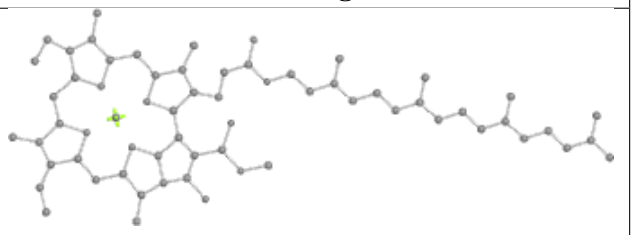
Bond lengths



Bond angles

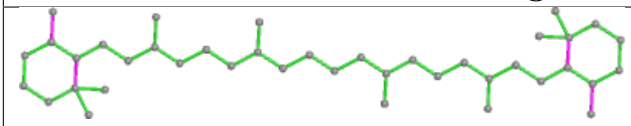


Torsions

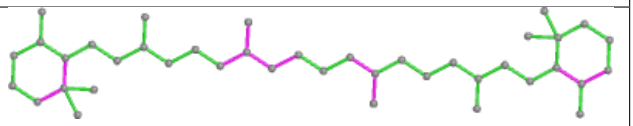


Rings

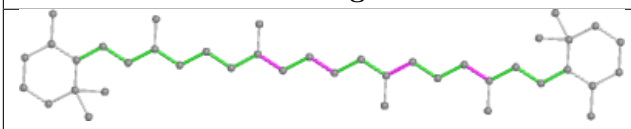
Ligand BCR c 515



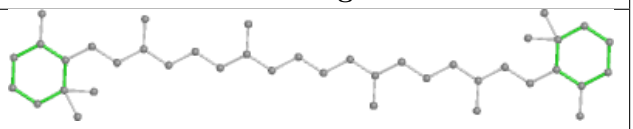
Bond lengths



Bond angles

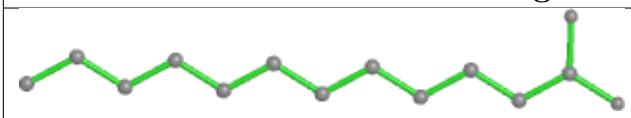


Torsions



Rings

Ligand STE t 102



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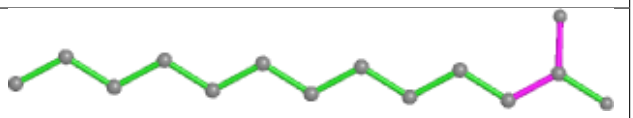
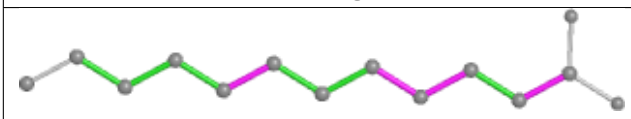


Bond angles



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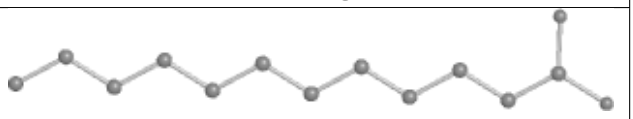
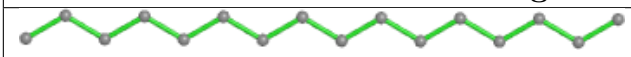


Rings

Ligand STE b 620



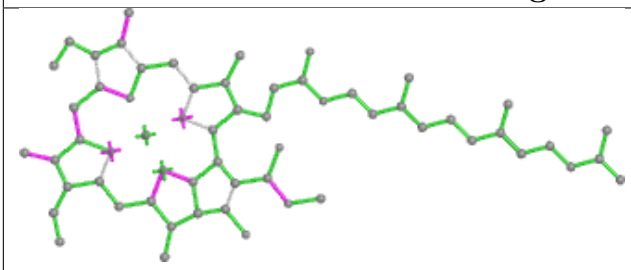
Bond lengths

Bond angles

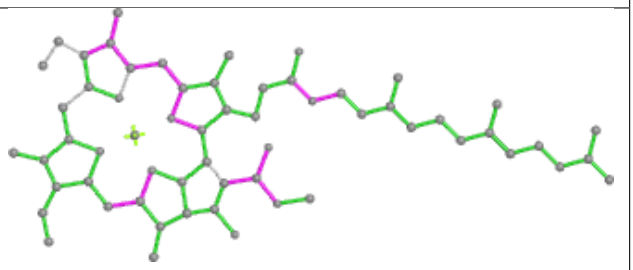
Torsions

Rings

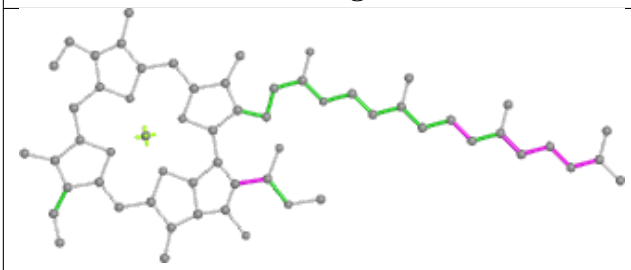
Ligand CLA c 504



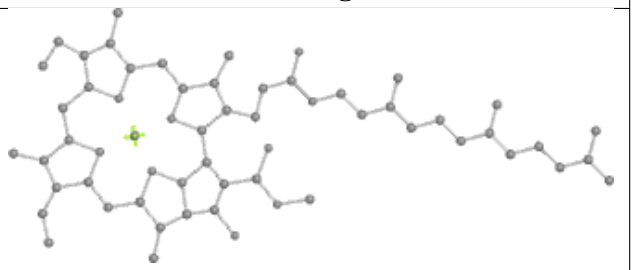
Bond lengths



Bond angles

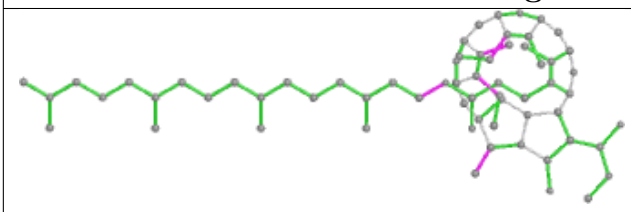


Torsions

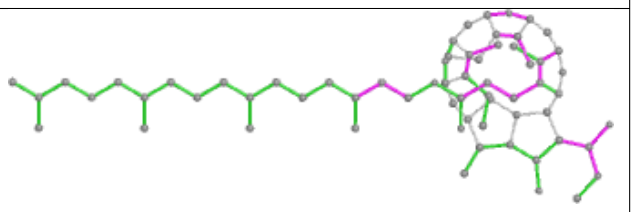


Rings

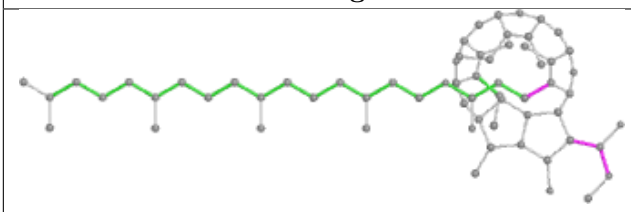
Ligand PHO d 401



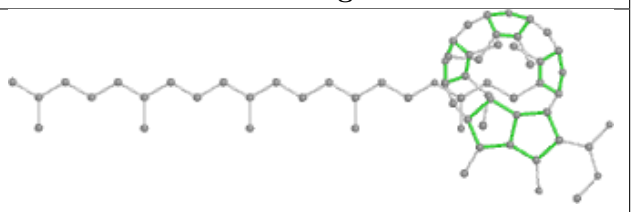
Bond lengths



Bond angles

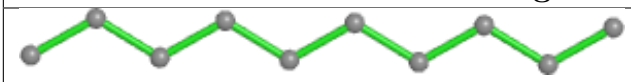


Torsions



Rings

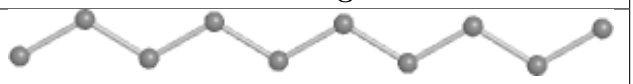
Ligand STE t 103



Bond lengths

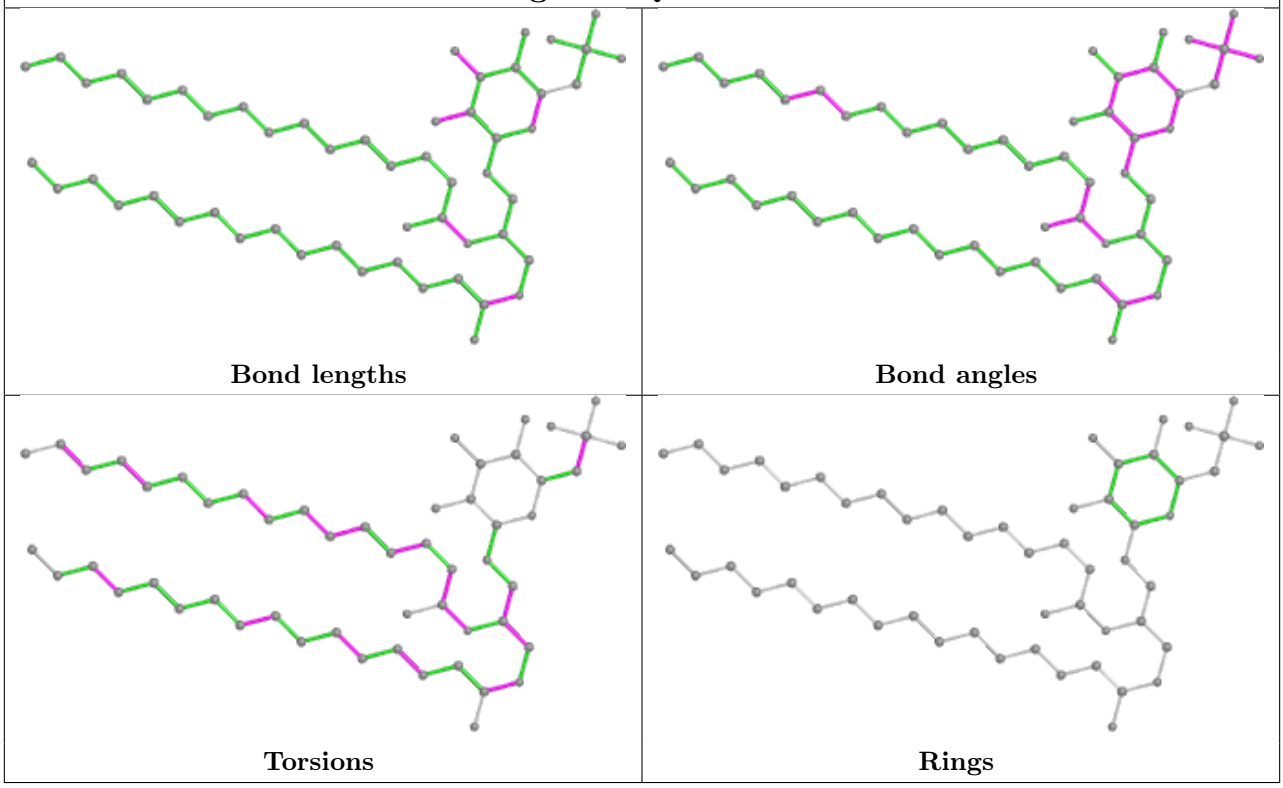
Bond angles

Torsions

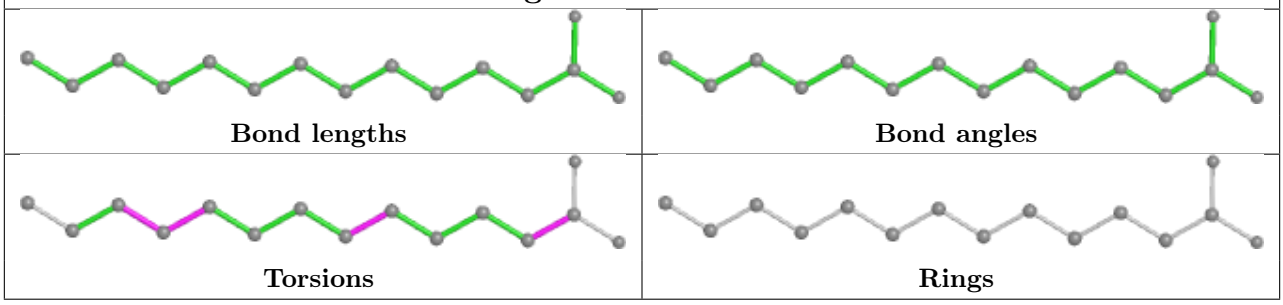


Rings

Ligand SQD a 411



Ligand STE M 102



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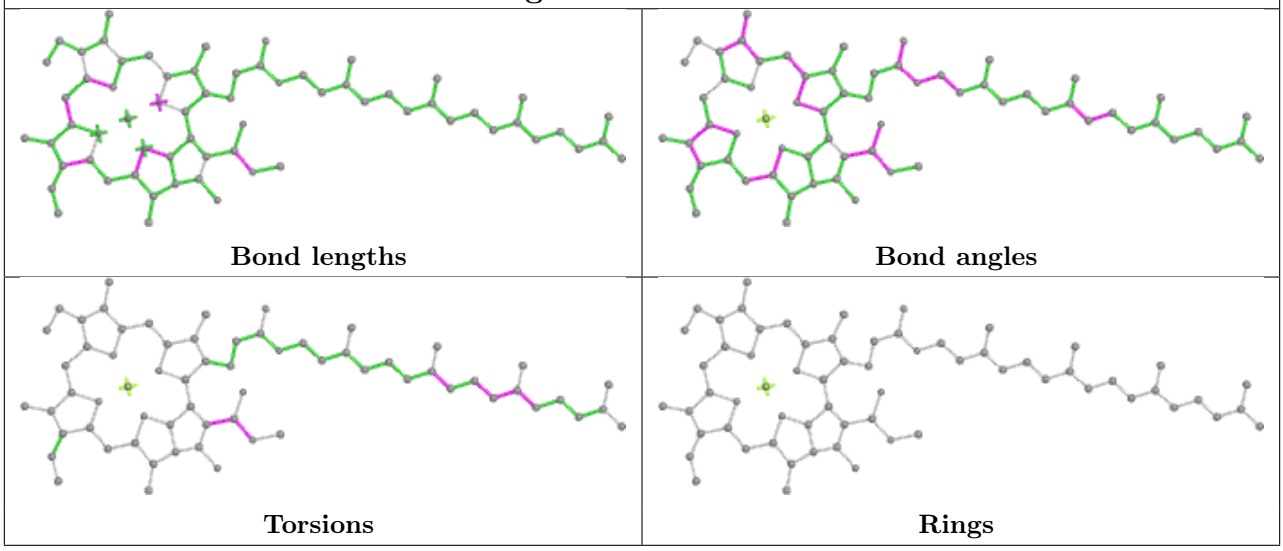
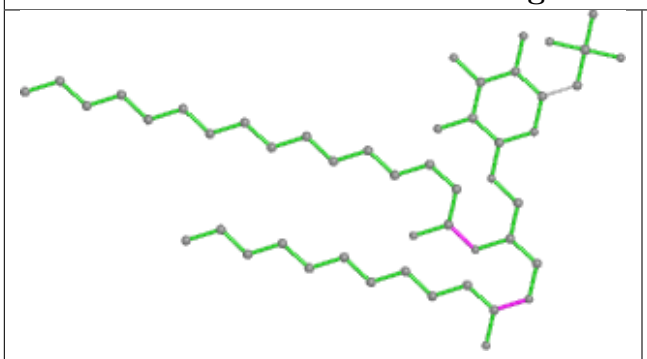
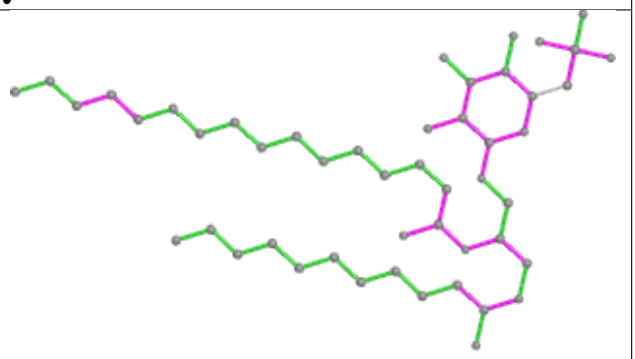


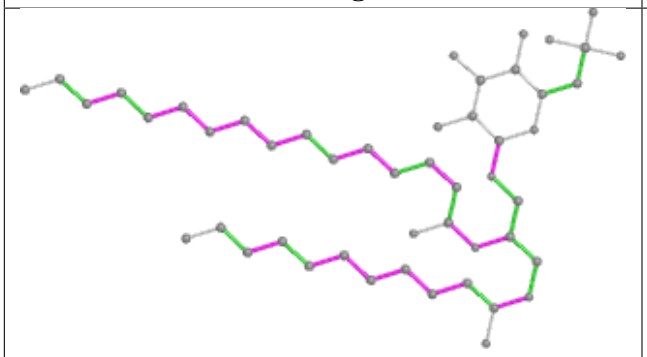
Ligand SQD L 101



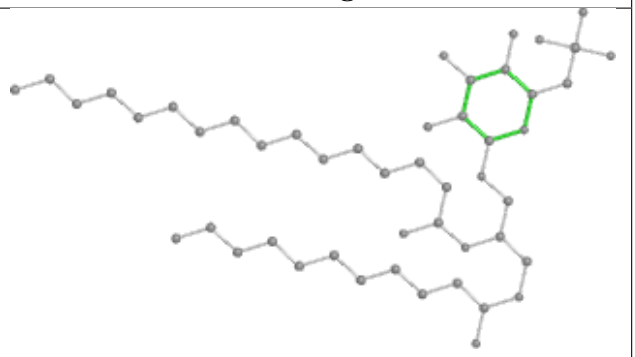
Bond lengths



Bond angles

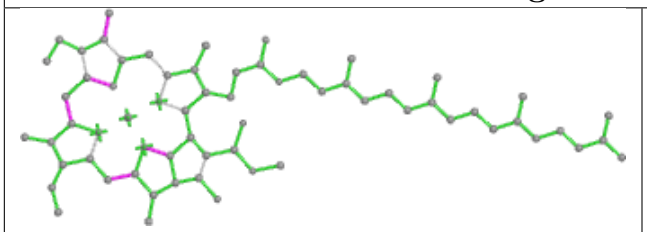


Torsions



Rings

Ligand CLA b 612



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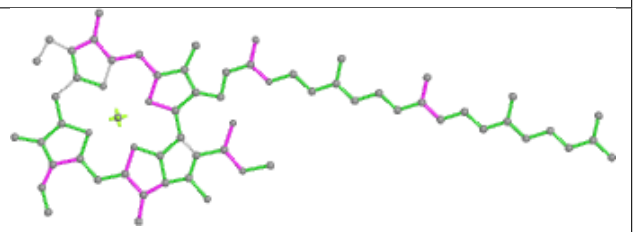
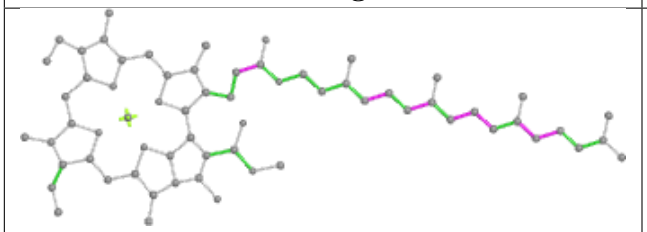


Bond angles



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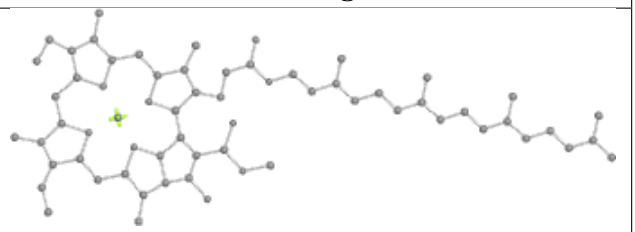
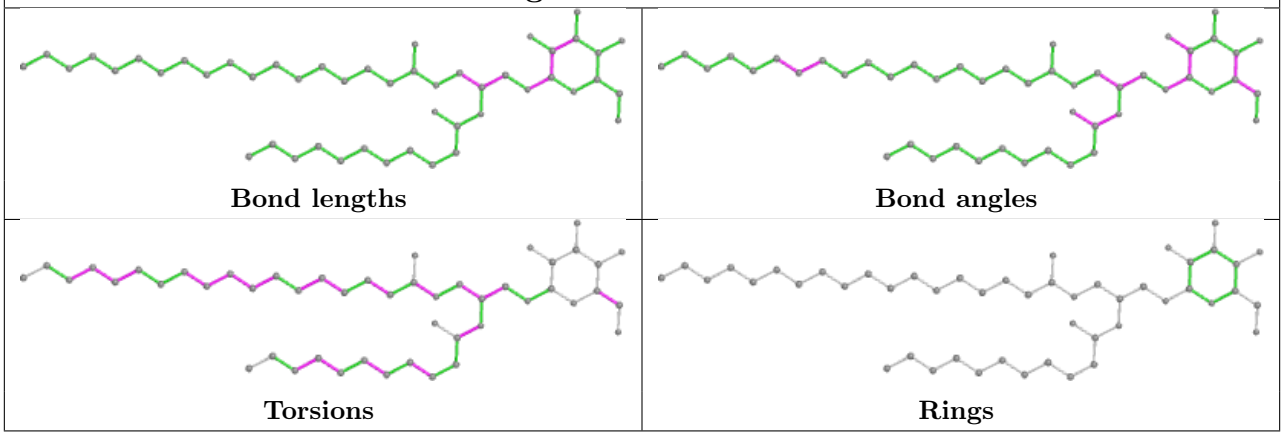


Rings

Ligand LMG c 521



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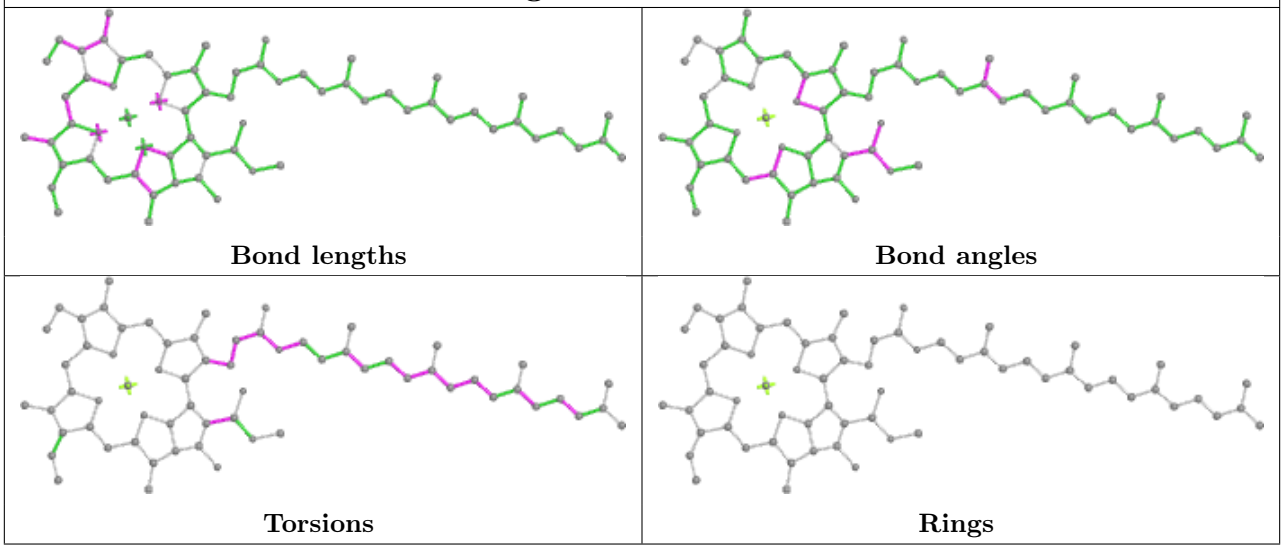
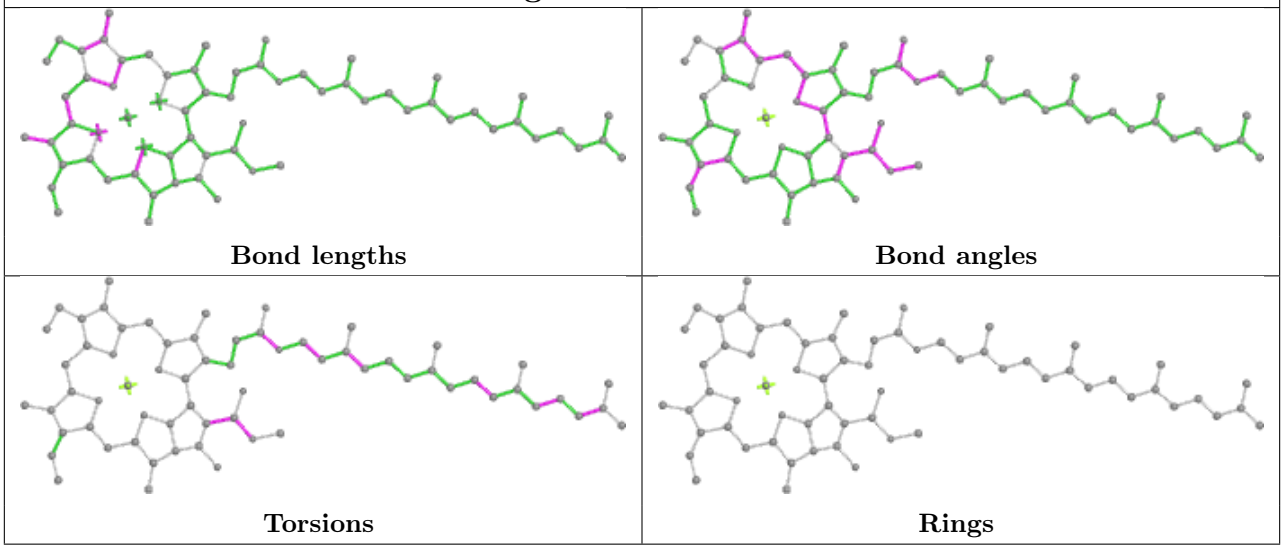
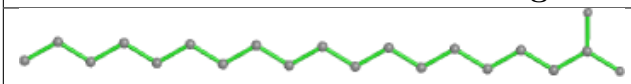


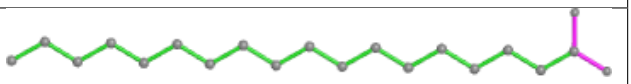
Ligand CLA D 404



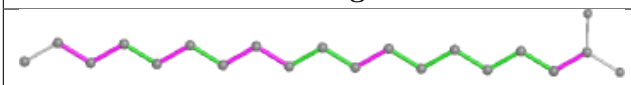
Ligand STE b 626



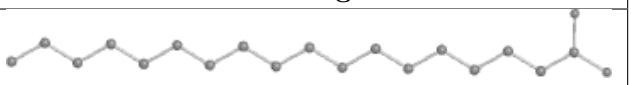
Bond lengths



Bond angles

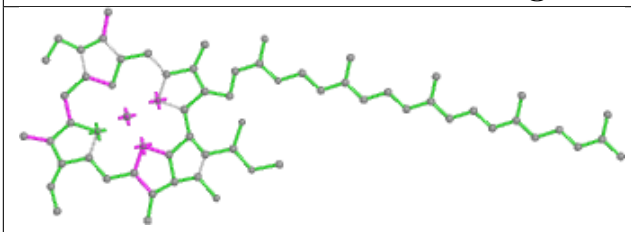


Torsions



Rings

Ligand CLA a 402



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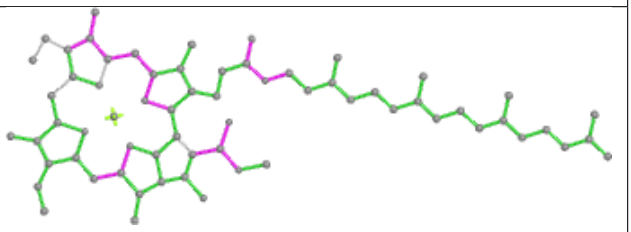

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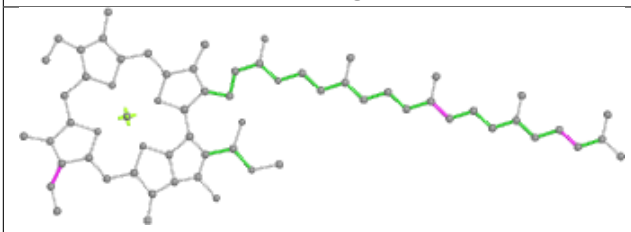

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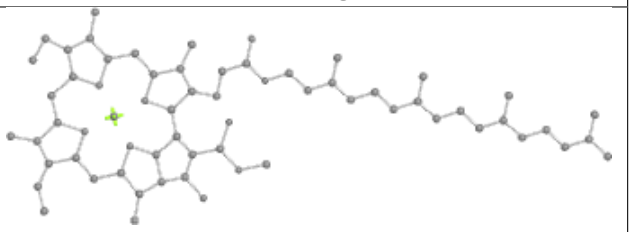
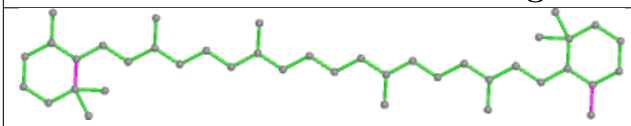


Rings

Ligand BCR a 406



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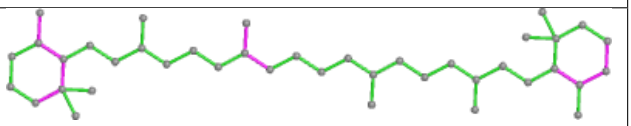
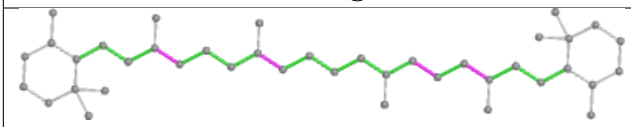


Bond angles



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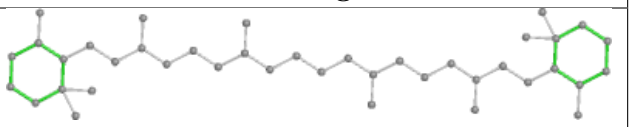
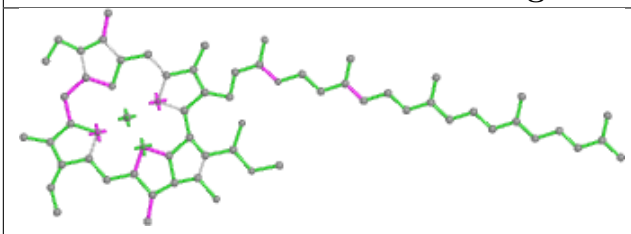


Rings

Ligand CLA b 613



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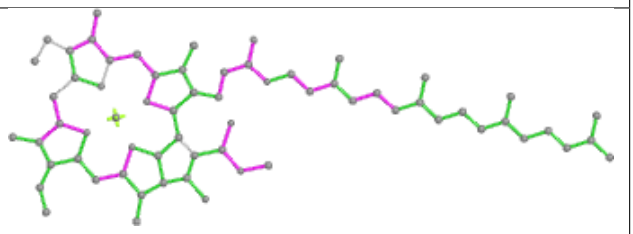

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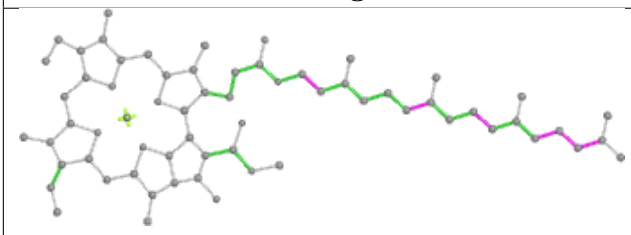

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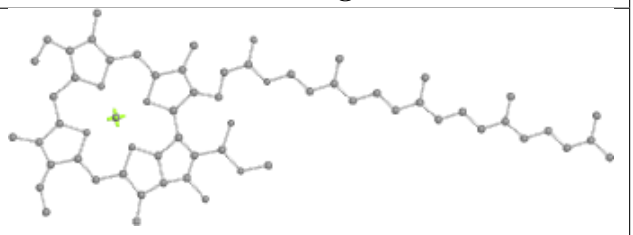
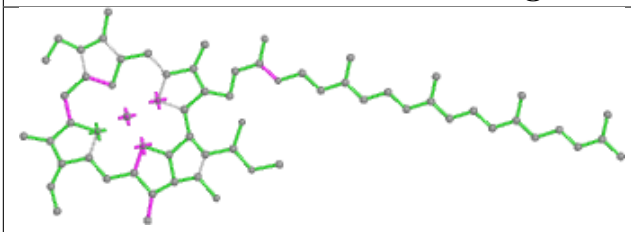


Rings

Ligand CLA C 509



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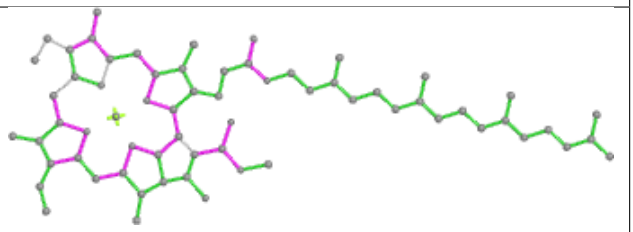
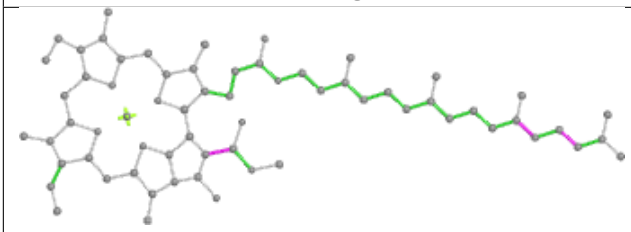


Bond angles



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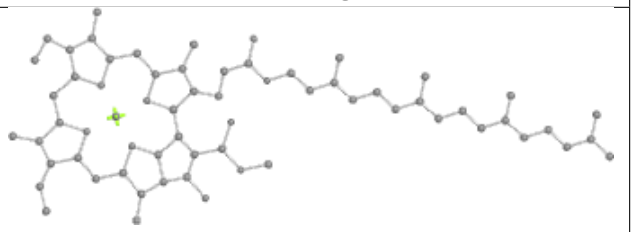
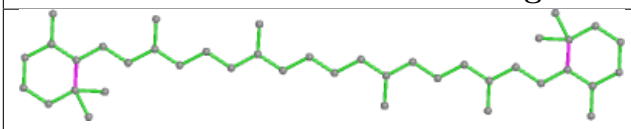


Rings

Ligand BCR Z 101



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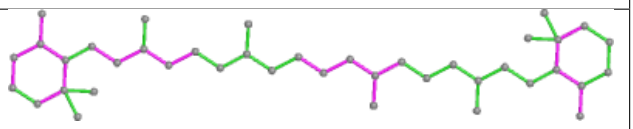
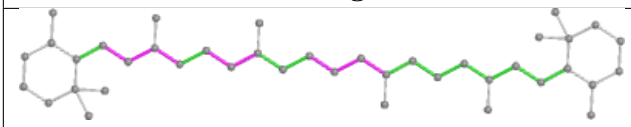


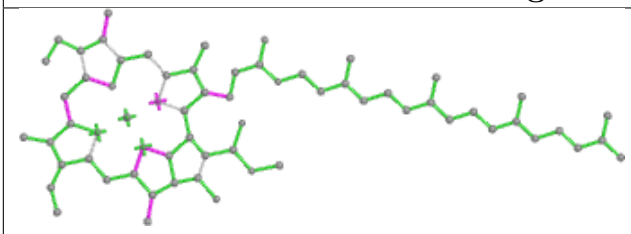
Bond angles



Torsions

Rings

Ligand CLA b 611



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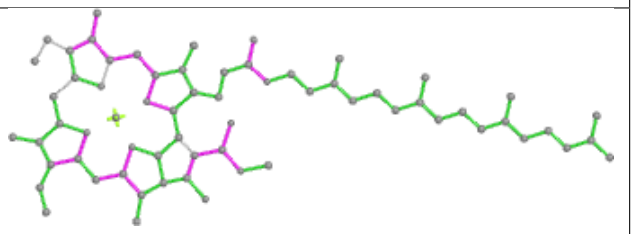
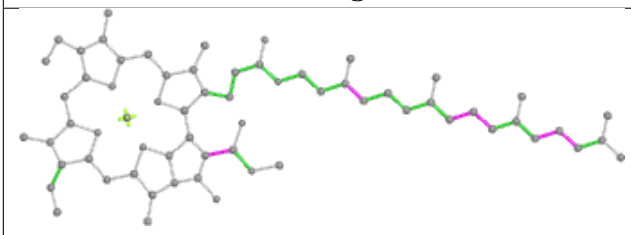


Bond angles



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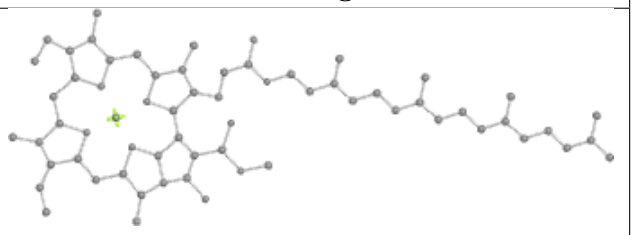
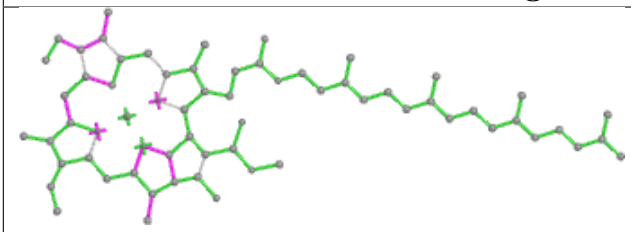


Rings

Ligand CLA C 504



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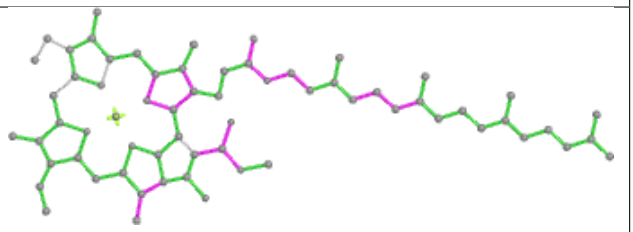

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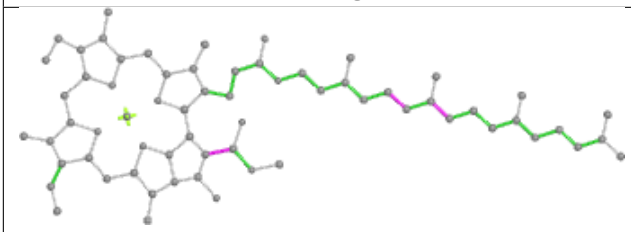

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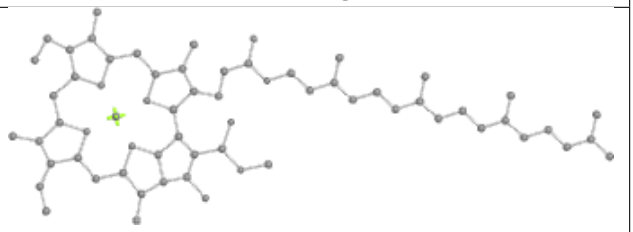
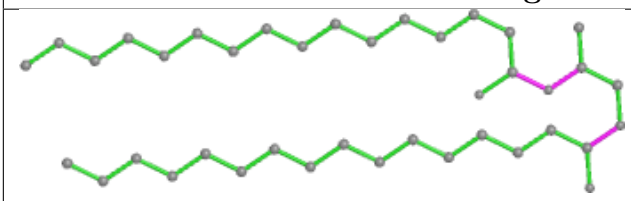


Rings

Ligand SQD A 414



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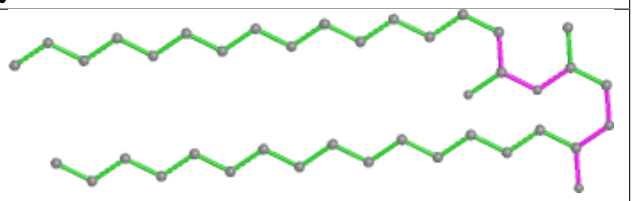
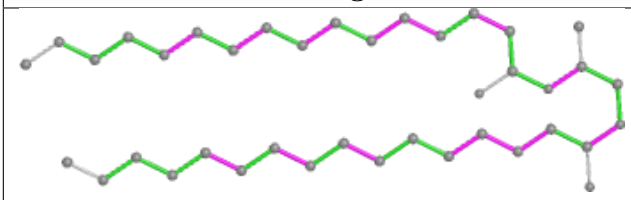
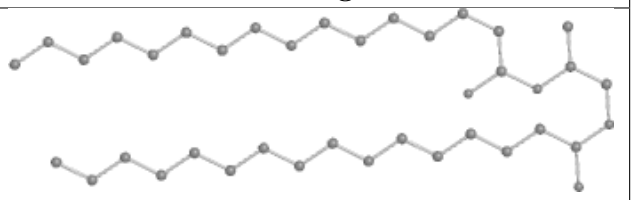


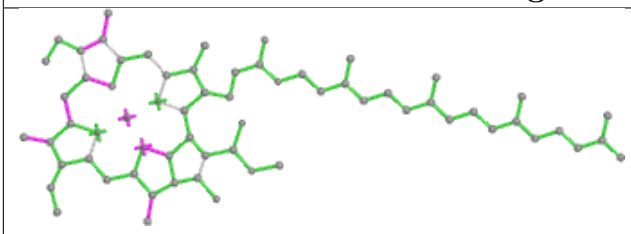
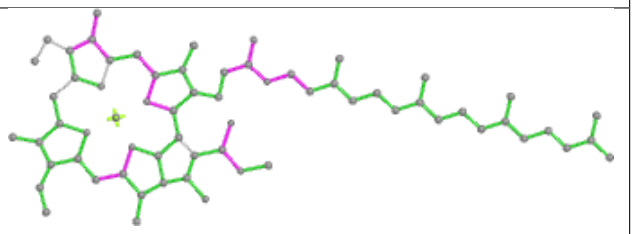
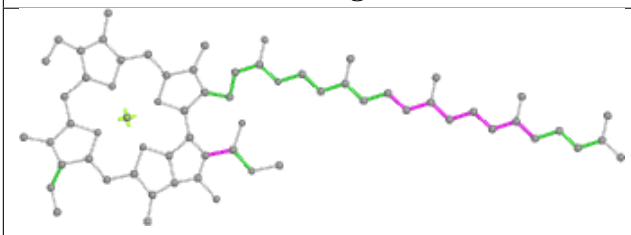
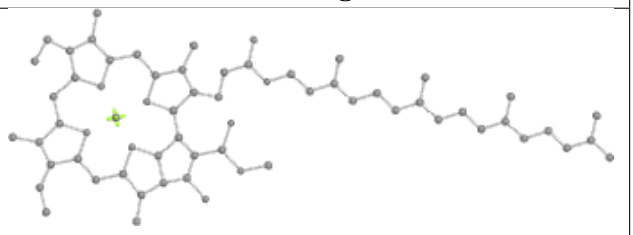
Bond angles

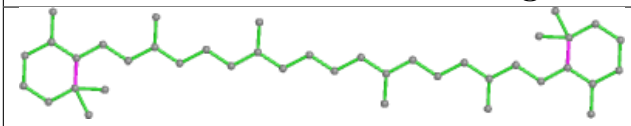
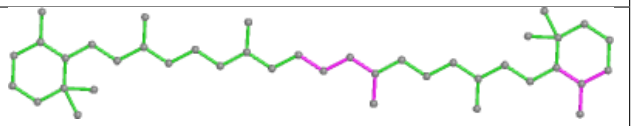
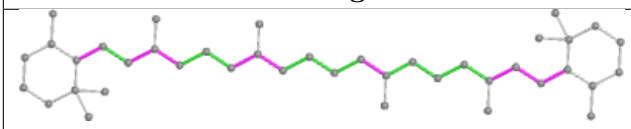
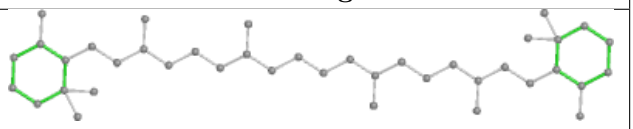


Torsions

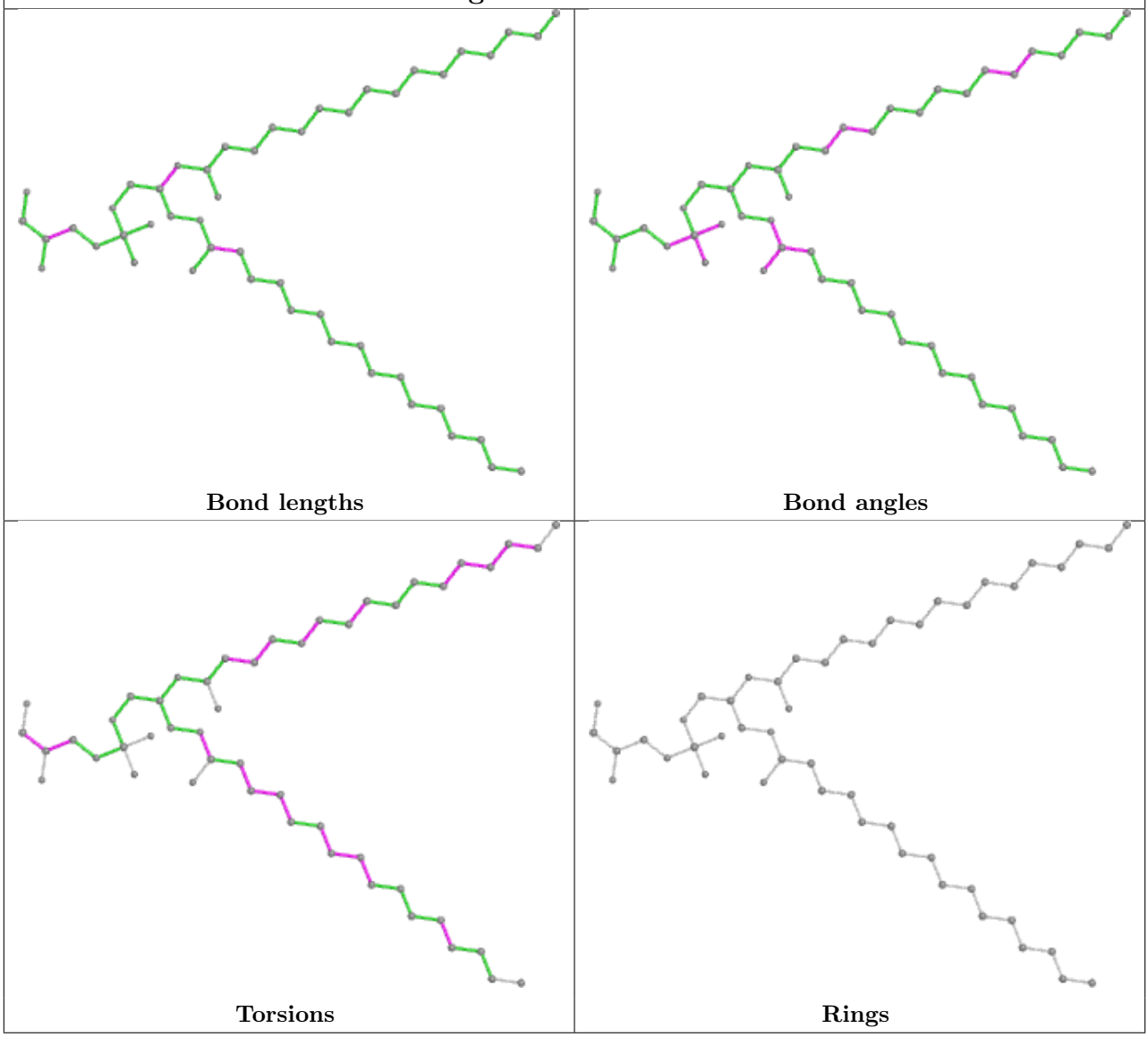


Rings

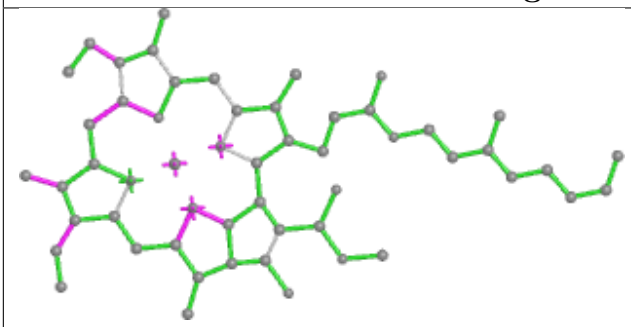
Ligand CLA b 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

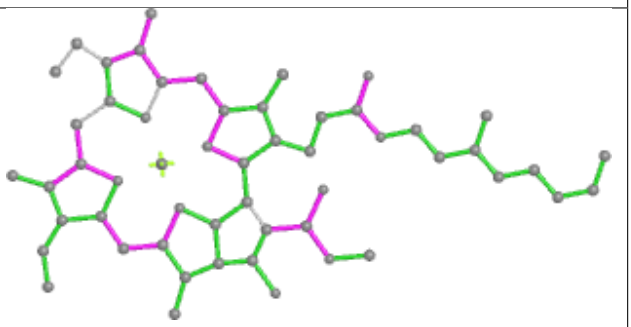
Ligand LHG B 622



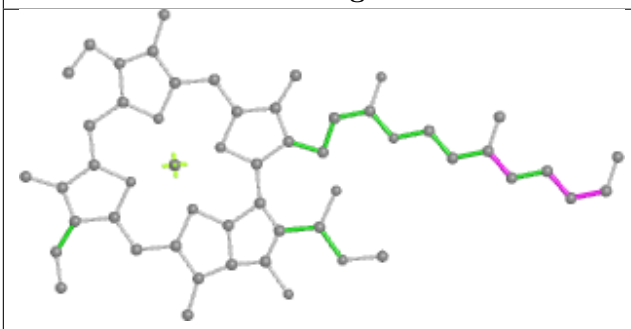
Ligand CLA A 405



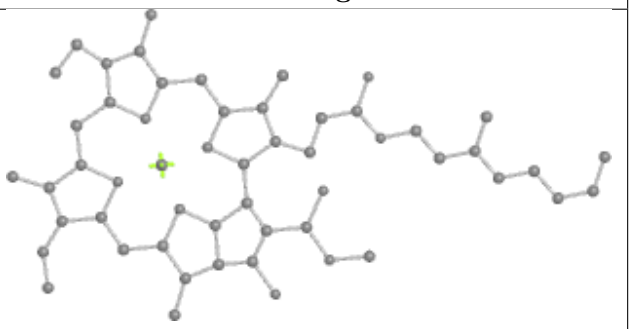
Bond lengths



Bond angles

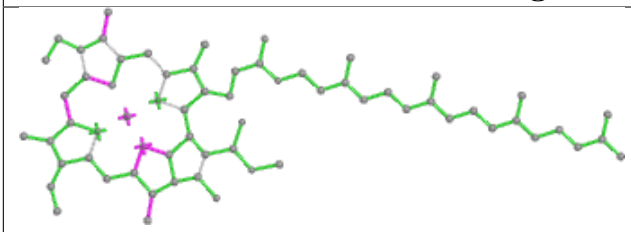


Torsions



Rings

Ligand CLA c 509



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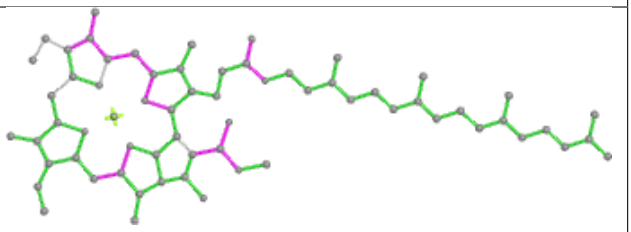

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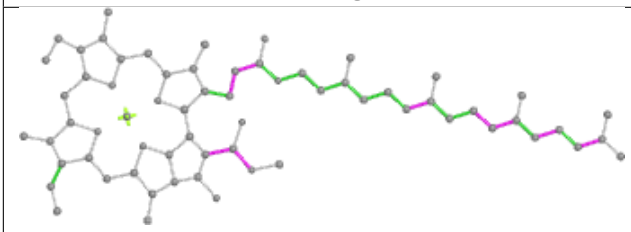

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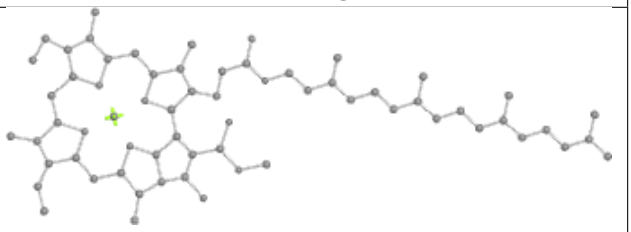
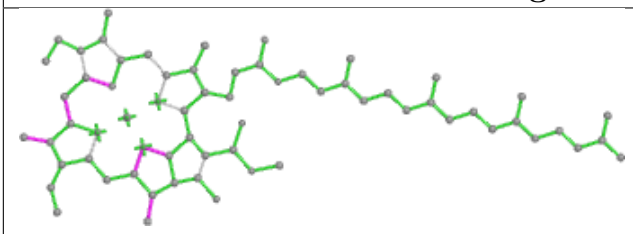


Rings

Ligand CLA c 502



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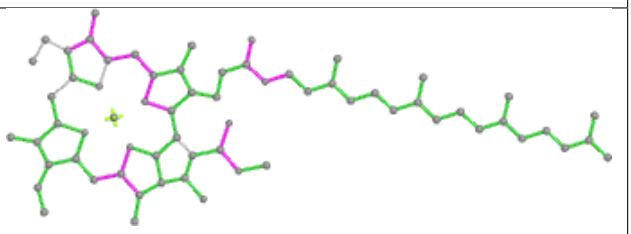
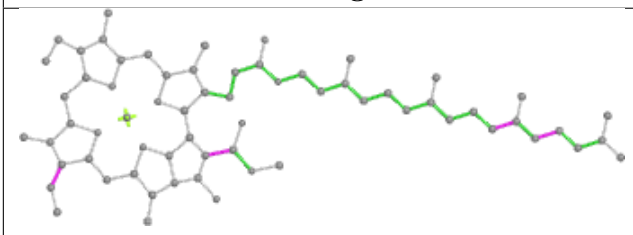


Bond angles



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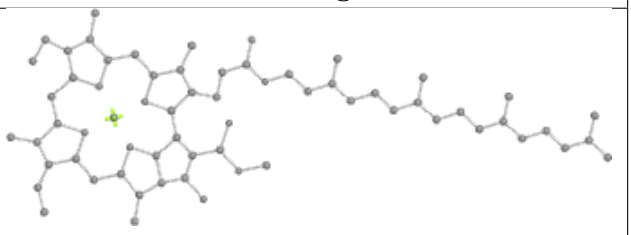
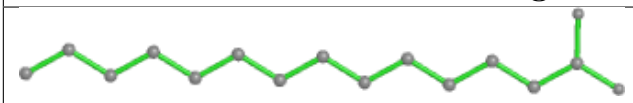


Rings

Ligand STE b 623



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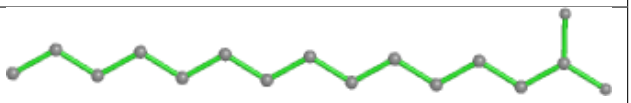
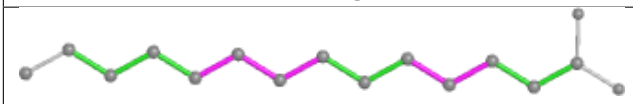


Bond angles



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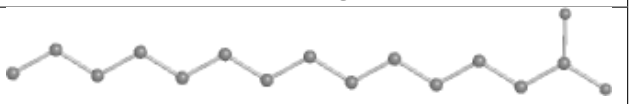

Rings

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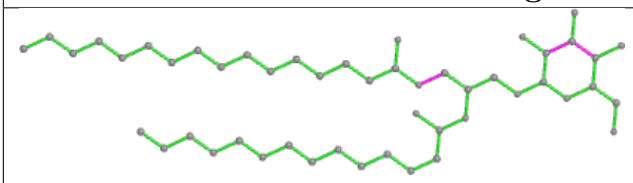

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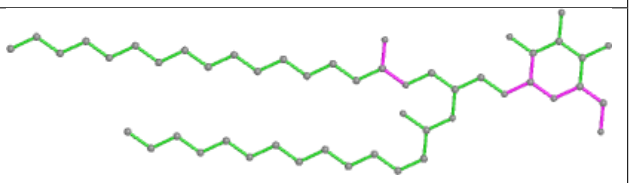
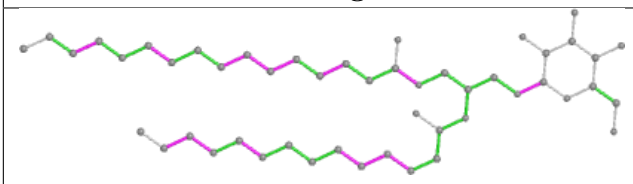


Bond angles



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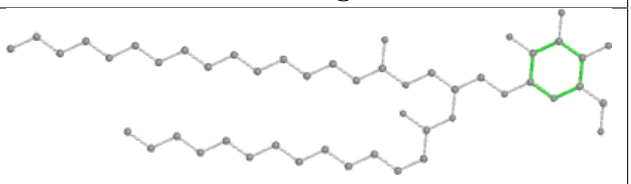

Rings

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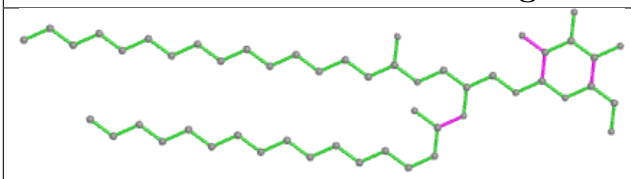

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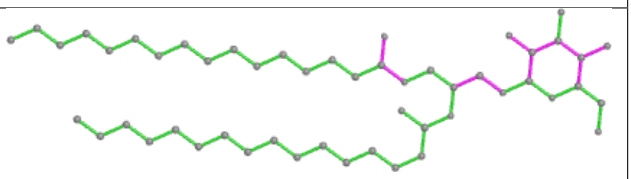

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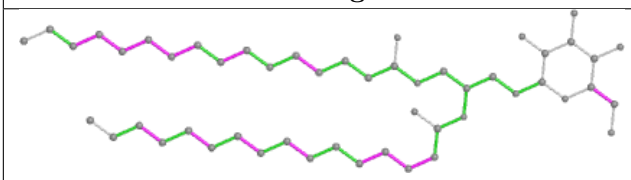

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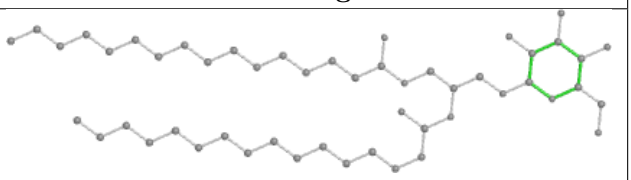

Rings

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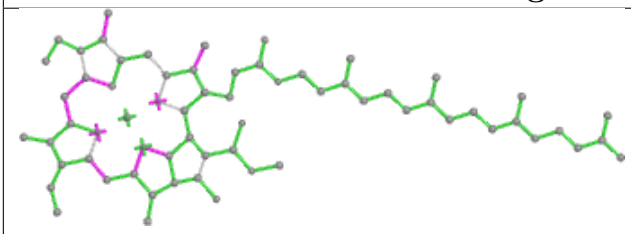

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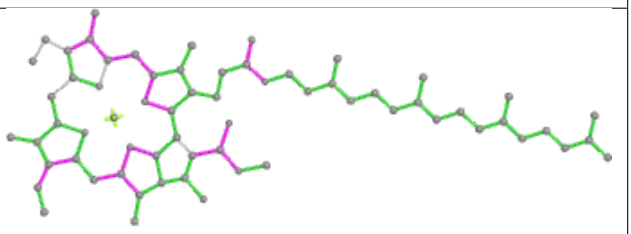

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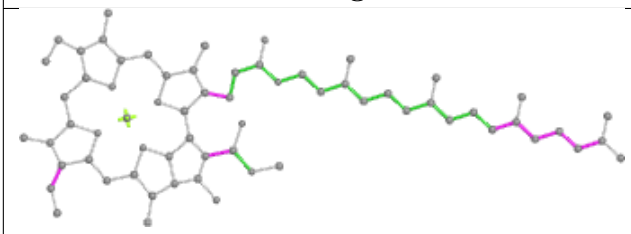

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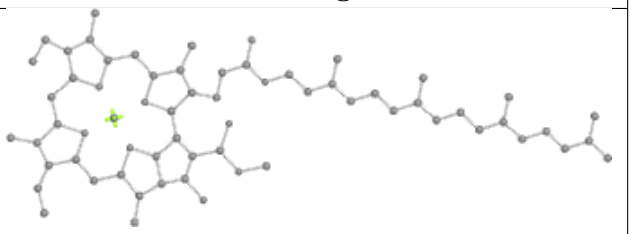

Rings

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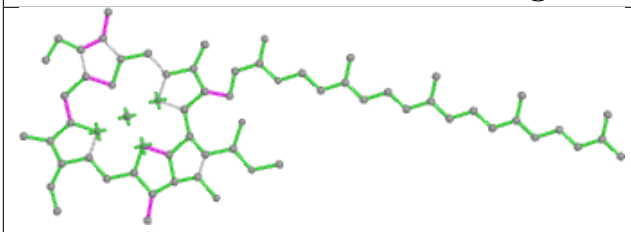

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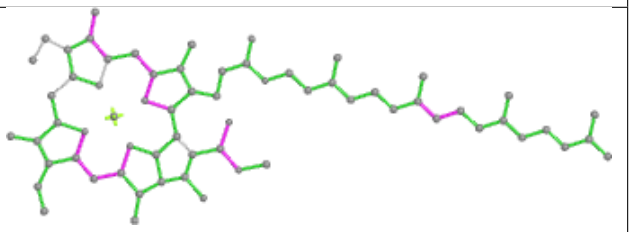

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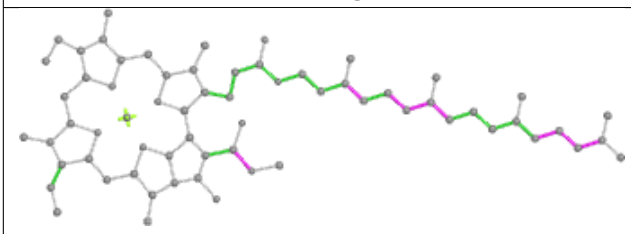

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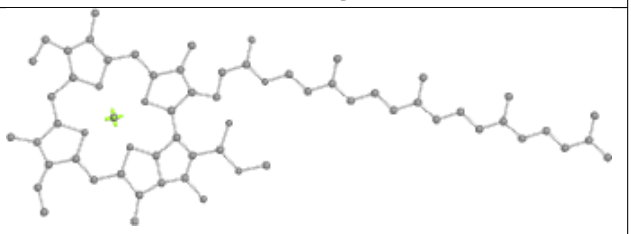
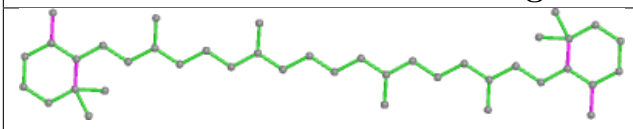


Rings

Ligand BCR k 102



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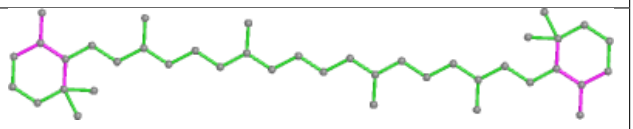

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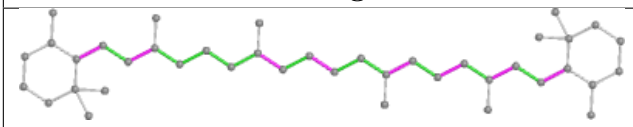

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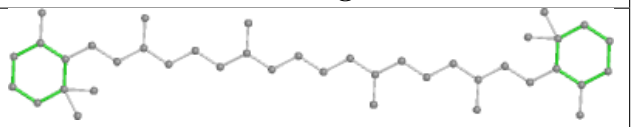

Rings

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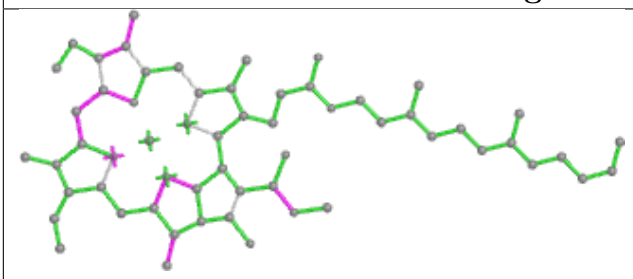

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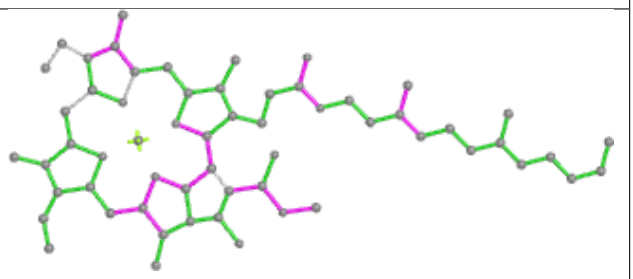

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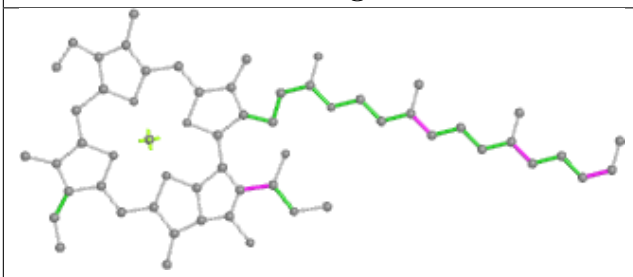

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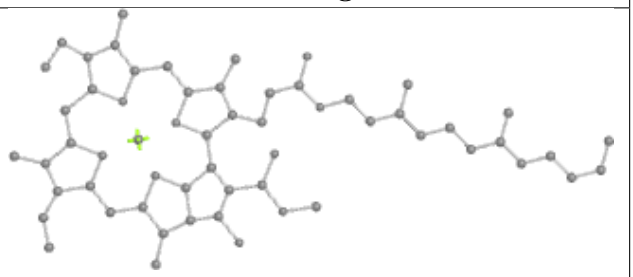
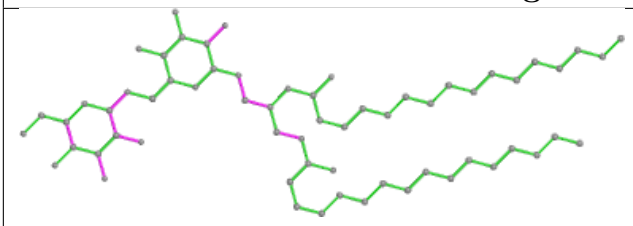


Rings

Ligand DGD h 101



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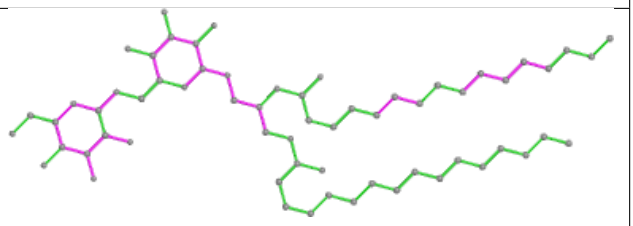

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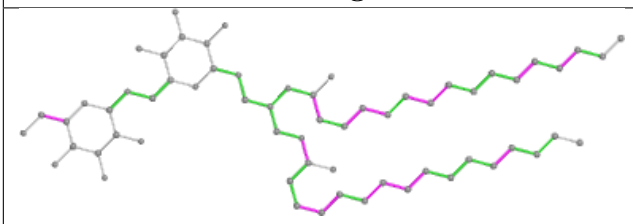

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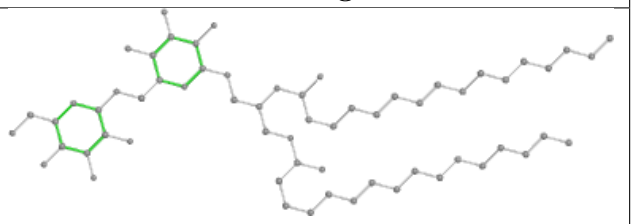

Rings

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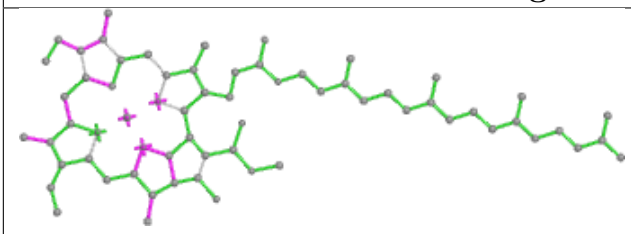
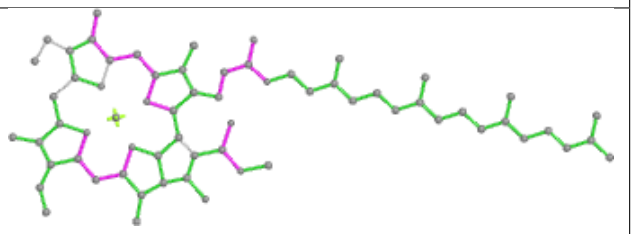
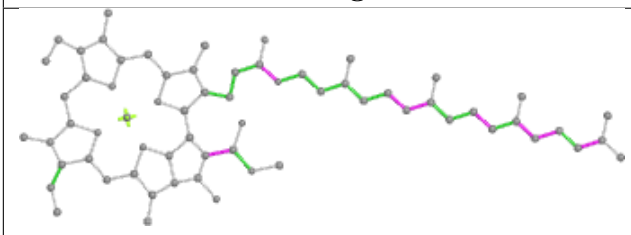


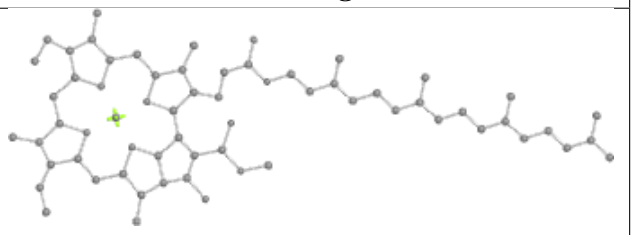
Bond lengths



Bond angles

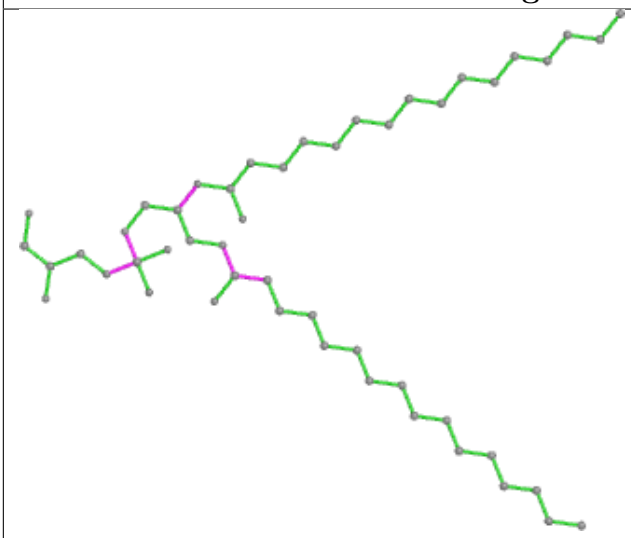


Torsions

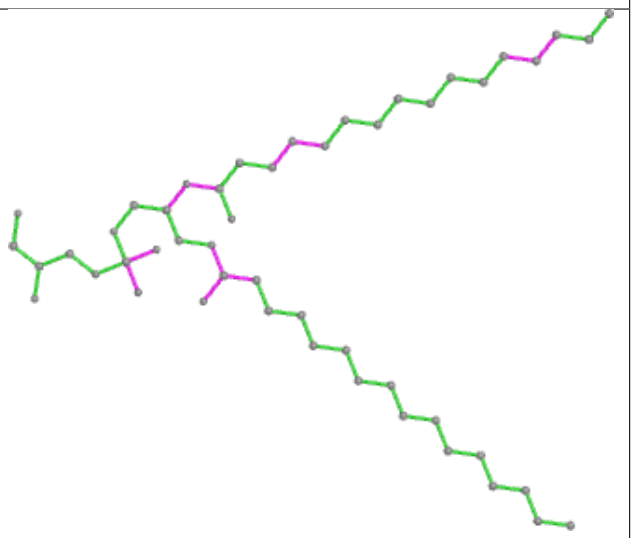


Rings

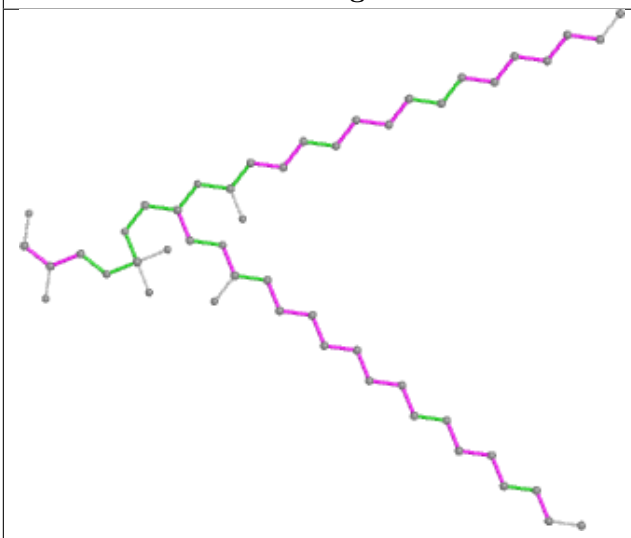
Ligand LHG A 413



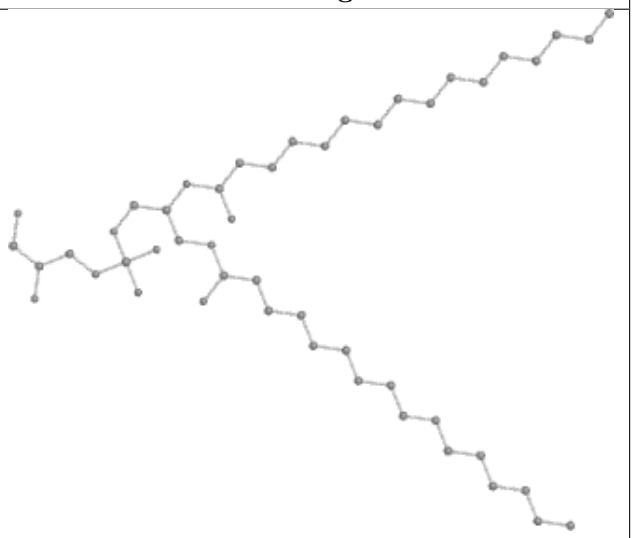
Bond lengths



Bond angles

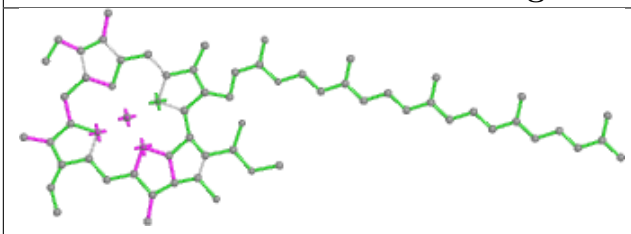


Torsions



Rings

Ligand CLA b 609



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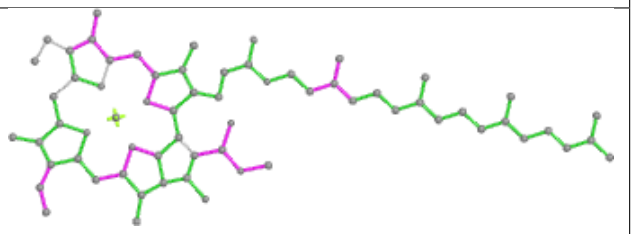
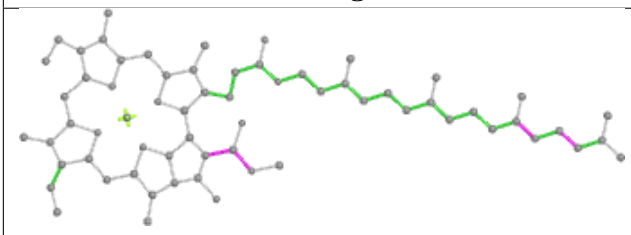
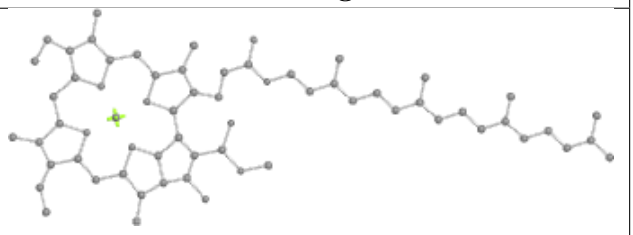


Bond angles

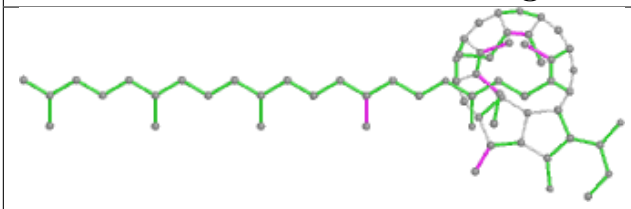


Torsions



Rings

Ligand PHO A 404



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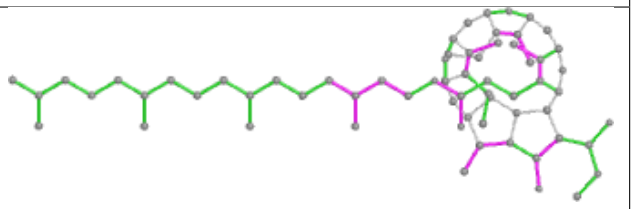
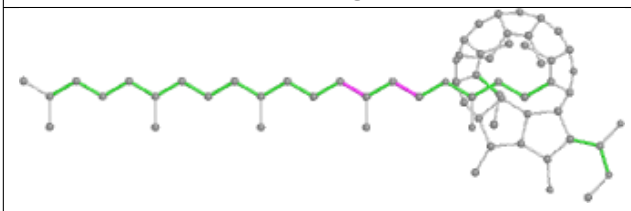


Bond angles



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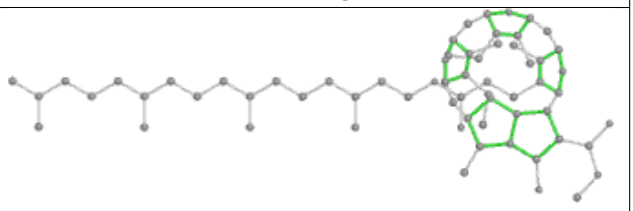
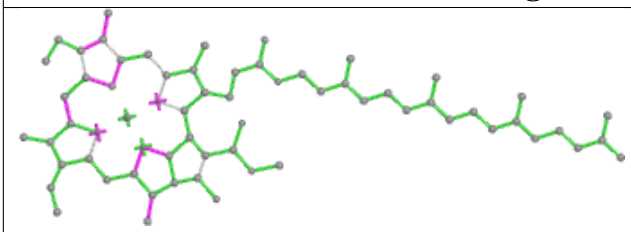


Rings

Ligand CLA C 512



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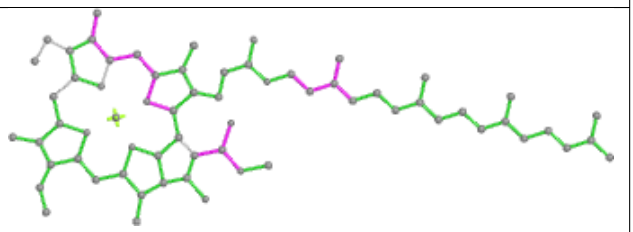
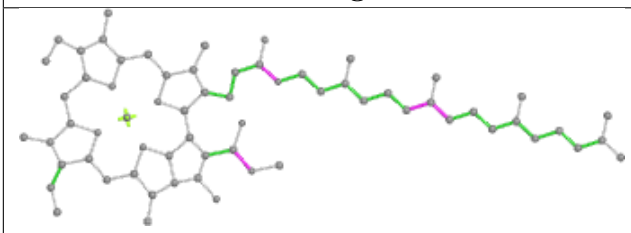


Bond angles



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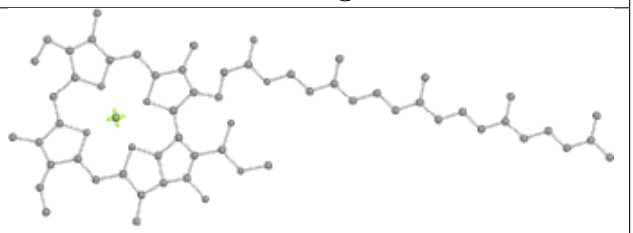
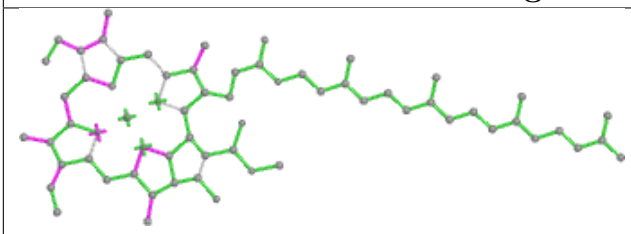


Rings

Ligand CLA B 608



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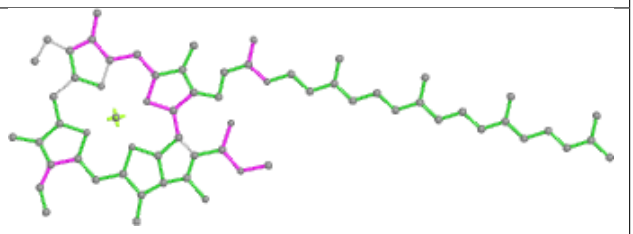
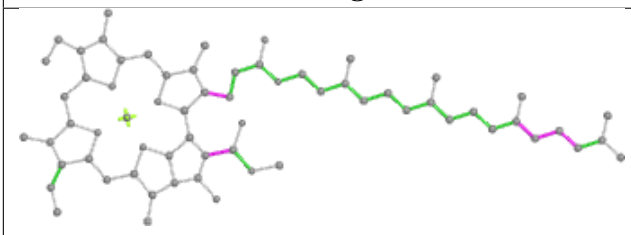


Bond angles



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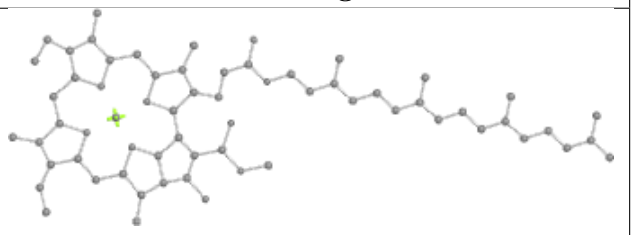
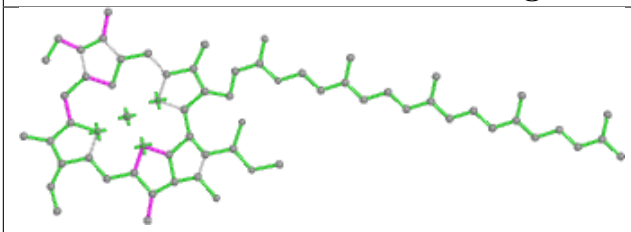


Rings

Ligand CLA D 403



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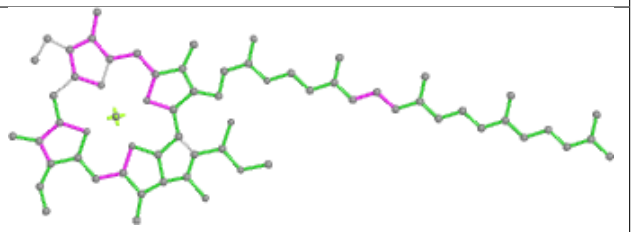
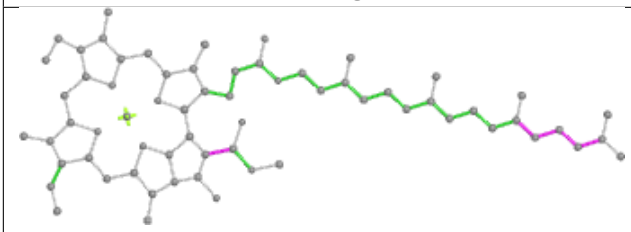


Bond angles



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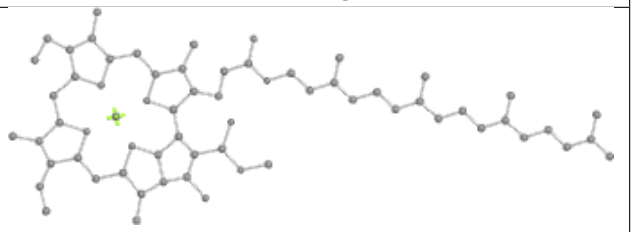
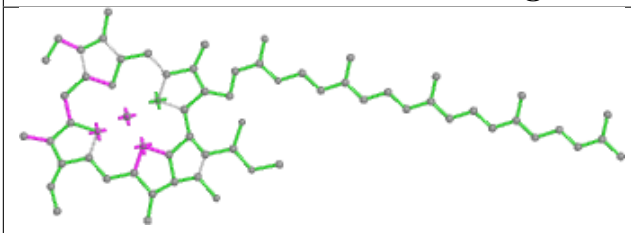


Rings

Ligand CLA C 506



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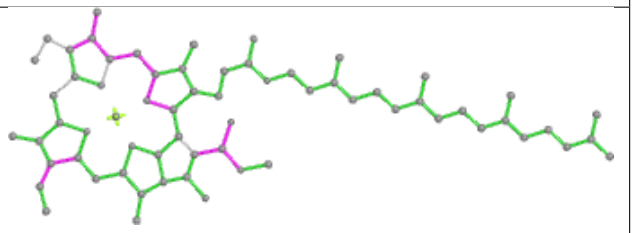
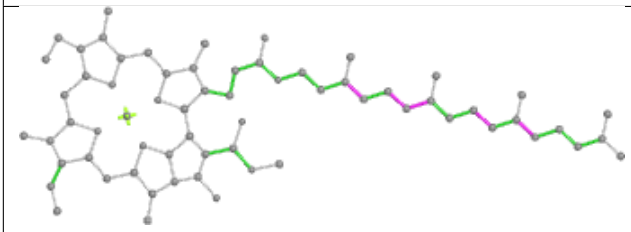


Bond angles



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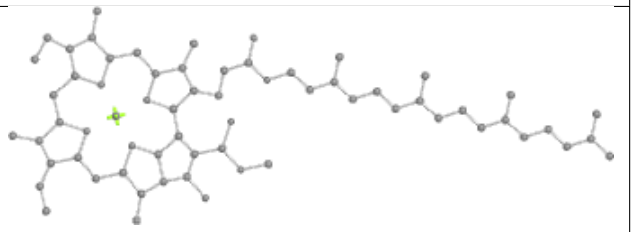

Rings

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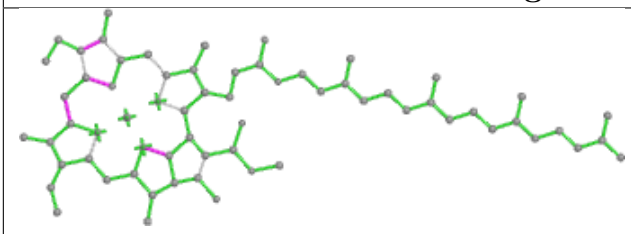

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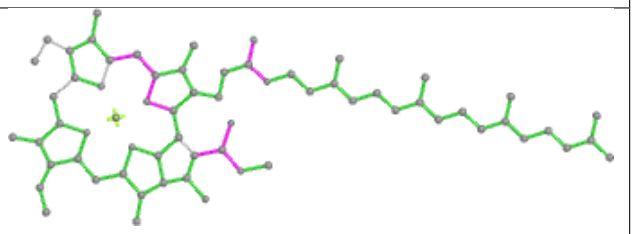
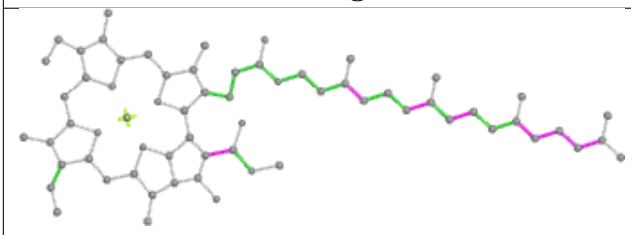


Bond angles



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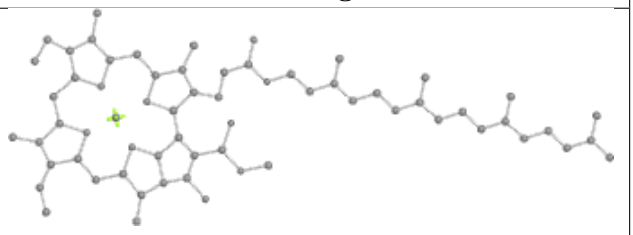
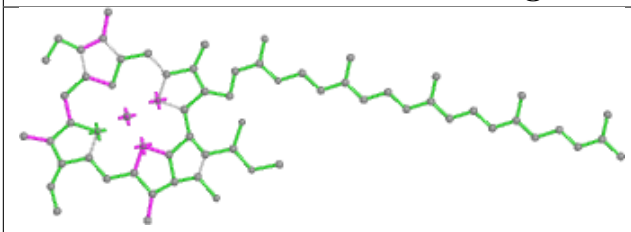


Rings

Ligand CLA C 502



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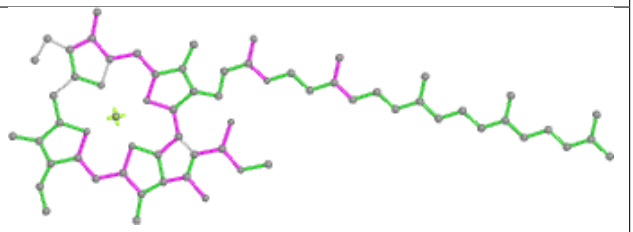
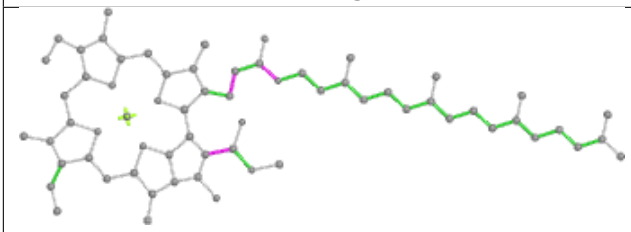


Bond angles



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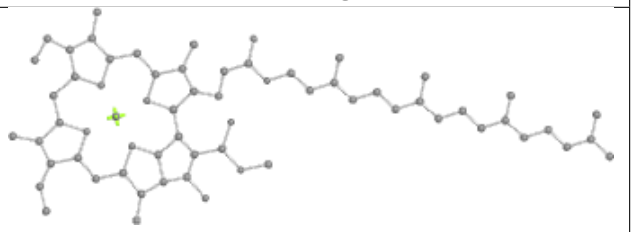
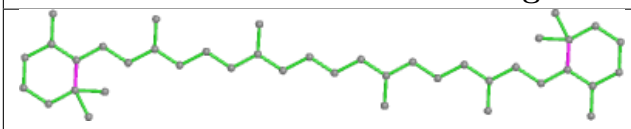


Rings

Ligand BCR B 620



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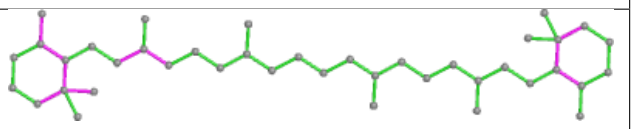
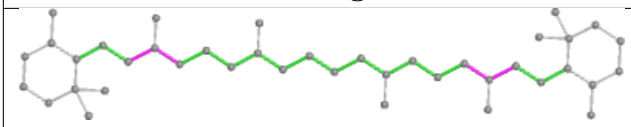


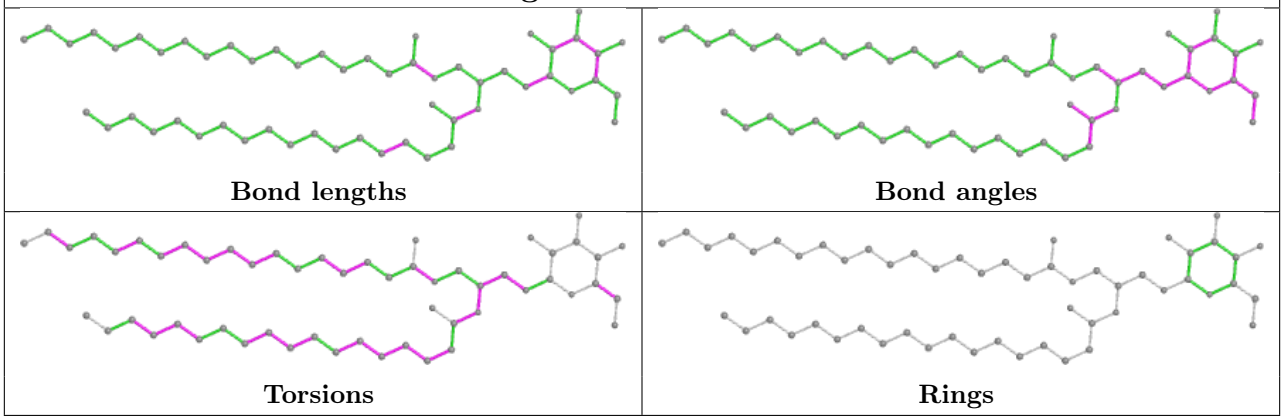
Bond angles



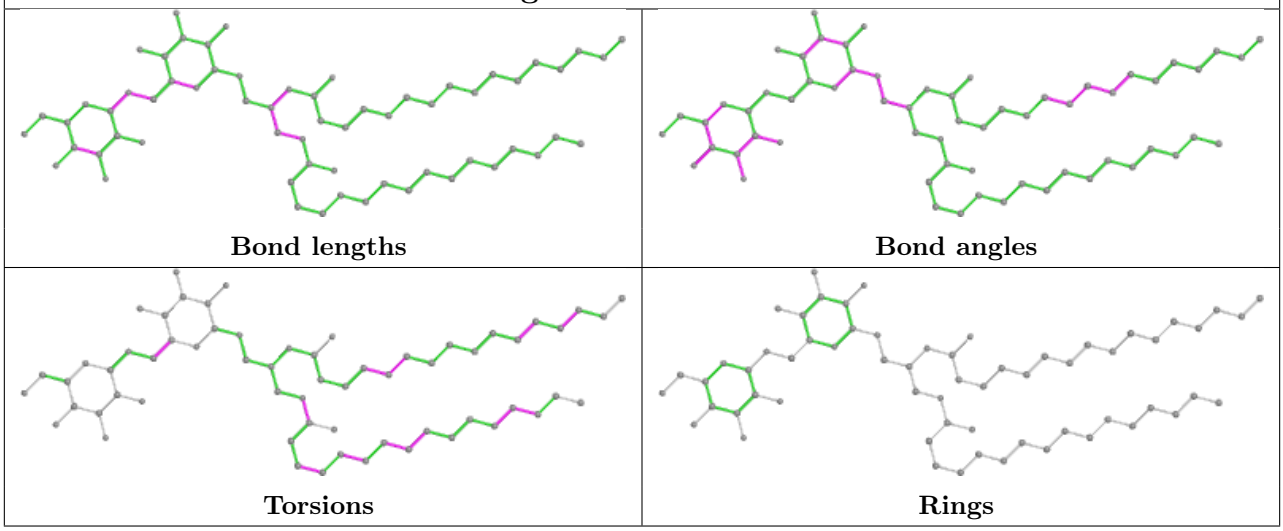
Torsions

Rings

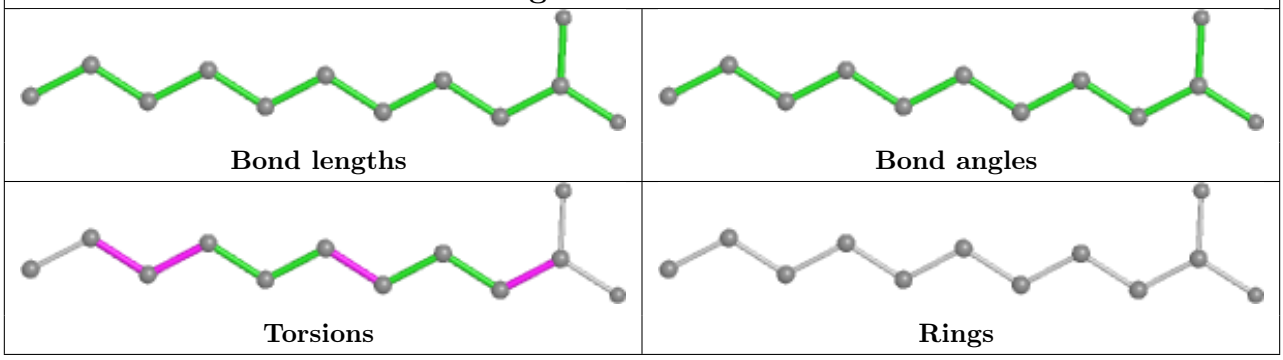
Ligand LMG B 627



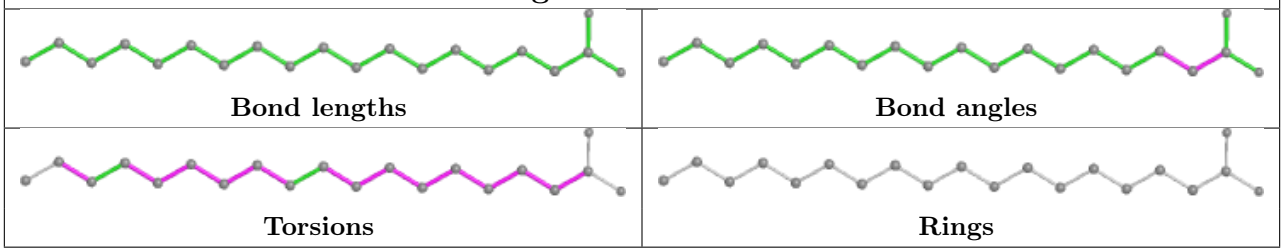
Ligand DGD C 519



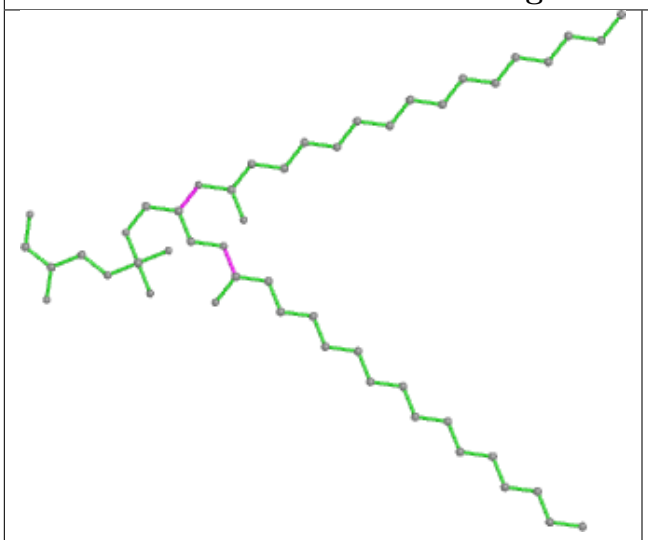
Ligand STE E 102



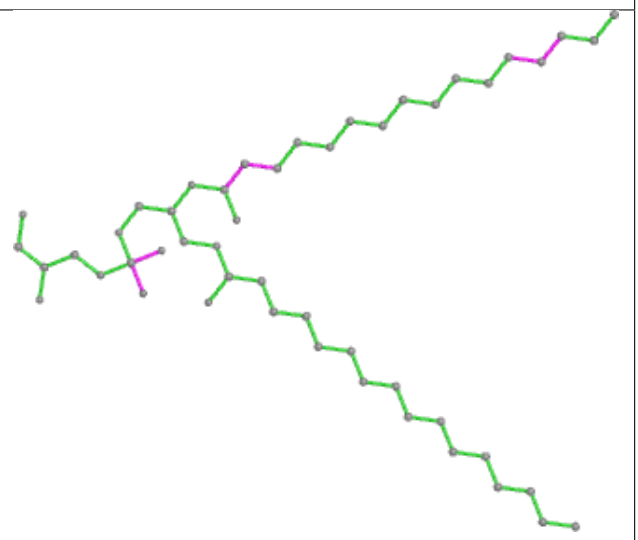
Ligand STE x 102



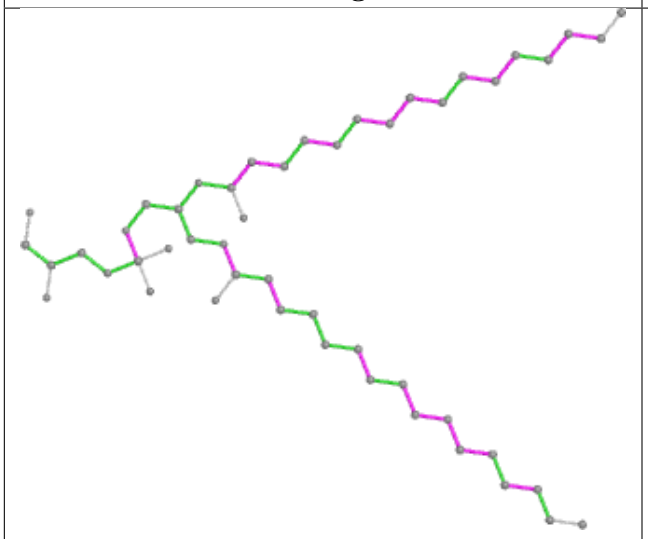
Ligand LHG L 102



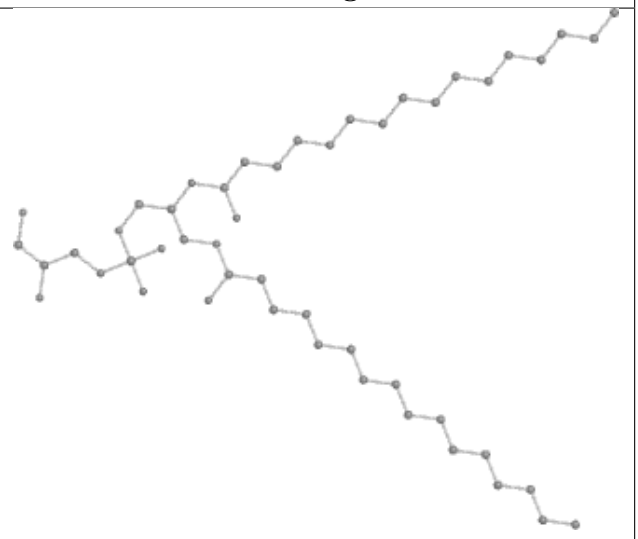
Bond lengths



Bond angles

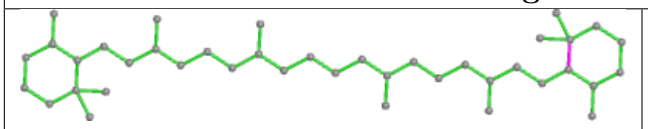


Torsions

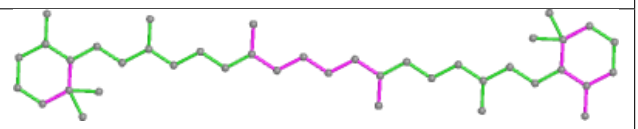


Rings

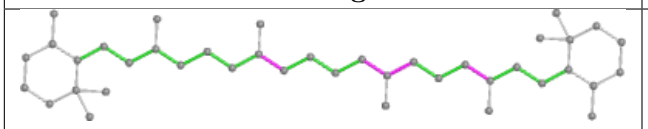
Ligand BCR H 101



Bond lengths



Bond angles



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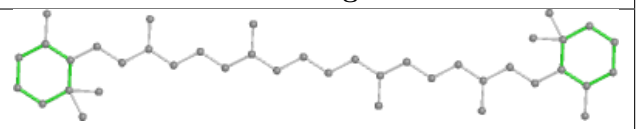
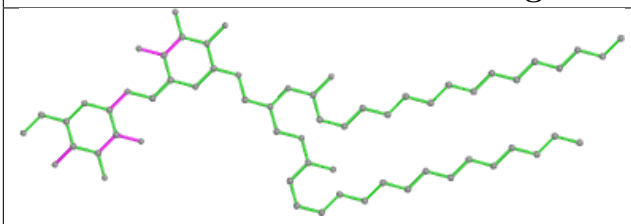
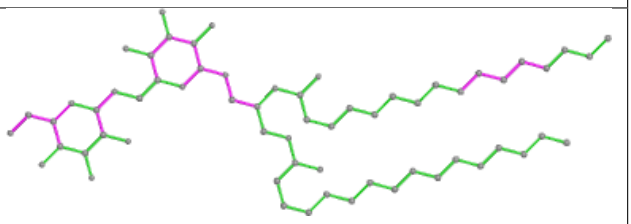


Rings

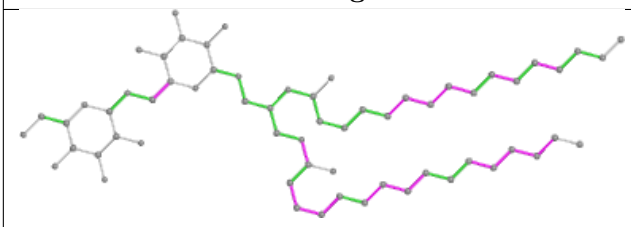
Ligand DGD c 518



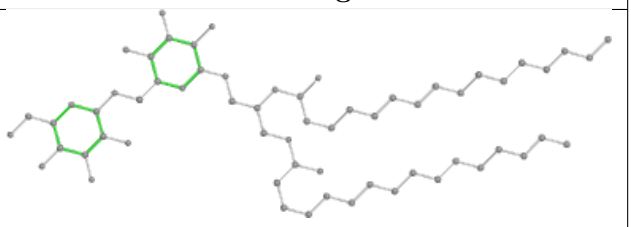
Bond lengths



Bond angles

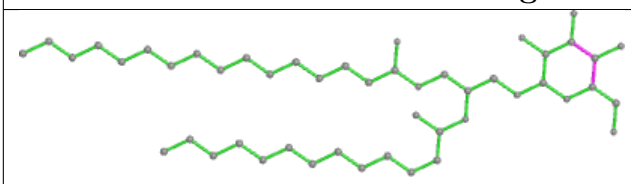


Torsions



Rings

Ligand LMG C 516



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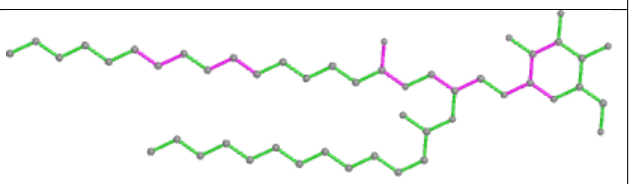

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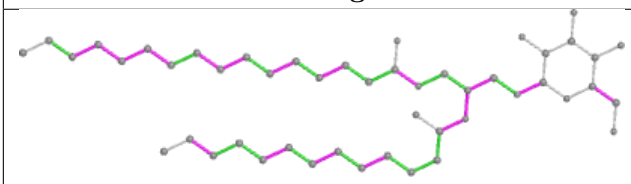

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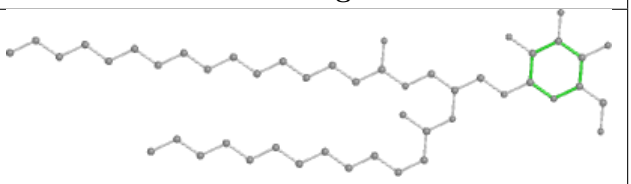
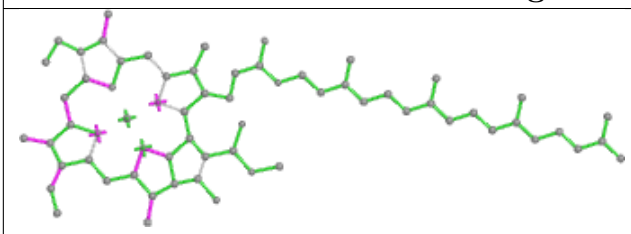


Rings

Ligand CLA b 602



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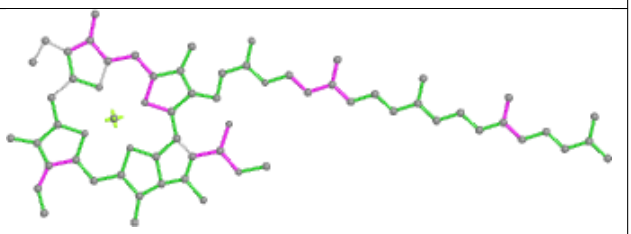
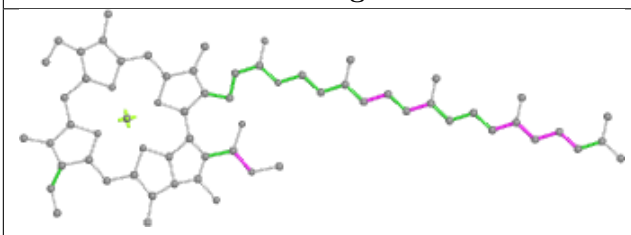


Bond angles



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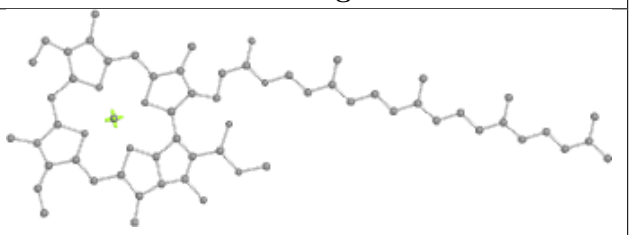
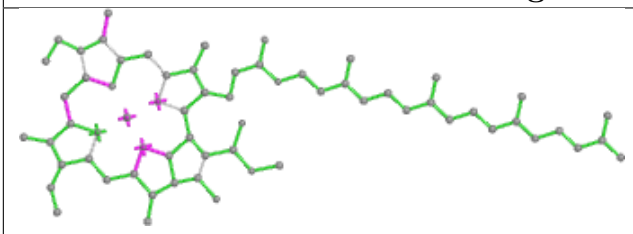


Rings

Ligand CLA d 402



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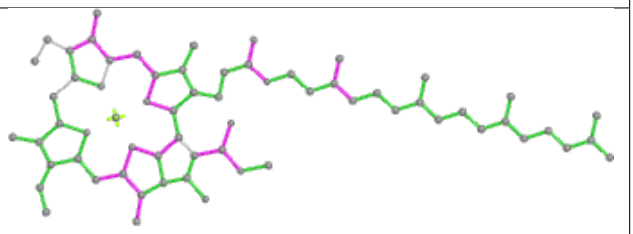

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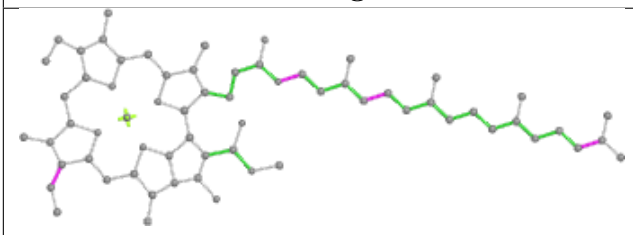

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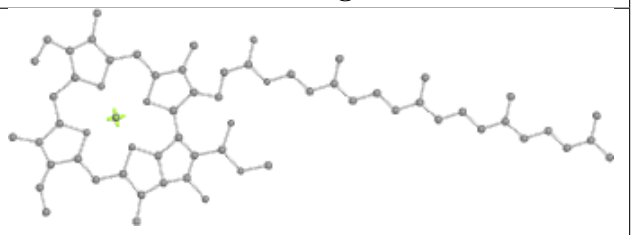
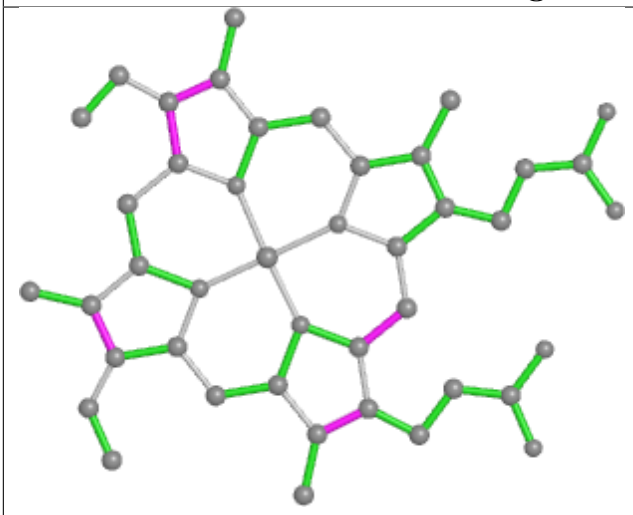


Rings

Ligand HEC e 101



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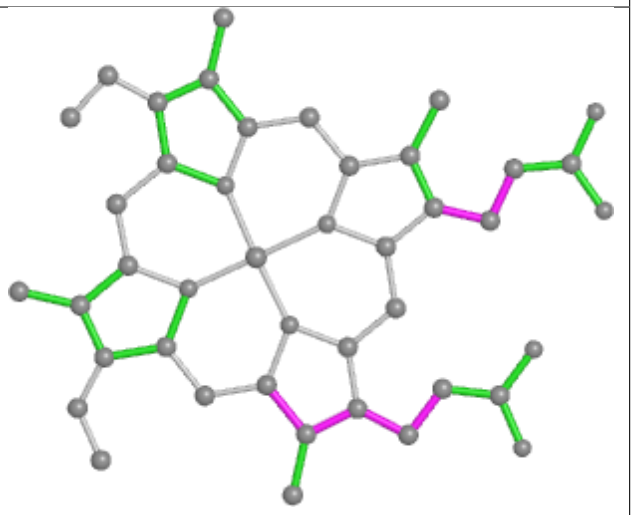
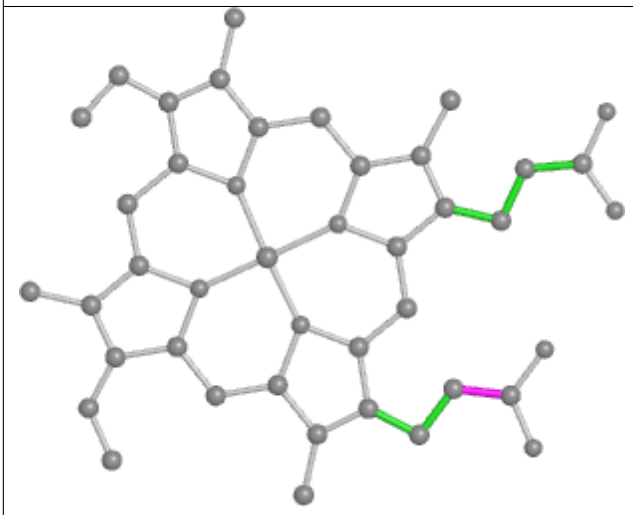


Bond angles



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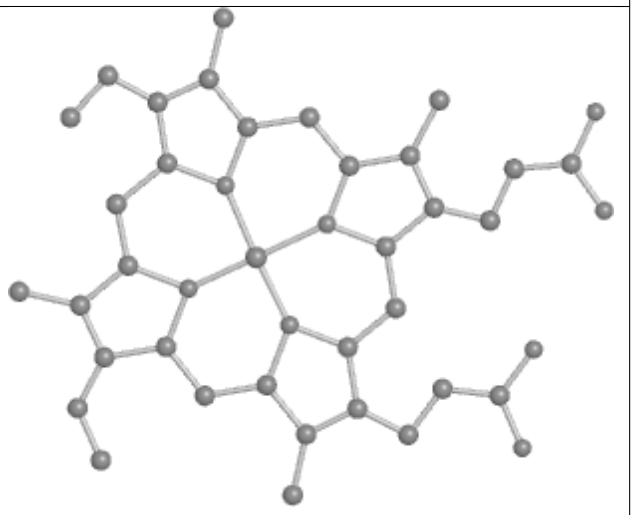
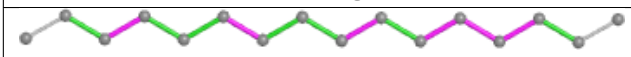


Rings

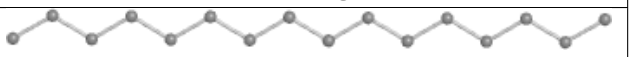
Ligand STE B 625

Bond lengths

Bond angles

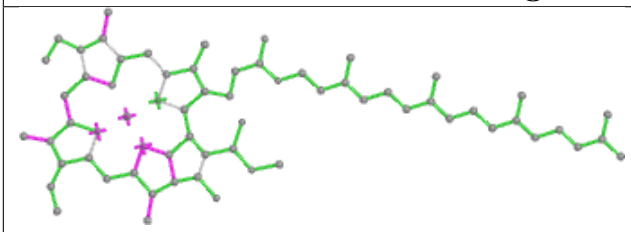


Torsions



Rings

Ligand CLA C 511



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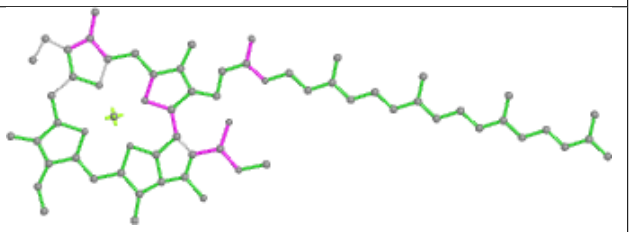
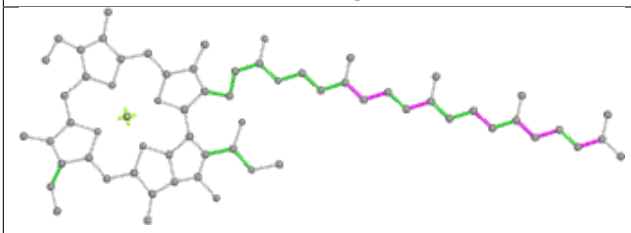


Bond angles



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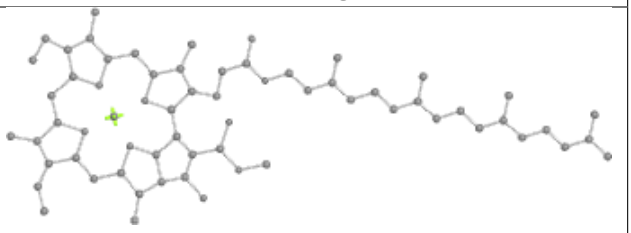
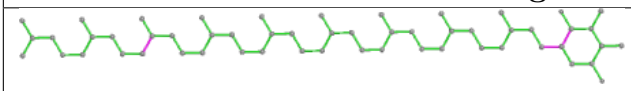


Rings

Ligand PL9 A 410



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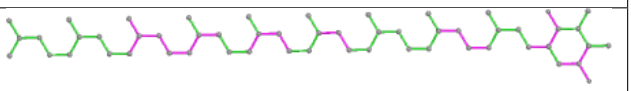
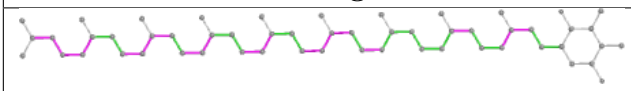
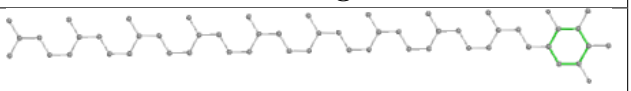


Bond angles

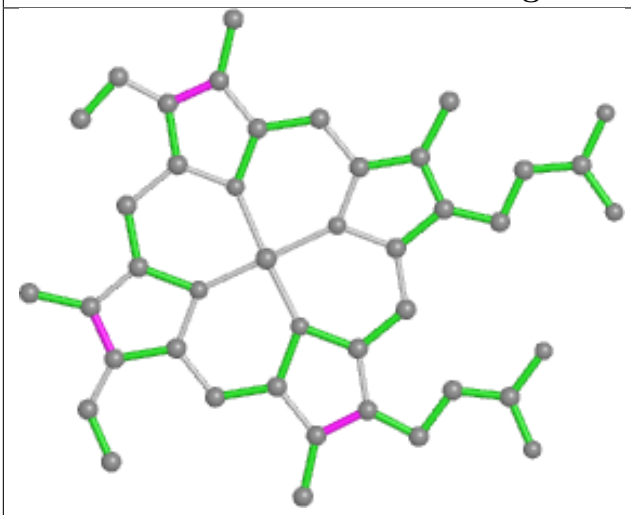


Torsions



Rings

Ligand HEC V 201



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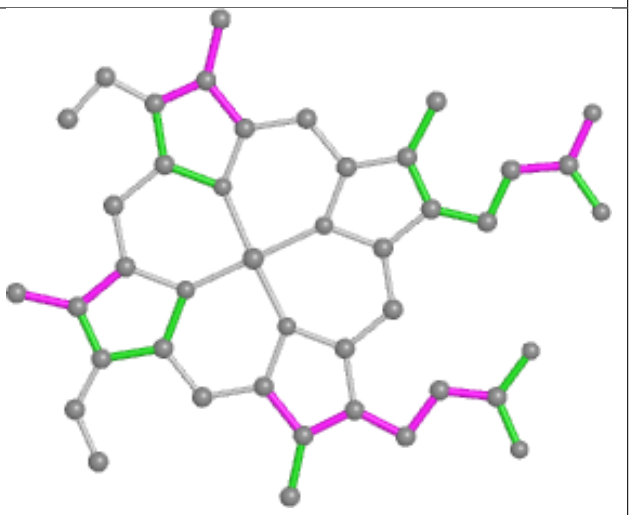
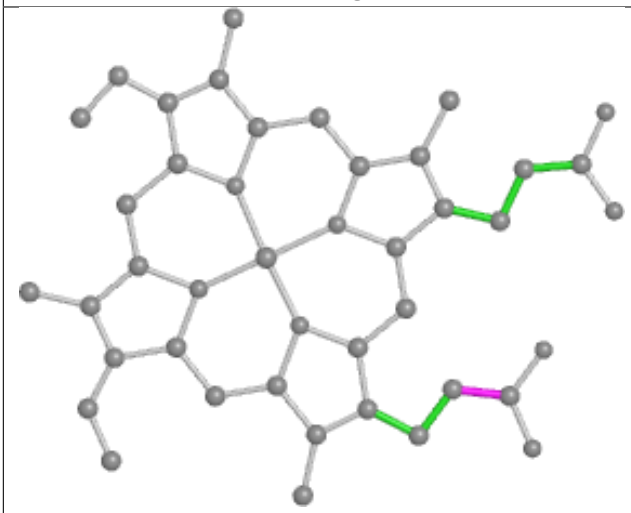
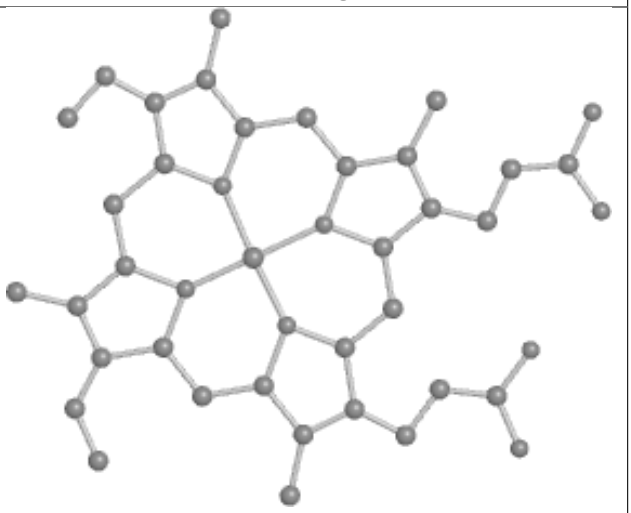


Bond angles

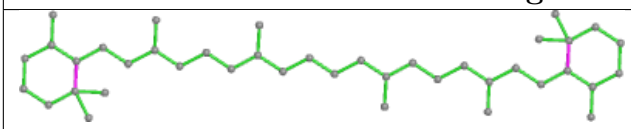


Torsions



Rings

Ligand BCR k 103



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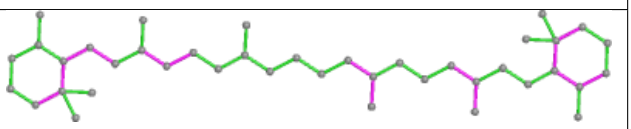
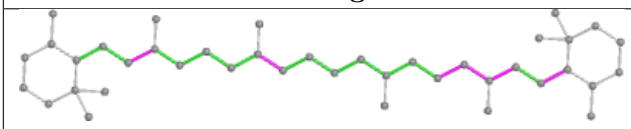
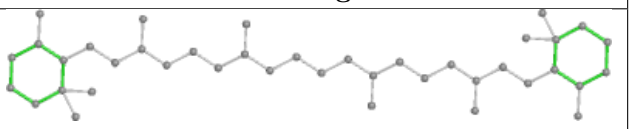


Bond angles

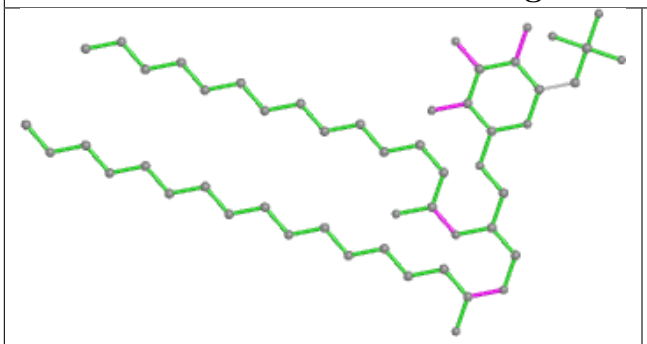


Torsions



Rings

Ligand SQD A 412



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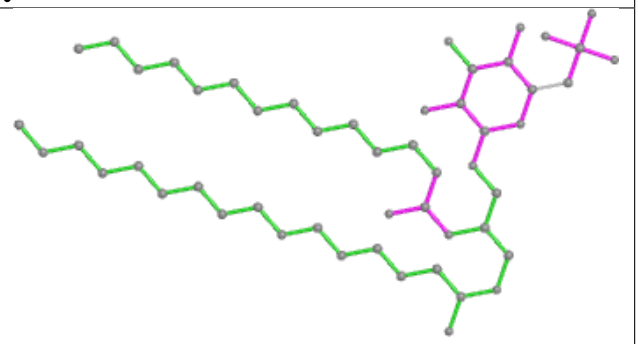
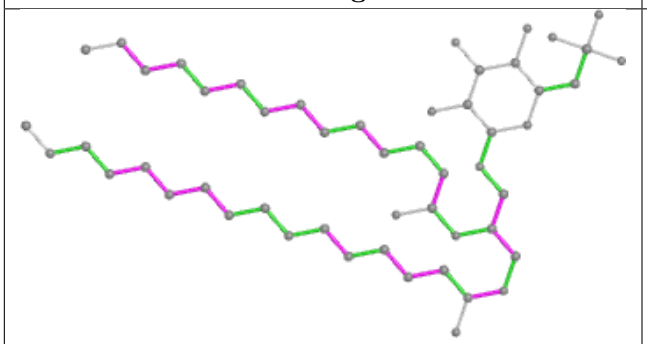
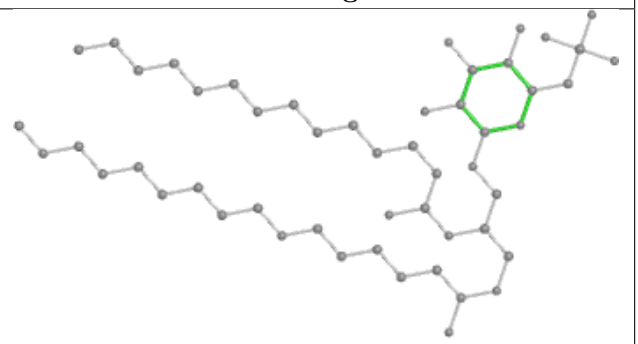


Bond angles

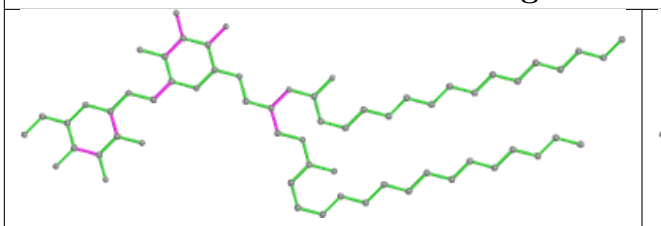


Torsions



Rings

Ligand DGD C 518



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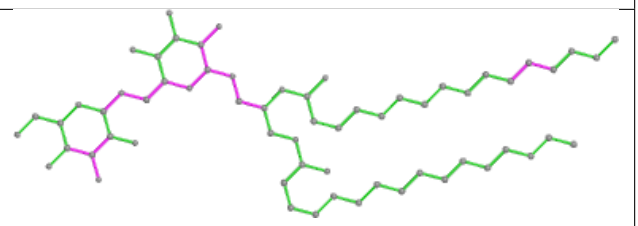
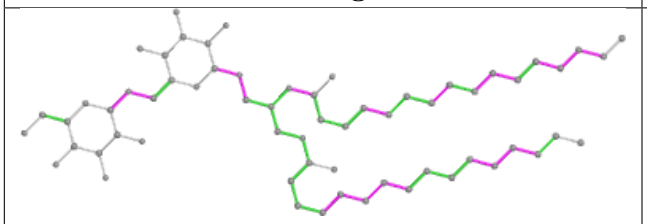
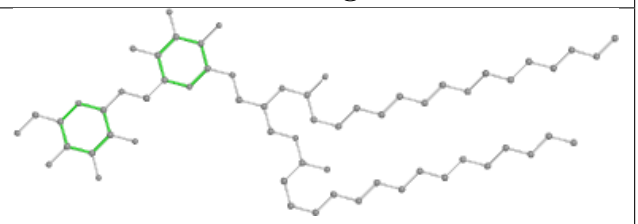


Bond angles

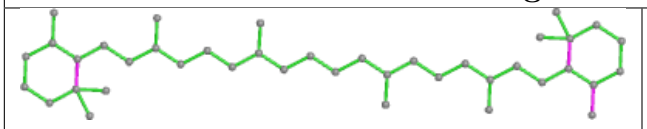


Torsions

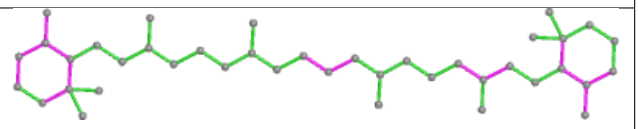


Rings

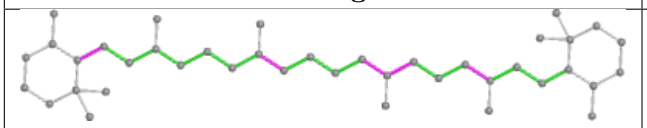
Ligand BCR B 618



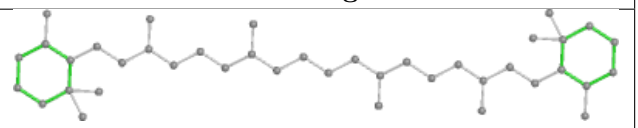
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	334/334 (100%)	-0.48	3 (0%)	84	85	25, 31, 49, 74	0
1	a	334/334 (100%)	-0.51	1 (0%)	94	94	24, 33, 58, 85	0
2	B	505/506 (99%)	-0.45	5 (0%)	82	84	25, 35, 62, 85	0
2	b	505/506 (99%)	-0.27	17 (3%)	45	47	27, 38, 71, 104	0
3	C	442/461 (95%)	-0.36	4 (0%)	84	85	27, 38, 54, 78	0
3	c	451/461 (97%)	-0.32	6 (1%)	77	79	27, 41, 61, 93	0
4	D	341/352 (96%)	-0.43	1 (0%)	94	94	24, 32, 48, 82	0
4	d	341/352 (96%)	-0.36	2 (0%)	89	89	26, 36, 59, 85	0
5	E	82/84 (97%)	-0.12	2 (2%)	59	62	34, 52, 69, 83	0
5	e	82/84 (97%)	0.09	5 (6%)	21	23	43, 58, 78, 83	0
6	F	34/45 (75%)	-0.56	1 (2%)	51	55	36, 44, 63, 73	0
6	f	34/45 (75%)	-0.36	1 (2%)	51	55	43, 50, 78, 84	0
7	H	65/66 (98%)	-0.14	1 (1%)	73	75	34, 41, 59, 80	0
7	h	63/66 (95%)	0.20	4 (6%)	20	22	43, 53, 66, 69	0
8	I	35/38 (92%)	-0.32	2 (5%)	23	25	35, 41, 68, 78	0
8	i	35/38 (92%)	-0.02	3 (8%)	10	11	34, 41, 79, 91	0
9	J	36/40 (90%)	0.01	4 (11%)	5	5	36, 49, 73, 87	0
9	j	36/40 (90%)	0.09	4 (11%)	5	5	38, 51, 85, 94	0
10	K	37/46 (80%)	0.07	2 (5%)	25	28	46, 53, 74, 77	0
10	k	37/46 (80%)	-0.13	0	100	100	48, 54, 67, 81	0
11	L	37/37 (100%)	-0.59	0	100	100	26, 33, 63, 79	0
11	l	36/37 (97%)	-0.29	3 (8%)	11	12	28, 33, 69, 81	0
12	M	32/36 (88%)	-0.17	1 (3%)	49	52	29, 36, 60, 71	0
12	m	31/36 (86%)	-0.19	0	100	100	29, 36, 55, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.15	10 (4%)	37	40	27, 44, 78, 124	0
13	o	244/272 (89%)	-0.19	13 (5%)	26	29	28, 42, 76, 118	0
14	R	34/40 (85%)	1.79	11 (32%)	0	0	57, 72, 91, 102	0
14	r	31/40 (77%)	3.41	23 (74%)	0	0	75, 92, 106, 121	0
15	T	29/30 (96%)	-0.59	1 (3%)	45	47	27, 33, 63, 78	0
15	t	29/30 (96%)	-0.34	3 (10%)	6	6	29, 35, 82, 91	0
16	U	97/134 (72%)	-0.34	3 (3%)	49	52	34, 44, 69, 84	0
16	u	97/134 (72%)	-0.53	0	100	100	31, 42, 60, 81	0
17	V	137/163 (84%)	-0.61	0	100	100	32, 42, 57, 77	0
17	v	137/163 (84%)	-0.28	3 (2%)	62	65	34, 47, 68, 81	0
18	X	38/41 (92%)	0.01	3 (7%)	12	14	40, 51, 71, 79	0
18	x	39/41 (95%)	0.44	5 (12%)	3	3	48, 59, 87, 102	0
19	Y	27/46 (58%)	1.23	9 (33%)	0	0	55, 71, 90, 94	0
19	y	30/46 (65%)	0.57	4 (13%)	3	3	58, 73, 85, 96	0
20	Z	62/62 (100%)	0.71	11 (17%)	1	1	52, 65, 108, 123	0
20	z	62/62 (100%)	0.72	11 (17%)	1	1	51, 71, 104, 112	0
All	All	5302/5666 (93%)	-0.26	182 (3%)	45	47	24, 40, 73, 124	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.4
14	r	14	LEU	7.3
2	b	495	PHE	7.1
14	r	9	LEU	6.7
14	r	10	LEU	6.5
20	z	33	TRP	6.2
13	o	60	ARG	6.0
8	i	36	ASP	5.8
1	A	13	LEU	5.8
14	r	3	TRP	5.7
13	O	56	PRO	5.6
13	o	57	LYS	5.6
20	Z	1	MET	5.5
14	r	29	LYS	5.5
14	r	13	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
13	O	3	GLN	5.2
13	O	62	GLU	5.1
20	Z	62	VAL	5.1
13	o	61	GLN	5.0
20	Z	35	ARG	4.9
14	r	5	VAL	4.9
13	o	4	THR	4.9
2	b	127	ARG	4.9
9	j	6	GLY	4.8
14	r	24	LEU	4.8
20	Z	33	TRP	4.8
14	r	25	PRO	4.6
5	e	79	PHE	4.5
13	o	3	GLN	4.5
13	O	4	THR	4.5
5	e	61	ARG	4.5
13	o	62	GLU	4.4
14	R	6	LEU	4.4
14	r	6	LEU	4.4
14	r	28	VAL	4.4
14	r	31	VAL	4.4
14	R	3	TRP	4.4
10	K	17	ILE	4.3
15	t	29	ILE	4.2
13	O	63	ALA	4.2
13	o	56	PRO	4.2
20	z	60	PHE	4.1
14	R	2	ASP	4.1
9	J	7	ARG	4.1
9	j	7	ARG	4.1
18	X	2	THR	4.0
13	o	59	LYS	4.0
19	Y	43	ARG	3.9
20	Z	34	ASP	3.8
9	j	8	ILE	3.8
13	O	60	ARG	3.8
14	R	25	PRO	3.8
9	J	6	GLY	3.7
18	x	2	THR	3.7
7	H	66	GLY	3.7
14	r	26	TYR	3.7
20	Z	3	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
20	Z	32	ASP	3.6
20	z	3	ILE	3.6
15	t	30	THR	3.6
1	A	11	ALA	3.6
9	J	8	ILE	3.6
14	r	21	ARG	3.6
1	a	11	ALA	3.6
14	R	29	LYS	3.5
19	y	37	PHE	3.5
14	R	32	GLN	3.5
19	Y	25	ILE	3.4
9	j	5	GLY	3.4
19	y	19	ILE	3.4
7	h	21	VAL	3.4
9	J	5	GLY	3.3
14	r	2	ASP	3.3
2	b	494	GLY	3.2
13	o	5	LEU	3.2
2	b	505	ARG	3.2
20	z	30	PRO	3.2
5	E	84	LYS	3.2
19	Y	37	PHE	3.2
2	B	293	ALA	3.2
18	x	38	GLN	3.2
2	b	506	ARG	3.1
18	x	39	ARG	3.1
2	b	128	THR	3.1
20	Z	42	LEU	3.1
20	z	34	ASP	3.0
2	b	486	LEU	3.0
14	r	15	ALA	3.0
2	b	502	VAL	3.0
10	K	14	ALA	2.9
18	x	40	SER	2.9
19	Y	20	ALA	2.9
8	i	34	ARG	2.9
14	R	14	LEU	2.9
2	b	295	GLY	2.9
2	b	289	GLN	2.9
19	Y	40	ALA	2.9
2	b	129	GLY	2.8
3	c	23	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
19	Y	41	VAL	2.8
20	Z	61	VAL	2.8
20	Z	4	LEU	2.8
13	O	5	LEU	2.8
3	c	143	TYR	2.8
5	e	74	GLN	2.8
3	c	262	ARG	2.8
18	X	34	ILE	2.8
15	T	30	THR	2.7
17	v	17	LYS	2.7
13	o	63	ALA	2.7
14	R	20	VAL	2.7
14	r	4	ARG	2.7
2	B	505	ARG	2.7
20	z	35	ARG	2.7
1	A	12	ASN	2.7
13	O	61	GLN	2.7
11	l	3	PRO	2.7
14	r	8	VAL	2.7
4	D	12	ARG	2.6
14	r	18	TRP	2.6
14	r	7	VAL	2.6
3	C	57	ALA	2.6
5	e	82	GLN	2.6
7	h	20	LYS	2.6
5	e	84	LYS	2.6
3	C	146	PHE	2.5
5	E	79	PHE	2.5
14	R	5	VAL	2.5
20	z	41	PHE	2.5
16	U	68	THR	2.5
2	b	288	VAL	2.5
11	l	2	GLU	2.5
19	y	18	VAL	2.5
13	o	55	GLU	2.5
19	Y	21	GLN	2.5
20	Z	38	GLN	2.5
7	h	6	TRP	2.5
14	R	26	TYR	2.5
8	i	35	LYS	2.5
18	X	3	ILE	2.5
14	r	30	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
6	f	12	SER	2.4
17	v	21	LEU	2.4
11	l	7	ARG	2.4
3	c	146	PHE	2.4
12	M	33	GLN	2.4
6	F	12	SER	2.4
2	B	485	GLU	2.4
20	z	37	LYS	2.4
14	R	21	ARG	2.4
7	h	10	ILE	2.3
14	r	17	GLY	2.3
2	b	487	SER	2.3
8	I	6	ILE	2.3
3	C	106	VAL	2.3
19	Y	42	ARG	2.3
19	Y	22	LEU	2.2
3	c	142	GLU	2.2
2	b	503	THR	2.2
15	t	28	ARG	2.2
4	d	12	ARG	2.2
8	I	34	ARG	2.2
2	b	293	ALA	2.2
2	b	126	PRO	2.2
20	z	2	THR	2.2
2	B	127	ARG	2.1
14	r	12	VAL	2.1
13	O	57	LYS	2.1
19	y	43	ARG	2.1
17	v	15	GLU	2.1
3	C	62	PHE	2.1
2	B	489	GLU	2.1
16	U	8	GLU	2.1
13	o	246	ALA	2.1
13	O	184	ARG	2.1
4	d	227[A]	GLU	2.0
2	b	86	ILE	2.0
3	c	25	ASN	2.0
20	z	36	SER	2.0
16	U	65	PRO	2.0
18	x	37	VAL	2.0
20	z	62	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
15	FME	t	1	10/11	0.93	0.09	36,49,70,70	0
15	FME	T	1	10/11	0.95	0.10	33,45,71,71	0
12	FME	m	1	10/11	0.95	0.14	36,55,70,84	0
12	FME	M	1	10/11	0.96	0.14	45,54,77,86	0
8	FME	i	1	10/11	0.96	0.17	45,57,75,77	0
8	FME	I	1	10/11	0.97	0.15	42,54,64,72	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
32	STE	H	103	18/20	0.71	0.34	42,77,99,99	0
32	STE	E	102	12/20	0.74	0.27	50,78,89,94	0
32	STE	k	101	12/20	0.76	0.25	49,73,89,92	0
32	STE	b	624	20/20	0.77	0.21	46,70,82,93	0
32	STE	B	625	16/20	0.77	0.24	47,64,74,78	0
32	STE	a	414	12/20	0.80	0.28	45,68,75,81	0
33	LMG	c	521	48/55	0.80	0.26	40,79,111,123	0
32	STE	c	520	20/20	0.81	0.23	42,61,83,84	0
28	LHG	a	412	42/49	0.83	0.25	54,83,108,130	0
22	CLA	C	513	65/65	0.83	0.21	38,56,101,105	0
32	STE	x	102	20/20	0.83	0.19	36,63,81,81	0
28	LHG	A	413	49/49	0.83	0.23	56,78,116,120	0
32	STE	d	411	17/20	0.84	0.18	44,58,70,77	0
29	SQD	a	413	36/54	0.84	0.19	27,65,92,100	0
32	STE	t	104	18/20	0.84	0.17	42,62,76,80	0
32	STE	C	521	16/20	0.84	0.17	43,59,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMG	D	409	33/55	0.84	0.17	34,56,86,94	0
32	STE	M	104	18/20	0.84	0.18	37,54,88,89	0
32	STE	j	101	12/20	0.85	0.17	39,61,75,80	0
27	PL9	A	410	55/55	0.85	0.24	37,69,85,95	0
24	BCR	H	101	40/40	0.85	0.16	32,48,64,73	0
32	STE	J	101	12/20	0.85	0.16	48,62,72,84	0
33	LMG	B	627	55/55	0.85	0.16	34,60,84,99	0
24	BCR	x	101	40/40	0.85	0.16	37,56,74,79	0
33	LMG	b	622	55/55	0.85	0.29	47,74,101,110	0
32	STE	h	102	14/20	0.85	0.24	47,67,84,84	0
32	STE	B	626	15/20	0.86	0.17	42,65,83,83	0
33	LMG	D	410	28/55	0.86	0.16	31,51,69,73	0
30	DGD	A	415	66/66	0.86	0.17	44,65,85,95	0
32	STE	I	101	15/20	0.86	0.13	44,58,80,81	0
22	CLA	c	512	65/65	0.87	0.16	45,61,100,112	0
22	CLA	C	514	65/65	0.87	0.21	44,64,100,106	0
22	CLA	b	601	65/65	0.87	0.18	46,71,90,108	0
32	STE	b	623	16/20	0.87	0.17	49,62,84,86	0
29	SQD	A	414	39/54	0.87	0.18	37,66,87,95	0
32	STE	b	626	20/20	0.87	0.18	46,73,96,101	0
29	SQD	L	101	49/54	0.88	0.14	45,61,96,100	0
32	STE	b	625	10/20	0.88	0.25	44,54,67,68	0
32	STE	B	621	17/20	0.88	0.17	35,53,68,75	0
32	STE	b	621	20/20	0.88	0.23	37,58,76,81	0
27	PL9	a	410	55/55	0.88	0.20	41,70,89,102	0
32	STE	B	601	12/20	0.89	0.44	48,70,94,97	0
29	SQD	B	623	54/54	0.89	0.15	34,65,92,110	0
24	BCR	K	101	40/40	0.89	0.13	40,56,73,77	0
24	BCR	d	405	40/40	0.89	0.15	31,52,87,102	0
33	LMG	Y	101	48/55	0.89	0.17	43,75,97,104	0
24	BCR	k	102	40/40	0.89	0.14	46,63,80,82	0
32	STE	Z	102	8/20	0.89	0.15	43,60,72,72	0
33	LMG	c	522	49/55	0.89	0.14	32,58,90,114	0
22	CLA	B	602	65/65	0.90	0.14	34,60,89,98	0
32	STE	T	102	15/20	0.90	0.16	42,58,81,89	0
32	STE	C	522	12/20	0.90	0.10	33,45,57,61	0
24	BCR	k	103	40/40	0.90	0.18	39,55,69,76	0
33	LMG	M	101	51/55	0.90	0.12	33,52,76,86	0
32	STE	b	620	16/20	0.90	0.17	33,55,75,78	0
22	CLA	a	405	65/65	0.90	0.15	22,42,90,105	0
22	CLA	c	513	65/65	0.90	0.20	44,68,109,121	0
32	STE	C	520	12/20	0.90	0.15	37,53,65,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	STE	D	411	20/20	0.91	0.14	35,55,70,74	0
32	STE	L	103	12/20	0.91	0.20	52,64,88,89	0
32	STE	t	102	14/20	0.91	0.13	35,53,60,65	0
32	STE	B	624	12/20	0.91	0.10	35,53,67,74	0
29	SQD	f	101	41/54	0.91	0.19	60,81,107,111	0
22	CLA	D	404	65/65	0.91	0.14	24,46,105,117	0
33	LMG	C	516	48/55	0.91	0.13	36,58,77,83	0
22	CLA	C	503	65/65	0.92	0.14	32,45,65,79	0
22	CLA	B	616	65/65	0.92	0.14	27,40,69,86	0
32	STE	M	102	15/20	0.92	0.14	36,49,63,72	0
33	LMG	D	407	51/55	0.92	0.17	31,58,97,101	0
22	CLA	d	404	65/65	0.92	0.15	32,52,97,105	0
22	CLA	b	616	60/65	0.92	0.14	29,48,91,98	0
22	CLA	c	502	65/65	0.92	0.16	32,47,64,70	0
30	DGD	C	518	62/66	0.92	0.15	34,53,108,130	0
24	BCR	Z	101	40/40	0.92	0.16	38,60,75,77	0
24	BCR	c	514	40/40	0.92	0.19	45,58,79,80	0
22	CLA	c	508	64/65	0.92	0.15	32,46,83,100	0
30	DGD	c	517	62/66	0.93	0.13	33,55,98,104	0
24	BCR	C	501	40/40	0.93	0.18	40,53,72,81	0
24	BCR	D	405	40/40	0.93	0.13	28,47,85,101	0
22	CLA	c	510	65/65	0.93	0.15	33,51,65,73	0
22	CLA	C	508	65/65	0.93	0.15	26,45,61,66	0
22	CLA	B	617	60/65	0.93	0.15	26,43,92,113	0
22	CLA	b	615	65/65	0.93	0.14	28,43,64,70	0
32	STE	t	103	10/20	0.93	0.17	41,58,70,73	0
33	LMG	c	519	37/55	0.93	0.15	43,67,84,87	0
24	BCR	B	620	40/40	0.93	0.12	24,47,67,76	0
32	STE	M	103	10/20	0.93	0.15	35,45,55,66	0
33	LMG	m	101	51/55	0.93	0.12	34,54,73,90	0
24	BCR	b	617	40/40	0.94	0.12	27,45,60,60	0
30	DGD	c	518	62/66	0.94	0.14	28,56,95,100	0
30	DGD	h	101	62/66	0.94	0.13	33,51,67,72	0
24	BCR	b	619	40/40	0.94	0.10	33,50,65,70	0
22	CLA	A	405	54/65	0.94	0.13	20,36,63,73	0
22	CLA	c	509	65/65	0.94	0.19	33,51,70,75	0
22	CLA	C	512	65/65	0.94	0.14	35,55,72,85	0
22	CLA	c	511	65/65	0.94	0.13	38,56,77,82	0
22	CLA	b	602	65/65	0.94	0.15	24,46,67,75	0
22	CLA	b	606	65/65	0.94	0.12	28,43,79,93	0
27	PL9	D	406	55/55	0.94	0.12	23,37,53,55	0
22	CLA	B	605	65/65	0.94	0.14	23,36,74,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	B	618	40/40	0.94	0.12	26,43,64,65	0
24	BCR	B	619	40/40	0.94	0.11	23,39,54,57	0
22	CLA	B	607	65/65	0.94	0.11	22,38,76,83	0
22	CLA	C	507	65/65	0.94	0.13	27,48,95,114	0
29	SQD	F	101	36/54	0.94	0.17	46,73,94,100	0
24	BCR	C	515	40/40	0.94	0.12	27,45,58,67	0
29	SQD	a	411	54/54	0.94	0.15	41,67,95,97	0
22	CLA	c	503	65/65	0.94	0.16	35,48,61,67	0
22	CLA	c	505	65/65	0.94	0.17	30,45,72,77	0
22	CLA	c	506	65/65	0.94	0.14	30,54,101,105	0
22	CLA	c	507	65/65	0.94	0.15	28,48,63,65	0
30	DGD	C	519	62/66	0.94	0.12	28,54,75,83	0
33	LMG	d	410	44/55	0.94	0.15	36,55,89,104	0
30	DGD	H	102	62/66	0.94	0.11	29,47,62,66	0
22	CLA	B	611	65/65	0.95	0.15	21,34,48,55	0
29	SQD	A	412	52/54	0.95	0.15	36,61,94,98	0
22	CLA	C	505	59/65	0.95	0.12	28,45,82,99	0
22	CLA	c	504	60/65	0.95	0.11	33,48,83,88	0
22	CLA	C	506	65/65	0.95	0.14	23,41,72,82	0
22	CLA	a	403	65/65	0.95	0.14	25,43,98,116	0
24	BCR	T	101	40/40	0.95	0.09	28,44,60,68	0
22	CLA	B	615	65/65	0.95	0.15	26,41,84,94	0
22	CLA	A	403	65/65	0.95	0.14	22,37,87,101	0
22	CLA	C	509	65/65	0.95	0.12	34,46,105,121	0
30	DGD	C	517	62/66	0.95	0.13	22,43,84,95	0
22	CLA	b	604	65/65	0.95	0.14	23,40,82,97	0
24	BCR	c	515	40/40	0.95	0.10	30,44,65,69	0
22	CLA	C	510	65/65	0.95	0.18	28,48,68,74	0
30	DGD	c	516	62/66	0.95	0.13	23,45,81,92	0
22	CLA	b	608	65/65	0.95	0.14	27,44,70,75	0
22	CLA	b	609	65/65	0.95	0.14	27,47,81,86	0
22	CLA	b	613	65/65	0.95	0.14	23,37,82,87	0
23	PHO	a	404	64/64	0.95	0.13	21,33,41,46	0
22	CLA	b	614	65/65	0.95	0.14	23,42,80,89	0
22	CLA	C	511	65/65	0.95	0.14	29,48,70,77	0
22	CLA	B	603	65/65	0.95	0.17	23,41,59,61	0
22	CLA	C	504	65/65	0.96	0.14	33,47,56,61	0
22	CLA	d	402	65/65	0.96	0.12	21,37,65,68	0
22	CLA	d	403	65/65	0.96	0.12	20,34,52,56	0
22	CLA	B	614	65/65	0.96	0.15	22,36,73,83	0
23	PHO	A	404	64/64	0.96	0.11	21,30,42,45	0
22	CLA	c	501	65/65	0.96	0.13	28,44,56,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	t	101	40/40	0.96	0.09	29,42,56,57	0
23	PHO	d	401	64/64	0.96	0.11	26,42,52,62	0
24	BCR	A	406	40/40	0.96	0.09	24,38,47,56	0
22	CLA	b	603	65/65	0.96	0.15	24,40,71,82	0
22	CLA	B	608	65/65	0.96	0.11	20,36,65,71	0
27	PL9	d	406	55/55	0.96	0.11	19,37,48,56	0
28	LHG	A	411	47/49	0.96	0.13	31,52,79,95	0
22	CLA	b	605	65/65	0.96	0.13	23,38,53,61	0
28	LHG	B	622	49/49	0.96	0.11	31,47,68,81	0
22	CLA	B	610	65/65	0.96	0.11	26,38,61,72	0
28	LHG	d	407	49/49	0.96	0.13	34,52,74,84	0
28	LHG	d	409	39/49	0.96	0.11	32,51,66,69	0
28	LHG	l	101	49/49	0.96	0.11	25,48,61,78	0
22	CLA	D	403	65/65	0.96	0.11	20,33,54,61	0
22	CLA	B	604	65/65	0.96	0.16	23,36,64,67	0
22	CLA	b	610	65/65	0.96	0.18	27,40,52,62	0
22	CLA	b	611	65/65	0.96	0.13	21,36,56,68	0
22	CLA	b	612	65/65	0.96	0.17	22,36,52,56	0
22	CLA	C	502	65/65	0.96	0.12	25,37,54,57	0
24	BCR	a	406	40/40	0.96	0.09	23,38,49,54	0
22	CLA	B	613	65/65	0.96	0.14	20,34,53,58	0
24	BCR	b	618	40/40	0.96	0.09	27,42,54,58	0
34	HEC	E	101	43/43	0.96	0.12	36,50,69,75	0
34	HEC	e	101	43/43	0.96	0.12	44,61,79,83	0
22	CLA	B	612	65/65	0.97	0.13	22,34,50,54	0
22	CLA	a	402	65/65	0.97	0.10	19,33,47,55	0
22	CLA	B	609	65/65	0.97	0.12	23,36,56,62	0
28	LHG	D	408	49/49	0.97	0.10	24,41,54,60	0
28	LHG	L	102	49/49	0.97	0.10	27,42,59,71	0
23	PHO	D	401	64/64	0.97	0.11	22,35,45,50	0
22	CLA	A	402	65/65	0.97	0.10	21,29,43,61	0
28	LHG	d	408	49/49	0.97	0.10	27,43,59,66	0
22	CLA	b	607	65/65	0.97	0.12	21,39,70,81	0
22	CLA	D	402	65/65	0.97	0.11	17,32,59,66	0
34	HEC	V	201	43/43	0.97	0.13	25,37,45,53	0
22	CLA	B	606	65/65	0.97	0.13	22,36,52,56	0
26	BCT	A	409	4/4	0.98	0.16	26,33,35,42	0
34	HEC	v	201	43/43	0.98	0.13	32,39,52,59	0
31	OEX	A	416	10/10	0.99	0.13	25,31,33,37	0
31	OEX	a	415	10/10	0.99	0.12	22,30,32,33	0
25	CL	a	407	1/1	0.99	0.05	32,32,32,32	0
25	CL	a	408	1/1	0.99	0.07	32,32,32,32	0

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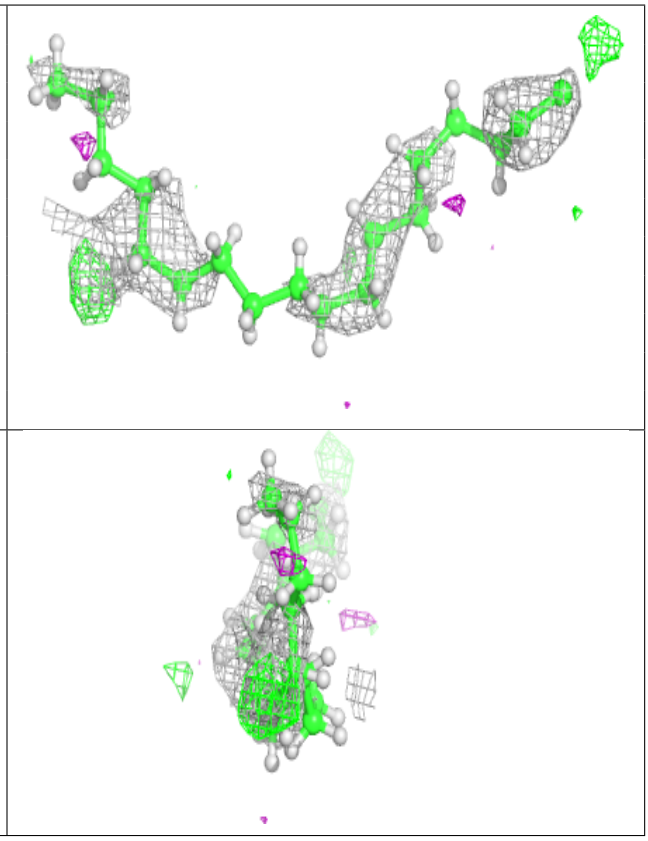
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	FE2	A	401	1/1	0.99	0.09	30,30,30,30	0
26	BCT	a	409	4/4	0.99	0.22	31,31,44,52	0
21	FE2	a	401	1/1	0.99	0.10	38,38,38,38	0
25	CL	A	407	1/1	0.99	0.07	32,32,32,32	0
25	CL	A	408	1/1	0.99	0.06	32,32,32,32	0

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.

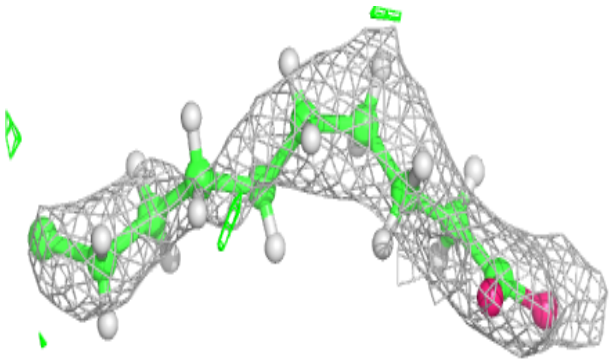
Electron density around STE H 103:

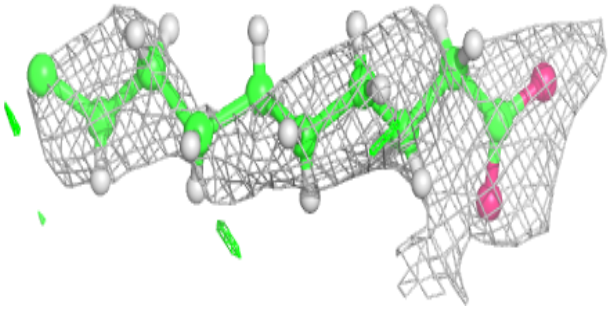
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

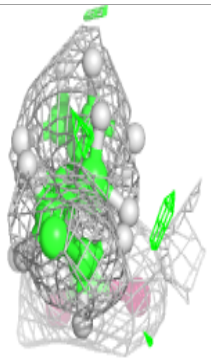


Electron density around STE E 102:

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

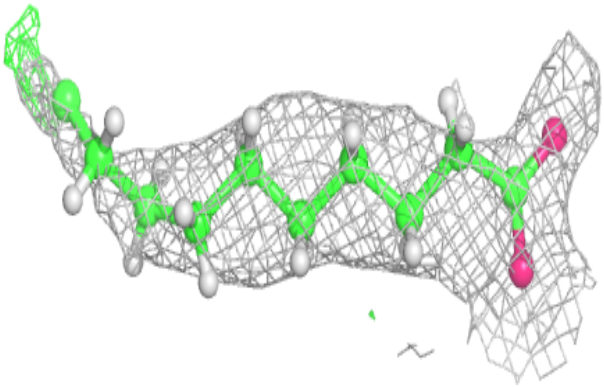


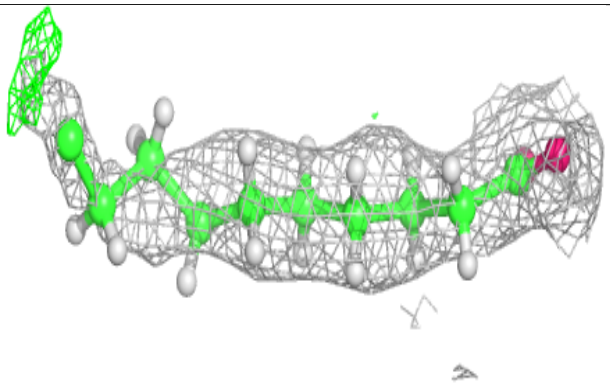


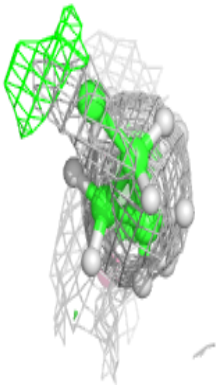


Electron density around STE k 101:

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

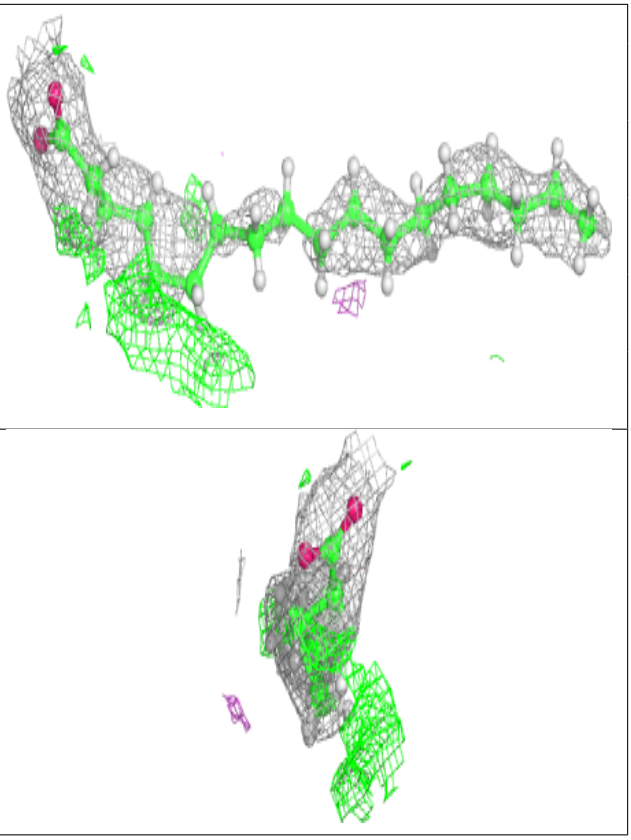


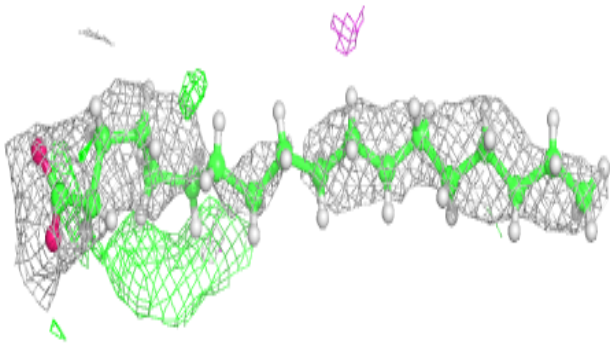




Electron density around STE b 624:

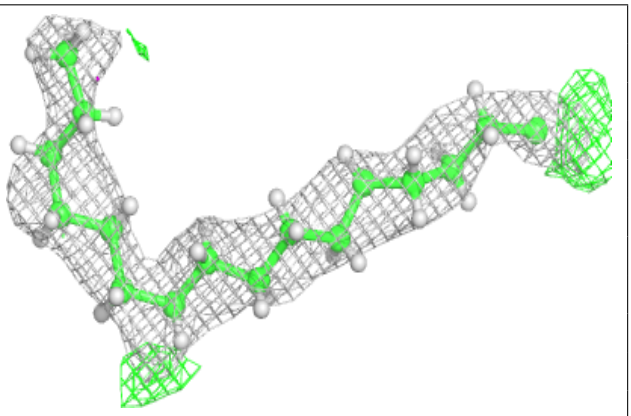
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

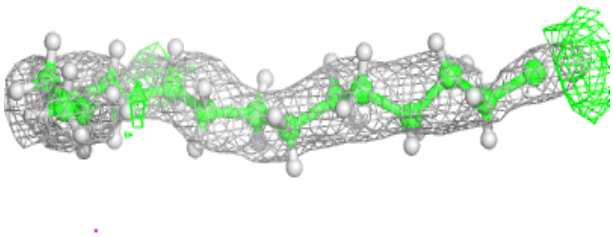


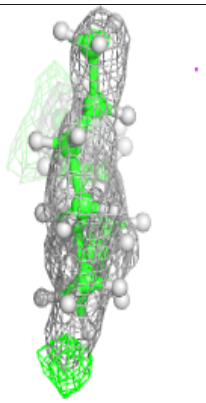


Electron density around STE B 625:

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

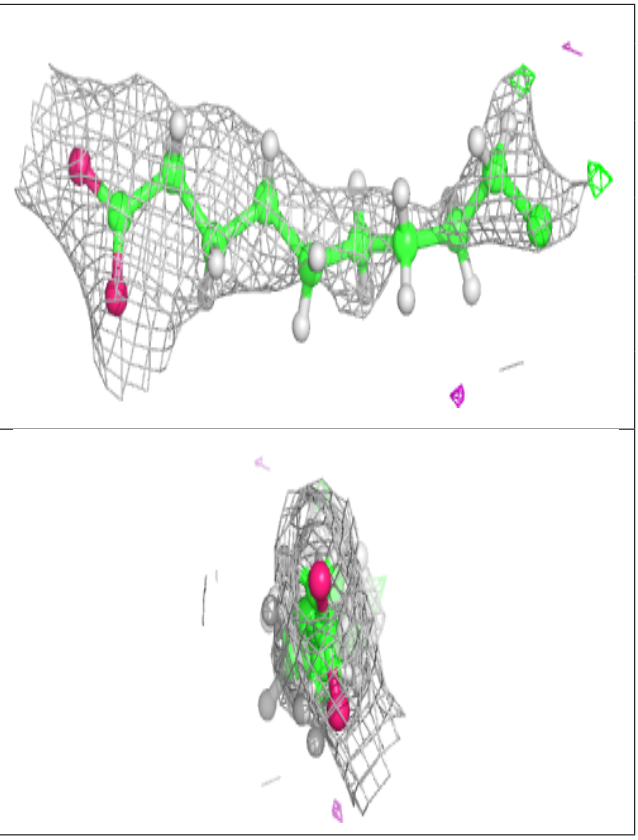






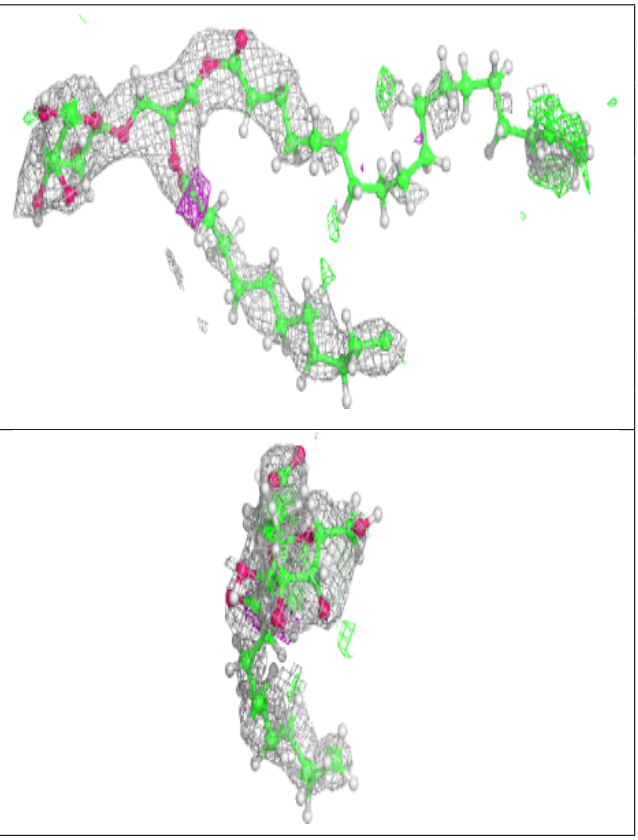
Electron density around STE a 414:

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



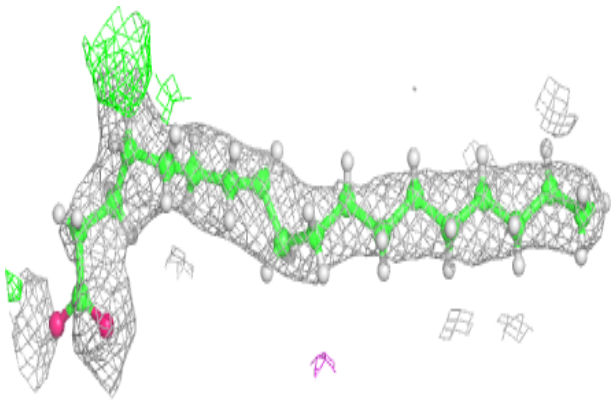
Electron density around LMG c 521:

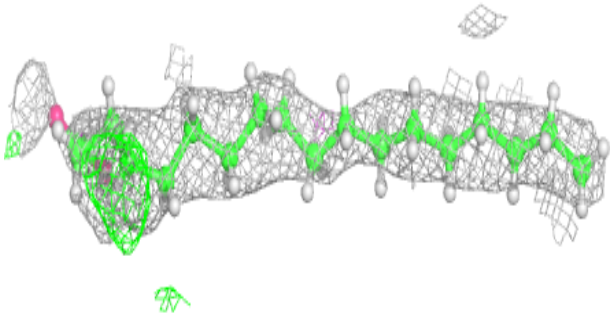
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

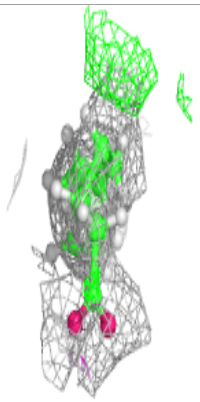


Electron density around STE c 520:

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

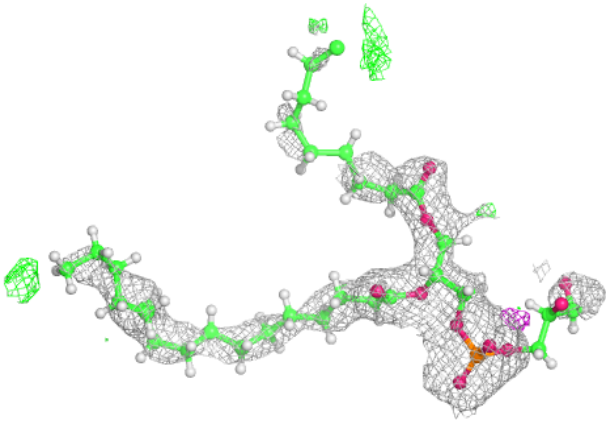


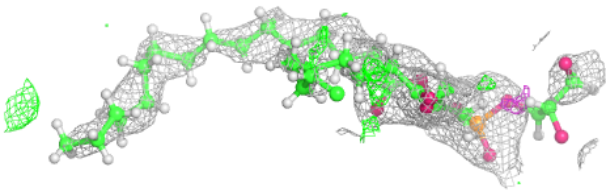


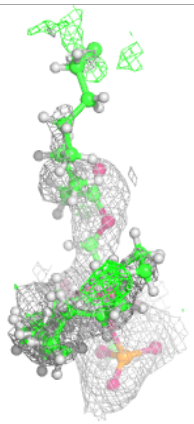


Electron density around LHG a 412:

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

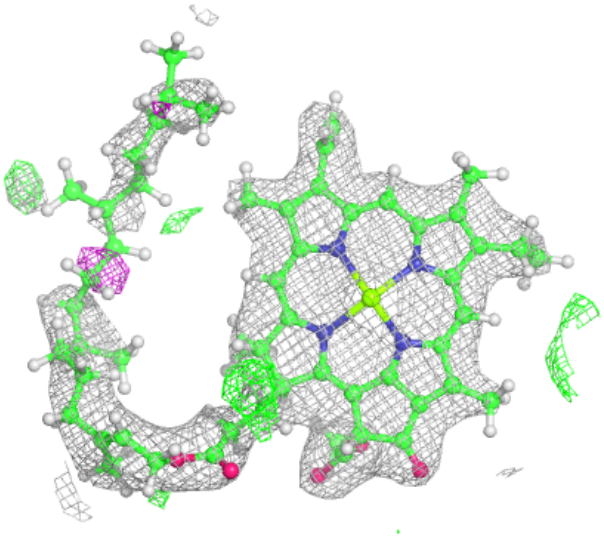


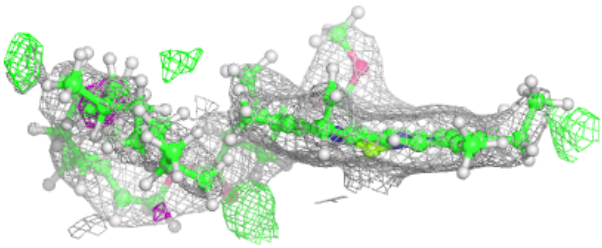




Electron density around CLA C 513:

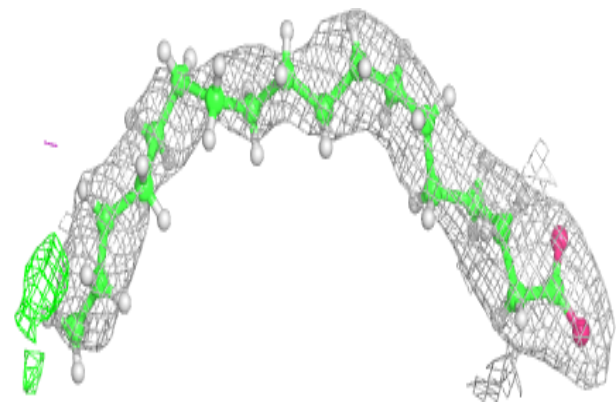
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

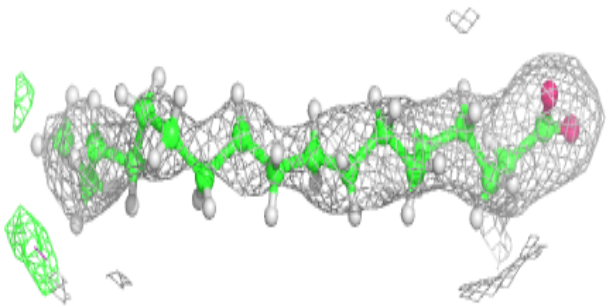


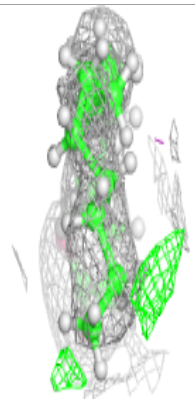


Electron density around STE x 102:

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

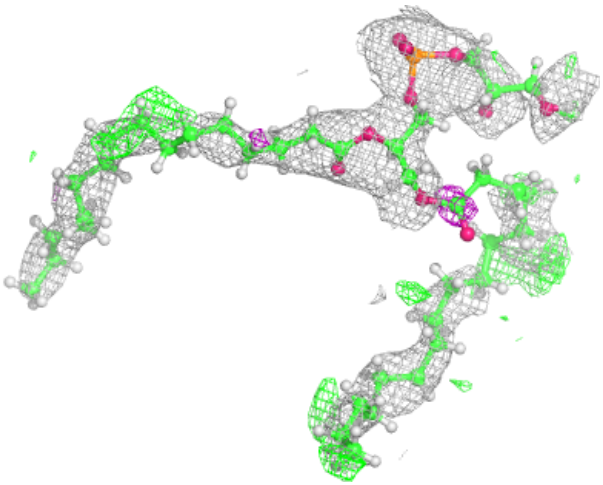


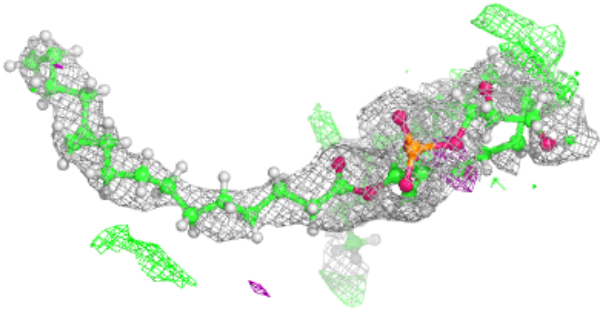


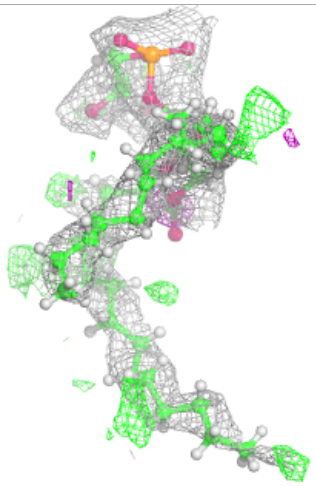


Electron density around LHG A 413:

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

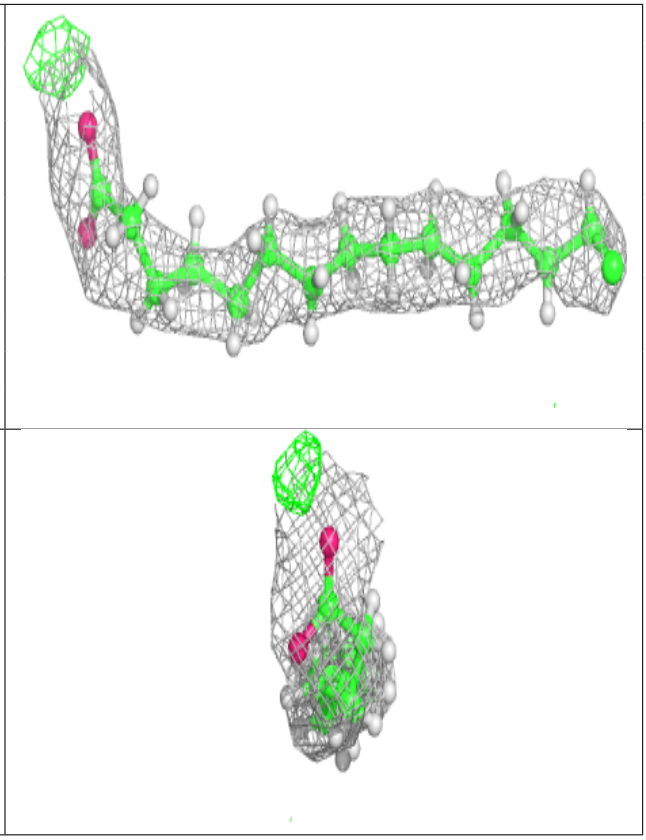


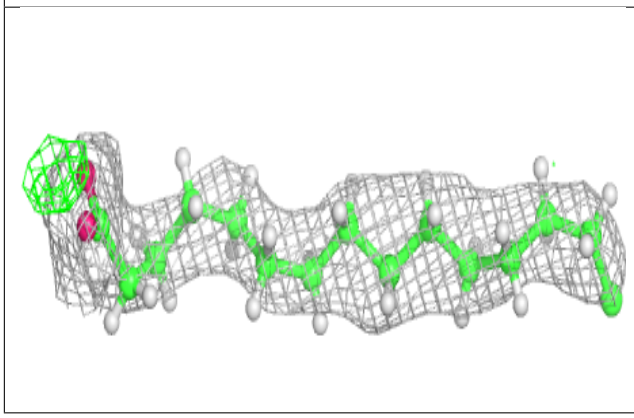




Electron density around STE d 411:

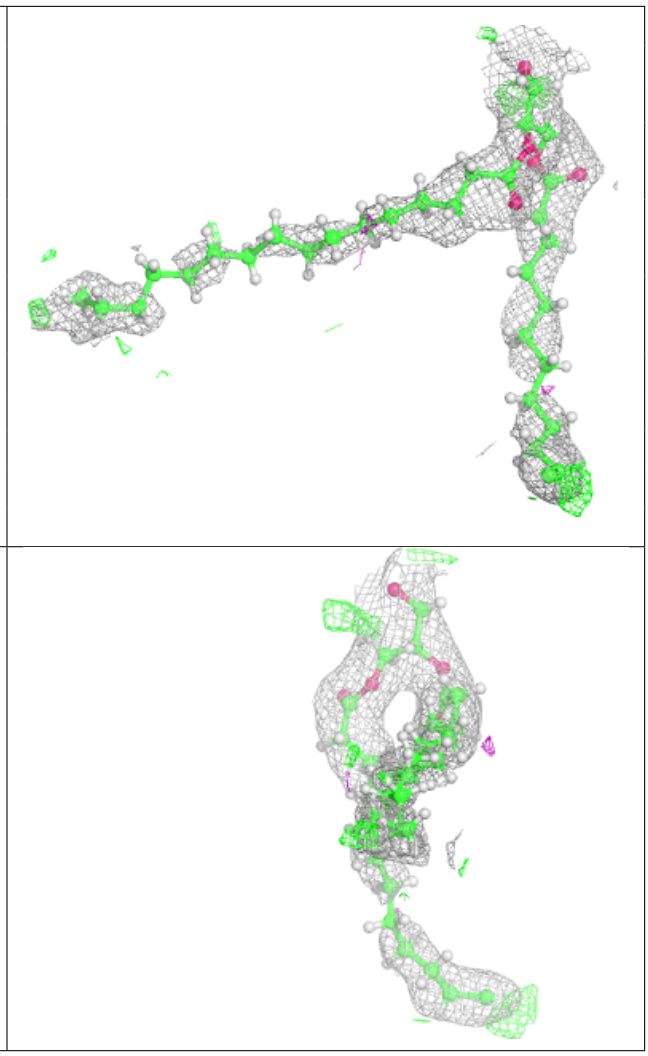
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





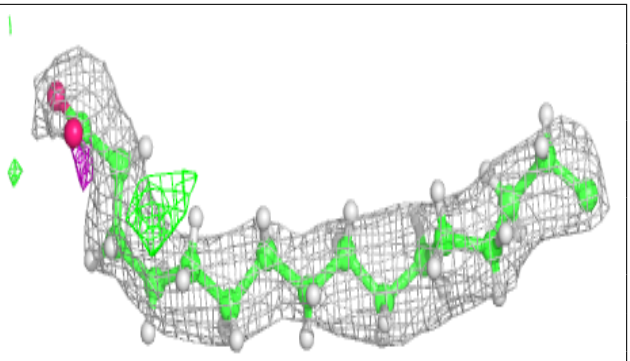
Electron density around SQD a 413:

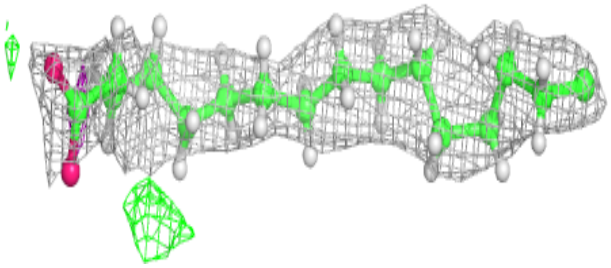
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

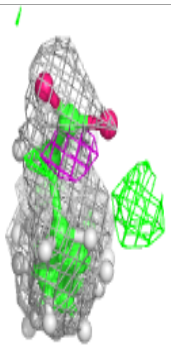


Electron density around STE t 104:

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

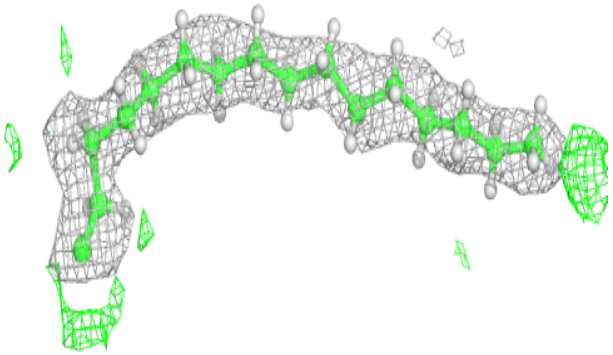


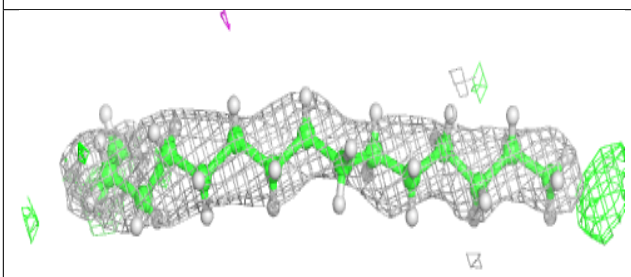


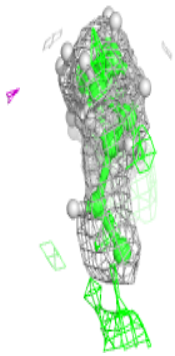


Electron density around STE C 521:

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

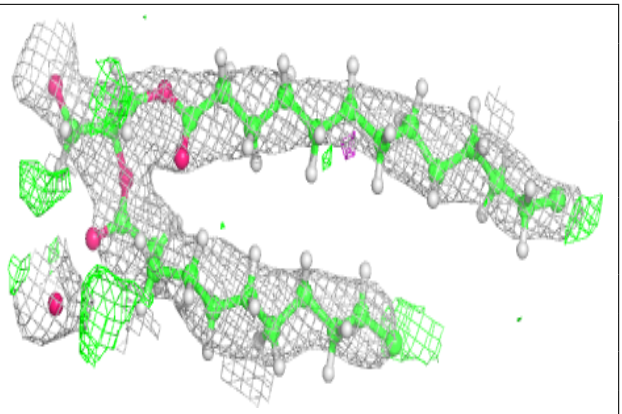


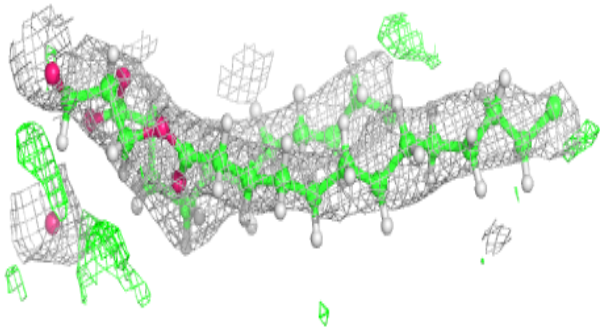


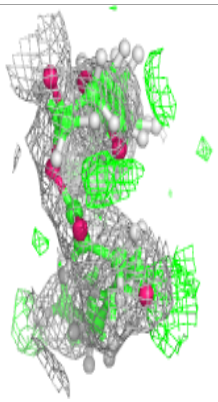


Electron density around LMG D 409:

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

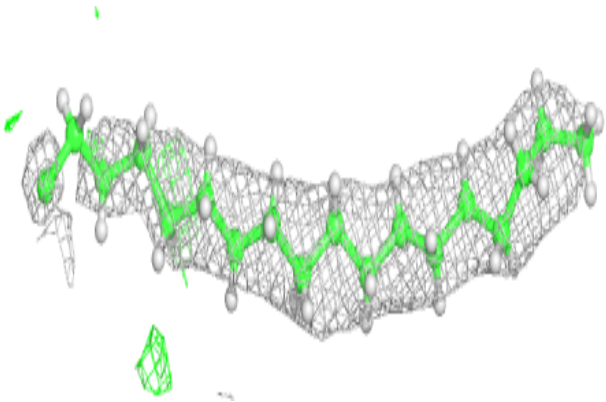


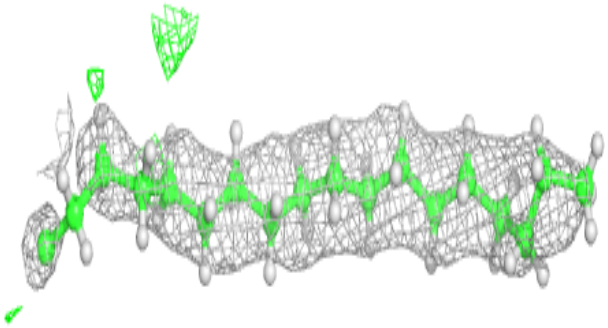


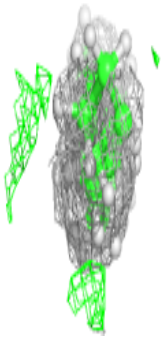


Electron density around STE M 104:

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

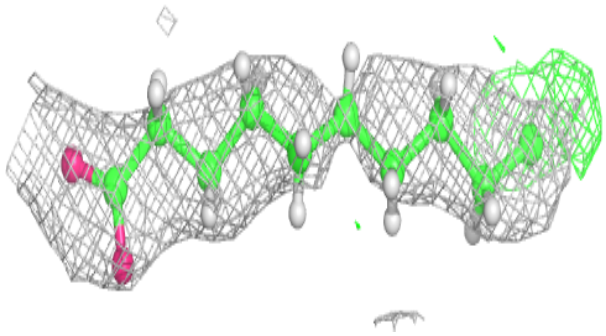


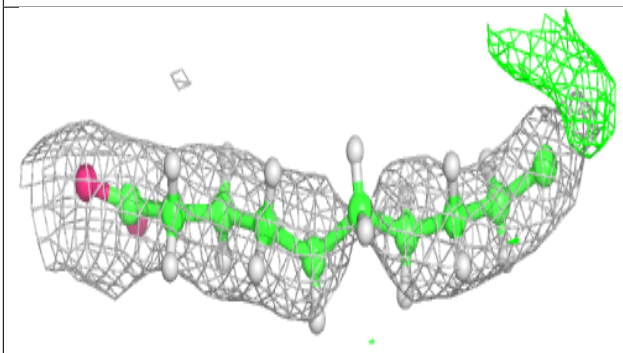


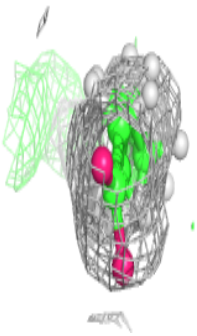


Electron density around STE j 101:

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

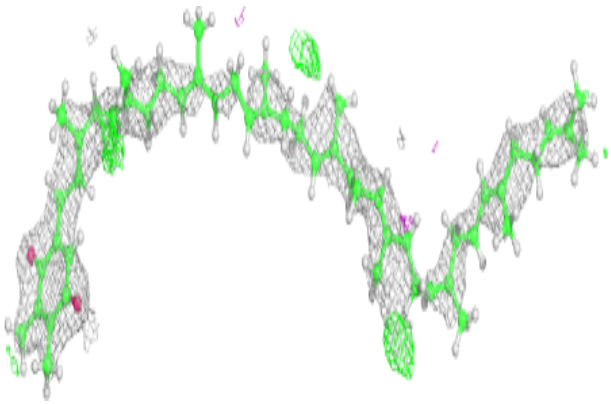


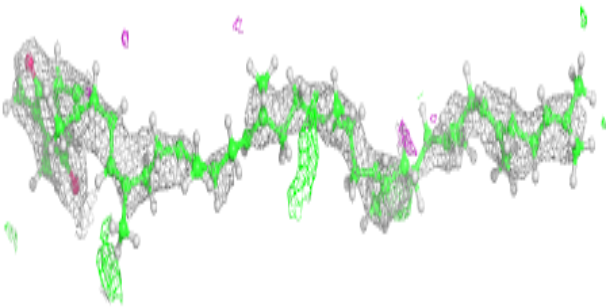




Electron density around PL9 A 410:

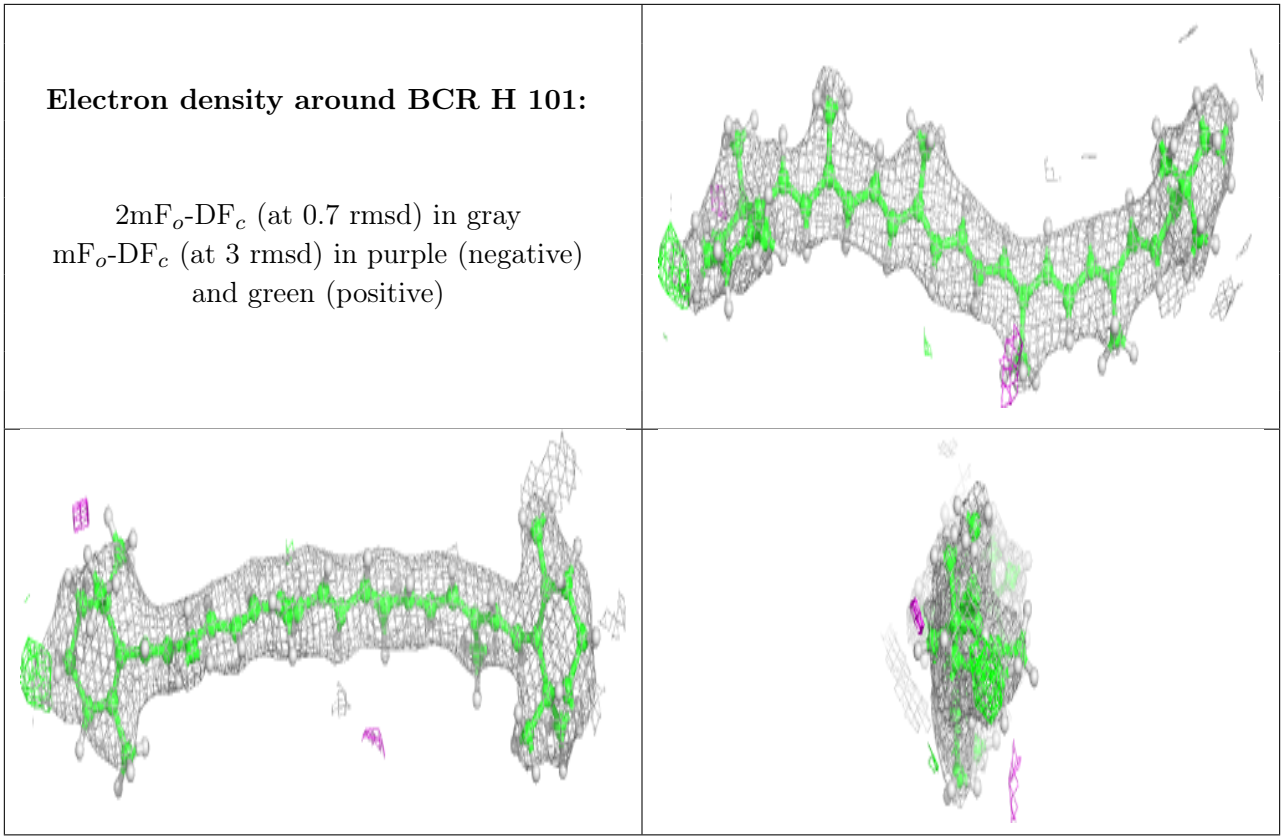
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





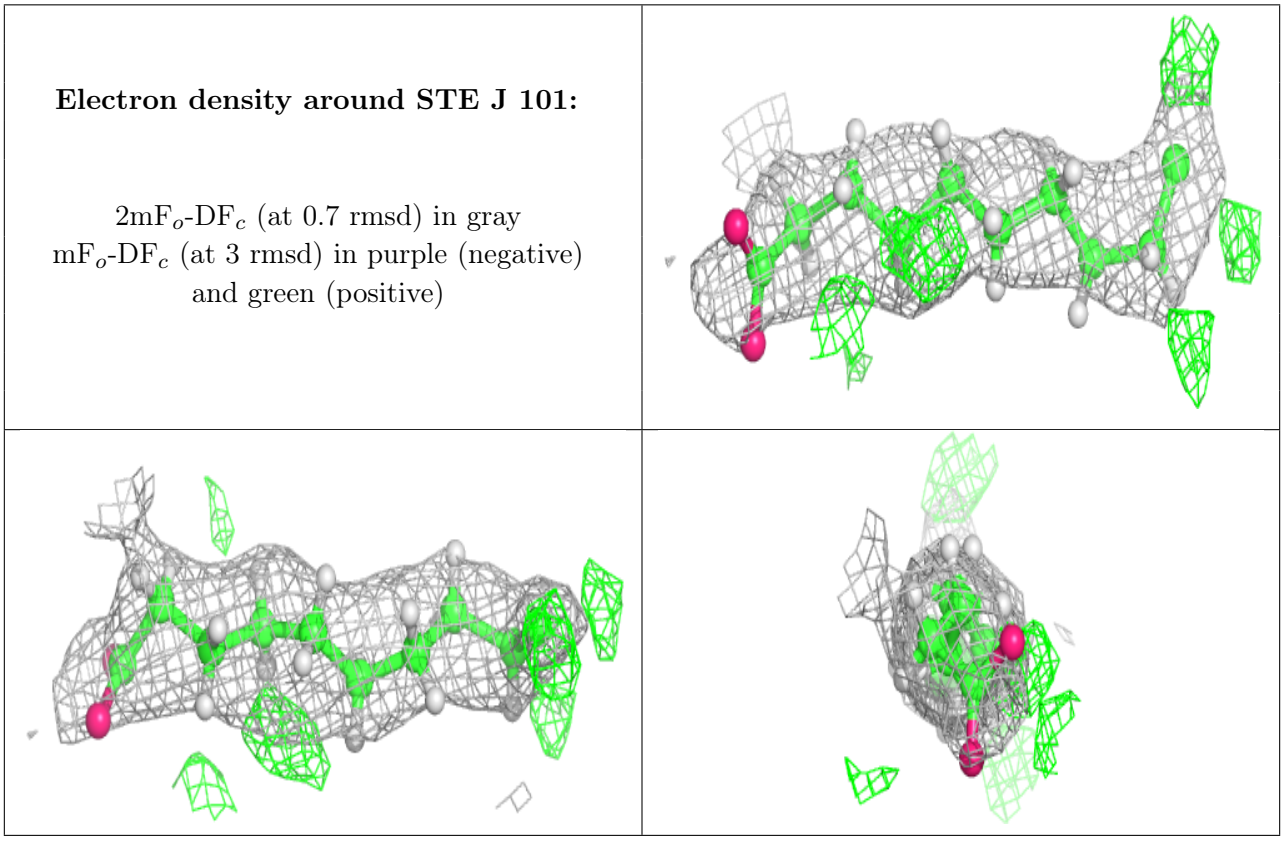
Electron density around BCR H 101:

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



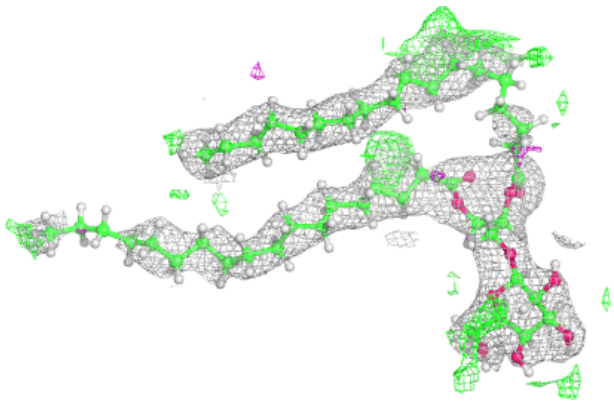
Electron density around STE J 101:

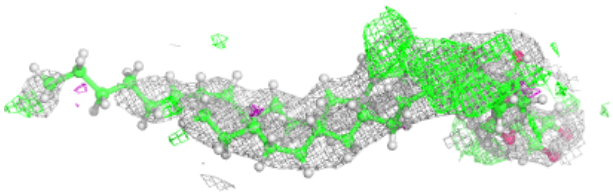
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

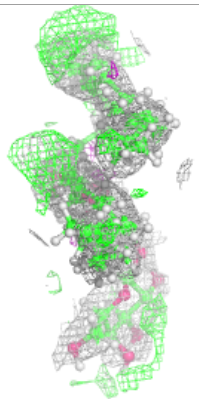


Electron density around LMG B 627:

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

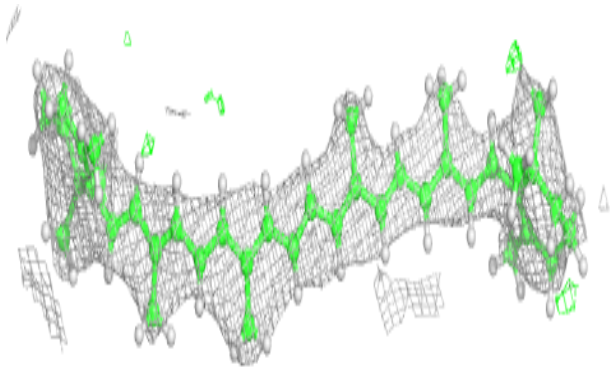


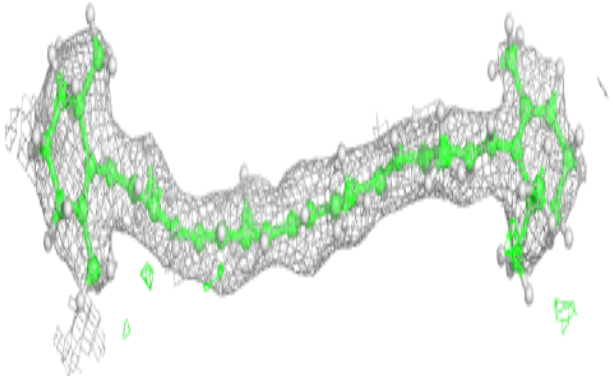


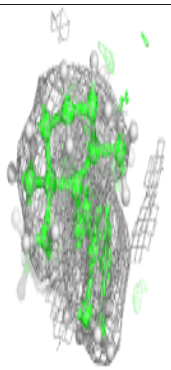


Electron density around BCR x 101:

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

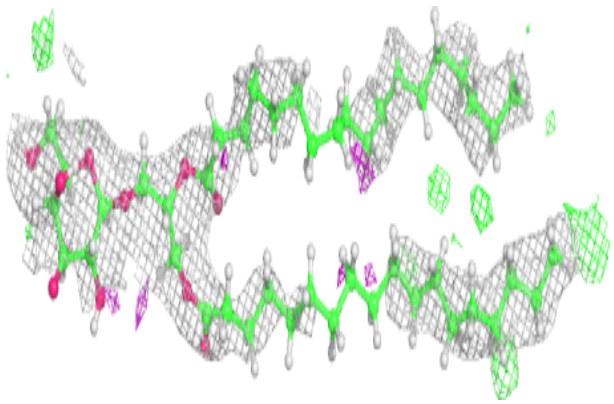


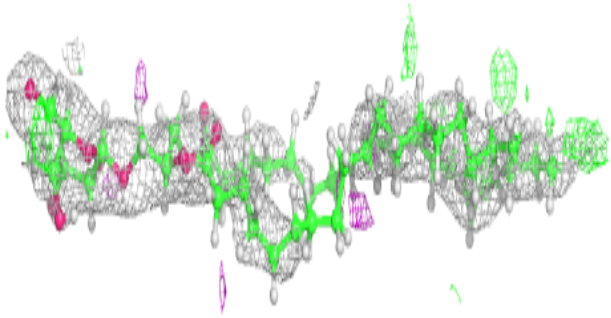


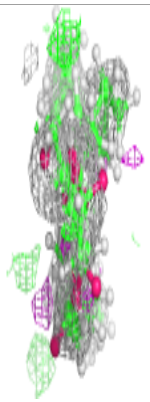


Electron density around LMG b 622:

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

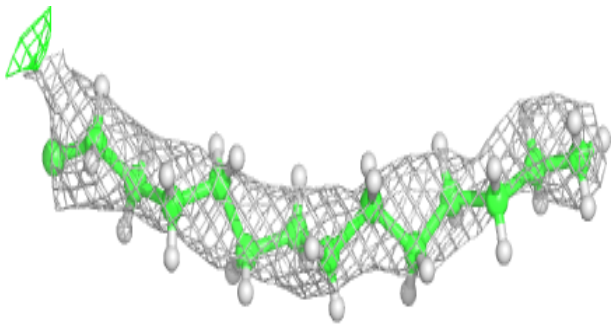


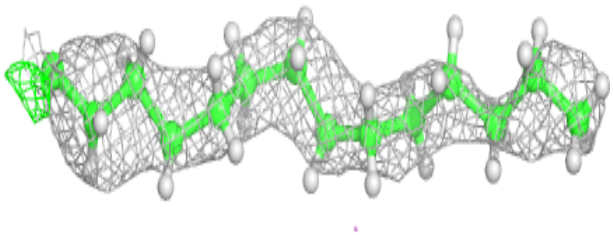


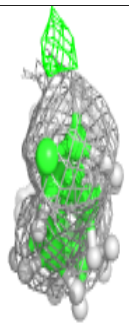


Electron density around STE h 102:

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

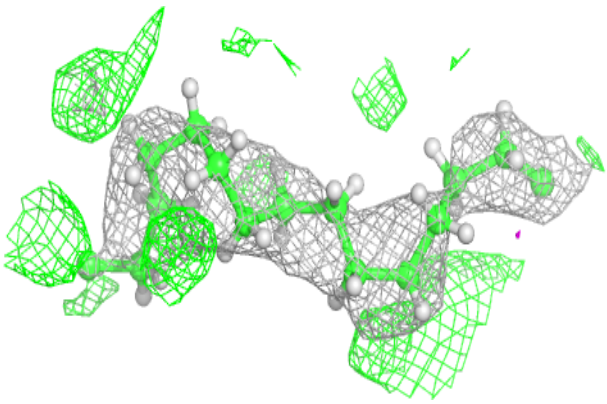


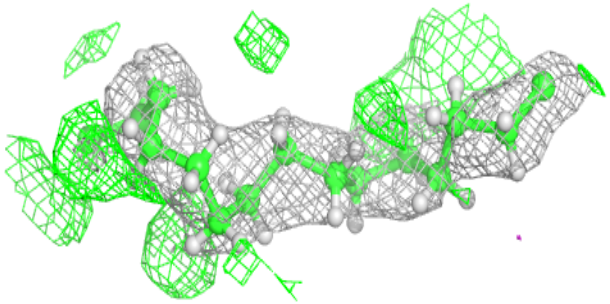


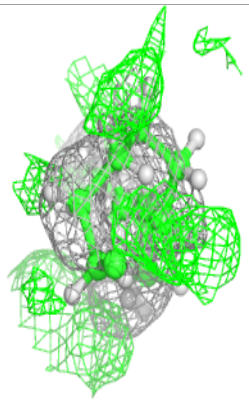


Electron density around STE B 626:

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

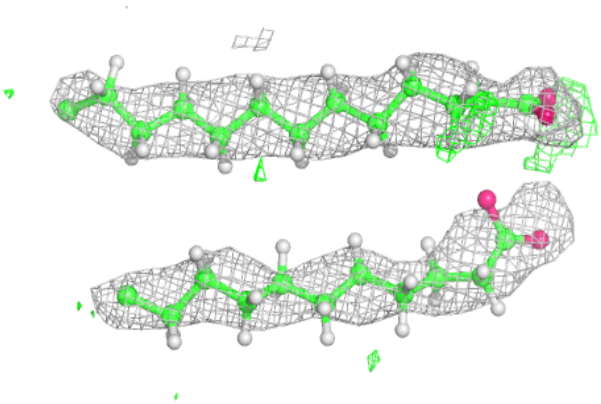


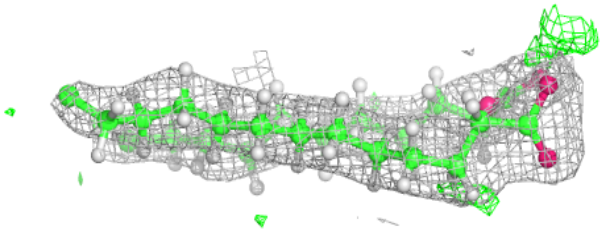


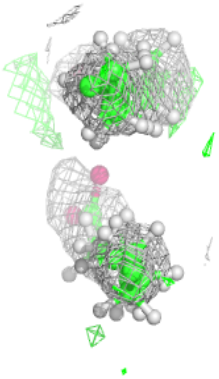


Electron density around LMG D 410:

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

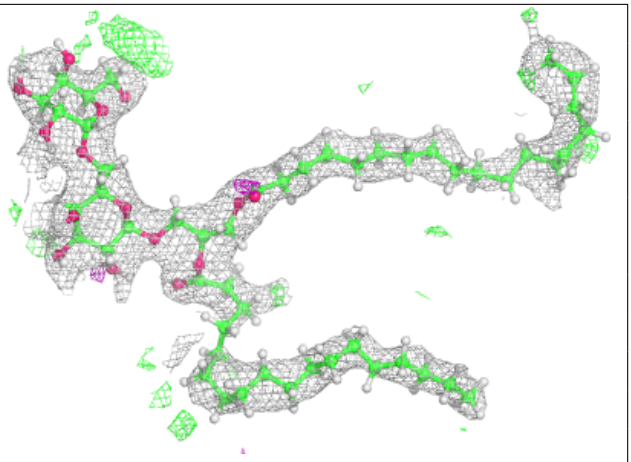


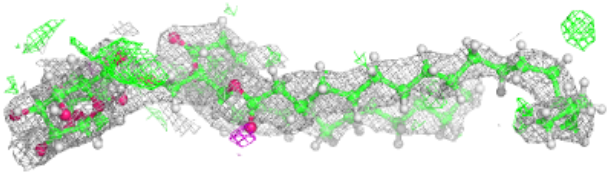


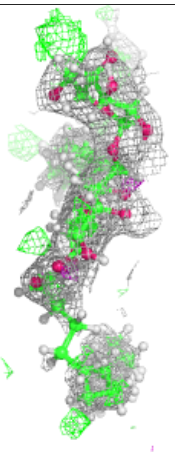


Electron density around DGD A 415:

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

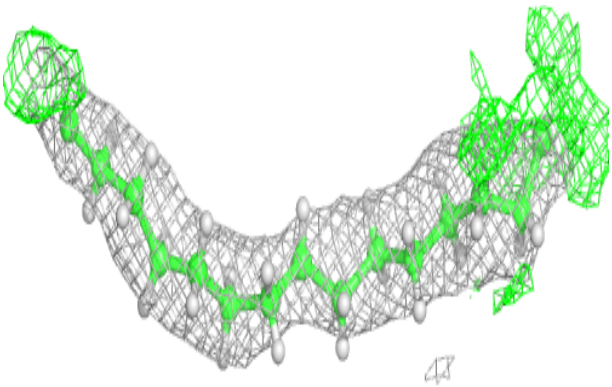


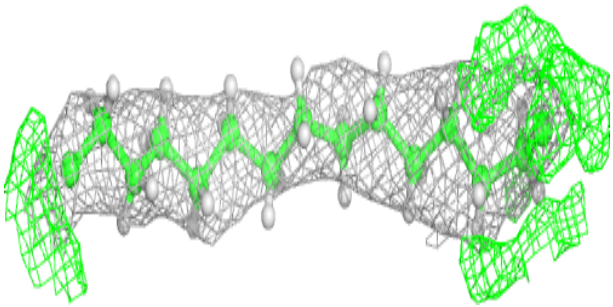


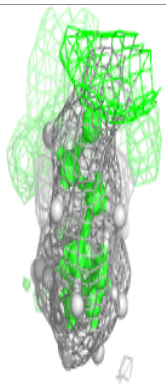


Electron density around STE I 101:

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

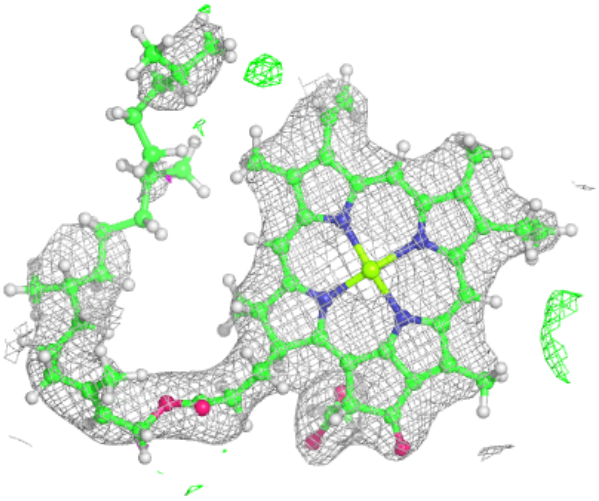


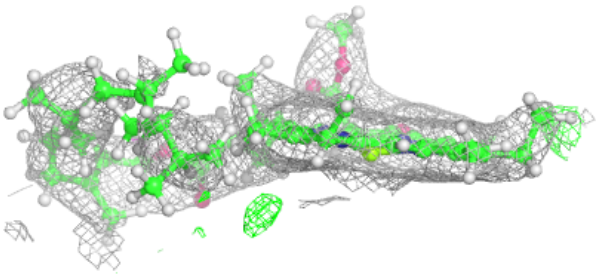


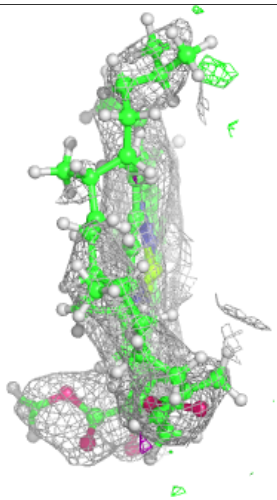


Electron density around CLA c 512:

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

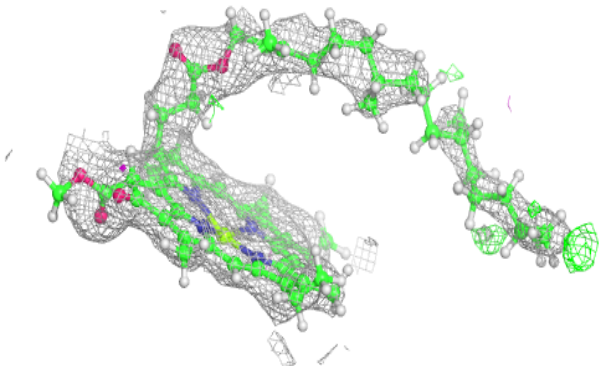


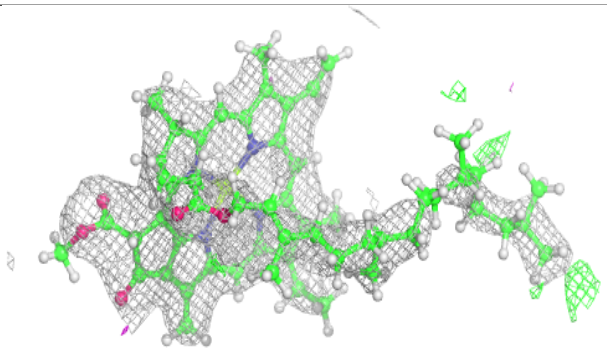


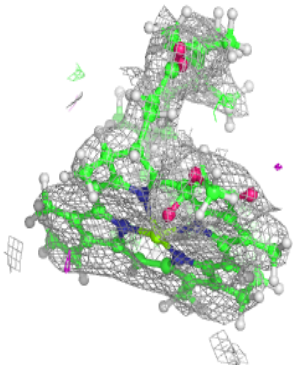


Electron density around CLA C 514:

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

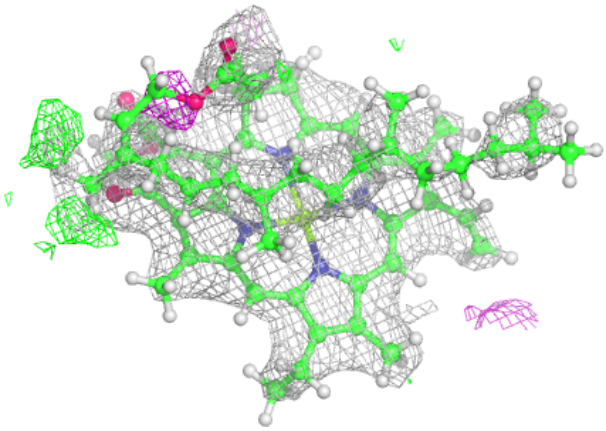


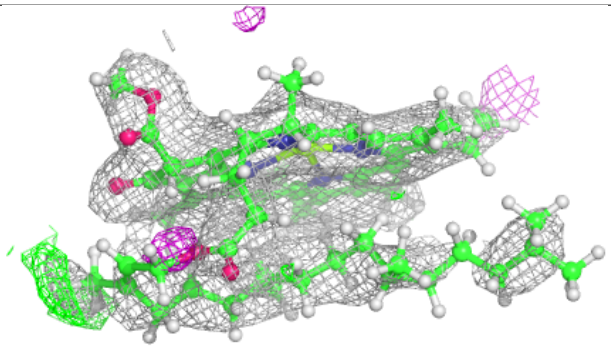


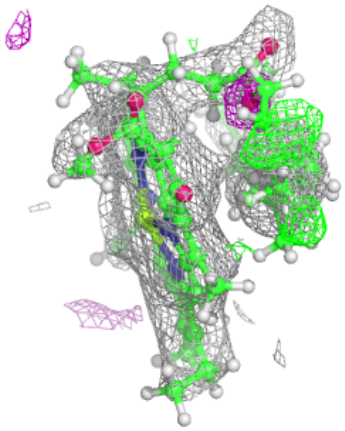


Electron density around CLA b 601:

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

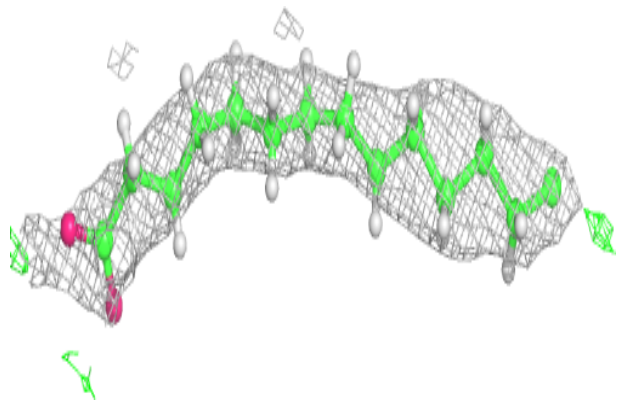


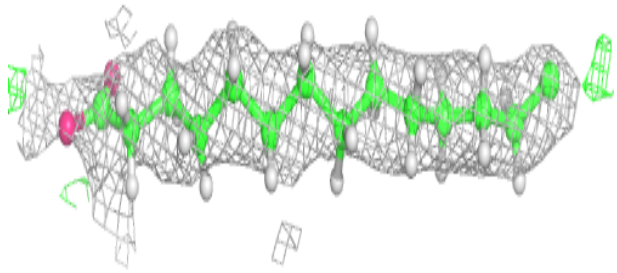


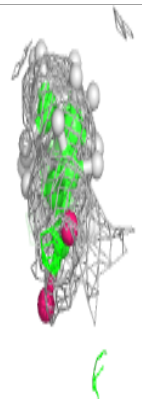


Electron density around STE b 623:

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

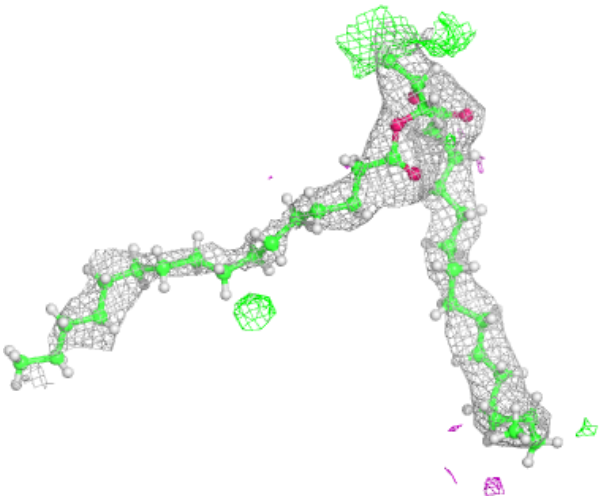


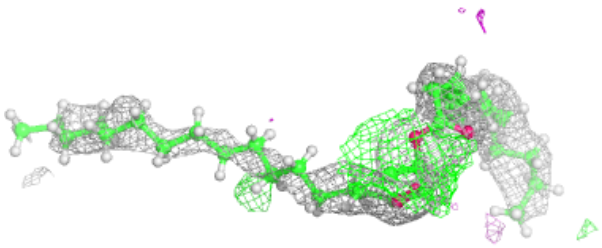


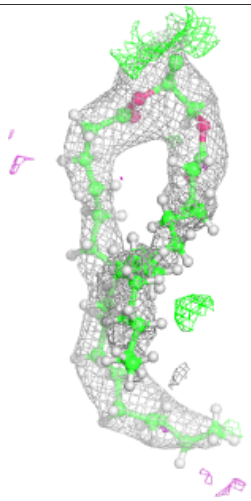


Electron density around SQD A 414:

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

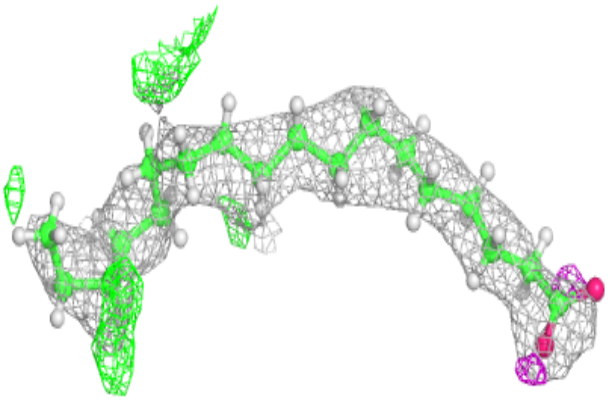


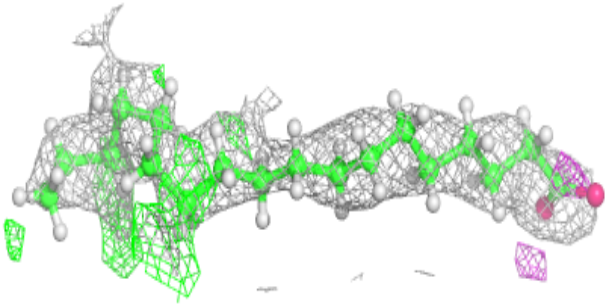


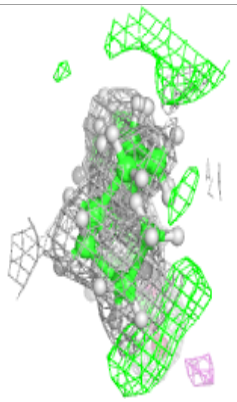


Electron density around STE b 626:

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

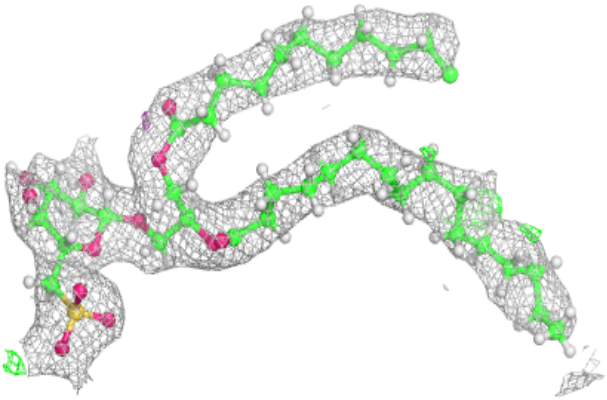


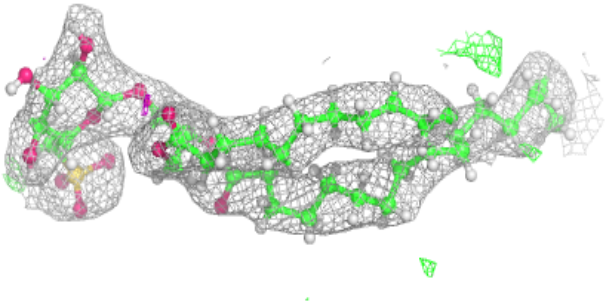


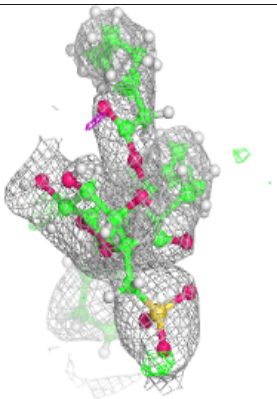


Electron density around SQD L 101:

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

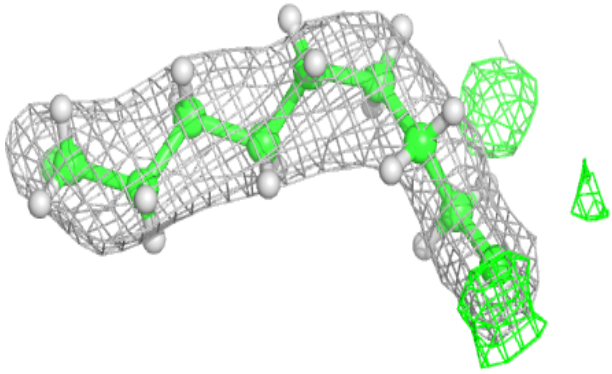


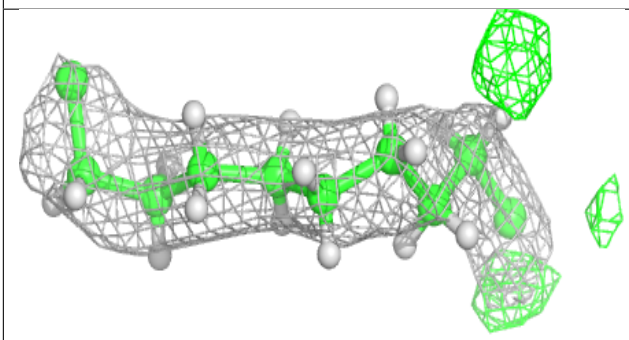


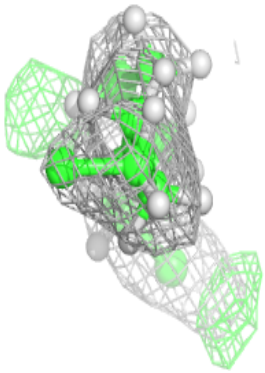


Electron density around STE b 625:

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

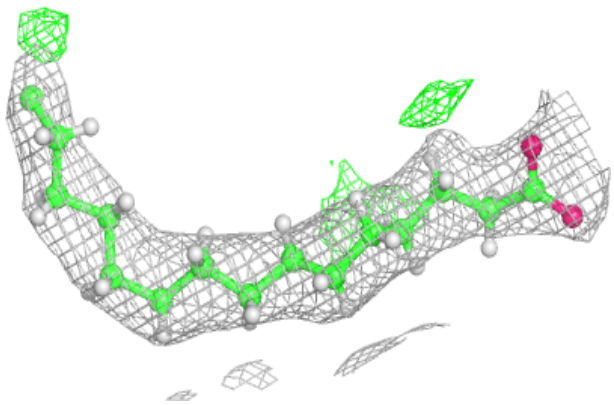


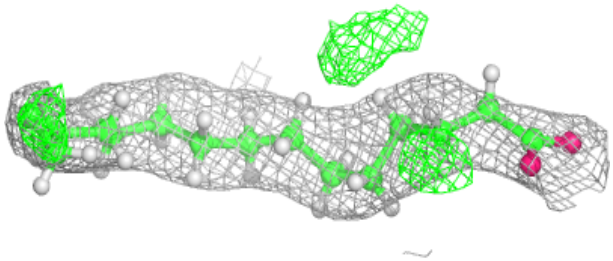


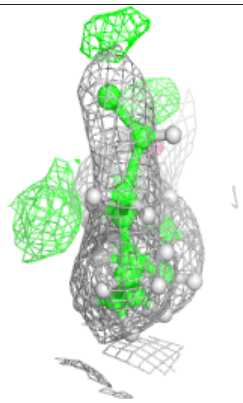


Electron density around STE B 621:

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

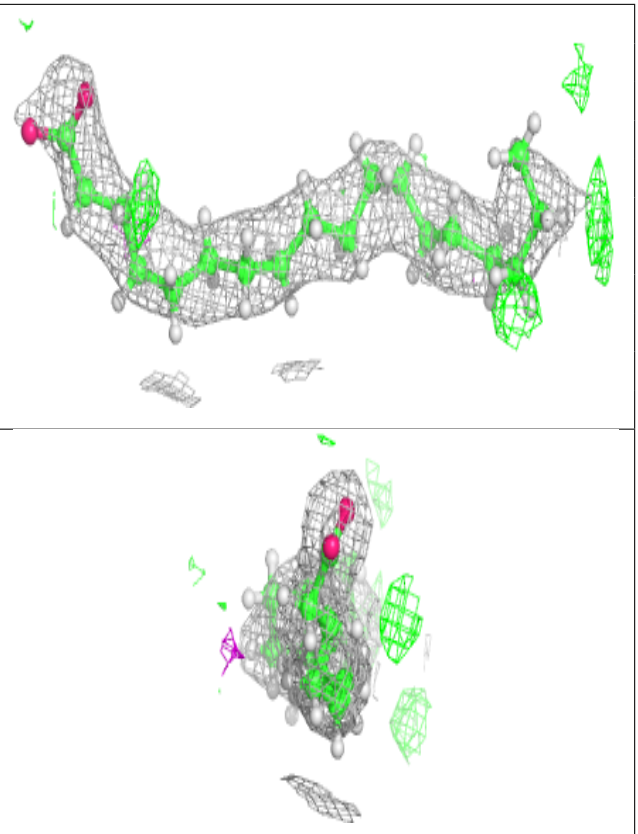


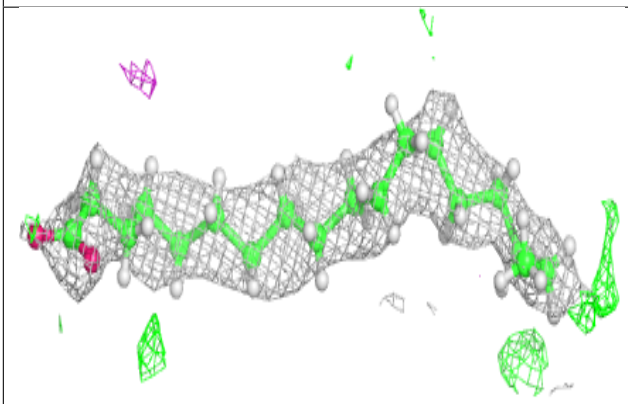




Electron density around STE b 621:

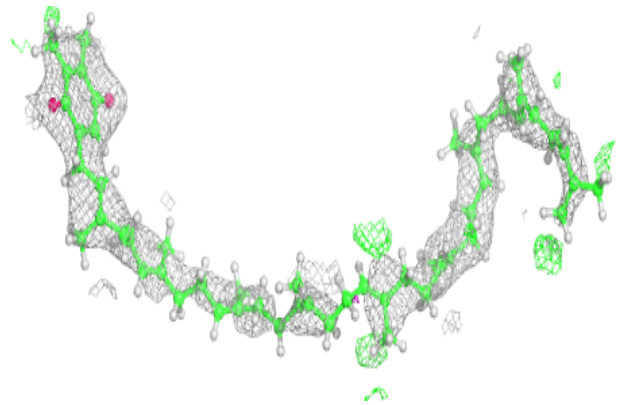
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

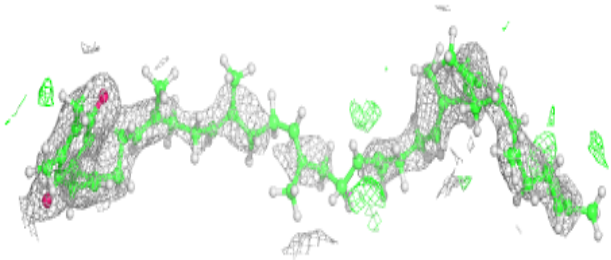


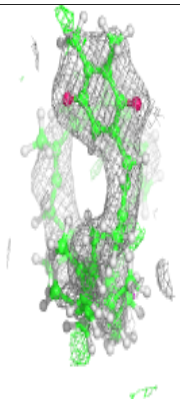


Electron density around PL9 a 410:

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

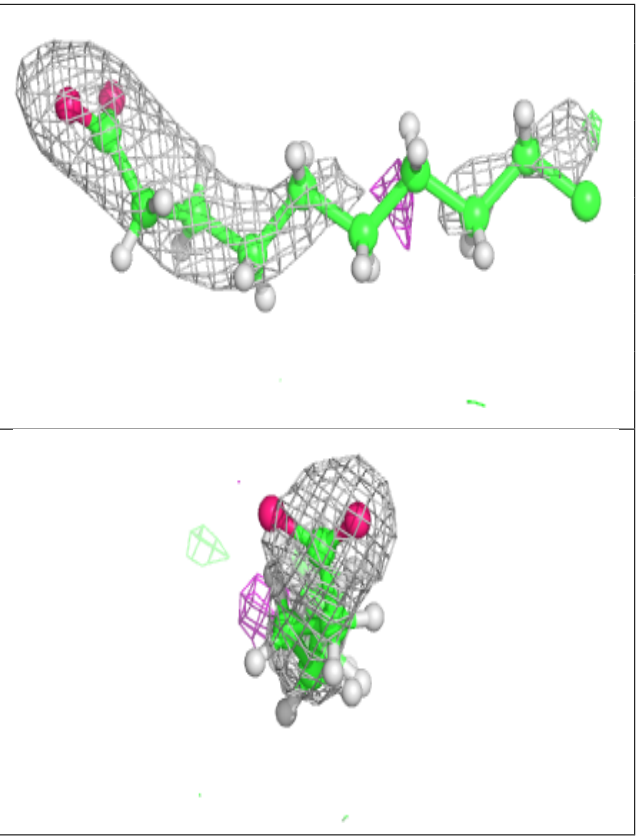






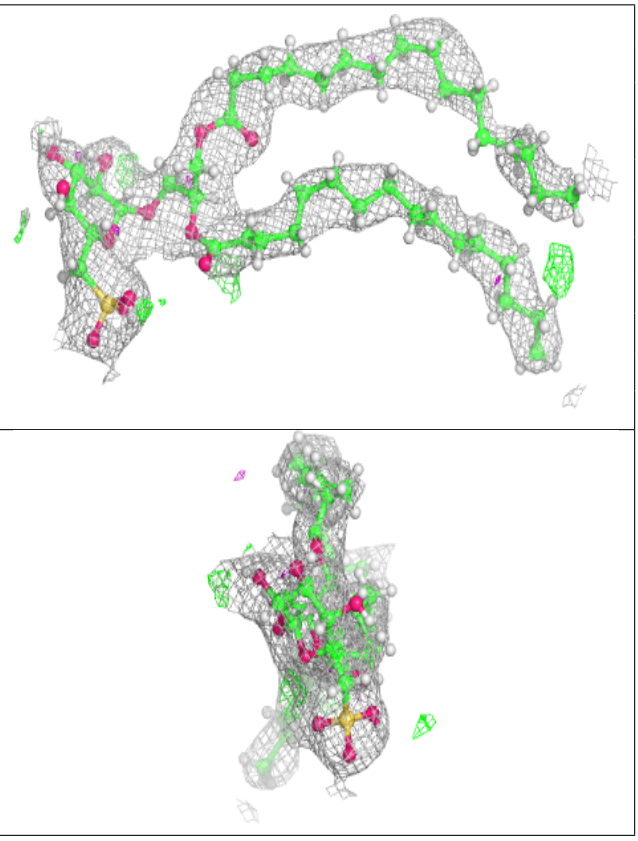
Electron density around STE B 601:

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



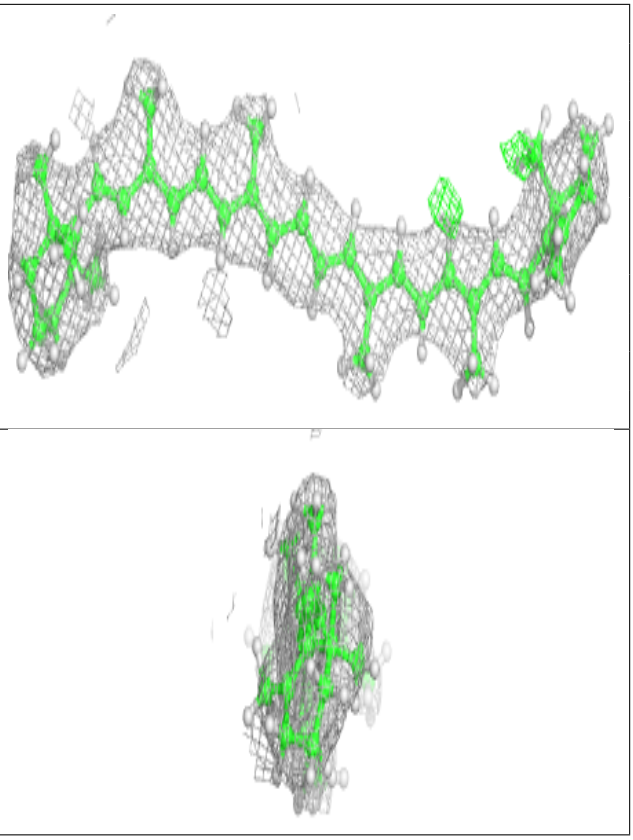
Electron density around SQD B 623:

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



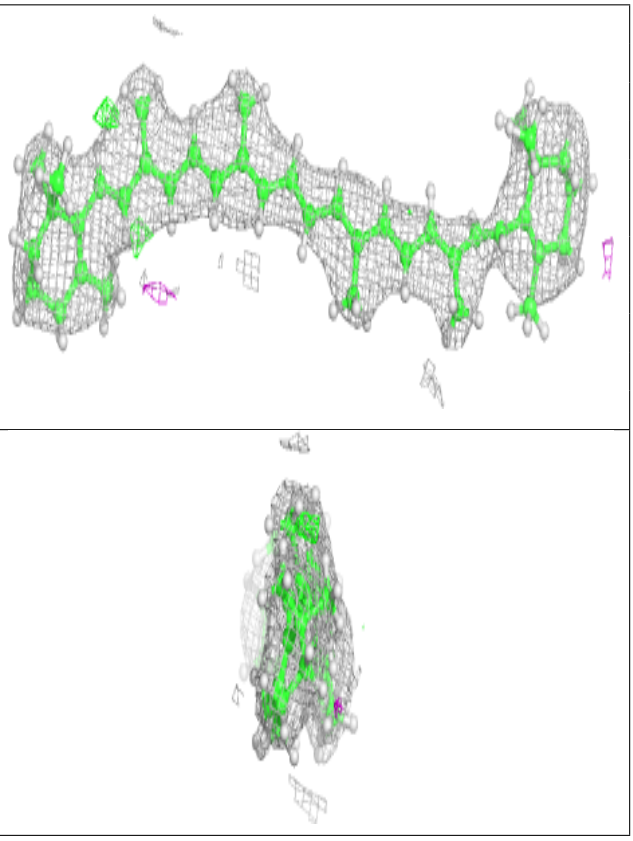
Electron density around BCR K 101:

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



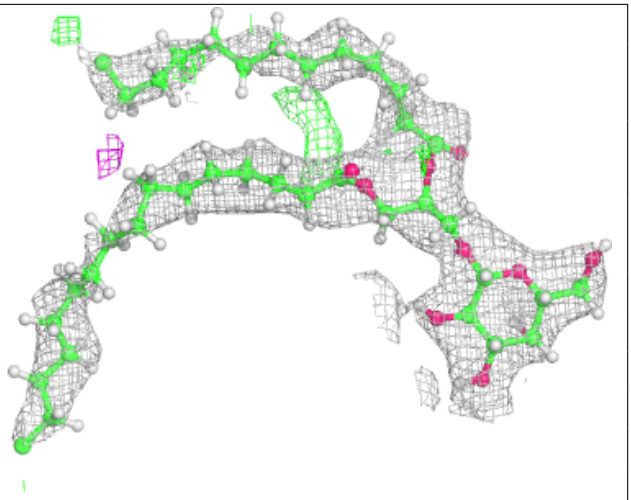
Electron density around BCR d 405:

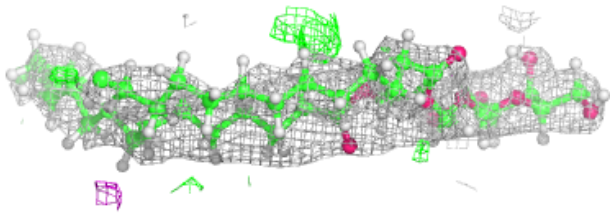
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

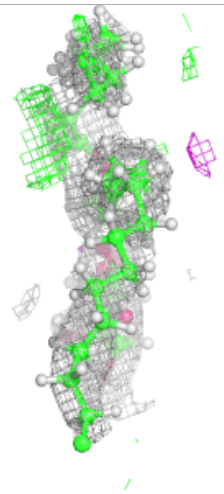


Electron density around LMG Y 101:

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

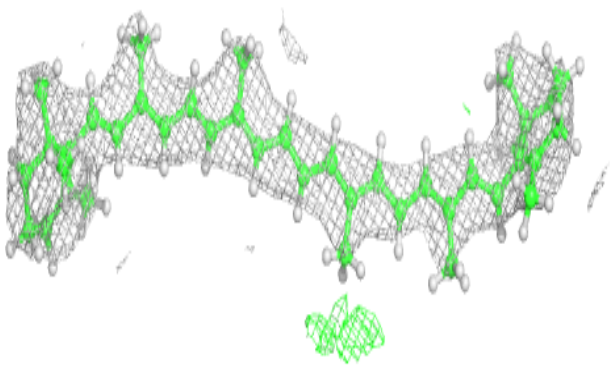


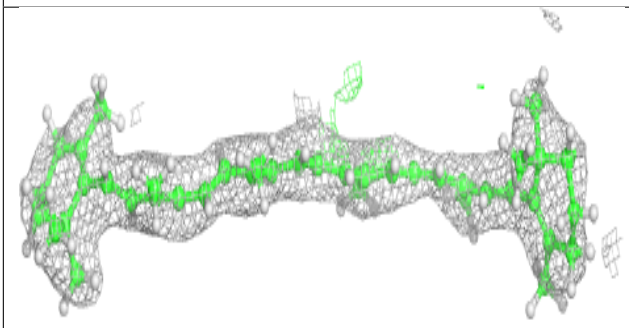


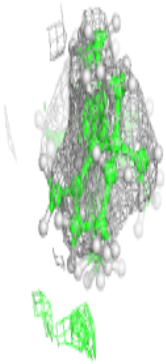


Electron density around BCR k 102:

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

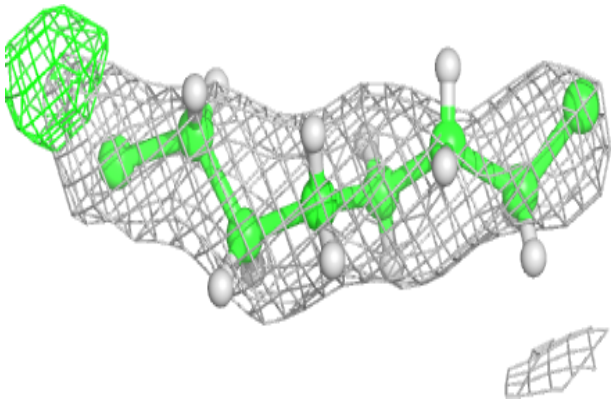


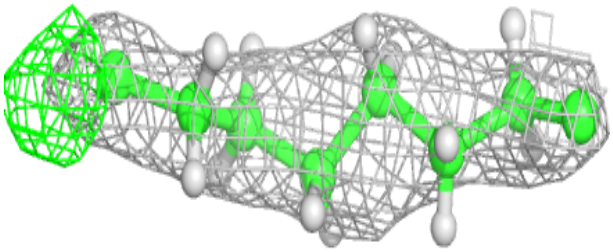


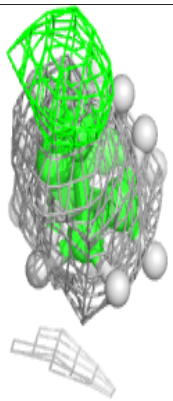


Electron density around STE Z 102:

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

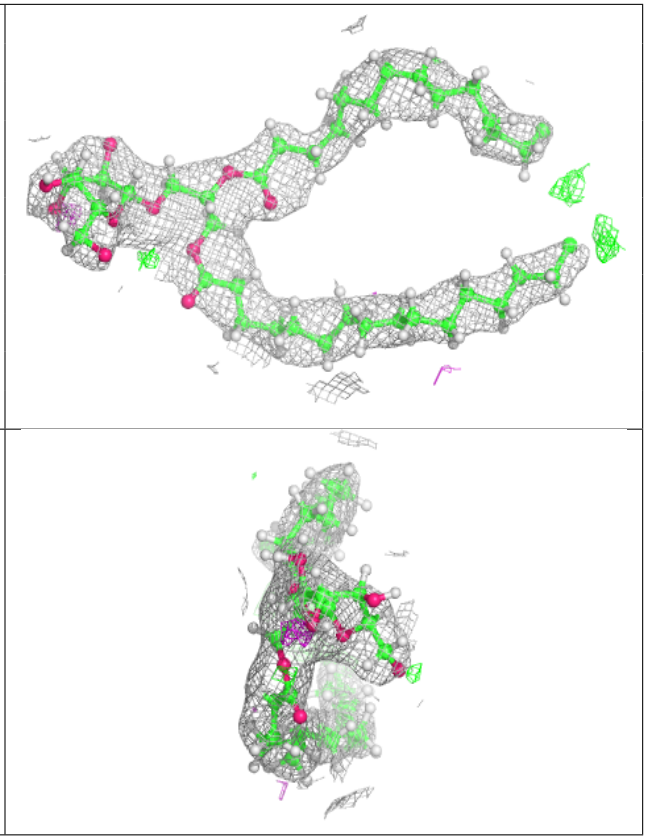






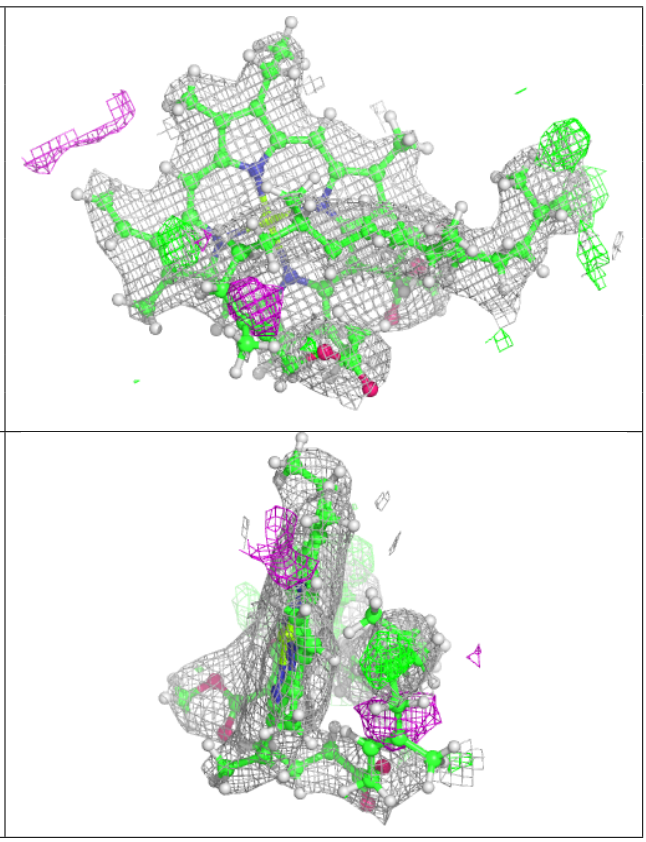
Electron density around LMG c 522:

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



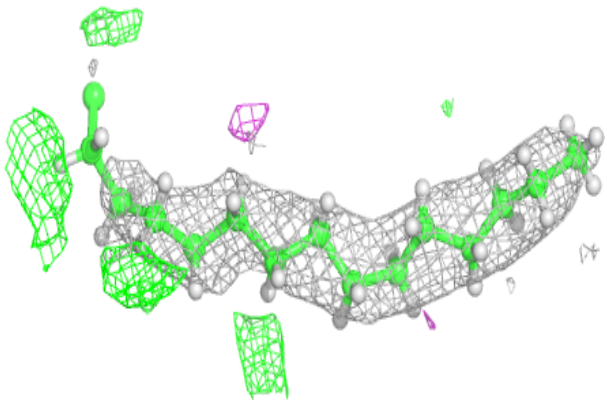
Electron density around CLA B 602:

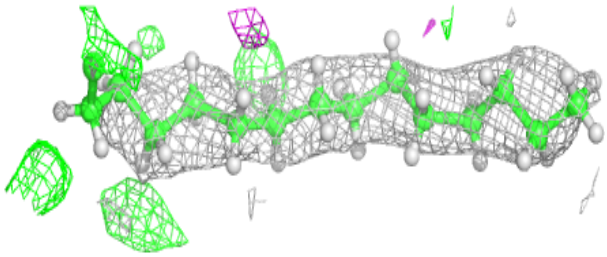
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

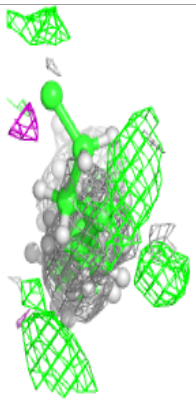


Electron density around STE T 102:

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

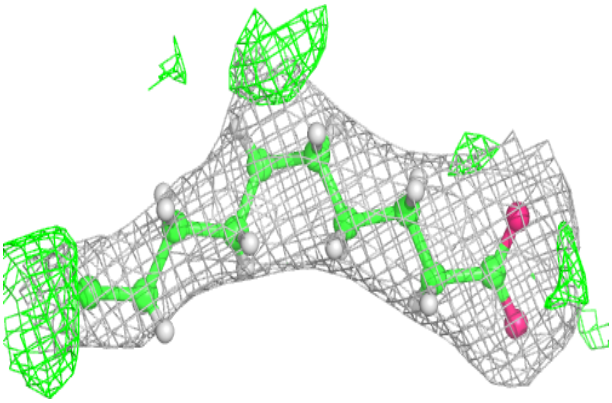


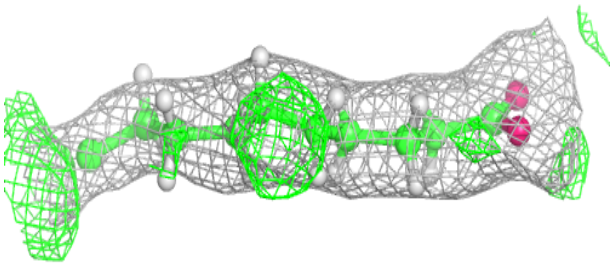


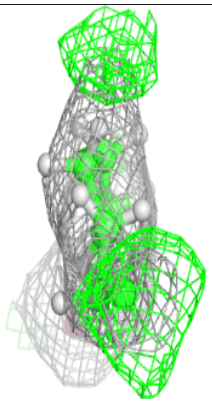


Electron density around STE C 522:

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

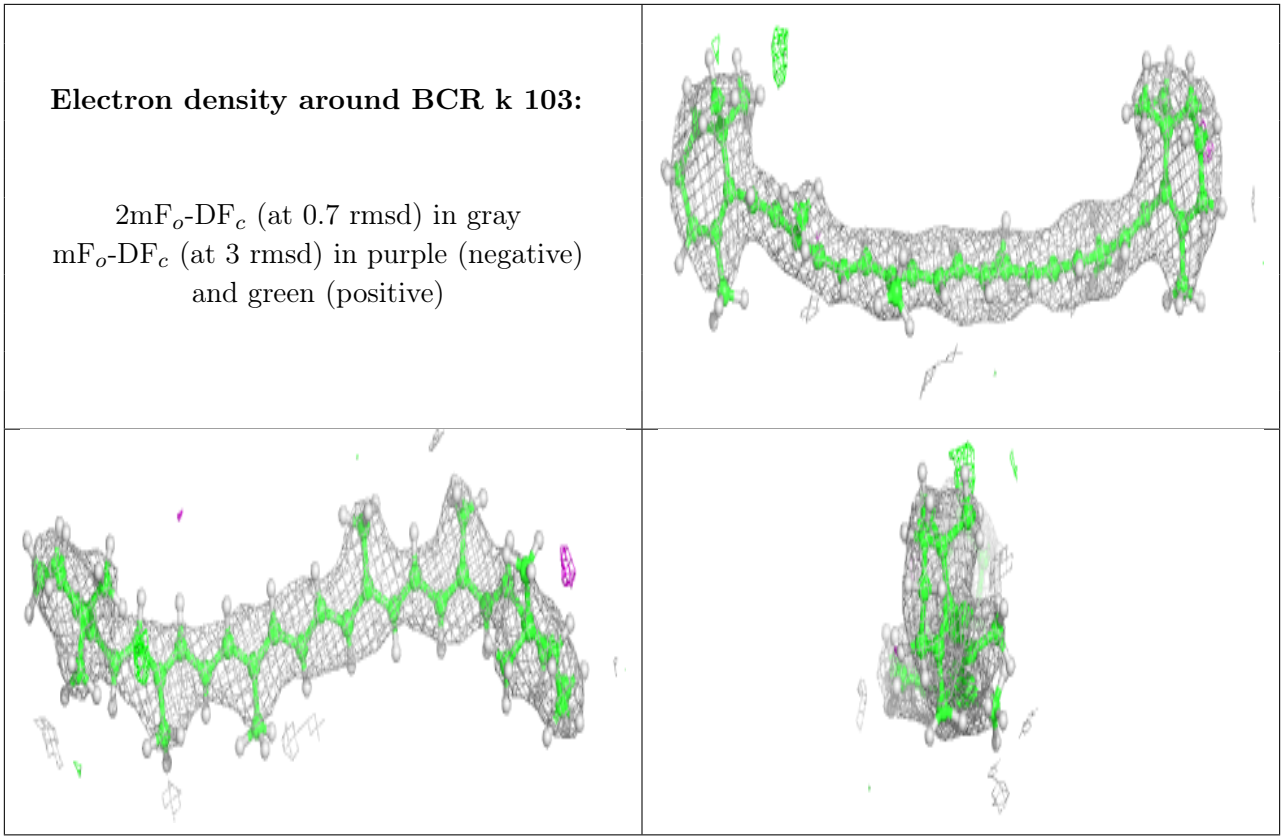






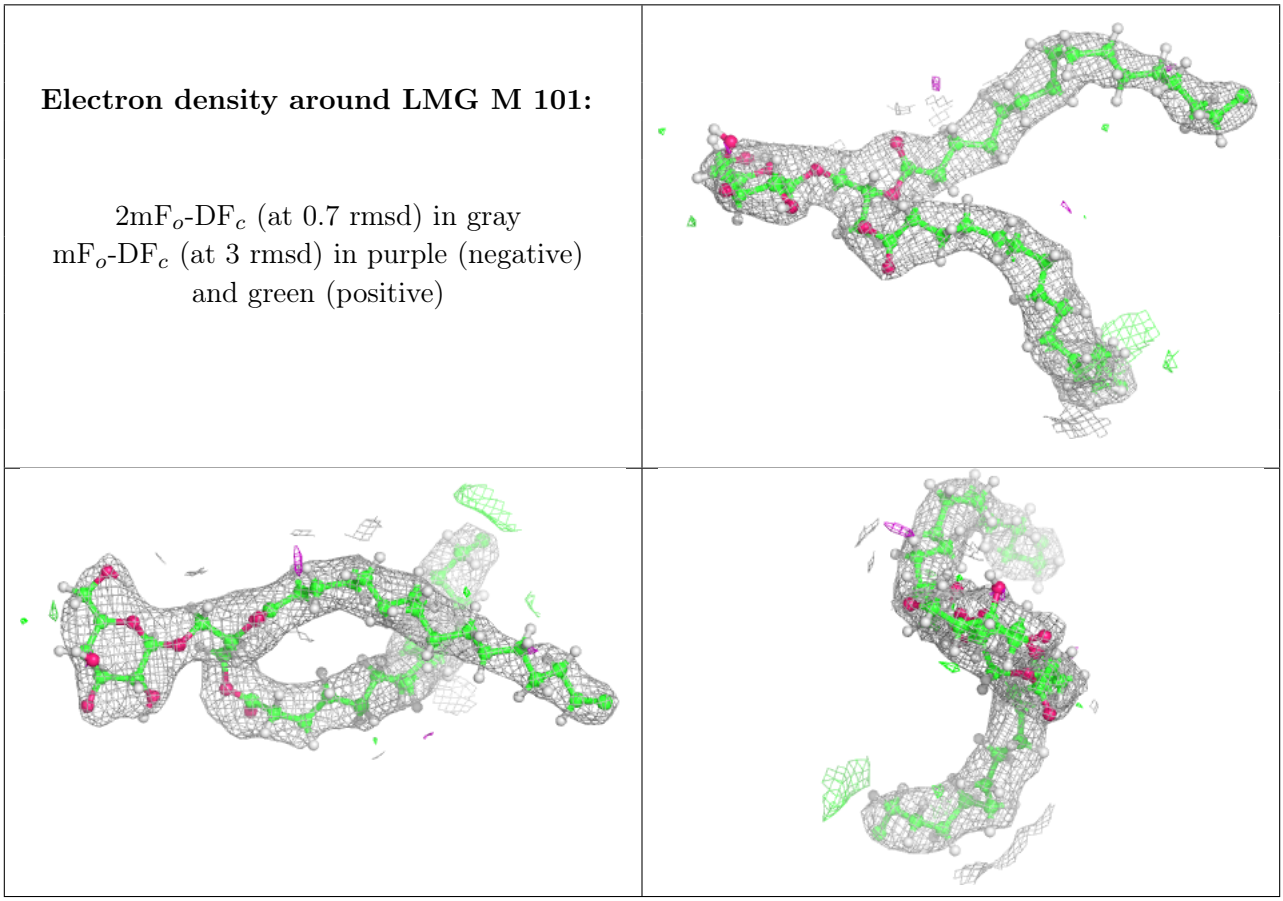
Electron density around BCR k 103:

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



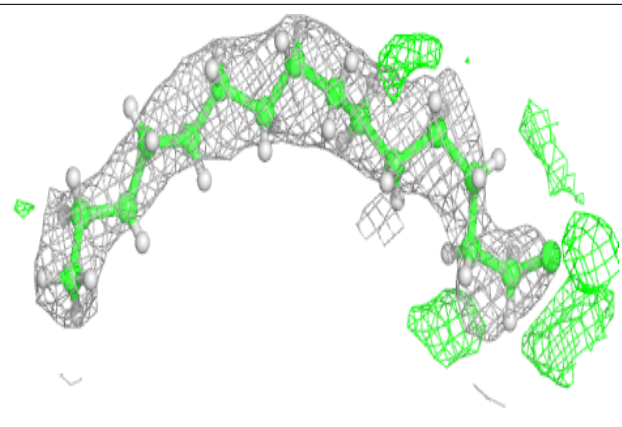
Electron density around LMG M 101:

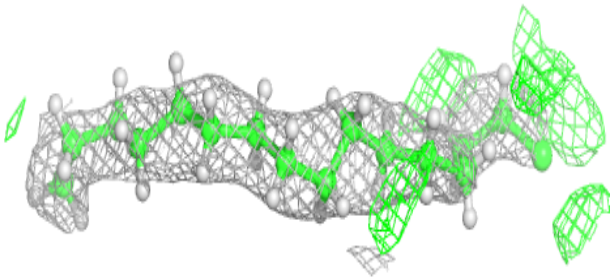
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

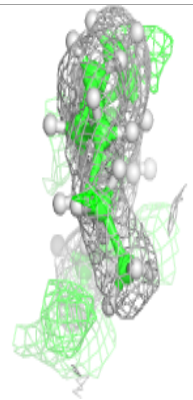


Electron density around STE b 620:

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

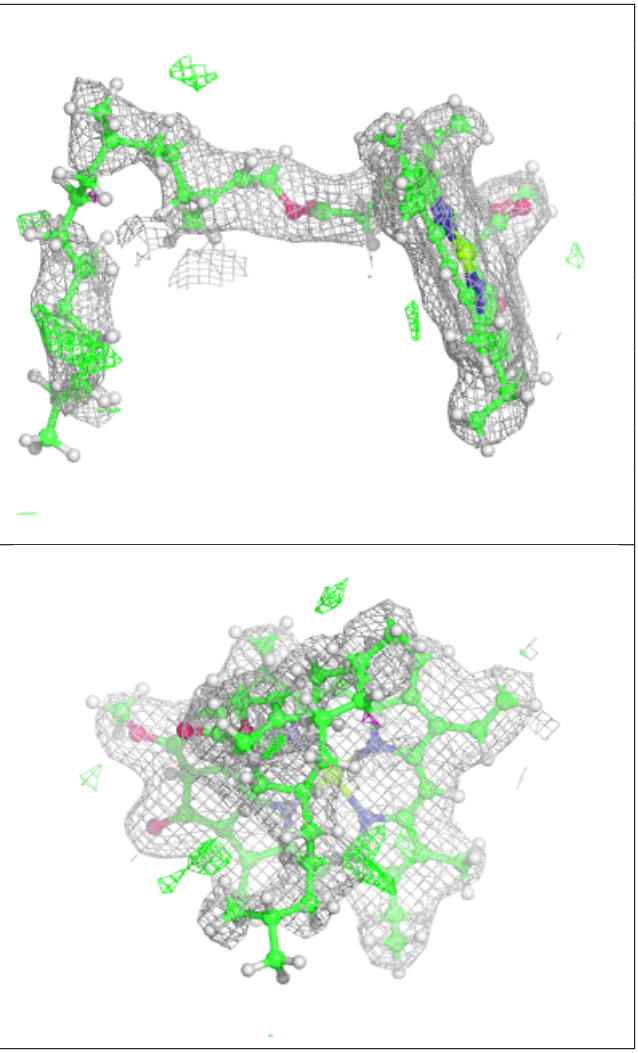






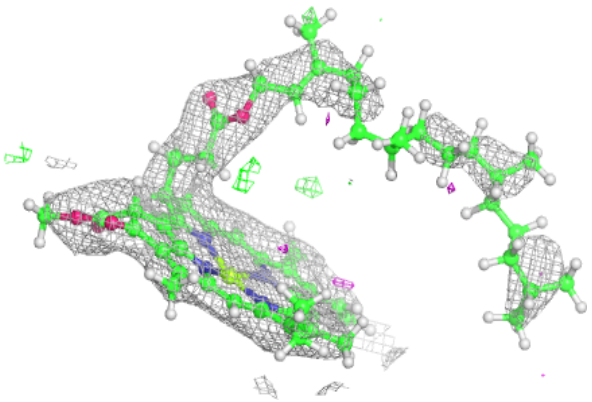
Electron density around CLA a 405:

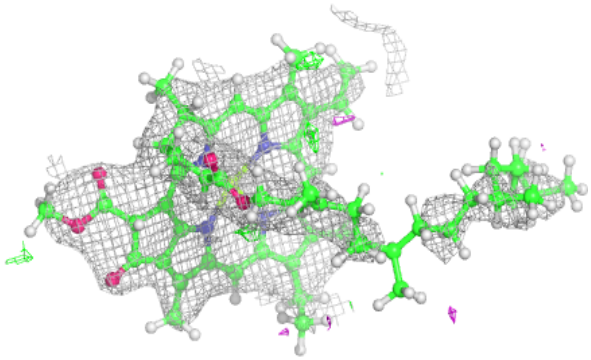
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

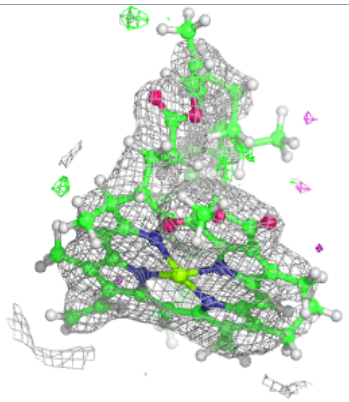


Electron density around CLA c 513:

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

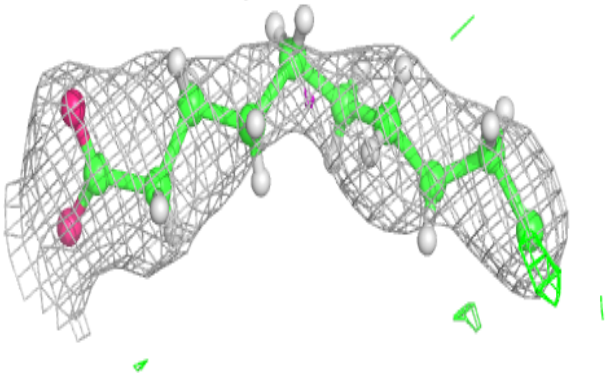


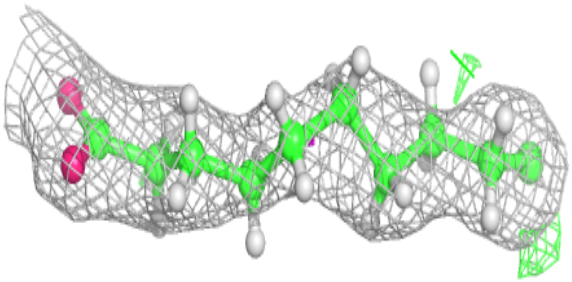


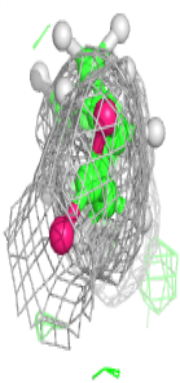


Electron density around STE C 520:

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

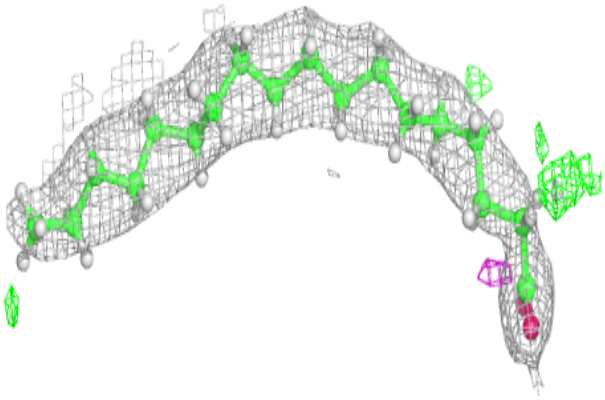


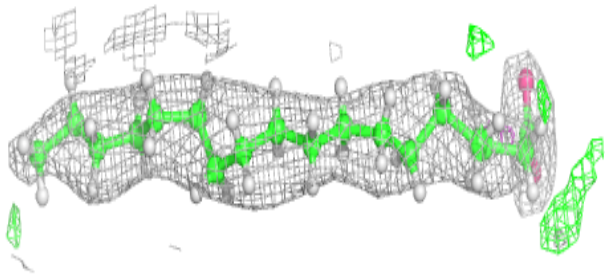


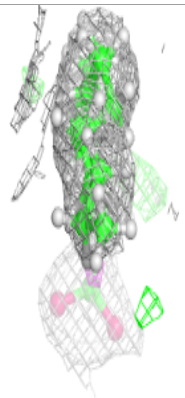


Electron density around STE D 411:

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

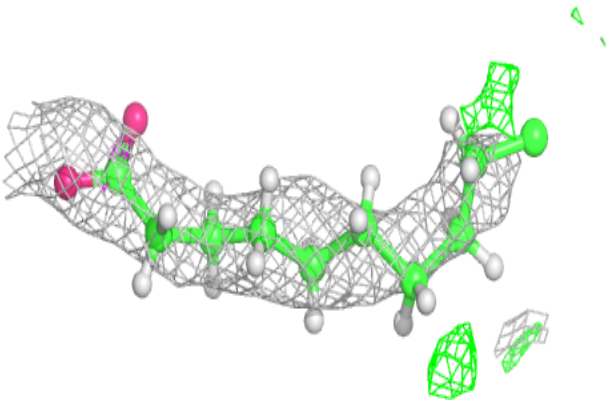


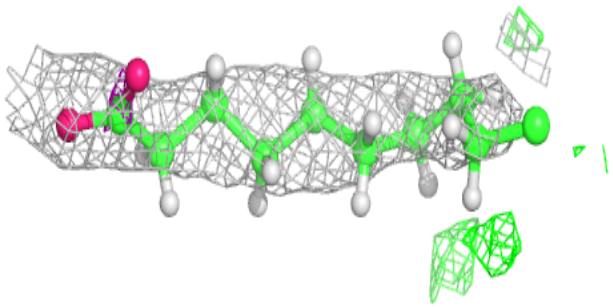


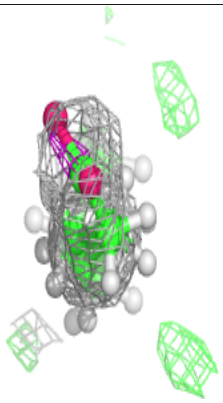


Electron density around STE L 103:

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

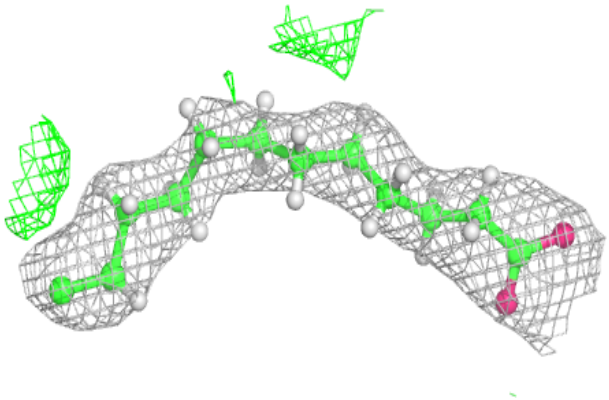


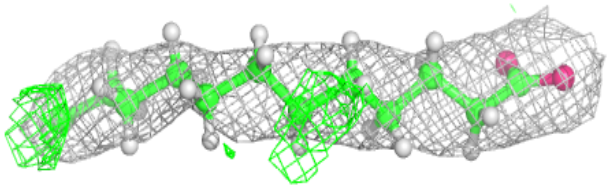


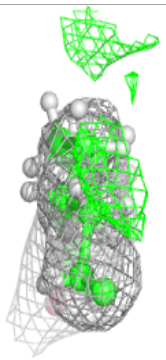


Electron density around STE t 102:

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

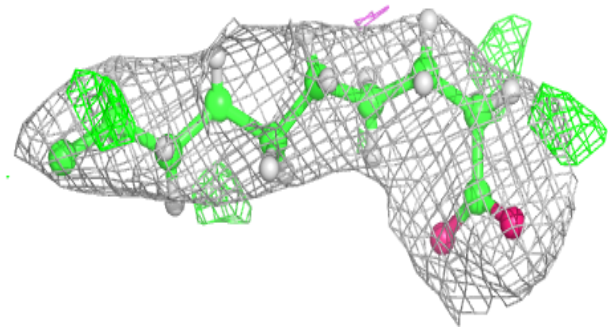


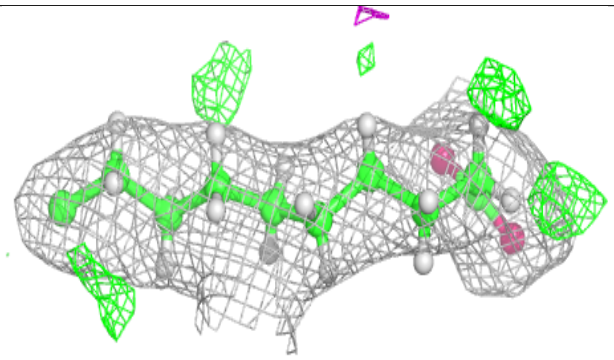


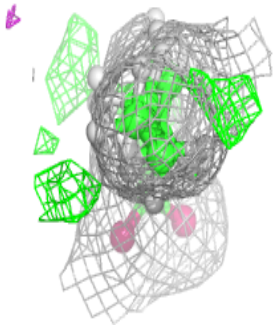


Electron density around STE B 624:

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

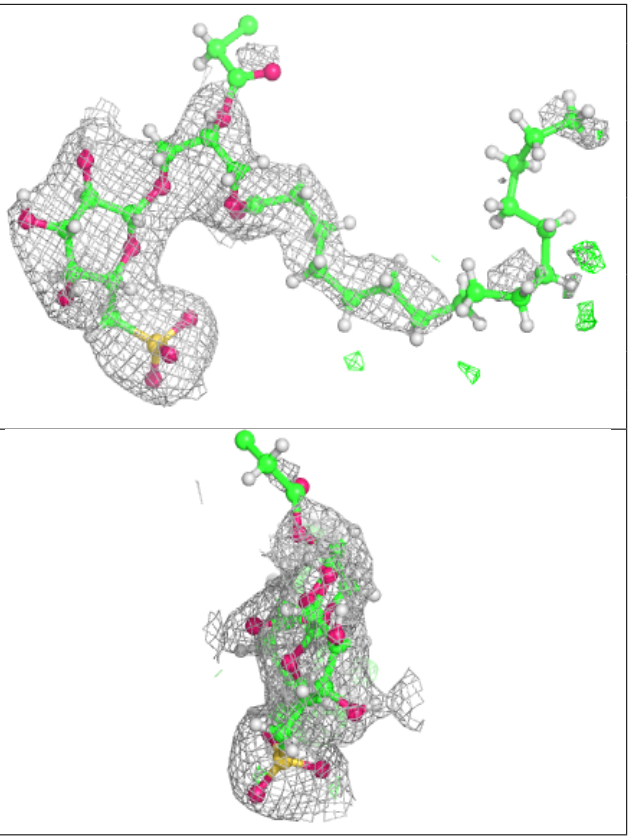


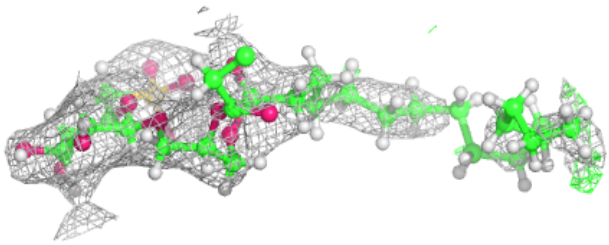




Electron density around SQD f 101:

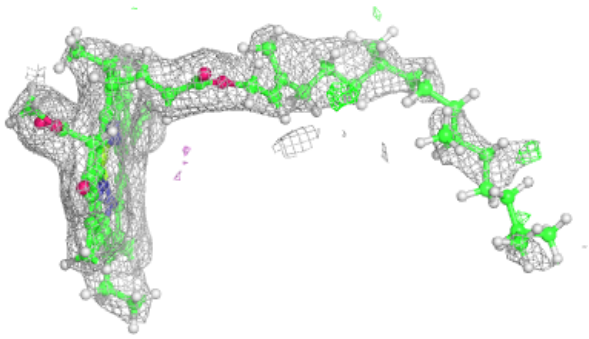
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

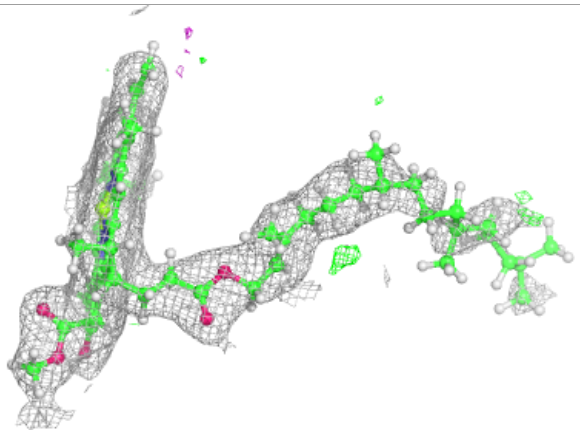


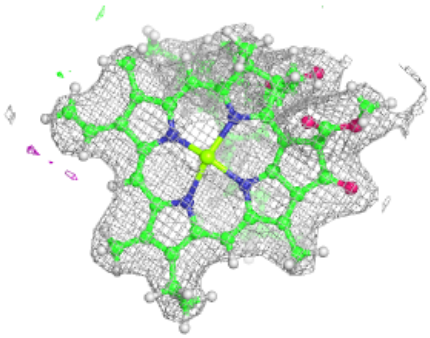


Electron density around CLA D 404:

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

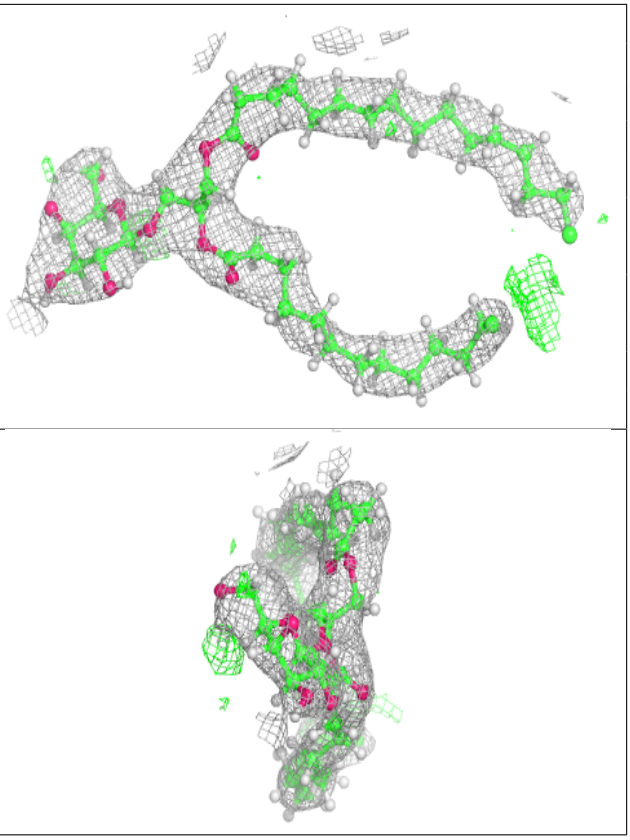


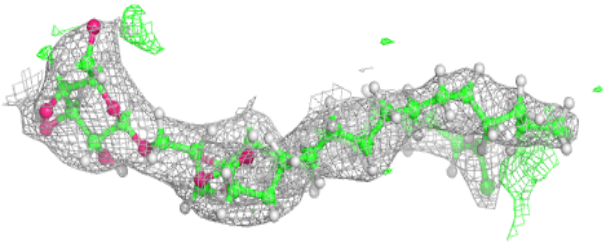




Electron density around LMG C 516:

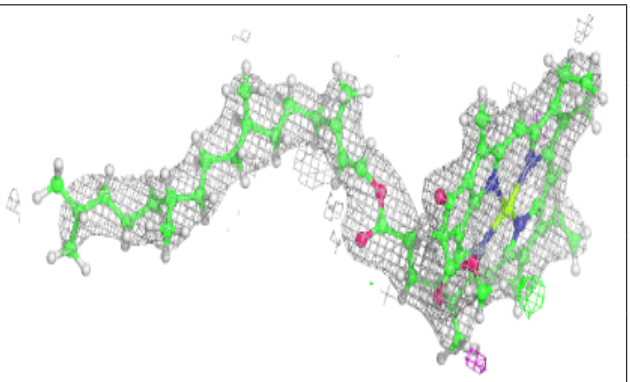
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

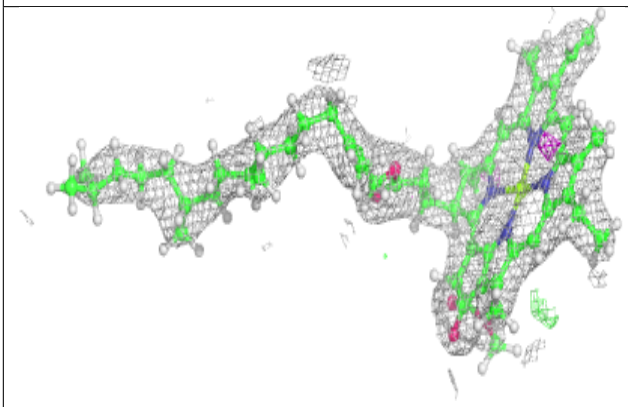


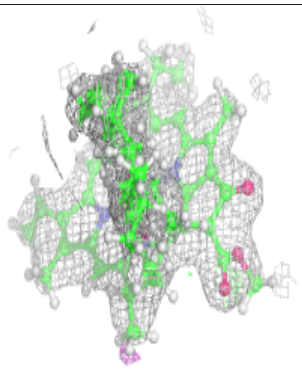


Electron density around CLA C 503:

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

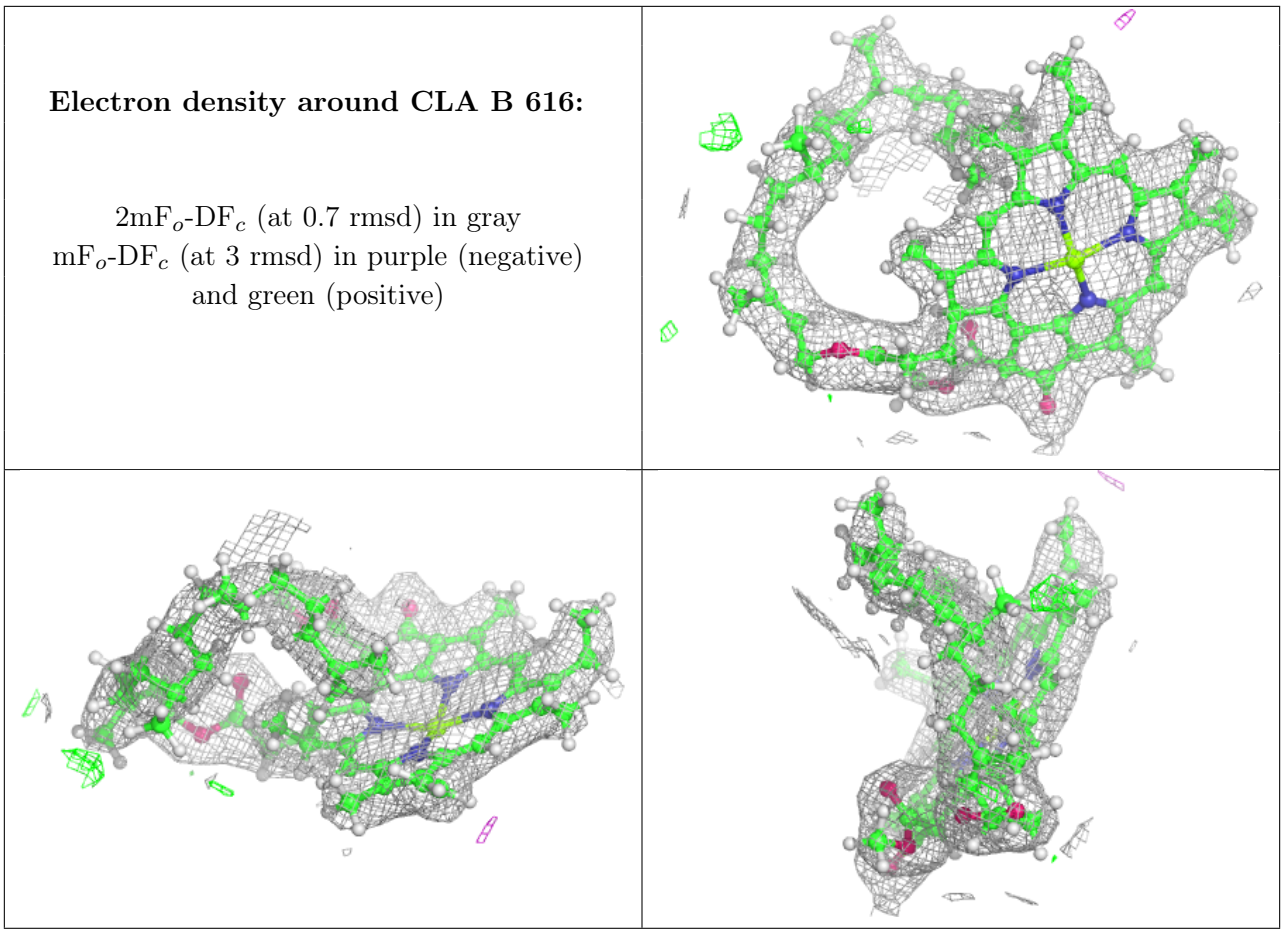






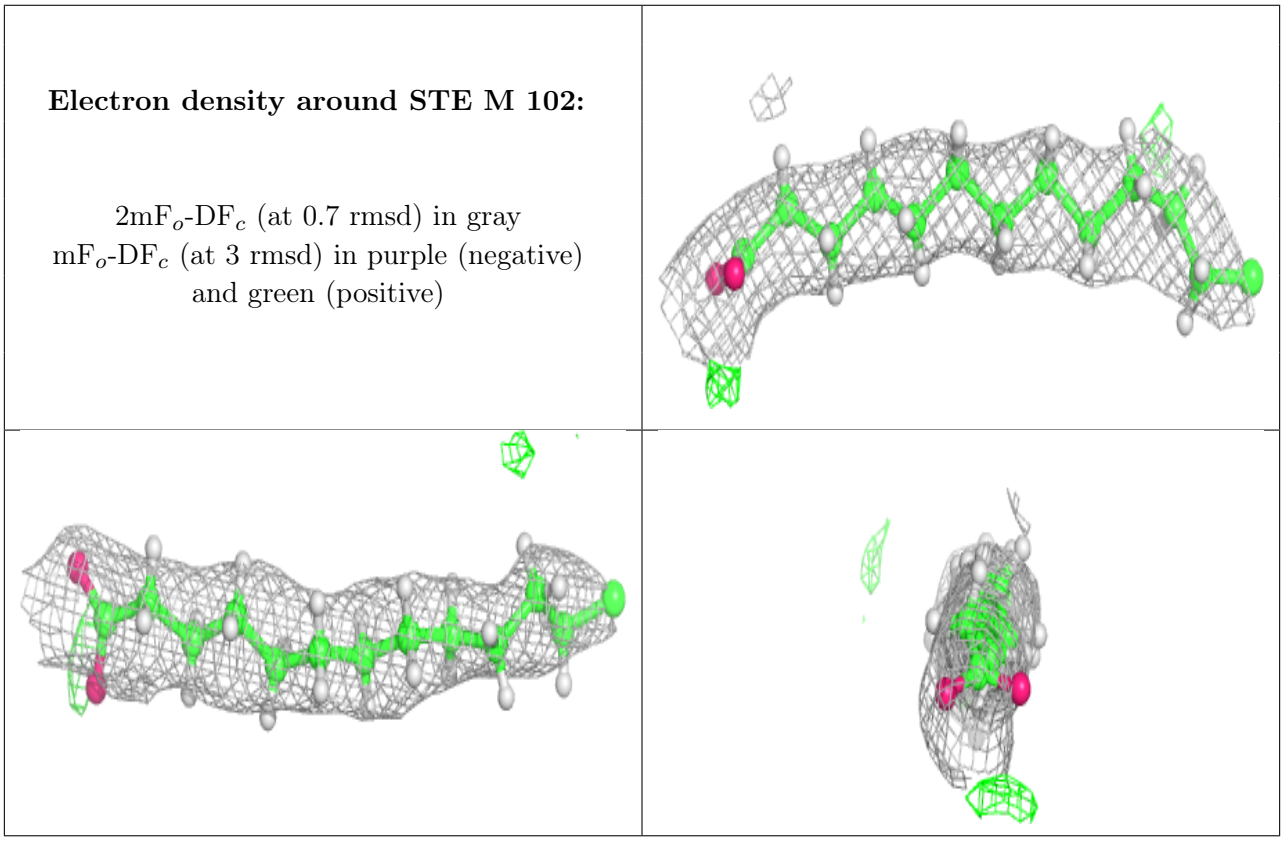
Electron density around CLA B 616:

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



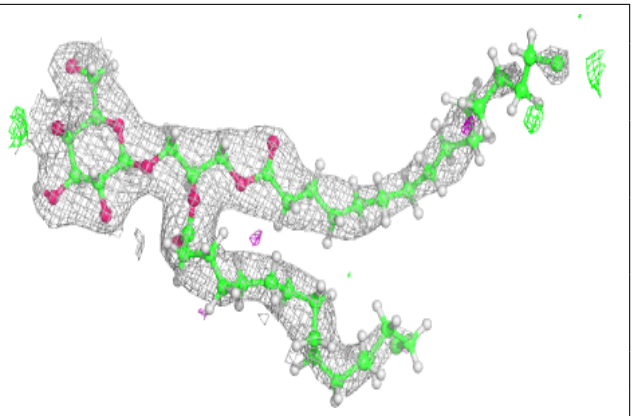
Electron density around STE M 102:

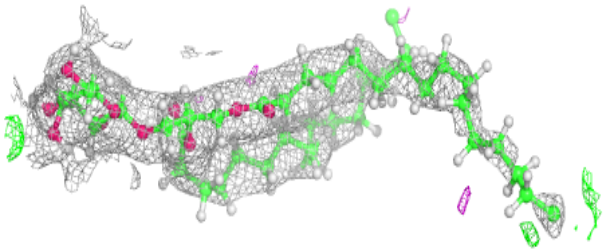
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

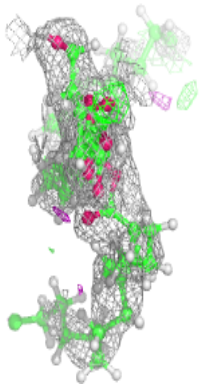


Electron density around LMG D 407:

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

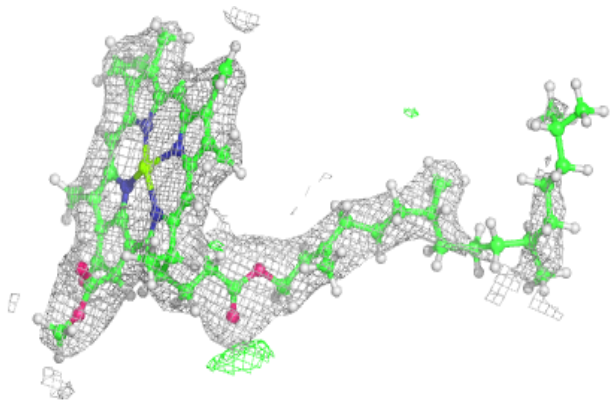


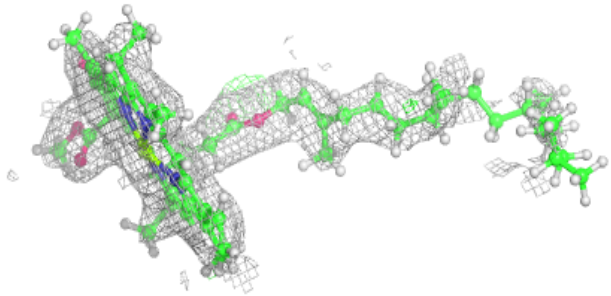


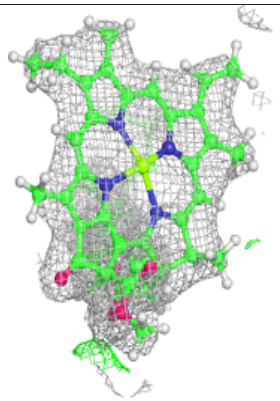


Electron density around CLA d 404:

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

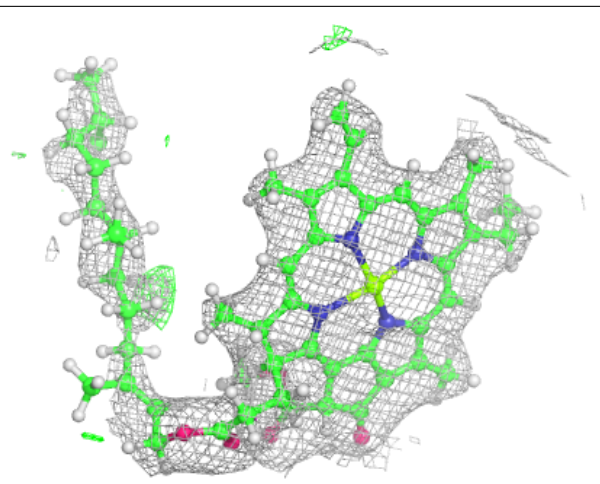


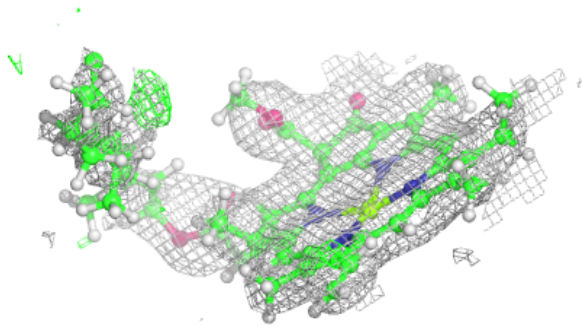


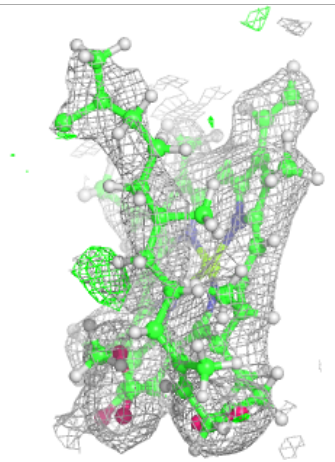


Electron density around CLA b 616:

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

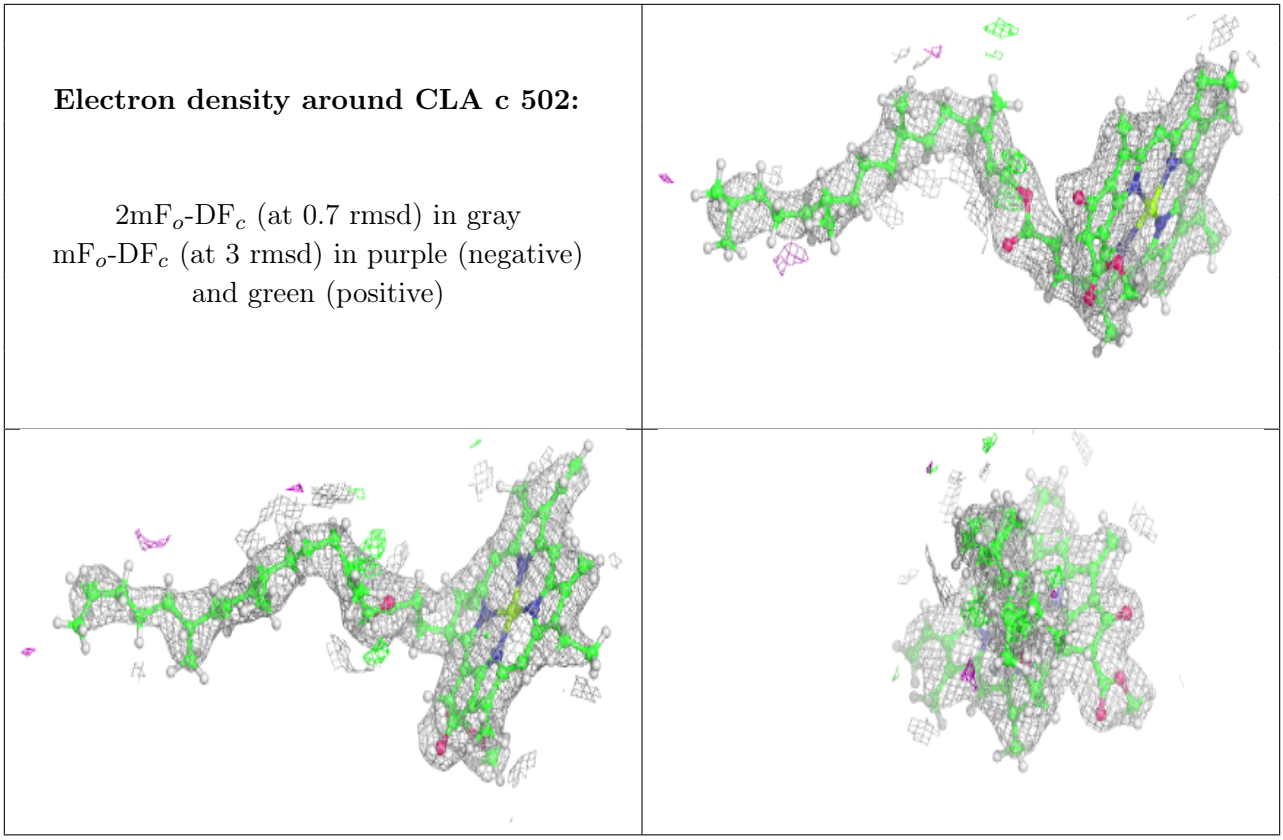






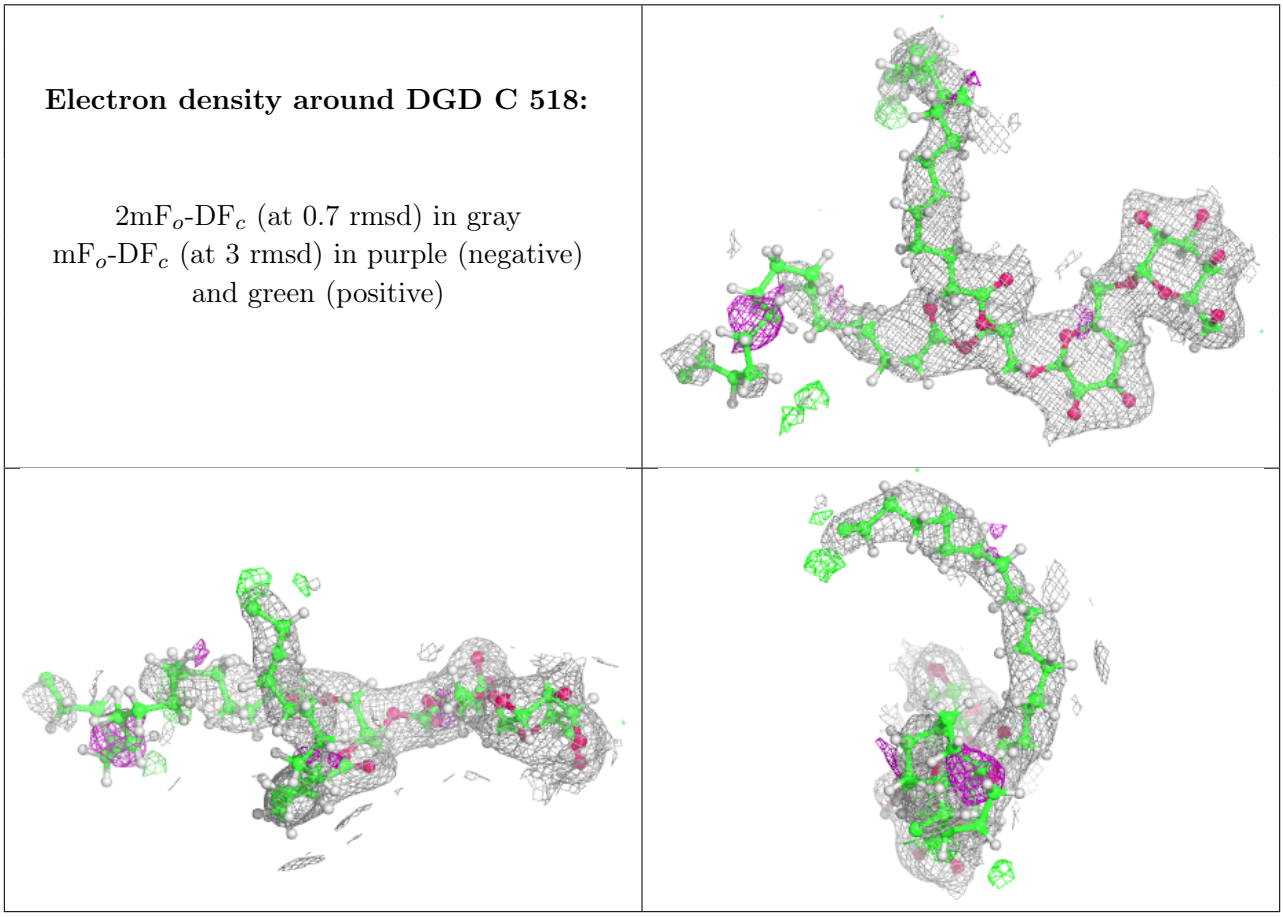
Electron density around CLA c 502:

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



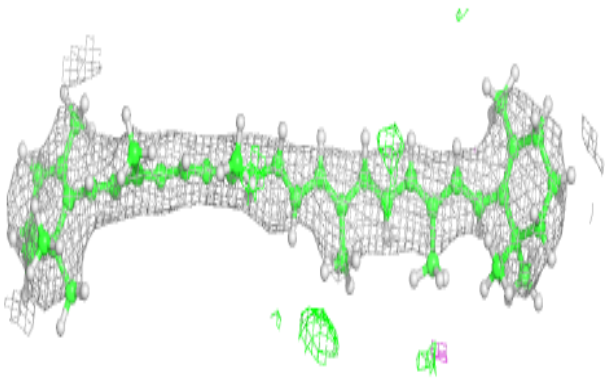
Electron density around DGD C 518:

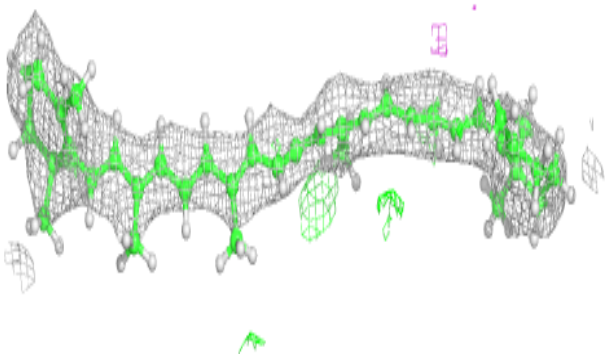
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

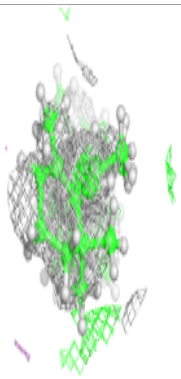


Electron density around BCR Z 101:

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

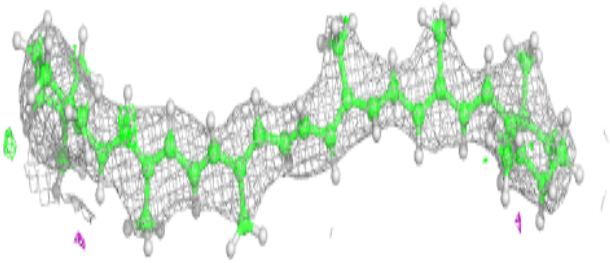


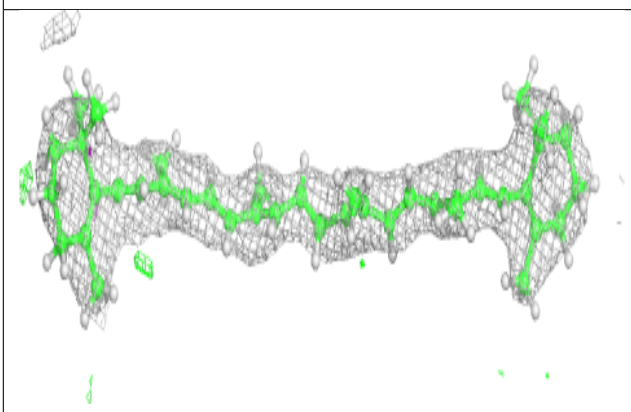


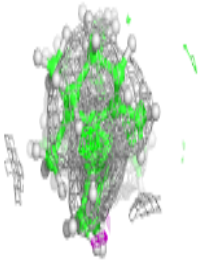


Electron density around BCR c 514:

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

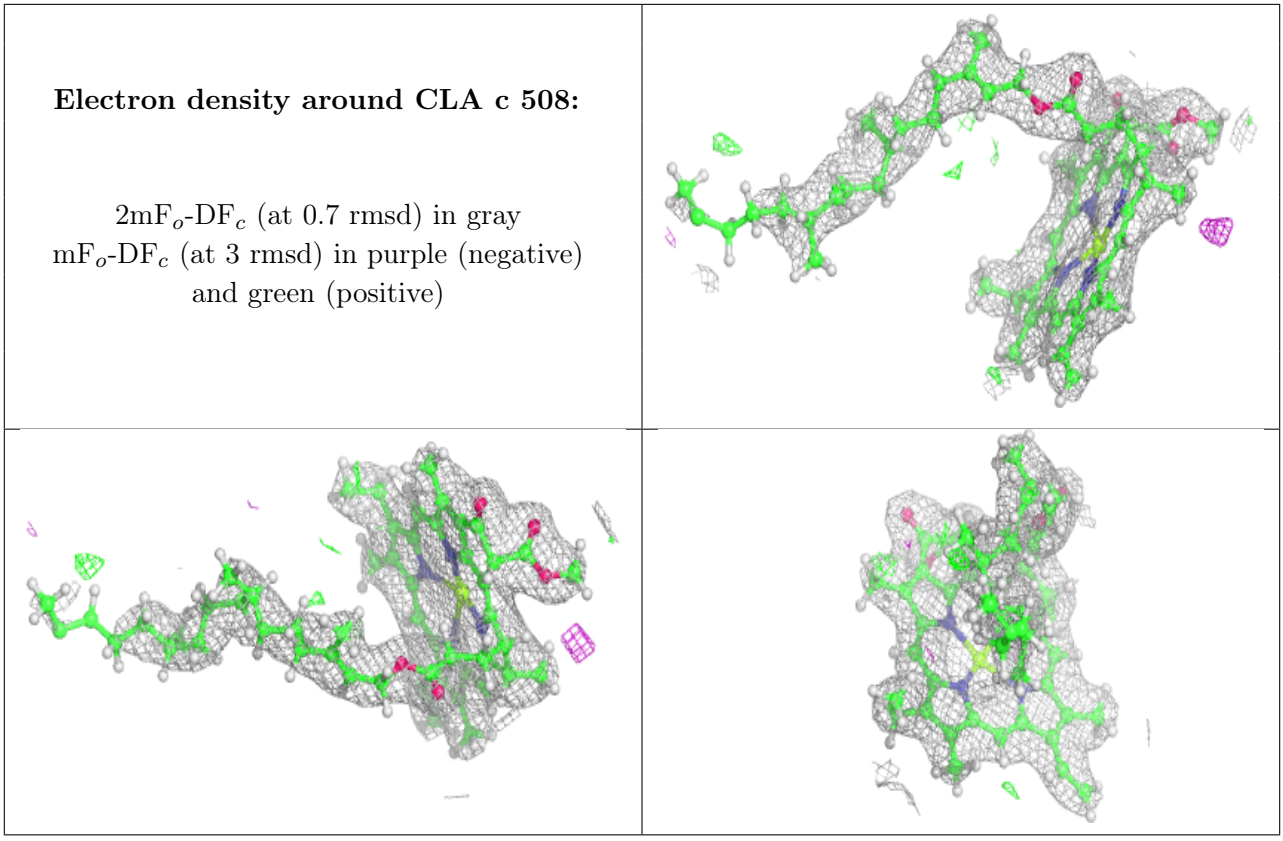






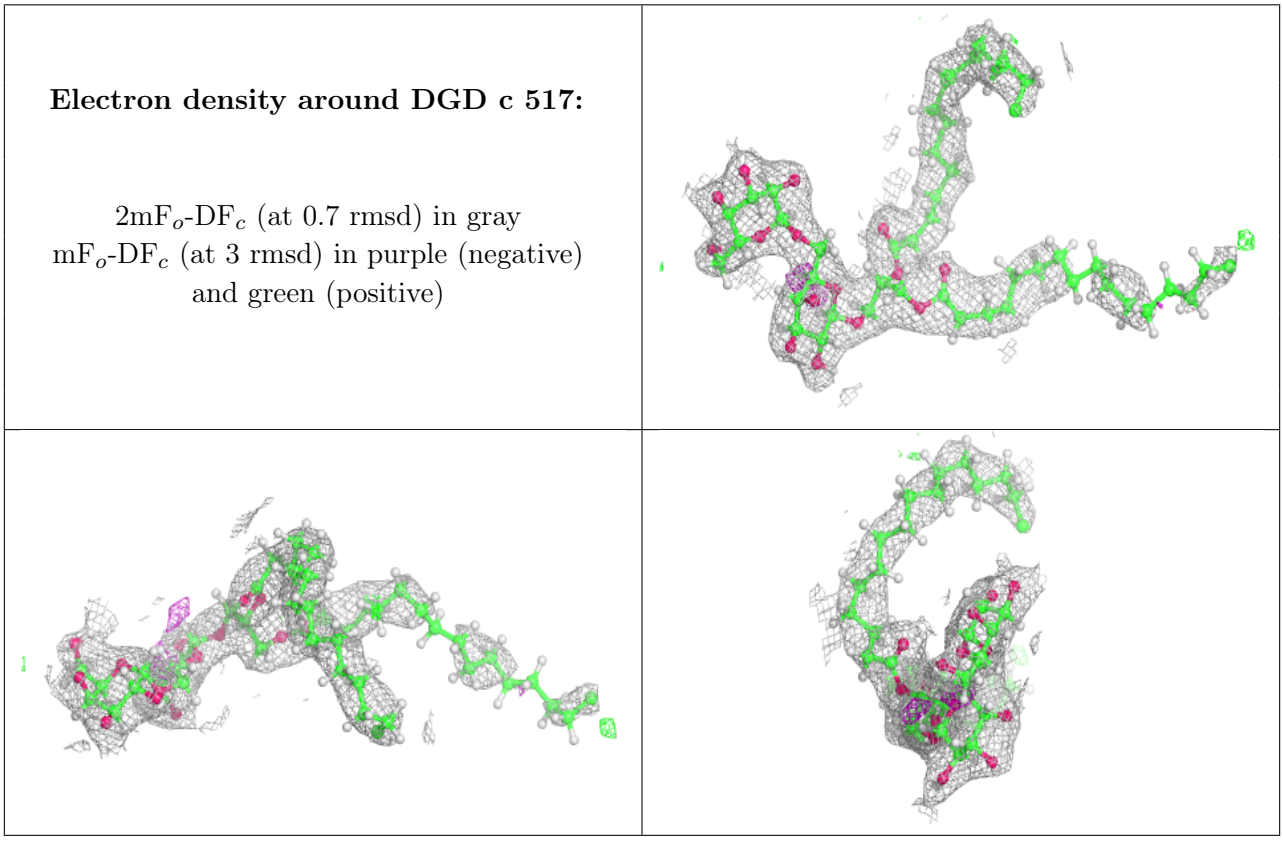
Electron density around CLA c 508:

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



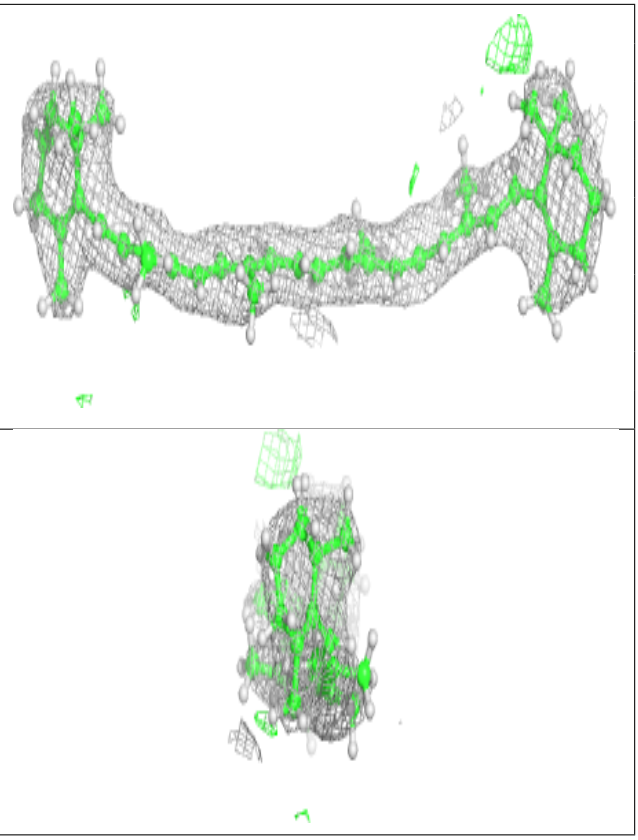
Electron density around DGD c 517:

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



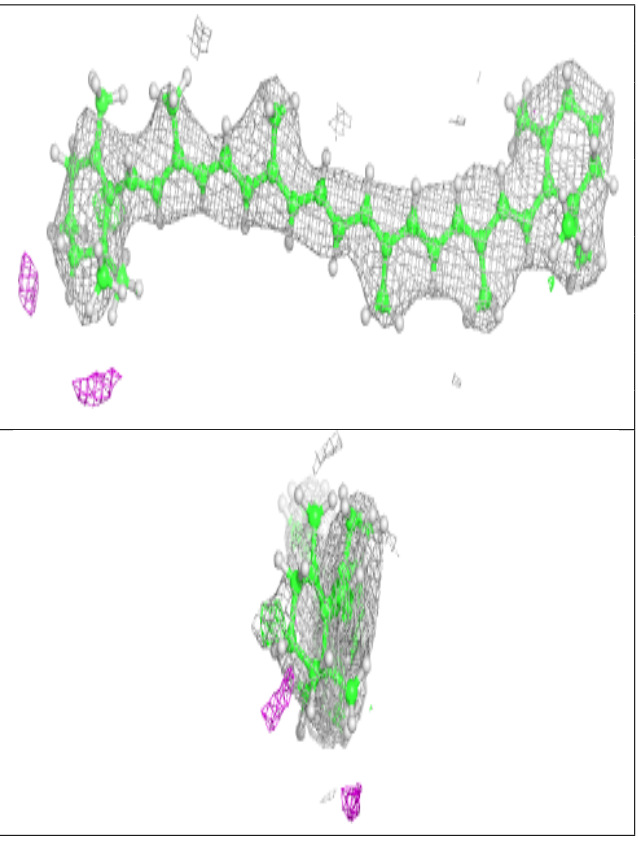
Electron density around BCR C 501:

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



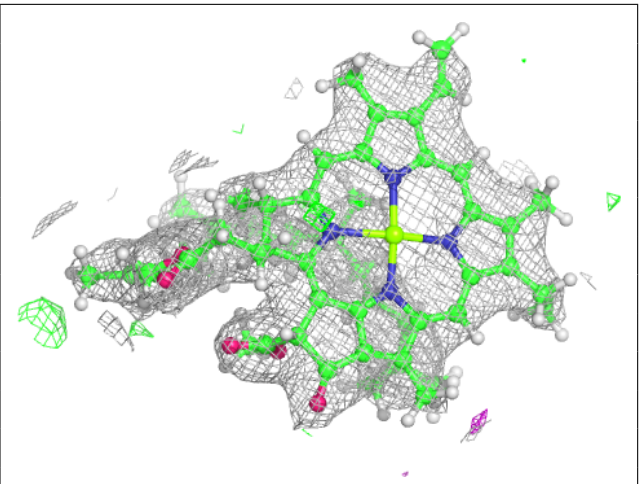
Electron density around BCR D 405:

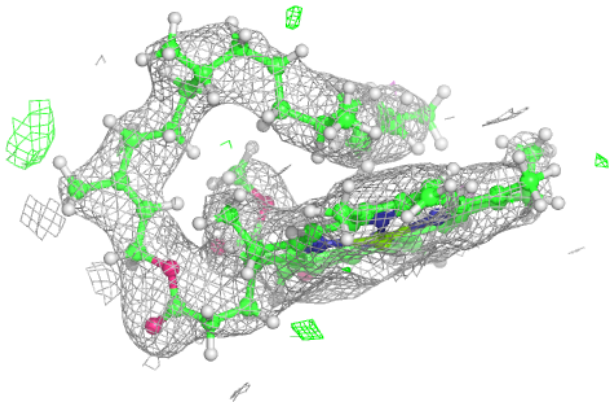
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

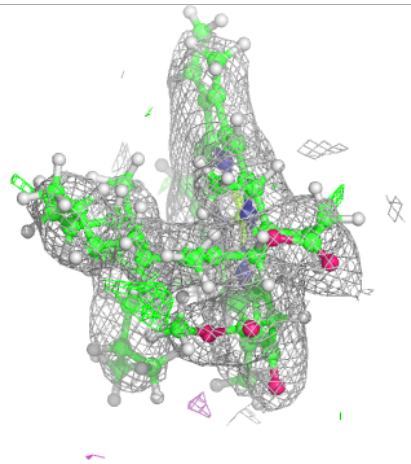


Electron density around CLA c 510:

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

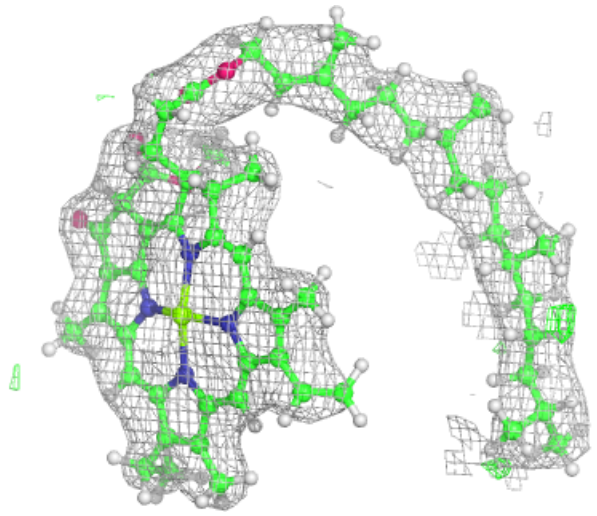


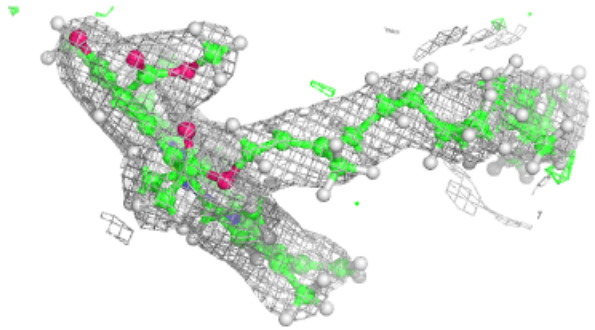


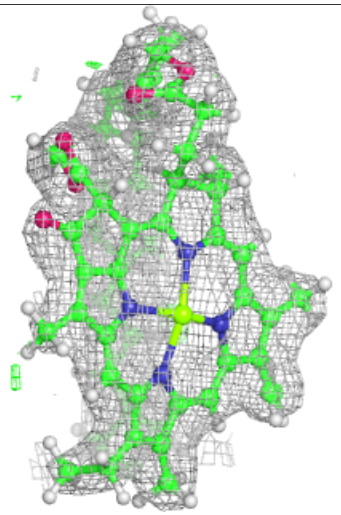


Electron density around CLA C 508:

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

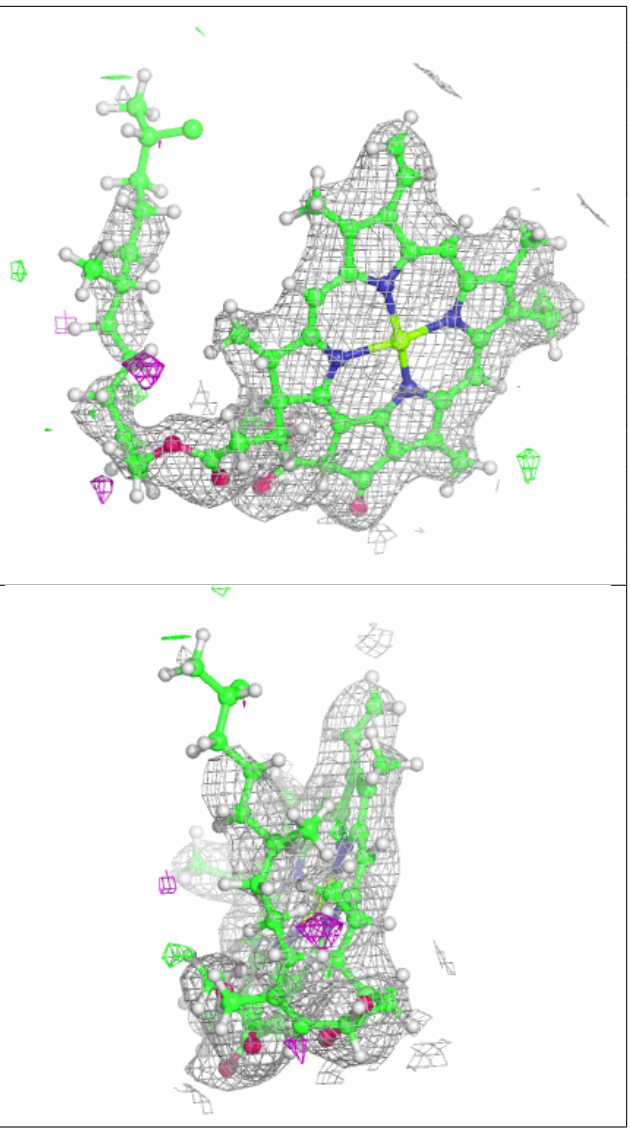






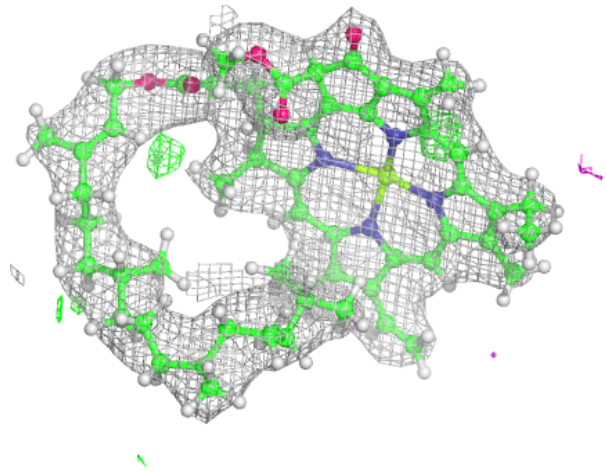
Electron density around CLA B 617:

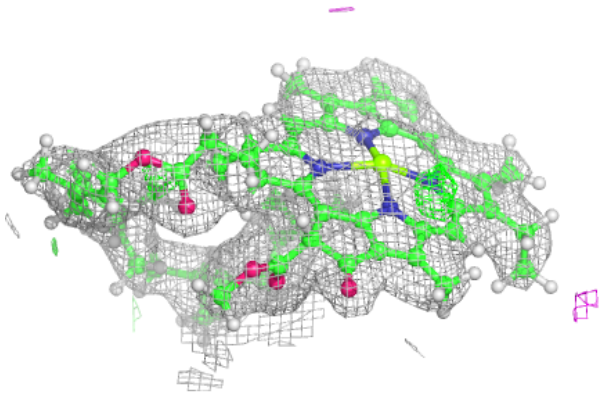
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

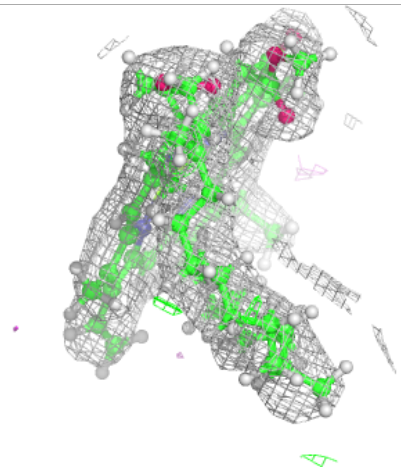


Electron density around CLA b 615:

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

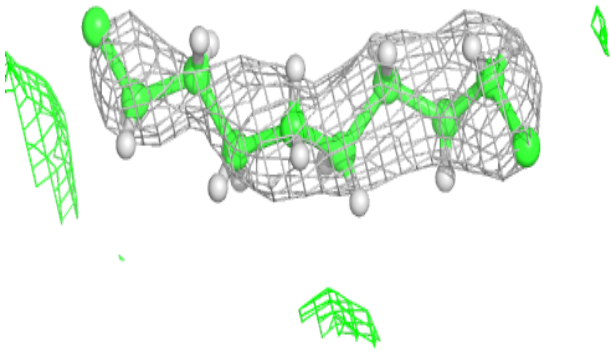


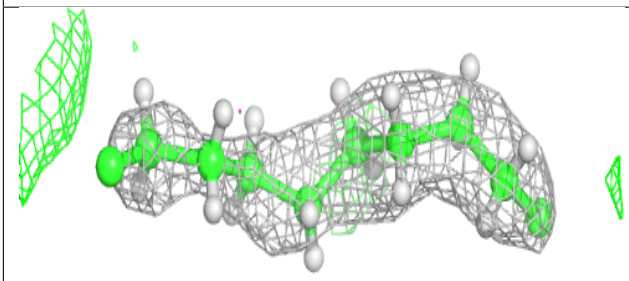


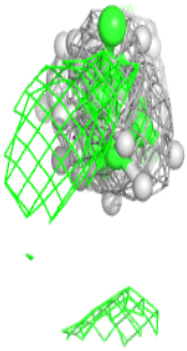


Electron density around STE t 103:

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

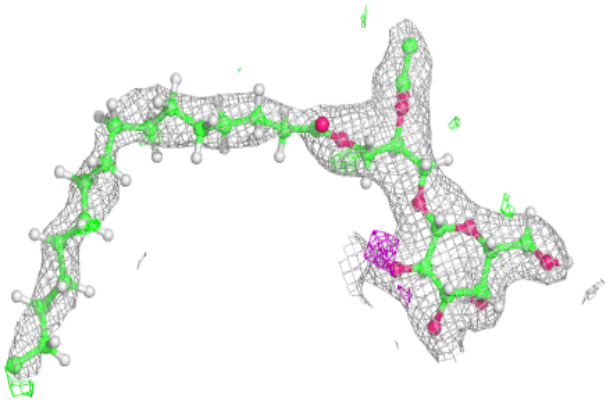


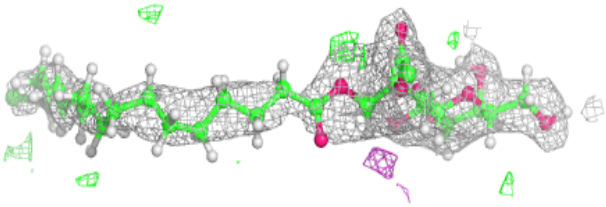


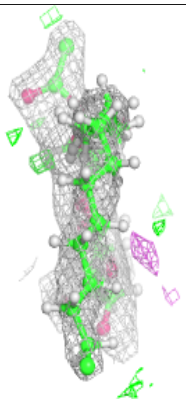


Electron density around LMG c 519:

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

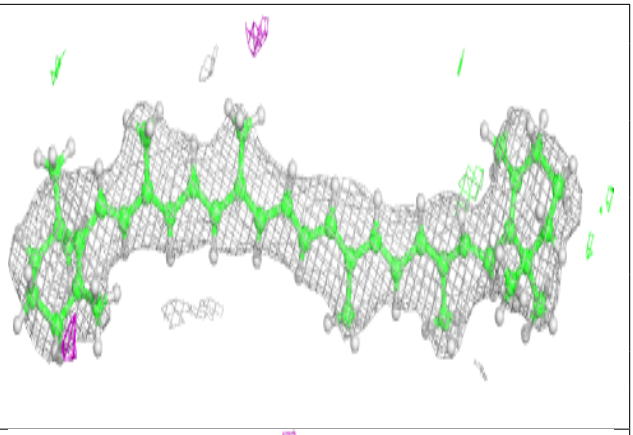


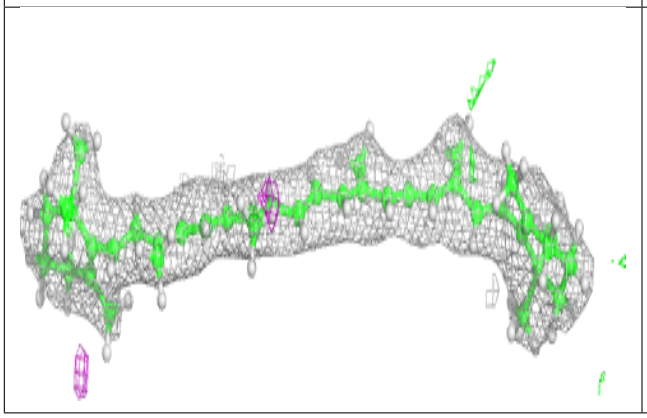


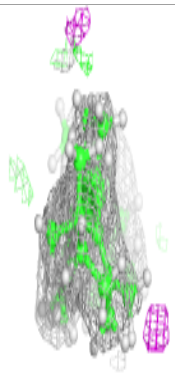


Electron density around BCR B 620:

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

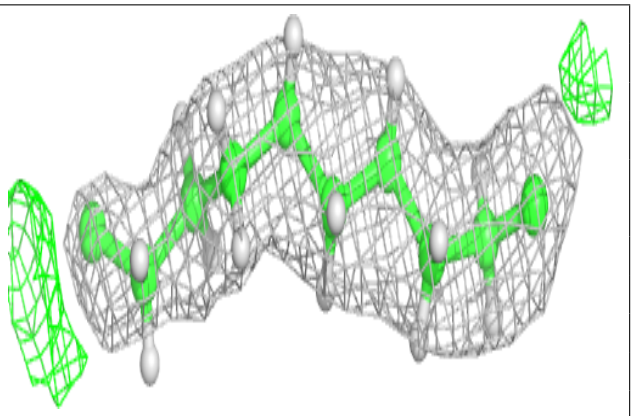


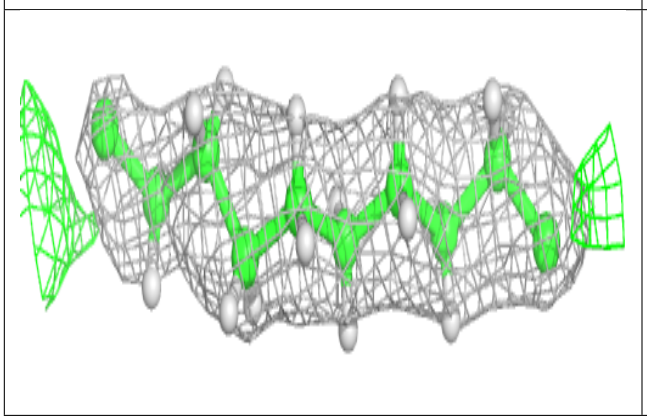


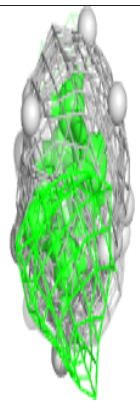


Electron density around STE M 103:

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

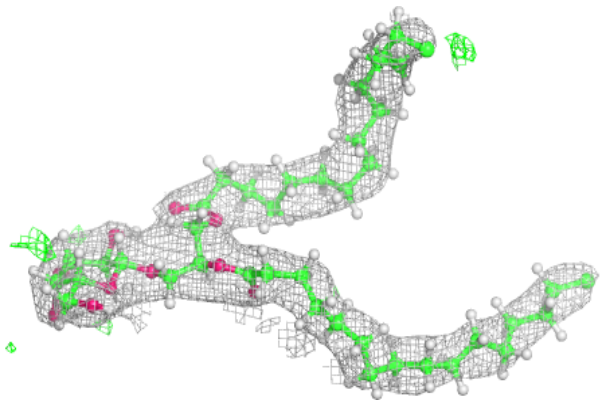


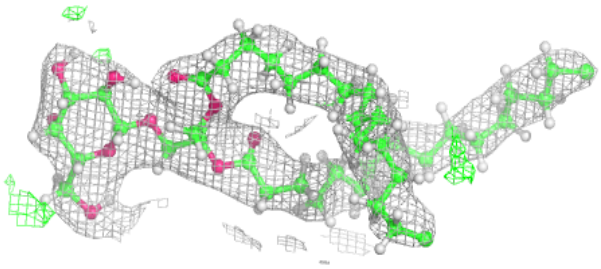


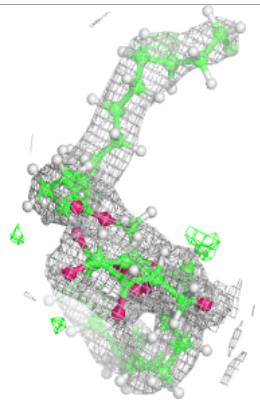


Electron density around LMG m 101:

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

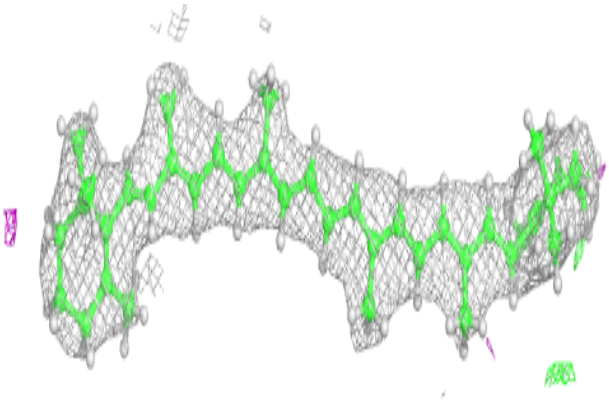


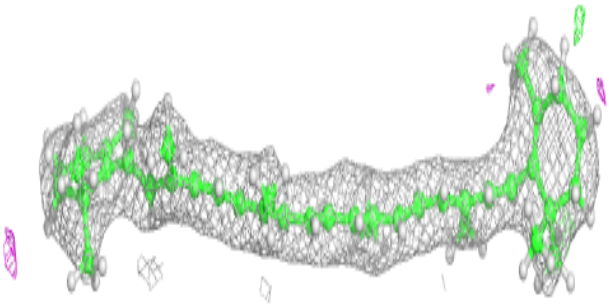


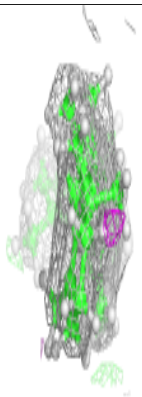


Electron density around BCR b 617:

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

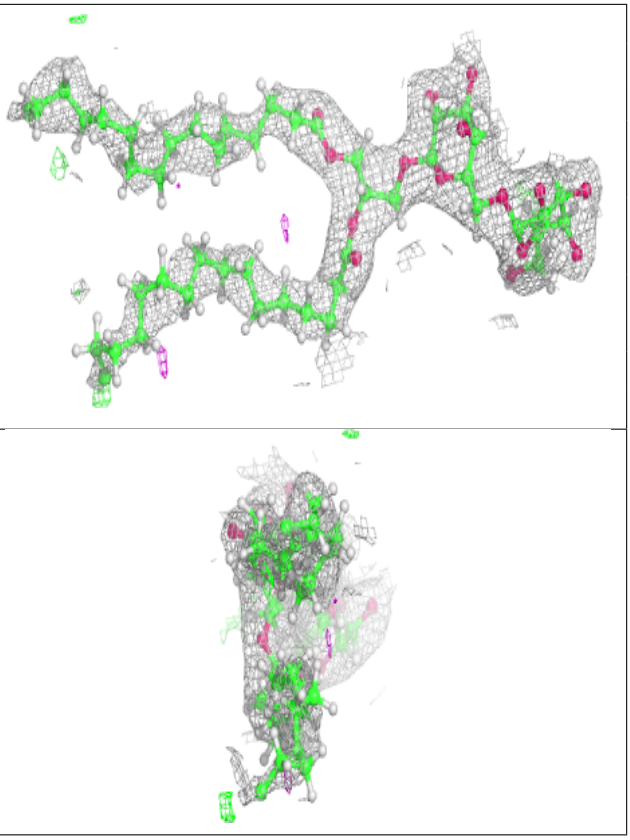






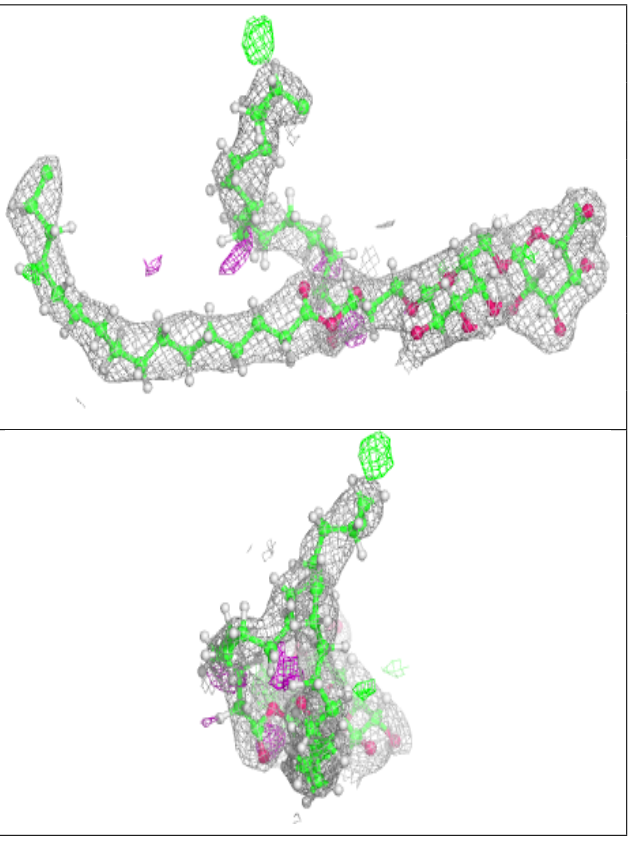
Electron density around DGD c 518:

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



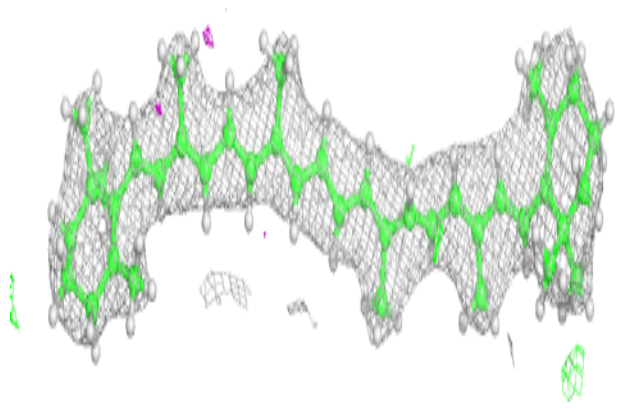
Electron density around DGD h 101:

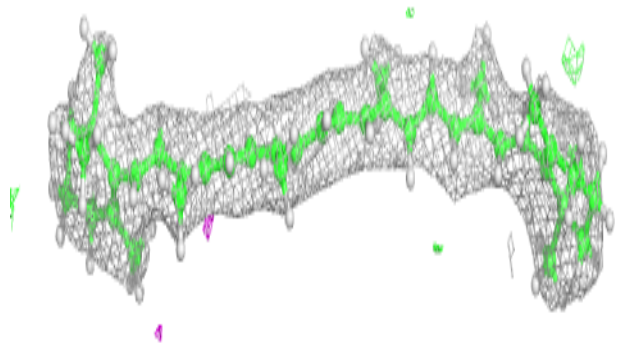
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

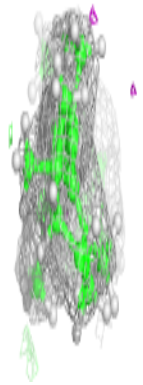


Electron density around BCR b 619:

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

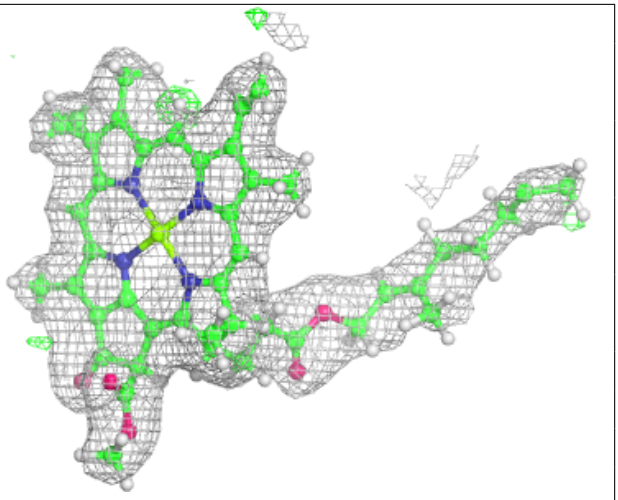


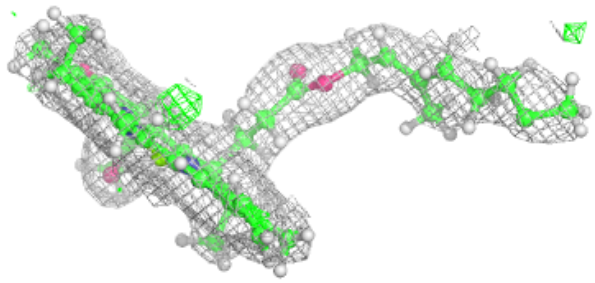


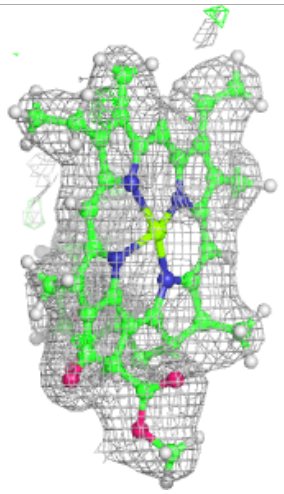


Electron density around CLA A 405:

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

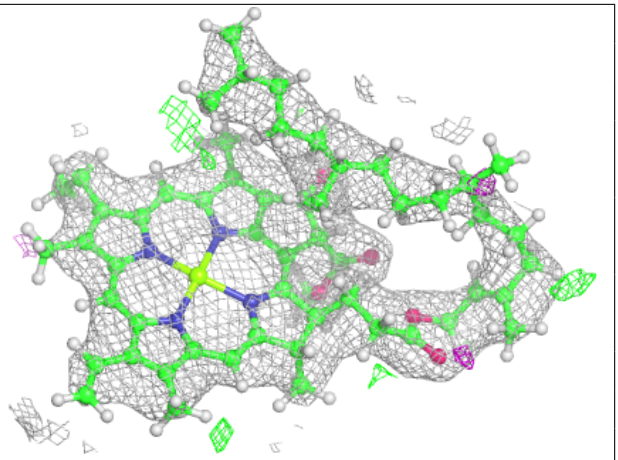


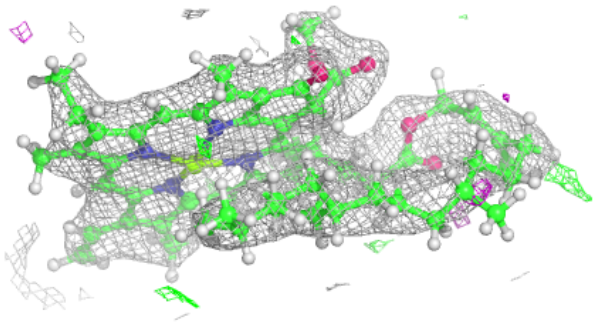


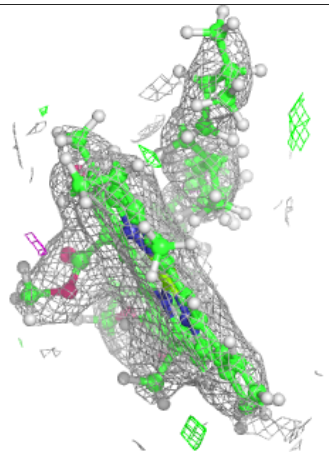


Electron density around CLA c 509:

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

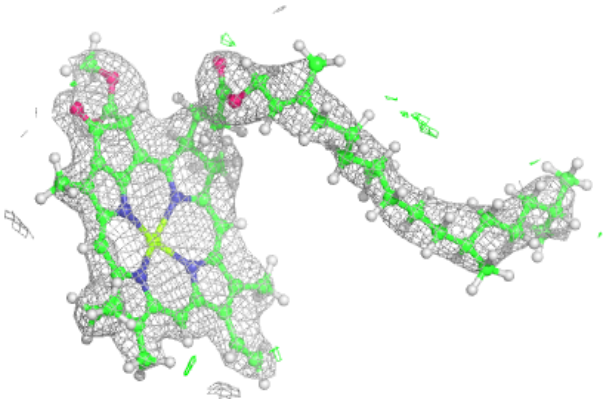


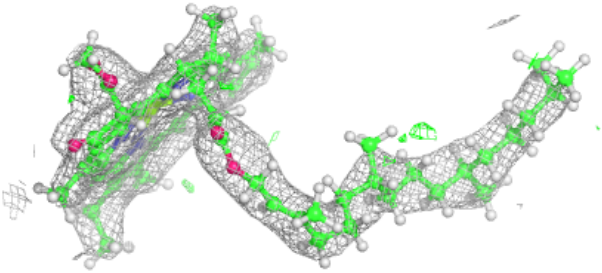


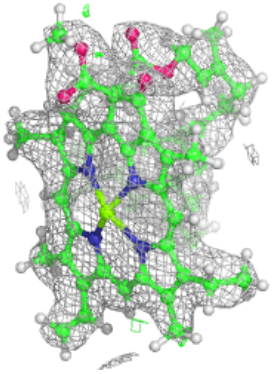


Electron density around CLA C 512:

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

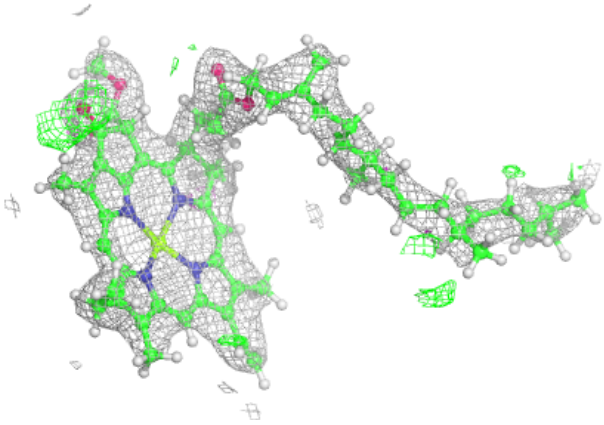


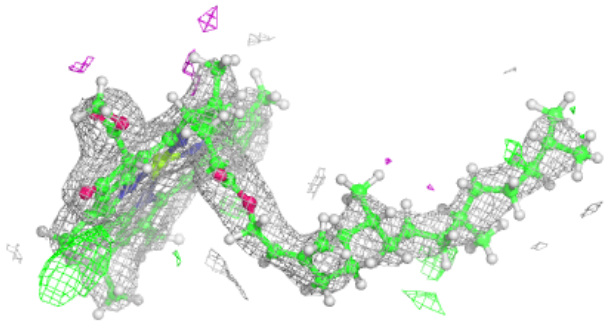


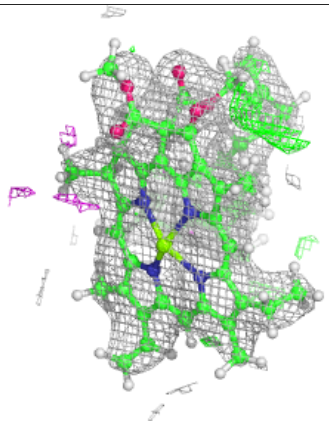


Electron density around CLA c 511:

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

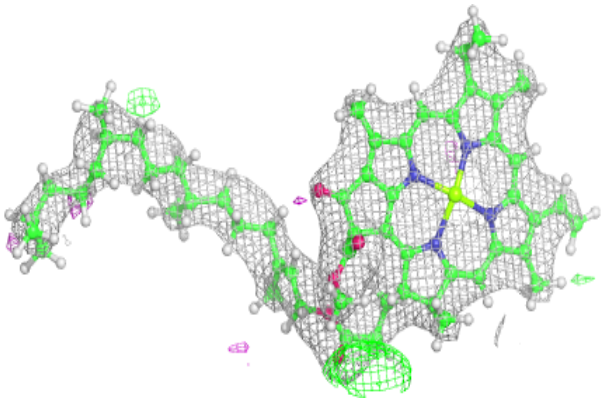


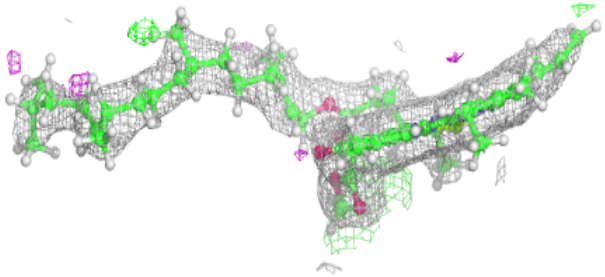


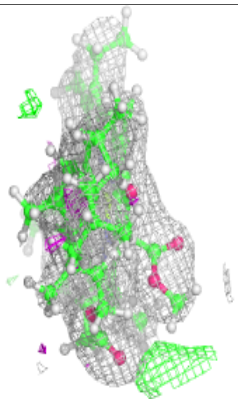


Electron density around CLA b 602:

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

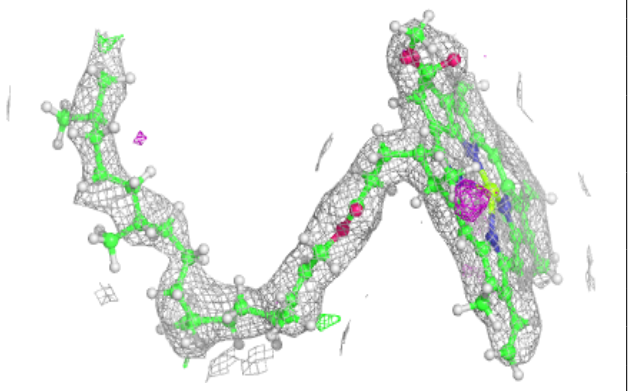


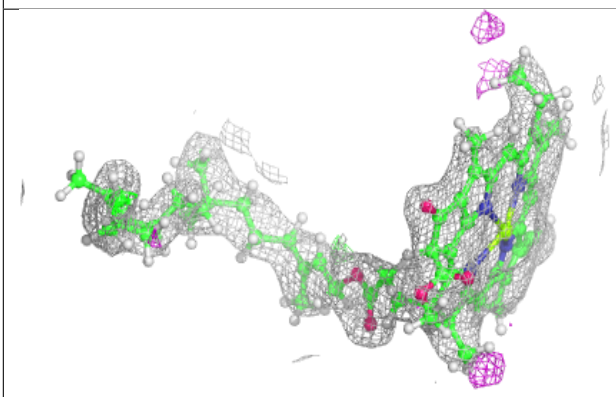


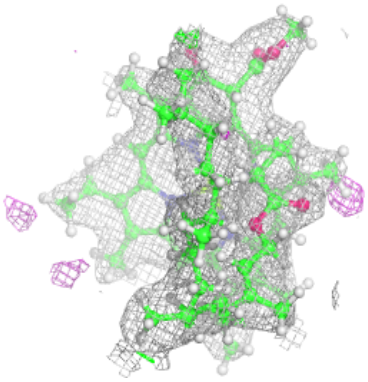


Electron density around CLA b 606:

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

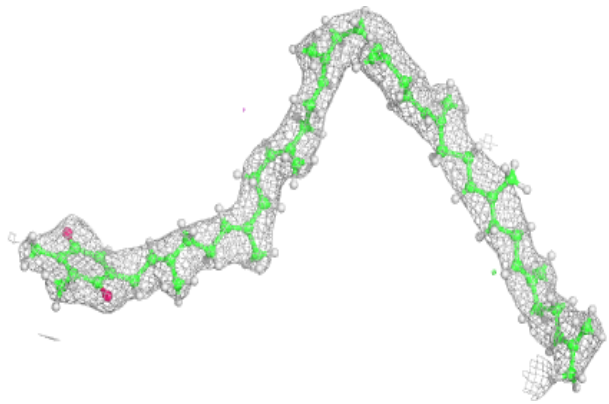


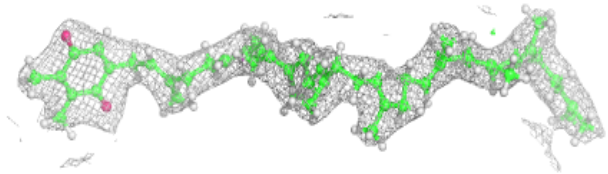


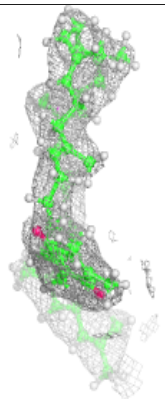


Electron density around PL9 D 406:

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

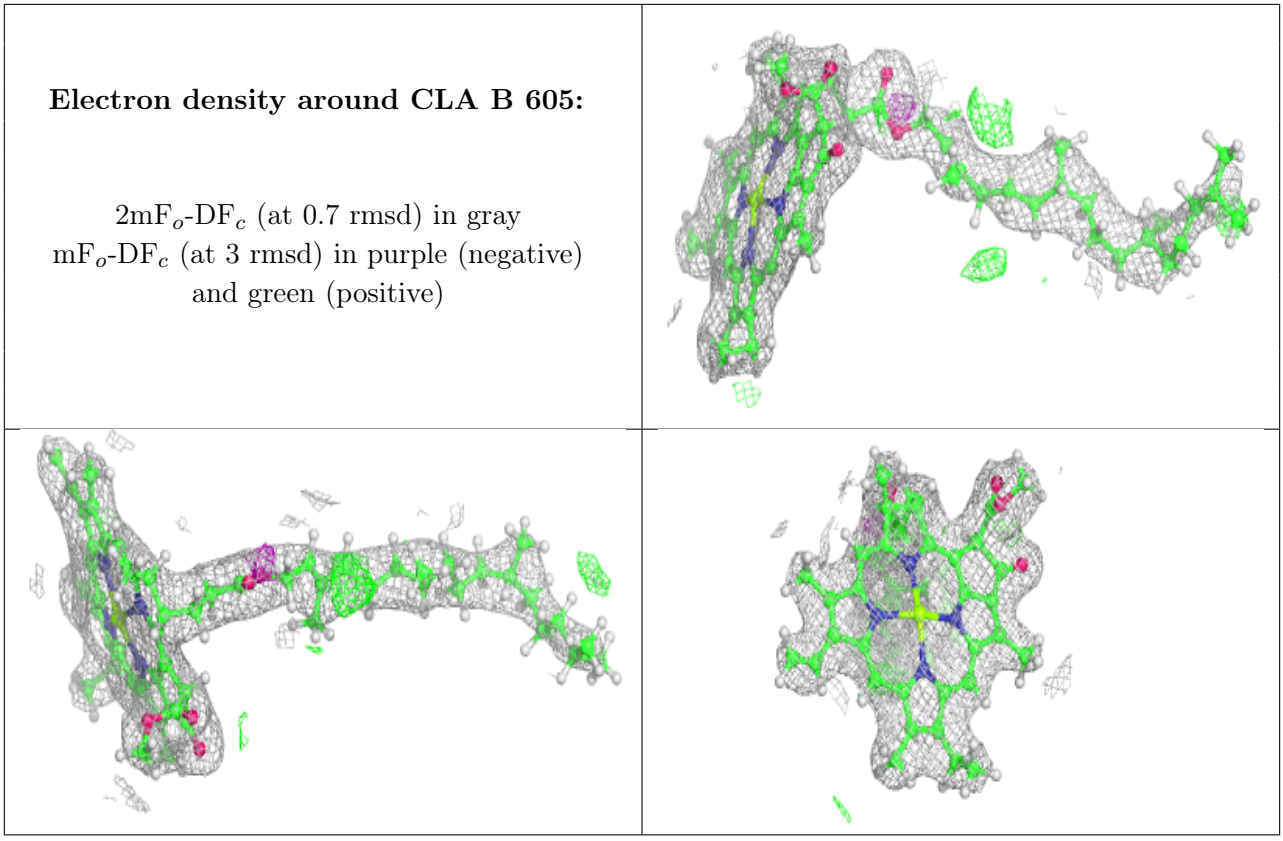






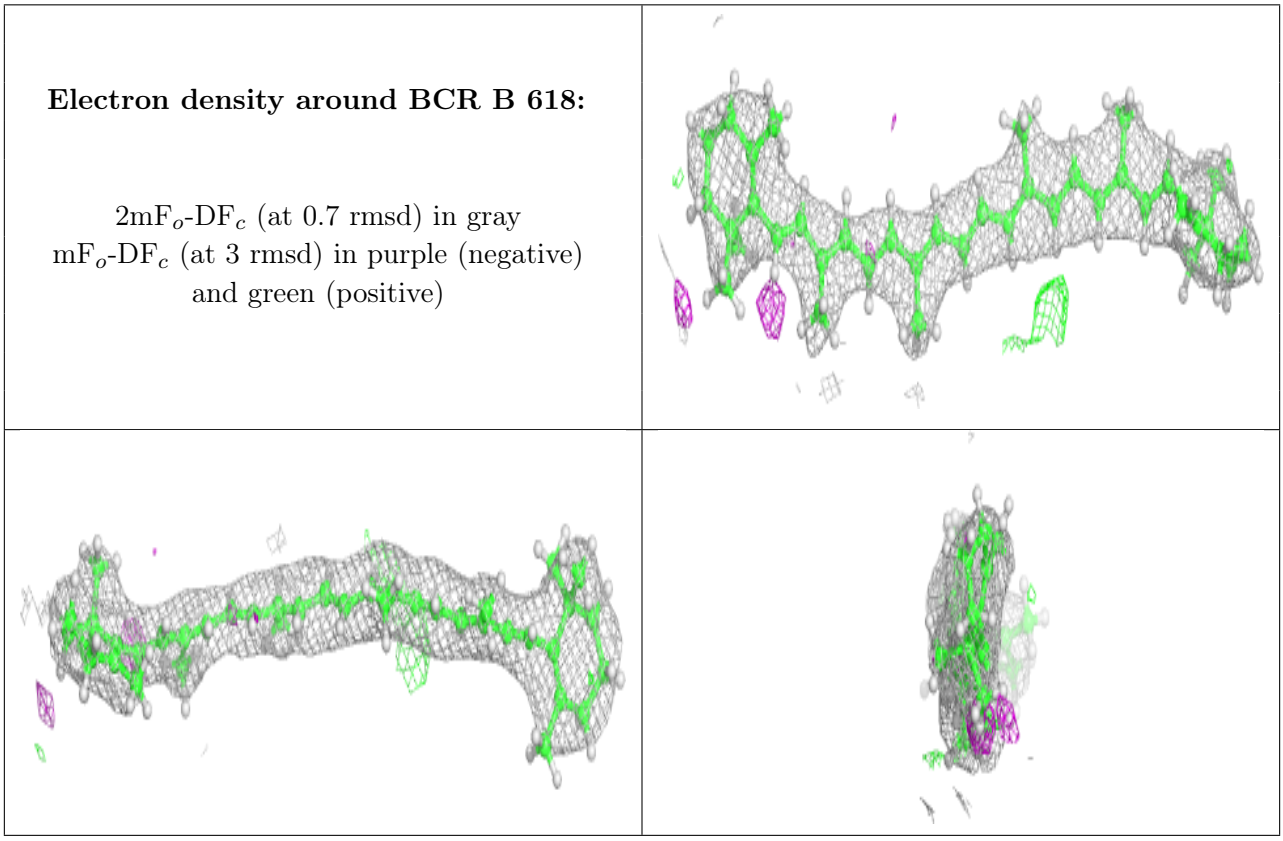
Electron density around CLA B 605:

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



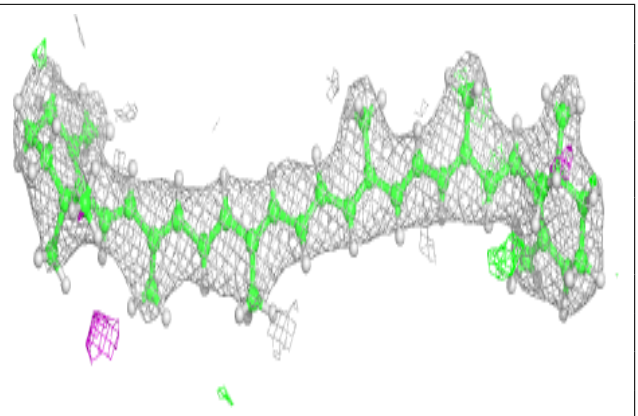
Electron density around BCR B 618:

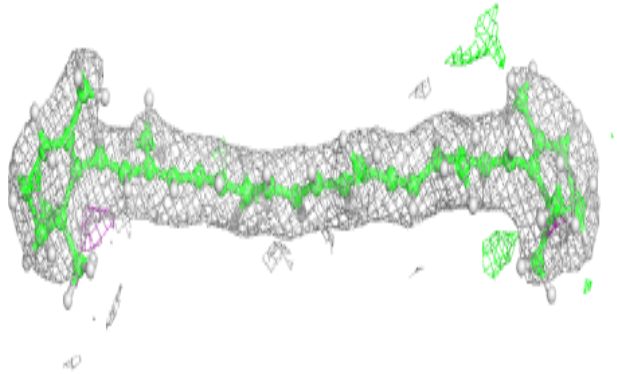
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

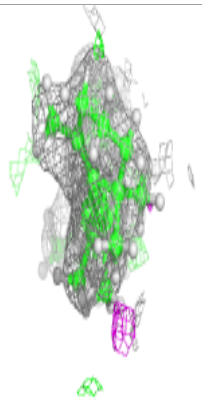


Electron density around BCR B 619:

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

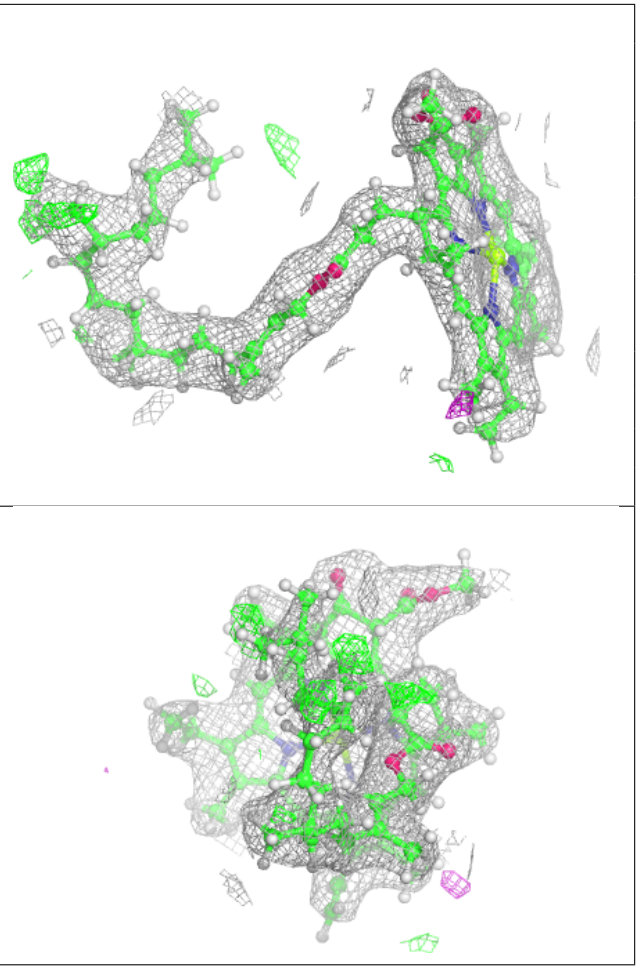






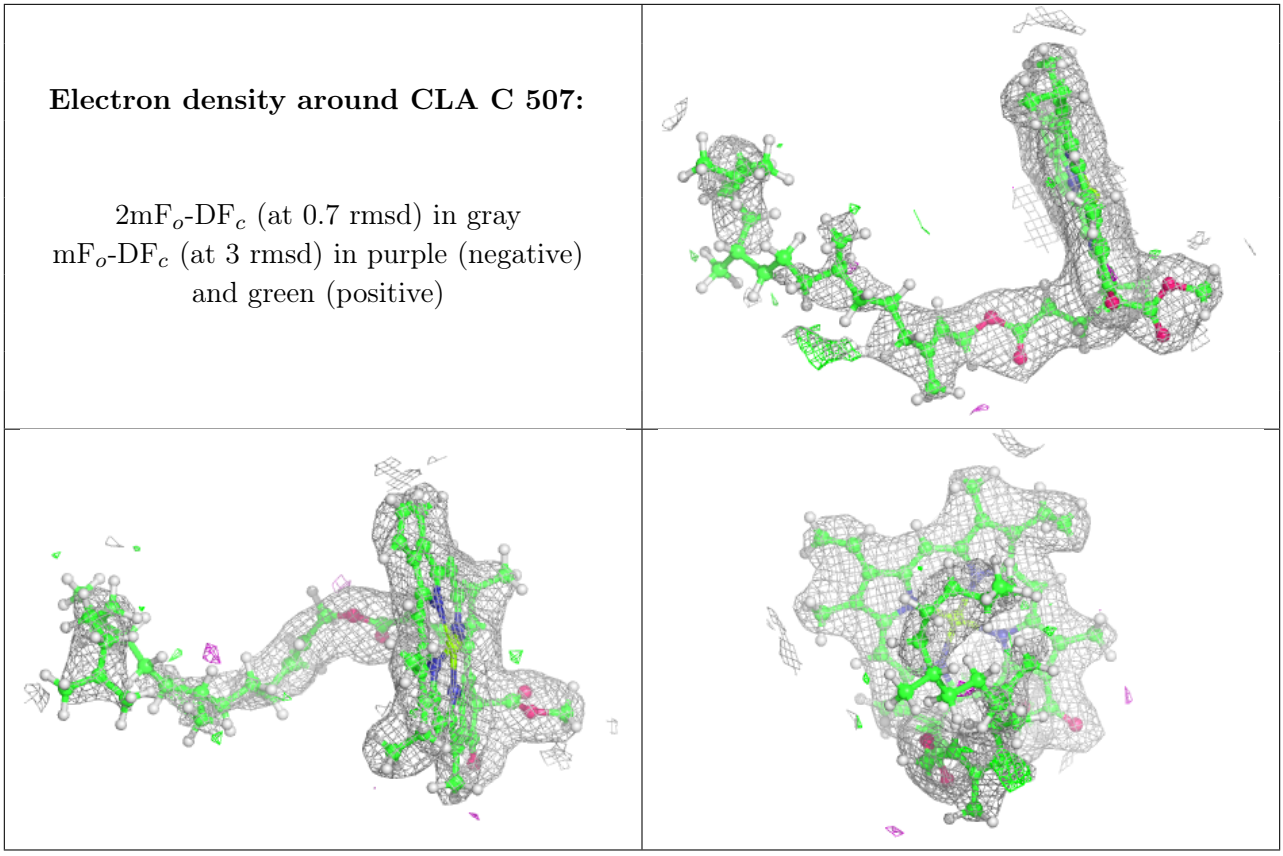
Electron density around CLA B 607:

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



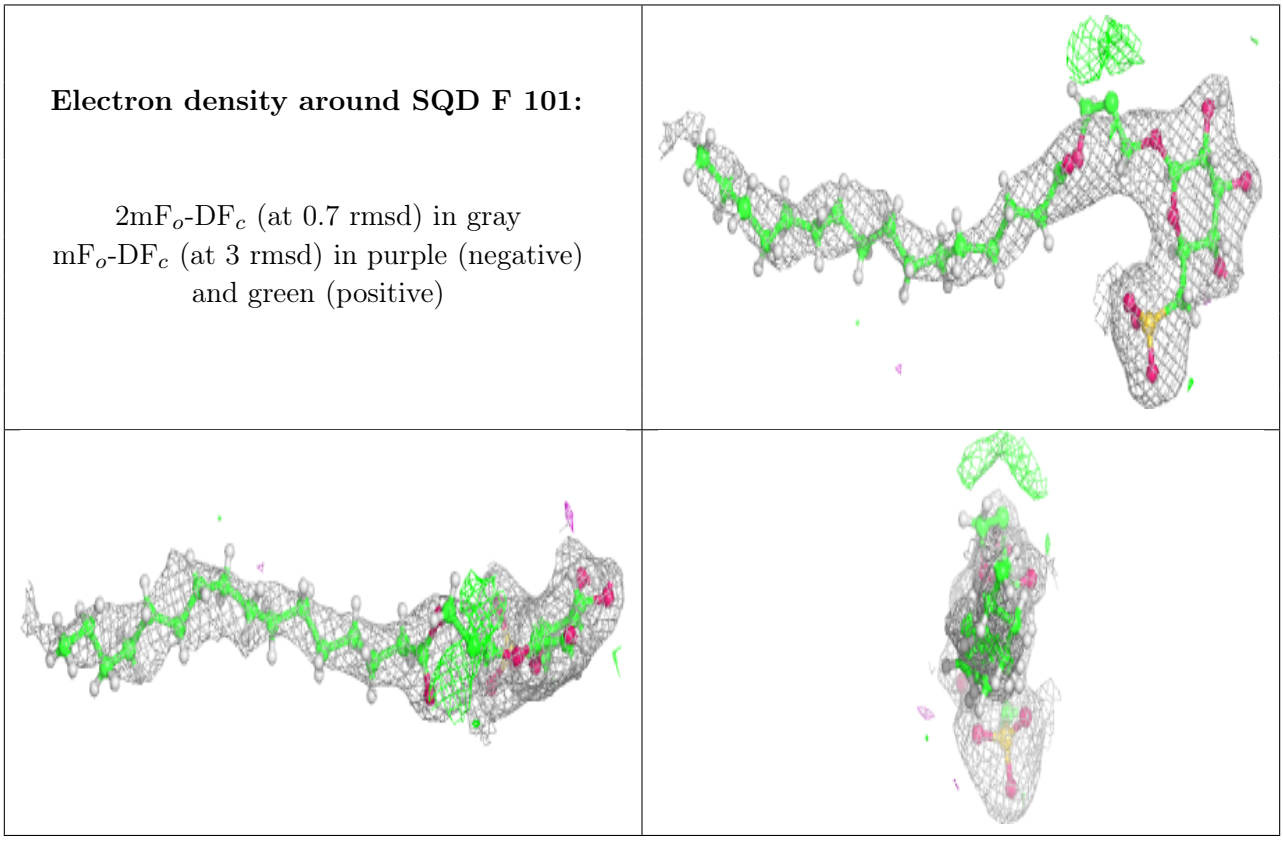
Electron density around CLA C 507:

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



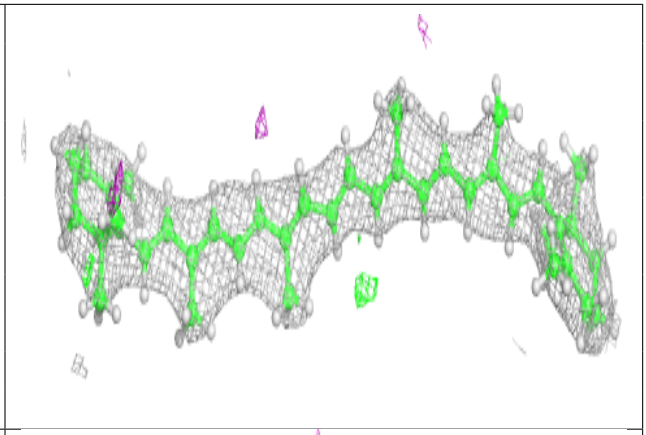
Electron density around SQD F 101:

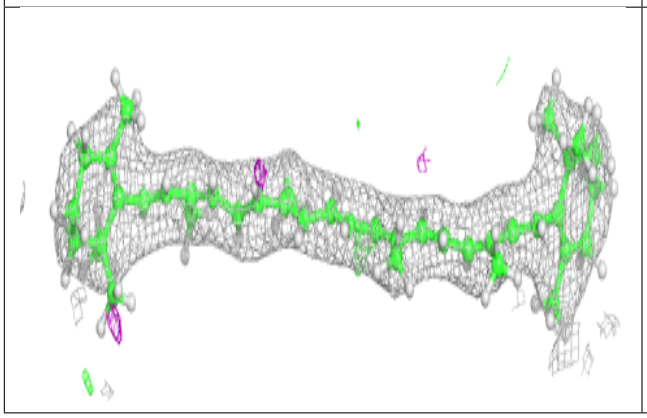
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

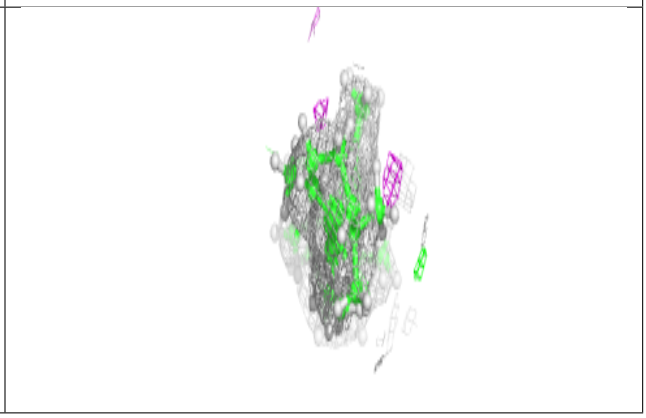


Electron density around BCR C 515:

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

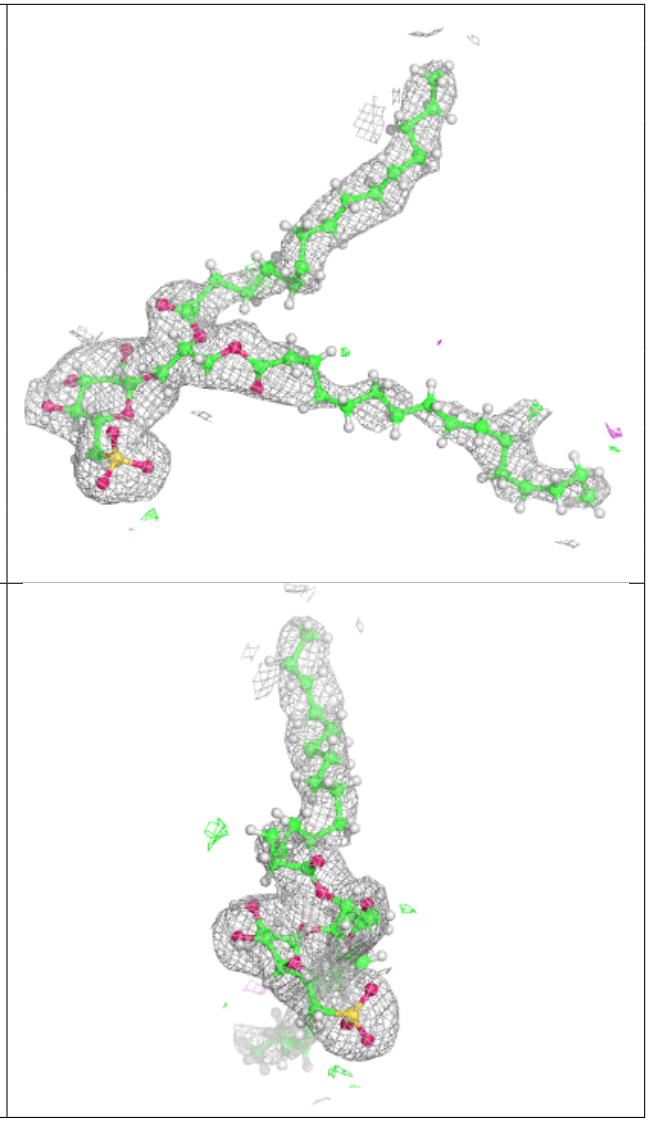






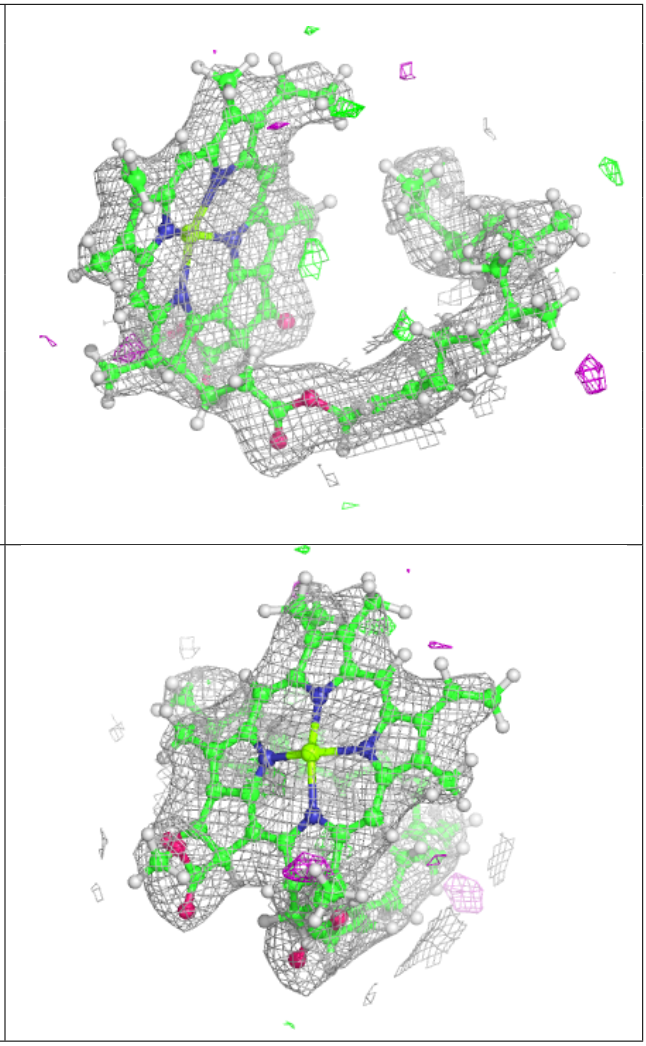
Electron density around SQD a 411:

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



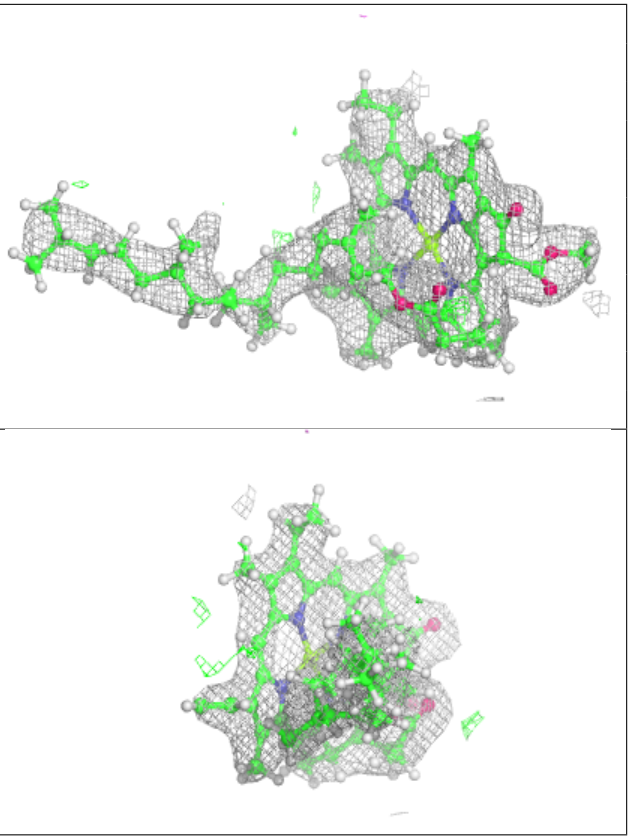
Electron density around CLA c 503:

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



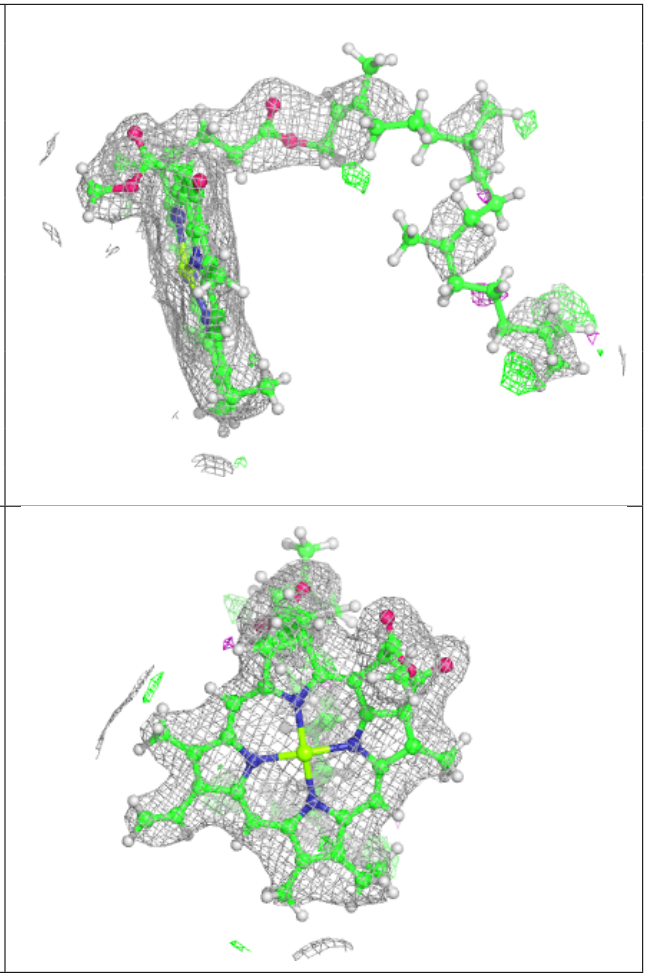
Electron density around CLA c 505:

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



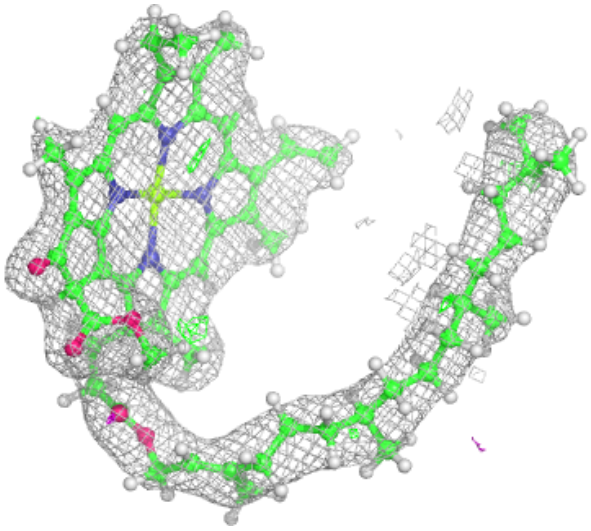
Electron density around CLA c 506:

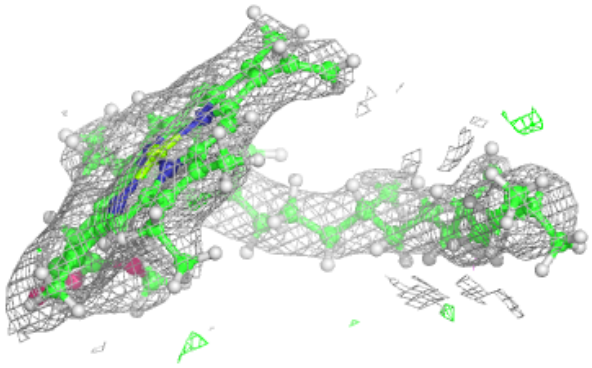
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

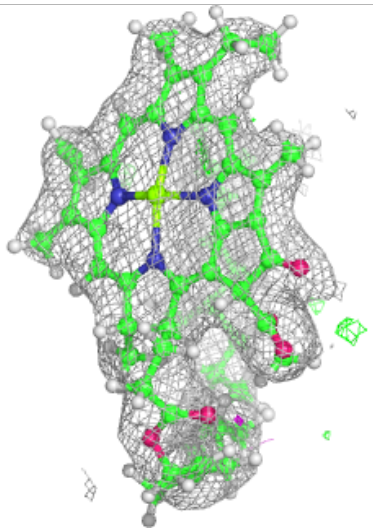


Electron density around CLA c 507:

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

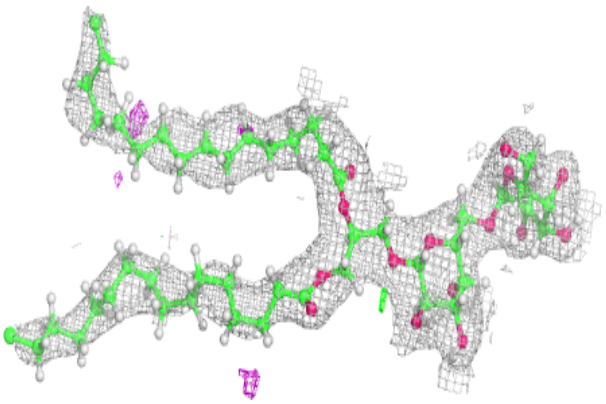


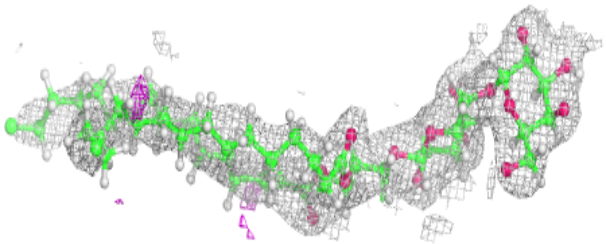




Electron density around DGD C 519:

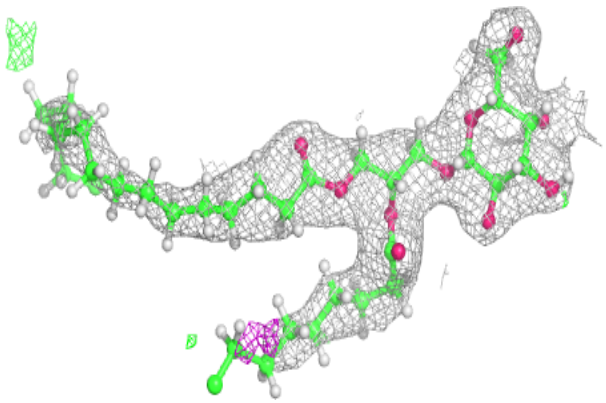
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

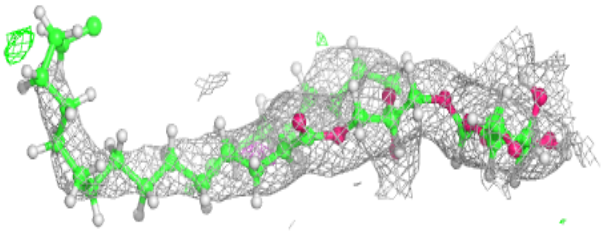


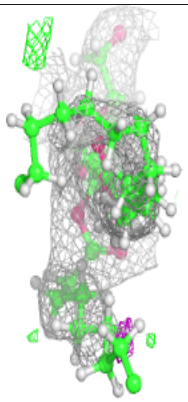


Electron density around LMG d 410:

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

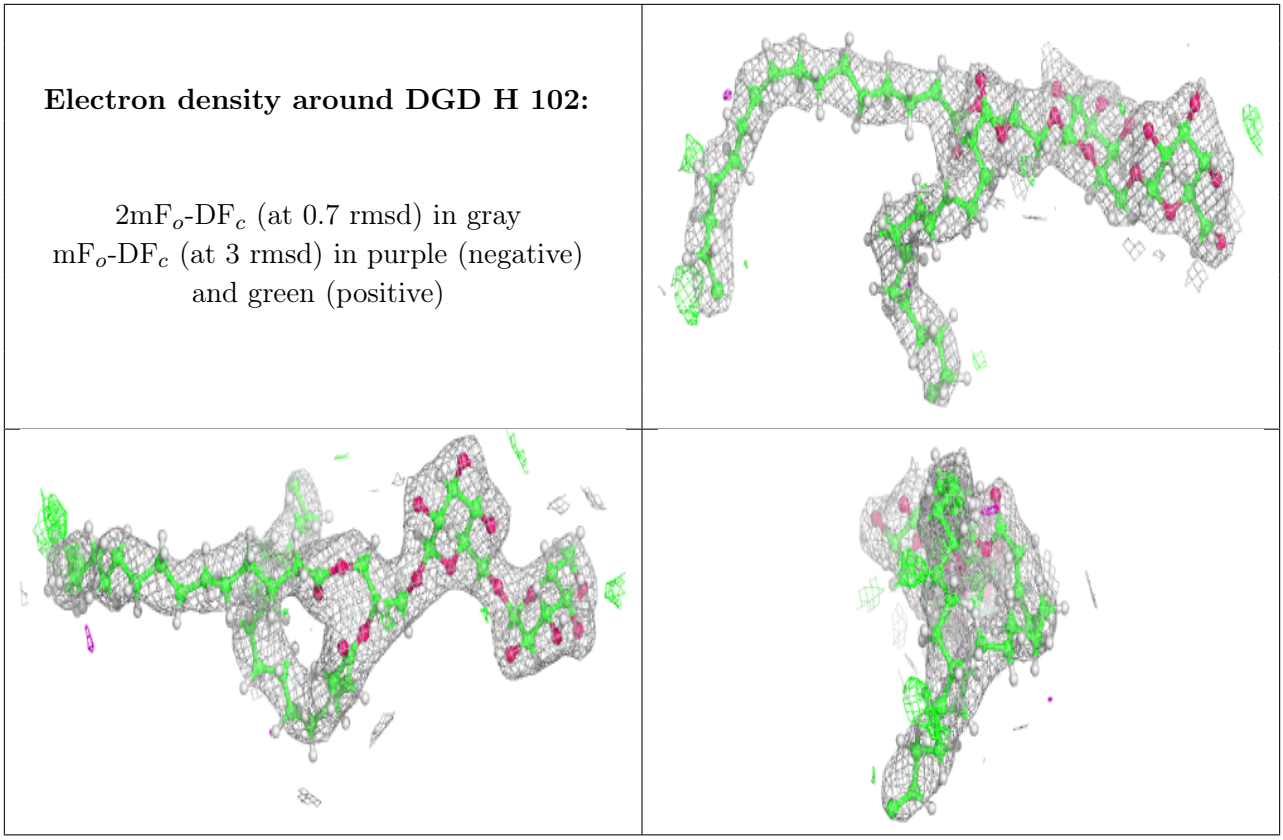






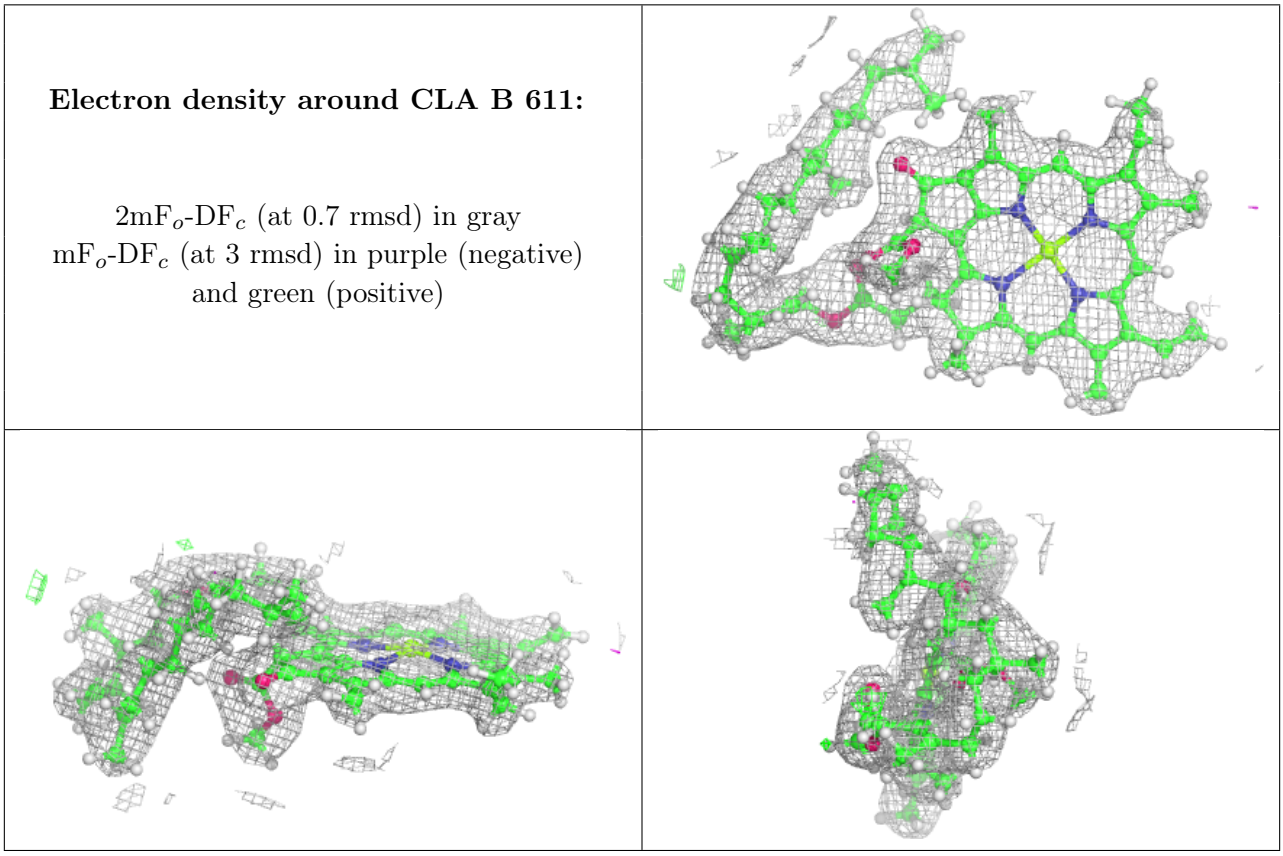
Electron density around DGD H 102:

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



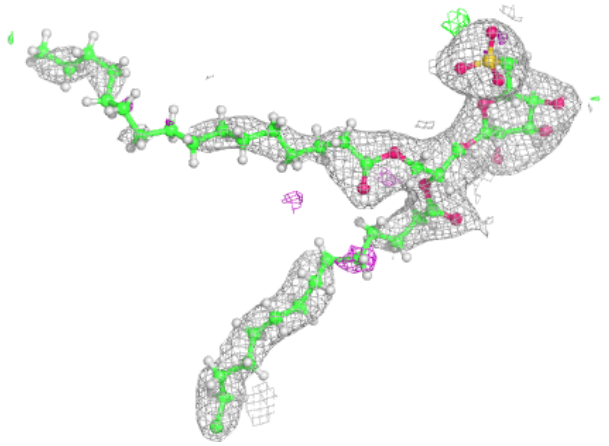
Electron density around CLA B 611:

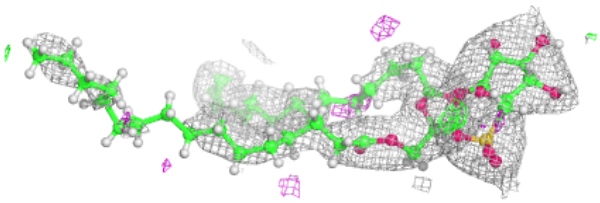
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

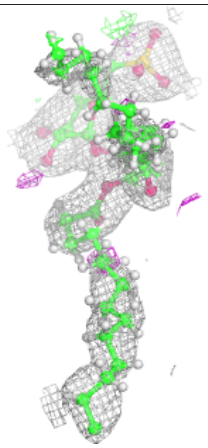


Electron density around SQD A 412:

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

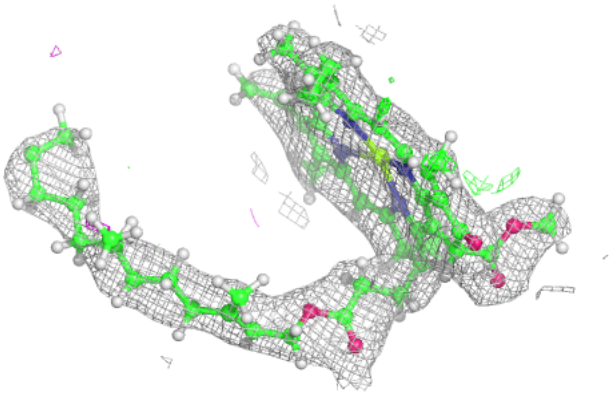


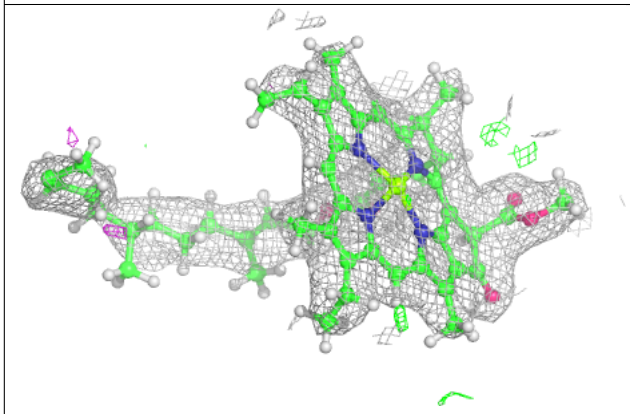


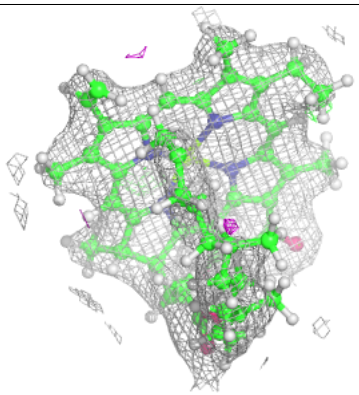


Electron density around CLA C 505:

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

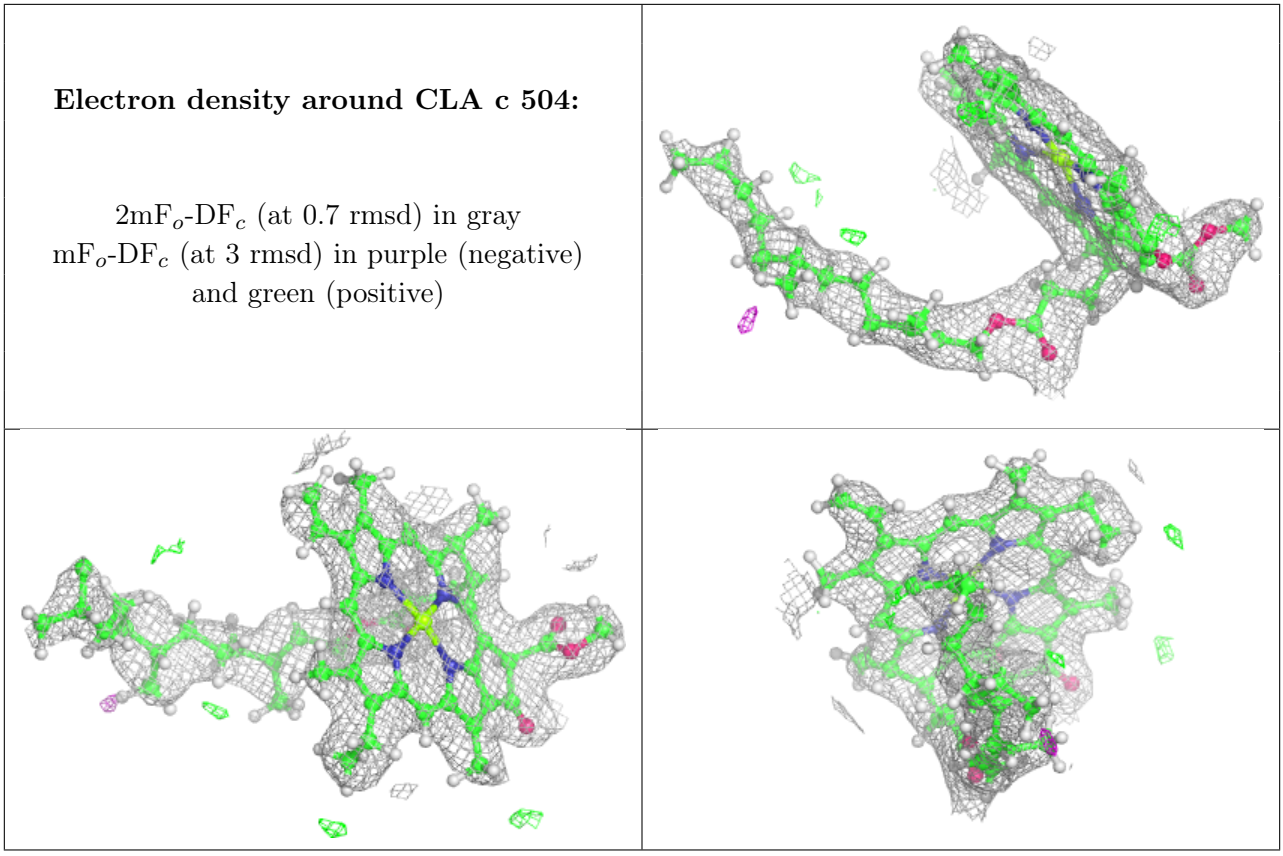






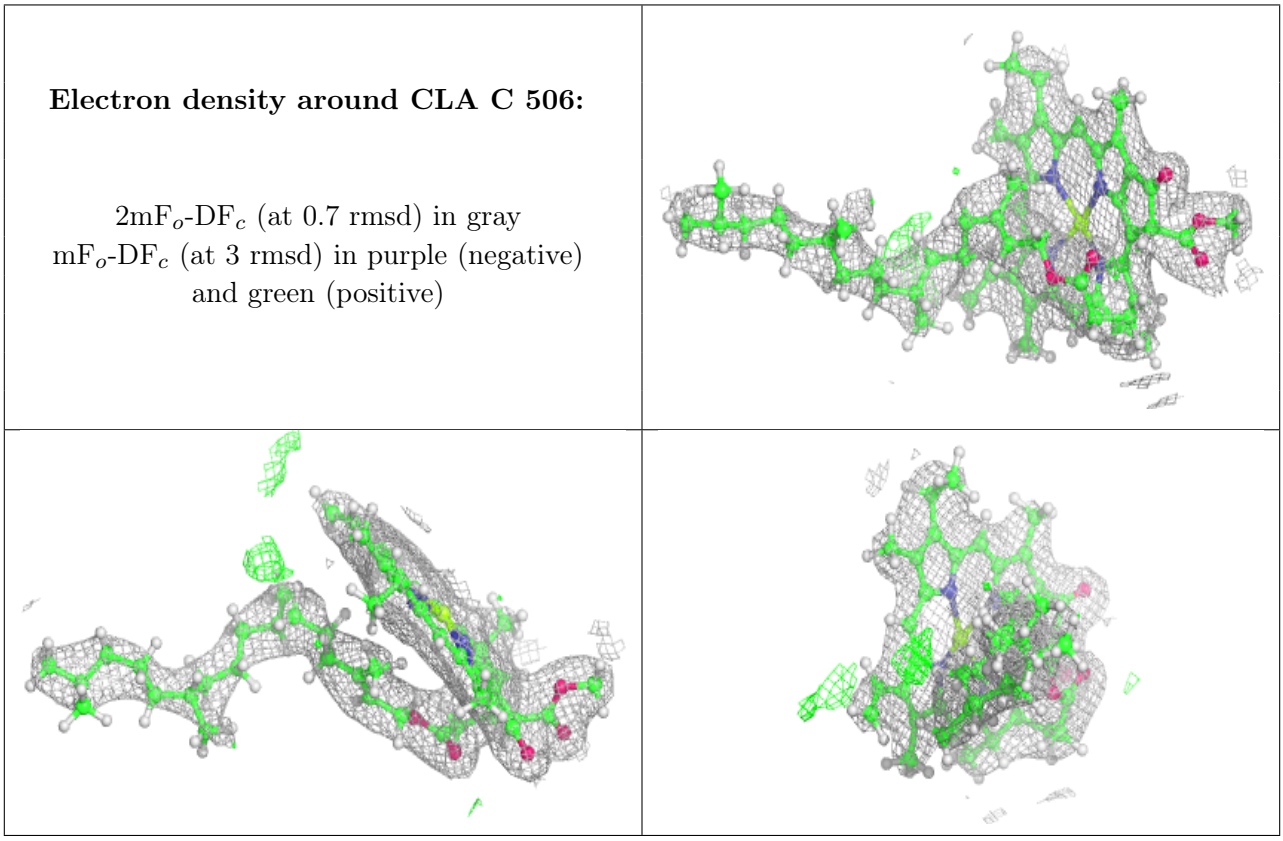
Electron density around CLA c 504:

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



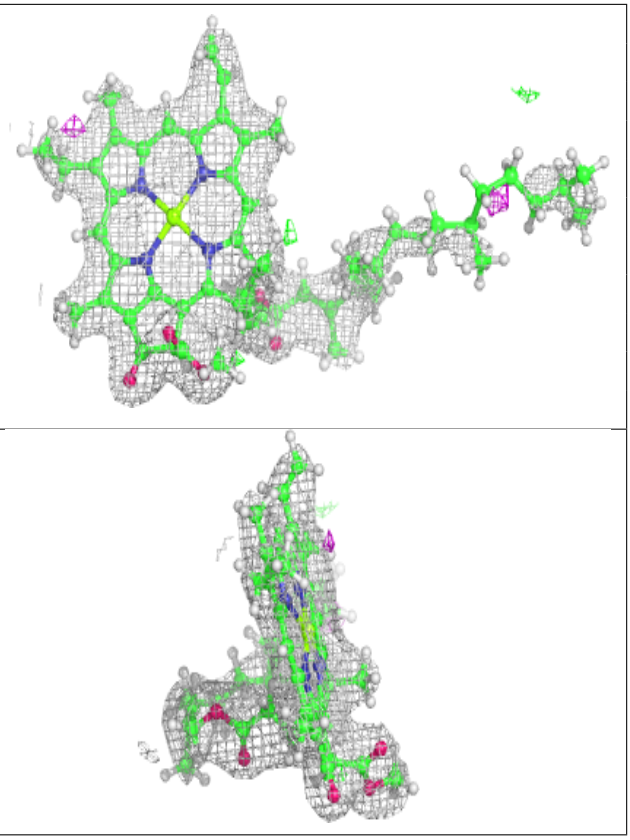
Electron density around CLA C 506:

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



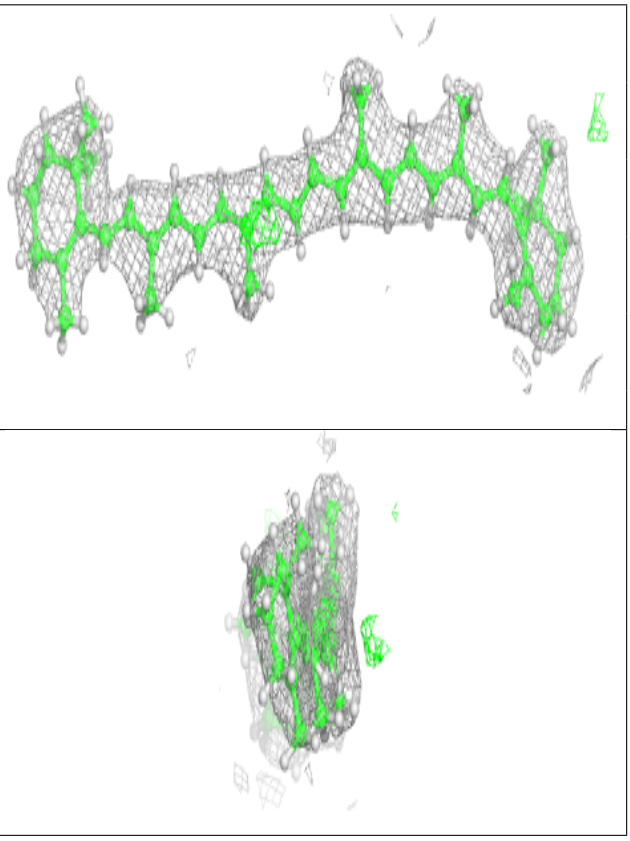
Electron density around CLA a 403:

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



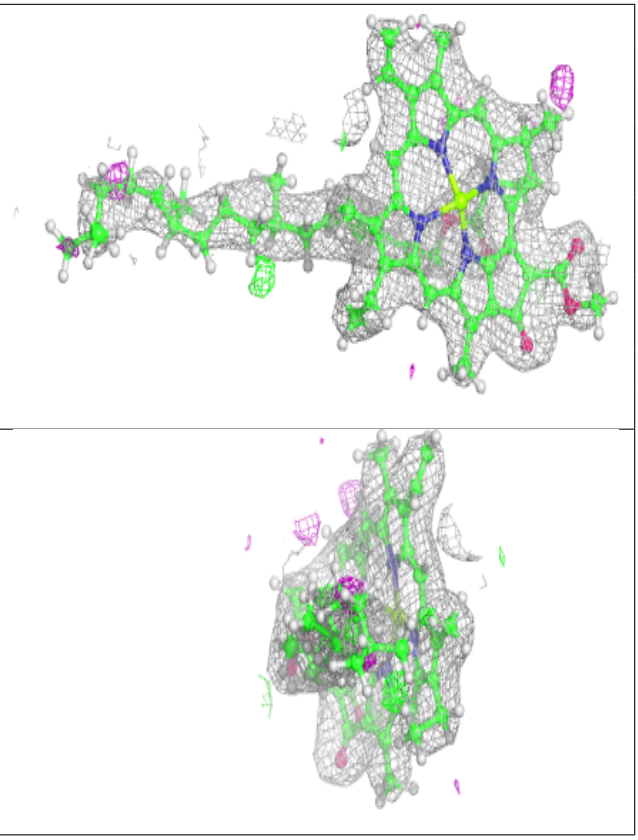
Electron density around BCR T 101:

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



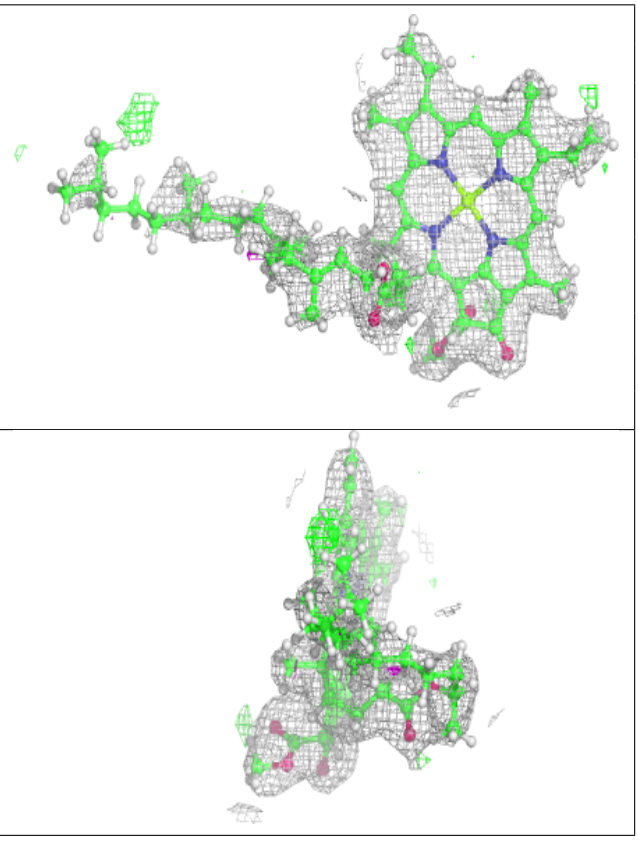
Electron density around CLA B 615:

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



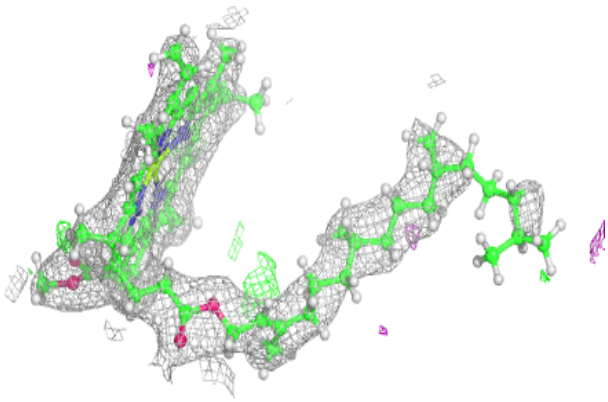
Electron density around CLA A 403:

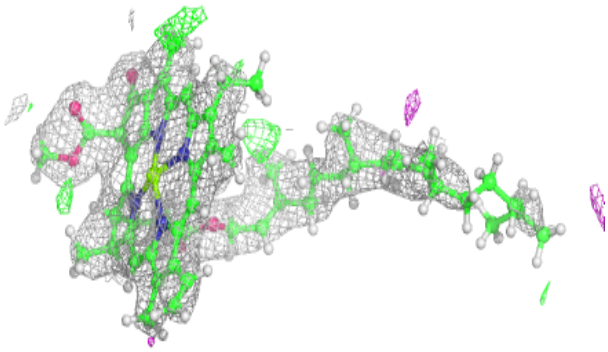
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

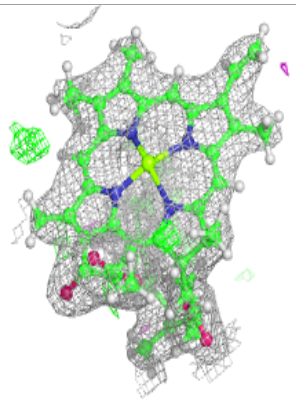


Electron density around CLA C 509:

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

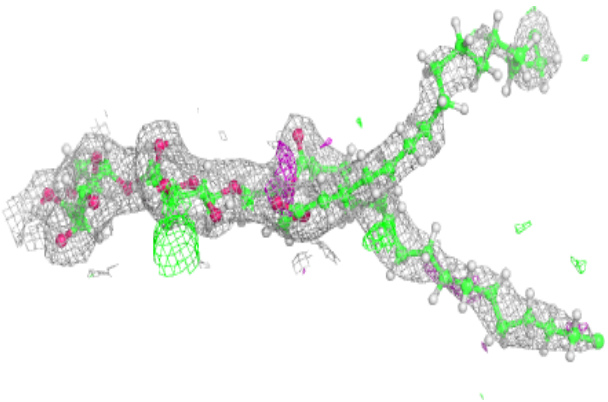


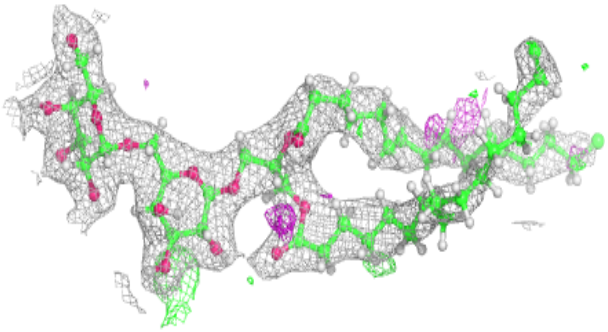


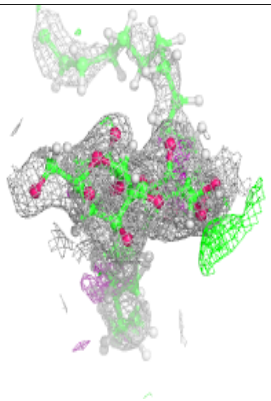


Electron density around DGD C 517:

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

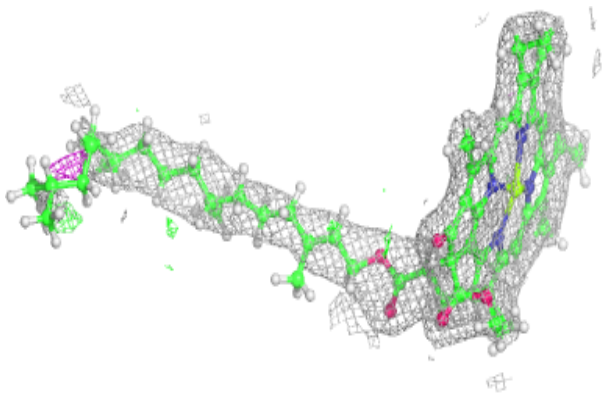


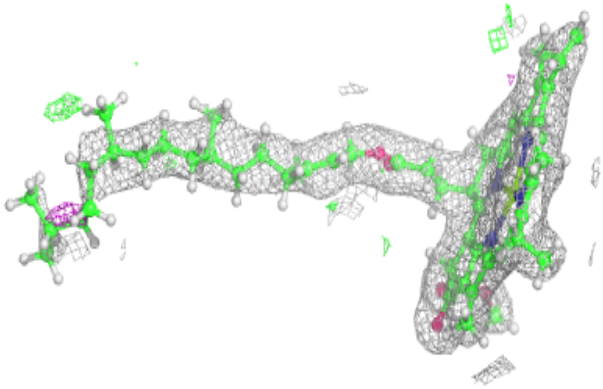


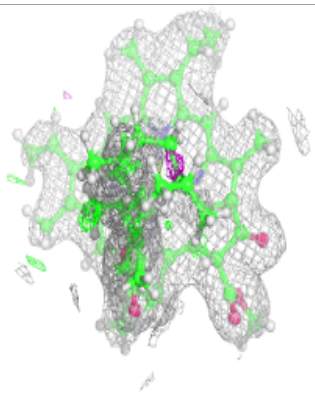


Electron density around CLA b 604:

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

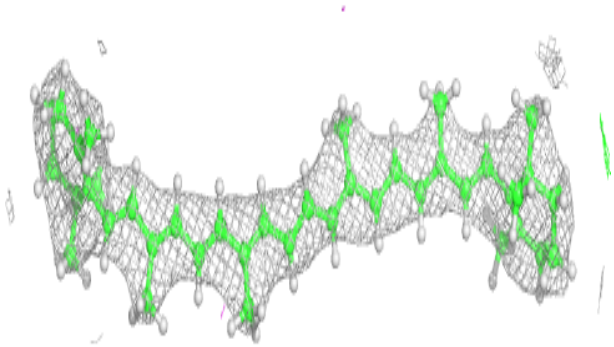


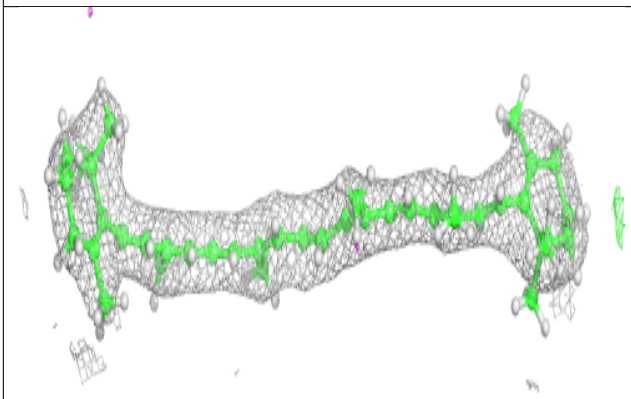


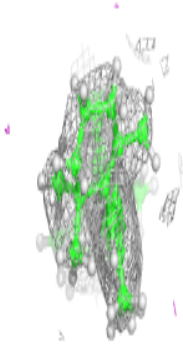


Electron density around BCR c 515:

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

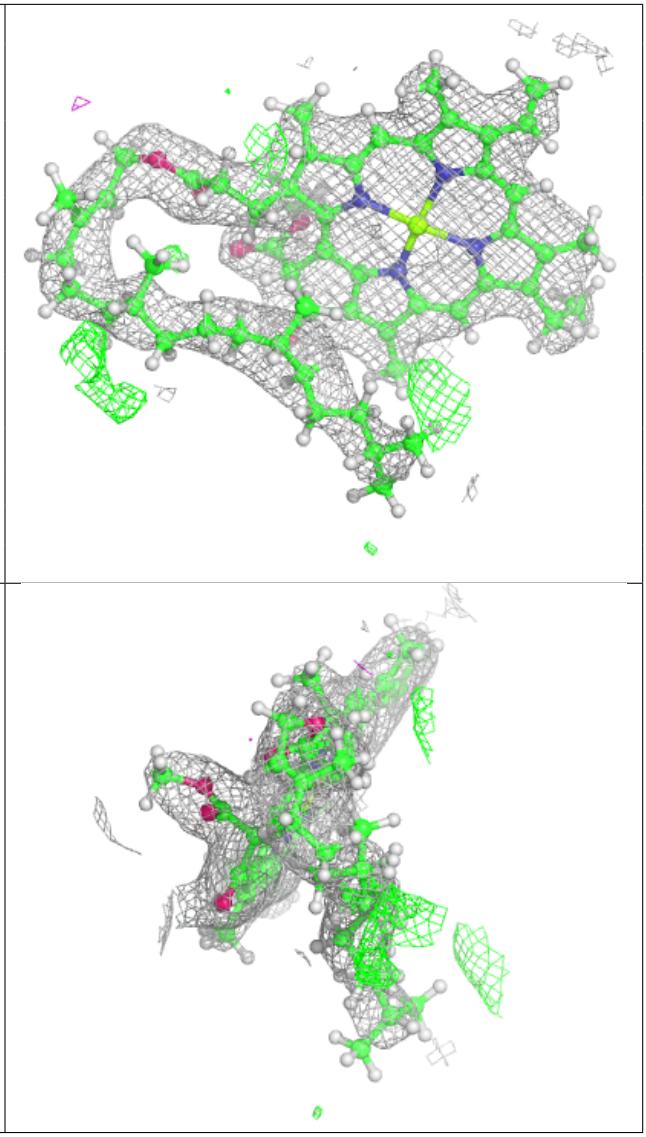






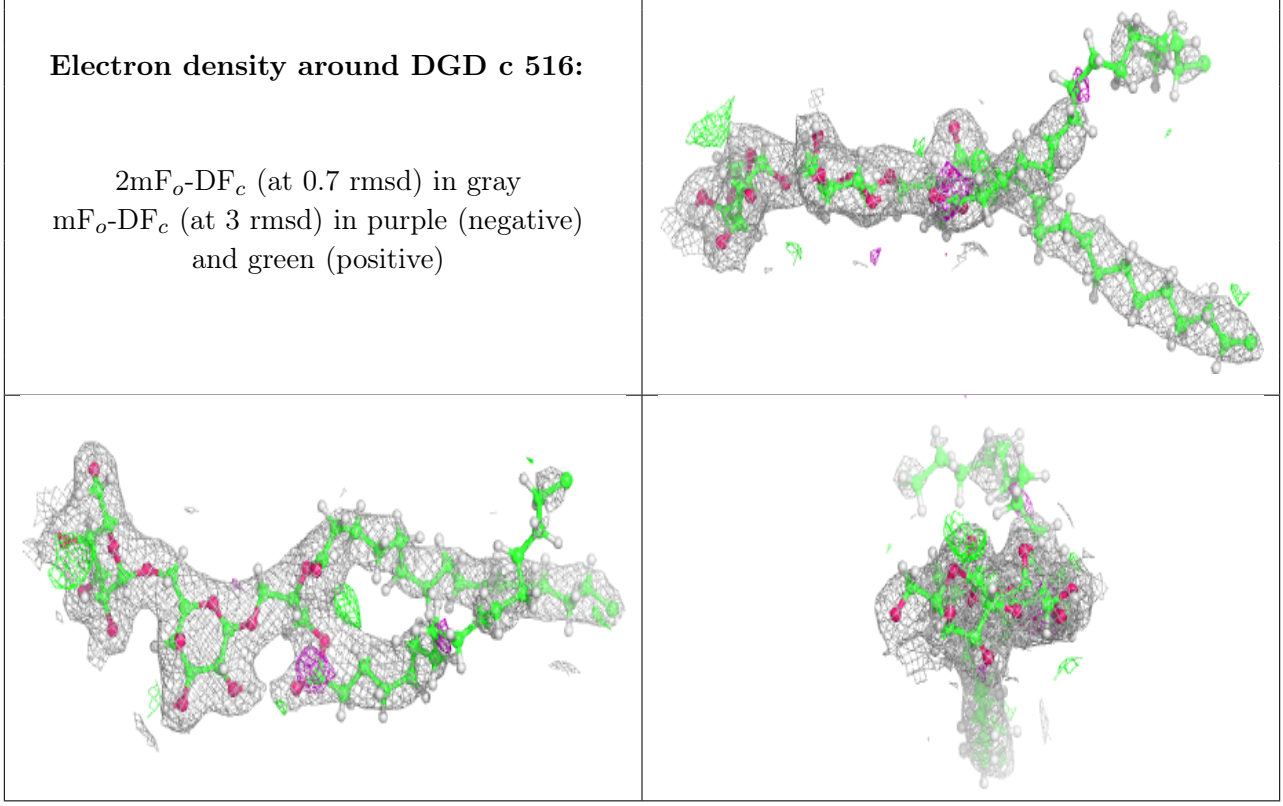
Electron density around CLA C 510:

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



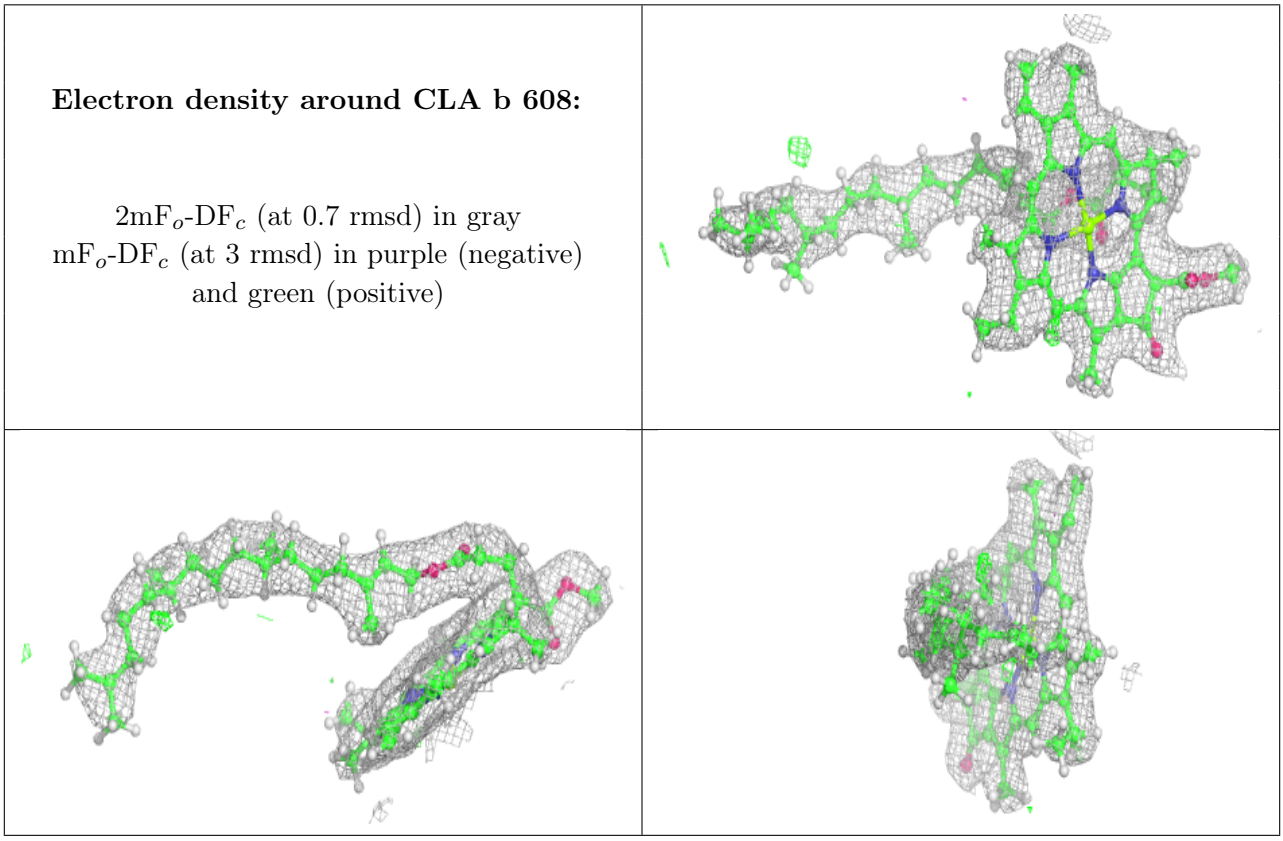
Electron density around DGD c 516:

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



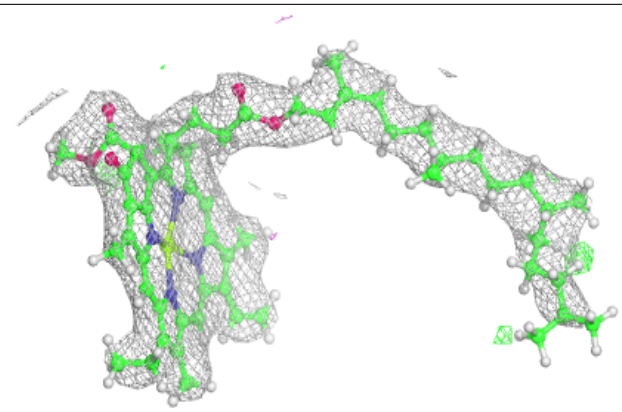
Electron density around CLA b 608:

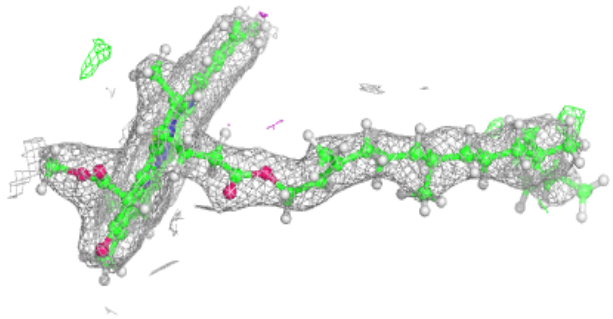
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

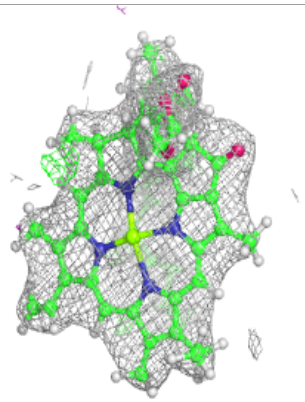


Electron density around CLA b 609:

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

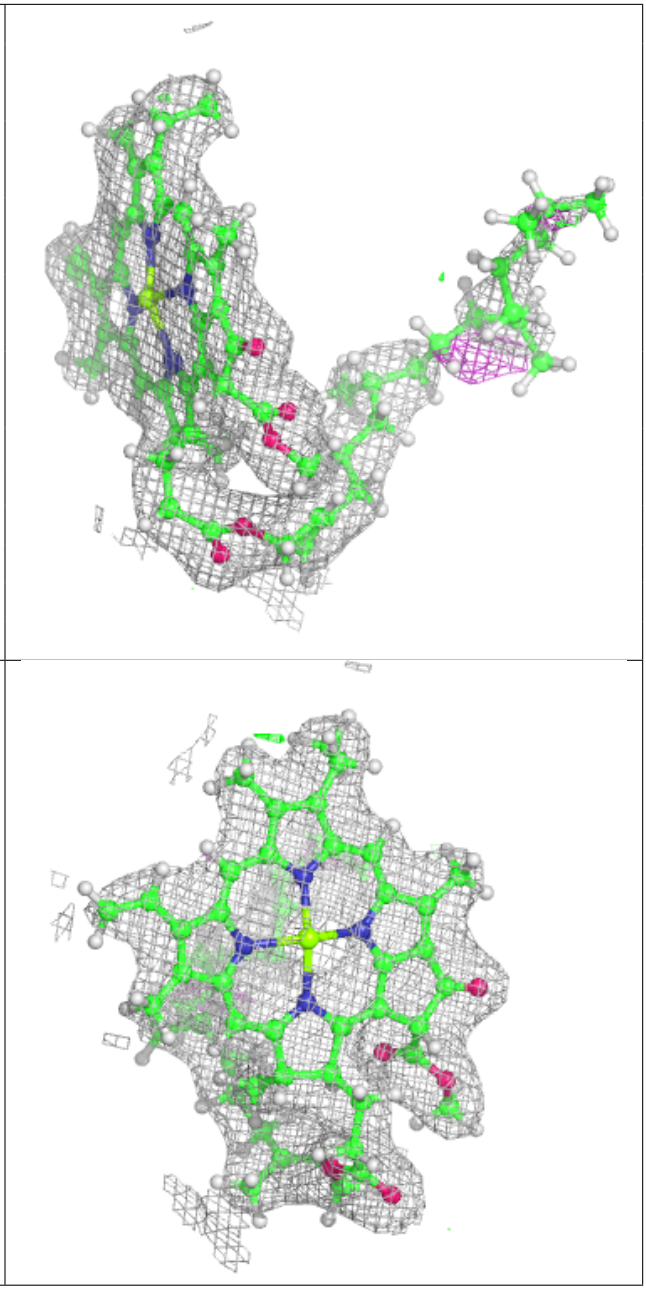






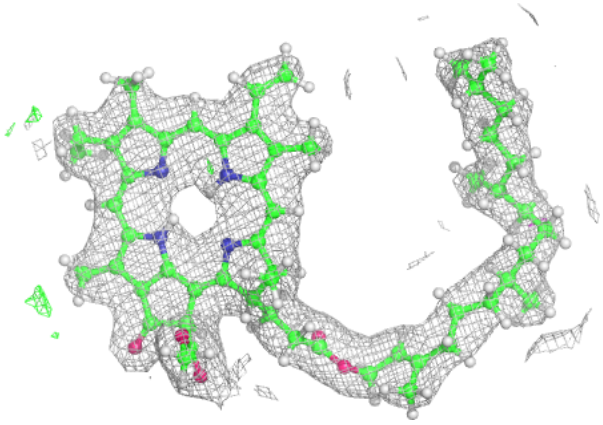
Electron density around CLA b 613:

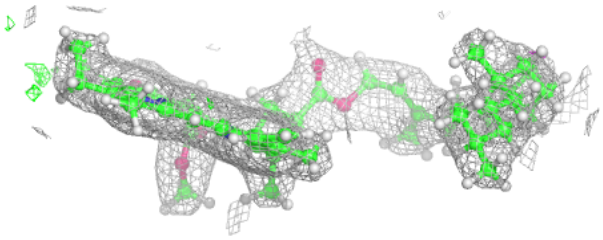
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

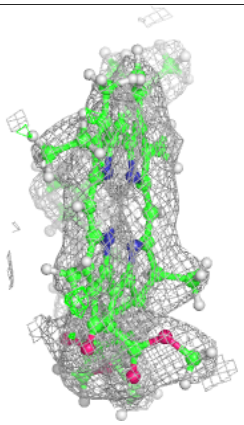


Electron density around PHO a 404:

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

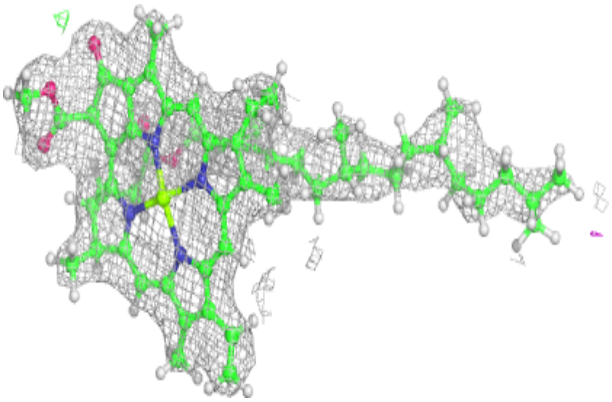


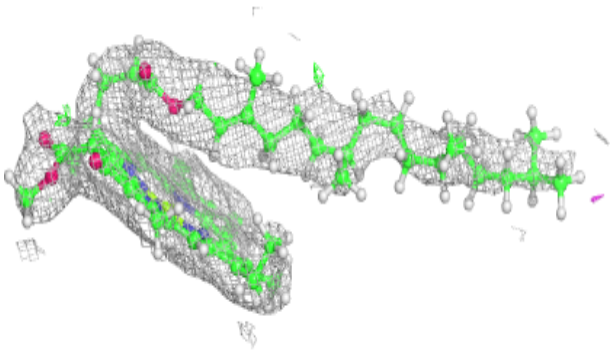


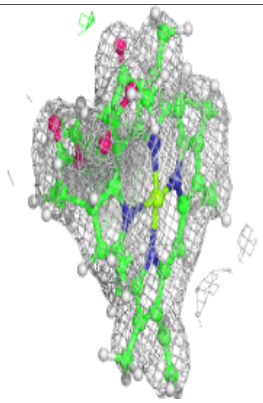


Electron density around CLA b 614:

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

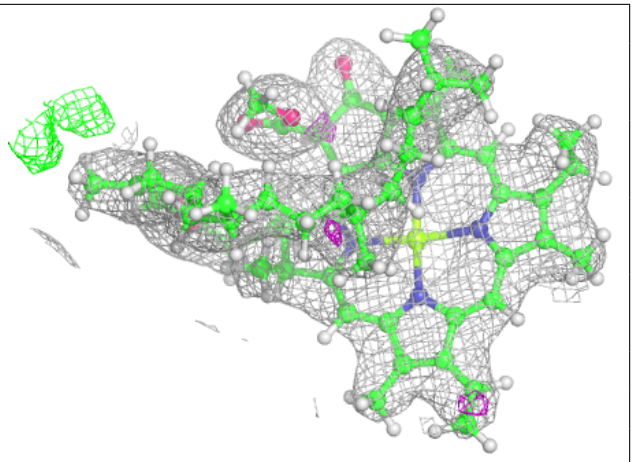


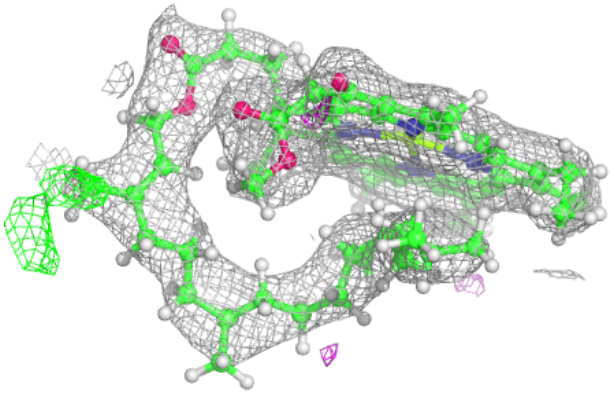


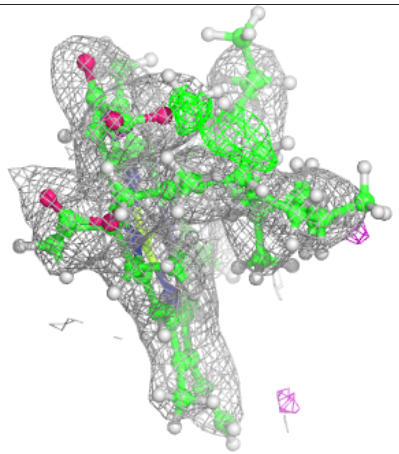


Electron density around CLA C 511:

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

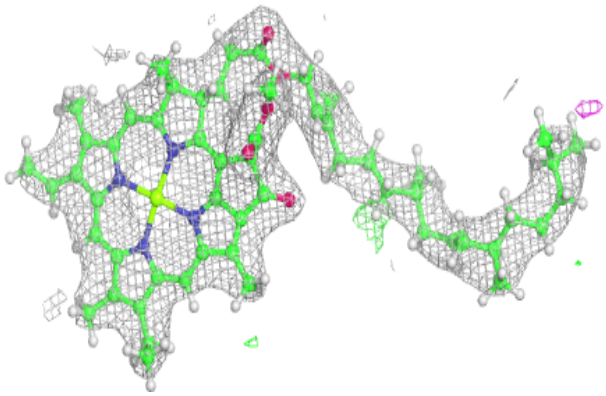


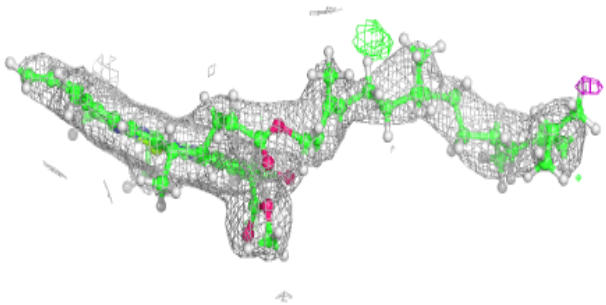


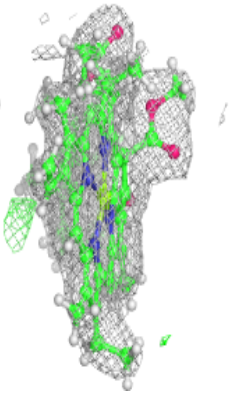


Electron density around CLA B 603:

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

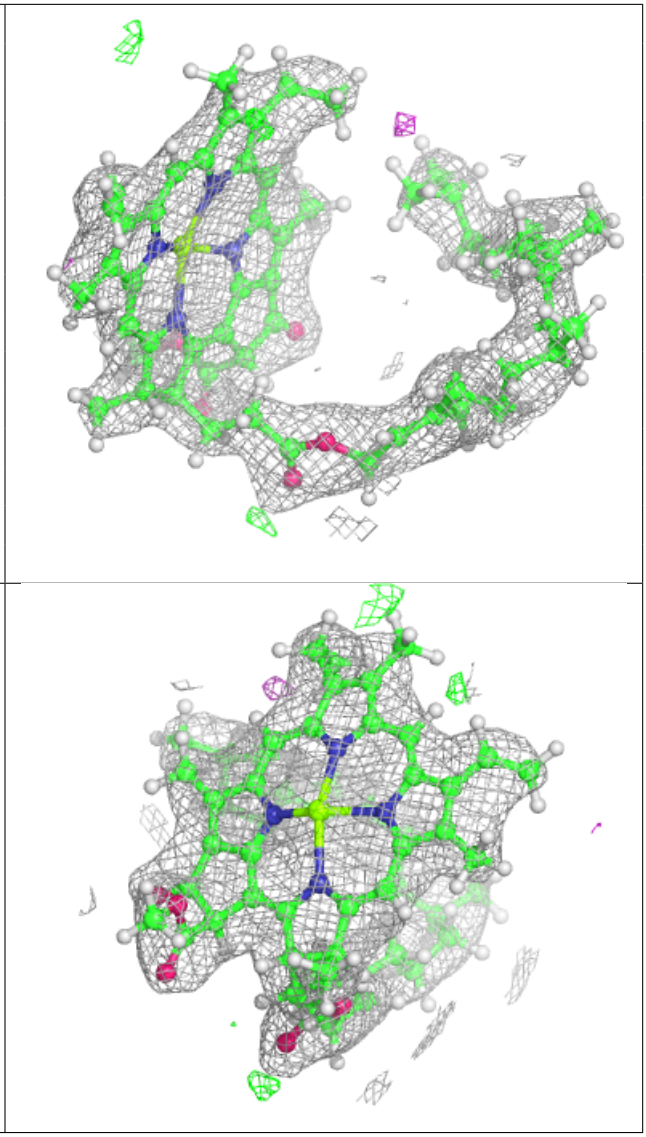






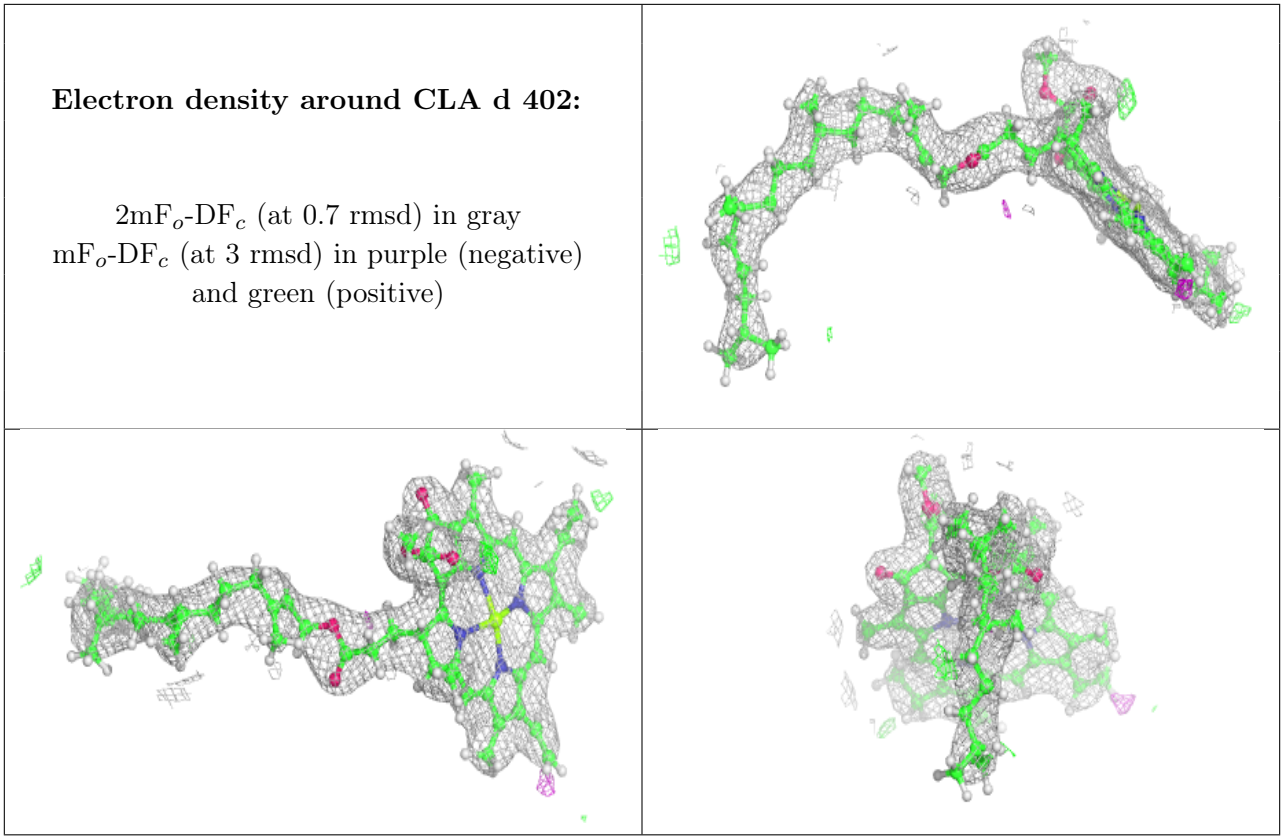
Electron density around CLA C 504:

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



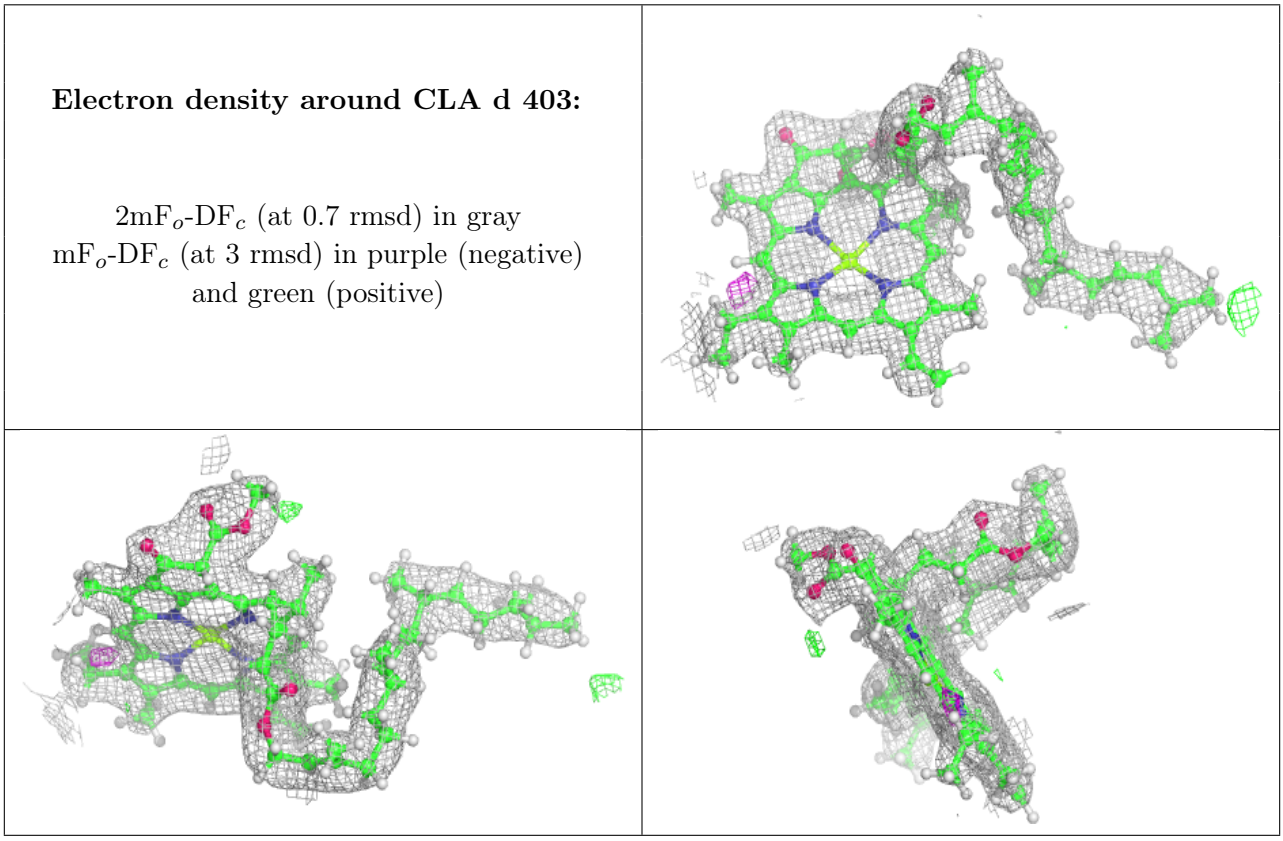
Electron density around CLA d 402:

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



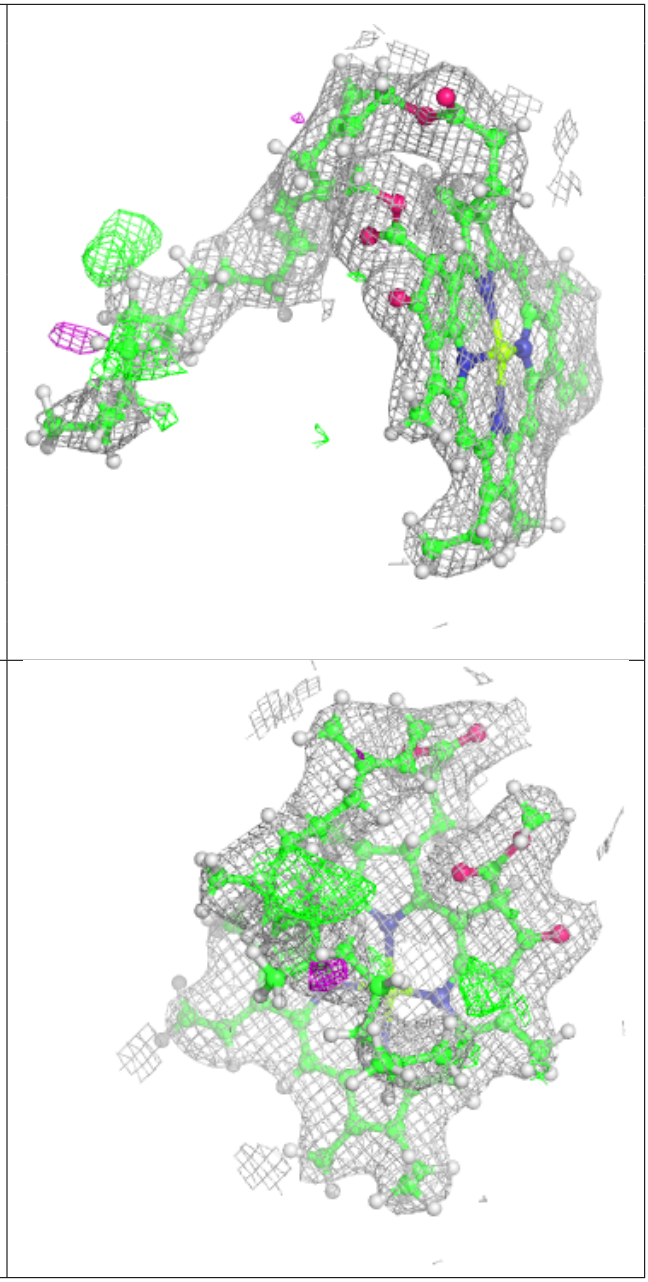
Electron density around CLA d 403:

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



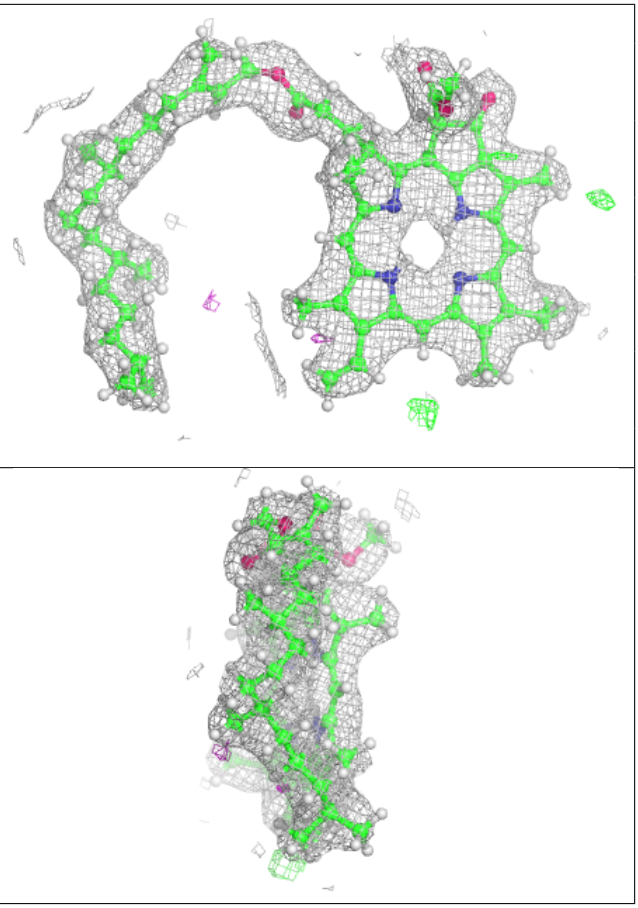
Electron density around CLA B 614:

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



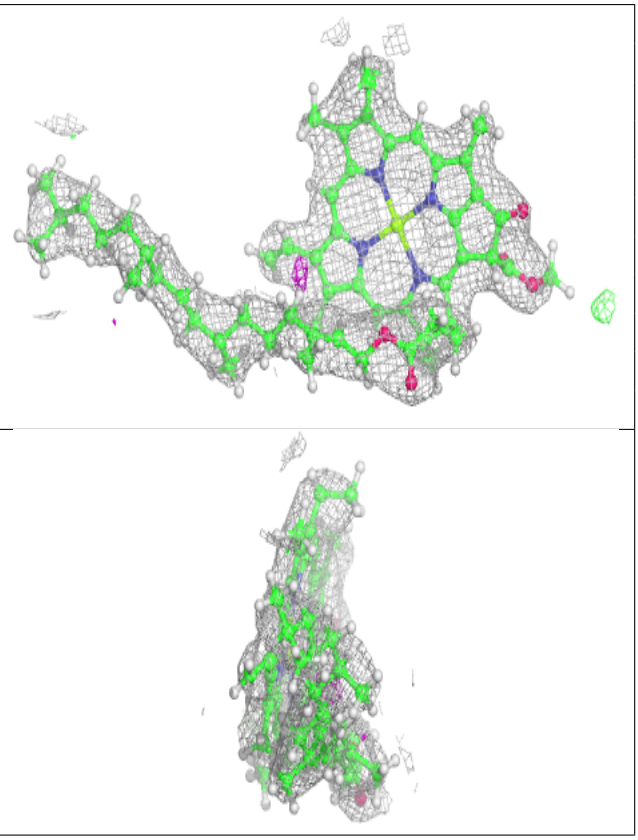
Electron density around PHO A 404:

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



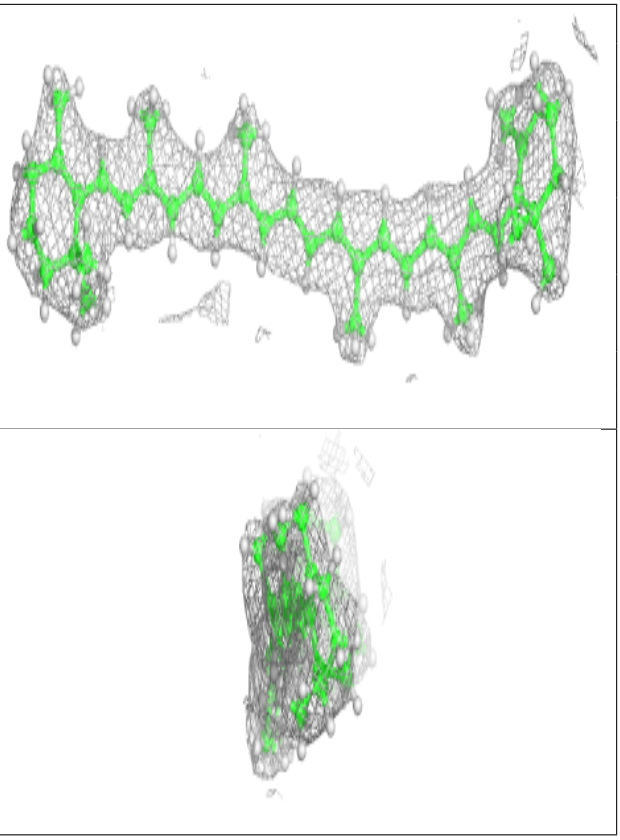
Electron density around CLA c 501:

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



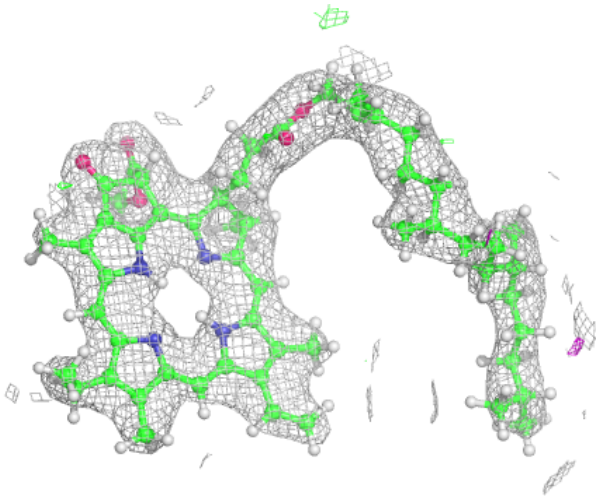
Electron density around BCR t 101:

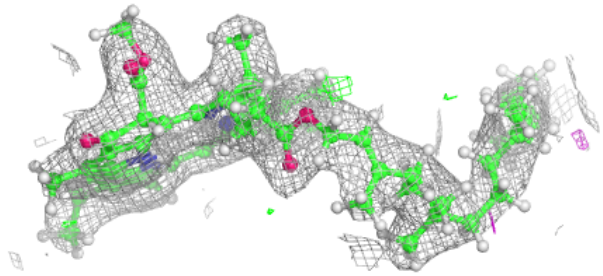
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

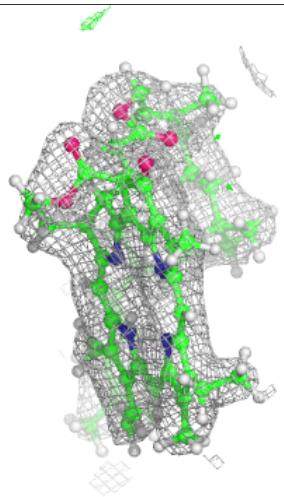


Electron density around PHO d 401:

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

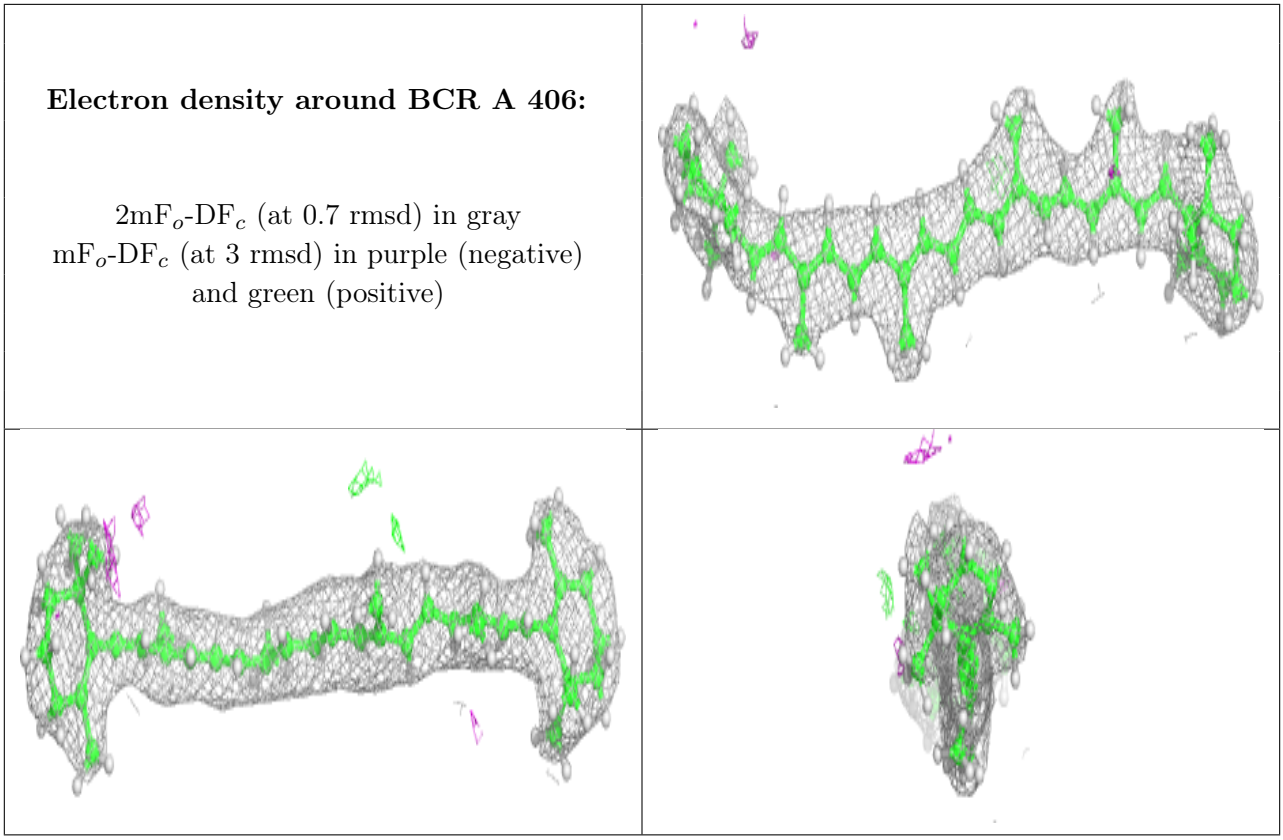






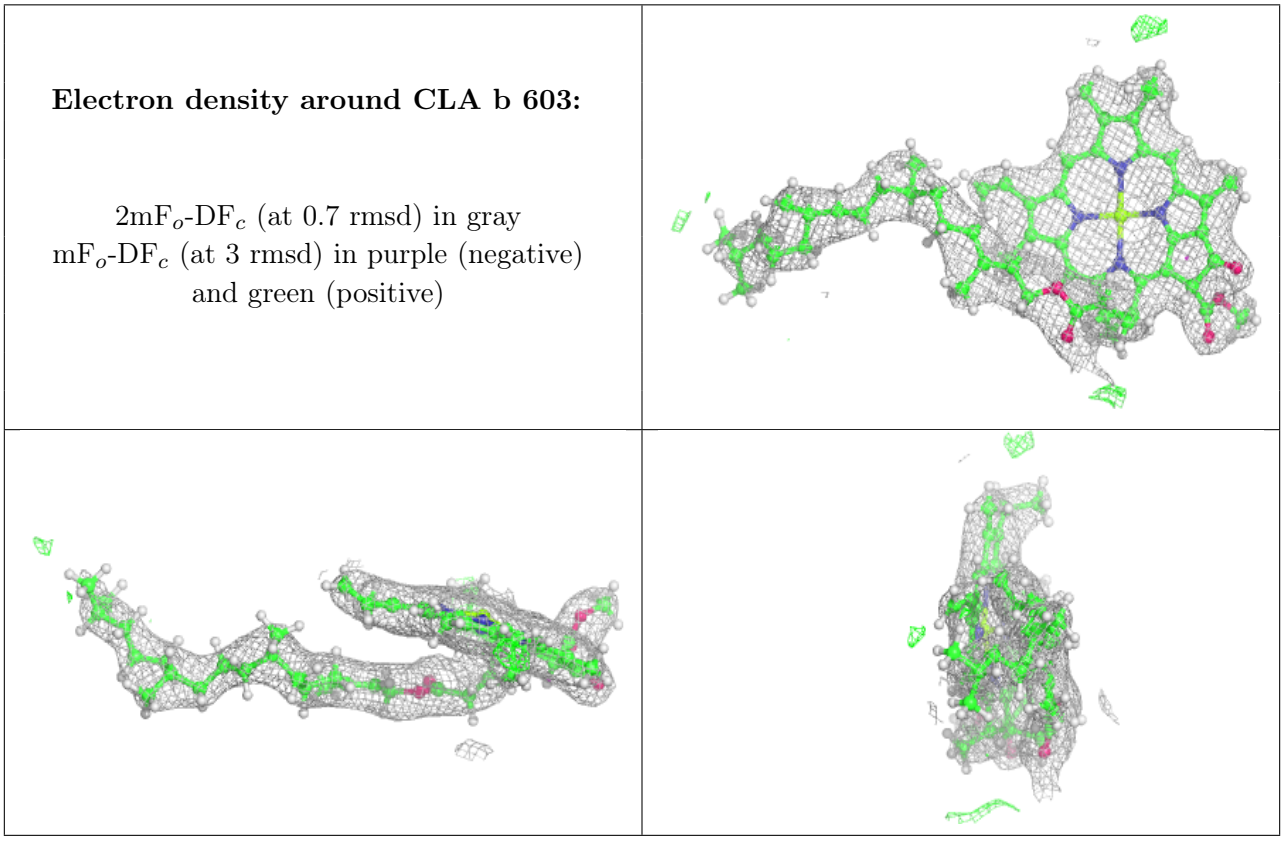
Electron density around BCR A 406:

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



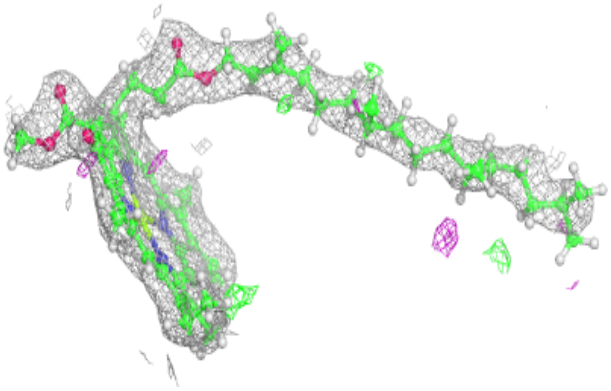
Electron density around CLA b 603:

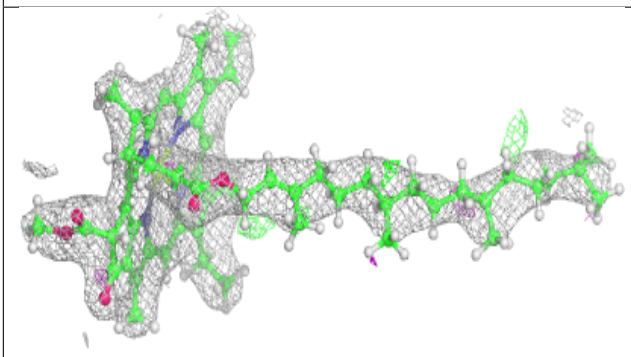
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

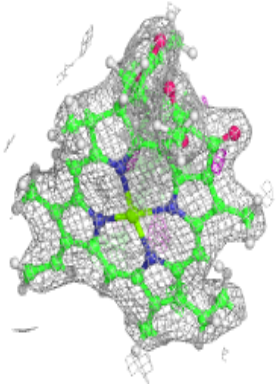


Electron density around CLA B 608:

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

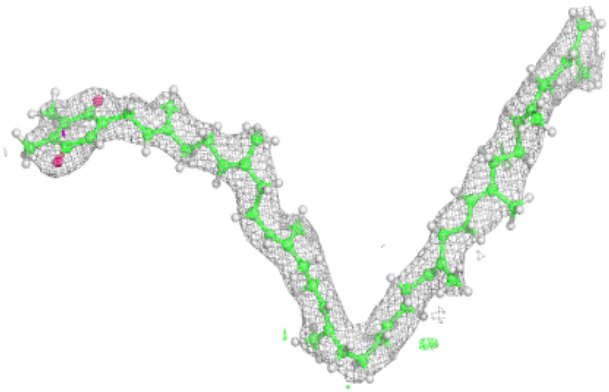


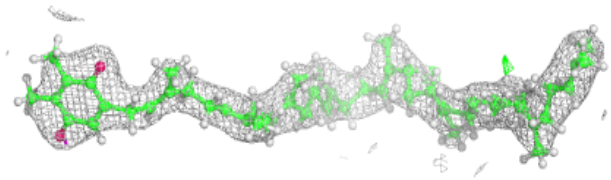


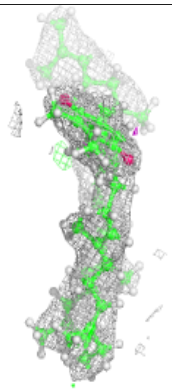


Electron density around PL9 d 406:

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

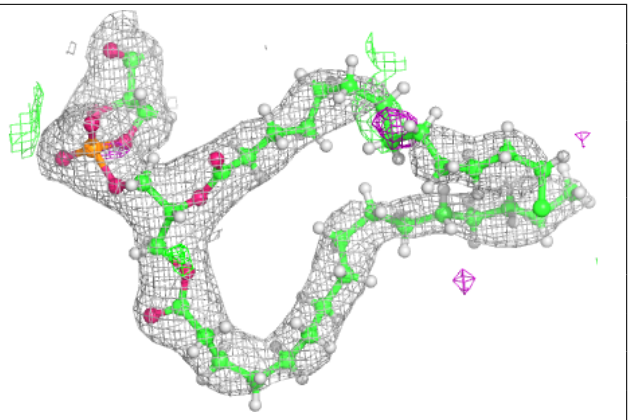


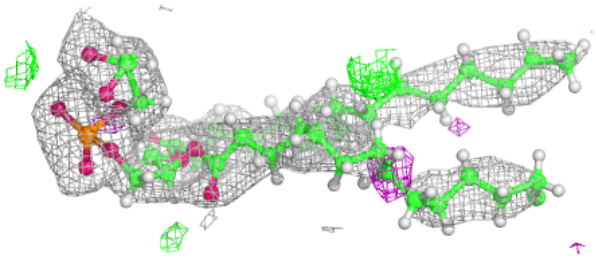


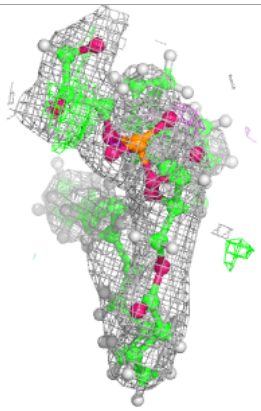


Electron density around LHG A 411:

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

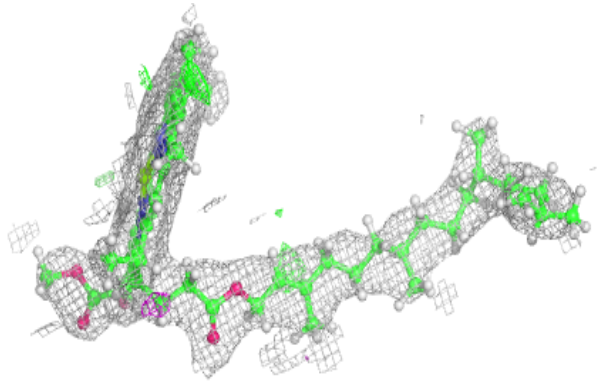


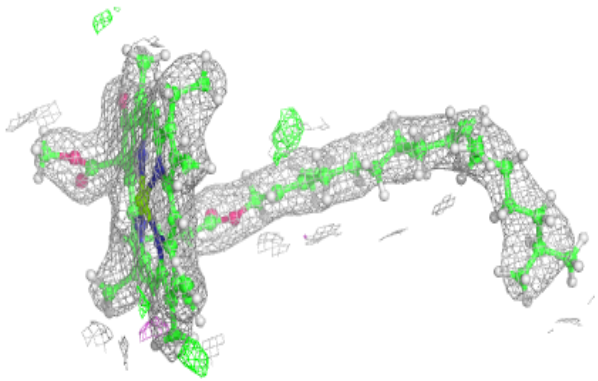


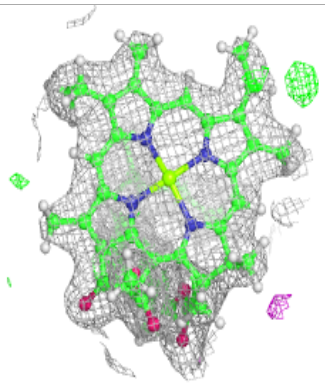


Electron density around CLA b 605:

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

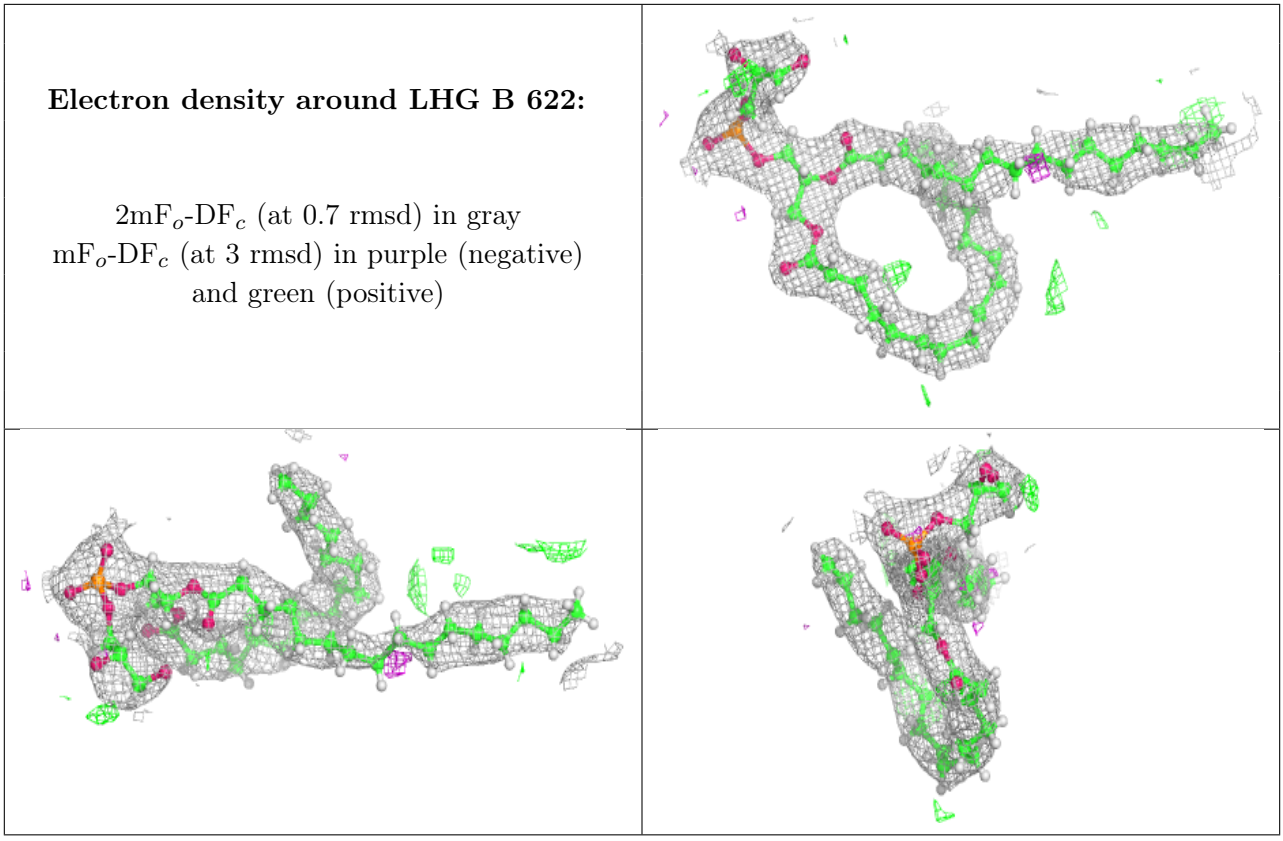






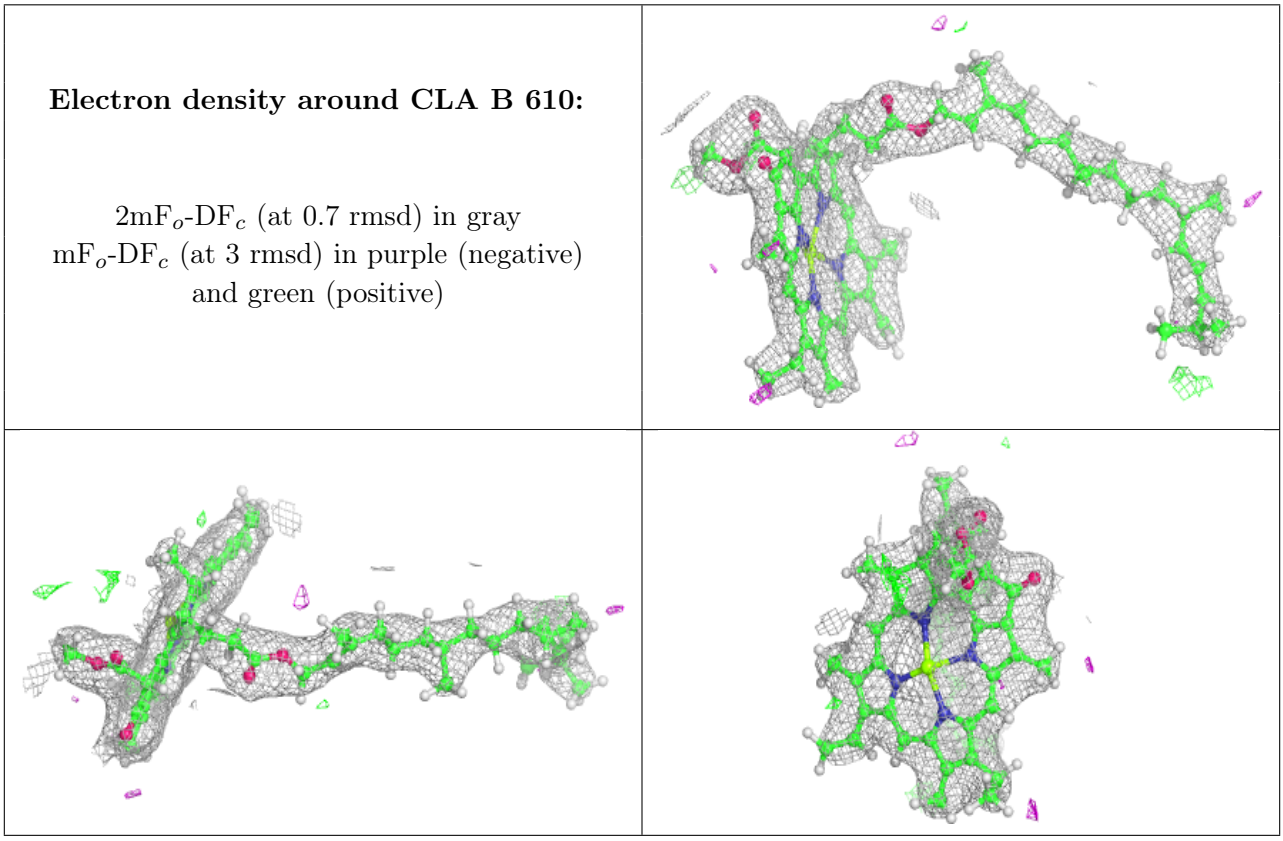
Electron density around LHG B 622:

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



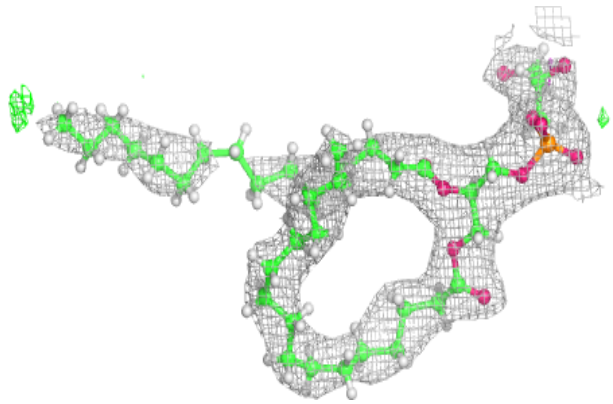
Electron density around CLA B 610:

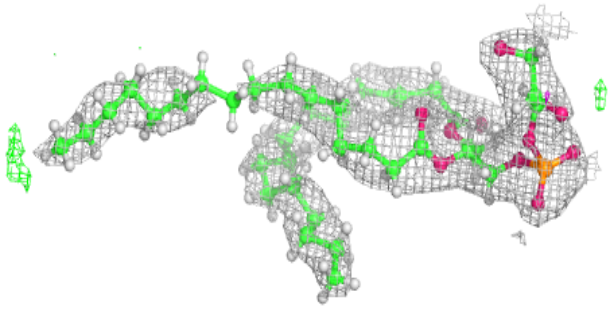
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

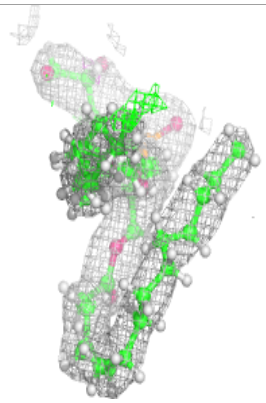


Electron density around LHG d 407:

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

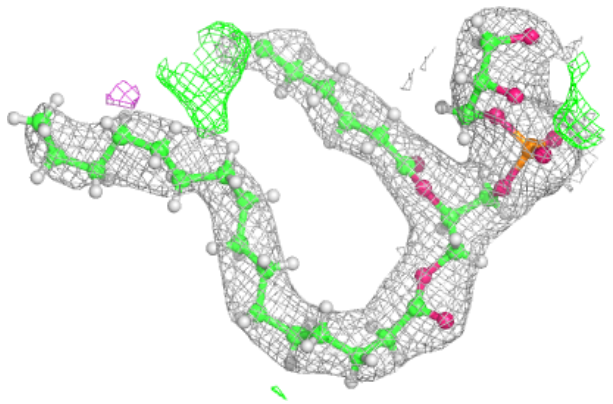


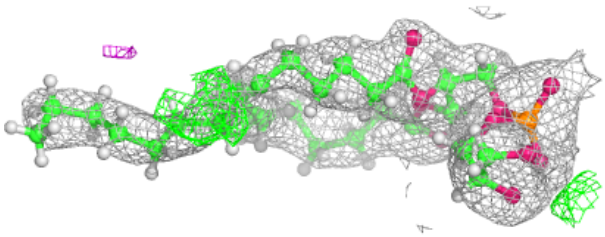


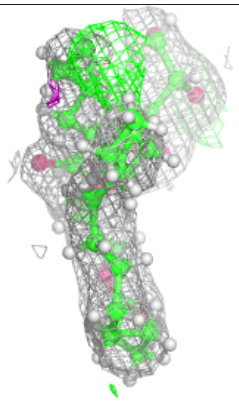


Electron density around LHG d 409:

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

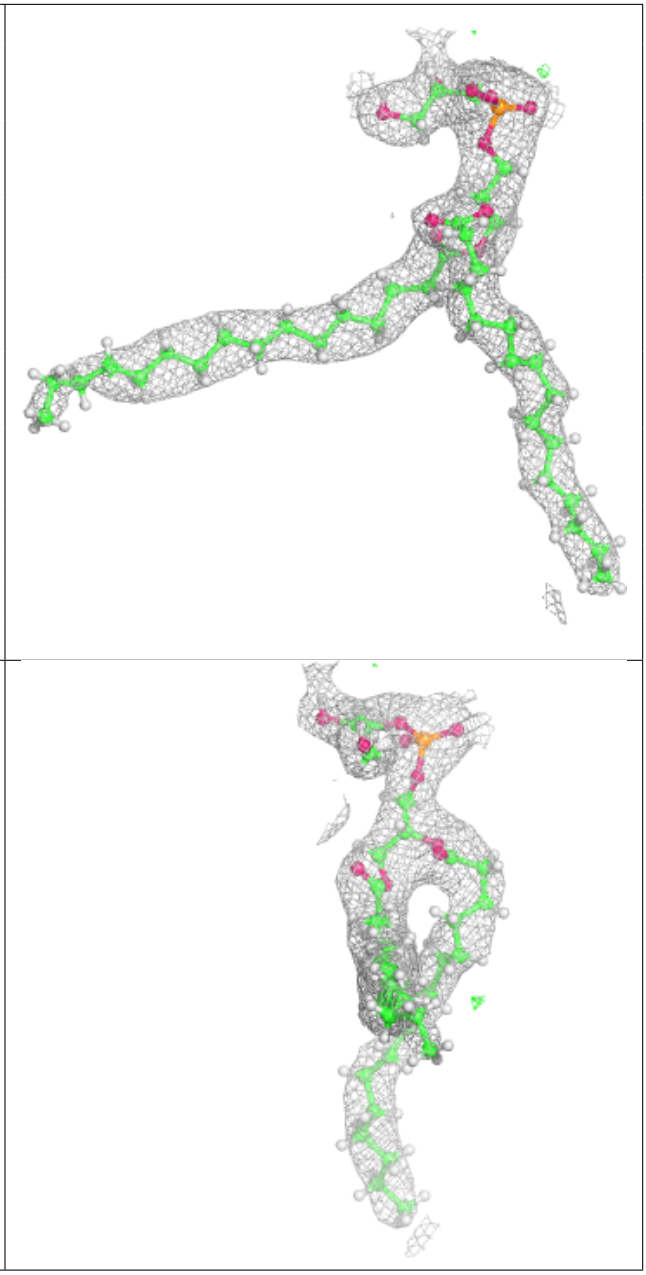






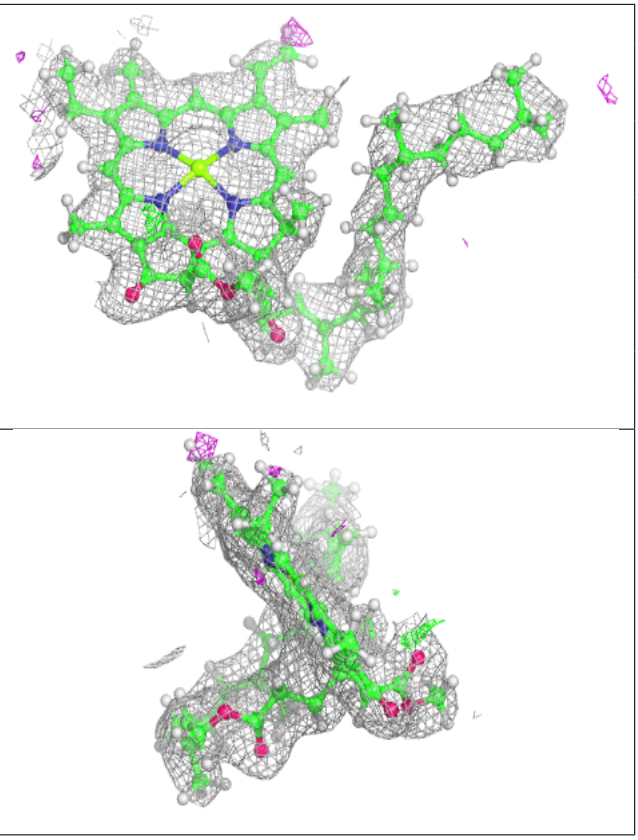
Electron density around LHG l 101:

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



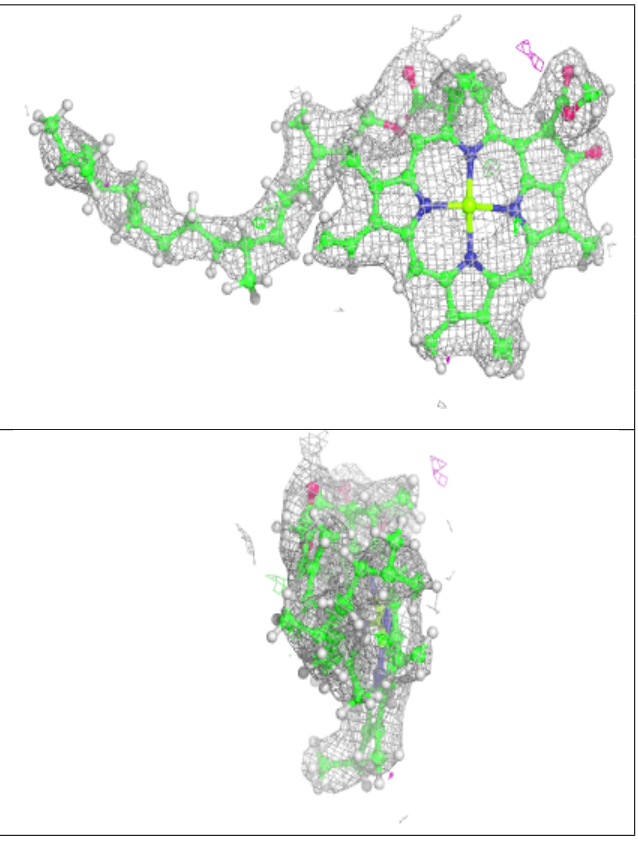
Electron density around CLA D 403:

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



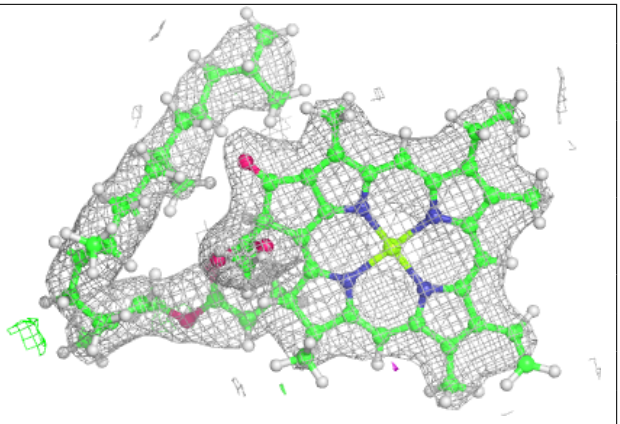
Electron density around CLA B 604:

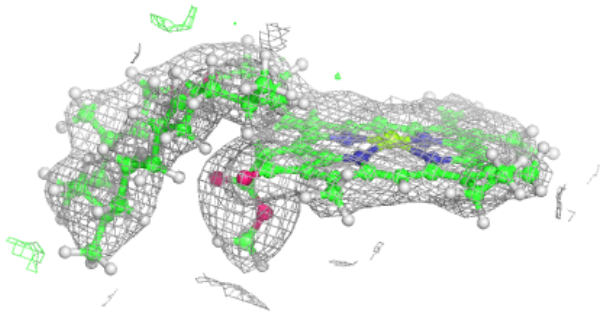
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

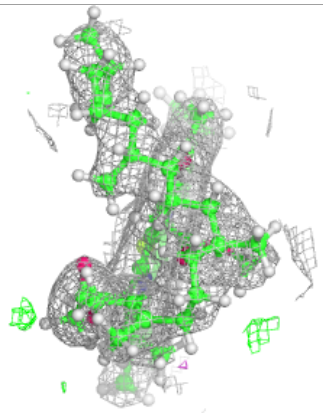


Electron density around CLA b 610:

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

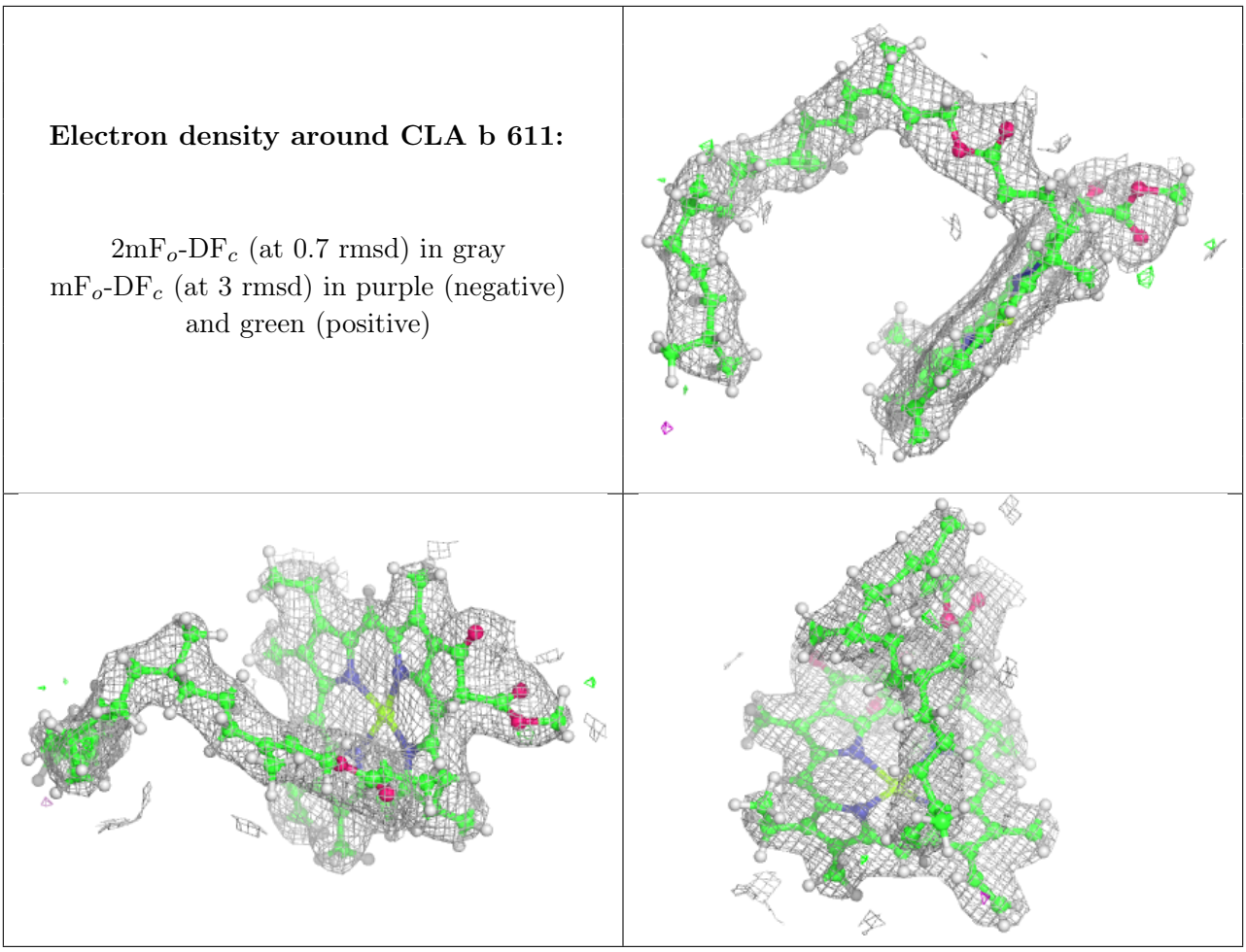






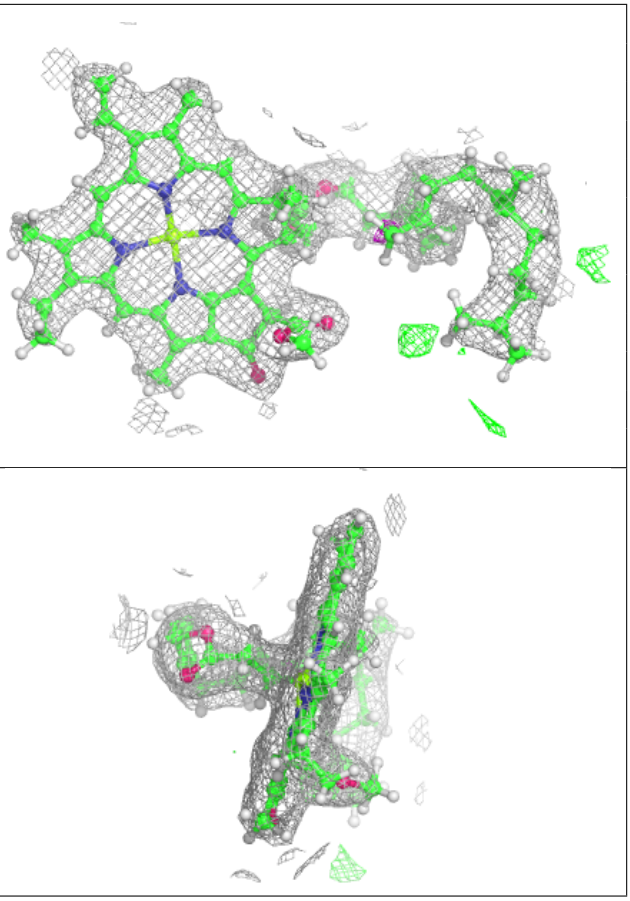
Electron density around CLA b 611:

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



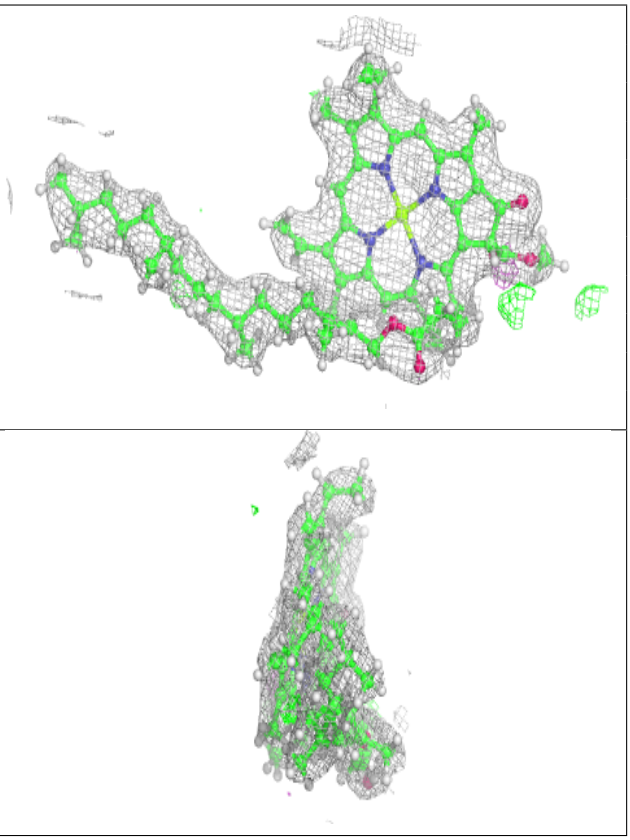
Electron density around CLA b 612:

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



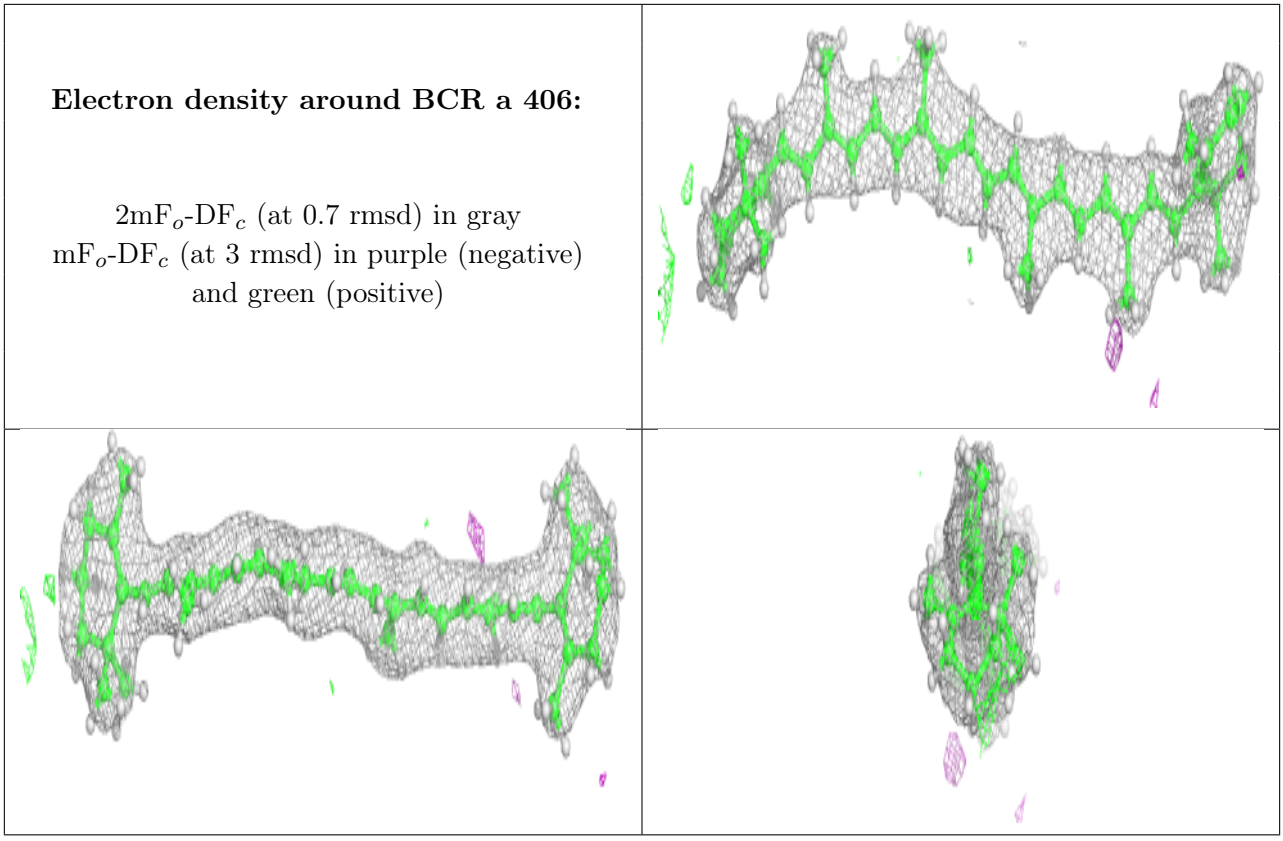
Electron density around CLA C 502:

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



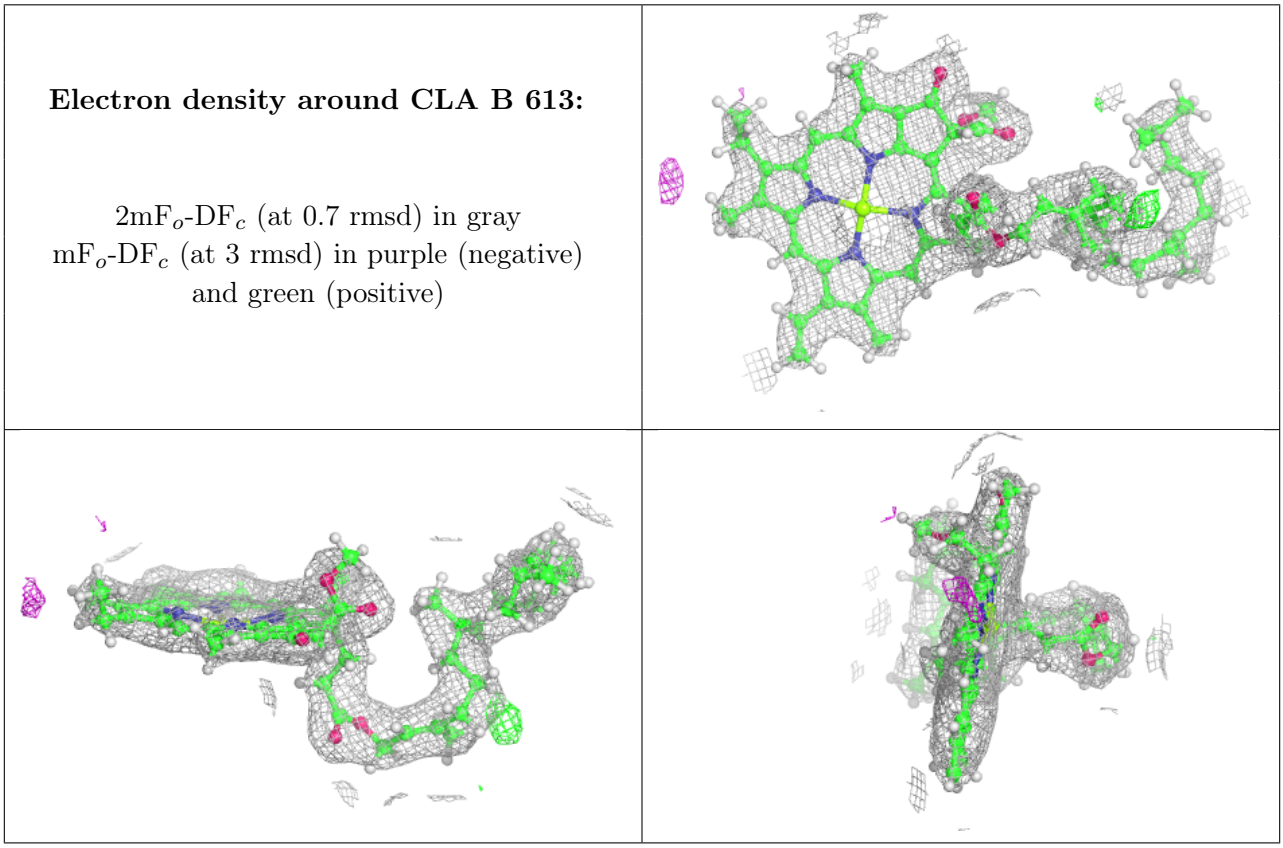
Electron density around BCR a 406:

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



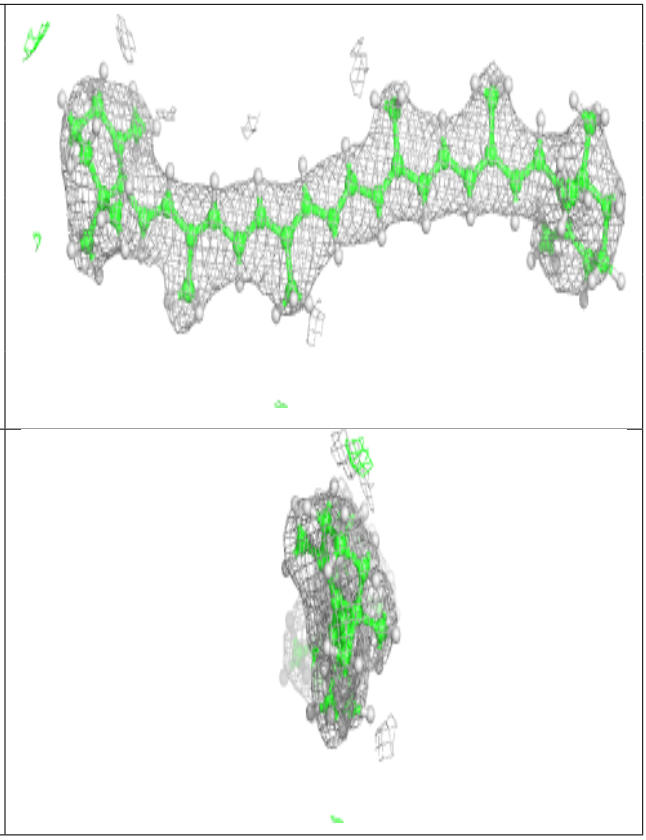
Electron density around CLA B 613:

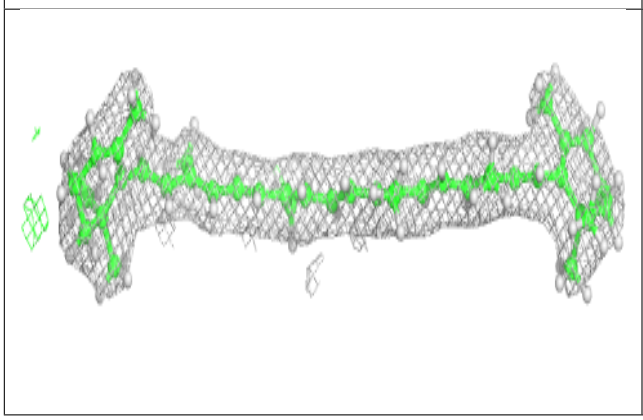
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCR b 618:

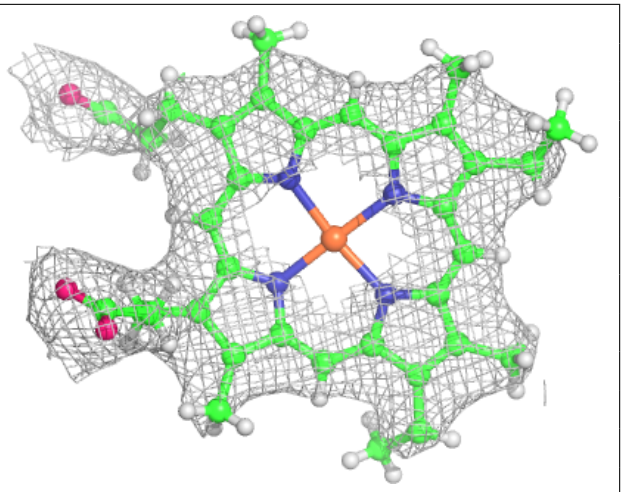
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

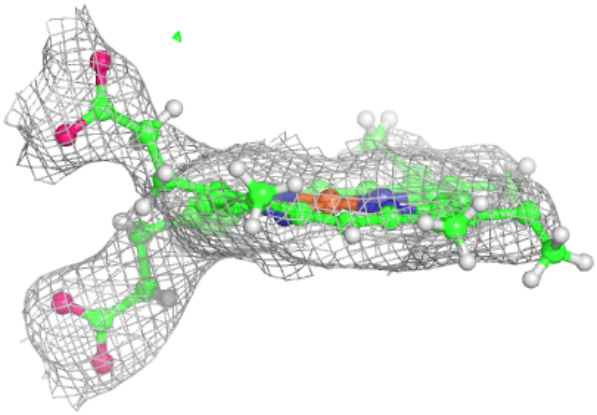


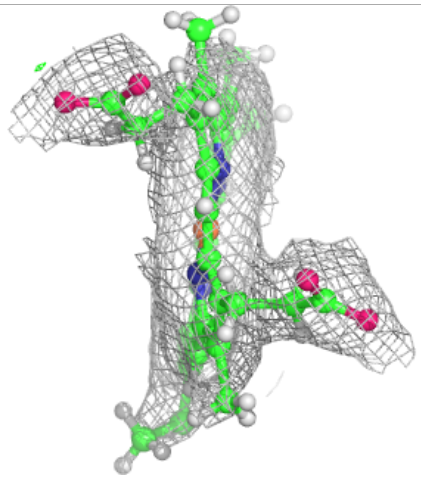


Electron density around HEC E 101:

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

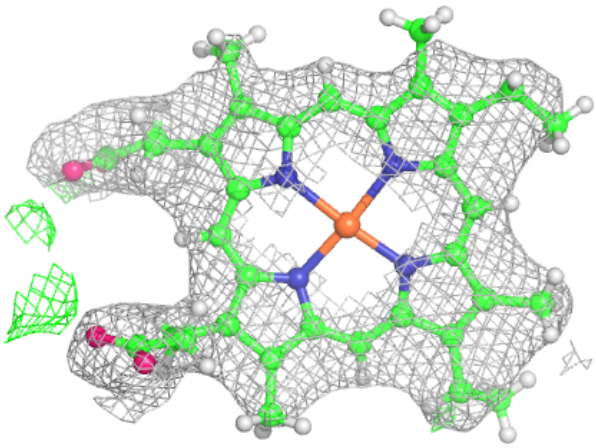


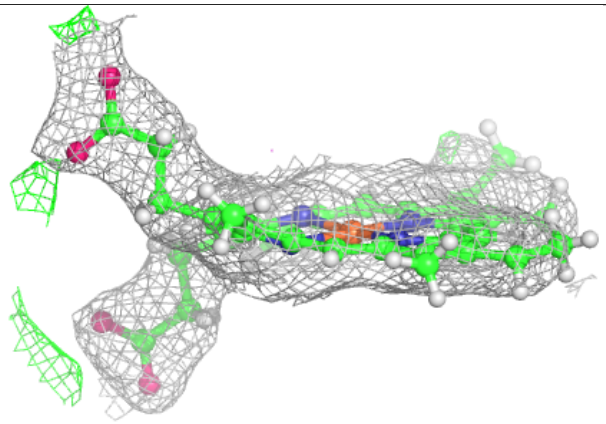


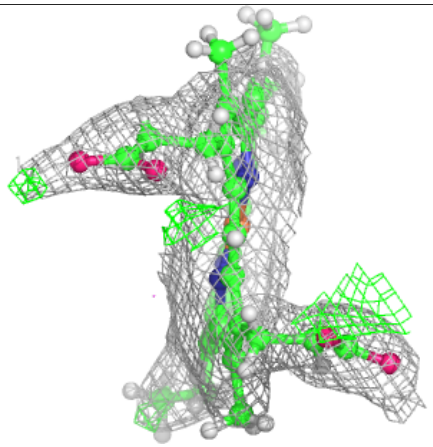


Electron density around HEC e 101:

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

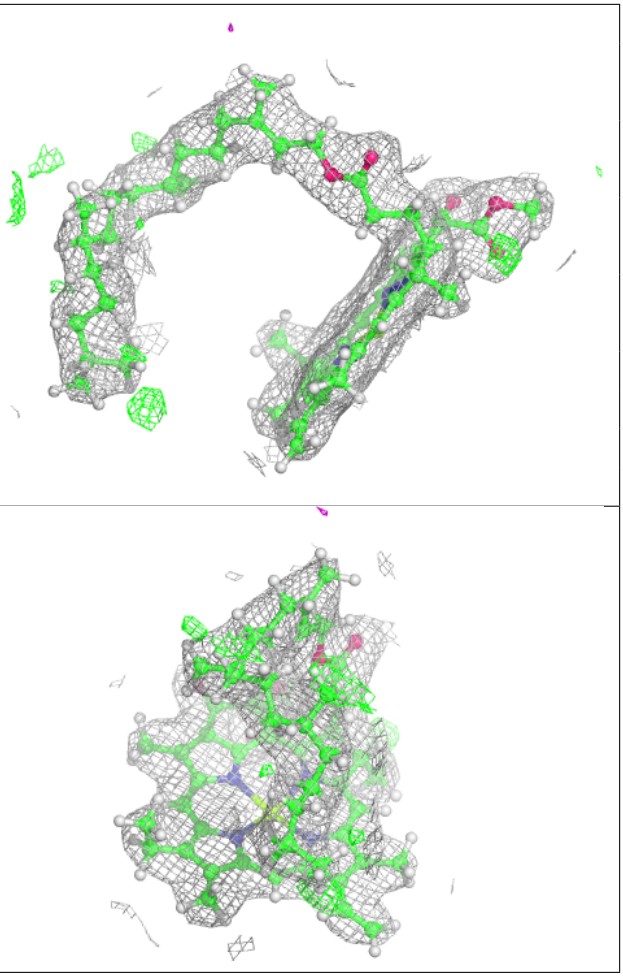






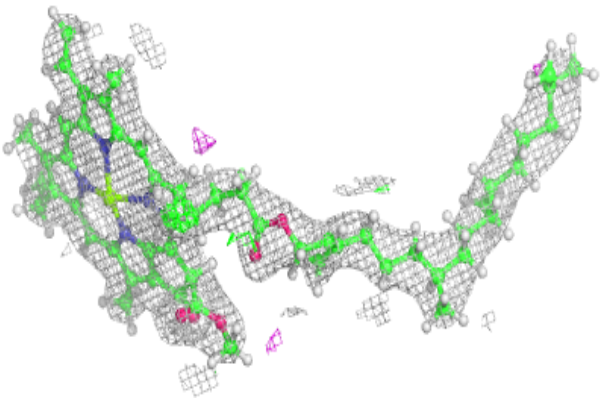
Electron density around CLA B 612:

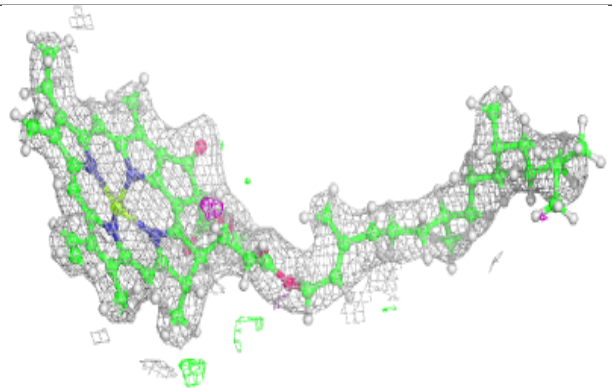
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

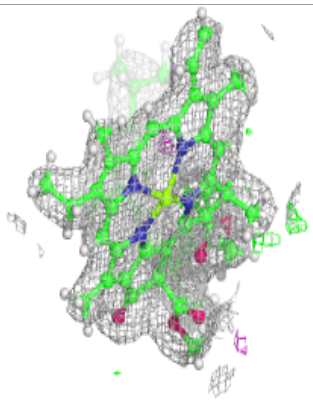


Electron density around CLA a 402:

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

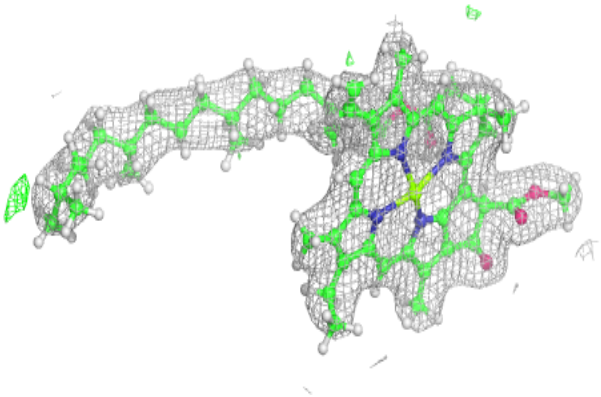


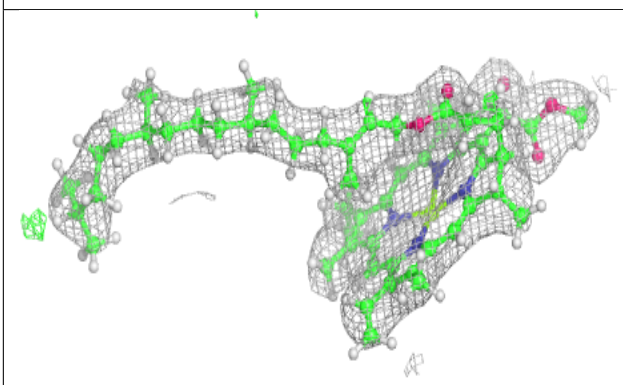


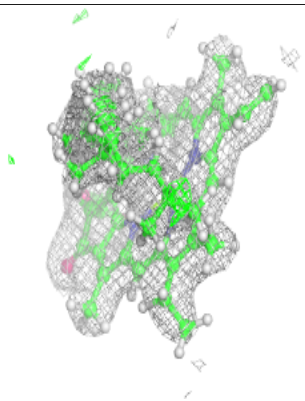


Electron density around CLA B 609:

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

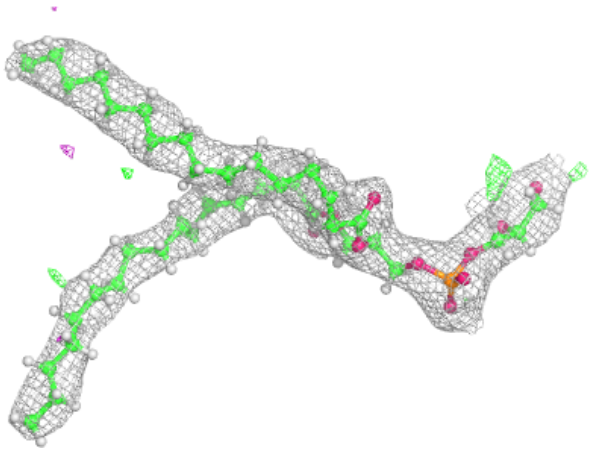


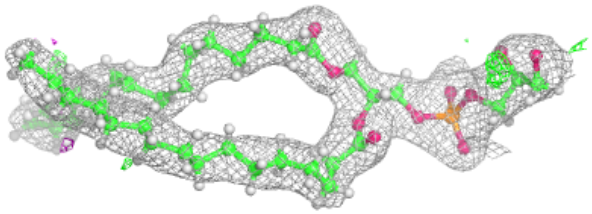


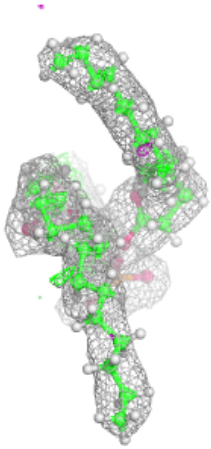


Electron density around LHG D 408:

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

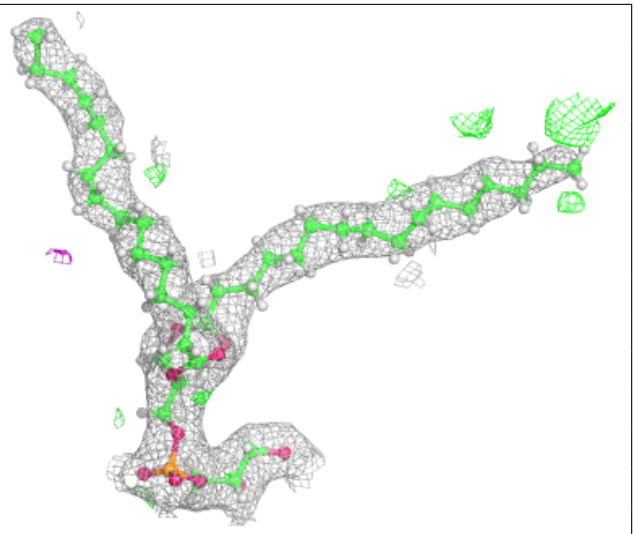


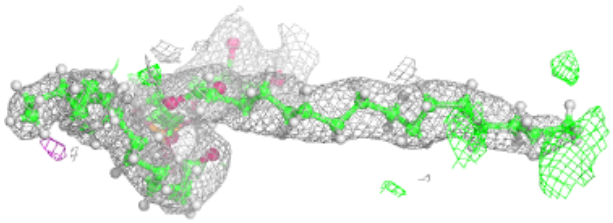


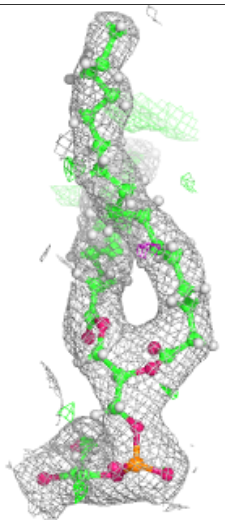


Electron density around LHG L 102:

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

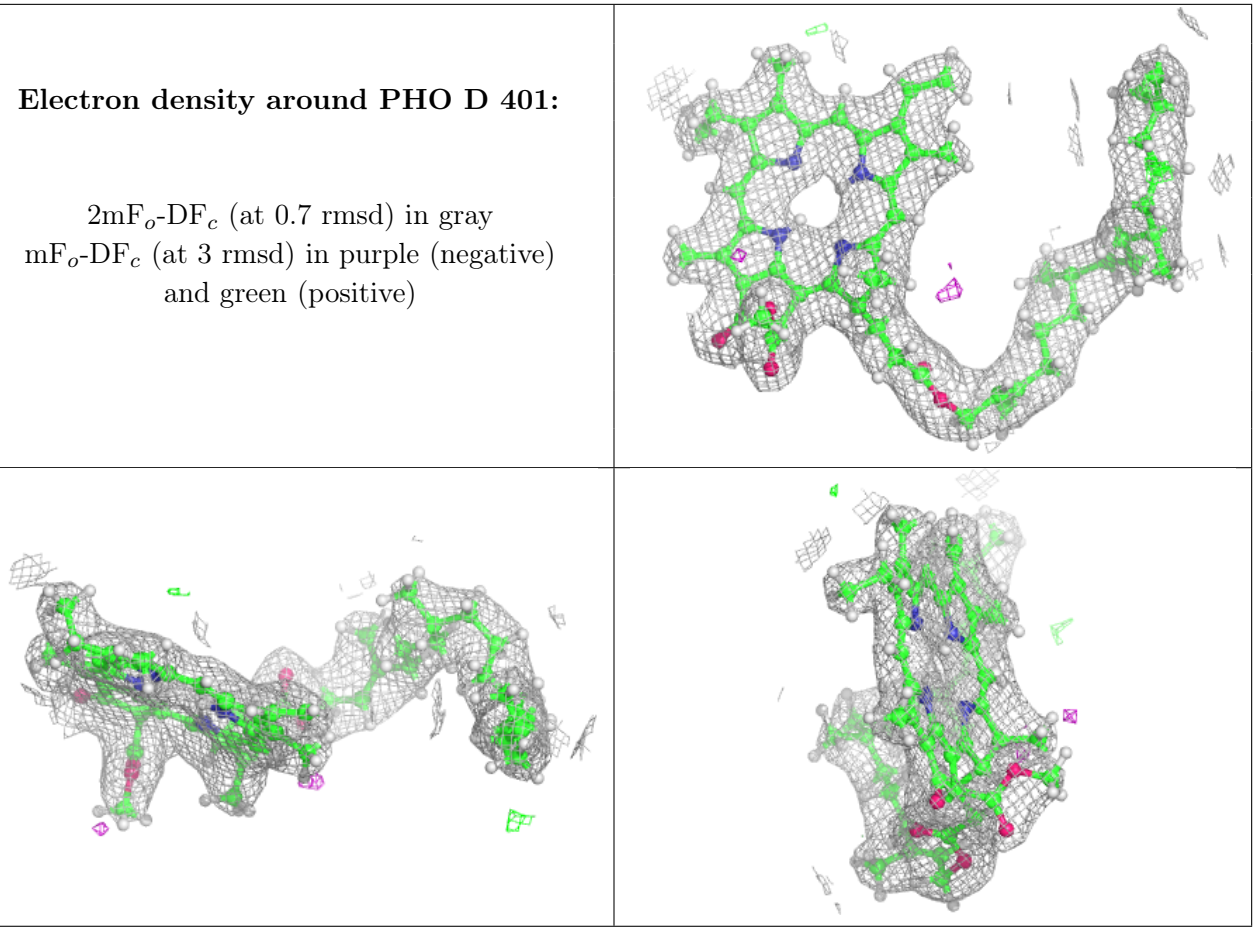






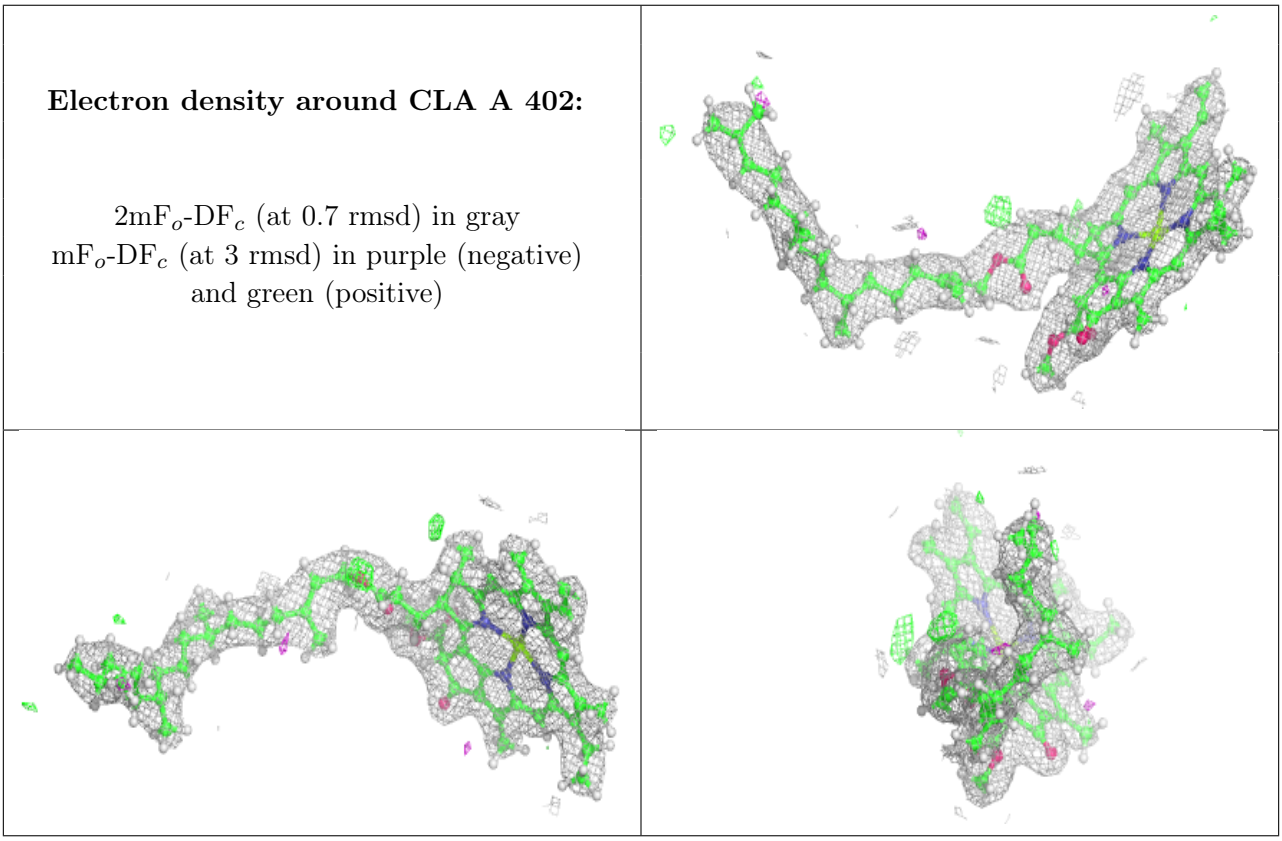
Electron density around PHO D 401:

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



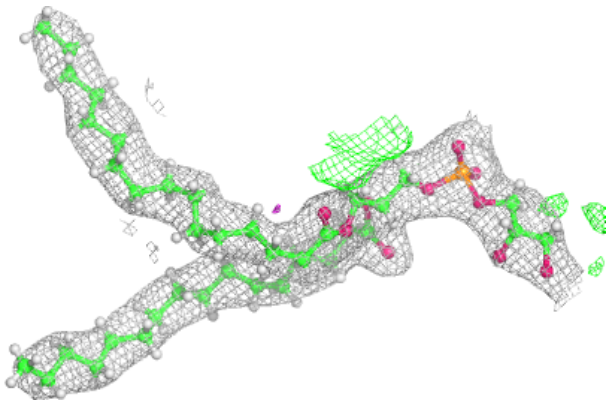
Electron density around CLA A 402:

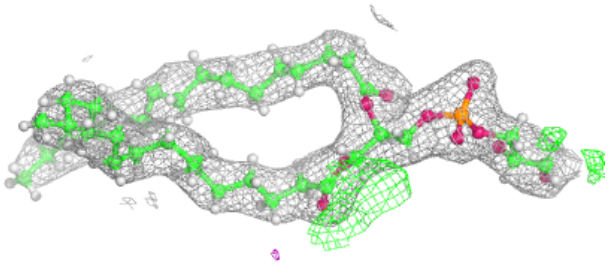
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

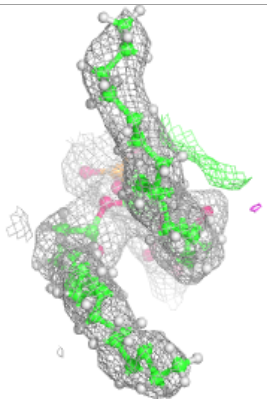


Electron density around LHG d 408:

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

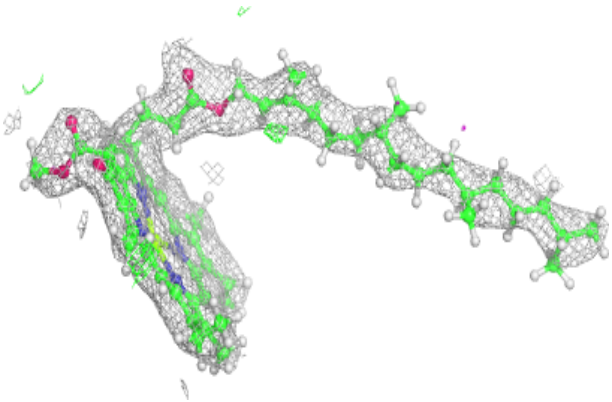


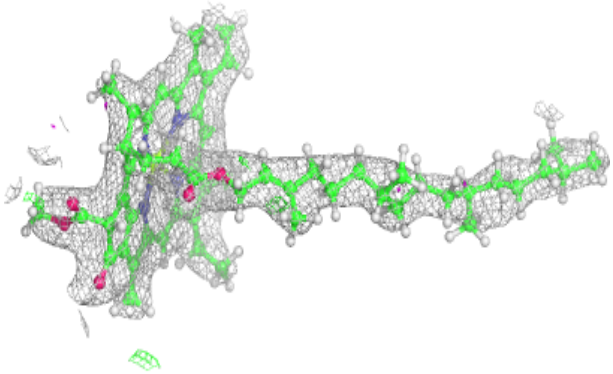


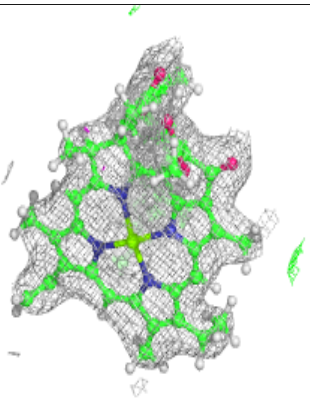


Electron density around CLA b 607:

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

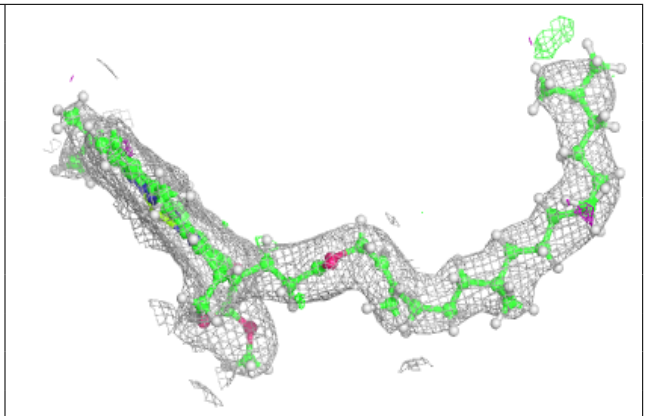


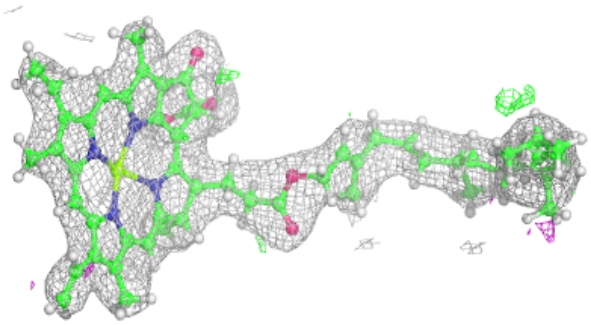


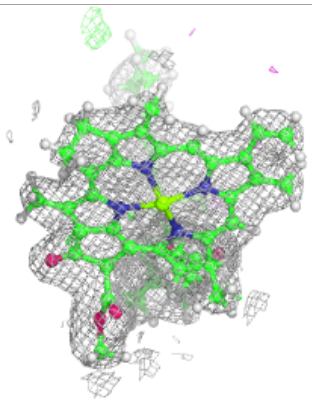


Electron density around CLA D 402:

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

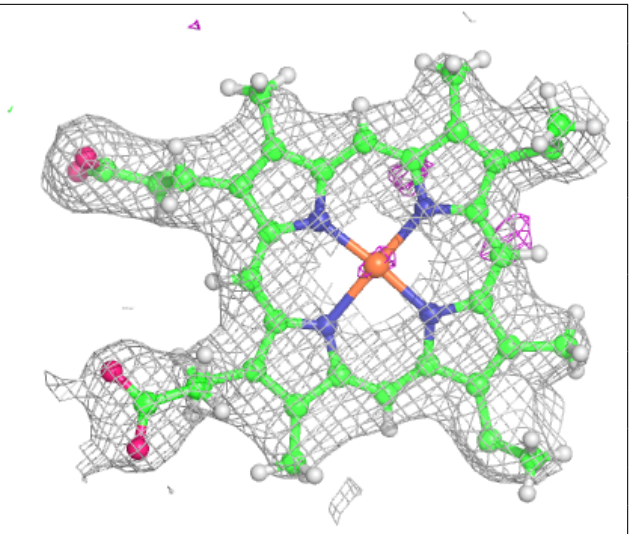


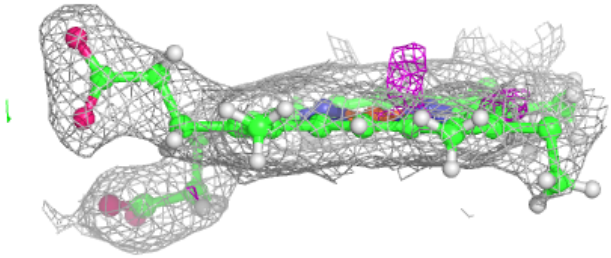


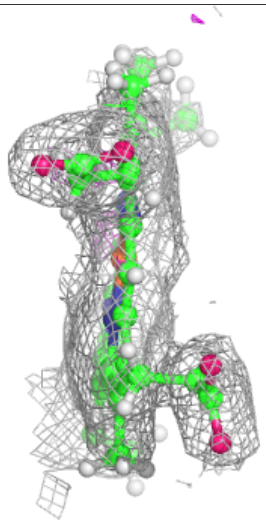


Electron density around HEC V 201:

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

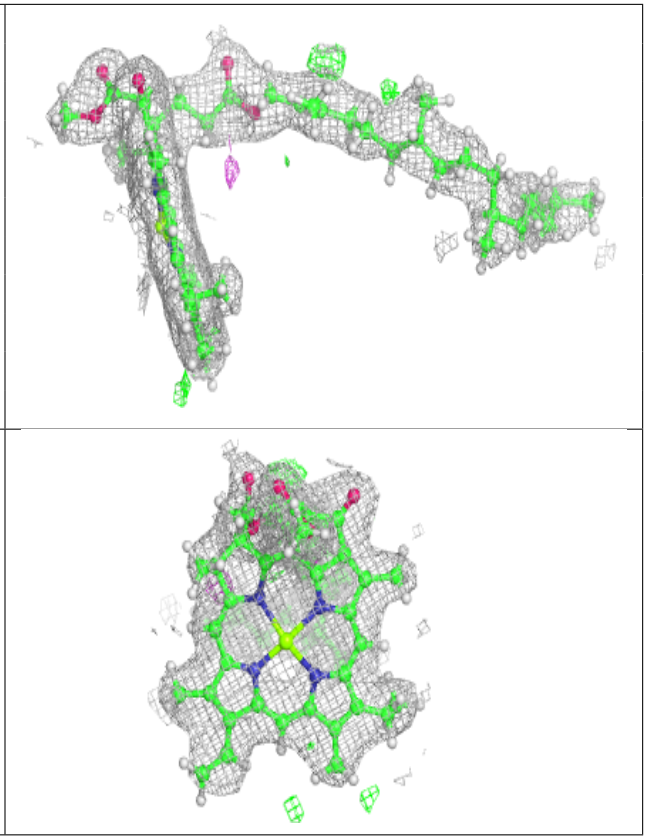


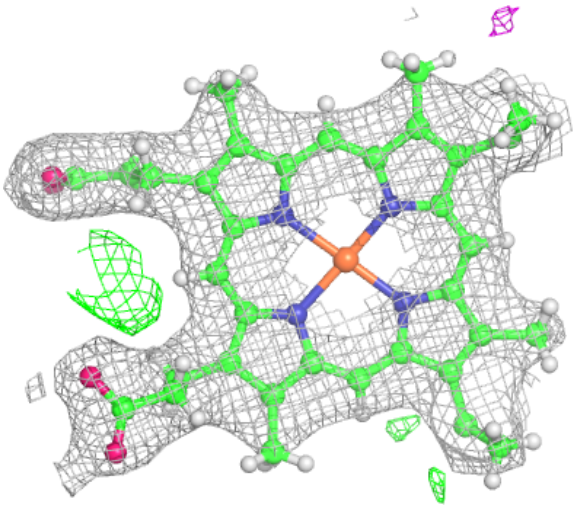
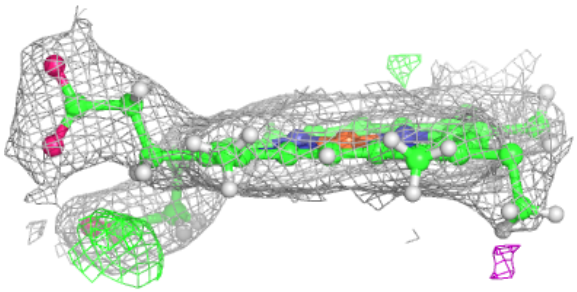
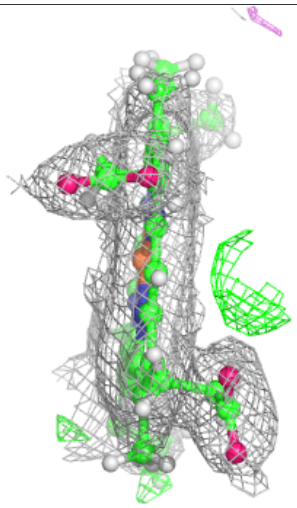




Electron density around CLA B 606:

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



Electron density around 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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.