Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 08:51 PM EDT

PDB ID	:	6W1Q
Title	:	RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 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	:	2.27 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:

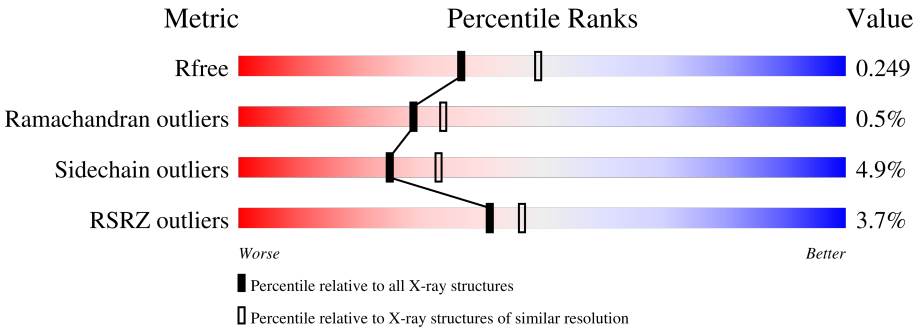
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

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 2.27 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	6980 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	344	% 94%
1	a	344	93%
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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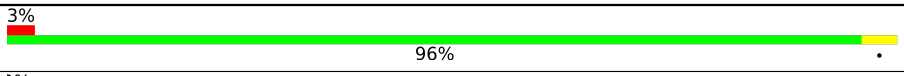
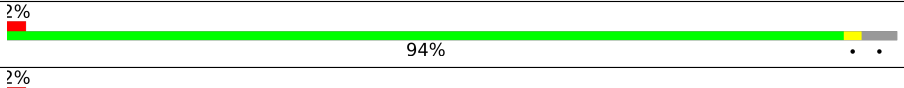
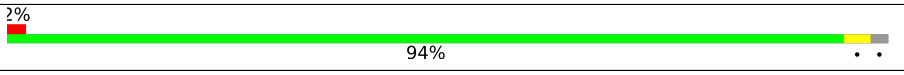
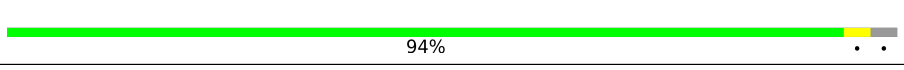
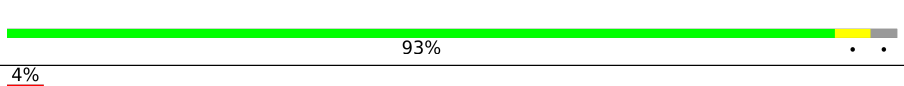
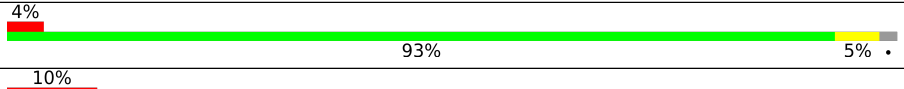
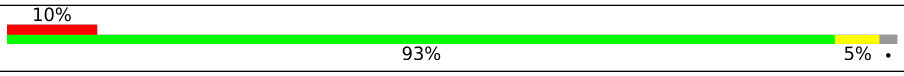
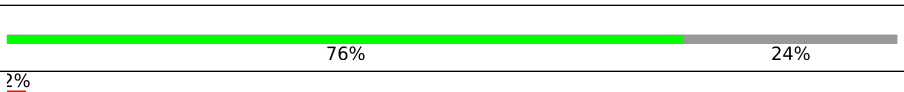
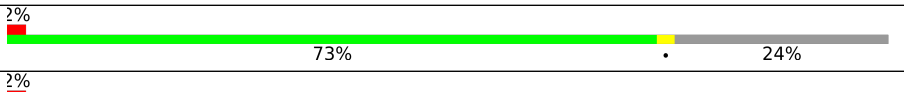
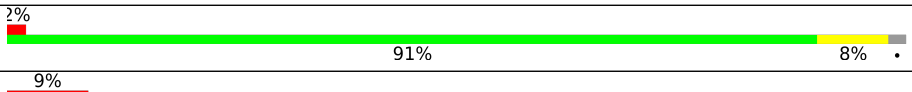
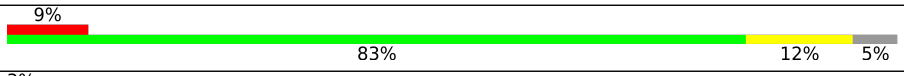
Mol	Chain	Length	Quality of chain
2	b	506	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
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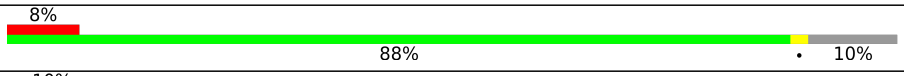
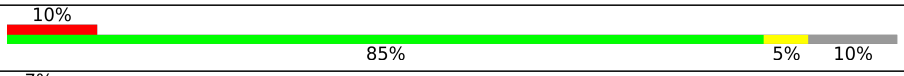
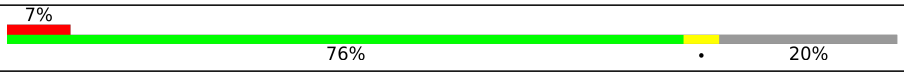
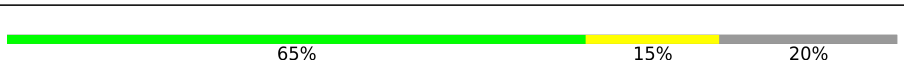
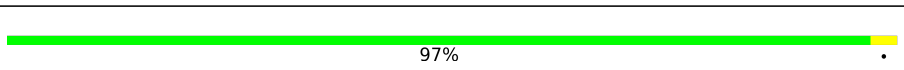
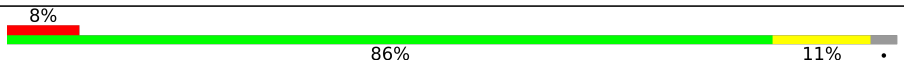
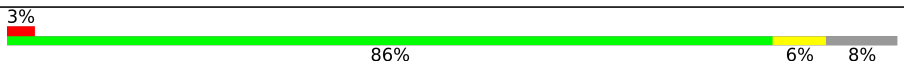
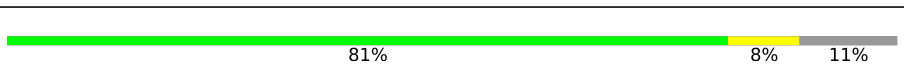
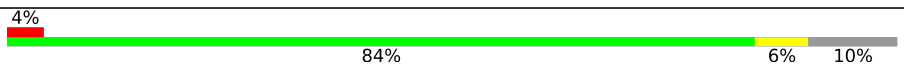
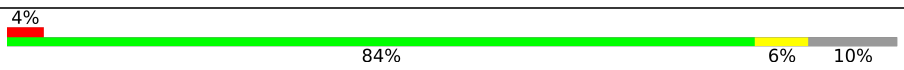
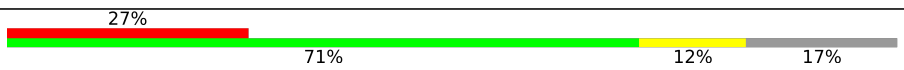
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	
14	r	41	

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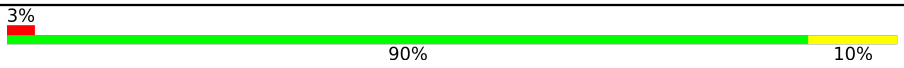
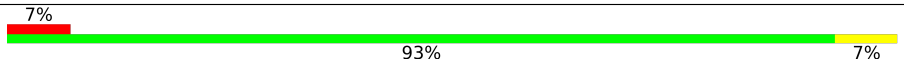
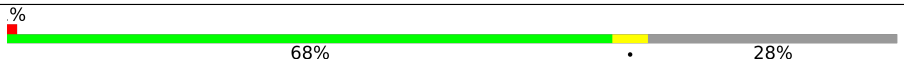
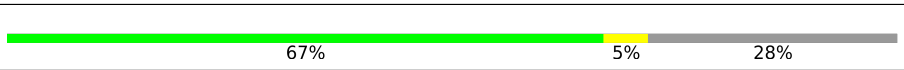
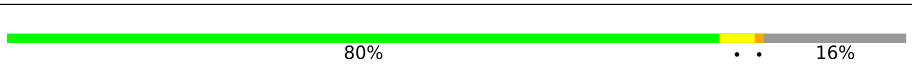
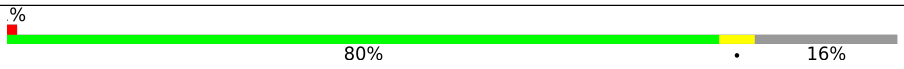
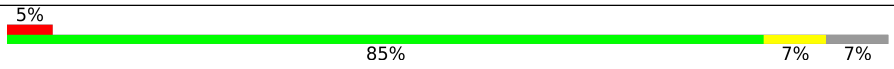
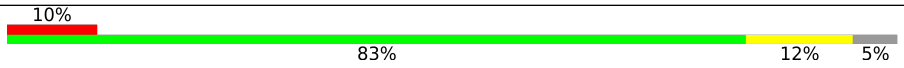
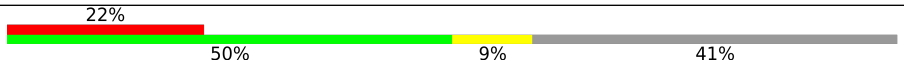
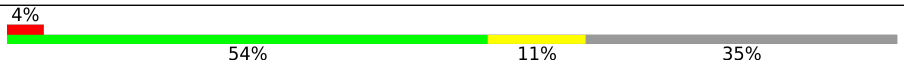
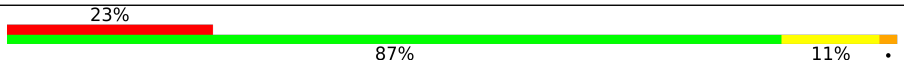
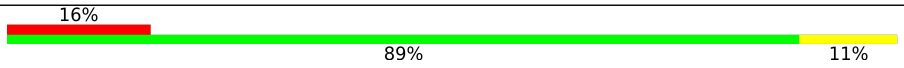
Mol	Chain	Length	Quality of chain
15	T	30	
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	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	609	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	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	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	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	H	101	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	-	-	-
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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	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	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	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	STE	a	412	-	-	-	X

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 103197 atoms, of which 51556 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
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6767	2249	3341	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	587	610	13			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	S	0	0	0
			1042	341	532	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

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
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

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

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

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

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
13	O	244	Total	C	H	N	O	S	0	1	0
			3698	1168	1828	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

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

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

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

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

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

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
16	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

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

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

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

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

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

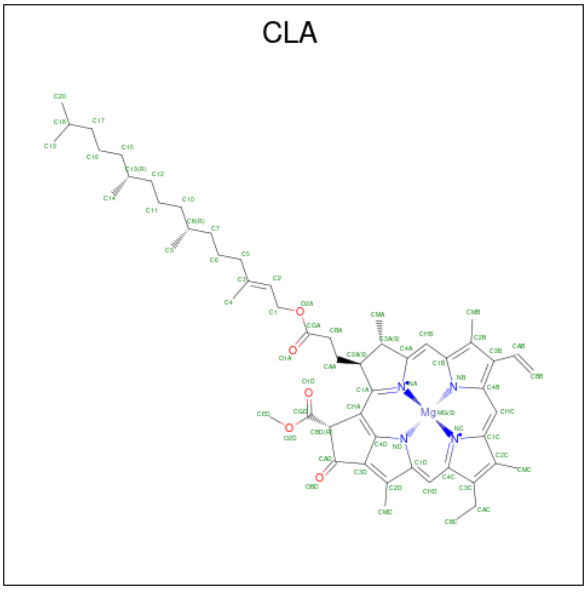
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		

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

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

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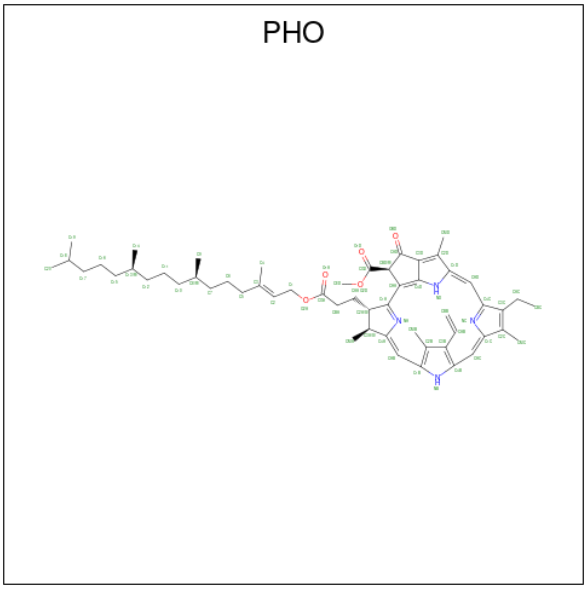
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total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

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

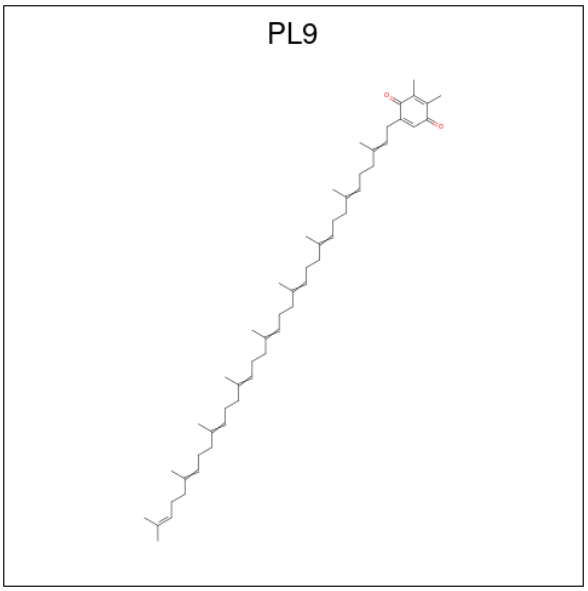


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

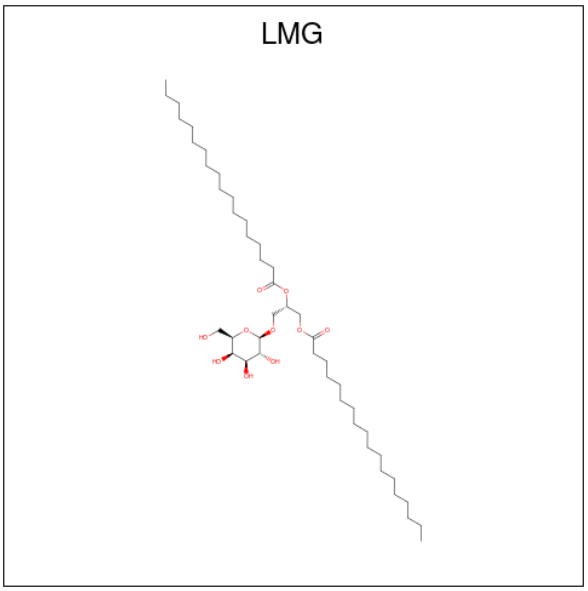
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 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
25	A	1	Total C H O 135 53 80 2	0	0
25	D	1	Total C H O 135 53 80 2	0	0
25	a	1	Total C H O 135 53 80 2	0	0
25	d	1	Total C H O 135 53 80 2	0	0

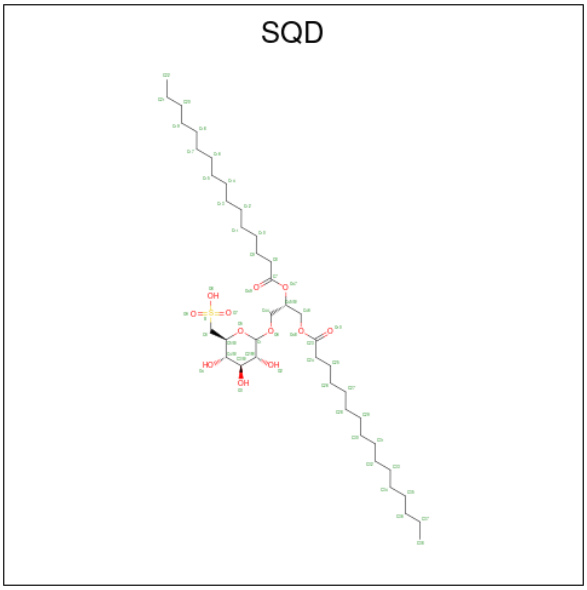
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			114	38	66	10		
26	B	1	Total	C	H	O	0	0
			68	24	40	4		
26	D	1	Total	C	H	O	0	0
			120	41	69	10		
26	D	1	Total	C	H	O	0	0
			78	27	45	6		
26	M	1	Total	C	H	O	0	0
			120	41	69	10		
26	Y	1	Total	C	H	O	0	0
			114	38	66	10		
26	a	1	Total	C	H	O	0	0
			140	45	85	10		
26	b	1	Total	C	H	O	0	0
			141	45	86	10		
26	c	1	Total	C	H	O	0	0
			79	27	42	10		
26	c	1	Total	C	H	O	0	0
			116	38	68	10		
26	c	1	Total	C	H	O	0	0
			117	39	68	10		
26	d	1	Total	C	H	O	0	0
			101	34	57	10		
26	m	1	Total	C	H	O	0	0
			122	41	71	10		

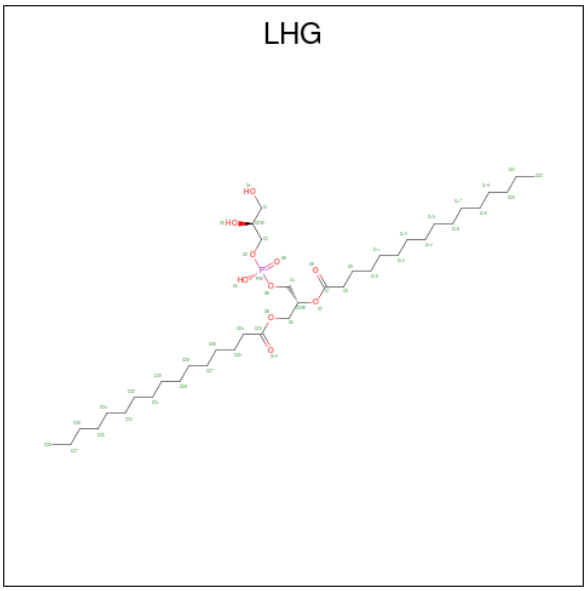
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



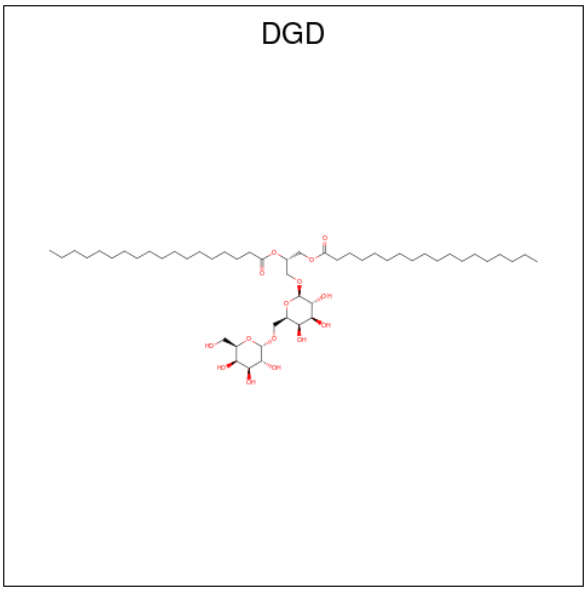
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C H O S 121 39 69 12 1	0	0
27	A	1	Total C H O 104 35 65 4	0	0
27	B	1	Total C H O S 131 41 77 12 1	0	0
27	D	1	Total C H O S 81 25 45 10 1	0	0
27	L	1	Total C H O S 114 36 65 12 1	0	0
27	a	1	Total C H O S 131 41 77 12 1	0	0
27	f	1	Total C H O S 89 28 48 12 1	0	0
27	t	1	Total C H O 92 31 56 5	0	0

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



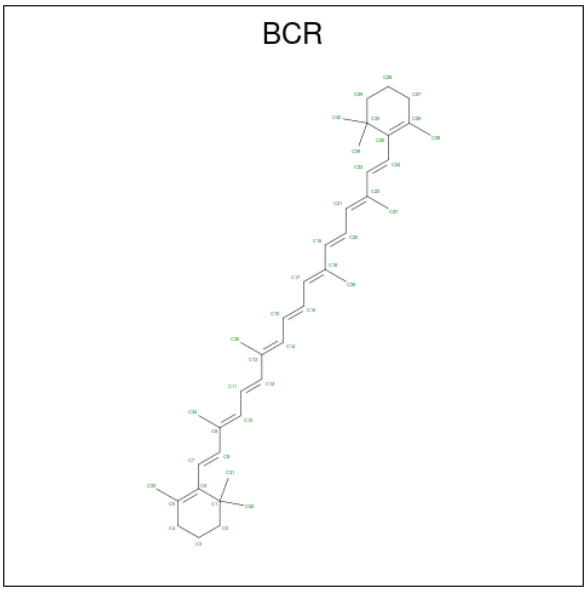
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	D	1	Total	C	H	O	P	0	0
			113	36	66	10	1		
28	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	b	1	Total	C	H	O	P	0	0
			122	38	73	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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			160	51	94	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			141	47	79	15		
29	H	1	Total	C	H	O	0	0
			139	47	77	15		
29	c	1	Total	C	H	O	0	0
			141	47	79	15		
29	c	1	Total	C	H	O	0	0
			140	47	78	15		
29	c	1	Total	C	H	O	0	0
			139	47	77	15		
29	h	1	Total	C	H	O	0	0
			141	47	79	15		

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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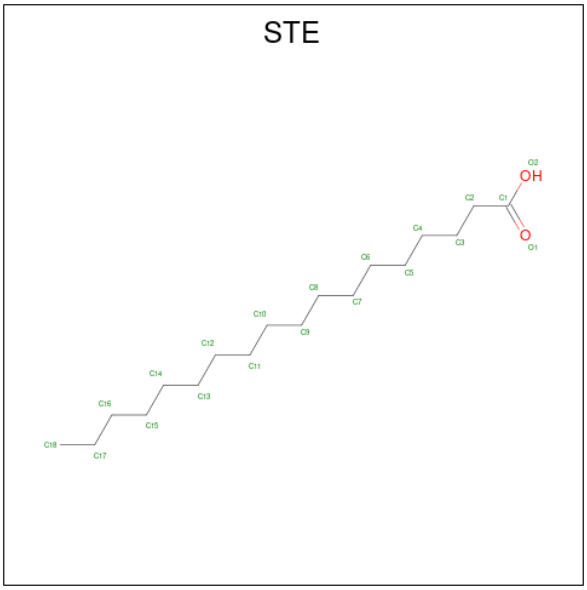
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	b	1	Total C H 96 40 56	0	0
30	c	1	Total C H 96 40 56	0	0
30	d	1	Total C H 96 40 56	0	0
30	k	1	Total C H 96 40 56	0	0
30	k	1	Total C H 96 40 56	0	0
30	k	1	Total C H 96 40 56	0	0
30	t	1	Total C H 96 40 56	0	0
30	x	1	Total C H 96 40 56	0	0

- Molecule 31 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C H O 43 15 26 2	0	0
31	B	1	Total C H O 28 10 16 2	0	0
31	B	1	Total C H O 46 16 28 2	0	0

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

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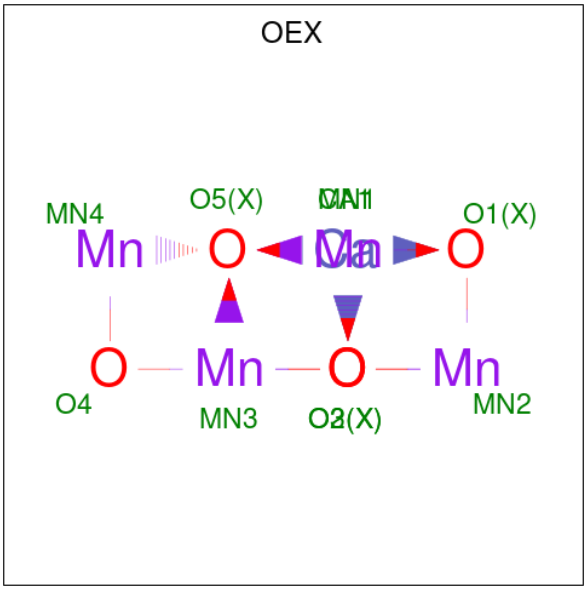
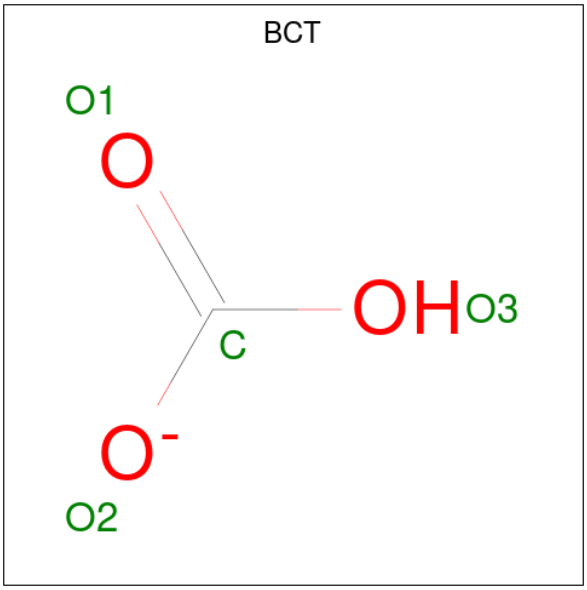
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	b	1	Total C H 41 14 27	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	j	1	Total C H O 28 10 16 2	0	0
31	k	1	Total C H O 28 10 16 2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

- Molecule 32 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



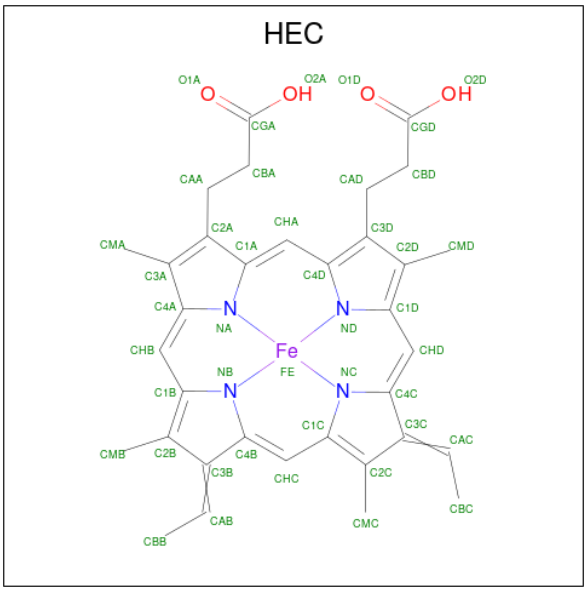
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	C	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
32	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	d	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	V	1	Total	Na	0	0
			1	1		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	112	Total	O	0	0
			112	112		
36	B	142	Total	O	0	0
			142	142		
36	C	125	Total	O	0	0
			125	125		
36	D	96	Total	O	0	0
			96	96		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	E	22	Total O 22 22	0	0
36	F	6	Total O 6 6	0	0
36	H	16	Total O 16 16	0	0
36	I	10	Total O 10 10	0	0
36	J	14	Total O 14 14	0	0
36	K	3	Total O 3 3	0	0
36	L	10	Total O 10 10	0	0
36	M	9	Total O 9 9	0	0
36	O	60	Total O 60 60	0	0
36	R	11	Total O 11 11	0	0
36	T	8	Total O 8 8	0	0
36	U	28	Total O 28 28	0	0
36	V	49	Total O 49 49	0	0
36	X	10	Total O 10 10	0	0
36	Y	2	Total O 2 2	0	0
36	Z	7	Total O 7 7	0	0
36	a	96	Total O 96 96	0	0
36	b	116	Total O 116 116	0	0
36	c	108	Total O 108 108	0	0
36	d	87	Total O 87 87	0	0
36	e	11	Total O 11 11	0	0

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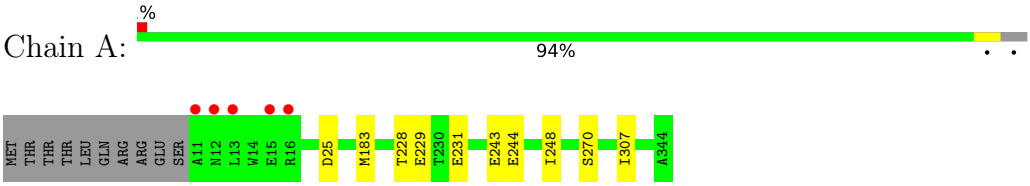
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	f	7	Total O 7 7	0	0
36	h	17	Total O 17 17	0	0
36	i	14	Total O 14 14	0	0
36	j	8	Total O 8 8	0	0
36	k	7	Total O 7 7	0	0
36	l	11	Total O 11 11	0	0
36	m	4	Total O 4 4	0	0
36	o	67	Total O 67 67	0	0
36	r	3	Total O 3 3	0	0
36	t	8	Total O 8 8	0	0
36	u	34	Total O 34 34	0	0
36	v	30	Total O 30 30	0	0
36	x	6	Total O 6 6	0	0
36	y	12	Total O 12 12	0	0
36	z	6	Total O 6 6	0	0

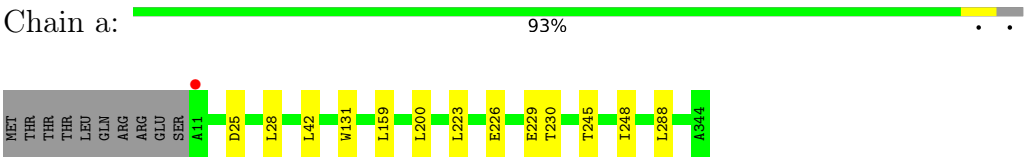
3 Residue-property plots (i)

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

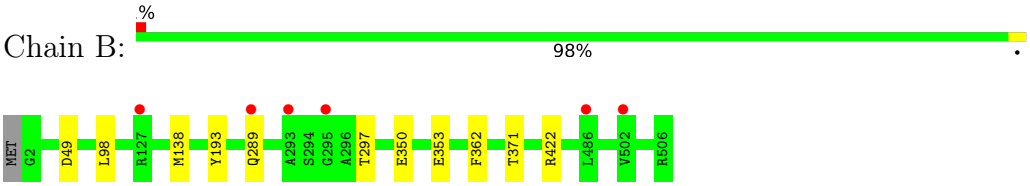
• Molecule 1: Photosystem II protein D1 1



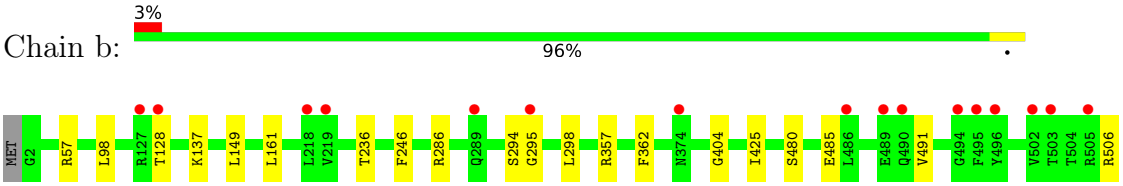
• Molecule 1: Photosystem II protein D1 1



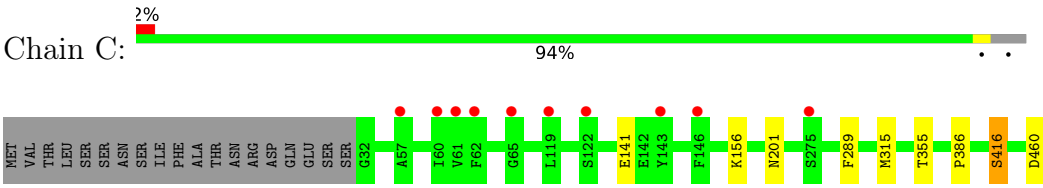
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

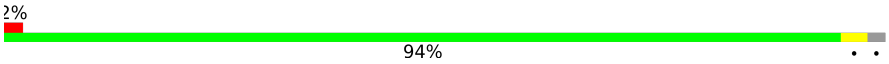


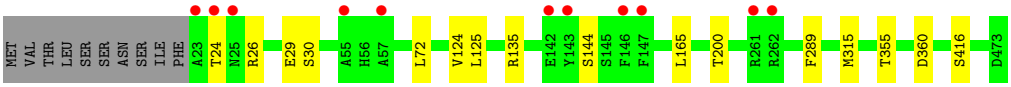
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

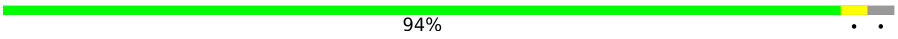
Chain c:

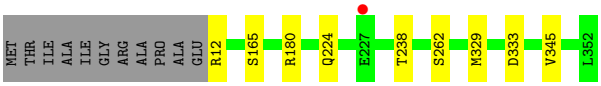




• Molecule 4: Photosystem II D2 protein

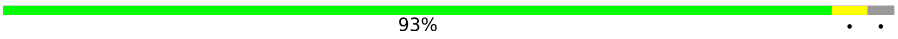
Chain D:

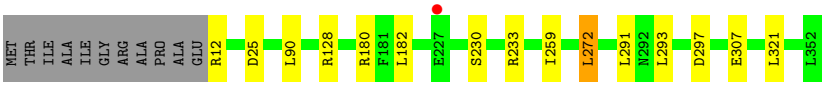




• Molecule 4: Photosystem II D2 protein

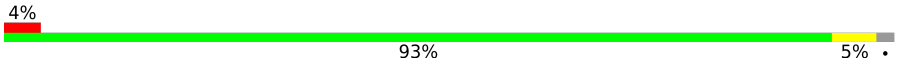
Chain d:





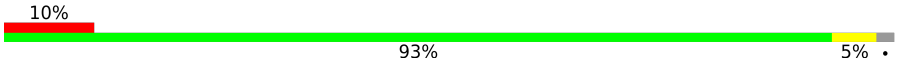
• Molecule 5: Cytochrome b559 subunit alpha

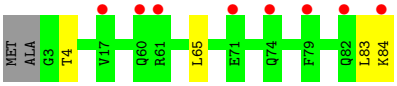
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



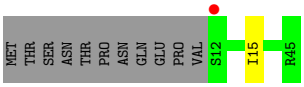


• Molecule 6: Cytochrome b559 subunit beta

Chain F:

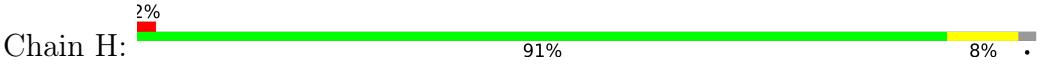
• Molecule 6: Cytochrome b559 subunit beta

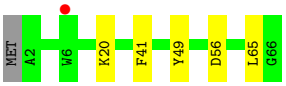
Chain f:



• Molecule 7: Photosystem II reaction center protein H

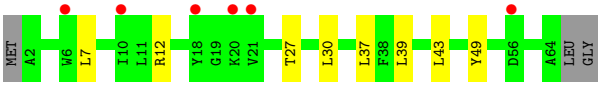
Chain H:





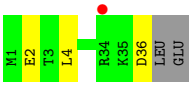
• Molecule 7: Photosystem II reaction center protein H

Chain h:



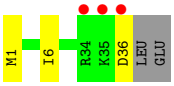
• Molecule 8: Photosystem II reaction center protein I

Chain I:



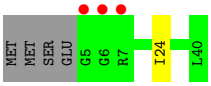
• Molecule 8: Photosystem II reaction center protein I

Chain i:



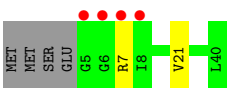
• Molecule 9: Photosystem II reaction center protein J

Chain J:



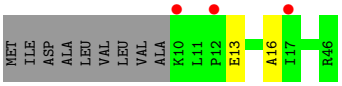
• Molecule 9: Photosystem II reaction center protein J

Chain j:



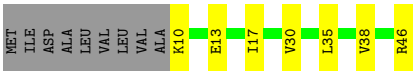
• Molecule 10: Photosystem II reaction center protein K

Chain K:



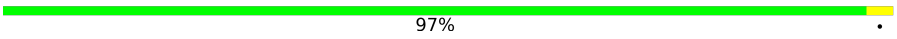
• Molecule 10: Photosystem II reaction center protein K

Chain k:



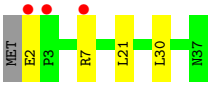
• Molecule 11: Photosystem II reaction center protein L

Chain L:



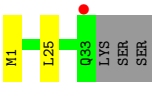
• Molecule 11: Photosystem II reaction center protein L

Chain l:



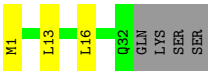
• Molecule 12: Photosystem II reaction center protein M

Chain M:



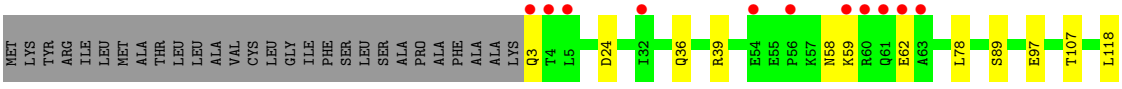
• Molecule 12: Photosystem II reaction center protein M

Chain m:



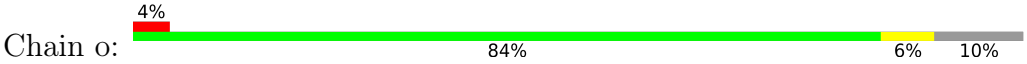
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

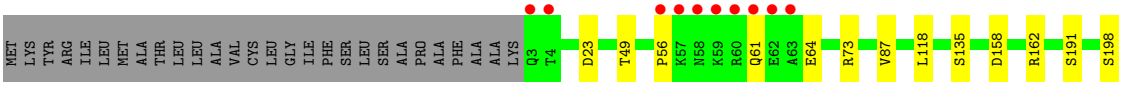
Chain O:

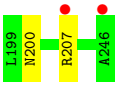


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

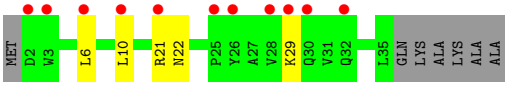






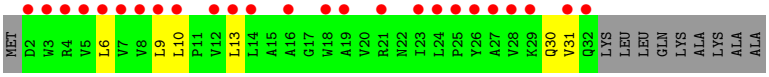
• Molecule 14: Photosystem II protein Y

Chain R:



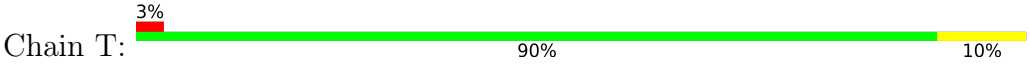
• Molecule 14: Photosystem II protein Y

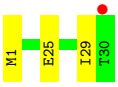
Chain r:



• Molecule 15: Photosystem II reaction center protein T

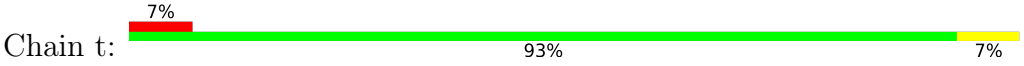
Chain T:





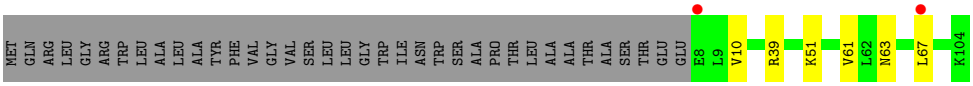
• Molecule 15: Photosystem II reaction center protein T

Chain t:



• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:



• Molecule 16: Photosystem II 12 kDa extrinsic protein

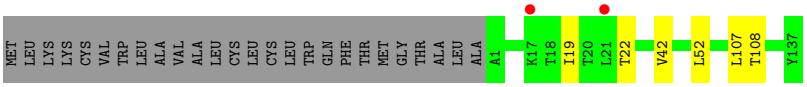
Chain u:

• Molecule 17: Cytochrome c-550

Chain V:

• Molecule 17: Cytochrome c-550

Chain v:

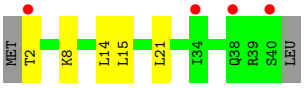


• Molecule 18: Photosystem II reaction center X protein

Chain X:

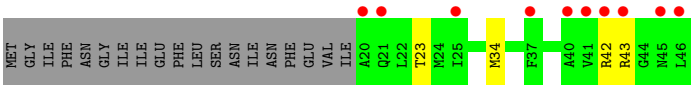
• Molecule 18: Photosystem II reaction center X protein

Chain x:



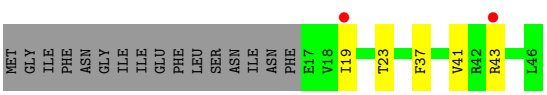
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



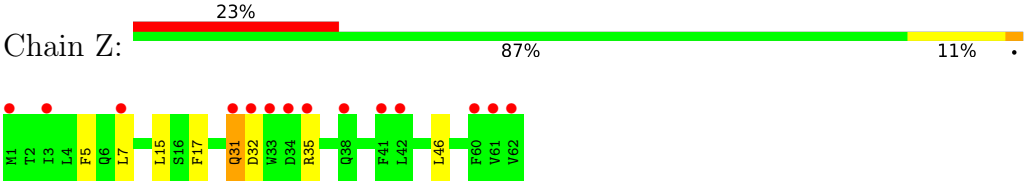
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:



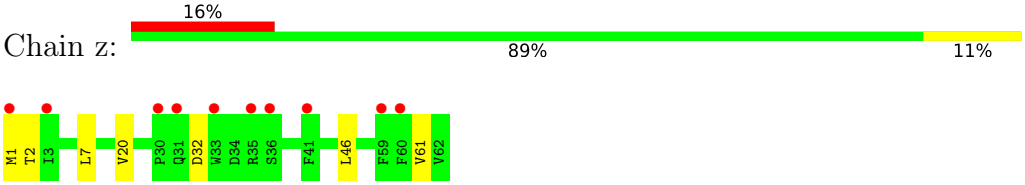
• Molecule 20: Photosystem II reaction center protein Z

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	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.3 (33.45-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.178 , 0.249 0.178 , 0.249	Depositor DCC
R_{free} test set	3275 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.1	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	103197	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: FE2, STE, BCR, PL9, CLA, LMG, CL, LHG, NA, OEX, HEC, BCT, SQD, DGD, PHO, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.70	0/2707	0.75	2/3692 (0.1%)
1	a	0.71	0/2704	0.73	2/3688 (0.1%)
2	B	0.70	1/4161 (0.0%)	0.72	2/5669 (0.0%)
2	b	0.67	0/4118	0.72	1/5611 (0.0%)
3	C	0.67	1/3547 (0.0%)	0.72	1/4830 (0.0%)
3	c	0.64	0/3619	0.72	1/4926 (0.0%)
4	D	0.72	0/2812	0.73	2/3832 (0.1%)
4	d	0.70	0/2821	0.75	4/3844 (0.1%)
5	E	0.64	0/688	0.65	0/940
5	e	0.60	0/683	0.65	0/932
6	F	0.53	0/284	0.62	0/387
6	f	0.50	0/284	0.67	0/387
7	H	0.70	1/523 (0.2%)	0.73	0/713
7	h	0.60	0/511	0.72	0/697
8	I	0.67	0/293	0.72	0/396
8	i	0.69	0/293	0.69	0/396
9	J	0.58	0/263	0.67	0/356
9	j	0.57	0/263	0.63	0/356
10	K	0.64	0/303	0.67	0/416
10	k	0.52	0/303	0.64	0/416
11	L	0.69	0/311	0.77	0/422
11	l	0.75	0/303	0.73	0/412
12	M	0.68	0/249	0.66	0/341
12	m	0.73	0/244	0.77	0/334
13	O	0.66	0/1904	0.77	0/2585
13	o	0.69	0/1905	0.81	2/2583 (0.1%)
14	R	0.50	0/277	0.60	0/380
14	r	0.43	0/246	0.54	0/339
15	T	0.83	0/257	0.80	0/349
15	t	0.78	0/255	0.67	0/346
16	U	0.60	0/785	0.71	0/1064
16	u	0.67	0/785	0.78	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	V	0.62	0/1085	0.74	1/1473 (0.1%)
17	v	0.59	0/1085	0.71	0/1473
18	X	0.62	0/284	0.74	0/384
18	x	0.51	0/289	0.68	0/391
19	Y	0.49	0/197	0.71	0/264
19	y	0.41	0/219	0.59	0/294
20	Z	0.50	0/490	0.60	0/669
20	z	0.49	0/488	0.59	0/666
All	All	0.67	3/42838 (0.0%)	0.72	18/58317 (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
16	u	0	1
17	V	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-7.38	1.17	1.34
2	B	193	TYR	CD2-CE2	-6.56	1.29	1.39
7	H	41	PHE	CB-CG	-5.27	1.42	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	57	ARG	NE-CZ-NH1	-7.43	116.59	120.30
17	V	63	THR	C-N-CD	-7.34	104.45	120.60
3	C	460	ASP	CB-CG-OD1	6.72	124.35	118.30
4	d	128	ARG	NE-CZ-NH2	-6.60	117.00	120.30
13	o	162	ARG	NE-CZ-NH2	6.60	123.60	120.30
13	o	158	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	183	MET	CA-CB-CG	6.51	124.36	113.30
4	d	297	ASP	CB-CG-OD1	6.36	124.02	118.30
4	d	272	LEU	CB-CG-CD1	-5.94	100.90	111.00
2	B	422	ARG	NE-CZ-NH1	-5.76	117.42	120.30
4	D	333	ASP	CB-CG-OD2	-5.76	113.12	118.30
4	D	333	ASP	CB-CG-OD1	5.70	123.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	49	ASP	CB-CG-OD1	5.53	123.28	118.30
3	c	360	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	a	25	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	25	ASP	CB-CG-OD1	5.23	123.01	118.30
4	d	272	LEU	CA-CB-CG	5.18	127.22	115.30
1	a	131	TRP	CA-CB-CG	-5.11	103.99	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	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	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
1	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100
2	B	508/506 (100%)	494 (97%)	14 (3%)	0	100	100
2	b	503/506 (99%)	484 (96%)	16 (3%)	3 (1%)	25	29
3	C	442/461 (96%)	423 (96%)	18 (4%)	1 (0%)	47	57
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	47	57
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	327 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	81/84 (96%)	78 (96%)	2 (2%)	1 (1%)	13 12
5	e	80/84 (95%)	78 (98%)	1 (1%)	1 (1%)	12 11
6	F	32/45 (71%)	32 (100%)	0	0	100 100
6	f	32/45 (71%)	28 (88%)	4 (12%)	0	100 100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100 100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100 100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100 100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100 100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100 100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100 100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	4 2
10	k	35/46 (76%)	32 (91%)	2 (6%)	1 (3%)	4 2
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%)	29 (97%)	1 (3%)	0	100 100
13	O	243/272 (89%)	227 (93%)	13 (5%)	3 (1%)	13 12
13	o	242/272 (89%)	224 (93%)	15 (6%)	3 (1%)	13 12
14	R	32/41 (78%)	31 (97%)	1 (3%)	0	100 100
14	r	29/41 (71%)	25 (86%)	2 (7%)	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%)	89 (94%)	5 (5%)	1 (1%)	14 14
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22 25
17	v	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22 25
18	X	36/41 (88%)	36 (100%)	0	0	100 100
18	x	37/41 (90%)	37 (100%)	0	0	100 100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	3 1
19	y	28/46 (61%)	20 (71%)	6 (21%)	2 (7%)	1 0
20	Z	60/62 (97%)	56 (93%)	2 (3%)	2 (3%)	4 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	z	60/62 (97%)	53 (88%)	5 (8%)	2 (3%)	4 2
All	All	5240/5688 (92%)	5024 (96%)	189 (4%)	27 (0%)	29 34

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	58	ASN
13	O	62	GLU
17	V	64	PRO
20	Z	31	GLN
20	Z	32	ASP
3	c	416	SER
14	r	31	VAL
16	u	53	ALA
19	y	41	VAL
19	y	43	ARG
20	z	2	THR
19	Y	43	ARG
2	b	294	SER
2	b	295	GLY
2	b	404	GLY
5	E	58	GLN
13	o	61	GLN
14	r	30	GLN
13	O	59	LYS
5	e	83	LEU
13	o	73	ARG
13	o	56	PRO
10	k	38	VAL
20	z	61	VAL
17	v	42	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	262 (97%)	8 (3%)	41	54
1	a	269/280 (96%)	258 (96%)	11 (4%)	30	41
2	B	408/404 (101%)	400 (98%)	8 (2%)	55	70
2	b	402/404 (100%)	386 (96%)	16 (4%)	31	42
3	C	346/362 (96%)	338 (98%)	8 (2%)	50	65
3	c	354/362 (98%)	340 (96%)	14 (4%)	31	42
4	D	276/283 (98%)	268 (97%)	8 (3%)	42	56
4	d	277/283 (98%)	264 (95%)	13 (5%)	26	34
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	27
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	39
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	47
7	H	54/55 (98%)	50 (93%)	4 (7%)	13	16
7	h	53/55 (96%)	45 (85%)	8 (15%)	3	2
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	9
8	i	32/34 (94%)	30 (94%)	2 (6%)	18	22
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	39
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	12
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	51
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	56
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	47
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	17
13	O	206/228 (90%)	193 (94%)	13 (6%)	18	22
13	o	207/228 (91%)	197 (95%)	10 (5%)	25	34
14	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
14	r	23/33 (70%)	19 (83%)	4 (17%)	2	1
15	T	26/26 (100%)	24 (92%)	2 (8%)	13	15
15	t	25/26 (96%)	24 (96%)	1 (4%)	31	42
16	U	84/112 (75%)	78 (93%)	6 (7%)	14	17
16	u	84/112 (75%)	79 (94%)	5 (6%)	19	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	V	117/138 (85%)	112 (96%)	5 (4%)	29 38
17	v	117/138 (85%)	112 (96%)	5 (4%)	29 38
18	X	31/34 (91%)	28 (90%)	3 (10%)	8 8
18	x	31/34 (91%)	26 (84%)	5 (16%)	2 2
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2 2
19	y	22/37 (60%)	19 (86%)	3 (14%)	3 3
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4 3
20	z	51/52 (98%)	46 (90%)	5 (10%)	8 8
All	All	4328/4644 (93%)	4117 (95%)	211 (5%)	25 33

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	229	GLU
1	A	231	GLU
1	A	243	GLU
1	A	244	GLU
1	A	248	ILE
1	A	270	SER
1	A	307	ILE
2	B	98	LEU
2	B	138	MET
2	B	289	GLN
2	B	297	THR
2	B	350	GLU
2	B	353	GLU
2	B	362	PHE
2	B	371	THR
3	C	141	GLU
3	C	156	LYS
3	C	201	ASN
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	386	PRO
3	C	416	SER
4	D	12	ARG
4	D	165	SER

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Mol	Chain	Res	Type
4	D	180	ARG
4	D	224	GLN
4	D	238	THR
4	D	262	SER
4	D	329	MET
4	D	345	VAL
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	61	ARG
7	H	20	LYS
7	H	49	TYR
7	H	56	ASP
7	H	65	LEU
8	I	2	GLU
8	I	4	LEU
8	I	36	ASP
9	J	24	ILE
10	K	13	GLU
11	L	11	GLU
12	M	25	LEU
13	O	3	GLN
13	O	24	ASP
13	O	36	GLN
13	O	39	ARG
13	O	78	LEU
13	O	89	SER
13	O	97	GLU
13	O	107	THR
13	O	118	LEU
13	O	191	SER
13	O	198	SER
13	O	214	THR
13	O	225	MET
14	R	6	LEU
14	R	10	LEU
14	R	21	ARG
14	R	22	ASN
14	R	29	LYS
15	T	25	GLU
15	T	29	ILE
16	U	10	VAL

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Mol	Chain	Res	Type
16	U	39	ARG
16	U	51	LYS
16	U	61	VAL
16	U	63	ASN
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	17	LYS
17	V	19	ILE
17	V	24	LYS
18	X	3	ILE
18	X	29	ILE
18	X	37	VAL
19	Y	23	THR
19	Y	34	MET
19	Y	42	ARG
20	Z	5	PHE
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN
20	Z	35	ARG
20	Z	46	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	230	THR
1	a	245	THR
1	a	248	ILE
1	a	288	LEU
2	b	98	LEU
2	b	128	THR
2	b	137	LYS
2	b	149	LEU
2	b	161	LEU
2	b	236	THR
2	b	246	PHE
2	b	286	ARG

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Mol	Chain	Res	Type
2	b	298	LEU
2	b	357	ARG
2	b	362	PHE
2	b	425	ILE
2	b	480	SER
2	b	485	GLU
2	b	491	VAL
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	29	GLU
3	c	30	SER
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	144	SER
3	c	165	LEU
3	c	200	THR
3	c	289	PHE
3	c	315	MET
3	c	355	THR
4	d	12	ARG
4	d	25	ASP
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	230	SER
4	d	233	ARG
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	65	LEU
5	e	84	LYS
6	f	15	ILE
7	h	7	LEU
7	h	12	ARG
7	h	27	THR

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Mol	Chain	Res	Type
7	h	30	LEU
7	h	37	LEU
7	h	39	LEU
7	h	43	LEU
7	h	49	TYR
8	i	6	ILE
8	i	36	ASP
9	j	7	ARG
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	17	ILE
10	k	30	VAL
10	k	35	LEU
10	k	46	ARG
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	23	ASP
13	o	49	THR
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	135	SER
13	o	191	SER
13	o	198	SER
13	o	200	ASN
13	o	207	ARG
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
14	r	13	LEU
15	t	29	ILE
16	u	10	VAL
16	u	23	GLU
16	u	51	LYS
16	u	77	GLU
16	u	80	GLU
17	v	19	ILE

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Mol	Chain	Res	Type
17	v	22	THR
17	v	52	LEU
17	v	107	LEU
17	v	108	THR
18	x	2	THR
18	x	8	LYS
18	x	14	LEU
18	x	15	LEU
18	x	21	LEU
19	y	19	ILE
19	y	23	THR
19	y	37	PHE
20	z	1	MET
20	z	7	LEU
20	z	20	VAL
20	z	32	ASP
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
2	B	289	GLN
3	C	327	ASN
5	E	60	GLN
13	O	36	GLN
13	O	88	ASN
18	X	38	GLN
19	Y	45	ASN
20	Z	6	GLN
20	Z	31	GLN
1	a	234	ASN
3	c	28	GLN
13	o	61	GLN
13	o	130	GLN

5.3.3 RNA

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	$\#\|Z\| > 2$
15	FME	T	1	15	8,9,10	1.11	1 (12%)	7,9,11	0.94	1 (14%)
12	FME	M	1	12	8,9,10	1.17	1 (12%)	7,9,11	1.09	1 (14%)
8	FME	I	1	8	8,9,10	1.06	0	7,9,11	0.66	0
8	FME	i	1	8	8,9,10	1.28	1 (12%)	7,9,11	1.24	1 (14%)
15	FME	t	1	15	8,9,10	1.56	1 (12%)	7,9,11	1.18	0
12	FME	m	1	12	8,9,10	0.89	0	7,9,11	1.36	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	T	1	15	-	4/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	3/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
15	FME	t	1	15	-	4/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-4.11	1.40	1.46
8	i	1	FME	CA-N	-2.73	1.42	1.46
12	M	1	FME	CA-N	-2.62	1.42	1.46
15	T	1	FME	CA-N	-2.10	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	1	FME	CA-N-CN	2.85	127.20	122.82
8	i	1	FME	CA-N-CN	-2.39	119.14	122.82
12	M	1	FME	CA-N-CN	-2.06	119.65	122.82
15	T	1	FME	CG-CB-CA	2.03	118.59	112.95

There are no chirality outliers.

All (15) 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
8	I	1	FME	N-CA-CB-CG
15	T	1	FME	N-CA-CB-CG
15	T	1	FME	CB-CG-SD-CE
8	I	1	FME	CB-CG-SD-CE
15	T	1	FME	C-CA-CB-CG
15	t	1	FME	N-CA-CB-CG
15	t	1	FME	C-CA-CB-CG
8	i	1	FME	CB-CG-SD-CE
12	m	1	FME	CB-CG-SD-CE
8	I	1	FME	CB-CA-N-CN
8	i	1	FME	CB-CA-N-CN
12	M	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 190 ligands modelled in this entry, 7 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	$\#\|Z\| > 2$
22	CLA	C	506	-	65,73,73	1.87	11 (16%)	76,113,113	1.44	11 (14%)
22	CLA	C	501	-	65,73,73	1.64	10 (15%)	76,113,113	1.57	10 (13%)
22	CLA	B	614	-	65,73,73	1.76	11 (16%)	76,113,113	1.50	10 (13%)
22	CLA	c	501	-	65,73,73	1.67	9 (13%)	76,113,113	1.62	10 (13%)
30	BCR	B	616	-	41,41,41	1.07	3 (7%)	56,56,56	1.40	9 (16%)
28	LHG	d	409	-	38,38,48	1.06	4 (10%)	41,44,54	1.21	5 (12%)
26	LMG	b	622	-	55,55,55	1.16	5 (9%)	63,63,63	1.45	5 (7%)
34	HEC	F	101	5,6	32,50,50	2.29	3 (9%)	24,82,82	2.02	7 (29%)
22	CLA	C	505	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	10 (13%)
22	CLA	a	405	-	65,73,73	1.65	9 (13%)	76,113,113	1.40	11 (14%)
22	CLA	c	505	-	65,73,73	1.54	7 (10%)	76,113,113	1.48	10 (13%)
31	STE	b	621	-	19,19,19	0.72	0	19,19,19	0.96	1 (5%)
22	CLA	B	609	36	65,73,73	1.55	11 (16%)	76,113,113	1.65	10 (13%)
22	CLA	B	604	-	65,73,73	1.26	5 (7%)	76,113,113	1.53	13 (17%)
22	CLA	C	509	-	65,73,73	1.55	10 (15%)	76,113,113	1.38	11 (14%)
22	CLA	D	403	-	65,73,73	1.59	8 (12%)	76,113,113	1.37	10 (13%)
30	BCR	D	406	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
22	CLA	c	509	-	65,73,73	1.55	9 (13%)	76,113,113	1.66	13 (17%)
22	CLA	C	511	3	65,73,73	1.73	11 (16%)	76,113,113	1.54	6 (7%)
30	BCR	b	618	-	41,41,41	1.46	4 (9%)	56,56,56	1.36	9 (16%)
30	BCR	H	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.24	8 (14%)
22	CLA	b	615	-	65,73,73	2.34	12 (18%)	76,113,113	1.42	8 (10%)
30	BCR	K	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.54	12 (21%)
27	SQD	t	102	-	35,35,54	1.19	3 (8%)	37,37,65	1.46	4 (10%)
31	STE	d	411	-	16,16,19	0.78	0	16,16,19	0.98	1 (6%)
22	CLA	C	510	-	65,73,73	1.56	10 (15%)	76,113,113	1.78	11 (14%)
22	CLA	c	510	-	65,73,73	1.41	7 (10%)	76,113,113	1.50	9 (11%)
30	BCR	k	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	6 (10%)
30	BCR	a	406	-	41,41,41	1.09	3 (7%)	56,56,56	1.53	12 (21%)
22	CLA	a	403	36	65,73,73	1.58	10 (15%)	76,113,113	1.48	12 (15%)
25	PL9	A	408	-	55,55,55	1.65	4 (7%)	68,69,69	1.54	15 (22%)
34	HEC	V	201	17	32,50,50	1.97	3 (9%)	24,82,82	1.89	6 (25%)
22	CLA	b	601	36	65,73,73	1.60	9 (13%)	76,113,113	1.58	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	BCR	K	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	9 (16%)
33	BCT	d	402	21	2,3,3	1.20	0	2,3,3	3.06	1 (50%)
22	CLA	C	507	36	65,73,73	1.44	10 (15%)	76,113,113	1.51	7 (9%)
31	STE	C	520	-	15,15,19	0.55	0	14,14,19	0.52	0
22	CLA	b	608	-	65,73,73	1.42	9 (13%)	76,113,113	1.43	12 (15%)
23	PHO	D	401	-	51,69,69	1.24	6 (11%)	47,99,99	1.36	6 (12%)
31	STE	L	103	-	11,11,19	0.75	0	11,11,19	1.68	2 (18%)
22	CLA	A	403	36	65,73,73	1.94	10 (15%)	76,113,113	1.52	13 (17%)
23	PHO	A	404	-	51,69,69	1.22	7 (13%)	47,99,99	1.43	8 (17%)
28	LHG	a	411	-	41,41,48	1.15	6 (14%)	44,47,54	1.24	4 (9%)
22	CLA	C	512	-	65,73,73	1.41	7 (10%)	76,113,113	1.57	11 (14%)
31	STE	B	624	-	15,15,19	0.47	0	14,14,19	0.84	0
22	CLA	B	607	-	65,73,73	1.60	11 (16%)	76,113,113	1.25	8 (10%)
27	SQD	D	409	-	35,36,54	1.09	4 (11%)	42,45,65	1.97	11 (26%)
22	CLA	H	101	36	65,73,73	1.80	8 (12%)	76,113,113	1.48	5 (6%)
30	BCR	b	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	9 (16%)
27	SQD	L	101	-	48,49,54	1.00	2 (4%)	57,60,65	2.32	18 (31%)
32	OEX	C	522	3,36,1	0,15,15	-	-	-		
23	PHO	a	404	-	51,69,69	1.00	5 (9%)	47,99,99	1.44	8 (17%)
26	LMG	D	412	-	31,31,55	1.24	3 (9%)	33,33,63	1.11	2 (6%)
31	STE	C	521	-	11,11,19	0.66	0	11,11,19	1.44	2 (18%)
30	BCR	C	514	-	41,41,41	1.24	2 (4%)	56,56,56	1.56	12 (21%)
31	STE	Z	101	-	7,7,19	0.52	0	6,6,19	0.26	0
31	STE	b	626	-	19,19,19	0.82	0	19,19,19	0.53	0
22	CLA	b	612	-	65,73,73	1.61	9 (13%)	76,113,113	1.59	12 (15%)
25	PL9	a	409	-	55,55,55	1.13	4 (7%)	68,69,69	1.53	12 (17%)
27	SQD	f	102	-	40,41,54	1.13	4 (10%)	49,52,65	2.02	12 (24%)
28	LHG	A	411	-	48,48,48	1.01	2 (4%)	51,54,54	1.22	5 (9%)
29	DGD	H	103	-	63,63,67	1.34	9 (14%)	77,77,81	1.58	13 (16%)
26	LMG	c	521	-	49,49,55	1.13	6 (12%)	57,57,63	1.34	8 (14%)
34	HEC	v	201	17	32,50,50	2.31	5 (15%)	24,82,82	2.21	4 (16%)
26	LMG	B	620	-	26,26,55	1.38	4 (15%)	26,26,63	1.08	2 (7%)
22	CLA	B	615	-	60,68,73	1.80	13 (21%)	70,107,113	1.57	10 (14%)
22	CLA	b	613	-	65,73,73	1.47	9 (13%)	76,113,113	1.60	10 (13%)
22	CLA	b	602	-	65,73,73	1.73	11 (16%)	76,113,113	1.65	13 (17%)
30	BCR	k	102	-	41,41,41	1.04	3 (7%)	56,56,56	1.16	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	STE	b	629	-	19,19,19	0.77	1 (5%)	19,19,19	0.93	0
22	CLA	a	402	-	65,73,73	1.39	9 (13%)	76,113,113	1.56	10 (13%)
22	CLA	B	602	-	65,73,73	1.39	10 (15%)	76,113,113	1.58	17 (22%)
26	LMG	c	518	-	37,37,55	1.44	7 (18%)	45,45,63	1.31	5 (11%)
31	STE	b	620	-	15,15,19	0.54	0	14,14,19	0.72	0
22	CLA	B	605	-	65,73,73	1.90	10 (15%)	76,113,113	1.42	9 (11%)
22	CLA	C	502	-	65,73,73	1.50	8 (12%)	76,113,113	1.41	9 (11%)
22	CLA	c	507	36	65,73,73	1.77	12 (18%)	76,113,113	1.54	12 (15%)
31	STE	B	625	-	11,11,19	0.81	0	11,11,19	1.49	3 (27%)
29	DGD	C	518	-	63,63,67	1.11	6 (9%)	77,77,81	1.53	11 (14%)
31	STE	b	624	-	15,15,19	0.86	0	15,15,19	0.90	0
22	CLA	b	610	36	65,73,73	1.52	11 (16%)	76,113,113	1.44	12 (15%)
22	CLA	B	611	-	65,73,73	1.63	10 (15%)	76,113,113	1.46	11 (14%)
26	LMG	m	101	-	51,51,55	1.25	4 (7%)	59,59,63	1.49	8 (13%)
29	DGD	c	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.38	8 (10%)
28	LHG	L	102	-	48,48,48	0.88	2 (4%)	51,54,54	1.17	4 (7%)
29	DGD	h	101	-	63,63,67	1.03	4 (6%)	77,77,81	1.46	14 (18%)
28	LHG	D	410	-	48,48,48	0.96	3 (6%)	51,54,54	1.22	5 (9%)
22	CLA	B	610	-	65,73,73	1.66	10 (15%)	76,113,113	1.78	13 (17%)
22	CLA	b	604	-	65,73,73	1.57	7 (10%)	76,113,113	1.60	14 (18%)
30	BCR	d	406	-	41,41,41	1.08	2 (4%)	56,56,56	1.39	8 (14%)
22	CLA	d	405	-	65,73,73	1.86	14 (21%)	76,113,113	1.31	9 (11%)
26	LMG	D	408	-	51,51,55	1.18	4 (7%)	59,59,63	1.35	6 (10%)
30	BCR	x	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.47	11 (19%)
31	STE	M	104	-	17,17,19	0.41	0	16,16,19	0.85	0
22	CLA	D	405	-	65,73,73	1.84	12 (18%)	76,113,113	1.21	6 (7%)
30	BCR	c	514	-	41,41,41	1.16	3 (7%)	56,56,56	1.65	12 (21%)
22	CLA	B	603	-	65,73,73	1.47	8 (12%)	76,113,113	1.81	14 (18%)
31	STE	t	103	-	13,13,19	0.87	0	13,13,19	1.10	2 (15%)
28	LHG	D	413	-	48,48,48	1.00	3 (6%)	51,54,54	1.40	7 (13%)
30	BCR	b	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.36	9 (16%)
31	STE	a	412	-	11,11,19	0.81	0	11,11,19	0.95	0
29	DGD	C	516	-	63,63,67	1.37	9 (14%)	77,77,81	1.39	11 (14%)
29	DGD	c	516	-	63,63,67	1.10	7 (11%)	77,77,81	1.55	16 (20%)
31	STE	B	622	-	11,11,19	0.77	0	11,11,19	1.41	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	SQD	a	410	-	53,54,54	1.04	3 (5%)	62,65,65	1.78	13 (20%)
28	LHG	D	411	-	46,46,48	1.05	3 (6%)	49,52,54	1.21	5 (10%)
28	LHG	d	408	-	48,48,48	0.77	1 (2%)	51,54,54	1.12	3 (5%)
30	BCR	t	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.44	10 (17%)
31	STE	H	104	-	17,17,19	0.46	0	16,16,19	0.64	0
22	CLA	c	506	-	65,73,73	1.79	8 (12%)	76,113,113	1.62	16 (21%)
22	CLA	c	502	-	65,73,73	1.62	11 (16%)	76,113,113	1.51	13 (17%)
27	SQD	A	410	-	51,52,54	1.12	4 (7%)	60,63,65	2.08	16 (26%)
22	CLA	b	606	-	65,73,73	2.00	12 (18%)	76,113,113	1.56	12 (15%)
33	BCT	D	402	21	2,3,3	0.96	0	2,3,3	3.91	2 (100%)
22	CLA	C	508	-	65,73,73	1.72	10 (15%)	76,113,113	1.53	14 (18%)
25	PL9	d	407	-	55,55,55	1.58	11 (20%)	68,69,69	1.52	15 (22%)
30	BCR	k	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.44	10 (17%)
31	STE	k	104	-	11,11,19	0.92	0	11,11,19	0.87	0
31	STE	t	104	-	9,9,19	0.56	0	8,8,19	0.37	0
31	STE	x	102	-	19,19,19	0.76	0	19,19,19	0.96	2 (10%)
32	OEX	a	415	3,36,1	0,15,15	-	-	-		
22	CLA	c	511	3	65,73,73	1.83	7 (10%)	76,113,113	1.59	11 (14%)
22	CLA	A	405	-	54,62,73	1.62	8 (14%)	62,99,113	1.70	12 (19%)
22	CLA	b	609	-	65,73,73	1.92	12 (18%)	76,113,113	1.50	12 (15%)
22	CLA	d	403	-	65,73,73	1.72	10 (15%)	76,113,113	1.45	7 (9%)
30	BCR	T	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	4 (7%)
31	STE	X	101	-	19,19,19	0.62	0	19,19,19	1.24	2 (10%)
29	DGD	c	515	-	63,63,67	1.31	8 (12%)	77,77,81	1.45	13 (16%)
22	CLA	d	404	36	65,73,73	1.81	8 (12%)	76,113,113	1.72	15 (19%)
27	SQD	A	412	-	38,38,54	1.09	2 (5%)	40,40,65	1.44	5 (12%)
31	STE	I	102	-	14,14,19	0.66	0	13,13,19	0.40	0
26	LMG	a	414	-	55,55,55	1.50	8 (14%)	63,63,63	1.30	7 (11%)
31	STE	J	101	-	11,11,19	0.67	0	11,11,19	1.29	1 (9%)
29	DGD	C	517	-	63,63,67	1.24	10 (15%)	77,77,81	1.39	10 (12%)
29	DGD	A	413	-	67,67,67	1.39	10 (14%)	81,81,81	1.33	14 (17%)
26	LMG	d	410	-	44,44,55	1.18	4 (9%)	52,52,63	1.26	6 (11%)
22	CLA	B	606	36	65,73,73	1.62	12 (18%)	76,113,113	1.50	8 (10%)
30	BCR	I	101	-	41,41,41	1.19	4 (9%)	56,56,56	1.57	11 (19%)
31	STE	M	102	-	14,14,19	0.90	0	14,14,19	1.02	1 (7%)
31	STE	a	413	-	14,14,19	0.46	0	13,13,19	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HEC	f	101	5,6	32,50,50	2.30	4 (12%)	24,82,82	2.39	5 (20%)
30	BCR	B	618	-	41,41,41	1.22	2 (4%)	56,56,56	1.59	10 (17%)
31	STE	R	101	-	11,11,19	0.74	0	11,11,19	1.09	1 (9%)
26	LMG	A	409	-	48,48,55	1.16	5 (10%)	56,56,63	1.42	8 (14%)
31	STE	b	627	-	9,9,19	0.57	0	8,8,19	0.44	0
22	CLA	C	513	-	65,73,73	1.55	11 (16%)	76,113,113	1.58	13 (17%)
22	CLA	b	616	-	60,68,73	1.46	7 (11%)	70,107,113	1.64	10 (14%)
22	CLA	B	612	-	65,73,73	2.23	11 (16%)	76,113,113	1.39	11 (14%)
22	CLA	C	503	-	65,73,73	1.71	10 (15%)	76,113,113	1.82	15 (19%)
22	CLA	b	603	-	65,73,73	1.76	10 (15%)	76,113,113	1.86	16 (21%)
22	CLA	c	513	-	65,73,73	1.57	7 (10%)	76,113,113	1.38	8 (10%)
25	PL9	D	407	-	55,55,55	1.58	13 (23%)	68,69,69	1.70	17 (25%)
22	CLA	c	503	-	65,73,73	1.49	9 (13%)	76,113,113	1.42	15 (19%)
30	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.44	11 (19%)
22	CLA	D	404	36	65,73,73	1.79	10 (15%)	76,113,113	1.31	10 (13%)
31	STE	M	103	-	9,9,19	0.71	0	8,8,19	0.40	0
31	STE	b	628	-	13,13,19	0.56	0	12,12,19	0.37	0
26	LMG	M	101	-	51,51,55	1.10	4 (7%)	59,59,63	1.39	8 (13%)
31	STE	j	101	-	11,11,19	1.00	1 (9%)	11,11,19	0.73	0
22	CLA	B	601	-	65,73,73	1.75	9 (13%)	76,113,113	1.48	14 (18%)
22	CLA	b	607	36	65,73,73	1.50	12 (18%)	76,113,113	1.30	7 (9%)
27	SQD	B	621	-	53,54,54	1.02	3 (5%)	62,65,65	1.93	14 (22%)
30	BCR	C	515	-	41,41,41	1.00	2 (4%)	56,56,56	1.30	9 (16%)
22	CLA	A	402	-	65,73,73	1.56	6 (9%)	76,113,113	1.69	18 (23%)
22	CLA	c	512	-	65,73,73	1.95	13 (20%)	76,113,113	1.52	12 (15%)
28	LHG	b	623	-	48,48,48	0.93	2 (4%)	51,54,54	1.24	3 (5%)
26	LMG	c	520	-	48,48,55	1.06	5 (10%)	56,56,63	1.29	7 (12%)
31	STE	b	625	-	14,14,19	0.38	0	13,13,19	0.92	0
22	CLA	b	605	-	65,73,73	1.43	11 (16%)	76,113,113	1.64	14 (18%)
28	LHG	l	101	-	48,48,48	0.90	3 (6%)	51,54,54	1.11	2 (3%)
31	STE	C	519	-	11,11,19	0.99	0	11,11,19	1.42	2 (18%)
31	STE	c	519	-	19,19,19	0.76	1 (5%)	19,19,19	0.84	0
31	STE	B	619	-	16,16,19	0.86	1 (6%)	16,16,19	0.91	0
22	CLA	B	613	-	65,73,73	1.66	6 (9%)	76,113,113	1.26	9 (11%)
23	PHO	d	401	-	51,69,69	1.13	5 (9%)	47,99,99	1.50	7 (14%)
31	STE	B	623	-	17,17,19	0.76	0	17,17,19	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	504	36	59,67,73	1.59	9 (15%)	68,105,113	1.46	9 (13%)
22	CLA	c	504	36	60,68,73	1.57	8 (13%)	70,107,113	1.43	13 (18%)
22	CLA	c	508	-	64,72,73	1.52	7 (10%)	74,111,113	1.40	10 (13%)
26	LMG	Y	101	-	48,48,55	1.10	7 (14%)	56,56,63	1.26	6 (10%)
22	CLA	B	608	-	65,73,73	1.49	7 (10%)	76,113,113	1.51	11 (14%)
22	CLA	b	611	-	65,73,73	1.54	9 (13%)	76,113,113	1.65	17 (22%)
22	CLA	b	614	-	65,73,73	1.78	11 (16%)	76,113,113	1.53	12 (15%)

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
22	CLA	C	506	-	1/1/20/20	23/37/115/115	-
22	CLA	C	501	-	1/1/20/20	5/37/115/115	-
22	CLA	B	614	-	1/1/20/20	7/37/115/115	-
22	CLA	c	501	-	1/1/20/20	5/37/115/115	-
30	BCR	B	616	-	-	8/29/63/63	0/2/2/2
28	LHG	d	409	-	-	13/43/43/53	-
26	LMG	b	622	-	-	28/50/70/70	0/1/1/1
34	HEC	F	101	5,6	-	3/10/54/54	-
22	CLA	C	505	-	1/1/20/20	9/37/115/115	-
22	CLA	a	405	-	1/1/20/20	7/37/115/115	-
22	CLA	c	505	-	1/1/20/20	14/37/115/115	-
31	STE	b	621	-	-	10/17/17/17	-
22	CLA	B	609	36	1/1/20/20	6/37/115/115	-
22	CLA	B	604	-	1/1/20/20	12/37/115/115	-
22	CLA	C	509	-	1/1/20/20	16/37/115/115	-
22	CLA	D	403	-	1/1/20/20	6/37/115/115	-
30	BCR	D	406	-	-	8/29/63/63	0/2/2/2
22	CLA	c	509	-	1/1/20/20	8/37/115/115	-
22	CLA	C	511	3	1/1/20/20	7/37/115/115	-
30	BCR	b	618	-	-	5/29/63/63	0/2/2/2
30	BCR	H	102	-	-	11/29/63/63	0/2/2/2
22	CLA	b	615	-	1/1/20/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	K	101	-	-	12/29/63/63	0/2/2/2
27	SQD	t	102	-	-	12/37/37/69	-
31	STE	d	411	-	-	9/14/14/17	-
22	CLA	C	510	-	1/1/20/20	14/37/115/115	-
22	CLA	c	510	-	1/1/20/20	13/37/115/115	-
30	BCR	k	103	-	-	7/29/63/63	0/2/2/2
30	BCR	a	406	-	-	2/29/63/63	0/2/2/2
22	CLA	a	403	36	-	10/37/115/115	-
25	PL9	A	408	-	-	21/53/73/73	0/1/1/1
34	HEC	V	201	17	-	2/10/54/54	-
22	CLA	b	601	36	1/1/20/20	22/37/115/115	-
30	BCR	K	102	-	-	13/29/63/63	0/2/2/2
22	CLA	C	507	36	1/1/20/20	6/37/115/115	-
31	STE	C	520	-	-	4/13/13/17	-
22	CLA	b	608	-	1/1/20/20	7/37/115/115	-
23	PHO	D	401	-	-	5/37/103/103	0/5/6/6
31	STE	L	103	-	-	5/9/9/17	-
22	CLA	A	403	36	-	10/37/115/115	-
23	PHO	A	404	-	-	6/37/103/103	0/5/6/6
28	LHG	a	411	-	-	26/46/46/53	-
22	CLA	C	512	-	1/1/20/20	9/37/115/115	-
31	STE	B	624	-	-	7/13/13/17	-
22	CLA	B	607	-	1/1/20/20	8/37/115/115	-
27	SQD	D	409	-	-	14/28/48/69	0/1/1/1
22	CLA	H	101	36	1/1/20/20	20/37/115/115	-
30	BCR	b	619	-	-	3/29/63/63	0/2/2/2
27	SQD	L	101	-	-	24/44/64/69	0/1/1/1
23	PHO	a	404	-	-	3/37/103/103	0/5/6/6
26	LMG	D	412	-	-	19/33/33/70	-
31	STE	C	521	-	-	2/9/9/17	-
30	BCR	C	514	-	-	8/29/63/63	0/2/2/2
31	STE	Z	101	-	-	4/5/5/17	-
31	STE	b	626	-	-	9/17/17/17	-
22	CLA	b	612	-	1/1/20/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PL9	a	409	-	-	26/53/73/73	0/1/1/1
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1
28	LHG	A	411	-	-	23/53/53/53	-
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2
26	LMG	c	521	-	-	24/44/64/70	0/1/1/1
34	HEC	v	201	17	-	2/10/54/54	-
26	LMG	B	620	-	-	8/22/22/70	-
22	CLA	B	615	-	1/1/19/20	9/31/109/115	-
22	CLA	b	613	-	1/1/20/20	10/37/115/115	-
22	CLA	b	602	-	1/1/20/20	10/37/115/115	-
30	BCR	k	102	-	-	14/29/63/63	0/2/2/2
31	STE	b	629	-	-	6/17/17/17	-
22	CLA	a	402	-	-	1/37/115/115	-
22	CLA	B	602	-	1/1/20/20	12/37/115/115	-
26	LMG	c	518	-	-	12/31/51/70	0/1/1/1
31	STE	b	620	-	-	6/13/13/17	-
22	CLA	B	605	-	1/1/20/20	10/37/115/115	-
22	CLA	C	502	-	1/1/20/20	11/37/115/115	-
22	CLA	c	507	36	1/1/20/20	11/37/115/115	-
31	STE	B	625	-	-	4/9/9/17	-
29	DGD	C	518	-	-	15/51/91/95	0/2/2/2
31	STE	b	624	-	-	10/13/13/17	-
22	CLA	b	610	36	1/1/20/20	7/37/115/115	-
22	CLA	B	611	-	1/1/20/20	8/37/115/115	-
26	LMG	m	101	-	-	17/46/66/70	0/1/1/1
29	DGD	c	517	-	-	14/51/91/95	0/2/2/2
28	LHG	L	102	-	-	25/53/53/53	-
29	DGD	h	101	-	-	17/51/91/95	0/2/2/2
28	LHG	D	410	-	-	23/53/53/53	-
22	CLA	B	610	-	-	6/37/115/115	-
22	CLA	b	604	-	1/1/20/20	12/37/115/115	-
30	BCR	d	406	-	-	8/29/63/63	0/2/2/2
22	CLA	d	405	-	1/1/20/20	7/37/115/115	-
26	LMG	D	408	-	-	17/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	x	101	-	-	7/29/63/63	0/2/2/2
31	STE	M	104	-	-	9/15/15/17	-
22	CLA	D	405	-	-	12/37/115/115	-
30	BCR	c	514	-	-	7/29/63/63	0/2/2/2
22	CLA	B	603	-	1/1/20/20	14/37/115/115	-
31	STE	t	103	-	-	5/11/11/17	-
28	LHG	D	413	-	-	19/53/53/53	-
30	BCR	b	617	-	-	13/29/63/63	0/2/2/2
31	STE	a	412	-	-	4/9/9/17	-
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
29	DGD	c	516	-	-	18/51/91/95	0/2/2/2
31	STE	B	622	-	-	5/9/9/17	-
27	SQD	a	410	-	-	22/49/69/69	0/1/1/1
28	LHG	D	411	-	-	21/51/51/53	-
28	LHG	d	408	-	-	22/53/53/53	-
30	BCR	t	101	-	-	13/29/63/63	0/2/2/2
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	c	506	-	1/1/20/20	14/37/115/115	-
22	CLA	c	502	-	1/1/20/20	13/37/115/115	-
27	SQD	A	410	-	-	23/47/67/69	0/1/1/1
22	CLA	b	606	-	1/1/20/20	8/37/115/115	-
22	CLA	C	508	-	-	11/37/115/115	-
25	PL9	d	407	-	-	18/53/73/73	0/1/1/1
30	BCR	k	101	-	-	10/29/63/63	0/2/2/2
31	STE	k	104	-	-	5/9/9/17	-
31	STE	t	104	-	-	3/7/7/17	-
31	STE	x	102	-	-	11/17/17/17	-
22	CLA	c	511	3	1/1/20/20	9/37/115/115	-
22	CLA	A	405	-	1/1/17/20	3/24/102/115	-
22	CLA	b	609	-	1/1/20/20	8/37/115/115	-
22	CLA	d	403	-	1/1/20/20	9/37/115/115	-
30	BCR	T	101	-	-	11/29/63/63	0/2/2/2
31	STE	X	101	-	-	10/17/17/17	-
29	DGD	c	515	-	-	22/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	404	36	1/1/20/20	3/37/115/115	-
27	SQD	A	412	-	-	19/39/39/69	-
31	STE	I	102	-	-	5/12/12/17	-
26	LMG	a	414	-	-	31/50/70/70	0/1/1/1
31	STE	J	101	-	-	5/9/9/17	-
29	DGD	C	517	-	-	22/51/91/95	0/2/2/2
29	DGD	A	413	-	-	28/55/95/95	0/2/2/2
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
22	CLA	B	606	36	1/1/20/20	18/37/115/115	-
30	BCR	I	101	-	-	7/29/63/63	0/2/2/2
31	STE	M	102	-	-	6/12/12/17	-
31	STE	a	413	-	-	9/12/12/17	-
34	HEC	f	101	5,6	-	2/10/54/54	-
30	BCR	B	618	-	-	9/29/63/63	0/2/2/2
31	STE	R	101	-	-	5/9/9/17	-
26	LMG	A	409	-	-	15/43/63/70	0/1/1/1
31	STE	b	627	-	-	5/7/7/17	-
22	CLA	C	513	-	1/1/20/20	7/37/115/115	-
22	CLA	b	616	-	1/1/19/20	6/31/109/115	-
22	CLA	B	612	-	1/1/20/20	12/37/115/115	-
22	CLA	C	503	-	1/1/20/20	5/37/115/115	-
22	CLA	b	603	-	1/1/20/20	8/37/115/115	-
22	CLA	c	513	-	1/1/20/20	10/37/115/115	-
25	PL9	D	407	-	-	14/53/73/73	0/1/1/1
22	CLA	c	503	-	-	10/37/115/115	-
30	BCR	B	617	-	-	10/29/63/63	0/2/2/2
22	CLA	D	404	36	1/1/20/20	10/37/115/115	-
31	STE	M	103	-	-	2/7/7/17	-
31	STE	b	628	-	-	7/11/11/17	-
26	LMG	M	101	-	-	17/46/66/70	0/1/1/1
31	STE	j	101	-	-	4/9/9/17	-
22	CLA	B	601	-	-	10/37/115/115	-
22	CLA	b	607	36	1/1/20/20	16/37/115/115	-
27	SQD	B	621	-	-	27/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
22	CLA	A	402	-	1/1/20/20	5/37/115/115	-
22	CLA	c	512	-	1/1/20/20	20/37/115/115	-
28	LHG	b	623	-	-	26/53/53/53	-
26	LMG	c	520	-	-	20/43/63/70	0/1/1/1
31	STE	b	625	-	-	7/12/12/17	-
22	CLA	b	605	-	1/1/20/20	13/37/115/115	-
28	LHG	l	101	-	-	18/53/53/53	-
31	STE	C	519	-	-	5/9/9/17	-
31	STE	c	519	-	-	7/17/17/17	-
31	STE	B	619	-	-	6/14/14/17	-
22	CLA	B	613	-	1/1/20/20	16/37/115/115	-
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
31	STE	B	623	-	-	11/15/15/17	-
22	CLA	C	504	36	1/1/18/20	6/30/108/115	-
22	CLA	c	504	36	1/1/19/20	7/31/109/115	-
22	CLA	c	508	-	-	13/36/114/115	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
22	CLA	B	608	-	-	7/37/115/115	-
22	CLA	b	611	-	-	9/37/115/115	-
22	CLA	b	614	-	1/1/20/20	20/37/115/115	-

All (984) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	MG-ND	-12.14	1.81	2.05
22	A	403	CLA	C4B-NB	11.07	1.45	1.35
22	b	615	CLA	MG-ND	-10.89	1.84	2.05
22	B	613	CLA	C4B-NB	9.31	1.43	1.35
22	B	605	CLA	MG-NA	9.19	2.28	2.06
22	b	606	CLA	MG-NA	9.02	2.27	2.06
22	c	512	CLA	C4B-NB	8.96	1.43	1.35
22	c	511	CLA	C4B-NB	8.80	1.43	1.35
22	b	609	CLA	C4B-NB	8.54	1.42	1.35
34	v	201	HEC	C2B-C3B	-8.40	1.32	1.40
22	B	601	CLA	C4B-NB	8.32	1.42	1.35
22	b	615	CLA	MG-NA	8.29	2.26	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	C4B-NB	8.16	1.42	1.35
34	f	101	HEC	C2B-C3B	-8.06	1.32	1.40
22	C	506	CLA	C4B-NB	8.06	1.42	1.35
22	b	602	CLA	C4B-NB	8.05	1.42	1.35
34	F	101	HEC	C2B-C3B	-8.03	1.32	1.40
22	b	615	CLA	C4B-NB	7.80	1.42	1.35
22	A	402	CLA	C4B-NB	7.72	1.42	1.35
22	c	504	CLA	C4B-NB	7.71	1.42	1.35
22	c	501	CLA	C4B-NB	7.69	1.42	1.35
22	H	101	CLA	MG-NA	7.61	2.24	2.06
22	B	611	CLA	C4B-NB	7.61	1.42	1.35
22	b	601	CLA	C4B-NB	7.61	1.42	1.35
22	c	513	CLA	C4B-NB	7.59	1.42	1.35
22	b	603	CLA	MG-NA	7.51	2.24	2.06
22	d	404	CLA	MG-NA	7.50	2.24	2.06
22	H	101	CLA	C4B-NB	7.47	1.41	1.35
22	b	606	CLA	C4B-NB	7.44	1.41	1.35
22	C	510	CLA	C4B-NB	7.25	1.41	1.35
22	c	505	CLA	C4B-NB	7.25	1.41	1.35
22	b	604	CLA	C4B-NB	7.20	1.41	1.35
22	B	614	CLA	C4B-NB	7.20	1.41	1.35
25	A	408	PL9	C7-C3	-7.15	1.44	1.51
22	d	404	CLA	C4B-NB	7.12	1.41	1.35
22	C	513	CLA	C4B-NB	7.12	1.41	1.35
22	D	405	CLA	C4B-NB	6.94	1.41	1.35
22	d	405	CLA	MG-NA	6.92	2.22	2.06
22	C	504	CLA	C4B-NB	6.90	1.41	1.35
22	a	403	CLA	C4B-NB	6.87	1.41	1.35
22	C	506	CLA	MG-ND	-6.85	1.92	2.05
22	b	611	CLA	C4B-NB	6.85	1.41	1.35
22	c	511	CLA	MG-NA	6.81	2.22	2.06
22	C	511	CLA	C4B-NB	6.78	1.41	1.35
22	B	608	CLA	C4B-NB	6.75	1.41	1.35
22	b	612	CLA	C4B-NB	6.73	1.41	1.35
22	C	503	CLA	C4B-NB	6.69	1.41	1.35
22	c	507	CLA	MG-NA	6.69	2.22	2.06
22	C	505	CLA	C4B-NB	6.62	1.41	1.35
22	c	506	CLA	MG-ND	-6.47	1.93	2.05
22	D	403	CLA	C4B-NB	6.42	1.40	1.35
22	b	607	CLA	C4B-NB	6.42	1.40	1.35
22	C	508	CLA	C4B-NB	6.40	1.40	1.35
22	b	609	CLA	MG-NC	6.40	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C4B-NB	6.38	1.40	1.35
22	B	610	CLA	MG-NA	6.37	2.21	2.06
22	b	605	CLA	C4B-NB	6.37	1.40	1.35
22	d	403	CLA	C4B-NB	6.36	1.40	1.35
22	a	405	CLA	MG-ND	-6.33	1.93	2.05
22	D	404	CLA	C4B-NB	6.29	1.40	1.35
22	c	502	CLA	C4B-NB	6.23	1.40	1.35
22	D	404	CLA	MG-NA	6.20	2.21	2.06
22	B	615	CLA	MG-NC	6.18	2.20	2.06
22	C	508	CLA	MG-NA	6.17	2.20	2.06
34	V	201	HEC	C2B-C3B	-6.12	1.34	1.40
22	B	607	CLA	MG-NA	6.12	2.20	2.06
22	c	506	CLA	C4B-NB	6.11	1.40	1.35
22	B	615	CLA	C4B-NB	6.11	1.40	1.35
22	C	502	CLA	C4B-NB	6.10	1.40	1.35
22	c	508	CLA	C4B-NB	6.09	1.40	1.35
22	b	613	CLA	C4B-NB	6.09	1.40	1.35
22	b	608	CLA	C4B-NB	6.06	1.40	1.35
22	C	511	CLA	MG-NA	6.06	2.20	2.06
22	C	509	CLA	C4B-NB	6.06	1.40	1.35
22	c	503	CLA	C4B-NB	6.05	1.40	1.35
34	v	201	HEC	C3C-C2C	-6.05	1.34	1.40
22	B	605	CLA	C4B-NB	6.04	1.40	1.35
22	b	614	CLA	C4B-NB	6.04	1.40	1.35
22	b	614	CLA	MG-NC	6.01	2.20	2.06
22	b	616	CLA	C4B-NB	6.01	1.40	1.35
34	V	201	HEC	C3C-C2C	-5.95	1.34	1.40
22	B	607	CLA	MG-NC	-5.90	1.92	2.06
34	f	101	HEC	C3C-C2C	-5.85	1.34	1.40
22	B	610	CLA	C4B-NB	5.82	1.40	1.35
22	C	501	CLA	MG-NA	5.80	2.20	2.06
22	b	614	CLA	MG-ND	5.79	2.17	2.05
22	b	603	CLA	C4B-NB	5.68	1.40	1.35
22	C	508	CLA	MG-ND	5.66	2.17	2.05
22	c	510	CLA	C4B-NB	5.63	1.40	1.35
30	b	618	BCR	C30-C25	-5.57	1.46	1.53
34	F	101	HEC	C3C-C2C	-5.55	1.35	1.40
22	C	503	CLA	MG-NC	5.51	2.19	2.06
22	d	405	CLA	C4B-NB	5.51	1.40	1.35
22	c	507	CLA	C4B-NB	5.49	1.40	1.35
22	C	512	CLA	C4B-NB	5.47	1.40	1.35
22	c	501	CLA	MG-NA	5.43	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	C4D-ND	-5.42	1.30	1.37
22	C	507	CLA	C4B-NB	5.41	1.40	1.35
22	d	405	CLA	MG-NC	-5.38	1.93	2.06
22	B	603	CLA	MG-NA	5.37	2.19	2.06
22	c	512	CLA	MG-NC	5.33	2.18	2.06
22	a	405	CLA	C4B-NB	5.32	1.40	1.35
26	m	101	LMG	C4-C3	5.30	1.65	1.52
34	F	101	HEC	C3D-C2D	5.30	1.53	1.37
22	B	601	CLA	C1D-ND	5.27	1.44	1.37
30	C	514	BCR	C1-C6	-5.19	1.46	1.53
22	C	501	CLA	C4B-NB	5.11	1.39	1.35
22	B	604	CLA	C4B-NB	5.08	1.39	1.35
22	c	509	CLA	C4B-NB	5.06	1.39	1.35
22	c	512	CLA	MG-ND	5.05	2.15	2.05
22	B	602	CLA	C4B-NB	5.05	1.39	1.35
22	a	405	CLA	C1D-ND	5.05	1.44	1.37
22	B	606	CLA	MG-NC	-5.02	1.94	2.06
22	D	405	CLA	MG-NC	4.96	2.18	2.06
22	D	405	CLA	MG-ND	-4.94	1.96	2.05
25	A	408	PL9	C7-C8	-4.90	1.43	1.50
22	B	603	CLA	C4B-NB	4.89	1.39	1.35
22	c	507	CLA	MG-NC	-4.88	1.94	2.06
22	a	403	CLA	C4D-ND	-4.88	1.31	1.37
22	D	404	CLA	C4D-ND	-4.88	1.31	1.37
34	v	201	HEC	C3D-C2D	4.87	1.52	1.37
22	D	405	CLA	C1D-ND	4.86	1.43	1.37
22	D	403	CLA	MG-NA	4.84	2.17	2.06
22	b	611	CLA	MG-NA	4.81	2.17	2.06
22	c	505	CLA	C4D-ND	-4.81	1.31	1.37
22	B	609	CLA	C4B-NB	4.80	1.39	1.35
22	b	602	CLA	C1D-ND	4.79	1.43	1.37
22	c	509	CLA	MG-NC	-4.78	1.94	2.06
34	f	101	HEC	C3D-C2D	4.78	1.51	1.37
22	c	506	CLA	C1D-ND	4.72	1.43	1.37
22	b	610	CLA	MG-ND	4.72	2.15	2.05
22	a	402	CLA	C4B-NB	4.71	1.39	1.35
22	b	606	CLA	C1B-NB	4.69	1.39	1.35
22	b	610	CLA	C4D-ND	-4.66	1.31	1.37
22	b	613	CLA	MG-ND	4.64	2.15	2.05
22	B	606	CLA	C4B-NB	4.62	1.39	1.35
22	c	509	CLA	MG-ND	4.58	2.14	2.05
22	d	403	CLA	C1D-ND	4.58	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	MG-NC	-4.57	1.95	2.06
25	A	408	PL9	C3-C4	-4.57	1.42	1.49
22	B	606	CLA	MG-NA	4.54	2.17	2.06
22	B	611	CLA	C4D-ND	-4.53	1.31	1.37
22	b	610	CLA	C4B-NB	4.52	1.39	1.35
22	b	609	CLA	MG-ND	-4.50	1.96	2.05
25	D	407	PL9	C52-C5	-4.47	1.41	1.50
22	c	510	CLA	C4D-ND	-4.46	1.31	1.37
22	B	609	CLA	MG-NA	4.44	2.16	2.06
22	C	505	CLA	CHC-C1C	4.43	1.46	1.35
22	D	403	CLA	C1D-ND	4.42	1.43	1.37
22	a	405	CLA	C4D-ND	-4.40	1.31	1.37
22	b	606	CLA	C1D-ND	4.40	1.43	1.37
22	A	402	CLA	C4D-ND	-4.40	1.31	1.37
22	B	604	CLA	C4D-ND	-4.40	1.31	1.37
22	c	508	CLA	C4D-ND	-4.38	1.31	1.37
29	H	103	DGD	C1E-C2E	4.38	1.65	1.52
22	b	602	CLA	MG-NA	4.36	2.16	2.06
22	b	609	CLA	C1D-ND	4.35	1.43	1.37
22	a	402	CLA	MG-NA	4.35	2.16	2.06
26	a	414	LMG	C4-C5	4.34	1.62	1.53
22	C	509	CLA	MG-NA	4.34	2.16	2.06
22	d	405	CLA	C1D-ND	4.34	1.43	1.37
29	c	515	DGD	O5D-C6D	-4.33	1.35	1.43
22	c	509	CLA	C4D-ND	-4.31	1.31	1.37
22	b	604	CLA	MG-NC	4.31	2.16	2.06
29	A	413	DGD	C4D-C5D	4.30	1.62	1.53
22	B	613	CLA	C4D-ND	-4.26	1.31	1.37
22	B	614	CLA	CMB-C2B	-4.23	1.42	1.51
22	D	404	CLA	C1D-ND	4.22	1.43	1.37
22	A	403	CLA	C4D-ND	-4.21	1.31	1.37
22	B	606	CLA	C4D-ND	-4.21	1.31	1.37
22	D	403	CLA	C4D-ND	-4.18	1.32	1.37
25	d	407	PL9	C3-C4	-4.18	1.42	1.49
22	c	502	CLA	MG-NC	-4.16	1.96	2.06
22	c	512	CLA	CHC-C1C	4.14	1.45	1.35
22	C	507	CLA	C1D-ND	4.14	1.42	1.37
25	d	407	PL9	C53-C6	-4.14	1.42	1.50
22	d	404	CLA	C4D-ND	-4.14	1.32	1.37
22	c	502	CLA	MG-NA	4.09	2.16	2.06
22	B	601	CLA	C4D-ND	-4.09	1.32	1.37
22	C	513	CLA	C1D-ND	4.08	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	LMG	O1-C7	-4.08	1.36	1.43
22	b	615	CLA	C1D-ND	4.06	1.42	1.37
22	d	403	CLA	MG-NC	4.06	2.15	2.06
22	d	403	CLA	C4D-ND	-4.05	1.32	1.37
29	A	413	DGD	C3G-C2G	4.03	1.63	1.50
34	V	201	HEC	C3D-C2D	4.01	1.49	1.37
22	C	502	CLA	MG-NA	4.01	2.15	2.06
30	b	619	BCR	C1-C6	-4.01	1.48	1.53
22	c	513	CLA	MG-ND	-4.00	1.97	2.05
25	a	409	PL9	C53-C6	-4.00	1.42	1.50
22	b	605	CLA	MG-ND	4.00	2.13	2.05
22	b	614	CLA	C4D-ND	-3.99	1.32	1.37
22	c	506	CLA	MG-NA	3.98	2.15	2.06
23	D	401	PHO	CAC-C3C	-3.97	1.45	1.52
30	k	101	BCR	C1-C6	-3.97	1.48	1.53
22	c	508	CLA	C1D-ND	3.95	1.42	1.37
22	A	405	CLA	C4D-ND	-3.94	1.32	1.37
22	b	601	CLA	MG-NA	3.94	2.15	2.06
22	b	608	CLA	C4D-ND	-3.93	1.32	1.37
30	K	102	BCR	C1-C6	-3.93	1.48	1.53
22	C	512	CLA	MG-ND	3.93	2.13	2.05
30	K	102	BCR	C30-C25	-3.92	1.48	1.53
22	B	611	CLA	C1D-ND	3.91	1.42	1.37
26	D	408	LMG	C4-C5	3.90	1.61	1.53
30	b	617	BCR	C1-C6	-3.89	1.48	1.53
25	D	407	PL9	C11-C9	-3.88	1.43	1.51
26	M	101	LMG	C1-C2	3.87	1.63	1.52
22	b	603	CLA	MG-NC	-3.86	1.97	2.06
22	C	501	CLA	C1D-ND	3.86	1.42	1.37
22	c	507	CLA	MG-ND	3.86	2.13	2.05
22	B	611	CLA	MG-NA	3.86	2.15	2.06
22	b	612	CLA	MG-ND	-3.86	1.98	2.05
22	c	503	CLA	C4D-ND	-3.85	1.32	1.37
26	c	521	LMG	C3-C2	3.84	1.62	1.52
30	H	102	BCR	C30-C25	-3.83	1.48	1.53
22	D	405	CLA	C3B-C2B	-3.82	1.35	1.40
22	c	510	CLA	C1D-ND	3.82	1.42	1.37
26	D	412	LMG	C7-C8	3.82	1.60	1.51
22	B	612	CLA	C4D-ND	-3.81	1.32	1.37
26	d	410	LMG	C4-C5	3.81	1.61	1.53
22	B	610	CLA	C4D-ND	-3.81	1.32	1.37
22	B	609	CLA	C3B-C2B	-3.80	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	MG-ND	3.80	2.13	2.05
22	c	501	CLA	C4D-ND	-3.80	1.32	1.37
22	C	503	CLA	C4D-ND	-3.80	1.32	1.37
22	C	511	CLA	C4D-ND	-3.80	1.32	1.37
26	B	620	LMG	O8-C28	3.79	1.43	1.30
22	B	615	CLA	MG-ND	3.78	2.13	2.05
22	b	612	CLA	C1D-ND	3.78	1.42	1.37
30	t	101	BCR	C30-C25	-3.77	1.48	1.53
22	b	612	CLA	MG-NC	3.77	2.15	2.06
22	C	503	CLA	MG-ND	3.77	2.13	2.05
26	c	518	LMG	C4-C5	3.76	1.60	1.53
22	b	608	CLA	CHC-C1C	3.75	1.44	1.35
30	B	618	BCR	C1-C6	-3.74	1.48	1.53
22	c	502	CLA	C1D-ND	3.72	1.42	1.37
22	c	511	CLA	C1D-ND	3.72	1.42	1.37
27	A	412	SQD	O48-C23	3.72	1.44	1.33
27	A	412	SQD	O47-C7	3.71	1.44	1.34
30	K	101	BCR	C30-C25	-3.68	1.48	1.53
22	c	512	CLA	C4D-ND	-3.68	1.32	1.37
22	b	614	CLA	CHC-C1C	3.67	1.44	1.35
30	D	406	BCR	C30-C25	-3.67	1.48	1.53
22	b	616	CLA	C4D-ND	-3.67	1.32	1.37
27	L	101	SQD	O48-C23	3.66	1.44	1.33
30	c	514	BCR	C1-C6	-3.66	1.48	1.53
22	b	603	CLA	C3B-C2B	-3.65	1.35	1.40
22	B	615	CLA	C1D-ND	3.63	1.42	1.37
22	C	502	CLA	C4D-ND	-3.63	1.32	1.37
27	a	410	SQD	O48-C23	3.63	1.43	1.33
26	m	101	LMG	O1-C7	-3.63	1.37	1.43
22	C	501	CLA	C4D-ND	-3.62	1.32	1.37
22	B	609	CLA	C1D-ND	3.62	1.42	1.37
22	b	604	CLA	C4D-ND	-3.61	1.32	1.37
22	a	402	CLA	C1D-ND	3.61	1.42	1.37
22	c	502	CLA	C4D-ND	-3.61	1.32	1.37
27	B	621	SQD	O47-C7	3.60	1.44	1.34
26	a	414	LMG	O1-C7	3.60	1.50	1.43
29	C	516	DGD	O5D-C6D	-3.59	1.37	1.43
22	c	512	CLA	MG-NA	-3.58	1.97	2.06
27	A	410	SQD	O47-C7	3.58	1.44	1.34
22	B	614	CLA	C3B-C2B	-3.58	1.35	1.40
22	H	101	CLA	CHC-C1C	3.57	1.44	1.35
22	A	403	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	b	618	BCR	C1-C6	-3.55	1.48	1.53
22	B	614	CLA	C3B-CAB	-3.54	1.40	1.47
22	C	501	CLA	C3B-C2B	-3.54	1.35	1.40
22	d	405	CLA	C4D-ND	-3.54	1.32	1.37
29	C	518	DGD	O1G-C1G	-3.53	1.37	1.45
27	D	409	SQD	O48-C23	3.53	1.43	1.33
22	C	506	CLA	CHC-C1C	3.53	1.44	1.35
22	B	605	CLA	C3B-C2B	-3.53	1.35	1.40
26	D	412	LMG	C9-C8	3.52	1.61	1.50
22	b	616	CLA	MG-ND	-3.52	1.98	2.05
22	a	403	CLA	CHC-C1C	3.52	1.44	1.35
22	C	511	CLA	C1D-ND	3.52	1.42	1.37
22	C	510	CLA	MG-NA	3.51	2.14	2.06
25	d	407	PL9	C16-C14	-3.51	1.44	1.51
22	B	603	CLA	C1D-ND	3.50	1.42	1.37
22	c	508	CLA	CHC-C1C	3.50	1.43	1.35
22	C	506	CLA	MG-NC	3.50	2.14	2.06
28	D	411	LHG	P-O6	3.49	1.73	1.59
29	H	103	DGD	C4E-C5E	3.47	1.60	1.53
27	t	102	SQD	O48-C23	3.47	1.43	1.33
22	A	405	CLA	C1D-ND	3.47	1.42	1.37
30	T	101	BCR	C30-C25	-3.46	1.49	1.53
22	b	604	CLA	MG-NA	-3.46	1.98	2.06
22	C	501	CLA	CHC-C1C	3.45	1.43	1.35
22	B	606	CLA	C3B-C2B	-3.44	1.35	1.40
30	x	101	BCR	C30-C25	-3.44	1.49	1.53
29	C	516	DGD	O1G-C1A	3.44	1.43	1.33
28	D	411	LHG	O3-C3	-3.43	1.31	1.44
22	c	503	CLA	MG-NA	3.43	2.14	2.06
22	C	504	CLA	MG-ND	-3.43	1.99	2.05
22	c	501	CLA	CMB-C2B	-3.42	1.44	1.51
22	C	509	CLA	C4D-ND	-3.42	1.33	1.37
27	t	102	SQD	O47-C7	3.42	1.44	1.34
27	L	101	SQD	O47-C7	3.42	1.43	1.34
23	D	401	PHO	CMD-C2D	-3.41	1.43	1.51
22	B	609	CLA	C4D-ND	-3.41	1.33	1.37
22	B	610	CLA	MG-NC	-3.41	1.98	2.06
22	B	612	CLA	C1D-ND	3.40	1.42	1.37
22	B	605	CLA	CHC-C1C	3.40	1.43	1.35
22	B	609	CLA	MG-NC	-3.40	1.98	2.06
27	A	410	SQD	O48-C23	3.39	1.43	1.33
30	k	102	BCR	C30-C25	-3.39	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	409	LHG	P-O6	3.37	1.73	1.59
22	D	404	CLA	CHC-C1C	3.37	1.43	1.35
22	c	513	CLA	CHC-C1C	3.37	1.43	1.35
27	B	621	SQD	O48-C23	3.37	1.43	1.33
30	I	101	BCR	C1-C6	-3.36	1.49	1.53
22	d	403	CLA	CMB-C2B	-3.36	1.44	1.51
22	b	609	CLA	CMB-C2B	-3.35	1.44	1.51
22	b	607	CLA	C3B-C2B	-3.35	1.35	1.40
22	B	610	CLA	CMD-C2D	-3.34	1.43	1.50
22	B	607	CLA	C4B-NB	3.34	1.38	1.35
30	d	406	BCR	C30-C25	-3.33	1.49	1.53
22	B	609	CLA	CMB-C2B	-3.33	1.44	1.51
22	b	614	CLA	C1D-ND	3.32	1.41	1.37
29	c	517	DGD	O2E-C2E	-3.32	1.35	1.43
22	A	402	CLA	MG-NC	-3.32	1.98	2.06
22	c	511	CLA	CHC-C1C	3.32	1.43	1.35
22	C	512	CLA	CHC-C1C	3.32	1.43	1.35
22	B	608	CLA	C4D-ND	-3.32	1.33	1.37
23	d	401	PHO	CAC-C3C	-3.32	1.46	1.52
22	b	606	CLA	CHC-C1C	3.31	1.43	1.35
22	c	501	CLA	CMC-C2C	-3.31	1.43	1.50
25	D	407	PL9	C6-C1	-3.31	1.42	1.48
30	a	406	BCR	C30-C25	-3.31	1.49	1.53
22	A	402	CLA	C1D-ND	3.30	1.41	1.37
22	c	507	CLA	C3B-C2B	-3.29	1.35	1.40
26	c	520	LMG	C3-C2	3.29	1.60	1.52
22	B	601	CLA	CMB-C2B	-3.29	1.44	1.51
22	C	512	CLA	C4D-ND	-3.28	1.33	1.37
22	A	403	CLA	CMB-C2B	-3.28	1.44	1.51
30	k	103	BCR	C30-C25	-3.28	1.49	1.53
26	c	518	LMG	C1-C2	3.28	1.61	1.52
28	A	411	LHG	C24-C23	3.27	1.60	1.50
22	c	507	CLA	C4D-ND	-3.27	1.33	1.37
29	c	515	DGD	O2G-C2G	-3.27	1.38	1.46
22	c	501	CLA	C1D-ND	3.27	1.41	1.37
26	a	414	LMG	O8-C9	-3.27	1.37	1.45
22	d	403	CLA	CHC-C1C	3.26	1.43	1.35
29	C	518	DGD	O3G-C3G	-3.26	1.37	1.43
26	Y	101	LMG	C4-C5	3.25	1.59	1.53
22	b	607	CLA	C1D-ND	3.25	1.41	1.37
22	C	503	CLA	CHC-C1C	3.25	1.43	1.35
22	B	615	CLA	CMB-C2B	-3.25	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	404	CLA	CMB-C2B	-3.25	1.44	1.51
22	b	605	CLA	CMC-C2C	-3.24	1.43	1.50
26	A	409	LMG	C4-C3	3.24	1.60	1.52
22	c	503	CLA	C1D-ND	3.23	1.41	1.37
22	C	510	CLA	CHC-C1C	3.23	1.43	1.35
22	d	405	CLA	C3B-CAB	-3.23	1.41	1.47
22	B	615	CLA	C4D-ND	-3.23	1.33	1.37
22	c	508	CLA	MG-NC	3.23	2.13	2.06
22	C	513	CLA	CMB-C2B	-3.21	1.45	1.51
22	C	503	CLA	CMB-C2B	-3.21	1.45	1.51
22	a	403	CLA	C1D-ND	3.21	1.41	1.37
29	c	516	DGD	O2E-C2E	-3.21	1.35	1.43
22	c	512	CLA	C1D-ND	3.21	1.41	1.37
22	C	508	CLA	C4D-ND	-3.21	1.33	1.37
22	B	603	CLA	C4D-ND	-3.21	1.33	1.37
22	c	505	CLA	CHC-C1C	3.21	1.43	1.35
29	A	413	DGD	O5D-C1E	3.20	1.45	1.40
22	A	403	CLA	MG-NA	3.20	2.13	2.06
22	b	609	CLA	CHC-C1C	3.19	1.43	1.35
22	b	610	CLA	MG-NC	-3.18	1.98	2.06
26	c	521	LMG	C1-C2	3.18	1.61	1.52
22	B	608	CLA	CMD-C2D	-3.18	1.44	1.50
22	C	510	CLA	C4D-ND	-3.17	1.33	1.37
22	b	610	CLA	C3B-C2B	-3.17	1.36	1.40
22	b	602	CLA	C4D-ND	-3.15	1.33	1.37
22	H	101	CLA	C1D-ND	3.15	1.41	1.37
22	B	613	CLA	MG-NA	3.15	2.13	2.06
29	C	516	DGD	C3G-C2G	3.14	1.60	1.50
22	H	101	CLA	CMB-C2B	-3.14	1.45	1.51
22	B	603	CLA	CHC-C1C	3.14	1.43	1.35
29	A	413	DGD	C1E-C2E	3.13	1.61	1.52
22	b	601	CLA	C1D-ND	3.12	1.41	1.37
22	B	607	CLA	C4D-ND	-3.12	1.33	1.37
22	c	513	CLA	C1D-ND	3.11	1.41	1.37
22	b	603	CLA	CMC-C2C	-3.11	1.44	1.50
26	b	622	LMG	O6-C1	3.11	1.49	1.41
26	M	101	LMG	C7-C8	3.11	1.60	1.50
22	C	507	CLA	MG-ND	-3.11	1.99	2.05
22	D	405	CLA	MG-NA	-3.11	1.98	2.06
22	b	602	CLA	CMD-C2D	-3.10	1.44	1.50
22	C	513	CLA	CHC-C1C	3.10	1.42	1.35
22	b	612	CLA	CMB-C2B	-3.10	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	517	DGD	C1E-C2E	3.09	1.61	1.52
22	b	601	CLA	CHC-C1C	3.09	1.42	1.35
22	c	506	CLA	CMB-C2B	-3.09	1.45	1.51
22	c	504	CLA	C4D-ND	-3.09	1.33	1.37
22	c	513	CLA	C4D-ND	-3.08	1.33	1.37
28	L	102	LHG	O7-C5	-3.08	1.38	1.46
22	B	602	CLA	C3B-CAB	-3.08	1.41	1.47
22	b	603	CLA	CMB-C2B	-3.08	1.45	1.51
27	f	102	SQD	O47-C7	3.07	1.43	1.34
26	d	410	LMG	O1-C7	-3.07	1.38	1.43
22	B	608	CLA	MG-NA	3.07	2.13	2.06
25	d	407	PL9	C21-C19	-3.07	1.44	1.51
28	D	413	LHG	O7-C5	-3.07	1.38	1.46
22	C	507	CLA	C1B-NB	-3.07	1.32	1.35
22	C	504	CLA	C1D-ND	3.07	1.41	1.37
22	b	616	CLA	C1D-ND	3.06	1.41	1.37
22	b	603	CLA	CMD-C2D	-3.06	1.44	1.50
29	H	103	DGD	C6D-C5D	3.06	1.61	1.51
22	C	503	CLA	C1D-ND	3.06	1.41	1.37
29	c	517	DGD	C3G-C2G	3.05	1.60	1.50
26	M	101	LMG	O7-C8	-3.05	1.39	1.46
22	B	612	CLA	CMD-C2D	-3.05	1.44	1.50
22	H	101	CLA	C3B-C2B	-3.04	1.36	1.40
22	C	506	CLA	C1D-ND	3.04	1.41	1.37
22	b	611	CLA	C4D-ND	-3.04	1.33	1.37
30	k	103	BCR	C1-C6	-3.03	1.49	1.53
25	D	407	PL9	C26-C24	-3.03	1.45	1.51
22	c	503	CLA	CHC-C1C	3.03	1.42	1.35
22	b	613	CLA	C1D-ND	3.03	1.41	1.37
30	K	101	BCR	C1-C6	-3.02	1.49	1.53
22	c	509	CLA	CHC-C1C	3.02	1.42	1.35
22	B	602	CLA	C3B-C2B	-3.02	1.36	1.40
22	c	510	CLA	CHC-C1C	3.01	1.42	1.35
22	b	611	CLA	CHC-C1C	3.01	1.42	1.35
28	a	411	LHG	P-O6	3.01	1.71	1.59
22	B	602	CLA	C1D-ND	3.01	1.41	1.37
22	B	614	CLA	C1D-ND	3.00	1.41	1.37
22	D	405	CLA	CMD-C2D	-3.00	1.44	1.50
22	B	606	CLA	C1D-ND	3.00	1.41	1.37
22	B	601	CLA	CHC-C1C	2.99	1.42	1.35
22	c	510	CLA	CMB-C2B	-2.99	1.45	1.51
22	b	615	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	616	BCR	C30-C25	-2.99	1.49	1.53
22	B	614	CLA	MG-ND	2.99	2.11	2.05
25	d	407	PL9	C7-C8	-2.98	1.46	1.50
22	c	509	CLA	C1D-ND	2.98	1.41	1.37
22	B	607	CLA	CHC-C1C	2.98	1.42	1.35
30	B	616	BCR	C1-C6	-2.98	1.49	1.53
22	b	615	CLA	CMB-C2B	-2.97	1.45	1.51
30	k	101	BCR	C30-C25	-2.97	1.49	1.53
27	a	410	SQD	O47-C7	2.96	1.42	1.34
22	C	511	CLA	CMB-C2B	-2.95	1.45	1.51
27	f	102	SQD	O48-C23	2.95	1.42	1.33
29	C	517	DGD	C6D-C5D	2.95	1.60	1.51
22	C	511	CLA	C1B-NB	2.94	1.37	1.35
22	B	612	CLA	C3B-C2B	-2.94	1.36	1.40
22	B	614	CLA	CHC-C1C	2.93	1.42	1.35
22	b	602	CLA	C3B-C2B	-2.93	1.36	1.40
29	c	515	DGD	C3D-C2D	2.92	1.59	1.52
22	B	601	CLA	MG-NA	2.92	2.13	2.06
22	C	502	CLA	C3B-C2B	-2.92	1.36	1.40
22	c	506	CLA	CHC-C1C	2.92	1.42	1.35
29	A	413	DGD	C4E-C5E	2.91	1.59	1.53
22	B	610	CLA	CHC-C1C	2.90	1.42	1.35
25	D	407	PL9	C53-C6	-2.89	1.44	1.50
22	C	504	CLA	C1B-NB	-2.89	1.32	1.35
29	C	516	DGD	C4E-C3E	2.89	1.59	1.52
22	C	506	CLA	C4D-ND	-2.88	1.33	1.37
22	d	404	CLA	CHC-C1C	2.88	1.42	1.35
22	a	402	CLA	CMB-C2B	-2.88	1.45	1.51
22	H	101	CLA	MG-ND	-2.88	2.00	2.05
22	B	608	CLA	C1D-ND	2.88	1.41	1.37
28	A	411	LHG	P-O6	2.87	1.70	1.59
22	C	501	CLA	MG-ND	2.86	2.11	2.05
29	c	516	DGD	C3D-C2D	2.85	1.59	1.52
22	b	603	CLA	CHC-C1C	2.85	1.42	1.35
22	b	607	CLA	C4D-ND	-2.85	1.33	1.37
26	a	414	LMG	C3-C2	2.85	1.59	1.52
22	B	610	CLA	MG-ND	2.85	2.11	2.05
22	C	511	CLA	C3B-C2B	-2.85	1.36	1.40
22	b	611	CLA	CMD-C2D	-2.85	1.44	1.50
23	D	401	PHO	C3B-CAB	-2.84	1.42	1.47
22	b	606	CLA	C4D-ND	-2.84	1.33	1.37
22	c	513	CLA	CMB-C2B	-2.84	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	103	DGD	O2D-C2D	-2.84	1.36	1.43
22	C	512	CLA	MG-NA	2.84	2.13	2.06
22	C	509	CLA	CMB-C2B	-2.84	1.45	1.51
22	b	615	CLA	MG-NC	-2.83	1.99	2.06
29	H	103	DGD	O5D-C1E	2.83	1.45	1.40
22	B	606	CLA	C3B-CAB	-2.83	1.42	1.47
22	C	501	CLA	CMD-C2D	-2.82	1.44	1.50
22	C	509	CLA	CMD-C2D	-2.82	1.44	1.50
28	b	623	LHG	O7-C5	-2.82	1.39	1.46
26	b	622	LMG	O8-C28	2.81	1.41	1.33
22	D	403	CLA	CHC-C1C	2.81	1.42	1.35
28	l	101	LHG	O7-C5	-2.81	1.39	1.46
22	c	502	CLA	CMD-C2D	-2.81	1.44	1.50
22	b	612	CLA	C4D-ND	-2.81	1.33	1.37
22	b	601	CLA	CMB-C2B	-2.81	1.45	1.51
22	C	509	CLA	MG-NC	-2.81	1.99	2.06
29	c	517	DGD	O4E-C4E	-2.80	1.36	1.43
22	b	607	CLA	CMB-C2B	-2.80	1.45	1.51
29	c	517	DGD	C4D-C5D	2.80	1.58	1.53
22	c	511	CLA	MG-ND	-2.80	2.00	2.05
22	B	611	CLA	CHC-C1C	2.80	1.42	1.35
28	a	411	LHG	O8-C23	2.79	1.41	1.33
22	C	513	CLA	C4D-ND	-2.79	1.33	1.37
28	D	410	LHG	O7-C5	-2.79	1.39	1.46
30	I	101	BCR	C33-C5	-2.79	1.46	1.50
30	C	515	BCR	C1-C6	-2.78	1.49	1.53
26	A	409	LMG	O8-C9	-2.78	1.38	1.45
30	t	101	BCR	C1-C6	-2.78	1.50	1.53
22	D	405	CLA	CMB-C2B	-2.77	1.45	1.51
22	b	604	CLA	CHC-C1C	2.77	1.42	1.35
22	B	615	CLA	CMD-C2D	-2.77	1.44	1.50
22	B	602	CLA	C4D-ND	-2.77	1.33	1.37
26	a	414	LMG	C1-C2	2.77	1.60	1.52
22	b	610	CLA	C4B-CHC	-2.76	1.33	1.41
22	C	506	CLA	C3B-C2B	-2.76	1.36	1.40
22	c	506	CLA	C4D-ND	-2.75	1.33	1.37
22	b	605	CLA	C1D-ND	2.75	1.41	1.37
22	c	504	CLA	C1D-ND	2.75	1.41	1.37
22	c	504	CLA	CMD-C2D	-2.75	1.45	1.50
26	a	414	LMG	O7-C10	2.75	1.42	1.34
22	c	503	CLA	C3B-C2B	-2.75	1.36	1.40
29	A	413	DGD	O1G-C1A	2.75	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	CMD-C2D	-2.74	1.45	1.50
22	B	609	CLA	CHC-C1C	2.74	1.42	1.35
22	b	602	CLA	CMB-C2B	-2.74	1.45	1.51
22	c	506	CLA	C3B-C2B	-2.73	1.36	1.40
22	b	616	CLA	CMD-C2D	-2.73	1.45	1.50
30	D	406	BCR	C1-C6	-2.73	1.50	1.53
22	B	601	CLA	C1B-NB	2.73	1.37	1.35
23	A	404	PHO	C1C-NC	-2.73	1.30	1.38
22	C	505	CLA	CMB-C2B	-2.73	1.46	1.51
30	B	618	BCR	C30-C25	-2.73	1.50	1.53
22	D	405	CLA	C4D-ND	-2.73	1.33	1.37
22	c	507	CLA	C1D-ND	2.72	1.41	1.37
22	b	602	CLA	CHC-C1C	2.72	1.41	1.35
22	c	513	CLA	CMD-C2D	-2.72	1.45	1.50
22	A	402	CLA	CHC-C1C	2.72	1.41	1.35
29	C	518	DGD	O2D-C2D	-2.71	1.36	1.43
25	A	408	PL9	C6-C1	-2.70	1.43	1.48
26	d	410	LMG	O7-C8	-2.70	1.39	1.46
22	B	614	CLA	C4B-CHC	-2.70	1.33	1.41
26	Y	101	LMG	C3-C2	2.70	1.59	1.52
22	c	502	CLA	CHC-C1C	2.70	1.41	1.35
26	c	518	LMG	O2-C2	-2.69	1.36	1.43
22	b	609	CLA	C4D-ND	-2.69	1.34	1.37
22	b	615	CLA	C1B-NB	2.69	1.37	1.35
22	B	612	CLA	CHC-C1C	2.69	1.41	1.35
22	c	502	CLA	CMC-C2C	-2.69	1.45	1.50
28	D	410	LHG	O8-C6	-2.69	1.39	1.45
22	c	511	CLA	C4D-ND	-2.69	1.34	1.37
22	a	403	CLA	C3B-CAB	-2.69	1.42	1.47
22	a	403	CLA	CMB-C2B	-2.68	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.68	1.46	1.51
26	Y	101	LMG	C6-C5	2.68	1.60	1.51
22	c	504	CLA	CHC-C1C	2.68	1.41	1.35
29	C	517	DGD	C4D-C3D	2.67	1.59	1.52
29	c	516	DGD	C3E-C2E	2.67	1.59	1.52
26	c	518	LMG	O1-C1	2.67	1.44	1.40
23	A	404	PHO	C3B-C2B	-2.66	1.36	1.40
28	L	102	LHG	P-O6	2.66	1.70	1.59
22	b	610	CLA	C3B-CAB	-2.66	1.42	1.47
22	C	505	CLA	C4D-ND	-2.66	1.34	1.37
22	b	608	CLA	C3B-CAB	-2.66	1.42	1.47
29	C	516	DGD	C1D-C2D	2.66	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	518	DGD	O2G-C2G	-2.65	1.40	1.46
22	b	601	CLA	O2A-CGA	2.65	1.41	1.33
22	d	403	CLA	C3D-C4D	2.64	1.50	1.44
22	A	403	CLA	CMD-C2D	-2.64	1.45	1.50
26	b	622	LMG	C9-C8	2.64	1.58	1.50
22	C	507	CLA	CHC-C1C	2.63	1.41	1.35
22	C	507	CLA	C3B-C2B	-2.63	1.36	1.40
22	C	509	CLA	CHC-C1C	2.63	1.41	1.35
26	c	520	LMG	O1-C1	2.63	1.44	1.40
22	A	403	CLA	MG-ND	-2.63	2.00	2.05
22	C	509	CLA	C1D-ND	2.62	1.41	1.37
22	c	512	CLA	CMB-C2B	-2.62	1.46	1.51
30	b	619	BCR	C30-C25	-2.62	1.50	1.53
22	C	508	CLA	CHC-C1C	2.62	1.41	1.35
22	B	610	CLA	CMB-C2B	-2.60	1.46	1.51
22	B	611	CLA	MG-ND	-2.60	2.00	2.05
22	b	613	CLA	MG-NC	2.60	2.12	2.06
30	d	406	BCR	C1-C6	-2.60	1.50	1.53
22	b	605	CLA	CHC-C1C	2.60	1.41	1.35
22	a	402	CLA	C3D-C4D	2.60	1.50	1.44
22	b	602	CLA	MG-ND	2.59	2.10	2.05
27	A	410	SQD	O2-C2	-2.59	1.36	1.43
22	d	405	CLA	CMD-C2D	-2.59	1.45	1.50
22	a	402	CLA	CHC-C1C	2.59	1.41	1.35
22	a	403	CLA	CMD-C2D	-2.59	1.45	1.50
28	d	409	LHG	C6-C5	2.58	1.58	1.50
22	A	405	CLA	C3B-CAB	-2.58	1.42	1.47
26	Y	101	LMG	O8-C9	-2.58	1.39	1.45
23	A	404	PHO	C3B-CAB	-2.58	1.42	1.47
22	c	505	CLA	MG-NC	-2.57	2.00	2.06
26	Y	101	LMG	O7-C8	-2.57	1.40	1.46
22	A	405	CLA	CMC-C2C	-2.57	1.45	1.50
29	c	517	DGD	C2A-C1A	-2.56	1.43	1.50
22	b	606	CLA	C3B-C2B	-2.56	1.36	1.40
22	A	405	CLA	CMD-C2D	-2.56	1.45	1.50
22	d	403	CLA	C1B-NB	-2.56	1.32	1.35
22	b	613	CLA	C4D-ND	-2.56	1.34	1.37
25	D	407	PL9	C45-C44	-2.56	1.44	1.50
27	a	410	SQD	O3-C3	-2.56	1.36	1.43
22	A	403	CLA	CHC-C1C	2.56	1.41	1.35
22	b	614	CLA	C3B-C2B	-2.56	1.36	1.40
29	H	103	DGD	O6E-C1E	2.56	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	PHO	C1C-NC	-2.55	1.30	1.38
30	I	101	BCR	C34-C9	-2.55	1.45	1.50
29	c	516	DGD	O3D-C3D	-2.55	1.37	1.43
22	B	605	CLA	C1D-ND	2.54	1.40	1.37
22	C	502	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.53	1.46	1.51
26	B	620	LMG	O7-C10	2.53	1.39	1.30
22	B	615	CLA	CMC-C2C	-2.53	1.45	1.50
30	a	406	BCR	C38-C26	-2.52	1.46	1.50
29	C	517	DGD	O3G-C3G	-2.52	1.39	1.43
29	C	518	DGD	C2A-C1A	-2.52	1.43	1.50
22	C	507	CLA	C3B-CAB	-2.51	1.42	1.47
22	b	604	CLA	C1D-ND	2.51	1.40	1.37
22	B	608	CLA	C3B-CAB	-2.51	1.42	1.47
22	C	502	CLA	C1D-ND	2.51	1.40	1.37
26	D	412	LMG	O8-C28	2.51	1.40	1.33
29	C	517	DGD	C4E-C5E	2.51	1.58	1.53
22	C	505	CLA	C3B-CAB	-2.50	1.42	1.47
28	D	413	LHG	O8-C23	2.50	1.40	1.33
22	d	405	CLA	CHC-C1C	2.50	1.41	1.35
22	B	613	CLA	C3B-CAB	-2.50	1.42	1.47
22	c	507	CLA	C3D-C4D	2.50	1.49	1.44
29	C	516	DGD	O2G-C2G	-2.49	1.40	1.46
22	B	610	CLA	C4B-CHC	-2.49	1.34	1.41
22	d	405	CLA	CMB-C2B	-2.49	1.46	1.51
29	C	517	DGD	C1G-C2G	2.49	1.58	1.50
22	C	510	CLA	CMB-C2B	-2.48	1.46	1.51
28	b	623	LHG	C8-C7	-2.47	1.43	1.50
22	b	607	CLA	C4B-CHC	-2.47	1.34	1.41
22	C	502	CLA	CHC-C1C	2.47	1.41	1.35
22	C	509	CLA	MG-ND	-2.47	2.00	2.05
23	A	404	PHO	CMD-C2D	-2.46	1.45	1.51
22	B	605	CLA	C4D-ND	-2.46	1.34	1.37
28	l	101	LHG	P-O6	2.46	1.69	1.59
27	D	409	SQD	O4-C4	-2.46	1.37	1.43
22	C	510	CLA	C3C-C2C	2.46	1.41	1.36
29	C	516	DGD	O1A-C1A	2.46	1.29	1.22
23	A	404	PHO	CAC-C3C	-2.46	1.47	1.52
22	b	616	CLA	CMC-C2C	-2.45	1.45	1.50
22	c	507	CLA	C4B-CHC	-2.45	1.34	1.41
27	f	102	SQD	O3-C3	-2.45	1.37	1.43
25	d	407	PL9	C7-C3	-2.45	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	CMD-C2D	-2.44	1.45	1.50
22	c	507	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	507	CLA	C4D-ND	-2.44	1.34	1.37
22	B	605	CLA	CMA-C3A	-2.44	1.47	1.53
25	d	407	PL9	C10-C9	-2.44	1.44	1.50
22	B	606	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	613	CLA	C1D-ND	2.43	1.40	1.37
22	C	501	CLA	CAC-C3C	-2.43	1.44	1.51
23	D	401	PHO	C3B-C2B	-2.43	1.37	1.40
22	B	603	CLA	C3B-C2B	-2.43	1.37	1.40
22	c	511	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	513	CLA	C3B-C2B	-2.43	1.37	1.40
25	a	409	PL9	C7-C3	-2.43	1.48	1.51
28	d	409	LHG	O8-C6	2.43	1.50	1.45
29	h	101	DGD	C4E-C3E	2.42	1.58	1.52
22	b	612	CLA	CHC-C1C	2.42	1.41	1.35
22	C	504	CLA	C4D-ND	-2.42	1.34	1.37
22	c	503	CLA	CMC-C2C	-2.42	1.45	1.50
22	c	512	CLA	C3D-C4D	2.42	1.49	1.44
22	b	605	CLA	C1D-C2D	2.42	1.50	1.45
22	c	509	CLA	CMB-C2B	-2.42	1.46	1.51
29	c	515	DGD	C1E-C2E	2.41	1.59	1.52
22	b	611	CLA	C4B-CHC	-2.41	1.34	1.41
22	c	504	CLA	CAC-C3C	-2.41	1.44	1.51
25	d	407	PL9	C40-C39	-2.41	1.44	1.50
22	C	512	CLA	CMD-C2D	-2.41	1.45	1.50
22	B	602	CLA	C4B-CHC	-2.41	1.34	1.41
26	c	518	LMG	C7-C8	2.41	1.58	1.50
22	b	607	CLA	CHD-C1D	-2.40	1.33	1.38
22	B	614	CLA	O2A-CGA	2.40	1.40	1.33
29	c	516	DGD	C4E-C5E	2.40	1.58	1.53
22	D	405	CLA	CMC-C2C	-2.40	1.45	1.50
22	D	403	CLA	MG-NC	-2.40	2.00	2.06
29	c	517	DGD	O2G-C1B	2.40	1.41	1.34
22	C	511	CLA	MG-NC	2.39	2.11	2.06
22	c	504	CLA	CMB-C2B	-2.39	1.46	1.51
23	d	401	PHO	CBD-CGD	-2.39	1.49	1.52
22	b	611	CLA	C3B-C2B	-2.39	1.37	1.40
22	a	405	CLA	CMB-C2B	-2.39	1.46	1.51
22	c	505	CLA	C1D-ND	2.39	1.40	1.37
26	b	622	LMG	C3-C2	2.39	1.58	1.52
29	c	517	DGD	O3D-C3D	-2.38	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C3B-CAB	-2.38	1.43	1.47
22	a	405	CLA	C4B-CHC	-2.38	1.34	1.41
22	B	604	CLA	C5-C3	-2.38	1.46	1.51
30	T	101	BCR	C38-C26	-2.38	1.47	1.50
22	D	404	CLA	CMB-C2B	-2.38	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	601	CLA	C4D-ND	-2.37	1.34	1.37
22	A	403	CLA	C3B-CAB	-2.37	1.43	1.47
22	C	512	CLA	CMC-C2C	-2.37	1.45	1.50
29	A	413	DGD	O5D-C6D	-2.37	1.39	1.43
30	I	101	BCR	C38-C26	-2.37	1.47	1.50
22	b	603	CLA	C3B-CAB	-2.36	1.43	1.47
22	c	505	CLA	C3B-CAB	-2.36	1.43	1.47
22	C	507	CLA	CMB-C2B	-2.36	1.46	1.51
22	B	607	CLA	C4B-CHC	-2.36	1.34	1.41
30	B	617	BCR	C30-C25	-2.36	1.50	1.53
25	D	407	PL9	C26-C27	2.35	1.61	1.53
23	d	401	PHO	CMC-C2C	-2.35	1.46	1.51
26	b	622	LMG	C4-C3	2.35	1.58	1.52
22	C	504	CLA	C4B-CHC	-2.35	1.34	1.41
22	c	505	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.35	1.45	1.50
26	Y	101	LMG	C1-C2	2.35	1.59	1.52
22	a	402	CLA	C1D-C2D	2.35	1.50	1.45
22	C	503	CLA	C3D-C4D	2.35	1.49	1.44
22	C	510	CLA	CMD-C2D	-2.35	1.45	1.50
29	h	101	DGD	O5D-C6D	-2.34	1.39	1.43
29	A	413	DGD	O1G-C1G	-2.34	1.39	1.45
29	c	515	DGD	O3G-C1D	-2.33	1.36	1.40
22	b	612	CLA	CMC-C2C	-2.33	1.45	1.50
26	c	521	LMG	C4-C5	2.33	1.57	1.53
22	B	602	CLA	CHC-C1C	2.33	1.40	1.35
23	A	404	PHO	O2D-CGD	2.33	1.38	1.33
30	x	101	BCR	C1-C6	-2.33	1.50	1.53
26	m	101	LMG	C1-C2	2.33	1.59	1.52
29	H	103	DGD	C1G-C2G	2.33	1.57	1.50
22	A	405	CLA	C4B-CHC	-2.33	1.34	1.41
29	c	516	DGD	C1E-C2E	2.33	1.59	1.52
22	B	601	CLA	C4B-CHC	-2.33	1.34	1.41
30	t	101	BCR	C27-C26	-2.32	1.46	1.51
22	c	501	CLA	C4B-CHC	-2.32	1.34	1.41
22	b	606	CLA	C4B-CHC	-2.32	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	k	102	BCR	C1-C6	-2.32	1.50	1.53
25	D	407	PL9	C21-C19	-2.32	1.46	1.51
26	D	408	LMG	O4-C4	2.32	1.48	1.43
22	B	615	CLA	CHC-C1C	2.32	1.40	1.35
22	C	504	CLA	CHC-C1C	2.31	1.40	1.35
22	B	606	CLA	C4B-CHC	-2.31	1.34	1.41
22	d	405	CLA	C4B-CHC	-2.31	1.34	1.41
22	b	611	CLA	MG-NC	-2.31	2.00	2.06
26	c	518	LMG	C3-C2	2.30	1.58	1.52
22	b	613	CLA	CAA-C2A	-2.30	1.49	1.54
29	h	101	DGD	C4E-C5E	2.30	1.57	1.53
22	B	615	CLA	C3B-C2B	-2.30	1.37	1.40
22	A	405	CLA	CHC-C1C	2.30	1.40	1.35
30	b	617	BCR	C30-C25	-2.30	1.50	1.53
22	B	604	CLA	CMD-C2D	-2.30	1.45	1.50
28	l	101	LHG	C6-C5	2.30	1.57	1.50
22	b	614	CLA	C1B-NB	-2.30	1.33	1.35
26	c	518	LMG	C6-C5	2.30	1.59	1.51
22	b	605	CLA	C4D-ND	-2.29	1.34	1.37
25	d	407	PL9	C26-C24	-2.29	1.46	1.51
22	C	501	CLA	CMC-C2C	-2.29	1.45	1.50
22	B	606	CLA	CHC-C1C	2.29	1.40	1.35
22	b	603	CLA	C4D-ND	-2.29	1.34	1.37
22	B	606	CLA	CMC-C2C	-2.28	1.46	1.50
27	t	102	SQD	C24-C23	2.28	1.57	1.50
22	B	612	CLA	CMC-C2C	-2.28	1.46	1.50
22	b	614	CLA	CMB-C2B	-2.28	1.46	1.51
22	B	613	CLA	C1B-NB	2.28	1.37	1.35
22	B	603	CLA	C1D-C2D	2.28	1.49	1.45
22	b	608	CLA	CMB-C2B	-2.27	1.46	1.51
22	B	610	CLA	C1D-ND	2.27	1.40	1.37
22	B	607	CLA	C3B-CAB	-2.27	1.43	1.47
25	D	407	PL9	C7-C3	-2.27	1.49	1.51
29	C	518	DGD	O2E-C2E	-2.26	1.37	1.43
22	b	605	CLA	CMD-C2D	-2.26	1.46	1.50
22	a	402	CLA	CMC-C2C	-2.26	1.46	1.50
30	B	616	BCR	C33-C5	-2.26	1.47	1.50
22	b	606	CLA	CMD-C2D	-2.26	1.46	1.50
22	b	606	CLA	CMB-C2B	-2.26	1.46	1.51
22	C	510	CLA	C1D-ND	2.26	1.40	1.37
31	B	619	STE	C2-C1	2.25	1.55	1.50
22	B	601	CLA	CAC-C3C	-2.25	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	CMB-C2B	-2.25	1.47	1.51
22	B	605	CLA	CMB-C2B	-2.25	1.47	1.51
29	c	517	DGD	O2G-C2G	-2.24	1.41	1.46
30	C	514	BCR	C33-C5	-2.24	1.47	1.50
22	C	513	CLA	C4B-CHC	-2.24	1.34	1.41
22	b	607	CLA	CMD-C2D	-2.23	1.46	1.50
25	D	407	PL9	C16-C17	2.23	1.61	1.53
22	c	502	CLA	C4B-CHC	-2.23	1.34	1.41
30	c	514	BCR	C38-C26	-2.22	1.47	1.50
22	C	511	CLA	C4B-CHC	-2.22	1.34	1.41
22	d	405	CLA	O1D-CGD	2.22	1.26	1.21
22	b	609	CLA	C3B-C2B	-2.22	1.37	1.40
22	D	405	CLA	C4B-CHC	-2.22	1.34	1.41
22	c	503	CLA	CMB-C2B	-2.21	1.47	1.51
26	a	414	LMG	C7-C8	2.21	1.57	1.50
30	k	102	BCR	C38-C26	-2.21	1.47	1.50
22	C	505	CLA	CMC-C2C	-2.21	1.46	1.50
22	B	611	CLA	CMD-C2D	-2.21	1.46	1.50
22	b	602	CLA	C3B-CAB	-2.21	1.43	1.47
28	a	411	LHG	C24-C23	2.21	1.57	1.50
26	a	414	LMG	O1-C1	2.21	1.44	1.40
22	a	403	CLA	C3B-C2B	-2.21	1.37	1.40
22	b	607	CLA	CMC-C2C	-2.21	1.46	1.50
22	b	608	CLA	CMA-C3A	-2.21	1.48	1.53
22	b	606	CLA	O2D-CED	-2.20	1.40	1.45
22	C	506	CLA	CAC-C3C	-2.20	1.45	1.51
22	d	404	CLA	C3B-CAB	-2.20	1.43	1.47
22	C	509	CLA	O2D-CGD	2.20	1.38	1.33
22	b	605	CLA	C4B-CHC	-2.20	1.34	1.41
26	B	620	LMG	C11-C10	2.20	1.55	1.50
26	A	409	LMG	C4-C5	2.19	1.57	1.53
29	C	517	DGD	C2B-C1B	-2.19	1.44	1.50
22	D	404	CLA	C3C-C2C	2.19	1.41	1.36
27	A	410	SQD	O3-C3	-2.19	1.37	1.43
26	A	409	LMG	C1-C2	2.19	1.58	1.52
26	c	520	LMG	C4-C3	2.19	1.57	1.52
22	D	404	CLA	C3D-C4D	2.18	1.49	1.44
22	B	611	CLA	C1C-NC	-2.18	1.34	1.37
26	D	408	LMG	C7-C8	2.18	1.57	1.50
22	c	510	CLA	CMC-C2C	-2.18	1.46	1.50
22	a	403	CLA	C4B-CHC	-2.18	1.34	1.41
22	a	402	CLA	C4B-CHC	-2.18	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C3B-CAB	-2.17	1.43	1.47
22	b	608	CLA	C1C-C2C	2.17	1.48	1.44
22	B	615	CLA	C1D-C2D	2.17	1.49	1.45
22	b	610	CLA	CMD-C2D	-2.17	1.46	1.50
22	c	507	CLA	CMC-C2C	-2.17	1.46	1.50
34	v	201	HEC	C1D-CHD	-2.17	1.35	1.41
22	d	405	CLA	C3B-C2B	-2.17	1.37	1.40
22	b	615	CLA	C3B-C2B	-2.17	1.37	1.40
22	C	507	CLA	C3D-C4D	2.17	1.49	1.44
23	D	401	PHO	CMB-C2B	-2.17	1.46	1.51
22	B	603	CLA	MG-NC	2.16	2.11	2.06
22	B	607	CLA	O2A-CGA	2.16	1.39	1.33
22	B	607	CLA	CMC-C2C	-2.16	1.46	1.50
26	d	410	LMG	O2-C2	-2.16	1.37	1.43
22	C	503	CLA	C1D-C2D	2.16	1.49	1.45
22	d	404	CLA	CMA-C3A	-2.16	1.48	1.53
22	b	602	CLA	CAC-C3C	-2.16	1.45	1.51
22	B	612	CLA	C4-C3	-2.16	1.45	1.50
22	b	608	CLA	O2A-CGA	2.16	1.39	1.33
25	d	407	PL9	C11-C9	-2.15	1.46	1.51
22	a	405	CLA	CMC-C2C	-2.15	1.46	1.50
29	A	413	DGD	C3D-C2D	2.15	1.57	1.52
28	a	411	LHG	C3-C2	2.15	1.58	1.51
22	C	508	CLA	CMD-C2D	-2.15	1.46	1.50
22	A	403	CLA	CMC-C2C	-2.15	1.46	1.50
22	c	509	CLA	C4B-CHC	-2.15	1.35	1.41
22	B	611	CLA	MG-NC	2.15	2.11	2.06
22	B	615	CLA	C3B-CAB	-2.15	1.43	1.47
22	C	508	CLA	CMB-C2B	-2.15	1.47	1.51
22	b	604	CLA	CMC-C2C	-2.15	1.46	1.50
26	M	101	LMG	O6-C1	2.14	1.47	1.41
28	D	413	LHG	C24-C23	2.14	1.57	1.50
29	C	516	DGD	C1G-C2G	2.14	1.57	1.50
29	C	517	DGD	O1G-C1G	-2.14	1.40	1.45
30	C	515	BCR	C30-C25	-2.14	1.50	1.53
29	c	517	DGD	C1D-C2D	2.14	1.58	1.52
30	b	618	BCR	C33-C5	-2.14	1.47	1.50
22	c	512	CLA	C1D-C2D	2.14	1.49	1.45
27	f	102	SQD	O2-C2	-2.14	1.37	1.43
29	c	515	DGD	C3G-C2G	2.14	1.57	1.50
28	d	409	LHG	P-O3	2.14	1.67	1.59
22	c	503	CLA	CAC-C3C	-2.13	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	407	PL9	C2-C3	2.13	1.40	1.34
22	C	504	CLA	CMD-C2D	-2.13	1.46	1.50
22	b	609	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	509	CLA	C3B-CAB	-2.13	1.43	1.47
22	B	614	CLA	CMD-C2D	-2.13	1.46	1.50
22	d	403	CLA	C3B-C2B	-2.13	1.37	1.40
28	D	410	LHG	C8-C7	-2.13	1.44	1.50
22	b	609	CLA	CMC-C2C	-2.13	1.46	1.50
22	B	609	CLA	MG-ND	-2.13	2.01	2.05
22	c	501	CLA	CMD-C2D	-2.13	1.46	1.50
22	a	405	CLA	MG-NC	-2.13	2.01	2.06
27	B	621	SQD	O2-C2	-2.13	1.38	1.43
26	c	521	LMG	C4-C3	2.13	1.57	1.52
26	Y	101	LMG	O1-C1	2.13	1.43	1.40
22	C	505	CLA	C1D-ND	2.13	1.40	1.37
22	C	513	CLA	C3B-CAB	-2.13	1.43	1.47
22	b	613	CLA	CMC-C2C	-2.13	1.46	1.50
22	b	607	CLA	CHC-C1C	2.12	1.40	1.35
22	B	604	CLA	CHC-C1C	2.12	1.40	1.35
22	b	614	CLA	C5-C3	-2.12	1.46	1.51
22	b	607	CLA	C1A-CHA	-2.12	1.34	1.43
22	a	405	CLA	CMD-C2D	-2.12	1.46	1.50
22	b	606	CLA	O2A-CGA	2.12	1.39	1.33
22	c	508	CLA	CMB-C2B	-2.12	1.47	1.51
30	b	618	BCR	C36-C18	-2.12	1.46	1.50
30	c	514	BCR	C30-C25	-2.11	1.50	1.53
26	B	620	LMG	C29-C28	2.11	1.55	1.50
29	C	517	DGD	O2G-C2G	-2.11	1.41	1.46
22	B	607	CLA	CMB-C2B	-2.10	1.47	1.51
22	d	405	CLA	MG-ND	-2.10	2.01	2.05
22	b	614	CLA	CMC-C2C	-2.10	1.46	1.50
23	A	404	PHO	CMC-C2C	-2.10	1.46	1.51
26	m	101	LMG	C6-C5	2.10	1.58	1.51
22	C	510	CLA	O2A-CGA	2.10	1.39	1.33
26	c	521	LMG	O1-C1	2.10	1.43	1.40
28	d	408	LHG	C8-C7	-2.09	1.44	1.50
26	D	408	LMG	O7-C8	-2.09	1.41	1.46
22	B	612	CLA	C3B-CAB	-2.09	1.43	1.47
31	j	101	STE	O1-C1	2.09	1.29	1.22
22	C	508	CLA	C3B-C2B	-2.09	1.37	1.40
25	a	409	PL9	C3-C4	-2.09	1.46	1.49
22	b	611	CLA	CAA-C2A	-2.09	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	406	BCR	C1-C6	-2.08	1.50	1.53
27	D	409	SQD	O2-C2	-2.08	1.38	1.43
22	c	510	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	607	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	606	CLA	C3D-C4D	2.08	1.48	1.44
28	a	411	LHG	P-O3	2.08	1.67	1.59
22	b	601	CLA	C3D-C4D	2.08	1.48	1.44
22	C	502	CLA	CMC-C2C	-2.08	1.46	1.50
22	C	508	CLA	MG-NC	-2.08	2.01	2.06
22	b	615	CLA	C4D-ND	-2.08	1.34	1.37
22	B	611	CLA	CMC-C2C	-2.08	1.46	1.50
22	b	610	CLA	C1C-NC	-2.08	1.34	1.37
23	a	404	PHO	CMB-C2B	-2.08	1.46	1.51
30	D	406	BCR	C38-C26	-2.07	1.47	1.50
22	A	402	CLA	C3C-C2C	2.07	1.41	1.36
22	C	511	CLA	CMD-C2D	-2.07	1.46	1.50
22	c	512	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	615	CLA	C4B-CHC	-2.07	1.35	1.41
22	b	616	CLA	C3B-C2B	-2.07	1.37	1.40
22	C	506	CLA	O2D-CGD	2.07	1.38	1.33
22	C	513	CLA	CMC-C2C	-2.07	1.46	1.50
29	H	103	DGD	O4D-C4D	-2.07	1.38	1.43
23	a	404	PHO	CAC-C3C	-2.07	1.48	1.52
29	A	413	DGD	C6D-C5D	2.07	1.58	1.51
22	D	404	CLA	MG-NC	-2.07	2.01	2.06
22	B	608	CLA	CHC-C1C	2.07	1.40	1.35
31	c	519	STE	C2-C1	2.07	1.55	1.50
25	a	409	PL9	C6-C1	-2.07	1.44	1.48
22	b	607	CLA	C3B-CAB	-2.07	1.43	1.47
28	a	411	LHG	C4-C5	2.06	1.57	1.50
29	h	101	DGD	C4D-C3D	2.06	1.57	1.52
22	b	613	CLA	CMB-C2B	-2.06	1.47	1.51
29	c	516	DGD	O6D-C5D	-2.06	1.39	1.44
22	b	601	CLA	CMD-C2D	-2.06	1.46	1.50
25	d	407	PL9	C16-C17	2.06	1.60	1.53
22	a	403	CLA	MG-ND	-2.06	2.01	2.05
25	D	407	PL9	C46-C44	-2.06	1.47	1.51
29	c	515	DGD	C4D-C3D	2.06	1.57	1.52
29	C	517	DGD	O3E-C3E	-2.06	1.38	1.43
22	B	605	CLA	C3B-CAB	-2.06	1.43	1.47
25	D	407	PL9	C15-C14	2.05	1.56	1.50
22	b	610	CLA	C1D-ND	2.05	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	CMC-C2C	-2.05	1.46	1.50
28	D	411	LHG	C8-C7	-2.05	1.44	1.50
29	H	103	DGD	O3G-C1D	2.05	1.43	1.40
22	c	512	CLA	C3B-CAB	-2.05	1.43	1.47
22	B	609	CLA	CMD-C2D	-2.05	1.46	1.50
22	d	403	CLA	CMD-C2D	-2.05	1.46	1.50
22	D	403	CLA	C1A-CHA	-2.05	1.34	1.43
22	C	506	CLA	CMA-C3A	-2.05	1.48	1.53
22	C	513	CLA	C1D-C2D	2.05	1.49	1.45
34	f	101	HEC	C4B-C3B	2.05	1.46	1.43
22	b	605	CLA	C1A-CHA	-2.05	1.34	1.43
22	c	504	CLA	MG-NA	-2.04	2.01	2.06
29	C	516	DGD	C2A-C1A	-2.04	1.44	1.50
22	C	513	CLA	C3D-C4D	2.04	1.48	1.44
22	D	403	CLA	C4B-CHC	-2.04	1.35	1.41
31	b	629	STE	C2-C1	2.04	1.55	1.50
22	B	602	CLA	MG-NA	2.04	2.11	2.06
22	b	608	CLA	CMC-C2C	-2.04	1.46	1.50
34	v	201	HEC	CMD-C2D	2.04	1.55	1.51
26	c	521	LMG	O6-C5	-2.04	1.39	1.44
29	c	517	DGD	O3E-C3E	-2.03	1.38	1.43
26	c	520	LMG	C7-C8	2.03	1.56	1.50
22	c	508	CLA	C3B-C2B	-2.03	1.37	1.40
22	b	615	CLA	CAC-C3C	-2.03	1.45	1.51
22	B	609	CLA	CAC-C3C	-2.03	1.45	1.51
23	d	401	PHO	CMD-C2D	-2.03	1.46	1.51
22	D	405	CLA	CAA-C2A	-2.03	1.50	1.54
22	b	609	CLA	C3D-C4D	2.03	1.48	1.44
22	c	501	CLA	C3B-C2B	-2.03	1.37	1.40
23	a	404	PHO	O2D-CGD	2.02	1.38	1.33
22	b	609	CLA	C3B-CAB	-2.02	1.43	1.47
22	C	508	CLA	CMC-C2C	-2.02	1.46	1.50
22	d	405	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	602	CLA	CMA-C3A	-2.02	1.48	1.53
29	c	515	DGD	O3G-C3G	-2.02	1.40	1.43
22	c	502	CLA	C3B-C2B	-2.01	1.37	1.40
27	D	409	SQD	O3-C3	-2.01	1.38	1.43
22	C	511	CLA	CMC-C2C	-2.01	1.46	1.50
22	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
23	D	401	PHO	CBD-CGD	-2.01	1.49	1.52
22	b	605	CLA	C3D-C4D	2.01	1.48	1.44
22	C	503	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	404	CLA	MG-ND	2.00	2.09	2.05
26	c	520	LMG	C4-C5	2.00	1.57	1.53
23	a	404	PHO	CMC-C2C	-2.00	1.46	1.51
22	C	510	CLA	CAC-C3C	-2.00	1.46	1.51
22	c	502	CLA	C3B-CAB	-2.00	1.43	1.47
22	H	101	CLA	C3C-C2C	2.00	1.41	1.36

All (1446) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	C4A-NA-C1A	10.34	111.35	106.71
27	L	101	SQD	O6-C1-C2	10.31	124.40	108.30
22	C	503	CLA	C4A-NA-C1A	9.87	111.14	106.71
22	C	511	CLA	C4A-NA-C1A	9.09	110.79	106.71
22	H	101	CLA	C4A-NA-C1A	9.03	110.76	106.71
22	c	511	CLA	C4A-NA-C1A	8.73	110.63	106.71
34	f	101	HEC	CBD-CAD-C3D	-8.26	98.53	112.62
22	b	601	CLA	C4A-NA-C1A	8.25	110.42	106.71
22	C	501	CLA	C4A-NA-C1A	8.13	110.36	106.71
22	c	501	CLA	C4A-NA-C1A	7.88	110.25	106.71
22	a	402	CLA	C4A-NA-C1A	7.79	110.21	106.71
22	B	609	CLA	C4A-NA-C1A	7.77	110.20	106.71
22	B	603	CLA	C4A-NA-C1A	7.67	110.16	106.71
22	B	614	CLA	C4A-NA-C1A	7.42	110.04	106.71
22	C	502	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	C	507	CLA	C4A-NA-C1A	7.16	109.92	106.71
22	B	606	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	B	615	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	B	605	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	b	606	CLA	C4A-NA-C1A	6.38	109.58	106.71
22	C	513	CLA	C4A-NA-C1A	6.25	109.52	106.71
27	B	621	SQD	O6-C1-C2	6.25	118.06	108.30
22	d	404	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	B	608	CLA	C4A-NA-C1A	6.21	109.50	106.71
27	D	409	SQD	O8-S-C6	6.19	115.60	105.74
22	b	603	CLA	O2D-CGD-O1D	-6.14	111.84	123.84
22	c	507	CLA	C4A-NA-C1A	6.10	109.45	106.71
27	f	102	SQD	O9-S-C6	5.99	114.06	106.94
22	B	610	CLA	CMB-C2B-C1B	-5.99	119.26	128.46
27	A	410	SQD	O7-S-C6	5.90	113.95	106.94
27	a	410	SQD	O6-C1-C2	5.90	117.51	108.30
34	F	101	HEC	CBD-CAD-C3D	-5.89	102.57	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	C4A-NA-C1A	5.88	109.35	106.71
22	c	510	CLA	C4A-NA-C1A	5.76	109.30	106.71
22	d	403	CLA	C4A-NA-C1A	5.68	109.26	106.71
34	v	201	HEC	C1D-C2D-C3D	-5.64	103.07	107.00
22	b	616	CLA	O2D-CGD-O1D	-5.64	112.81	123.84
27	D	409	SQD	O9-S-C6	5.63	113.63	106.94
22	b	606	CLA	O2D-CGD-O1D	-5.60	112.89	123.84
27	f	102	SQD	O7-S-C6	5.60	113.59	106.94
22	b	615	CLA	C4A-NA-C1A	5.58	109.22	106.71
22	A	402	CLA	C4A-NA-C1A	5.58	109.21	106.71
22	c	509	CLA	C4A-NA-C1A	5.55	109.20	106.71
22	a	403	CLA	C4A-NA-C1A	5.52	109.19	106.71
22	b	612	CLA	C4A-NA-C1A	5.47	109.16	106.71
27	B	621	SQD	O7-S-C6	5.45	113.42	106.94
22	b	603	CLA	O2D-CGD-CBD	5.45	120.95	111.27
22	c	501	CLA	O2D-CGD-O1D	-5.40	113.27	123.84
29	H	103	DGD	O3G-C3G-C2G	-5.37	97.93	110.90
22	c	513	CLA	C4A-NA-C1A	5.35	109.11	106.71
27	f	102	SQD	O6-C1-C2	5.30	116.58	108.30
30	c	514	BCR	C35-C13-C14	-5.28	115.53	122.92
22	B	604	CLA	O2D-CGD-O1D	-5.23	113.61	123.84
22	B	602	CLA	O2D-CGD-O1D	-5.22	113.64	123.84
34	v	201	HEC	CBD-CAD-C3D	-5.16	103.81	112.62
22	A	403	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
22	b	602	CLA	O2D-CGD-CBD	5.15	120.42	111.27
27	t	102	SQD	O47-C7-C8	5.15	122.60	111.50
27	B	621	SQD	O47-C7-C8	5.09	122.47	111.50
22	A	402	CLA	CHD-C1D-ND	-5.08	119.79	124.45
22	b	616	CLA	C4A-NA-C1A	5.05	108.98	106.71
22	c	506	CLA	C4A-NA-C1A	5.05	108.98	106.71
22	B	611	CLA	C4A-NA-C1A	5.04	108.97	106.71
22	b	605	CLA	C4A-NA-C1A	5.02	108.96	106.71
22	C	513	CLA	O2D-CGD-O1D	-5.02	114.03	123.84
22	b	605	CLA	CHD-C1D-ND	-4.97	119.89	124.45
25	a	409	PL9	C7-C3-C4	4.96	120.91	116.88
22	c	506	CLA	C2D-C1D-ND	-4.96	106.45	110.10
27	A	410	SQD	O6-C1-C2	4.94	116.01	108.30
22	C	512	CLA	C4A-NA-C1A	4.93	108.92	106.71
27	A	412	SQD	C45-O47-C7	4.93	124.22	117.88
33	D	402	BCT	O2-C-O1	4.90	132.24	119.55
27	D	409	SQD	O6-C1-C2	4.89	115.93	108.30
22	b	611	CLA	C4A-NA-C1A	4.88	108.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	611	CLA	CHD-C1D-ND	-4.88	119.97	124.45
26	b	622	LMG	C1-O6-C5	-4.87	104.14	113.69
22	B	610	CLA	O2D-CGD-CBD	4.86	119.91	111.27
22	b	614	CLA	CMB-C2B-C1B	-4.86	120.99	128.46
22	b	614	CLA	C4A-NA-C1A	4.85	108.89	106.71
22	c	508	CLA	C4A-NA-C1A	4.83	108.88	106.71
27	a	410	SQD	O8-S-C6	4.82	113.42	105.74
22	B	601	CLA	O2D-CGD-CBD	4.79	119.78	111.27
22	b	615	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
22	b	613	CLA	C4A-NA-C1A	4.76	108.85	106.71
22	B	610	CLA	O2D-CGD-O1D	-4.74	114.56	123.84
22	b	605	CLA	O2D-CGD-O1D	-4.74	114.57	123.84
22	C	504	CLA	CMB-C2B-C1B	-4.74	121.19	128.46
22	C	506	CLA	C4A-NA-C1A	4.68	108.81	106.71
27	A	410	SQD	O47-C7-C8	4.68	121.58	111.50
22	D	404	CLA	C4A-NA-C1A	4.66	108.80	106.71
34	V	201	HEC	CMC-C2C-C1C	-4.65	121.31	128.46
22	b	612	CLA	O2A-CGA-O1A	-4.65	111.85	123.59
22	b	602	CLA	O2D-CGD-O1D	-4.64	114.76	123.84
22	B	603	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
22	d	404	CLA	C1D-ND-C4D	4.64	109.63	106.33
22	B	610	CLA	CMB-C2B-C3B	4.62	133.33	124.68
22	C	508	CLA	C4A-NA-C1A	4.62	108.78	106.71
34	v	201	HEC	CMC-C2C-C1C	-4.61	121.38	128.46
29	h	101	DGD	C3D-C4D-C5D	-4.61	102.02	110.24
22	c	505	CLA	O2D-CGD-O1D	-4.59	114.86	123.84
22	b	613	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
29	C	518	DGD	O3G-C3G-C2G	-4.56	99.90	110.90
22	A	403	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	d	403	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
22	C	508	CLA	CHD-C1D-ND	-4.53	120.29	124.45
22	c	509	CLA	O2A-CGA-O1A	-4.49	112.26	123.59
22	C	505	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
25	D	407	PL9	C7-C3-C4	4.47	120.51	116.88
22	b	609	CLA	C4A-NA-C1A	4.47	108.71	106.71
22	b	609	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
22	C	512	CLA	CHB-C4A-NA	4.42	130.63	124.51
22	b	613	CLA	O2D-CGD-O1D	-4.41	115.21	123.84
22	c	502	CLA	C4A-NA-C1A	4.38	108.68	106.71
27	L	101	SQD	C1-C2-C3	-4.37	100.89	110.00
22	A	405	CLA	CHD-C1D-ND	-4.33	120.47	124.45
22	B	609	CLA	O2D-CGD-O1D	-4.32	115.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	411	LHG	O4-P-O5	4.30	133.49	112.24
22	B	603	CLA	O2A-CGA-O1A	-4.28	112.80	123.59
27	B	621	SQD	C3-C4-C5	4.27	117.86	110.24
22	B	604	CLA	O1D-CGD-CBD	4.27	133.23	124.48
26	m	101	LMG	O3-C3-C2	-4.27	100.47	110.35
22	B	609	CLA	CHD-C1D-ND	-4.25	120.55	124.45
22	b	604	CLA	C1-C2-C3	-4.25	118.69	126.04
22	C	508	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
28	A	411	LHG	O4-P-O5	4.24	133.19	112.24
22	c	512	CLA	CHD-C1D-ND	-4.23	120.56	124.45
22	b	610	CLA	C4A-NA-C1A	4.23	108.61	106.71
22	c	510	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
22	c	509	CLA	CHD-C1D-ND	-4.21	120.59	124.45
27	A	410	SQD	O9-S-O7	-4.21	99.39	113.95
27	A	410	SQD	C46-C45-C44	-4.20	101.86	111.79
22	b	602	CLA	C4A-NA-C1A	4.20	108.59	106.71
22	B	601	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
22	c	507	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
22	b	604	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
22	B	601	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
22	c	502	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
28	b	623	LHG	O4-P-O5	4.13	132.68	112.24
27	a	410	SQD	O9-S-C6	4.13	111.85	106.94
27	L	101	SQD	C45-O47-C7	4.13	127.96	117.79
33	d	402	BCT	O2-C-O1	4.10	130.17	119.55
22	c	508	CLA	CHD-C1D-ND	-4.09	120.70	124.45
22	D	403	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
22	c	505	CLA	O2D-CGD-CBD	4.07	118.50	111.27
28	D	413	LHG	O4-P-O5	4.07	132.36	112.24
25	A	408	PL9	C7-C3-C4	4.06	120.18	116.88
22	b	603	CLA	CHD-C1D-ND	-4.05	120.73	124.45
22	c	504	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
25	D	407	PL9	C36-C34-C33	-4.04	112.94	121.12
22	b	616	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
22	c	512	CLA	C4A-NA-C1A	4.03	108.52	106.71
26	b	622	LMG	O1-C1-C2	-4.03	102.01	108.30
29	c	516	DGD	O3G-C3G-C2G	-4.03	101.18	110.90
22	a	405	CLA	CHB-C4A-NA	4.02	130.07	124.51
22	c	506	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
34	V	201	HEC	C1D-C2D-C3D	-4.00	104.21	107.00
22	C	512	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
29	C	517	DGD	O3G-C3G-C2G	-4.00	101.25	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	502	CLA	CMB-C2B-C3B	3.99	132.15	124.68
22	A	402	CLA	CHB-C4A-NA	3.99	130.03	124.51
22	b	604	CLA	C4A-NA-C1A	3.98	108.50	106.71
30	b	617	BCR	C2-C1-C6	3.98	116.61	110.48
28	a	411	LHG	O4-P-O5	3.98	131.90	112.24
28	d	408	LHG	O4-P-O5	3.97	131.87	112.24
22	B	603	CLA	CMB-C2B-C3B	3.96	132.09	124.68
27	a	410	SQD	C1-C2-C3	-3.96	101.75	110.00
34	v	201	HEC	CBA-CAA-C2A	-3.95	105.94	112.60
27	t	102	SQD	O48-C23-O10	-3.93	113.67	123.59
28	D	410	LHG	O4-P-O5	3.91	131.55	112.24
22	c	509	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
31	L	103	STE	O2-C1-C2	3.90	126.57	114.03
25	A	408	PL9	C36-C34-C33	-3.89	113.24	121.12
22	a	403	CLA	CHB-C4A-NA	3.88	129.88	124.51
22	b	608	CLA	CHD-C1D-ND	-3.87	120.89	124.45
30	B	617	BCR	C29-C30-C25	3.86	116.42	110.48
30	B	618	BCR	C29-C30-C25	3.86	116.42	110.48
27	L	101	SQD	O5-C5-C4	3.85	116.69	109.69
22	c	507	CLA	CHD-C1D-ND	-3.85	120.92	124.45
27	a	410	SQD	C1-O5-C5	-3.85	106.14	113.69
27	f	102	SQD	O9-S-O7	-3.85	100.64	113.95
34	F	101	HEC	CMC-C2C-C1C	-3.85	122.55	128.46
22	b	616	CLA	O1D-CGD-CBD	3.84	132.34	124.48
22	B	614	CLA	C1B-CHB-C4A	-3.83	122.52	130.12
22	B	613	CLA	C4A-NA-C1A	3.83	108.43	106.71
27	L	101	SQD	O48-C23-C24	3.83	123.92	111.91
30	B	616	BCR	C2-C1-C6	3.83	116.37	110.48
22	c	502	CLA	CHD-C1D-ND	-3.82	120.94	124.45
22	B	607	CLA	CHD-C1D-ND	-3.82	120.94	124.45
22	D	405	CLA	C1B-CHB-C4A	-3.82	122.56	130.12
22	c	512	CLA	O2D-CGD-O1D	-3.82	116.38	123.84
28	l	101	LHG	O4-P-O5	3.81	131.09	112.24
34	V	201	HEC	CBD-CAD-C3D	-3.80	106.13	112.62
22	B	606	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
22	b	614	CLA	O2D-CGD-O1D	-3.79	116.44	123.84
22	d	403	CLA	CHD-C1D-ND	-3.77	120.99	124.45
30	B	618	BCR	C38-C26-C25	-3.77	120.30	124.53
22	b	604	CLA	C4-C3-C5	3.76	121.60	115.27
22	C	512	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
28	d	409	LHG	O4-P-O5	3.75	130.80	112.24
22	C	503	CLA	CHD-C1D-ND	-3.74	121.01	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
22	B	602	CLA	C6-C7-C8	-3.74	103.84	115.92
30	C	514	BCR	C33-C5-C6	-3.73	120.33	124.53
22	b	613	CLA	CMB-C2B-C3B	3.73	131.66	124.68
22	c	505	CLA	CHD-C1D-ND	-3.71	121.04	124.45
25	D	407	PL9	C40-C39-C41	3.71	121.51	115.27
25	A	408	PL9	O1-C4-C3	-3.70	116.64	120.72
22	B	603	CLA	CHB-C4A-NA	3.70	129.63	124.51
22	C	512	CLA	CHD-C1D-ND	-3.70	121.06	124.45
22	b	601	CLA	CHD-C1D-ND	-3.69	121.06	124.45
25	d	407	PL9	C22-C23-C24	-3.69	118.77	127.66
27	A	410	SQD	C45-O47-C7	3.69	126.88	117.79
22	B	609	CLA	CHB-C4A-NA	3.69	129.61	124.51
27	A	410	SQD	C1-O5-C5	-3.69	106.45	113.69
22	b	613	CLA	CHB-C4A-NA	3.68	129.61	124.51
22	b	603	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	a	402	CLA	O1D-CGD-CBD	3.68	132.02	124.48
28	L	102	LHG	O4-P-O5	3.68	130.43	112.24
26	A	409	LMG	O6-C1-O1	-3.68	101.26	109.97
29	C	516	DGD	O1G-C1A-C2A	-3.68	100.37	111.91
22	B	603	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
22	C	509	CLA	C4A-NA-C1A	3.67	108.35	106.71
30	B	617	BCR	C37-C22-C21	-3.66	117.79	122.92
26	c	521	LMG	C1-O6-C5	-3.66	106.50	113.69
22	B	611	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
22	c	503	CLA	CHD-C1D-ND	-3.66	121.09	124.45
22	c	509	CLA	CHB-C4A-NA	3.64	129.55	124.51
22	d	405	CLA	CMB-C2B-C3B	3.64	131.49	124.68
29	C	518	DGD	C4D-C3D-C2D	-3.63	104.48	110.82
34	f	101	HEC	CBA-CAA-C2A	-3.63	106.48	112.60
22	A	403	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
22	c	509	CLA	CMB-C2B-C3B	3.62	131.44	124.68
27	A	410	SQD	O9-S-C6	3.61	111.23	106.94
22	A	405	CLA	O2D-CGD-CBD	3.61	117.69	111.27
22	d	404	CLA	C2D-C1D-ND	-3.61	107.44	110.10
22	B	611	CLA	CMB-C2B-C3B	3.60	131.42	124.68
30	k	103	BCR	C39-C30-C25	-3.60	104.46	110.30
22	C	505	CLA	CMB-C2B-C3B	3.60	131.41	124.68
22	b	607	CLA	C4A-NA-C1A	3.60	108.32	106.71
27	B	621	SQD	O48-C23-C24	3.60	123.19	111.91
27	A	412	SQD	O47-C7-C8	3.59	119.25	111.50
22	C	505	CLA	CHB-C4A-NA	3.59	129.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	f	101	HEC	CMC-C2C-C1C	-3.59	122.94	128.46
22	d	404	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
31	B	625	STE	O2-C1-C2	3.59	125.56	114.03
23	d	401	PHO	O1D-CGD-CBD	3.59	130.71	124.74
27	L	101	SQD	O7-S-C6	3.58	111.19	106.94
22	b	612	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
30	K	101	BCR	C7-C8-C9	-3.57	120.84	126.23
22	c	504	CLA	CMB-C2B-C3B	3.56	131.35	124.68
22	c	512	CLA	C1-C2-C3	-3.56	119.89	126.04
22	b	601	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
29	c	517	DGD	O3G-C3G-C2G	-3.55	102.33	110.90
27	L	101	SQD	O9-S-C6	3.55	111.16	106.94
25	A	408	PL9	C22-C23-C24	-3.55	119.11	127.66
22	b	616	CLA	CMB-C2B-C3B	3.55	131.32	124.68
27	A	410	SQD	C1-C2-C3	-3.55	102.61	110.00
31	C	519	STE	O2-C1-O1	-3.55	114.46	123.30
22	d	404	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
22	c	510	CLA	CMB-C2B-C3B	3.54	131.31	124.68
22	C	509	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
29	c	517	DGD	C3D-C4D-C5D	-3.53	103.94	110.24
22	b	614	CLA	CMB-C2B-C3B	3.53	131.28	124.68
30	B	618	BCR	C36-C18-C17	-3.53	117.98	122.92
22	A	403	CLA	CMB-C2B-C3B	3.53	131.28	124.68
22	b	611	CLA	O2D-CGD-O1D	-3.53	116.95	123.84
22	c	505	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
25	a	409	PL9	C7-C3-C2	-3.52	118.67	123.30
23	A	404	PHO	C5-C3-C2	3.52	128.25	121.12
22	c	509	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	B	607	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	a	405	CLA	O2A-CGA-O1A	-3.51	114.74	123.59
30	C	514	BCR	C7-C8-C9	-3.50	120.94	126.23
22	C	504	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
30	K	101	BCR	C15-C16-C17	-3.49	116.32	123.47
29	h	101	DGD	C4D-C3D-C2D	-3.49	104.73	110.82
22	A	405	CLA	C4A-NA-C1A	3.49	108.27	106.71
22	A	405	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
22	b	605	CLA	O1D-CGD-CBD	3.48	131.61	124.48
29	C	518	DGD	O5D-C6D-C5D	-3.48	102.61	109.05
22	c	503	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
27	L	101	SQD	O5-C1-C2	-3.48	102.99	110.35
22	d	405	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
22	B	612	CLA	CHA-C1A-NA	-3.47	118.44	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	512	CLA	CHB-C4A-NA	3.47	129.32	124.51
22	C	510	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
30	d	406	BCR	C38-C26-C25	-3.47	120.63	124.53
22	c	511	CLA	O2A-C1-C2	-3.47	99.52	108.64
22	B	606	CLA	CHD-C1D-ND	-3.46	121.27	124.45
22	b	604	CLA	CMB-C2B-C3B	3.46	131.15	124.68
22	B	610	CLA	C4A-NA-C1A	3.45	108.26	106.71
23	A	404	PHO	C1-C2-C3	-3.45	120.07	126.04
26	m	101	LMG	O1-C7-C8	-3.45	102.57	110.90
26	m	101	LMG	O7-C10-O9	-3.45	115.37	123.70
27	D	409	SQD	O8-S-O9	-3.44	102.87	111.27
22	B	608	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
23	d	401	PHO	CMB-C2B-C3B	3.43	131.10	124.68
22	B	613	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
22	b	606	CLA	O2D-CGD-CBD	3.42	117.35	111.27
22	B	612	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	D	407	PL9	C50-C49-C48	-3.41	112.78	122.65
22	D	403	CLA	CMB-C2B-C3B	3.41	131.06	124.68
22	d	404	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
22	c	510	CLA	CHB-C4A-NA	3.41	129.22	124.51
22	B	607	CLA	CMB-C2B-C3B	3.40	131.04	124.68
22	b	612	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
22	A	402	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
22	C	507	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
22	C	506	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
22	b	613	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
27	t	102	SQD	O48-C23-C24	3.39	122.53	111.91
30	x	101	BCR	C27-C26-C25	3.38	127.64	122.73
30	t	101	BCR	C7-C8-C9	-3.37	121.14	126.23
27	L	101	SQD	O47-C7-C8	3.37	118.76	111.50
30	T	101	BCR	C7-C8-C9	-3.37	121.15	126.23
22	c	501	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
30	T	101	BCR	C27-C26-C25	3.36	127.61	122.73
22	b	608	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
22	C	508	CLA	CMB-C2B-C3B	3.36	130.96	124.68
22	b	613	CLA	O2D-CGD-CBD	3.36	117.23	111.27
22	b	610	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
22	C	503	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
26	M	101	LMG	C4-C3-C2	-3.35	104.97	110.82
30	D	406	BCR	C7-C8-C9	-3.35	121.18	126.23
22	D	405	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
22	c	501	CLA	O2D-CGD-CBD	3.35	117.21	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	622	STE	C3-C2-C1	-3.34	106.04	114.47
22	C	510	CLA	CHB-C4A-NA	3.34	129.14	124.51
22	A	402	CLA	C1D-ND-C4D	-3.34	103.96	106.33
22	c	513	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
29	c	516	DGD	O6D-C1D-O3G	-3.34	102.07	109.97
22	B	615	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
27	f	102	SQD	C1-C2-C3	-3.33	103.06	110.00
22	C	504	CLA	CMB-C2B-C3B	3.33	130.90	124.68
22	B	612	CLA	CHB-C4A-NA	3.33	129.11	124.51
22	B	615	CLA	C2C-C1C-NC	3.32	113.09	109.97
22	b	612	CLA	CAC-C3C-C4C	3.31	129.11	124.81
22	b	602	CLA	C2D-C1D-ND	-3.31	107.67	110.10
27	D	409	SQD	O48-C23-C24	3.31	122.28	111.91
22	b	602	CLA	O2A-CGA-O1A	-3.30	115.25	123.59
22	a	403	CLA	C2D-C1D-ND	-3.30	107.67	110.10
22	b	612	CLA	CHB-C4A-NA	3.30	129.07	124.51
22	B	601	CLA	C1B-CHB-C4A	-3.29	123.59	130.12
26	c	518	LMG	O6-C1-O1	-3.29	102.17	109.97
22	b	602	CLA	CMB-C2B-C3B	3.29	130.84	124.68
34	F	101	HEC	CBA-CAA-C2A	-3.29	107.06	112.60
22	D	403	CLA	O2A-CGA-O1A	-3.29	115.30	123.59
22	B	610	CLA	C1-C2-C3	-3.28	120.36	126.04
22	B	612	CLA	C1B-CHB-C4A	-3.28	123.61	130.12
23	d	401	PHO	CMC-C2C-C3C	3.28	131.13	124.94
22	B	608	CLA	C2C-C1C-NC	3.28	113.05	109.97
28	D	413	LHG	O8-C23-C24	3.28	122.20	111.91
26	a	414	LMG	C7-O1-C1	3.28	120.14	113.74
22	b	602	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
26	D	408	LMG	C3-C4-C5	-3.27	104.41	110.24
22	b	612	CLA	CMB-C2B-C3B	3.27	130.79	124.68
30	I	101	BCR	C27-C26-C25	3.27	127.47	122.73
22	C	507	CLA	CHB-C4A-NA	3.27	129.03	124.51
22	C	502	CLA	O1D-CGD-CBD	3.26	131.16	124.48
30	k	101	BCR	C15-C14-C13	-3.26	122.65	127.31
22	c	506	CLA	CHB-C4A-NA	3.26	129.02	124.51
25	D	407	PL9	C30-C29-C31	-3.26	109.79	115.27
28	D	413	LHG	O8-C23-O10	-3.25	115.38	123.59
25	d	407	PL9	C37-C38-C39	-3.25	119.83	127.66
22	b	609	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
22	c	502	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
22	B	603	CLA	C2D-C1D-ND	-3.24	107.72	110.10
26	m	101	LMG	O6-C1-O1	-3.24	102.30	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	613	CLA	CAC-C3C-C4C	3.24	129.01	124.81
29	c	515	DGD	O6D-C1D-O3G	-3.24	102.31	109.97
30	C	514	BCR	C35-C13-C14	-3.24	118.39	122.92
27	L	101	SQD	O2-C2-C1	3.23	117.89	110.05
22	c	503	CLA	C4A-NA-C1A	3.23	108.16	106.71
26	d	410	LMG	O6-C1-O1	-3.23	102.33	109.97
22	b	614	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
30	B	618	BCR	C15-C14-C13	-3.22	122.71	127.31
22	b	602	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
22	c	507	CLA	O2A-CGA-O1A	-3.22	115.46	123.59
22	A	405	CLA	CMB-C2B-C3B	3.22	130.70	124.68
22	B	601	CLA	CMB-C2B-C3B	3.22	130.70	124.68
22	B	611	CLA	C11-C12-C13	-3.21	105.53	115.92
22	b	605	CLA	CHB-C4A-NA	3.21	128.96	124.51
22	C	506	CLA	C2D-C1D-ND	-3.21	107.74	110.10
22	b	615	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
23	a	404	PHO	CMB-C2B-C3B	3.21	130.68	124.68
22	b	603	CLA	CED-O2D-CGD	-3.20	108.69	115.94
22	b	611	CLA	O2D-CGD-CBD	3.20	116.96	111.27
23	d	401	PHO	O2D-CGD-O1D	-3.20	117.58	123.84
22	B	606	CLA	CMB-C2B-C3B	3.20	130.66	124.68
22	c	508	CLA	O2A-CGA-O1A	-3.19	115.54	123.59
22	B	607	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
30	C	514	BCR	C36-C18-C17	-3.18	118.47	122.92
27	f	102	SQD	O48-C23-O10	-3.18	115.58	123.59
22	A	405	CLA	C1B-CHB-C4A	-3.18	123.83	130.12
22	d	404	CLA	O2D-CGD-CBD	3.17	116.91	111.27
29	c	516	DGD	C3D-C4D-C5D	-3.17	104.58	110.24
22	c	512	CLA	CHD-C4C-NC	3.17	129.20	124.20
30	x	101	BCR	C35-C13-C14	-3.17	118.48	122.92
29	H	103	DGD	O2D-C2D-C1D	-3.17	102.36	110.05
22	B	602	CLA	C4-C3-C5	3.16	120.58	115.27
22	b	607	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
25	D	407	PL9	C22-C23-C24	-3.15	120.07	127.66
22	d	403	CLA	CMB-C2B-C3B	3.15	130.57	124.68
27	B	621	SQD	C1-O5-C5	-3.15	107.51	113.69
22	b	609	CLA	O1D-CGD-CBD	3.15	130.93	124.48
22	C	501	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
22	C	513	CLA	O1D-CGD-CBD	3.15	130.92	124.48
22	B	602	CLA	CMB-C2B-C3B	3.14	130.56	124.68
22	b	608	CLA	CHB-C4A-NA	3.14	128.86	124.51
22	b	602	CLA	CHB-C4A-NA	3.14	128.85	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	610	CLA	CHB-C4A-NA	3.14	128.85	124.51
30	D	406	BCR	C2-C1-C6	3.13	115.31	110.48
22	B	605	CLA	CHD-C1D-ND	-3.13	121.58	124.45
29	H	103	DGD	C1D-C2D-C3D	-3.13	103.48	110.00
30	C	514	BCR	C15-C16-C17	-3.13	117.07	123.47
34	f	101	HEC	C1D-C2D-C3D	-3.12	104.82	107.00
22	C	513	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	b	607	CLA	CHD-C1D-ND	-3.12	121.59	124.45
22	C	512	CLA	CMB-C2B-C3B	3.12	130.51	124.68
22	c	505	CLA	CMB-C2B-C3B	3.12	130.51	124.68
29	C	516	DGD	O5D-C6D-C5D	-3.12	103.28	109.05
30	B	617	BCR	C35-C13-C14	-3.12	118.56	122.92
30	k	102	BCR	C2-C1-C6	3.11	115.27	110.48
27	A	410	SQD	O5-C5-C4	3.11	115.33	109.69
22	C	510	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
22	C	509	CLA	CMB-C2B-C3B	3.10	130.49	124.68
30	I	101	BCR	C40-C30-C25	3.10	115.33	110.30
30	I	101	BCR	C11-C10-C9	-3.10	122.88	127.31
30	a	406	BCR	C38-C26-C27	-3.10	107.66	113.62
22	D	404	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
30	K	101	BCR	C11-C10-C9	-3.10	122.89	127.31
22	C	506	CLA	C4-C3-C5	3.10	120.48	115.27
29	c	516	DGD	C3E-C4E-C5E	-3.10	104.72	110.24
23	A	404	PHO	CMC-C2C-C3C	3.09	130.77	124.94
22	a	403	CLA	CED-O2D-CGD	-3.09	108.95	115.94
27	f	102	SQD	C1-O5-C5	-3.08	107.64	113.69
29	A	413	DGD	O6E-C5E-C4E	3.08	115.29	109.69
22	B	615	CLA	CHB-C4A-NA	3.08	128.77	124.51
22	b	604	CLA	CHB-C4A-NA	3.08	128.77	124.51
29	H	103	DGD	C3E-C4E-C5E	-3.08	104.75	110.24
30	I	101	BCR	C38-C26-C27	-3.08	107.71	113.62
22	c	501	CLA	CED-O2D-CGD	-3.07	108.98	115.94
27	L	101	SQD	O47-C45-C46	3.07	119.50	108.40
22	b	608	CLA	C3B-C4B-NB	-3.07	105.25	109.21
22	c	513	CLA	CHD-C1D-ND	-3.06	121.64	124.45
30	k	101	BCR	C24-C23-C22	-3.06	121.61	126.23
22	c	509	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
22	b	601	CLA	CHB-C4A-NA	3.05	128.74	124.51
27	a	410	SQD	O9-S-O7	-3.05	103.38	113.95
22	B	610	CLA	CHB-C4A-NA	3.05	128.74	124.51
23	a	404	PHO	O2D-CGD-CBD	3.05	114.86	111.00
29	C	518	DGD	O6D-C1D-O3G	-3.05	102.75	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	501	CLA	C4-C3-C5	3.05	120.40	115.27
30	B	618	BCR	C2-C1-C6	3.05	115.18	110.48
30	c	514	BCR	C27-C26-C25	3.05	127.16	122.73
22	b	603	CLA	O2A-CGA-O1A	-3.04	115.91	123.59
27	A	410	SQD	O8-S-C6	3.04	110.59	105.74
22	b	606	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
22	b	616	CLA	CHB-C4A-NA	3.04	128.72	124.51
31	L	103	STE	O1-C1-C2	-3.04	113.31	123.08
26	M	101	LMG	O6-C1-O1	-3.04	102.77	109.97
28	a	411	LHG	O8-C23-C24	3.04	121.45	111.91
30	a	406	BCR	C37-C22-C21	-3.04	118.67	122.92
22	d	405	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
30	d	406	BCR	C3-C4-C5	-3.03	108.66	114.08
23	D	401	PHO	CMB-C2B-C3B	3.03	130.35	124.68
23	a	404	PHO	OBD-CAD-CBD	-3.03	121.38	125.82
22	b	611	CLA	CHD-C1D-C2D	3.03	131.83	125.48
22	C	502	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	d	407	PL9	C40-C39-C41	3.02	120.35	115.27
22	B	610	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
30	K	101	BCR	C35-C13-C14	-3.02	118.70	122.92
22	b	615	CLA	CMB-C2B-C3B	3.01	130.32	124.68
22	d	404	CLA	C2C-C1C-NC	3.01	112.80	109.97
22	c	511	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	B	604	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
22	c	504	CLA	C4A-NA-C1A	3.01	108.06	106.71
22	a	403	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
28	b	623	LHG	C11-C10-C9	-3.01	99.15	114.42
22	c	507	CLA	O2D-CGD-CBD	3.01	116.61	111.27
22	c	513	CLA	C1-C2-C3	-3.01	120.84	126.04
22	C	502	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
22	C	503	CLA	C4-C3-C5	3.00	120.33	115.27
27	B	621	SQD	O8-S-C6	3.00	110.52	105.74
22	A	402	CLA	O1D-CGD-CBD	3.00	130.62	124.48
27	B	621	SQD	O48-C23-O10	-2.99	116.03	123.59
29	C	517	DGD	C1D-C2D-C3D	-2.99	103.76	110.00
22	A	405	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
22	c	513	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
22	C	507	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
22	C	509	CLA	CHB-C4A-NA	2.99	128.64	124.51
30	c	514	BCR	C34-C9-C10	-2.99	118.74	122.92
22	B	613	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	D	403	CLA	C4-C3-C5	2.98	120.29	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	m	101	LMG	O1-C1-C2	-2.98	103.64	108.30
22	c	503	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
22	c	510	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
28	D	413	LHG	O3-P-O5	-2.98	97.43	109.07
26	b	622	LMG	O2-C2-C1	-2.97	102.83	110.05
22	B	604	CLA	CHD-C1D-ND	-2.97	121.72	124.45
27	a	410	SQD	O47-C7-O49	-2.97	116.53	123.70
30	c	514	BCR	C36-C18-C17	-2.97	118.77	122.92
22	b	610	CLA	C6-C5-C3	2.96	121.23	113.45
29	c	515	DGD	O3G-C3G-C2G	-2.96	103.75	110.90
22	B	614	CLA	CHB-C4A-NA	2.96	128.60	124.51
22	b	606	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
22	c	507	CLA	C2C-C1C-NC	2.95	112.74	109.97
30	H	102	BCR	C24-C23-C22	-2.95	121.77	126.23
22	d	404	CLA	CHB-C4A-NA	2.95	128.59	124.51
22	C	507	CLA	CMB-C2B-C3B	2.95	130.20	124.68
29	C	516	DGD	O6D-C1D-O3G	-2.94	103.00	109.97
22	B	613	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
22	B	609	CLA	O2A-CGA-O1A	-2.94	116.16	123.59
22	b	609	CLA	CMB-C2B-C3B	2.94	130.18	124.68
28	d	409	LHG	C26-C25-C24	2.94	123.76	113.19
22	B	614	CLA	CHD-C1D-ND	-2.94	121.75	124.45
29	c	517	DGD	O6D-C1D-O3G	-2.94	103.01	109.97
29	C	516	DGD	O3G-C3G-C2G	-2.94	103.81	110.90
22	B	608	CLA	CMB-C2B-C3B	2.94	130.17	124.68
30	k	101	BCR	C15-C16-C17	-2.93	117.46	123.47
22	B	612	CLA	O1D-CGD-CBD	2.93	130.49	124.48
22	b	604	CLA	C6-C7-C8	-2.93	106.44	115.92
22	c	506	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
27	L	101	SQD	O8-S-C6	2.93	110.41	105.74
22	B	612	CLA	C4-C3-C5	2.93	120.20	115.27
30	K	101	BCR	C36-C18-C17	-2.93	118.82	122.92
22	c	506	CLA	C1D-ND-C4D	2.92	108.41	106.33
27	D	409	SQD	C1-C2-C3	-2.92	103.91	110.00
22	c	512	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	c	511	CLA	C4-C3-C5	2.92	120.18	115.27
27	L	101	SQD	C3-C4-C5	2.92	115.44	110.24
30	b	619	BCR	C29-C30-C25	2.92	114.97	110.48
23	D	401	PHO	O1D-CGD-CBD	2.92	129.60	124.74
22	B	604	CLA	CMB-C2B-C3B	2.92	130.13	124.68
22	a	403	CLA	CAC-C3C-C4C	2.92	128.59	124.81
22	B	602	CLA	O2D-CGD-CBD	2.92	116.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	C6-C7-C8	-2.91	106.50	115.92
30	H	102	BCR	C2-C1-C6	2.91	114.97	110.48
27	B	621	SQD	C46-C45-C44	-2.91	104.90	111.79
22	C	504	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
22	b	616	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
29	C	516	DGD	O3E-C3E-C2E	-2.91	103.62	110.35
22	b	608	CLA	O2D-CGD-CBD	2.91	116.44	111.27
22	b	605	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
22	D	403	CLA	C1-C2-C3	-2.91	121.02	126.04
22	c	510	CLA	C16-C15-C13	-2.90	106.53	115.92
30	b	618	BCR	C35-C13-C14	-2.90	118.86	122.92
29	c	516	DGD	O5D-C6D-C5D	-2.90	103.68	109.05
30	a	406	BCR	C27-C26-C25	2.90	126.94	122.73
22	H	101	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	C	509	CLA	C1-O2A-CGA	2.89	124.04	116.44
27	f	102	SQD	O5-C1-O6	2.89	116.82	109.97
22	d	405	CLA	O2A-CGA-O1A	-2.89	116.29	123.59
30	K	102	BCR	C8-C7-C6	-2.89	119.09	127.20
22	d	405	CLA	CHD-C1D-ND	-2.89	121.80	124.45
22	D	405	CLA	C2D-C1D-ND	-2.88	107.98	110.10
22	C	511	CLA	CAC-C3C-C4C	2.88	128.55	124.81
30	b	617	BCR	C38-C26-C25	-2.88	121.29	124.53
31	C	519	STE	O2-C1-C2	2.88	123.28	114.03
30	k	101	BCR	C7-C8-C9	-2.88	121.88	126.23
22	H	101	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
22	C	501	CLA	O2D-CGD-CBD	2.88	116.38	111.27
25	a	409	PL9	C37-C38-C39	-2.87	120.74	127.66
28	D	410	LHG	C11-C10-C9	-2.87	99.84	114.42
22	B	611	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
22	b	603	CLA	CMB-C2B-C3B	2.87	130.05	124.68
34	V	201	HEC	CAD-CBD-CGD	-2.87	105.72	113.76
29	H	103	DGD	C4E-C3E-C2E	-2.87	105.81	110.82
27	A	410	SQD	O48-C23-C24	2.87	120.91	111.91
22	d	405	CLA	CED-O2D-CGD	2.87	122.42	115.94
27	A	410	SQD	O5-C1-O6	2.86	116.75	109.97
30	x	101	BCR	C36-C18-C17	-2.86	118.92	122.92
22	c	512	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
22	c	502	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
22	C	510	CLA	CMB-C2B-C3B	2.86	130.02	124.68
22	B	615	CLA	C2A-C3A-C4A	2.85	106.48	101.87
26	b	622	LMG	O6-C5-C6	2.85	113.53	106.44
22	b	601	CLA	O2D-CGD-O1D	-2.85	118.26	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	514	BCR	C15-C14-C13	-2.85	123.24	127.31
22	A	402	CLA	C16-C15-C13	-2.85	106.72	115.92
26	c	521	LMG	C1-C2-C3	2.84	115.91	110.00
30	K	102	BCR	C27-C26-C25	2.84	126.85	122.73
30	b	618	BCR	C8-C7-C6	-2.83	119.24	127.20
25	D	407	PL9	C7-C8-C9	-2.83	122.08	126.79
22	a	405	CLA	C2C-C1C-NC	2.83	112.62	109.97
22	b	611	CLA	CAA-C2A-C1A	-2.83	102.70	111.97
22	b	607	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
30	k	101	BCR	C11-C10-C9	-2.82	123.28	127.31
23	a	404	PHO	CMD-C2D-C3D	2.82	129.96	124.68
22	B	609	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
22	C	506	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	b	611	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
30	c	514	BCR	C30-C25-C26	-2.81	118.65	122.61
30	c	514	BCR	C33-C5-C6	-2.81	121.38	124.53
22	C	513	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
22	B	605	CLA	CHB-C4A-NA	2.80	128.39	124.51
30	d	406	BCR	C27-C26-C25	2.80	126.80	122.73
22	a	402	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	B	604	CLA	C16-C15-C13	-2.80	106.88	115.92
27	B	621	SQD	C4-C3-C2	2.79	115.69	110.82
30	K	101	BCR	C27-C26-C25	2.79	126.78	122.73
22	D	403	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
29	C	516	DGD	CDB-CCB-CBB	-2.78	100.29	114.42
22	B	612	CLA	O2A-C1-C2	-2.78	101.33	108.64
30	k	103	BCR	C1-C6-C5	-2.78	118.70	122.61
25	a	409	PL9	C30-C29-C28	-2.78	116.56	123.68
22	b	611	CLA	CMB-C2B-C3B	2.78	129.87	124.68
29	H	103	DGD	O2G-C1B-O1B	-2.78	117.00	123.70
22	c	505	CLA	C4A-NA-C1A	2.77	107.95	106.71
22	C	506	CLA	O2A-C1-C2	-2.77	101.35	108.64
22	A	402	CLA	C2D-C1D-ND	2.77	112.15	110.10
30	D	406	BCR	C3-C4-C5	-2.77	109.13	114.08
22	C	508	CLA	C3C-C4C-NC	-2.76	107.47	110.57
26	b	622	LMG	C3-C4-C5	-2.76	105.31	110.24
22	A	402	CLA	CMD-C2D-C1D	2.76	129.58	124.71
29	C	516	DGD	C6D-O5D-C1E	2.76	119.13	113.74
29	A	413	DGD	O5D-C6D-C5D	-2.76	103.94	109.05
30	b	617	BCR	C34-C9-C10	-2.76	119.06	122.92
27	B	621	SQD	O9-S-O7	-2.76	104.41	113.95
29	H	103	DGD	O6D-C1D-O3G	-2.76	103.45	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	405	CLA	CMA-C3A-C4A	-2.76	104.37	111.77
26	A	409	LMG	C9-C8-C7	-2.75	105.28	111.79
22	C	512	CLA	C1-C2-C3	-2.75	121.29	126.04
22	A	402	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
30	B	616	BCR	C15-C16-C17	-2.75	117.85	123.47
29	h	101	DGD	O1G-C1A-O1A	-2.75	116.66	123.59
22	C	503	CLA	O2A-C1-C2	-2.74	101.42	108.64
30	a	406	BCR	C7-C8-C9	-2.74	122.09	126.23
30	b	619	BCR	C12-C13-C14	-2.74	114.74	118.94
22	b	609	CLA	CHB-C4A-NA	2.74	128.30	124.51
30	D	406	BCR	C24-C23-C22	-2.73	122.11	126.23
30	c	514	BCR	C2-C1-C6	2.73	114.69	110.48
22	b	610	CLA	CAA-CBA-CGA	-2.73	105.27	113.25
29	c	515	DGD	O2D-C2D-C1D	-2.73	103.41	110.05
34	V	201	HEC	CMC-C2C-C3C	2.73	129.03	125.82
22	c	506	CLA	CMB-C2B-C3B	2.72	129.77	124.68
22	B	608	CLA	CHD-C4C-NC	2.72	128.49	124.20
22	B	611	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	B	615	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
22	c	508	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	a	402	CLA	CHD-C1D-ND	-2.71	121.96	124.45
22	B	607	CLA	O2D-CGD-CBD	2.71	116.09	111.27
26	D	408	LMG	O4-C4-C5	2.71	116.03	109.30
30	b	617	BCR	C27-C26-C25	2.71	126.67	122.73
26	c	520	LMG	O7-C10-O9	-2.71	117.16	123.70
25	A	408	PL9	C11-C9-C8	-2.71	115.64	121.12
26	B	620	LMG	O7-C10-O9	-2.71	116.55	123.30
22	c	512	CLA	O1D-CGD-CBD	2.71	130.02	124.48
23	a	404	PHO	O2D-CGD-O1D	-2.71	118.55	123.84
27	f	102	SQD	O47-C7-C8	2.70	118.33	110.80
30	d	406	BCR	C16-C15-C14	-2.70	117.94	123.47
22	C	508	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
29	c	516	DGD	CBB-CAB-C9B	-2.70	100.73	114.42
22	b	611	CLA	C2D-C1D-ND	-2.70	108.12	110.10
23	D	401	PHO	CMA-C3A-C4A	-2.70	108.47	114.38
30	B	618	BCR	C30-C25-C26	-2.69	118.82	122.61
30	b	619	BCR	C16-C15-C14	-2.69	117.96	123.47
30	k	101	BCR	C33-C5-C6	-2.69	121.51	124.53
26	c	521	LMG	O8-C28-O10	-2.69	116.80	123.59
25	A	408	PL9	C7-C3-C2	-2.69	119.76	123.30
26	a	414	LMG	O6-C5-C4	2.69	114.58	109.69
26	Y	101	LMG	O2-C2-C1	-2.69	103.52	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	x	101	BCR	C38-C26-C25	-2.69	121.51	124.53
26	D	408	LMG	O8-C28-O10	-2.68	116.82	123.59
23	D	401	PHO	C1-C2-C3	-2.68	121.40	126.04
22	B	612	CLA	CMB-C2B-C3B	2.68	129.69	124.68
22	C	504	CLA	C4-C3-C5	2.68	119.78	115.27
22	b	604	CLA	C11-C12-C13	-2.68	107.26	115.92
27	L	101	SQD	O9-S-O7	-2.68	104.68	113.95
22	b	605	CLA	C4-C3-C5	2.68	119.77	115.27
22	c	512	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
29	h	101	DGD	C1D-C2D-C3D	-2.68	104.42	110.00
30	b	619	BCR	C1-C6-C5	-2.68	118.84	122.61
22	a	402	CLA	CHB-C4A-NA	2.68	128.21	124.51
22	b	608	CLA	CHD-C4C-C3C	-2.67	120.91	124.84
26	D	408	LMG	O2-C2-C1	-2.67	103.56	110.05
30	H	102	BCR	C16-C15-C14	-2.67	118.01	123.47
22	d	404	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
22	b	615	CLA	CAA-CBA-CGA	-2.67	105.45	113.25
22	C	508	CLA	CHD-C1D-C2D	2.67	131.07	125.48
22	c	505	CLA	CHB-C4A-NA	2.67	128.20	124.51
29	c	515	DGD	O5D-C6D-C5D	-2.67	104.11	109.05
22	b	613	CLA	CBC-CAC-C3C	2.67	119.78	112.43
22	A	403	CLA	CAC-C3C-C4C	2.66	128.27	124.81
23	A	404	PHO	OBD-CAD-CBD	-2.66	121.92	125.82
22	A	403	CLA	O2D-CGD-CBD	2.66	116.00	111.27
26	c	520	LMG	O2-C2-C1	-2.66	103.59	110.05
27	L	101	SQD	O47-C7-O49	-2.66	117.28	123.70
26	c	521	LMG	O3-C3-C2	-2.66	104.21	110.35
22	b	612	CLA	C11-C12-C13	-2.66	107.33	115.92
26	a	414	LMG	O7-C10-C11	2.66	117.22	111.50
22	B	613	CLA	CMB-C2B-C1B	-2.65	124.38	128.46
22	B	602	CLA	O1D-CGD-CBD	2.65	129.91	124.48
22	b	608	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
22	D	404	CLA	C16-C15-C13	-2.65	107.35	115.92
22	B	605	CLA	CHD-C4C-NC	2.65	128.38	124.20
30	C	515	BCR	C15-C16-C17	-2.65	118.05	123.47
27	A	412	SQD	O47-C45-C46	2.65	112.27	106.13
25	D	407	PL9	C12-C13-C14	-2.65	121.29	127.66
22	D	404	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	a	409	PL9	C12-C13-C14	-2.65	121.29	127.66
29	c	515	DGD	C4E-C3E-C2E	-2.64	106.21	110.82
22	c	508	CLA	CMD-C2D-C1D	2.64	129.37	124.71
26	c	520	LMG	O6-C1-O1	-2.64	103.72	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	403	CLA	C1D-ND-C4D	2.64	108.21	106.33
25	A	408	PL9	O2-C1-C2	-2.63	115.75	121.78
22	b	605	CLA	CHD-C4C-NC	2.63	128.35	124.20
22	C	512	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
22	b	610	CLA	C2C-C1C-NC	2.63	112.44	109.97
23	A	404	PHO	C1B-NB-C4B	2.63	112.49	107.09
22	b	607	CLA	CMB-C2B-C3B	2.63	129.59	124.68
29	A	413	DGD	O6D-C1D-O3G	-2.63	103.75	109.97
22	D	404	CLA	CHB-C4A-NA	2.63	128.14	124.51
23	d	401	PHO	O2A-CGA-O1A	-2.63	116.97	123.59
29	h	101	DGD	O3G-C3G-C2G	-2.62	104.57	110.90
22	c	503	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
27	a	410	SQD	O48-C23-C24	2.62	120.14	111.91
22	c	506	CLA	CHD-C1D-C2D	2.62	130.98	125.48
30	c	514	BCR	C38-C26-C27	-2.62	108.58	113.62
22	B	602	CLA	C5-C3-C2	-2.62	115.81	121.12
30	t	101	BCR	C35-C13-C14	-2.62	119.25	122.92
22	C	513	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	k	101	BCR	C36-C18-C17	-2.62	119.26	122.92
30	b	618	BCR	C15-C16-C17	-2.62	118.11	123.47
22	B	608	CLA	CBC-CAC-C3C	-2.61	105.22	112.43
22	a	402	CLA	C2A-C1A-CHA	2.61	128.43	123.86
30	I	101	BCR	C37-C22-C21	-2.61	119.26	122.92
28	d	409	LHG	O8-C23-C24	2.61	120.10	111.91
31	x	102	STE	O2-C1-C2	2.61	122.42	114.03
26	c	520	LMG	O3-C3-C2	-2.61	104.31	110.35
22	A	402	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
30	k	102	BCR	C38-C26-C25	-2.61	121.60	124.53
22	C	504	CLA	C2C-C1C-NC	2.60	112.41	109.97
30	C	515	BCR	C40-C30-C25	2.60	114.52	110.30
26	c	518	LMG	O2-C2-C3	-2.60	104.33	110.35
22	B	611	CLA	O1D-CGD-CBD	2.60	129.81	124.48
30	b	617	BCR	C15-C16-C17	-2.60	118.15	123.47
22	c	502	CLA	O1D-CGD-CBD	2.60	129.80	124.48
22	D	404	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
25	D	407	PL9	C45-C44-C43	-2.60	117.01	123.68
22	c	503	CLA	C7-C6-C5	-2.60	106.30	113.36
26	a	414	LMG	C1-C2-C3	-2.60	104.59	110.00
22	B	602	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
30	H	102	BCR	C27-C26-C25	2.59	126.49	122.73
22	C	503	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	B	608	CLA	C1C-C2C-C3C	-2.59	104.24	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	619	BCR	C37-C22-C21	-2.59	119.30	122.92
26	M	101	LMG	C3-C4-C5	-2.59	105.63	110.24
22	D	405	CLA	O1D-CGD-CBD	2.59	129.78	124.48
22	C	513	CLA	CHC-C1C-NC	2.59	128.13	124.20
30	c	514	BCR	C32-C1-C6	-2.59	106.11	110.30
22	C	501	CLA	CED-O2D-CGD	-2.58	110.10	115.94
22	B	611	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	602	CLA	O2A-C1-C2	-2.58	101.85	108.64
30	c	514	BCR	C15-C14-C13	-2.58	123.63	127.31
26	a	414	LMG	C6-C5-C4	-2.58	106.96	113.00
29	C	516	DGD	O2D-C2D-C1D	-2.58	103.78	110.05
30	k	103	BCR	C27-C26-C25	2.57	126.47	122.73
22	b	606	CLA	C3C-C4C-NC	-2.57	107.69	110.57
22	b	605	CLA	CHD-C4C-C3C	-2.57	121.06	124.84
22	c	511	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	b	609	CLA	C7-C6-C5	-2.57	106.39	113.36
27	D	409	SQD	C46-C45-C44	-2.57	105.16	113.70
25	a	409	PL9	C7-C8-C9	-2.57	122.52	126.79
33	D	402	BCT	O3-C-O1	-2.57	112.89	119.55
22	C	506	CLA	CMB-C2B-C3B	2.56	129.47	124.68
26	d	410	LMG	O1-C1-C2	-2.56	104.31	108.30
30	I	101	BCR	C8-C7-C6	-2.56	120.02	127.20
22	c	504	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
22	B	609	CLA	C1-C2-C3	-2.56	121.62	126.04
22	D	403	CLA	C11-C12-C13	-2.55	107.66	115.92
22	b	604	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	C	502	CLA	CHA-C1A-NA	-2.55	120.56	126.40
22	C	502	CLA	CMB-C2B-C3B	2.55	129.45	124.68
22	b	608	CLA	CMB-C2B-C3B	2.55	129.44	124.68
30	a	406	BCR	C2-C1-C6	2.55	114.40	110.48
22	a	402	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
22	b	608	CLA	CMA-C3A-C4A	-2.54	104.94	111.77
30	T	101	BCR	C38-C26-C27	-2.54	108.73	113.62
29	C	518	DGD	O3E-C3E-C2E	-2.54	104.47	110.35
22	c	508	CLA	C7-C6-C5	-2.54	106.47	113.36
22	D	403	CLA	CHD-C1D-ND	-2.54	122.12	124.45
22	B	602	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	C	510	CLA	CHD-C1D-ND	-2.54	122.12	124.45
22	B	615	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	A	405	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
27	A	410	SQD	O48-C23-O10	-2.53	117.20	123.59
22	C	505	CLA	C1-O2A-CGA	-2.53	109.81	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	505	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
22	c	504	CLA	CHD-C1D-ND	-2.52	122.13	124.45
30	a	406	BCR	C20-C21-C22	-2.52	123.71	127.31
22	A	403	CLA	CED-O2D-CGD	-2.52	110.24	115.94
22	C	505	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
25	a	409	PL9	C32-C33-C34	-2.52	121.59	127.66
29	h	101	DGD	O6D-C1D-O3G	-2.52	104.01	109.97
22	b	606	CLA	O1D-CGD-CBD	2.52	129.64	124.48
22	C	504	CLA	O2D-CGD-CBD	2.52	115.74	111.27
22	B	615	CLA	CMB-C2B-C3B	2.52	129.39	124.68
30	b	618	BCR	C37-C22-C21	-2.52	119.40	122.92
28	D	410	LHG	O8-C23-C24	2.51	119.79	111.91
22	B	608	CLA	C2A-C3A-C4A	2.51	105.93	101.87
22	B	608	CLA	CHA-C1A-NA	-2.51	120.64	126.40
22	a	403	CLA	O2D-CGD-CBD	2.51	115.73	111.27
22	c	506	CLA	C3C-C4C-NC	-2.51	107.76	110.57
22	B	605	CLA	C2A-C3A-C4A	2.51	105.92	101.87
22	C	503	CLA	CMB-C2B-C3B	2.51	129.37	124.68
22	C	509	CLA	O2D-CGD-CBD	2.51	115.72	111.27
22	c	503	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
22	C	503	CLA	C4D-CHA-C1A	2.51	124.30	121.25
30	t	101	BCR	C15-C16-C17	-2.51	118.34	123.47
30	K	101	BCR	C34-C9-C8	-2.50	114.13	118.08
22	A	403	CLA	CHA-C1A-NA	-2.49	120.69	126.40
30	c	514	BCR	C29-C30-C25	2.49	114.32	110.48
22	c	503	CLA	C4D-CHA-C1A	2.49	124.28	121.25
29	c	517	DGD	CDB-CCB-CBB	-2.49	101.77	114.42
22	C	504	CLA	CED-O2D-CGD	2.49	121.57	115.94
22	C	513	CLA	CBC-CAC-C3C	2.49	119.29	112.43
27	B	621	SQD	O5-C5-C4	2.49	114.21	109.69
22	A	402	CLA	CMB-C2B-C3B	2.49	129.33	124.68
22	B	609	CLA	CHC-C1C-NC	2.49	127.97	124.20
23	d	401	PHO	C1-C2-C3	-2.48	121.75	126.04
30	k	101	BCR	C35-C13-C14	-2.48	119.45	122.92
22	B	613	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
22	b	611	CLA	CAC-C3C-C4C	2.48	128.03	124.81
30	B	618	BCR	C11-C10-C9	-2.48	123.77	127.31
22	B	613	CLA	O2D-CGD-CBD	2.48	115.67	111.27
22	c	510	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	b	605	CLA	C1D-ND-C4D	-2.48	104.58	106.33
22	B	609	CLA	O1D-CGD-CBD	2.48	129.55	124.48
25	D	407	PL9	C25-C24-C26	2.48	119.44	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	409	LMG	C3-C4-C5	-2.48	105.82	110.24
30	x	101	BCR	C33-C5-C6	-2.48	121.75	124.53
25	D	407	PL9	C42-C43-C44	-2.47	121.70	127.66
23	d	401	PHO	C1B-NB-C4B	2.47	112.17	107.09
30	x	101	BCR	C2-C1-C6	2.47	114.29	110.48
29	A	413	DGD	O3E-C3E-C2E	-2.47	104.63	110.35
22	a	405	CLA	CHA-C1A-NA	-2.47	120.74	126.40
22	b	611	CLA	CMD-C2D-C1D	2.47	129.06	124.71
22	b	603	CLA	CHD-C1D-C2D	2.47	130.66	125.48
22	b	612	CLA	C11-C10-C8	-2.47	107.94	115.92
29	c	516	DGD	O6E-C1E-O5D	-2.47	104.13	109.97
29	c	517	DGD	C3E-C4E-C5E	-2.47	105.84	110.24
22	B	603	CLA	O1D-CGD-CBD	2.46	129.53	124.48
28	d	409	LHG	O8-C23-O10	-2.46	117.38	123.59
22	c	503	CLA	O1D-CGD-CBD	2.46	129.52	124.48
22	b	604	CLA	C1-O2A-CGA	-2.46	110.00	116.44
30	x	101	BCR	C15-C16-C17	-2.46	118.44	123.47
26	Y	101	LMG	C3-C4-C5	-2.46	105.86	110.24
22	b	614	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	t	101	BCR	C34-C9-C10	-2.46	119.48	122.92
22	c	513	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	B	604	CLA	CAA-CBA-CGA	-2.45	106.08	113.25
31	R	101	STE	O2-C1-C2	2.45	121.91	114.03
22	C	503	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
22	C	503	CLA	C3A-C2A-C1A	2.45	105.01	101.34
26	d	410	LMG	O6-C5-C4	2.45	114.14	109.69
22	B	605	CLA	C6-C5-C3	-2.45	107.03	113.45
30	D	406	BCR	C27-C26-C25	2.45	126.29	122.73
22	B	605	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
22	b	606	CLA	C2D-C1D-ND	-2.45	108.30	110.10
29	c	515	DGD	C2G-O2G-C1B	2.45	123.82	117.79
22	C	505	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	B	601	CLA	C1-C2-C3	-2.44	121.81	126.04
22	d	403	CLA	CMD-C2D-C1D	2.44	129.02	124.71
29	c	515	DGD	C3G-C2G-C1G	-2.44	106.01	111.79
30	K	102	BCR	C16-C15-C14	-2.44	118.47	123.47
30	B	616	BCR	C11-C10-C9	-2.44	123.82	127.31
25	d	407	PL9	C50-C49-C48	-2.44	115.59	122.65
22	d	404	CLA	C16-C15-C13	-2.44	108.04	115.92
30	d	406	BCR	C11-C10-C9	-2.44	123.83	127.31
22	c	501	CLA	O1D-CGD-CBD	2.44	129.47	124.48
22	b	611	CLA	C3A-C2A-C1A	2.43	104.98	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	PL9	O2-C1-C6	2.43	124.80	120.59
22	C	502	CLA	C2A-C1A-CHA	2.43	128.11	123.86
26	M	101	LMG	C38-C37-C36	-2.43	102.08	114.42
26	c	521	LMG	O2-C2-C1	-2.43	104.14	110.05
22	C	512	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
30	b	618	BCR	C36-C18-C17	-2.43	119.52	122.92
22	B	602	CLA	CHD-C1D-ND	-2.43	122.22	124.45
22	B	606	CLA	CED-O2D-CGD	2.43	121.43	115.94
22	C	505	CLA	C4A-NA-C1A	2.43	107.80	106.71
22	c	513	CLA	O1D-CGD-CBD	2.43	129.45	124.48
30	K	102	BCR	C1-C6-C5	-2.43	119.20	122.61
30	H	102	BCR	C29-C30-C25	2.43	114.22	110.48
30	b	618	BCR	C15-C14-C13	-2.42	123.85	127.31
22	A	405	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	C	515	BCR	C37-C22-C21	-2.42	119.53	122.92
31	X	101	STE	C11-C10-C9	-2.42	102.14	114.42
30	d	406	BCR	C30-C25-C26	-2.42	119.20	122.61
30	t	101	BCR	C2-C1-C6	2.42	114.20	110.48
30	b	619	BCR	C31-C1-C6	2.42	114.22	110.30
22	c	507	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
34	V	201	HEC	CMB-C2B-C1B	-2.42	124.75	128.46
22	B	602	CLA	C4A-NA-C1A	2.42	107.79	106.71
22	b	606	CLA	CMB-C2B-C3B	2.41	129.19	124.68
26	c	520	LMG	O8-C28-O10	-2.41	117.50	123.59
22	C	503	CLA	CHD-C4C-NC	2.41	128.01	124.20
23	A	404	PHO	CMB-C2B-C3B	2.41	129.19	124.68
29	C	517	DGD	O2D-C2D-C1D	-2.41	104.19	110.05
22	a	403	CLA	C2A-C1A-CHA	2.41	128.07	123.86
30	b	619	BCR	C7-C8-C9	-2.41	122.59	126.23
23	D	401	PHO	C1B-NB-C4B	2.41	112.04	107.09
22	A	402	CLA	CHD-C4C-C3C	-2.41	121.30	124.84
22	c	511	CLA	CMB-C2B-C1B	-2.41	124.76	128.46
22	b	601	CLA	O2D-CGD-CBD	2.41	115.54	111.27
31	J	101	STE	O2-C1-C2	2.40	121.75	114.03
22	c	504	CLA	C4-C3-C5	2.40	119.31	115.27
26	D	408	LMG	C1-O6-C5	-2.40	108.97	113.69
22	B	604	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	d	407	PL9	C32-C33-C34	-2.40	121.88	127.66
29	A	413	DGD	O5D-C1E-C2E	2.40	112.05	108.30
29	C	518	DGD	C3G-C2G-C1G	-2.40	106.11	111.79
22	b	609	CLA	C2D-C1D-ND	-2.40	108.34	110.10
28	L	102	LHG	C5-O7-C7	-2.40	111.89	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	403	CLA	CHB-C4A-NA	2.40	127.83	124.51
29	C	518	DGD	O3D-C3D-C4D	-2.39	104.81	110.35
23	A	404	PHO	C1A-C2A-C3A	-2.39	100.56	102.84
22	A	402	CLA	C3D-C2D-C1D	-2.39	102.57	105.83
22	b	601	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
30	a	406	BCR	C35-C13-C14	-2.39	119.57	122.92
30	C	514	BCR	C11-C10-C9	-2.39	123.91	127.31
22	b	612	CLA	C1-C2-C3	-2.39	121.92	126.04
25	a	409	PL9	C42-C43-C44	-2.38	121.92	127.66
22	c	508	CLA	CHD-C1D-C2D	2.38	130.48	125.48
30	B	616	BCR	C37-C22-C23	2.38	121.83	118.08
28	a	411	LHG	C11-C10-C9	-2.38	102.34	114.42
34	F	101	HEC	CMD-C2D-C1D	-2.38	124.81	128.46
22	c	504	CLA	C6-C7-C8	-2.38	108.23	115.92
22	b	610	CLA	CHD-C1D-ND	-2.38	122.27	124.45
22	c	511	CLA	CMA-C3A-C4A	2.38	118.16	111.77
22	c	506	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
26	c	521	LMG	C4-C3-C2	2.38	114.97	110.82
30	B	617	BCR	C7-C8-C9	-2.38	122.64	126.23
29	H	103	DGD	CCB-CBB-CAB	-2.38	102.37	114.42
29	A	413	DGD	O3D-C3D-C4D	-2.37	104.86	110.35
22	B	612	CLA	C7-C6-C5	-2.37	106.91	113.36
22	A	402	CLA	CHD-C4C-NC	2.37	127.94	124.20
29	C	517	DGD	C7B-C6B-C5B	-2.37	102.38	114.42
29	C	517	DGD	O3G-C1D-C2D	-2.37	104.60	108.30
22	B	601	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	c	503	CLA	CMB-C2B-C3B	2.37	129.11	124.68
27	A	412	SQD	O49-C7-C8	-2.37	114.49	123.73
22	b	601	CLA	CMB-C2B-C3B	2.37	129.11	124.68
22	c	502	CLA	CHD-C1D-C2D	2.37	130.44	125.48
25	a	409	PL9	C20-C19-C21	2.36	119.25	115.27
22	a	405	CLA	CMB-C2B-C3B	2.36	129.10	124.68
22	b	610	CLA	CMB-C2B-C3B	2.36	129.10	124.68
22	a	402	CLA	C4-C3-C5	2.36	119.24	115.27
30	d	406	BCR	C19-C18-C17	-2.36	115.32	118.94
29	c	516	DGD	CDB-CCB-CBB	-2.36	102.45	114.42
30	B	617	BCR	C15-C14-C13	-2.36	123.94	127.31
22	b	601	CLA	CHD-C4C-NC	2.36	127.92	124.20
22	B	614	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
22	c	511	CLA	O1A-CGA-CBA	2.36	132.92	123.73
27	D	409	SQD	C3-C4-C5	2.35	114.44	110.24
29	A	413	DGD	C3E-C4E-C5E	-2.35	106.04	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	CMC-C2C-C1C	2.35	128.62	125.04
29	C	516	DGD	C5B-C4B-C3B	-2.35	102.49	114.42
23	a	404	PHO	C1B-NB-C4B	2.35	111.92	107.09
30	T	101	BCR	C3-C4-C5	-2.35	109.88	114.08
22	c	505	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
22	b	611	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
22	c	511	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
22	C	510	CLA	C1D-ND-C4D	2.35	108.00	106.33
29	h	101	DGD	C2G-O2G-C1B	2.35	123.57	117.79
29	h	101	DGD	O3E-C3E-C2E	-2.35	104.93	110.35
22	b	608	CLA	C4A-NA-C1A	2.34	107.76	106.71
22	A	403	CLA	C2D-C1D-ND	-2.34	108.38	110.10
26	d	410	LMG	O2-C2-C1	-2.34	104.36	110.05
22	A	405	CLA	C4-C3-C5	2.34	119.21	115.27
22	b	610	CLA	O1D-CGD-CBD	2.34	129.28	124.48
25	A	408	PL9	C40-C39-C38	-2.34	117.67	123.68
23	a	404	PHO	O2A-CGA-O1A	-2.34	117.68	123.59
22	b	616	CLA	C6-C5-C3	2.34	119.59	113.45
22	C	511	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	614	CLA	CMC-C2C-C1C	-2.34	121.47	125.04
27	A	410	SQD	O5-C1-C2	-2.34	105.40	110.35
29	C	518	DGD	O1G-C1A-O1A	-2.34	117.69	123.59
30	K	101	BCR	C40-C30-C25	2.33	114.09	110.30
29	C	517	DGD	C1D-O6D-C5D	-2.33	109.11	113.69
22	B	603	CLA	C1D-ND-C4D	2.33	107.99	106.33
30	I	101	BCR	C34-C9-C8	-2.33	114.40	118.08
31	X	101	STE	C3-C2-C1	-2.33	108.60	114.47
25	d	407	PL9	C27-C28-C29	-2.33	122.05	127.66
28	l	101	LHG	O8-C23-C24	2.33	119.22	111.91
22	C	507	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	A	403	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
30	k	103	BCR	C40-C30-C25	2.32	114.07	110.30
22	b	611	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	b	604	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	B	605	CLA	CHD-C4C-C3C	-2.32	121.43	124.84
29	h	101	DGD	C1E-O6E-C5E	2.32	118.24	113.69
22	b	611	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
30	k	102	BCR	C27-C26-C25	2.32	126.10	122.73
22	b	602	CLA	C4-C3-C5	2.32	119.17	115.27
28	b	623	LHG	O8-C23-C24	2.32	119.18	111.91
22	b	612	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
30	b	618	BCR	C28-C27-C26	-2.32	109.94	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	102	BCR	C12-C13-C14	-2.31	115.39	118.94
30	a	406	BCR	C39-C30-C25	-2.31	106.55	110.30
22	C	509	CLA	CHA-C1A-NA	-2.31	121.10	126.40
22	B	614	CLA	CMC-C2C-C3C	2.31	132.39	126.12
22	d	404	CLA	CMB-C2B-C3B	2.31	129.00	124.68
22	d	403	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
29	H	103	DGD	C6D-C5D-C4D	2.31	116.92	112.09
27	a	410	SQD	O5-C1-O6	2.31	115.44	109.97
34	F	101	HEC	CMC-C2C-C3C	2.31	128.53	125.82
25	d	407	PL9	C51-C49-C50	2.31	119.70	114.60
22	b	603	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
29	c	516	DGD	C3G-O3G-C1D	2.31	118.24	113.74
26	c	521	LMG	O2-C2-C3	-2.30	105.02	110.35
27	B	621	SQD	O49-C7-C8	-2.30	114.75	123.73
30	B	616	BCR	C29-C30-C25	2.30	114.03	110.48
22	c	501	CLA	C2C-C1C-NC	2.30	112.13	109.97
26	c	518	LMG	O8-C28-O10	-2.30	117.78	123.59
22	b	609	CLA	C6-C5-C3	2.30	119.49	113.45
22	a	403	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
29	C	517	DGD	CDB-CCB-CBB	-2.30	102.76	114.42
22	C	512	CLA	O1D-CGD-CBD	2.30	129.19	124.48
22	B	601	CLA	C4A-NA-C1A	2.30	107.74	106.71
22	b	614	CLA	O2A-C1-C2	-2.29	102.60	108.64
22	C	506	CLA	OBD-CAD-C3D	2.29	134.04	128.52
22	c	504	CLA	CED-O2D-CGD	2.29	121.12	115.94
22	b	609	CLA	CHA-C1A-NA	-2.29	121.15	126.40
26	A	409	LMG	O3-C3-C2	-2.29	105.06	110.35
29	c	516	DGD	O5D-C1E-C2E	2.29	111.88	108.30
22	c	512	CLA	C3C-C4C-NC	-2.29	108.00	110.57
27	a	410	SQD	O5-C5-C4	2.29	113.85	109.69
26	D	412	LMG	C38-C37-C36	-2.29	102.81	114.42
22	D	404	CLA	CMB-C2B-C3B	2.29	128.96	124.68
30	k	103	BCR	C35-C13-C14	-2.29	119.72	122.92
22	B	608	CLA	C6-C5-C3	2.29	119.45	113.45
30	C	514	BCR	C29-C30-C25	2.28	114.00	110.48
26	M	101	LMG	O5-C6-C5	-2.28	103.46	111.29
22	c	504	CLA	OBD-CAD-C3D	2.28	134.01	128.52
29	c	516	DGD	O2G-C1B-O1B	-2.28	118.19	123.70
22	C	511	CLA	C4-C3-C5	2.28	119.11	115.27
27	D	409	SQD	O9-S-O7	-2.28	106.05	113.95
22	C	508	CLA	C7-C6-C5	-2.28	107.16	113.36
23	D	401	PHO	CMD-C2D-C3D	2.28	128.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	402	CLA	CHC-C1C-NC	2.28	127.66	124.20
25	d	407	PL9	C7-C8-C9	-2.28	123.00	126.79
25	D	407	PL9	C8-C7-C3	2.27	118.40	111.98
25	d	407	PL9	C20-C19-C21	2.27	119.09	115.27
30	x	101	BCR	C7-C8-C9	-2.27	122.80	126.23
30	c	514	BCR	C11-C10-C9	-2.27	124.07	127.31
22	b	612	CLA	O2A-CGA-CBA	2.27	119.03	111.91
31	t	103	STE	C3-C2-C1	-2.27	108.75	114.47
22	c	504	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
26	c	520	LMG	O1-C1-C2	-2.27	104.76	108.30
25	a	409	PL9	O2-C1-C2	-2.27	116.58	121.78
29	c	515	DGD	C3D-C4D-C5D	-2.27	106.20	110.24
26	B	620	LMG	O8-C28-O10	-2.26	117.66	123.30
28	A	411	LHG	O8-C23-C24	2.26	119.01	111.91
22	B	602	CLA	CHC-C1C-NC	2.26	127.63	124.20
22	c	505	CLA	CHA-C1A-NA	-2.26	121.22	126.40
26	d	410	LMG	O3-C3-C2	-2.26	105.13	110.35
27	a	410	SQD	O47-C7-C8	2.26	116.37	111.50
22	C	502	CLA	CMD-C2D-C3D	2.26	132.81	127.61
22	B	613	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
29	c	516	DGD	O3D-C3D-C4D	-2.26	105.13	110.35
25	D	407	PL9	C11-C12-C13	-2.26	104.47	111.88
22	b	609	CLA	C4-C3-C5	-2.26	111.48	115.27
30	I	101	BCR	C16-C17-C18	-2.26	124.09	127.31
30	K	102	BCR	C39-C30-C25	-2.25	106.64	110.30
22	a	405	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
25	d	407	PL9	C7-C3-C4	2.25	118.71	116.88
22	c	506	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
22	b	607	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
22	b	610	CLA	C4-C3-C5	2.25	119.06	115.27
22	c	509	CLA	C16-C15-C13	-2.25	108.64	115.92
29	c	516	DGD	C7B-C6B-C5B	-2.25	103.00	114.42
22	c	502	CLA	C1-C2-C3	-2.25	122.15	126.04
22	d	404	CLA	C2A-C1A-CHA	2.25	127.79	123.86
30	k	103	BCR	C29-C30-C25	2.25	113.94	110.48
22	a	405	CLA	C4D-CHA-C1A	-2.25	118.51	121.25
22	C	501	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
22	C	501	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
26	Y	101	LMG	O6-C5-C6	2.25	112.02	106.44
22	B	603	CLA	C2A-C1A-CHA	2.25	127.78	123.86
30	B	616	BCR	C27-C26-C25	2.24	125.99	122.73
22	B	604	CLA	C2C-C1C-NC	2.24	112.07	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	621	STE	C3-C2-C1	-2.24	108.82	114.47
22	b	614	CLA	O2D-CGD-CBD	2.24	115.25	111.27
22	d	404	CLA	C1-C2-C3	-2.24	122.17	126.04
22	A	403	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	B	601	CLA	CHA-C4D-ND	2.24	137.18	132.50
27	D	409	SQD	O48-C23-O10	-2.24	117.95	123.59
29	C	517	DGD	O5D-C6D-C5D	-2.24	104.91	109.05
28	D	411	LHG	O8-C23-O10	-2.24	117.95	123.59
22	b	606	CLA	C1C-C2C-C3C	-2.24	104.61	106.96
22	c	501	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
22	B	610	CLA	C2C-C1C-NC	2.23	112.06	109.97
22	B	602	CLA	CHD-C4C-C3C	-2.23	121.56	124.84
25	A	408	PL9	C25-C24-C23	-2.23	117.95	123.68
25	d	407	PL9	C40-C39-C38	-2.23	117.96	123.68
22	B	611	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	B	603	CLA	O2A-CGA-CBA	2.23	118.90	111.91
22	b	616	CLA	C2C-C1C-NC	2.23	112.06	109.97
22	b	605	CLA	C3D-C4D-ND	2.23	113.84	110.24
26	Y	101	LMG	O1-C7-C8	-2.22	105.53	110.90
22	c	507	CLA	C1-C2-C3	-2.22	122.20	126.04
26	a	414	LMG	C9-C8-C7	-2.22	106.53	111.79
22	b	611	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
22	b	603	CLA	C1-C2-C3	-2.22	122.20	126.04
22	a	405	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
27	L	101	SQD	O48-C23-O10	-2.22	117.99	123.59
22	B	615	CLA	O1D-CGD-CBD	2.22	129.03	124.48
30	I	101	BCR	C15-C16-C17	-2.22	118.93	123.47
22	B	604	CLA	C2D-C1D-ND	-2.22	108.47	110.10
22	B	614	CLA	CHC-C1C-NC	2.22	127.57	124.20
22	C	501	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	C	508	CLA	O1D-CGD-CBD	2.22	129.03	124.48
22	C	502	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	D	407	PL9	C41-C39-C38	-2.22	116.63	121.12
26	c	520	LMG	C9-C8-C7	-2.22	106.54	111.79
29	h	101	DGD	O6E-C5E-C4E	2.22	113.72	109.69
22	c	501	CLA	CMB-C2B-C3B	2.22	128.82	124.68
22	C	506	CLA	CGD-CBD-CAD	-2.22	103.56	110.73
29	A	413	DGD	C3G-C2G-C1G	-2.21	106.55	111.79
29	c	516	DGD	O6E-C5E-C4E	2.21	113.71	109.69
22	b	603	CLA	C7-C6-C5	-2.21	107.35	113.36
30	B	617	BCR	C15-C16-C17	-2.21	118.94	123.47
22	A	405	CLA	CHD-C1D-C2D	2.21	130.12	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	102	BCR	C30-C25-C26	-2.21	119.50	122.61
27	a	410	SQD	O8-S-O7	2.21	116.68	111.27
22	B	605	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	a	405	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
26	A	409	LMG	O8-C28-O10	-2.21	118.02	123.59
26	M	101	LMG	O7-C10-O9	-2.21	118.37	123.70
22	b	615	CLA	C3A-C2A-C1A	2.21	104.65	101.34
26	A	409	LMG	O5-C6-C5	-2.21	103.72	111.29
22	C	511	CLA	C2A-C1A-CHA	2.21	127.72	123.86
29	c	515	DGD	O3D-C3D-C4D	-2.21	105.25	110.35
25	d	407	PL9	C8-C7-C3	2.21	118.21	111.98
28	D	411	LHG	O8-C23-C24	2.20	118.82	111.91
22	A	405	CLA	CHD-C4C-NC	2.20	127.68	124.20
30	b	617	BCR	C15-C14-C13	-2.20	124.17	127.31
29	c	515	DGD	C4D-C3D-C2D	-2.20	106.98	110.82
27	A	412	SQD	O48-C46-C45	2.20	114.72	108.38
30	K	102	BCR	C10-C11-C12	-2.20	116.35	123.22
22	C	509	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
22	B	614	CLA	C6-C7-C8	-2.20	108.81	115.92
22	d	405	CLA	O1D-CGD-CBD	2.20	128.98	124.48
22	B	610	CLA	O1A-CGA-CBA	2.20	132.31	123.73
22	c	504	CLA	O2D-CGD-CBD	2.20	115.17	111.27
22	c	502	CLA	C2D-C1D-ND	-2.20	108.48	110.10
26	Y	101	LMG	O6-C1-O1	-2.20	104.77	109.97
29	c	516	DGD	C9A-C8A-C7A	-2.20	103.27	114.42
30	C	515	BCR	C8-C7-C6	-2.20	121.03	127.20
26	c	518	LMG	O7-C10-O9	-2.20	118.60	122.96
27	t	102	SQD	O49-C7-C8	-2.20	115.17	123.73
22	c	504	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	b	610	CLA	CAC-C3C-C4C	2.19	127.66	124.81
23	A	404	PHO	O2D-CGD-O1D	-2.19	119.55	123.84
22	b	606	CLA	CED-O2D-CGD	-2.19	110.98	115.94
22	C	513	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	b	611	CLA	CGD-CBD-CAD	-2.19	103.64	110.73
22	B	610	CLA	C14-C13-C15	-2.19	103.36	111.29
30	I	101	BCR	C16-C15-C14	-2.19	118.99	123.47
27	D	409	SQD	C1-O5-C5	-2.19	109.39	113.69
22	B	610	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	B	611	CLA	O2A-C1-C2	-2.19	102.88	108.64
22	c	507	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
28	D	411	LHG	C18-C17-C16	-2.19	103.32	114.42
22	C	508	CLA	O2A-CGA-O1A	-2.18	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	617	BCR	C3-C4-C5	-2.18	110.18	114.08
28	D	410	LHG	C18-C17-C16	-2.18	103.35	114.42
22	D	405	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	d	407	PL9	C11-C9-C8	-2.18	116.70	121.12
30	B	617	BCR	C2-C1-C6	2.18	113.84	110.48
29	A	413	DGD	C1E-O6E-C5E	2.18	117.97	113.69
29	A	413	DGD	C1D-C2D-C3D	-2.18	105.46	110.00
30	t	101	BCR	C12-C13-C14	-2.18	115.60	118.94
31	d	411	STE	O2-C1-C2	2.18	121.03	114.03
22	B	614	CLA	CMD-C2D-C1D	2.18	128.55	124.71
22	c	507	CLA	O1A-CGA-CBA	2.18	132.23	123.73
25	D	407	PL9	C36-C37-C38	-2.18	104.72	111.88
29	C	516	DGD	CAB-C9B-C8B	-2.18	103.37	114.42
27	a	410	SQD	O8-S-O9	-2.18	105.95	111.27
22	B	615	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	K	101	BCR	C37-C22-C23	2.18	121.50	118.08
30	C	514	BCR	C38-C26-C27	-2.17	109.44	113.62
25	a	409	PL9	C21-C19-C18	-2.17	116.72	121.12
22	C	510	CLA	C11-C10-C8	-2.17	108.90	115.92
22	b	602	CLA	CHA-C4D-ND	2.17	137.04	132.50
22	b	615	CLA	C7-C6-C5	-2.17	107.46	113.36
28	D	411	LHG	O3-P-O5	-2.17	100.59	109.07
30	B	617	BCR	C40-C30-C29	-2.17	100.23	108.91
30	x	101	BCR	C36-C18-C19	2.17	121.49	118.08
31	C	521	STE	C4-C3-C2	-2.17	105.40	113.19
22	a	403	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
31	B	625	STE	O2-C1-O1	-2.16	117.90	123.30
22	B	608	CLA	CHB-C4A-NA	2.16	127.50	124.51
28	L	102	LHG	C12-C11-C10	-2.16	103.44	114.42
30	C	514	BCR	C31-C1-C6	-2.16	106.79	110.30
22	b	607	CLA	C3A-C2A-C1A	2.16	104.58	101.34
29	h	101	DGD	C7B-C6B-C5B	-2.16	103.45	114.42
30	B	618	BCR	C15-C16-C17	-2.16	119.05	123.47
22	a	403	CLA	CHA-C1A-NA	-2.16	121.45	126.40
22	b	603	CLA	OBD-CAD-C3D	2.16	133.72	128.52
30	B	616	BCR	C8-C7-C6	-2.16	121.14	127.20
26	Y	101	LMG	O7-C10-O9	-2.16	118.48	123.70
22	c	503	CLA	CHC-C1C-NC	2.16	127.48	124.20
22	c	512	CLA	C3B-C4B-NB	-2.16	106.42	109.21
31	M	102	STE	O2-C1-O1	-2.16	117.93	123.30
30	b	619	BCR	C20-C21-C22	-2.16	124.23	127.31
22	C	506	CLA	C1D-ND-C4D	2.16	107.87	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	CBC-CAC-C3C	-2.15	106.49	112.43
31	x	102	STE	O2-C1-O1	-2.15	117.93	123.30
30	t	101	BCR	C33-C5-C6	-2.15	122.11	124.53
22	c	501	CLA	CHA-C1A-NA	-2.15	121.47	126.40
25	d	407	PL9	C31-C29-C28	2.15	125.47	121.12
22	A	402	CLA	C7-C6-C5	-2.15	107.52	113.36
30	C	515	BCR	C27-C26-C25	2.15	125.85	122.73
25	A	408	PL9	C27-C28-C29	-2.15	122.48	127.66
30	x	101	BCR	C34-C9-C8	-2.15	114.69	118.08
22	B	601	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
31	t	103	STE	O2-C1-C2	2.15	120.93	114.03
22	D	404	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
26	A	409	LMG	C1-O6-C5	-2.15	109.47	113.69
22	C	501	CLA	CHD-C4C-NC	2.15	127.59	124.20
22	c	508	CLA	CHD-C4C-NC	2.15	127.59	124.20
30	b	617	BCR	C11-C10-C9	-2.15	124.25	127.31
26	M	101	LMG	C1-C2-C3	-2.14	105.53	110.00
25	A	408	PL9	C41-C39-C38	-2.14	116.78	121.12
22	C	510	CLA	C2D-C1D-ND	-2.14	108.53	110.10
22	C	503	CLA	C5-C3-C2	-2.14	116.78	121.12
26	D	412	LMG	O7-C10-O9	-2.14	118.53	123.70
30	C	515	BCR	C38-C26-C27	-2.14	109.51	113.62
28	a	411	LHG	C20-C19-C18	-2.14	103.57	114.42
27	f	102	SQD	O5-C1-C2	-2.14	105.83	110.35
22	C	505	CLA	C2D-C1D-ND	-2.14	108.53	110.10
29	C	517	DGD	C5B-C4B-C3B	-2.14	103.58	114.42
30	x	101	BCR	C35-C13-C12	2.14	121.44	118.08
30	K	101	BCR	C37-C22-C21	-2.13	119.93	122.92
22	c	507	CLA	C7-C6-C5	-2.13	107.56	113.36
29	c	515	DGD	O3E-C3E-C2E	-2.13	105.42	110.35
30	C	515	BCR	C2-C1-C6	2.13	113.77	110.48
22	b	603	CLA	C4-C3-C5	2.13	118.86	115.27
27	f	102	SQD	C45-O47-C7	2.13	123.04	117.79
29	A	413	DGD	CAB-C9B-C8B	-2.13	103.61	114.42
22	B	603	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	B	602	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
29	h	101	DGD	CBB-CAB-C9B	-2.13	103.62	114.42
30	I	101	BCR	C34-C9-C10	-2.13	119.94	122.92
22	C	513	CLA	O2D-CGD-CBD	2.13	115.05	111.27
30	a	406	BCR	C16-C17-C18	-2.13	124.27	127.31
22	c	503	CLA	CMA-C3A-C4A	2.13	117.49	111.77
22	C	506	CLA	CHA-C1A-NA	-2.13	121.53	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	618	BCR	C11-C10-C9	-2.13	124.28	127.31
29	C	516	DGD	O1G-C1A-O1A	2.13	128.96	123.59
29	A	413	DGD	C4E-C3E-C2E	-2.13	107.11	110.82
22	B	612	CLA	C2A-C1A-CHA	2.13	127.58	123.86
29	C	517	DGD	CAB-C9B-C8B	-2.13	103.63	114.42
22	B	602	CLA	CHD-C4C-NC	2.13	127.55	124.20
29	c	516	DGD	C4E-C3E-C2E	-2.12	107.11	110.82
22	b	614	CLA	C2D-C1D-ND	-2.12	108.54	110.10
22	B	601	CLA	C6-C5-C3	-2.12	107.89	113.45
22	D	403	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
22	B	607	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
22	c	509	CLA	O2D-CGD-CBD	2.12	115.04	111.27
22	c	510	CLA	C6-C5-C3	-2.12	107.90	113.45
30	t	101	BCR	C1-C6-C5	-2.12	119.63	122.61
29	H	103	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
22	B	609	CLA	O2D-CGD-CBD	2.12	115.03	111.27
29	c	517	DGD	C5B-C4B-C3B	-2.12	103.69	114.42
22	b	605	CLA	CHC-C1C-NC	2.12	127.41	124.20
27	L	101	SQD	O10-C23-C24	-2.11	115.48	123.73
30	t	101	BCR	C29-C30-C25	2.11	113.73	110.48
22	B	601	CLA	CGD-CBD-CAD	-2.11	103.89	110.73
22	C	513	CLA	C2D-C1D-ND	-2.11	108.55	110.10
22	C	508	CLA	CHD-C4C-NC	2.11	127.53	124.20
22	B	607	CLA	CHD-C4C-NC	2.11	127.53	124.20
22	B	606	CLA	C2D-C1D-ND	2.11	111.66	110.10
27	L	101	SQD	O49-C7-C8	-2.11	115.50	123.73
22	B	606	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
22	c	504	CLA	C3D-C4D-ND	2.11	113.65	110.24
22	c	502	CLA	C4D-CHA-C1A	2.11	123.81	121.25
22	C	504	CLA	CHA-C1A-NA	-2.11	121.57	126.40
22	B	601	CLA	C16-C15-C13	-2.11	109.11	115.92
30	C	514	BCR	C34-C9-C10	-2.11	119.97	122.92
29	A	413	DGD	O5E-C6E-C5E	-2.10	104.07	111.29
22	b	603	CLA	C1-O2A-CGA	2.10	121.96	116.44
22	c	502	CLA	C1D-ND-C4D	2.10	107.83	106.33
26	a	414	LMG	O7-C10-O9	-2.10	118.62	123.70
28	D	410	LHG	C27-C26-C25	-2.10	103.76	114.42
30	D	406	BCR	C28-C27-C26	-2.10	110.33	114.08
30	b	617	BCR	C3-C4-C5	-2.10	110.33	114.08
22	B	607	CLA	CHB-C4A-NA	2.10	127.41	124.51
28	D	413	LHG	C11-C10-C9	-2.10	103.78	114.42
29	C	518	DGD	O2D-C2D-C1D	-2.10	104.95	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	616	BCR	C37-C22-C21	-2.10	119.99	122.92
22	c	511	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
26	A	409	LMG	C20-C19-C18	-2.09	103.80	114.42
25	A	408	PL9	C12-C13-C14	-2.09	122.63	127.66
22	B	601	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
30	K	102	BCR	C8-C9-C10	-2.09	115.73	118.94
27	A	410	SQD	O47-C45-C44	2.09	115.97	108.40
22	b	602	CLA	C1-C2-C3	-2.09	122.43	126.04
22	c	509	CLA	O1D-CGD-CBD	2.09	128.76	124.48
22	C	513	CLA	CHD-C1D-C2D	2.09	129.86	125.48
22	C	505	CLA	CBA-CAA-C2A	2.09	120.02	113.86
22	D	404	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
22	b	614	CLA	C11-C10-C8	-2.08	109.18	115.92
26	m	101	LMG	O8-C28-O10	-2.08	118.34	123.59
22	H	101	CLA	C4-C3-C5	2.08	118.77	115.27
30	K	101	BCR	C30-C25-C26	-2.08	119.68	122.61
22	C	509	CLA	CED-O2D-CGD	2.08	120.64	115.94
22	b	605	CLA	C4D-C3D-CAD	-2.08	105.64	108.10
30	b	619	BCR	C11-C10-C9	-2.08	124.34	127.31
22	c	502	CLA	C4D-C3D-CAD	-2.08	105.64	108.10
28	d	408	LHG	C20-C19-C18	-2.08	103.87	114.42
22	c	506	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	C	515	BCR	C35-C13-C14	-2.08	120.01	122.92
22	b	601	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
30	B	618	BCR	C27-C26-C25	2.08	125.74	122.73
29	A	413	DGD	C6D-O5D-C1E	2.07	117.79	113.74
26	c	521	LMG	O6-C1-O1	-2.07	105.06	109.97
22	b	608	CLA	CHD-C1D-C2D	2.07	129.83	125.48
31	C	521	STE	O2-C1-C2	2.07	120.68	114.03
28	d	409	LHG	C29-C28-C27	-2.07	103.91	114.42
22	c	513	CLA	CMB-C2B-C3B	2.07	128.55	124.68
22	c	508	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	c	507	CLA	CHA-C1A-NA	-2.07	121.66	126.40
22	b	604	CLA	CBA-CAA-C2A	-2.07	107.76	113.86
28	A	411	LHG	O8-C23-O10	-2.07	118.38	123.59
29	H	103	DGD	O2E-C2E-C3E	-2.07	105.57	110.35
22	b	615	CLA	CHA-C4D-ND	2.07	136.82	132.50
28	A	411	LHG	C20-C19-C18	-2.06	103.94	114.42
27	B	621	SQD	O47-C45-C46	2.06	115.87	108.40
28	D	413	LHG	C18-C17-C16	-2.06	103.95	114.42
22	d	405	CLA	CHA-C1A-NA	-2.06	121.67	126.40
30	b	618	BCR	C16-C15-C14	-2.06	119.25	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	k	101	BCR	C20-C21-C22	-2.06	124.37	127.31
22	b	604	CLA	C4D-C3D-CAD	-2.06	105.67	108.10
22	b	608	CLA	CBA-CAA-C2A	2.06	119.95	113.86
22	C	503	CLA	O1D-CGD-CBD	2.06	128.70	124.48
30	H	102	BCR	C38-C26-C25	-2.06	122.21	124.53
22	c	508	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
22	a	402	CLA	C1D-CHD-C4C	-2.06	121.61	126.06
22	c	506	CLA	CAC-C3C-C4C	2.06	127.48	124.81
22	A	403	CLA	C2C-C1C-NC	2.06	111.90	109.97
23	a	404	PHO	C1-C2-C3	-2.06	122.48	126.04
30	B	618	BCR	C1-C6-C5	-2.06	119.71	122.61
22	c	503	CLA	CHD-C4C-NC	2.06	127.44	124.20
22	B	602	CLA	C1B-CHB-C4A	-2.06	126.05	130.12
22	C	508	CLA	CMD-C2D-C1D	2.06	128.34	124.71
22	A	402	CLA	CBC-CAC-C3C	2.06	118.10	112.43
22	B	604	CLA	CHD-C1D-C2D	2.06	129.79	125.48
34	F	101	HEC	CMB-C2B-C1B	-2.06	125.31	128.46
22	B	612	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
22	c	510	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
22	C	503	CLA	CHB-C4A-NA	2.05	127.35	124.51
22	b	602	CLA	C3C-C4C-NC	-2.05	108.27	110.57
22	C	513	CLA	CMB-C2B-C3B	2.05	128.52	124.68
27	f	102	SQD	O5-C5-C4	2.05	113.42	109.69
22	c	509	CLA	CHC-C1C-C2C	-2.05	121.05	126.72
25	a	409	PL9	C45-C44-C43	-2.05	118.42	123.68
22	H	101	CLA	O2D-CGD-CBD	2.05	114.91	111.27
26	m	101	LMG	C1-O6-C5	-2.05	109.66	113.69
22	D	404	CLA	C11-C12-C13	-2.05	109.29	115.92
22	C	501	CLA	CAC-C3C-C4C	2.05	127.47	124.81
22	b	606	CLA	CHD-C1D-ND	-2.05	122.57	124.45
30	b	617	BCR	C32-C1-C6	-2.05	106.97	110.30
30	K	101	BCR	C15-C14-C13	-2.05	124.39	127.31
22	b	604	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	M	101	LMG	C37-C36-C35	-2.05	104.03	114.42
30	k	102	BCR	C33-C5-C6	-2.05	122.23	124.53
29	c	515	DGD	O6E-C1E-O5D	-2.05	105.13	109.97
22	b	605	CLA	CMB-C2B-C3B	2.05	128.51	124.68
29	H	103	DGD	C9A-C8A-C7A	-2.05	104.04	114.42
22	C	505	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
30	k	101	BCR	C27-C26-C25	2.04	125.70	122.73
30	B	617	BCR	C38-C26-C25	-2.04	122.23	124.53
22	C	512	CLA	C2A-C3A-C4A	2.04	105.17	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	406	BCR	C7-C8-C9	-2.04	123.15	126.23
29	C	518	DGD	C8B-C7B-C6B	-2.04	104.06	114.42
22	B	613	CLA	C6-C7-C8	-2.04	109.32	115.92
29	H	103	DGD	C8B-C7B-C6B	-2.04	104.07	114.42
29	h	101	DGD	CDB-CCB-CBB	-2.04	104.07	114.42
31	B	625	STE	O1-C1-C2	-2.04	116.53	123.08
22	B	604	CLA	CHD-C4C-NC	2.04	127.42	124.20
30	a	406	BCR	C33-C5-C6	-2.04	122.24	124.53
30	B	616	BCR	C30-C25-C26	-2.04	119.75	122.61
22	a	402	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
26	d	410	LMG	C40-C39-C38	-2.04	104.09	114.42
22	b	603	CLA	C2D-C1D-ND	-2.03	108.61	110.10
28	D	413	LHG	O10-C23-C24	-2.03	115.80	123.73
28	L	102	LHG	C20-C19-C18	-2.03	104.10	114.42
22	C	508	CLA	CHA-C4D-ND	2.03	136.75	132.50
22	c	506	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	d	403	CLA	C1-C2-C3	-2.03	122.53	126.04
25	D	407	PL9	C7-C3-C2	-2.03	120.63	123.30
22	C	507	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
22	b	614	CLA	CHA-C4D-ND	2.03	136.75	132.50
22	B	606	CLA	C2C-C1C-NC	2.03	111.87	109.97
29	c	517	DGD	C7B-C6B-C5B	-2.03	104.12	114.42
22	b	614	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
22	a	405	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	b	601	CLA	O2A-CGA-CBA	2.03	118.27	111.91
22	C	509	CLA	C2A-C3A-C4A	2.03	105.14	101.87
26	D	408	LMG	O7-C10-O9	-2.03	118.80	123.70
30	a	406	BCR	C29-C30-C25	2.03	113.60	110.48
30	C	515	BCR	C30-C25-C26	-2.03	119.76	122.61
22	A	403	CLA	C4-C3-C5	-2.03	111.86	115.27
22	c	503	CLA	C3A-C2A-C1A	2.03	104.37	101.34
29	h	101	DGD	O2E-C2E-C1E	-2.03	105.13	110.05
28	A	411	LHG	C11-C10-C9	-2.03	104.14	114.42
22	c	506	CLA	C1-O2A-CGA	2.02	121.76	116.44
22	c	509	CLA	CHC-C1C-NC	2.02	127.27	124.20
22	B	610	CLA	C9-C8-C10	-2.02	103.97	111.29
30	a	406	BCR	C30-C25-C26	-2.02	119.77	122.61
22	C	511	CLA	C2D-C1D-ND	-2.02	108.61	110.10
29	c	515	DGD	C4A-C3A-C2A	-2.02	105.93	113.19
28	d	408	LHG	C27-C26-C25	-2.02	104.17	114.42
22	c	503	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
29	c	517	DGD	O5E-C6E-C5E	-2.02	104.36	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	514	BCR	C36-C18-C19	2.02	121.26	118.08
25	A	408	PL9	C31-C32-C33	-2.02	105.25	111.88
22	d	405	CLA	CMA-C3A-C2A	-2.02	105.69	113.83
34	f	101	HEC	C4C-C3C-C2C	2.02	108.53	106.35
30	t	101	BCR	C11-C10-C9	-2.02	124.43	127.31
30	H	102	BCR	C35-C13-C14	-2.01	120.10	122.92
26	m	101	LMG	C38-C37-C36	-2.01	104.20	114.42
29	C	518	DGD	CDB-CCB-CBB	-2.01	104.20	114.42
26	c	518	LMG	C9-C8-C7	-2.01	107.03	111.79
30	B	617	BCR	C28-C27-C26	-2.01	110.48	114.08
22	D	405	CLA	O1A-CGA-CBA	2.01	131.58	123.73
22	b	610	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
22	b	616	CLA	O2D-CGD-CBD	2.01	114.84	111.27
25	d	407	PL9	C11-C12-C13	-2.01	105.27	111.88
22	B	603	CLA	C1C-C2C-C3C	-2.01	104.84	106.96
30	H	102	BCR	C36-C18-C17	-2.01	120.11	122.92
22	c	506	CLA	O2A-CGA-CBA	-2.01	105.60	111.91
34	F	101	HEC	CMD-C2D-C3D	2.01	128.73	124.94
22	b	613	CLA	C1D-ND-C4D	-2.01	104.91	106.33
22	C	508	CLA	C2D-C1D-ND	-2.01	108.62	110.10
22	b	609	CLA	C5-C3-C2	2.01	125.18	121.12
22	B	611	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
22	d	404	CLA	CMC-C2C-C1C	2.01	128.09	125.04
22	c	511	CLA	C3A-C2A-C1A	2.01	104.34	101.34
25	A	408	PL9	C20-C19-C18	-2.00	118.54	123.68
22	C	503	CLA	C1-O2A-CGA	2.00	121.70	116.44
25	D	407	PL9	C37-C38-C39	-2.00	122.84	127.66
22	C	510	CLA	C1-O2A-CGA	2.00	121.69	116.44

All (59) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	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
22	B	609	CLA	ND
22	B	611	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	C	501	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	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
22	D	404	CLA	ND
22	H	101	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	608	CLA	ND
22	b	609	CLA	ND
22	b	610	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
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	509	CLA	ND

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Mol	Chain	Res	Type	Atom
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
22	d	404	CLA	ND
22	d	405	CLA	ND

All (2018) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	C2-C3-C5-C6
22	B	602	CLA	C4-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6
22	B	603	CLA	C4-C3-C5-C6
22	B	604	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	611	CLA	CHA-CBD-CGD-O1D
22	B	611	CLA	CHA-CBD-CGD-O2D
22	B	613	CLA	CHA-CBD-CGD-O1D
22	B	613	CLA	C2-C3-C5-C6
22	B	613	CLA	C4-C3-C5-C6
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	C14-C13-C15-C16
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	C2-C1-O2A-CGA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C11-C10-C8-C9
22	D	404	CLA	CHA-CBD-CGD-O2D
22	D	405	CLA	O2A-C1-C2-C3
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	C2-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C4-C3-C5-C6
22	b	614	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	C2-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	c	504	CLA	C2-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
22	c	506	CLA	CHA-CBD-CGD-O1D
22	c	506	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C6-C7-C8-C9
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
22	d	404	CLA	CHA-CBD-CGD-O1D
22	d	404	CLA	CHA-CBD-CGD-O2D
25	A	408	PL9	C17-C18-C19-C20
25	A	408	PL9	C23-C24-C26-C27
25	A	408	PL9	C24-C26-C27-C28
25	A	408	PL9	C32-C33-C34-C36
25	A	408	PL9	C34-C36-C37-C38
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C40-C39-C41-C42
25	D	407	PL9	C42-C43-C44-C45
25	D	407	PL9	C47-C48-C49-C51
25	a	409	PL9	C9-C11-C12-C13
25	a	409	PL9	C12-C13-C14-C15
25	a	409	PL9	C12-C13-C14-C16
25	a	409	PL9	C17-C18-C19-C21
25	a	409	PL9	C19-C21-C22-C23
25	a	409	PL9	C24-C26-C27-C28
25	a	409	PL9	C27-C28-C29-C30
25	a	409	PL9	C32-C33-C34-C35
25	a	409	PL9	C37-C38-C39-C40
25	a	409	PL9	C42-C43-C44-C45
25	a	409	PL9	C42-C43-C44-C46
25	d	407	PL9	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
25	d	407	PL9	C32-C33-C34-C36
25	d	407	PL9	C37-C38-C39-C41
25	d	407	PL9	C38-C39-C41-C42
25	d	407	PL9	C42-C43-C44-C46
25	d	407	PL9	C47-C48-C49-C50
26	A	409	LMG	O9-C10-O7-C8
26	a	414	LMG	C8-C7-O1-C1
26	b	622	LMG	C11-C10-O7-C8
26	c	521	LMG	O6-C1-O1-C7
27	A	412	SQD	C46-C45-O47-C7
27	B	621	SQD	C2-C1-O6-C44
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	D	409	SQD	C45-C44-O6-C1
27	L	101	SQD	O49-C7-O47-C45
27	f	102	SQD	C2-C1-O6-C44
27	f	102	SQD	O5-C1-O6-C44
27	t	102	SQD	O49-C7-O47-C45
27	t	102	SQD	C8-C7-O47-C45
28	A	411	LHG	O1-C1-C2-C3
28	A	411	LHG	C3-O3-P-O5
28	A	411	LHG	C3-O3-P-O6
28	D	410	LHG	O1-C1-C2-C3
28	D	410	LHG	C3-O3-P-O5
28	D	410	LHG	C4-O6-P-O4
28	D	411	LHG	C3-O3-P-O5
28	D	411	LHG	C3-O3-P-O6
28	D	413	LHG	O1-C1-C2-O2
28	D	413	LHG	O1-C1-C2-C3
28	D	413	LHG	C1-C2-C3-O3
28	L	102	LHG	C3-O3-P-O4
28	L	102	LHG	C4-O6-P-O4
28	a	411	LHG	O1-C1-C2-O2
28	a	411	LHG	O1-C1-C2-C3
28	a	411	LHG	C3-O3-P-O4
28	a	411	LHG	O6-C4-C5-O7
28	a	411	LHG	O10-C23-O8-C6
28	a	411	LHG	C24-C23-O8-C6
28	b	623	LHG	O1-C1-C2-C3
28	b	623	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
28	b	623	LHG	C4-O6-P-O4
28	d	408	LHG	O1-C1-C2-C3
28	d	408	LHG	C3-O3-P-O4
28	d	408	LHG	C4-O6-P-O4
29	A	413	DGD	C2B-C1B-O2G-C2G
29	A	413	DGD	O1B-C1B-O2G-C2G
29	A	413	DGD	O2G-C2G-C3G-O3G
30	B	616	BCR	C35-C13-C14-C15
30	B	616	BCR	C16-C17-C18-C36
30	B	616	BCR	C20-C21-C22-C37
30	B	617	BCR	C11-C10-C9-C34
30	B	617	BCR	C10-C11-C12-C13
30	B	617	BCR	C37-C22-C23-C24
30	B	618	BCR	C7-C8-C9-C34
30	B	618	BCR	C11-C10-C9-C8
30	B	618	BCR	C35-C13-C14-C15
30	C	514	BCR	C1-C6-C7-C8
30	C	514	BCR	C5-C6-C7-C8
30	C	514	BCR	C7-C8-C9-C10
30	C	515	BCR	C7-C8-C9-C34
30	C	515	BCR	C11-C12-C13-C14
30	D	406	BCR	C7-C8-C9-C10
30	D	406	BCR	C11-C10-C9-C34
30	D	406	BCR	C37-C22-C23-C24
30	D	406	BCR	C22-C23-C24-C25
30	H	102	BCR	C11-C12-C13-C14
30	H	102	BCR	C36-C18-C19-C20
30	H	102	BCR	C37-C22-C23-C24
30	I	101	BCR	C11-C10-C9-C34
30	I	101	BCR	C11-C12-C13-C35
30	I	101	BCR	C14-C15-C16-C17
30	I	101	BCR	C16-C17-C18-C19
30	I	101	BCR	C20-C21-C22-C37
30	K	101	BCR	C6-C7-C8-C9
30	K	101	BCR	C7-C8-C9-C34
30	K	101	BCR	C11-C10-C9-C8
30	K	101	BCR	C14-C15-C16-C17
30	K	101	BCR	C16-C17-C18-C36
30	K	101	BCR	C36-C18-C19-C20
30	K	102	BCR	C1-C6-C7-C8
30	K	102	BCR	C5-C6-C7-C8
30	K	102	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
30	K	102	BCR	C11-C12-C13-C14
30	K	102	BCR	C11-C12-C13-C35
30	K	102	BCR	C16-C17-C18-C36
30	K	102	BCR	C21-C22-C23-C24
30	K	102	BCR	C37-C22-C23-C24
30	T	101	BCR	C7-C8-C9-C10
30	T	101	BCR	C7-C8-C9-C34
30	T	101	BCR	C9-C10-C11-C12
30	T	101	BCR	C11-C12-C13-C14
30	a	406	BCR	C37-C22-C23-C24
30	b	617	BCR	C7-C8-C9-C34
30	b	617	BCR	C11-C10-C9-C8
30	b	617	BCR	C11-C12-C13-C35
30	b	617	BCR	C12-C13-C14-C15
30	b	617	BCR	C35-C13-C14-C15
30	b	617	BCR	C20-C21-C22-C37
30	b	617	BCR	C21-C22-C23-C24
30	b	619	BCR	C11-C12-C13-C35
30	c	514	BCR	C11-C12-C13-C35
30	c	514	BCR	C12-C13-C14-C15
30	c	514	BCR	C16-C17-C18-C36
30	d	406	BCR	C35-C13-C14-C15
30	d	406	BCR	C37-C22-C23-C24
30	d	406	BCR	C22-C23-C24-C25
30	k	101	BCR	C6-C7-C8-C9
30	k	101	BCR	C7-C8-C9-C10
30	k	101	BCR	C35-C13-C14-C15
30	k	101	BCR	C18-C19-C20-C21
30	k	101	BCR	C20-C21-C22-C37
30	k	102	BCR	C7-C8-C9-C10
30	k	102	BCR	C7-C8-C9-C34
30	k	102	BCR	C11-C12-C13-C35
30	k	102	BCR	C17-C18-C19-C20
30	k	102	BCR	C21-C22-C23-C24
30	k	102	BCR	C37-C22-C23-C24
30	k	102	BCR	C23-C24-C25-C30
30	k	103	BCR	C37-C22-C23-C24
30	t	101	BCR	C11-C10-C9-C34
30	t	101	BCR	C35-C13-C14-C15
30	t	101	BCR	C16-C17-C18-C19
30	t	101	BCR	C16-C17-C18-C36
30	x	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	O1D-CGD-O2D-CED
26	c	518	LMG	C11-C10-O7-C8
22	C	509	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	H	101	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
26	c	520	LMG	O10-C28-O8-C9
26	c	521	LMG	O10-C28-O8-C9
22	c	508	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
25	D	407	PL9	C47-C48-C49-C50
25	a	409	PL9	C47-C48-C49-C50
25	a	409	PL9	C47-C48-C49-C51
25	d	407	PL9	C47-C48-C49-C51
22	B	615	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	O1A-CGA-O2A-C1
22	H	101	CLA	O1A-CGA-O2A-C1
27	L	101	SQD	O10-C23-O48-C46
26	c	518	LMG	O9-C10-O7-C8
22	C	501	CLA	O1D-CGD-O2D-CED
22	H	101	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	CBD-CGD-O2D-CED
26	D	412	LMG	O9-C10-O7-C8
26	Y	101	LMG	O9-C10-O7-C8
26	b	622	LMG	O9-C10-O7-C8
27	f	102	SQD	O49-C7-O47-C45
26	M	101	LMG	O10-C28-O8-C9
22	B	603	CLA	C3-C5-C6-C7
22	B	604	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	c	510	CLA	C3-C5-C6-C7
26	c	521	LMG	C29-C28-O8-C9
27	L	101	SQD	C24-C23-O48-C46
27	f	102	SQD	C24-C23-O48-C46
26	A	409	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
26	D	412	LMG	C11-C10-O7-C8
26	Y	101	LMG	C11-C10-O7-C8
26	c	520	LMG	C11-C10-O7-C8
27	L	101	SQD	C8-C7-O47-C45
22	c	510	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
22	B	611	CLA	CBD-CGD-O2D-CED
25	A	408	PL9	C43-C44-C46-C47
22	b	605	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	C2A-CAA-CBA-CGA
22	d	405	CLA	C3-C5-C6-C7
22	B	603	CLA	CBA-CGA-O2A-C1
22	H	101	CLA	CBA-CGA-O2A-C1
26	a	414	LMG	C29-C28-O8-C9
26	c	520	LMG	C29-C28-O8-C9
25	a	409	PL9	C17-C18-C19-C20
29	h	101	DGD	O6E-C5E-C6E-O5E
26	c	520	LMG	O9-C10-O7-C8
25	A	408	PL9	C22-C23-C24-C26
25	A	408	PL9	C37-C38-C39-C41
25	D	407	PL9	C32-C33-C34-C36
25	a	409	PL9	C37-C38-C39-C41
22	C	502	CLA	CBD-CGD-O2D-CED
28	D	413	LHG	O2-C2-C3-O3
22	b	609	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
26	M	101	LMG	C29-C28-O8-C9
26	A	409	LMG	C4-C5-C6-O5
22	b	609	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
26	A	409	LMG	O6-C5-C6-O5
29	h	101	DGD	C4E-C5E-C6E-O5E
31	a	413	STE	C5-C6-C7-C8
26	a	414	LMG	O10-C28-O8-C9
27	f	102	SQD	O10-C23-O48-C46
29	c	517	DGD	O1A-C1A-O1G-C1G
31	b	621	STE	C14-C15-C16-C17
22	C	504	CLA	C4-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
25	a	409	PL9	C28-C29-C31-C32
22	b	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	B	624	STE	C11-C12-C13-C14
27	D	409	SQD	O10-C23-O48-C46
25	A	408	PL9	C29-C31-C32-C33
25	D	407	PL9	C34-C36-C37-C38
25	D	407	PL9	C44-C46-C47-C48
25	a	409	PL9	C14-C16-C17-C18
25	d	407	PL9	C44-C46-C47-C48
26	Y	101	LMG	O6-C5-C6-O5
22	B	615	CLA	O1D-CGD-O2D-CED
25	A	408	PL9	C47-C48-C49-C50
25	A	408	PL9	C7-C8-C9-C10
22	C	510	CLA	CBD-CGD-O2D-CED
26	d	410	LMG	C10-C11-C12-C13
28	a	411	LHG	C1-C2-C3-O3
25	a	409	PL9	C22-C23-C24-C26
27	B	621	SQD	C24-C23-O48-C46
27	D	409	SQD	C24-C23-O48-C46
22	c	507	CLA	C5-C6-C7-C8
26	B	620	LMG	C28-C29-C30-C31
22	c	510	CLA	C5-C6-C7-C8
22	c	512	CLA	C13-C15-C16-C17
28	d	409	LHG	C24-C25-C26-C27
22	B	610	CLA	C13-C15-C16-C17
22	C	506	CLA	C15-C16-C17-C18
28	D	411	LHG	O2-C2-C3-O3
28	a	411	LHG	O2-C2-C3-O3
31	c	519	STE	C2-C3-C4-C5
25	a	409	PL9	C30-C29-C31-C32
22	B	606	CLA	C14-C13-C15-C16
22	B	613	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	D	405	CLA	C11-C12-C13-C14
22	H	101	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	b	614	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C12-C13-C14
23	A	404	PHO	C14-C13-C15-C16
22	b	607	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	C10-C11-C12-C13
30	B	618	BCR	C37-C22-C23-C24
30	C	514	BCR	C7-C8-C9-C34
30	C	515	BCR	C11-C12-C13-C35
30	H	102	BCR	C7-C8-C9-C34
30	T	101	BCR	C11-C12-C13-C35
30	T	101	BCR	C37-C22-C23-C24
30	k	101	BCR	C7-C8-C9-C34
30	x	101	BCR	C36-C18-C19-C20
29	c	515	DGD	C1B-C2B-C3B-C4B
22	B	602	CLA	C8-C10-C11-C12
22	C	502	CLA	C15-C16-C17-C18
22	c	505	CLA	C15-C16-C17-C18
22	b	602	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
29	C	516	DGD	O6E-C5E-C6E-O5E
22	C	512	CLA	C3-C5-C6-C7
22	B	612	CLA	C8-C10-C11-C12
22	C	510	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
26	D	408	LMG	C10-C11-C12-C13
26	M	101	LMG	C10-C11-C12-C13
26	c	518	LMG	C28-C29-C30-C31
31	b	624	STE	C1-C2-C3-C4
31	x	102	STE	C1-C2-C3-C4
22	C	506	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	C5-C6-C7-C8
22	C	503	CLA	C5-C6-C7-C8
22	a	405	CLA	C5-C6-C7-C8
26	M	101	LMG	C28-C29-C30-C31
26	Y	101	LMG	C28-C29-C30-C31
26	a	414	LMG	C10-C11-C12-C13
27	A	410	SQD	C7-C8-C9-C10
28	d	409	LHG	C23-C24-C25-C26
28	l	101	LHG	C23-C24-C25-C26
29	C	517	DGD	C1B-C2B-C3B-C4B
31	B	623	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
31	L	103	STE	C1-C2-C3-C4
22	B	604	CLA	C8-C10-C11-C12
22	B	606	CLA	C8-C10-C11-C12
22	B	607	CLA	C15-C16-C17-C18
22	B	608	CLA	C15-C16-C17-C18
22	B	613	CLA	C8-C10-C11-C12
22	C	505	CLA	C10-C11-C12-C13
22	C	508	CLA	C15-C16-C17-C18
22	b	605	CLA	C5-C6-C7-C8
22	b	615	CLA	C8-C10-C11-C12
28	d	409	LHG	C30-C31-C32-C33
22	B	613	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	C15-C16-C17-C18
22	C	506	CLA	C8-C10-C11-C12
22	C	512	CLA	C8-C10-C11-C12
31	B	625	STE	C1-C2-C3-C4
31	b	626	STE	C4-C5-C6-C7
22	C	505	CLA	C5-C6-C7-C8
22	B	605	CLA	C12-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	b	602	CLA	C12-C13-C15-C16
22	b	608	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C10-C8-C7
22	d	405	CLA	C6-C7-C8-C10
26	m	101	LMG	O10-C28-O8-C9
22	d	405	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	C10-C11-C12-C13
22	D	405	CLA	C10-C11-C12-C13
22	b	608	CLA	C13-C15-C16-C17
22	b	615	CLA	C5-C6-C7-C8
22	c	509	CLA	C10-C11-C12-C13
26	Y	101	LMG	C4-C5-C6-O5
30	b	617	BCR	C6-C7-C8-C9
26	Y	101	LMG	O6-C1-O1-C7
26	b	622	LMG	O6-C1-O1-C7
29	A	413	DGD	O6E-C1E-O5D-C6D
25	A	408	PL9	C44-C46-C47-C48
30	B	617	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	C	515	BCR	C18-C19-C20-C21
30	T	101	BCR	C18-C19-C20-C21
30	k	102	BCR	C10-C11-C12-C13
30	k	103	BCR	C18-C19-C20-C21
30	t	101	BCR	C10-C11-C12-C13
29	A	413	DGD	O6D-C5D-C6D-O5D
22	b	611	CLA	C15-C16-C17-C18
29	C	518	DGD	C8A-C9A-CAA-CBA
26	d	410	LMG	C28-C29-C30-C31
27	B	621	SQD	C23-C24-C25-C26
22	B	606	CLA	C5-C6-C7-C8
22	C	513	CLA	C13-C15-C16-C17
22	C	513	CLA	C15-C16-C17-C18
22	D	403	CLA	C15-C16-C17-C18
22	b	606	CLA	C10-C11-C12-C13
22	b	614	CLA	C13-C15-C16-C17
29	H	103	DGD	C4E-C5E-C6E-O5E
22	B	603	CLA	CBD-CGD-O2D-CED
31	B	625	STE	C5-C6-C7-C8
22	B	605	CLA	C8-C10-C11-C12
22	C	509	CLA	C13-C15-C16-C17
22	C	510	CLA	C15-C16-C17-C18
22	b	603	CLA	C10-C11-C12-C13
22	b	611	CLA	C10-C11-C12-C13
22	b	614	CLA	C8-C10-C11-C12
22	c	507	CLA	C8-C10-C11-C12
28	a	411	LHG	C3-O3-P-O6
28	b	623	LHG	C4-O6-P-O3
28	d	408	LHG	C3-O3-P-O6
22	c	512	CLA	CBA-CGA-O2A-C1
27	a	410	SQD	C24-C23-O48-C46
25	D	407	PL9	C32-C33-C34-C35
22	b	616	CLA	C10-C11-C12-C13
22	c	511	CLA	C13-C15-C16-C17
26	D	412	LMG	C28-C29-C30-C31
25	a	409	PL9	C38-C39-C41-C42
22	D	404	CLA	C13-C15-C16-C17
22	c	503	CLA	C16-C17-C18-C20
29	c	517	DGD	C2A-C1A-O1G-C1G
22	b	613	CLA	C13-C15-C16-C17
27	B	621	SQD	C11-C10-C9-C8
26	Y	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	b	622	LMG	C11-C12-C13-C14
28	D	410	LHG	C29-C30-C31-C32
29	A	413	DGD	C2B-C3B-C4B-C5B
29	C	518	DGD	CBA-CCA-CDA-CEA
30	B	618	BCR	C11-C10-C9-C34
30	C	514	BCR	C16-C17-C18-C36
30	C	515	BCR	C11-C10-C9-C34
30	C	515	BCR	C20-C21-C22-C37
30	D	406	BCR	C35-C13-C14-C15
30	D	406	BCR	C20-C21-C22-C37
30	I	101	BCR	C16-C17-C18-C36
30	K	101	BCR	C20-C21-C22-C37
30	T	101	BCR	C16-C17-C18-C36
30	b	619	BCR	C35-C13-C14-C15
30	d	406	BCR	C20-C21-C22-C37
30	t	101	BCR	C20-C21-C22-C37
30	x	101	BCR	C11-C10-C9-C34
22	b	602	CLA	C3-C5-C6-C7
26	D	408	LMG	C17-C18-C19-C20
26	c	520	LMG	C15-C16-C17-C18
26	c	521	LMG	C11-C12-C13-C14
26	c	521	LMG	C34-C35-C36-C37
27	a	410	SQD	C9-C10-C11-C12
27	a	410	SQD	C10-C11-C12-C13
28	A	411	LHG	C26-C27-C28-C29
28	D	410	LHG	C28-C29-C30-C31
28	D	413	LHG	C9-C10-C11-C12
28	L	102	LHG	C30-C31-C32-C33
29	A	413	DGD	CEA-CFA-CGA-CHA
29	c	515	DGD	C3B-C4B-C5B-C6B
29	c	516	DGD	CCB-CDB-CEB-CFB
29	h	101	DGD	C5B-C6B-C7B-C8B
31	I	102	STE	C10-C11-C12-C13
31	R	101	STE	C2-C3-C4-C5
31	b	628	STE	C11-C12-C13-C14
22	B	611	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	b	613	CLA	C16-C17-C18-C19
23	D	401	PHO	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	A	410	SQD	C25-C26-C27-C28
27	f	102	SQD	C30-C31-C32-C33
28	A	411	LHG	C32-C33-C34-C35
28	b	623	LHG	C32-C33-C34-C35
29	A	413	DGD	CBA-CCA-CDA-CEA
31	B	622	STE	C6-C7-C8-C9
31	J	101	STE	C6-C7-C8-C9
31	Z	101	STE	C13-C14-C15-C16
31	a	413	STE	C7-C8-C9-C10
27	L	101	SQD	C46-C45-O47-C7
27	A	412	SQD	C24-C25-C26-C27
27	B	621	SQD	C11-C12-C13-C14
27	t	102	SQD	C15-C16-C17-C18
28	D	411	LHG	C12-C13-C14-C15
28	L	102	LHG	C31-C32-C33-C34
28	d	408	LHG	C11-C12-C13-C14
29	c	516	DGD	C8A-C9A-CAA-CBA
31	L	103	STE	C3-C4-C5-C6
31	b	620	STE	C4-C5-C6-C7
26	a	414	LMG	C12-C13-C14-C15
26	c	520	LMG	C34-C35-C36-C37
26	c	521	LMG	C30-C31-C32-C33
26	m	101	LMG	C17-C18-C19-C20
27	A	410	SQD	C14-C15-C16-C17
27	D	409	SQD	C25-C26-C27-C28
28	L	102	LHG	C24-C25-C26-C27
28	d	408	LHG	C29-C30-C31-C32
29	C	518	DGD	C4B-C5B-C6B-C7B
29	c	517	DGD	CCB-CDB-CEB-CFB
31	B	624	STE	C9-C10-C11-C12
31	M	104	STE	C4-C5-C6-C7
31	b	621	STE	C11-C12-C13-C14
31	b	628	STE	C9-C10-C11-C12
31	b	629	STE	C4-C5-C6-C7
22	C	510	CLA	C10-C11-C12-C13
26	c	518	LMG	C33-C34-C35-C36
27	t	102	SQD	C11-C10-C9-C8
28	A	411	LHG	C28-C29-C30-C31
28	D	410	LHG	C15-C16-C17-C18
31	B	623	STE	C10-C11-C12-C13
31	b	628	STE	C13-C14-C15-C16
27	A	412	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	L	101	SQD	C7-C8-C9-C10
26	Y	101	LMG	C2-C1-O1-C7
26	b	622	LMG	C2-C1-O1-C7
26	m	101	LMG	C2-C1-O1-C7
29	A	413	DGD	C2E-C1E-O5D-C6D
29	C	517	DGD	C2E-C1E-O5D-C6D
29	c	516	DGD	C2E-C1E-O5D-C6D
30	B	616	BCR	C12-C13-C14-C15
30	B	616	BCR	C16-C17-C18-C19
30	B	616	BCR	C20-C21-C22-C23
30	B	617	BCR	C11-C10-C9-C8
30	C	515	BCR	C11-C10-C9-C8
30	K	101	BCR	C16-C17-C18-C19
30	K	102	BCR	C11-C10-C9-C8
30	K	102	BCR	C16-C17-C18-C19
30	T	101	BCR	C12-C13-C14-C15
30	a	406	BCR	C20-C21-C22-C23
30	k	101	BCR	C20-C21-C22-C23
30	k	103	BCR	C16-C17-C18-C19
30	k	103	BCR	C20-C21-C22-C23
30	t	101	BCR	C11-C10-C9-C8
30	t	101	BCR	C12-C13-C14-C15
30	x	101	BCR	C11-C10-C9-C8
30	x	101	BCR	C16-C17-C18-C19
26	c	521	LMG	C17-C18-C19-C20
27	B	621	SQD	C17-C18-C19-C20
27	L	101	SQD	C12-C13-C14-C15
28	D	410	LHG	C17-C18-C19-C20
29	A	413	DGD	CCB-CDB-CEB-CFB
29	C	517	DGD	C6A-C7A-C8A-C9A
31	B	622	STE	C2-C3-C4-C5
31	C	519	STE	C5-C6-C7-C8
31	a	413	STE	C11-C10-C9-C8
31	b	620	STE	C6-C7-C8-C9
31	b	621	STE	C3-C4-C5-C6
26	D	412	LMG	O10-C28-O8-C9
22	B	605	CLA	C16-C17-C18-C20
22	b	603	CLA	O1D-CGD-O2D-CED
22	d	405	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	C4-C3-C5-C6
25	d	407	PL9	C15-C14-C16-C17
26	c	518	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
28	d	408	LHG	C33-C34-C35-C36
28	l	101	LHG	C28-C29-C30-C31
29	C	517	DGD	C3B-C4B-C5B-C6B
29	c	515	DGD	C4B-C5B-C6B-C7B
31	b	624	STE	C3-C4-C5-C6
31	b	629	STE	C12-C13-C14-C15
31	d	411	STE	C11-C12-C13-C14
31	k	104	STE	C5-C6-C7-C8
31	x	102	STE	C4-C5-C6-C7
31	x	102	STE	C9-C10-C11-C12
22	A	403	CLA	C14-C13-C15-C16
22	B	605	CLA	C14-C13-C15-C16
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C12-C13-C14
22	c	502	CLA	C11-C12-C13-C14
26	D	408	LMG	C30-C31-C32-C33
26	a	414	LMG	C13-C14-C15-C16
26	a	414	LMG	C39-C40-C41-C42
26	c	518	LMG	C39-C40-C41-C42
26	c	520	LMG	C30-C31-C32-C33
27	D	409	SQD	C29-C30-C31-C32
27	L	101	SQD	C24-C25-C26-C27
27	t	102	SQD	C11-C12-C13-C14
28	D	411	LHG	C11-C12-C13-C14
28	D	411	LHG	C25-C26-C27-C28
28	D	411	LHG	C32-C33-C34-C35
28	d	408	LHG	C14-C15-C16-C17
29	C	518	DGD	C6B-C7B-C8B-C9B
31	B	623	STE	C4-C5-C6-C7
31	H	104	STE	C4-C5-C6-C7
31	b	624	STE	C11-C10-C9-C8
31	c	519	STE	C9-C10-C11-C12
31	x	102	STE	C3-C4-C5-C6
22	a	405	CLA	C10-C11-C12-C13
22	b	607	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
26	M	101	LMG	C37-C38-C39-C40
26	a	414	LMG	C22-C23-C24-C25
26	a	414	LMG	C33-C34-C35-C36
27	A	410	SQD	C30-C31-C32-C33
27	B	621	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
27	D	409	SQD	C30-C31-C32-C33
27	L	101	SQD	C13-C14-C15-C16
29	h	101	DGD	C2B-C3B-C4B-C5B
28	d	409	LHG	O1-C1-C2-C3
28	a	411	LHG	O9-C7-O7-C5
22	a	403	CLA	C13-C15-C16-C17
22	c	506	CLA	C10-C11-C12-C13
26	a	414	LMG	C11-C10-O7-C8
26	c	521	LMG	C32-C33-C34-C35
27	f	102	SQD	C27-C28-C29-C30
28	D	410	LHG	C11-C12-C13-C14
28	D	413	LHG	C15-C16-C17-C18
28	D	413	LHG	C18-C19-C20-C21
28	b	623	LHG	C16-C17-C18-C19
29	A	413	DGD	C2A-C3A-C4A-C5A
29	A	413	DGD	C5B-C6B-C7B-C8B
29	c	516	DGD	C2A-C3A-C4A-C5A
29	c	517	DGD	C4B-C5B-C6B-C7B
28	d	408	LHG	C7-C8-C9-C10
22	B	606	CLA	O1D-CGD-O2D-CED
22	C	502	CLA	O1D-CGD-O2D-CED
26	b	622	LMG	C19-C20-C21-C22
26	c	520	LMG	C35-C36-C37-C38
26	d	410	LMG	C14-C15-C16-C17
27	A	410	SQD	C12-C13-C14-C15
27	D	409	SQD	C26-C27-C28-C29
28	A	411	LHG	C15-C16-C17-C18
28	D	413	LHG	C24-C25-C26-C27
28	l	101	LHG	C9-C10-C11-C12
28	l	101	LHG	C11-C12-C13-C14
28	l	101	LHG	C15-C16-C17-C18
29	C	517	DGD	C8B-C9B-CAB-CBB
29	H	103	DGD	C7A-C8A-C9A-CAA
29	c	515	DGD	C4A-C5A-C6A-C7A
31	M	104	STE	C13-C14-C15-C16
31	X	101	STE	C10-C11-C12-C13
31	b	624	STE	C6-C7-C8-C9
29	H	103	DGD	O6E-C5E-C6E-O5E
22	B	612	CLA	C16-C17-C18-C20
22	D	404	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C19
26	m	101	LMG	O6-C1-O1-C7
29	c	516	DGD	O6E-C1E-O5D-C6D
22	b	608	CLA	C8-C10-C11-C12
25	d	407	PL9	C34-C36-C37-C38
26	A	409	LMG	C11-C12-C13-C14
26	d	410	LMG	C34-C35-C36-C37
27	a	410	SQD	C12-C13-C14-C15
27	a	410	SQD	C26-C27-C28-C29
28	L	102	LHG	C12-C13-C14-C15
31	B	623	STE	C5-C6-C7-C8
31	M	102	STE	C2-C3-C4-C5
31	j	101	STE	C4-C5-C6-C7
29	A	413	DGD	C4D-C5D-C6D-O5D
22	b	609	CLA	O1D-CGD-O2D-CED
26	a	414	LMG	C35-C36-C37-C38
27	A	412	SQD	C12-C13-C14-C15
29	C	516	DGD	C6B-C7B-C8B-C9B
29	H	103	DGD	C4B-C5B-C6B-C7B
29	c	516	DGD	CBA-CCA-CDA-CEA
31	b	628	STE	C6-C7-C8-C9
22	c	512	CLA	O1A-CGA-O2A-C1
26	Y	101	LMG	O10-C28-O8-C9
27	t	102	SQD	C12-C13-C14-C15
28	D	411	LHG	C27-C28-C29-C30
29	A	413	DGD	CBB-CCB-CDB-CEB
29	h	101	DGD	C9A-CAA-CBA-CCA
31	J	101	STE	C2-C3-C4-C5
31	b	626	STE	C12-C13-C14-C15
22	b	614	CLA	CBA-CGA-O2A-C1
28	D	411	LHG	C24-C25-C26-C27
29	c	516	DGD	C7B-C8B-C9B-CAB
31	Z	101	STE	C11-C12-C13-C14
22	C	512	CLA	C3A-C2A-CAA-CBA
22	b	601	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	A	403	CLA	C15-C16-C17-C18
22	b	607	CLA	C8-C10-C11-C12
26	D	408	LMG	C36-C37-C38-C39
26	Y	101	LMG	C37-C38-C39-C40
26	a	414	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
26	b	622	LMG	C30-C31-C32-C33
26	c	518	LMG	C31-C32-C33-C34
26	m	101	LMG	C39-C40-C41-C42
27	f	102	SQD	C28-C29-C30-C31
27	t	102	SQD	C30-C31-C32-C33
29	C	517	DGD	C9B-CAB-CBB-CCB
29	c	515	DGD	CBA-CCA-CDA-CEA
29	c	516	DGD	C4A-C5A-C6A-C7A
22	H	101	CLA	C16-C17-C18-C19
22	H	101	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C20
26	A	409	LMG	C35-C36-C37-C38
26	A	409	LMG	C36-C37-C38-C39
26	D	412	LMG	C14-C15-C16-C17
27	A	412	SQD	C10-C11-C12-C13
28	a	411	LHG	C27-C28-C29-C30
31	M	104	STE	C2-C3-C4-C5
31	b	625	STE	C9-C10-C11-C12
31	b	628	STE	C10-C11-C12-C13
26	a	414	LMG	O1-C7-C8-C9
28	D	411	LHG	C16-C17-C18-C19
28	l	101	LHG	C24-C25-C26-C27
29	C	517	DGD	C6B-C7B-C8B-C9B
29	H	103	DGD	C6B-C7B-C8B-C9B
29	c	517	DGD	C6B-C7B-C8B-C9B
26	c	520	LMG	O6-C5-C6-O5
28	d	409	LHG	C29-C30-C31-C32
29	H	103	DGD	CBB-CCB-CDB-CEB
31	B	623	STE	C11-C10-C9-C8
22	c	507	CLA	C13-C15-C16-C17
22	B	610	CLA	C4-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
25	D	407	PL9	C13-C14-C16-C17
27	f	102	SQD	C8-C7-O47-C45
26	M	101	LMG	C12-C13-C14-C15
28	A	411	LHG	C13-C14-C15-C16
31	B	619	STE	C11-C12-C13-C14
31	B	623	STE	C3-C4-C5-C6
31	x	102	STE	C13-C14-C15-C16
28	D	410	LHG	O1-C1-C2-O2
28	d	408	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
26	a	414	LMG	C30-C31-C32-C33
26	c	521	LMG	C37-C38-C39-C40
28	A	411	LHG	C25-C26-C27-C28
28	L	102	LHG	C28-C29-C30-C31
28	d	408	LHG	C32-C33-C34-C35
29	C	518	DGD	CCB-CDB-CEB-CFB
23	D	401	PHO	C16-C17-C18-C20
26	a	414	LMG	C17-C18-C19-C20
26	b	622	LMG	C12-C13-C14-C15
26	c	521	LMG	C31-C32-C33-C34
28	a	411	LHG	C17-C18-C19-C20
22	a	403	CLA	C8-C10-C11-C12
22	c	508	CLA	C10-C11-C12-C13
29	C	517	DGD	C5A-C6A-C7A-C8A
29	c	516	DGD	C6A-C7A-C8A-C9A
26	A	409	LMG	C18-C19-C20-C21
26	M	101	LMG	C30-C31-C32-C33
28	L	102	LHG	C33-C34-C35-C36
29	A	413	DGD	C4B-C5B-C6B-C7B
29	C	516	DGD	CCB-CDB-CEB-CFB
26	A	409	LMG	C13-C14-C15-C16
27	a	410	SQD	C24-C25-C26-C27
29	C	516	DGD	C3B-C4B-C5B-C6B
22	c	506	CLA	C2-C1-O2A-CGA
26	D	412	LMG	C13-C14-C15-C16
26	D	412	LMG	C31-C32-C33-C34
26	c	520	LMG	C16-C17-C18-C19
27	f	102	SQD	C31-C32-C33-C34
28	l	101	LHG	C32-C33-C34-C35
29	A	413	DGD	CAA-CBA-CCA-CDA
29	A	413	DGD	C6B-C7B-C8B-C9B
31	B	624	STE	C7-C8-C9-C10
31	b	625	STE	C5-C6-C7-C8
31	d	411	STE	C5-C6-C7-C8
31	b	629	STE	C9-C10-C11-C12
22	D	404	CLA	C16-C17-C18-C19
27	A	410	SQD	C23-C24-C25-C26
30	B	617	BCR	C23-C24-C25-C26
30	B	617	BCR	C23-C24-C25-C30
30	D	406	BCR	C23-C24-C25-C26
30	D	406	BCR	C23-C24-C25-C30
30	H	102	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	H	102	BCR	C23-C24-C25-C30
30	T	101	BCR	C1-C6-C7-C8
30	k	102	BCR	C1-C6-C7-C8
30	k	102	BCR	C5-C6-C7-C8
30	k	102	BCR	C23-C24-C25-C26
30	x	101	BCR	C23-C24-C25-C26
29	c	517	DGD	C3A-C4A-C5A-C6A
31	H	104	STE	C2-C3-C4-C5
27	A	410	SQD	C24-C23-O48-C46
22	b	610	CLA	C13-C15-C16-C17
22	c	505	CLA	C5-C6-C7-C8
26	c	521	LMG	C11-C10-O7-C8
27	f	102	SQD	C25-C26-C27-C28
28	D	413	LHG	C17-C18-C19-C20
28	b	623	LHG	C15-C16-C17-C18
29	A	413	DGD	CCA-CDA-CEA-CFA
29	C	518	DGD	C3B-C4B-C5B-C6B
31	H	104	STE	C13-C14-C15-C16
31	b	629	STE	C2-C3-C4-C5
27	A	412	SQD	C34-C35-C36-C37
22	C	511	CLA	C8-C10-C11-C12
26	c	521	LMG	C13-C14-C15-C16
28	D	410	LHG	C30-C31-C32-C33
29	C	518	DGD	C5A-C6A-C7A-C8A
31	J	101	STE	C5-C6-C7-C8
22	A	403	CLA	C12-C13-C15-C16
22	B	610	CLA	C2-C3-C5-C6
22	C	509	CLA	C11-C10-C8-C7
22	C	510	CLA	C2-C3-C5-C6
22	H	101	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C10-C8-C7
22	b	611	CLA	C2-C3-C5-C6
22	b	613	CLA	C11-C12-C13-C15
22	b	614	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C12-C13-C15
22	b	615	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
22	c	505	CLA	C2-C3-C5-C6
25	D	407	PL9	C28-C29-C31-C32
25	d	407	PL9	C13-C14-C16-C17
25	d	407	PL9	C28-C29-C31-C32
25	d	407	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
28	a	411	LHG	C11-C10-C9-C8
28	l	101	LHG	C30-C31-C32-C33
31	a	413	STE	C11-C12-C13-C14
22	c	504	CLA	C10-C11-C12-C13
23	A	404	PHO	C15-C16-C17-C18
30	K	101	BCR	C15-C16-C17-C18
30	t	101	BCR	C15-C16-C17-C18
22	b	601	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C19
22	c	510	CLA	C16-C17-C18-C20
26	a	414	LMG	O9-C10-O7-C8
28	D	410	LHG	O9-C7-O7-C5
26	b	622	LMG	C10-C11-C12-C13
31	M	102	STE	C1-C2-C3-C4
26	m	101	LMG	C18-C19-C20-C21
27	a	410	SQD	C11-C10-C9-C8
28	l	101	LHG	C17-C18-C19-C20
31	k	104	STE	C6-C7-C8-C9
22	B	611	CLA	C10-C11-C12-C13
22	c	508	CLA	C8-C10-C11-C12
26	c	520	LMG	C33-C34-C35-C36
28	b	623	LHG	C11-C10-C9-C8
28	b	623	LHG	C23-C24-C25-C26
29	C	518	DGD	C1A-C2A-C3A-C4A
22	C	506	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	C10-C11-C12-C13
26	M	101	LMG	C38-C39-C40-C41
26	b	622	LMG	C31-C32-C33-C34
26	c	521	LMG	C12-C13-C14-C15
28	D	411	LHG	C14-C15-C16-C17
31	X	101	STE	C9-C10-C11-C12
31	d	411	STE	C2-C3-C4-C5
22	A	405	CLA	C3-C5-C6-C7
22	b	606	CLA	C3-C5-C6-C7
26	m	101	LMG	C33-C34-C35-C36
28	D	413	LHG	C13-C14-C15-C16
29	h	101	DGD	C6B-C7B-C8B-C9B
30	B	616	BCR	C6-C7-C8-C9
29	C	517	DGD	O6E-C1E-O5D-C6D
22	a	402	CLA	C15-C16-C17-C18
22	c	503	CLA	C5-C6-C7-C8
26	B	620	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	b	622	LMG	C18-C19-C20-C21
28	D	413	LHG	C16-C17-C18-C19
28	L	102	LHG	C15-C16-C17-C18
29	A	413	DGD	C7A-C8A-C9A-CAA
31	C	519	STE	C2-C3-C4-C5
27	a	410	SQD	C8-C7-O47-C45
28	A	411	LHG	C16-C17-C18-C19
29	C	516	DGD	C4B-C5B-C6B-C7B
31	B	619	STE	C11-C10-C9-C8
22	B	615	CLA	C5-C6-C7-C8
22	b	615	CLA	C15-C16-C17-C18
22	c	507	CLA	CBD-CGD-O2D-CED
26	c	521	LMG	C36-C37-C38-C39
27	D	409	SQD	C27-C28-C29-C30
28	D	410	LHG	C13-C14-C15-C16
31	b	625	STE	C7-C8-C9-C10
28	L	102	LHG	O9-C7-O7-C5
27	A	412	SQD	C9-C10-C11-C12
31	b	629	STE	C11-C12-C13-C14
22	H	101	CLA	C13-C15-C16-C17
26	a	414	LMG	O7-C8-C9-O8
27	A	410	SQD	O6-C44-C45-O47
27	a	410	SQD	O6-C44-C45-O47
26	a	414	LMG	O6-C5-C6-O5
28	a	411	LHG	C25-C26-C27-C28
31	a	412	STE	C2-C3-C4-C5
22	b	614	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	C16-C17-C18-C19
28	D	413	LHG	C31-C32-C33-C34
22	B	609	CLA	C8-C10-C11-C12
22	C	513	CLA	C10-C11-C12-C13
22	C	510	CLA	C4-C3-C5-C6
22	b	611	CLA	C4-C3-C5-C6
22	c	505	CLA	C4-C3-C5-C6
23	A	404	PHO	C2-C3-C5-C6
25	D	407	PL9	C4-C3-C7-C8
25	d	407	PL9	C4-C3-C7-C8
27	a	410	SQD	C13-C14-C15-C16
29	H	103	DGD	C8B-C9B-CAB-CBB
29	c	516	DGD	C2B-C3B-C4B-C5B
31	c	519	STE	C10-C11-C12-C13
22	A	403	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C11-C10-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	C	510	CLA	C6-C7-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	b	602	CLA	C14-C13-C15-C16
22	b	606	CLA	C14-C13-C15-C16
22	b	615	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C12-C13-C14
22	d	405	CLA	C6-C7-C8-C9
26	a	414	LMG	C23-C24-C25-C26
27	L	101	SQD	C9-C10-C11-C12
31	H	104	STE	C5-C6-C7-C8
31	b	627	STE	C4-C5-C6-C7
26	b	622	LMG	C38-C39-C40-C41
31	X	101	STE	C14-C15-C16-C17
31	a	412	STE	C6-C7-C8-C9
27	A	412	SQD	C16-C17-C18-C19
29	A	413	DGD	C5A-C6A-C7A-C8A
29	c	515	DGD	CAB-CBB-CCB-CDB
31	c	519	STE	C7-C8-C9-C10
22	H	101	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C16-C17-C18-C19
26	Y	101	LMG	C11-C12-C13-C14
26	b	622	LMG	C34-C35-C36-C37
28	D	413	LHG	C25-C26-C27-C28
29	c	517	DGD	C2A-C3A-C4A-C5A
29	c	517	DGD	CCA-CDA-CEA-CFA
31	b	628	STE	C7-C8-C9-C10
22	C	512	CLA	C15-C16-C17-C18
28	A	411	LHG	C4-O6-P-O3
28	D	410	LHG	C3-O3-P-O6
28	L	102	LHG	C3-O3-P-O6
28	d	408	LHG	C4-O6-P-O3
27	A	410	SQD	C11-C10-C9-C8
26	a	414	LMG	C15-C16-C17-C18
22	C	507	CLA	C10-C11-C12-C13
25	A	408	PL9	C22-C23-C24-C25
27	A	412	SQD	C11-C10-C9-C8
26	c	521	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	d	410	LMG	O6-C5-C6-O5
26	Y	101	LMG	C15-C16-C17-C18
26	b	622	LMG	O6-C5-C6-O5
27	A	412	SQD	C28-C29-C30-C31
31	c	519	STE	C4-C5-C6-C7
22	c	511	CLA	C3-C5-C6-C7
22	C	508	CLA	C13-C15-C16-C17
26	D	412	LMG	C36-C37-C38-C39
31	R	101	STE	C4-C5-C6-C7
23	A	404	PHO	C4-C3-C5-C6
25	d	407	PL9	C30-C29-C31-C32
25	d	407	PL9	C45-C44-C46-C47
26	D	412	LMG	C12-C13-C14-C15
26	Y	101	LMG	C14-C15-C16-C17
26	b	622	LMG	C16-C17-C18-C19
27	L	101	SQD	C26-C27-C28-C29
28	D	411	LHG	C30-C31-C32-C33
29	c	516	DGD	CAB-CBB-CCB-CDB
29	h	101	DGD	C3B-C4B-C5B-C6B
27	B	621	SQD	O10-C23-O48-C46
29	C	518	DGD	C6A-C7A-C8A-C9A
31	b	621	STE	C6-C7-C8-C9
22	D	405	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
26	c	518	LMG	O6-C5-C6-O5
22	C	510	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
26	Y	101	LMG	O1-C7-C8-C9
26	c	520	LMG	O1-C7-C8-C9
26	c	520	LMG	C7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-C9
27	B	621	SQD	O6-C44-C45-C46
27	a	410	SQD	C25-C26-C27-C28
29	A	413	DGD	C1G-C2G-C3G-O3G
29	C	516	DGD	O1G-C1G-C2G-C3G
31	X	101	STE	C3-C4-C5-C6
22	B	607	CLA	C10-C11-C12-C13
22	c	512	CLA	C8-C10-C11-C12
26	m	101	LMG	C12-C13-C14-C15
29	C	517	DGD	C2G-C3G-O3G-C1D
29	c	516	DGD	C2G-C3G-O3G-C1D
22	b	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	d	410	LMG	C15-C16-C17-C18
28	D	413	LHG	C32-C33-C34-C35
28	d	408	LHG	C11-C10-C9-C8
22	b	601	CLA	C10-C11-C12-C13
22	b	602	CLA	C15-C16-C17-C18
27	B	621	SQD	C32-C33-C34-C35
29	C	517	DGD	C2B-C3B-C4B-C5B
26	d	410	LMG	C30-C31-C32-C33
29	c	515	DGD	CBB-CCB-CDB-CEB
31	X	101	STE	C6-C7-C8-C9
31	b	624	STE	C7-C8-C9-C10
31	b	625	STE	C10-C11-C12-C13
31	t	104	STE	C7-C8-C9-C10
22	B	611	CLA	C3-C5-C6-C7
26	D	412	LMG	C34-C35-C36-C37
27	A	412	SQD	C15-C16-C17-C18
27	B	621	SQD	C13-C14-C15-C16
31	C	520	STE	C11-C10-C9-C8
31	k	104	STE	C4-C5-C6-C7
28	A	411	LHG	O1-C1-C2-O2
28	b	623	LHG	O1-C1-C2-O2
28	d	409	LHG	O1-C1-C2-O2
26	A	409	LMG	C37-C38-C39-C40
26	D	412	LMG	C37-C38-C39-C40
26	Y	101	LMG	C33-C34-C35-C36
25	D	407	PL9	C37-C38-C39-C40
22	B	613	CLA	C15-C16-C17-C18
27	L	101	SQD	C19-C20-C21-C22
27	L	101	SQD	C27-C28-C29-C30
31	R	101	STE	C3-C4-C5-C6
27	A	410	SQD	C8-C7-O47-C45
31	k	104	STE	C7-C8-C9-C10
29	c	515	DGD	O6E-C5E-C6E-O5E
30	b	618	BCR	C16-C17-C18-C36
22	H	101	CLA	C3-C5-C6-C7
25	A	408	PL9	C15-C14-C16-C17
25	D	407	PL9	C30-C29-C31-C32
26	D	408	LMG	C15-C16-C17-C18
22	C	509	CLA	C16-C17-C18-C19
29	C	517	DGD	CDA-CEA-CFA-CGA
22	C	507	CLA	C5-C6-C7-C8
22	C	510	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	m	101	LMG	C15-C16-C17-C18
29	C	517	DGD	C4A-C5A-C6A-C7A
31	b	620	STE	C3-C4-C5-C6
31	b	629	STE	C15-C16-C17-C18
26	D	408	LMG	O6-C5-C6-O5
22	D	403	CLA	C2-C1-O2A-CGA
28	A	411	LHG	C18-C19-C20-C21
31	J	101	STE	C3-C4-C5-C6
31	a	413	STE	C13-C14-C15-C16
31	b	627	STE	C7-C8-C9-C10
31	c	519	STE	C11-C12-C13-C14
29	C	517	DGD	CAA-CBA-CCA-CDA
29	c	517	DGD	C9B-CAB-CBB-CCB
31	a	412	STE	C3-C4-C5-C6
22	C	502	CLA	C16-C17-C18-C19
26	c	520	LMG	C32-C33-C34-C35
27	A	410	SQD	C17-C18-C19-C20
27	D	409	SQD	C28-C29-C30-C31
29	A	413	DGD	CEB-CFB-CGB-CHB
29	H	103	DGD	C5B-C6B-C7B-C8B
22	B	601	CLA	C8-C10-C11-C12
26	b	622	LMG	C15-C16-C17-C18
27	A	410	SQD	C29-C30-C31-C32
28	D	411	LHG	C13-C14-C15-C16
28	b	623	LHG	C19-C20-C21-C22
28	D	410	LHG	O2-C2-C3-O3
26	Y	101	LMG	C32-C33-C34-C35
27	a	410	SQD	C32-C33-C34-C35
27	B	621	SQD	C7-C8-C9-C10
22	B	605	CLA	C5-C6-C7-C8
22	B	612	CLA	C5-C6-C7-C8
22	b	611	CLA	C13-C15-C16-C17
26	c	521	LMG	C2-C1-O1-C7
30	d	406	BCR	C16-C17-C18-C19
28	d	408	LHG	C34-C35-C36-C37
31	B	623	STE	C12-C13-C14-C15
31	a	412	STE	C7-C8-C9-C10
29	C	516	DGD	O1G-C1A-C2A-C3A
27	a	410	SQD	O47-C45-C46-O48
26	c	521	LMG	C20-C21-C22-C23
27	t	102	SQD	C10-C11-C12-C13
29	c	515	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C5-C6-C7-C8
31	L	103	STE	C6-C7-C8-C9
31	M	102	STE	C4-C5-C6-C7
31	Z	101	STE	C12-C13-C14-C15
22	A	403	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	B	602	CLA	C6-C7-C8-C10
22	B	602	CLA	C11-C12-C13-C15
22	B	603	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C12-C13-C15
22	B	610	CLA	C11-C10-C8-C7
22	B	613	CLA	C11-C12-C13-C15
22	B	613	CLA	C12-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C15
22	B	615	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C12-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	D	403	CLA	C11-C12-C13-C15
22	D	405	CLA	C11-C12-C13-C15
22	a	403	CLA	C11-C10-C8-C7
22	a	403	CLA	C12-C13-C15-C16
22	b	604	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C6-C7-C8-C10
22	b	607	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C10-C8-C7
22	c	501	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	508	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	D	408	LMG	C35-C36-C37-C38
27	a	410	SQD	C14-C15-C16-C17
22	B	601	CLA	C11-C12-C13-C14
22	B	602	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	615	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	D	404	CLA	C11-C12-C13-C14
22	D	405	CLA	C6-C7-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	604	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C14
22	b	606	CLA	C6-C7-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	b	607	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C9
26	c	521	LMG	C39-C40-C41-C42
31	b	620	STE	C15-C16-C17-C18
31	b	624	STE	C4-C5-C6-C7
22	B	604	CLA	CBA-CGA-O2A-C1
22	b	607	CLA	CBA-CGA-O2A-C1
26	D	412	LMG	C29-C28-O8-C9
27	A	412	SQD	C24-C23-O48-C46
22	b	605	CLA	C13-C15-C16-C17
22	c	502	CLA	C15-C16-C17-C18
26	D	412	LMG	C16-C17-C18-C19
26	c	521	LMG	C35-C36-C37-C38
29	c	516	DGD	CBB-CCB-CDB-CEB
30	b	618	BCR	C37-C22-C23-C24
22	D	405	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C16-C17-C18-C20
29	h	101	DGD	CAB-CBB-CCB-CDB
31	M	104	STE	C3-C4-C5-C6
27	a	410	SQD	C16-C17-C18-C19
22	C	509	CLA	C3-C5-C6-C7
22	C	506	CLA	C10-C11-C12-C13
26	Y	101	LMG	C12-C13-C14-C15
31	a	413	STE	C10-C11-C12-C13
27	t	102	SQD	C24-C23-O48-C46
26	B	620	LMG	C37-C38-C39-C40
22	C	513	CLA	C8-C10-C11-C12
28	A	411	LHG	C10-C11-C12-C13
28	D	410	LHG	C25-C26-C27-C28
28	L	102	LHG	C13-C14-C15-C16
27	A	412	SQD	C44-C45-O47-C7
22	D	405	CLA	CBD-CGD-O2D-CED
28	l	101	LHG	C25-C26-C27-C28
22	c	509	CLA	C13-C15-C16-C17
28	a	411	LHG	C14-C15-C16-C17
29	c	517	DGD	C8B-C9B-CAB-CBB
28	l	101	LHG	C34-C35-C36-C37
22	C	506	CLA	CBA-CGA-O2A-C1
22	B	603	CLA	O1D-CGD-O2D-CED
29	H	103	DGD	CDB-CEB-CFB-CGB
29	c	515	DGD	C6B-C7B-C8B-C9B
25	d	407	PL9	C33-C34-C36-C37
28	D	411	LHG	C29-C30-C31-C32
29	A	413	DGD	C7B-C8B-C9B-CAB
22	B	607	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C19
31	B	619	STE	C9-C10-C11-C12
22	B	607	CLA	C5-C6-C7-C8
22	a	405	CLA	CBA-CGA-O2A-C1
22	c	509	CLA	CAA-CBA-CGA-O2A
28	b	623	LHG	C7-C8-C9-C10
27	f	102	SQD	C29-C30-C31-C32
22	C	506	CLA	C3A-C2A-CAA-CBA
26	a	414	LMG	C37-C38-C39-C40
28	D	410	LHG	C11-C10-C9-C8
29	h	101	DGD	CDB-CEB-CFB-CGB
30	k	102	BCR	C19-C20-C21-C22
28	b	623	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	H	103	DGD	CCA-CDA-CEA-CFA
26	c	521	LMG	C19-C20-C21-C22
27	L	101	SQD	C16-C17-C18-C19
31	b	621	STE	C5-C6-C7-C8
22	B	609	CLA	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C19
22	C	509	CLA	C16-C17-C18-C20
22	C	511	CLA	CBA-CGA-O2A-C1
29	c	515	DGD	C3A-C4A-C5A-C6A
26	M	101	LMG	C7-C8-C9-O8
26	a	414	LMG	C7-C8-C9-O8
27	A	410	SQD	O6-C44-C45-C46
27	L	101	SQD	C44-C45-C46-O48
27	a	410	SQD	O6-C44-C45-C46
29	c	517	DGD	C7B-C8B-C9B-CAB
28	D	413	LHG	C27-C28-C29-C30
27	A	412	SQD	C13-C14-C15-C16
27	B	621	SQD	C29-C30-C31-C32
26	D	408	LMG	C37-C38-C39-C40
29	h	101	DGD	C7B-C8B-C9B-CAB
22	B	606	CLA	C10-C11-C12-C13
22	c	503	CLA	C15-C16-C17-C18
23	A	404	PHO	C10-C11-C12-C13
26	a	414	LMG	C32-C33-C34-C35
31	t	104	STE	C3-C4-C5-C6
29	h	101	DGD	C1A-C2A-C3A-C4A
26	D	408	LMG	C40-C41-C42-C43
26	a	414	LMG	C24-C25-C26-C27
31	B	619	STE	C4-C5-C6-C7
22	b	604	CLA	C3-C5-C6-C7
26	b	622	LMG	C29-C30-C31-C32
26	Y	101	LMG	C29-C28-O8-C9
22	b	607	CLA	O1A-CGA-O2A-C1
28	D	410	LHG	C23-C24-C25-C26
27	a	410	SQD	C30-C31-C32-C33
29	c	515	DGD	CDB-CEB-CFB-CGB
31	k	104	STE	C2-C3-C4-C5
26	Y	101	LMG	O1-C7-C8-O7
26	c	520	LMG	O1-C7-C8-O7
29	A	413	DGD	O1G-C1G-C2G-O2G
22	b	612	CLA	C10-C11-C12-C13
27	B	621	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C19
26	a	414	LMG	C16-C17-C18-C19
31	B	624	STE	C11-C10-C9-C8
22	D	404	CLA	C15-C16-C17-C18
23	D	401	PHO	C13-C15-C16-C17
26	D	412	LMG	O1-C7-C8-C9
27	B	621	SQD	C24-C25-C26-C27
22	c	502	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
26	A	409	LMG	C14-C15-C16-C17
31	b	627	STE	C3-C4-C5-C6
22	B	606	CLA	C11-C12-C13-C14
22	C	506	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
23	d	401	PHO	CBD-CGD-O2D-CED
28	L	102	LHG	C35-C36-C37-C38
22	b	610	CLA	O1D-CGD-O2D-CED
28	b	623	LHG	C2-C3-O3-P
28	d	409	LHG	C2-C3-O3-P
27	A	410	SQD	C28-C29-C30-C31
29	C	517	DGD	C4B-C5B-C6B-C7B
29	H	103	DGD	C3B-C4B-C5B-C6B
31	b	627	STE	C1-C2-C3-C4
22	c	501	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C16-C17-C18-C19
22	b	609	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	A	403	CLA	C3-C5-C6-C7
30	K	102	BCR	C23-C24-C25-C30
30	T	101	BCR	C5-C6-C7-C8
30	k	103	BCR	C23-C24-C25-C26
27	A	412	SQD	C18-C19-C20-C21
29	C	516	DGD	C9A-CAA-CBA-CCA
31	H	104	STE	C11-C10-C9-C8
31	b	626	STE	C10-C11-C12-C13
26	m	101	LMG	C16-C17-C18-C19
28	d	408	LHG	C16-C17-C18-C19
31	Z	101	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	C	515	BCR	C7-C8-C9-C10
30	K	101	BCR	C11-C12-C13-C14
30	k	101	BCR	C21-C22-C23-C24
31	I	102	STE	C11-C10-C9-C8
22	c	502	CLA	CBD-CGD-O2D-CED
26	c	521	LMG	O6-C5-C6-O5
28	a	411	LHG	C8-C7-O7-C5
29	C	518	DGD	C3A-C4A-C5A-C6A
28	L	102	LHG	O10-C23-O8-C6
26	a	414	LMG	C34-C35-C36-C37
31	x	102	STE	C15-C16-C17-C18
22	B	604	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C20
28	D	410	LHG	C12-C13-C14-C15
27	D	409	SQD	O6-C44-C45-C46
28	l	101	LHG	O6-C4-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	c	511	CLA	C2C-C3C-CAC-CBC
31	b	628	STE	C12-C13-C14-C15
22	B	603	CLA	C11-C12-C13-C15
22	B	605	CLA	C11-C10-C8-C7
22	B	606	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
22	C	513	CLA	C11-C10-C8-C7
22	D	404	CLA	C11-C12-C13-C15
22	D	405	CLA	C6-C7-C8-C10
22	D	405	CLA	C11-C10-C8-C7
22	b	601	CLA	C11-C12-C13-C15
22	b	603	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
23	A	404	PHO	C12-C13-C15-C16
28	L	102	LHG	C17-C18-C19-C20
28	L	102	LHG	C18-C19-C20-C21
31	H	104	STE	C6-C7-C8-C9
31	a	413	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
26	D	412	LMG	O1-C7-C8-O7
22	b	609	CLA	C15-C16-C17-C18
30	H	102	BCR	C13-C14-C15-C16
30	H	102	BCR	C15-C16-C17-C18
22	B	614	CLA	C16-C17-C18-C19
22	C	508	CLA	C16-C17-C18-C19
27	A	412	SQD	C29-C30-C31-C32
29	A	413	DGD	C4A-C5A-C6A-C7A
31	I	102	STE	C2-C3-C4-C5
22	B	606	CLA	C15-C16-C17-C18
22	C	511	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	CBD-CGD-O2D-CED
31	H	104	STE	C10-C11-C12-C13
30	B	617	BCR	C20-C21-C22-C37
30	C	514	BCR	C35-C13-C14-C15
30	c	514	BCR	C20-C21-C22-C37
28	D	413	LHG	C7-C8-C9-C10
27	A	410	SQD	C11-C12-C13-C14
27	A	410	SQD	C26-C27-C28-C29
31	L	103	STE	C7-C8-C9-C10
22	C	502	CLA	C16-C17-C18-C20
22	c	506	CLA	CBA-CGA-O2A-C1
29	H	103	DGD	O2G-C1B-C2B-C3B
28	a	411	LHG	C26-C27-C28-C29
26	D	408	LMG	C20-C21-C22-C23
26	D	412	LMG	C11-C12-C13-C14
26	m	101	LMG	C32-C33-C34-C35
31	B	625	STE	C7-C8-C9-C10
31	b	621	STE	C2-C3-C4-C5
31	b	621	STE	C11-C10-C9-C8
22	b	604	CLA	C15-C16-C17-C18
27	A	410	SQD	C16-C17-C18-C19
28	A	411	LHG	C31-C32-C33-C34
29	H	103	DGD	CAB-CBB-CCB-CDB
31	b	625	STE	C12-C13-C14-C15
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	CAD-CBD-CGD-O2D
27	f	102	SQD	C46-C45-O47-C7
28	L	102	LHG	C32-C33-C34-C35
28	d	409	LHG	C35-C36-C37-C38
29	C	517	DGD	CBB-CCB-CDB-CEB
31	x	102	STE	C11-C10-C9-C8
22	d	404	CLA	C13-C15-C16-C17
31	b	621	STE	C10-C11-C12-C13
22	d	403	CLA	C16-C17-C18-C19
26	a	414	LMG	O6-C1-O1-C7
22	C	505	CLA	C2-C3-C5-C6
26	m	101	LMG	C7-C8-C9-O8
29	A	413	DGD	O1G-C1G-C2G-C3G
27	a	410	SQD	O10-C23-O48-C46
31	B	624	STE	C10-C11-C12-C13
27	D	409	SQD	O48-C23-C24-C25
22	b	610	CLA	C2A-CAA-CBA-CGA
31	M	104	STE	C12-C13-C14-C15
27	L	101	SQD	C23-C24-C25-C26
22	C	511	CLA	CBD-CGD-O2D-CED
22	D	403	CLA	C16-C17-C18-C19
27	A	410	SQD	C15-C16-C17-C18
27	f	102	SQD	C33-C34-C35-C36
29	C	516	DGD	O1B-C1B-O2G-C2G
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	613	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	H	101	CLA	CHA-CBD-CGD-O1D
22	H	101	CLA	CHA-CBD-CGD-O2D
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	c	502	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
28	d	408	LHG	C15-C16-C17-C18
22	B	604	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	O1A-CGA-O2A-C1
28	D	411	LHG	C11-C10-C9-C8
31	M	102	STE	C11-C10-C9-C8
30	B	617	BCR	C12-C13-C14-C15
30	B	618	BCR	C12-C13-C14-C15
30	c	514	BCR	C11-C10-C9-C8
22	B	609	CLA	C15-C16-C17-C18
26	Y	101	LMG	C17-C18-C19-C20
27	L	101	SQD	C18-C19-C20-C21
31	B	619	STE	C2-C3-C4-C5
31	B	624	STE	C14-C15-C16-C17
31	t	103	STE	C6-C7-C8-C9
26	c	520	LMG	O7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-O7
22	C	506	CLA	O1A-CGA-O2A-C1
29	C	517	DGD	O1A-C1A-O1G-C1G
26	D	408	LMG	C31-C32-C33-C34
22	B	602	CLA	C16-C17-C18-C19
27	a	410	SQD	C27-C28-C29-C30
29	H	103	DGD	CBA-CCA-CDA-CEA
22	b	601	CLA	C8-C10-C11-C12
25	a	409	PL9	C4-C3-C7-C8
27	B	621	SQD	C9-C10-C11-C12
22	B	614	CLA	C5-C6-C7-C8
22	H	101	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C10-C8-C9
26	M	101	LMG	C19-C20-C21-C22
26	b	622	LMG	C32-C33-C34-C35
27	L	101	SQD	C30-C31-C32-C33
27	a	410	SQD	C35-C36-C37-C38
29	H	103	DGD	CCB-CDB-CEB-CFB
27	t	102	SQD	C14-C15-C16-C17
28	D	410	LHG	C32-C33-C34-C35
31	I	102	STE	C12-C13-C14-C15
31	M	103	STE	C2-C3-C4-C5
30	I	101	BCR	C7-C8-C9-C34
31	X	101	STE	C7-C8-C9-C10
26	b	622	LMG	C42-C43-C44-C45
29	h	101	DGD	C7A-C8A-C9A-CAA
31	C	520	STE	C4-C5-C6-C7
31	M	104	STE	C9-C10-C11-C12
22	a	405	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C5-C6-C7-C8
31	M	104	STE	C5-C6-C7-C8
22	b	616	CLA	C8-C10-C11-C12
28	L	102	LHG	C4-O6-P-O3
28	l	101	LHG	C4-O6-P-O3
28	b	623	LHG	C33-C34-C35-C36
26	b	622	LMG	C35-C36-C37-C38
27	A	412	SQD	C27-C28-C29-C30
28	l	101	LHG	C18-C19-C20-C21
22	c	507	CLA	C4-C3-C5-C6
28	D	411	LHG	C15-C16-C17-C18
28	A	411	LHG	C4-O6-P-O5
28	b	623	LHG	C3-O3-P-O4
28	l	101	LHG	C4-O6-P-O4
22	B	614	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C20
28	a	411	LHG	C7-C8-C9-C10
28	a	411	LHG	O6-C4-C5-C6
26	D	412	LMG	C33-C34-C35-C36
29	c	515	DGD	C1A-C2A-C3A-C4A
26	a	414	LMG	C36-C37-C38-C39
28	a	411	LHG	C11-C12-C13-C14
28	l	101	LHG	C14-C15-C16-C17
31	C	520	STE	C6-C7-C8-C9
28	b	623	LHG	C14-C15-C16-C17
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	611	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	H	101	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
26	D	408	LMG	C16-C17-C18-C19
31	b	620	STE	C10-C11-C12-C13
26	D	408	LMG	C33-C34-C35-C36
29	c	515	DGD	C4D-C5D-C6D-O5D
26	c	520	LMG	C41-C42-C43-C44
31	b	620	STE	C11-C12-C13-C14
22	A	403	CLA	C11-C12-C13-C15
22	B	604	CLA	C6-C7-C8-C10
22	B	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	H	101	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C12-C13-C15
22	b	601	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C12-C13-C15
22	b	612	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C12-C13-C15
22	d	405	CLA	C11-C12-C13-C15
28	l	101	LHG	O6-C4-C5-O7
26	B	620	LMG	C36-C37-C38-C39
26	D	412	LMG	C15-C16-C17-C18
31	b	627	STE	C5-C6-C7-C8
25	D	407	PL9	C2-C3-C7-C8
22	b	611	CLA	C5-C6-C7-C8
22	c	512	CLA	C10-C11-C12-C13
28	b	623	LHG	C17-C18-C19-C20
29	C	516	DGD	C5A-C6A-C7A-C8A
29	C	516	DGD	CDA-CEA-CFA-CGA
22	B	601	CLA	C16-C17-C18-C19
26	M	101	LMG	O7-C8-C9-O8
26	a	414	LMG	O1-C7-C8-O7
27	L	101	SQD	O6-C44-C45-O47
27	L	101	SQD	O47-C45-C46-O48
27	t	102	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
28	l	101	LHG	C33-C34-C35-C36
28	D	410	LHG	C26-C27-C28-C29
29	A	413	DGD	CFB-CGB-CHB-CIB
29	C	517	DGD	C3A-C4A-C5A-C6A
29	C	517	DGD	C5D-C6D-O5D-C1E
22	B	602	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
28	d	409	LHG	C26-C27-C28-C29
22	c	507	CLA	O1D-CGD-O2D-CED
26	d	410	LMG	C12-C13-C14-C15
22	B	608	CLA	C4-C3-C5-C6
26	m	101	LMG	C29-C28-O8-C9
27	L	101	SQD	C29-C30-C31-C32
28	a	411	LHG	C28-C29-C30-C31
22	A	403	CLA	C11-C12-C13-C14
22	B	603	CLA	C11-C12-C13-C14
22	B	608	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C10-C8-C9
22	c	501	CLA	C11-C12-C13-C14
22	c	511	CLA	C11-C10-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	b	607	CLA	C16-C17-C18-C19
22	b	610	CLA	C16-C17-C18-C19
28	D	411	LHG	C9-C10-C11-C12
25	A	408	PL9	C19-C21-C22-C23
26	b	622	LMG	C28-C29-C30-C31
26	m	101	LMG	C37-C38-C39-C40
22	B	606	CLA	C13-C15-C16-C17
22	b	601	CLA	C13-C15-C16-C17
26	D	408	LMG	C12-C13-C14-C15
29	H	103	DGD	C9A-CAA-CBA-CCA
23	d	401	PHO	O1D-CGD-O2D-CED
26	c	518	LMG	C32-C33-C34-C35
28	A	411	LHG	C11-C10-C9-C8
31	t	103	STE	C7-C8-C9-C10
26	D	408	LMG	C21-C22-C23-C24
29	c	515	DGD	C9B-CAB-CBB-CCB
22	B	612	CLA	C13-C15-C16-C17
28	D	411	LHG	C31-C32-C33-C34
29	C	516	DGD	C2A-C3A-C4A-C5A
28	A	411	LHG	C17-C18-C19-C20
29	c	517	DGD	CAA-CBA-CCA-CDA
22	b	603	CLA	C13-C15-C16-C17
26	D	412	LMG	C9-C8-O7-C10
29	C	518	DGD	O1A-C1A-O1G-C1G
22	B	603	CLA	C2-C1-O2A-CGA
22	B	615	CLA	C2-C1-O2A-CGA
22	C	506	CLA	C2-C1-O2A-CGA
26	c	518	LMG	C34-C35-C36-C37
22	B	601	CLA	C16-C17-C18-C20
31	d	411	STE	C3-C4-C5-C6
22	c	502	CLA	O1D-CGD-O2D-CED
30	b	617	BCR	C5-C6-C7-C8
22	c	507	CLA	C2-C3-C5-C6
25	A	408	PL9	C13-C14-C16-C17
28	b	623	LHG	C30-C31-C32-C33
31	b	624	STE	C11-C12-C13-C14
28	d	408	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
30	B	618	BCR	C20-C21-C22-C23
30	C	514	BCR	C11-C10-C9-C8
30	b	618	BCR	C12-C13-C14-C15
30	d	406	BCR	C12-C13-C14-C15
22	b	604	CLA	C13-C15-C16-C17
28	d	409	LHG	C31-C32-C33-C34
27	B	621	SQD	C31-C32-C33-C34
29	c	515	DGD	O6D-C5D-C6D-O5D
28	L	102	LHG	C29-C30-C31-C32
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
26	b	622	LMG	O1-C7-C8-C9
27	a	410	SQD	C44-C45-C46-O48
22	c	512	CLA	C4-C3-C5-C6
31	B	623	STE	C2-C3-C4-C5
31	b	625	STE	C11-C10-C9-C8
22	C	505	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C15
22	C	510	CLA	C11-C10-C8-C7
22	C	513	CLA	C12-C13-C15-C16
22	B	603	CLA	C14-C13-C15-C16
22	C	509	CLA	C14-C13-C15-C16
22	a	403	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C12-C13-C14
30	c	514	BCR	C13-C14-C15-C16
30	k	101	BCR	C9-C10-C11-C12
25	a	409	PL9	C41-C42-C43-C44
31	b	626	STE	C14-C15-C16-C17
31	t	103	STE	C11-C10-C9-C8
30	b	618	BCR	C7-C8-C9-C34
30	k	102	BCR	C36-C18-C19-C20
27	B	621	SQD	C30-C31-C32-C33
31	x	102	STE	C14-C15-C16-C17
28	D	411	LHG	O9-C7-O7-C5
28	b	623	LHG	C28-C29-C30-C31
28	d	408	LHG	C17-C18-C19-C20
22	A	402	CLA	C15-C16-C17-C18
22	B	604	CLA	C10-C11-C12-C13
22	c	510	CLA	C15-C16-C17-C18
28	A	411	LHG	C23-C24-C25-C26
28	a	411	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	CCB-CDB-CEB-CFB
30	t	101	BCR	C13-C14-C15-C16
28	A	411	LHG	C27-C28-C29-C30
28	a	411	LHG	C15-C16-C17-C18
22	A	402	CLA	C13-C15-C16-C17
22	b	614	CLA	C5-C6-C7-C8
31	B	623	STE	C11-C12-C13-C14
28	L	102	LHG	C11-C12-C13-C14
22	C	508	CLA	C16-C17-C18-C20
26	a	414	LMG	O8-C28-C29-C30
26	M	101	LMG	C17-C18-C19-C20
31	t	104	STE	C4-C5-C6-C7
22	c	510	CLA	C8-C10-C11-C12
22	B	608	CLA	C2-C3-C5-C6
27	t	102	SQD	C24-C25-C26-C27
31	M	102	STE	O1-C1-C2-C3
31	d	411	STE	O1-C1-C2-C3
29	c	515	DGD	O1G-C1A-C2A-C3A
22	a	405	CLA	C15-C16-C17-C18
22	D	403	CLA	C16-C17-C18-C20
31	d	411	STE	C12-C13-C14-C15
22	B	613	CLA	C2A-CAA-CBA-CGA
26	m	101	LMG	O7-C8-C9-O8
26	M	101	LMG	C33-C34-C35-C36
27	A	410	SQD	C9-C10-C11-C12
27	A	412	SQD	C31-C32-C33-C34
23	D	401	PHO	C3A-C2A-CAA-CBA
31	B	622	STE	O1-C1-C2-C3
31	b	626	STE	O2-C1-C2-C3
30	C	515	BCR	C9-C10-C11-C12
22	C	501	CLA	C2C-C3C-CAC-CBC
28	b	623	LHG	C24-C25-C26-C27
28	d	408	LHG	C24-C25-C26-C27
25	A	408	PL9	C4-C3-C7-C8
22	A	402	CLA	C14-C13-C15-C16
22	B	609	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C9
22	c	502	CLA	C14-C13-C15-C16
22	d	403	CLA	C11-C10-C8-C9
23	d	401	PHO	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	501	CLA	C4C-C3C-CAC-CBC
26	D	408	LMG	C32-C33-C34-C35
31	B	619	STE	C12-C13-C14-C15
31	X	101	STE	C13-C14-C15-C16
29	c	516	DGD	C4E-C5E-C6E-O5E
31	C	521	STE	C5-C6-C7-C8
28	L	102	LHG	C10-C11-C12-C13
29	C	516	DGD	C2B-C3B-C4B-C5B
22	b	610	CLA	C16-C17-C18-C20
29	c	516	DGD	O6D-C1D-O3G-C3G
28	D	410	LHG	C9-C10-C11-C12
31	a	413	STE	C12-C13-C14-C15
30	t	101	BCR	C11-C12-C13-C35
31	b	626	STE	O1-C1-C2-C3
30	B	617	BCR	C14-C15-C16-C17
26	m	101	LMG	C14-C15-C16-C17
31	b	626	STE	C2-C3-C4-C5
22	d	403	CLA	C3-C5-C6-C7
26	M	101	LMG	C39-C40-C41-C42
29	h	101	DGD	CBB-CCB-CDB-CEB
26	a	414	LMG	C9-C8-O7-C10
22	C	506	CLA	C1A-C2A-CAA-CBA
22	C	508	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	B	614	CLA	C6-C7-C8-C10
22	D	405	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
31	b	621	STE	O1-C1-C2-C3
29	H	103	DGD	C9B-CAB-CBB-CCB
22	b	612	CLA	C15-C16-C17-C18
31	d	411	STE	O2-C1-C2-C3
34	f	101	HEC	CAD-CBD-CGD-O1D
26	c	520	LMG	C29-C30-C31-C32
22	B	613	CLA	C13-C15-C16-C17
22	B	614	CLA	C13-C15-C16-C17
29	C	518	DGD	C8B-C9B-CAB-CBB
22	C	507	CLA	C13-C15-C16-C17
22	b	603	CLA	C8-C10-C11-C12
34	f	101	HEC	CAD-CBD-CGD-O2D
27	A	410	SQD	C31-C32-C33-C34
22	D	404	CLA	C8-C10-C11-C12
28	A	411	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	C	516	DGD	O6D-C5D-C6D-O5D
31	M	102	STE	O2-C1-C2-C3
29	h	101	DGD	C9B-CAB-CBB-CCB
31	x	102	STE	C10-C11-C12-C13
29	C	518	DGD	CDA-CEA-CFA-CGA
31	X	101	STE	O1-C1-C2-C3
22	B	608	CLA	C13-C15-C16-C17
22	c	505	CLA	C10-C11-C12-C13
25	A	408	PL9	C47-C48-C49-C51
27	A	410	SQD	O49-C7-O47-C45
26	b	622	LMG	C14-C15-C16-C17
30	C	515	BCR	C13-C14-C15-C16
30	k	101	BCR	C13-C14-C15-C16
22	c	504	CLA	C11-C12-C13-C14
26	M	101	LMG	C18-C19-C20-C21
25	a	409	PL9	C29-C31-C32-C33
31	X	101	STE	O2-C1-C2-C3
22	B	607	CLA	C4-C3-C5-C6
26	D	408	LMG	C22-C23-C24-C25
22	d	403	CLA	C2-C1-O2A-CGA
27	A	412	SQD	C35-C36-C37-C38
30	K	101	BCR	C18-C19-C20-C21
28	b	623	LHG	C26-C27-C28-C29
29	C	516	DGD	C8A-C9A-CAA-CBA
31	M	104	STE	C11-C12-C13-C14
31	c	519	STE	C14-C15-C16-C17
22	b	602	CLA	C11-C10-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	c	505	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	C3-C5-C6-C7
31	B	622	STE	O2-C1-C2-C3
26	c	520	LMG	C39-C40-C41-C42
29	c	515	DGD	C6A-C7A-C8A-C9A
31	j	101	STE	C5-C6-C7-C8
22	d	403	CLA	C2C-C3C-CAC-CBC
30	b	617	BCR	C1-C6-C7-C8
30	b	617	BCR	C23-C24-C25-C30
30	b	618	BCR	C23-C24-C25-C30
30	d	406	BCR	C23-C24-C25-C30
30	k	103	BCR	C23-C24-C25-C30
30	t	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	t	101	BCR	C5-C6-C7-C8
22	c	513	CLA	C13-C15-C16-C17
22	A	402	CLA	C4C-C3C-CAC-CBC
27	D	409	SQD	C45-C46-O48-C23
30	k	103	BCR	C9-C10-C11-C12
22	b	615	CLA	C4-C3-C5-C6
30	H	102	BCR	C17-C18-C19-C20
30	H	102	BCR	C21-C22-C23-C24
29	c	517	DGD	C5A-C6A-C7A-C8A
22	c	512	CLA	C2-C3-C5-C6
25	a	409	PL9	C43-C44-C46-C47
29	c	516	DGD	C5D-C6D-O5D-C1E
26	M	101	LMG	O6-C5-C6-O5
31	J	101	STE	C7-C8-C9-C10
27	B	621	SQD	C34-C35-C36-C37
28	D	413	LHG	C29-C30-C31-C32
22	c	513	CLA	C8-C10-C11-C12
28	D	413	LHG	O6-C4-C5-O7
31	C	519	STE	O2-C1-C2-C3
29	C	518	DGD	CDB-CEB-CFB-CGB
26	b	622	LMG	C40-C41-C42-C43
31	b	625	STE	C11-C12-C13-C14
22	c	508	CLA	C4-C3-C5-C6
25	D	407	PL9	C33-C34-C36-C37
31	B	624	STE	C13-C14-C15-C16
29	h	101	DGD	O2G-C1B-C2B-C3B
26	b	622	LMG	O1-C7-C8-O7
26	c	518	LMG	C36-C37-C38-C39
28	A	411	LHG	C29-C30-C31-C32
22	c	505	CLA	CBA-CGA-O2A-C1
30	x	101	BCR	C35-C13-C14-C15
31	B	622	STE	C5-C6-C7-C8
22	b	601	CLA	CAA-CBA-CGA-O2A
22	A	405	CLA	C4-C3-C5-C6
22	d	403	CLA	C4-C3-C5-C6
25	a	409	PL9	C18-C19-C21-C22
22	B	612	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
28	D	410	LHG	C33-C34-C35-C36
31	b	624	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
34	F	101	HEC	CAD-CBD-CGD-O1D
34	F	101	HEC	C2A-CAA-CBA-CGA
26	d	410	LMG	O7-C10-C11-C12
31	x	102	STE	O1-C1-C2-C3
22	B	603	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
23	D	401	PHO	CAD-CBD-CGD-O2D
26	A	409	LMG	C7-C8-O7-C10
29	C	516	DGD	C4E-C5E-C6E-O5E
22	B	609	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
28	d	408	LHG	O9-C7-O7-C5
28	L	102	LHG	C11-C10-C9-C8
30	B	618	BCR	C6-C7-C8-C9
30	B	618	BCR	C22-C23-C24-C25
22	c	502	CLA	O1A-CGA-O2A-C1
31	C	519	STE	O1-C1-C2-C3
34	V	201	HEC	CAD-CBD-CGD-O2D
34	v	201	HEC	CAD-CBD-CGD-O2D
26	A	409	LMG	C39-C40-C41-C42
31	C	519	STE	C6-C7-C8-C9
22	B	607	CLA	C2-C3-C5-C6
28	a	411	LHG	O8-C23-C24-C25
29	C	517	DGD	O2G-C1B-C2B-C3B
29	c	516	DGD	O2G-C1B-C2B-C3B
22	C	507	CLA	CBD-CGD-O2D-CED
30	K	101	BCR	C7-C8-C9-C10
30	b	617	BCR	C11-C12-C13-C14
30	d	406	BCR	C21-C22-C23-C24
30	k	102	BCR	C11-C12-C13-C14
31	H	104	STE	C14-C15-C16-C17
31	b	626	STE	C11-C10-C9-C8
23	d	401	PHO	C2C-C3C-CAC-CBC
26	A	409	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
29	h	101	DGD	C1G-C2G-C3G-O3G
26	B	620	LMG	C17-C18-C19-C20
29	c	516	DGD	C9B-CAB-CBB-CCB
26	B	620	LMG	O10-C28-C29-C30
31	b	621	STE	O2-C1-C2-C3
34	V	201	HEC	CAD-CBD-CGD-O1D
22	H	101	CLA	O2A-C1-C2-C3
23	a	404	PHO	O2A-C1-C2-C3
29	A	413	DGD	C3B-C4B-C5B-C6B
31	d	411	STE	C6-C7-C8-C9
31	t	103	STE	O1-C1-C2-C3
31	t	103	STE	O2-C1-C2-C3
22	c	502	CLA	C13-C15-C16-C17
22	b	616	CLA	C11-C12-C13-C15
31	B	623	STE	C13-C14-C15-C16
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D
22	B	604	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	D	404	CLA	CHA-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O2D
30	C	515	BCR	C15-C16-C17-C18
31	x	102	STE	O2-C1-C2-C3
34	F	101	HEC	CAD-CBD-CGD-O2D
22	c	502	CLA	CBA-CGA-O2A-C1
22	b	615	CLA	C2-C3-C5-C6
22	b	605	CLA	C10-C11-C12-C13
28	b	623	LHG	O6-C4-C5-C6
31	b	624	STE	O2-C1-C2-C3
29	C	516	DGD	C9B-CAB-CBB-CCB
29	c	515	DGD	C9A-CAA-CBA-CCA
27	D	409	SQD	C44-C45-C46-O48
22	B	601	CLA	C15-C16-C17-C18
26	m	101	LMG	O8-C28-C29-C30
34	v	201	HEC	CAD-CBD-CGD-O1D
22	B	601	CLA	C10-C11-C12-C13
22	B	607	CLA	C13-C15-C16-C17
26	B	620	LMG	C16-C17-C18-C19
22	c	509	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	D	413	LHG	O10-C23-C24-C25
22	C	511	CLA	C3-C5-C6-C7
31	L	103	STE	C4-C5-C6-C7
22	B	602	CLA	C11-C10-C8-C7
23	a	404	PHO	C6-C7-C8-C10
29	C	518	DGD	CAB-CBB-CCB-CDB
31	a	413	STE	C9-C10-C11-C12
31	H	104	STE	C15-C16-C17-C18
22	C	505	CLA	C6-C7-C8-C9
22	b	612	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	508	CLA	C11-C12-C13-C14
30	b	619	BCR	C9-C10-C11-C12
30	c	514	BCR	C15-C16-C17-C18
26	M	101	LMG	C20-C21-C22-C23
27	B	621	SQD	C27-C28-C29-C30
27	D	409	SQD	C32-C33-C34-C35
26	B	620	LMG	O7-C10-C11-C12
22	C	503	CLA	C10-C11-C12-C13
27	L	101	SQD	C5-C6-S-O8
31	C	521	STE	C3-C4-C5-C6
22	B	612	CLA	CAA-CBA-CGA-O2A
28	L	102	LHG	O7-C7-C8-C9
31	X	101	STE	C15-C16-C17-C18
28	d	409	LHG	C9-C10-C11-C12
29	c	517	DGD	O1G-C1A-C2A-C3A
22	c	505	CLA	CBD-CGD-O2D-CED
30	C	514	BCR	C11-C12-C13-C14
22	c	507	CLA	CBA-CGA-O2A-C1
22	b	604	CLA	C8-C10-C11-C12
22	b	601	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C1A-C2A-CAA-CBA
22	b	602	CLA	C1A-C2A-CAA-CBA
22	b	604	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
31	M	103	STE	C1-C2-C3-C4
31	M	104	STE	C7-C8-C9-C10
22	C	501	CLA	C16-C17-C18-C20
26	d	410	LMG	O9-C10-C11-C12
28	A	411	LHG	C30-C31-C32-C33
22	B	612	CLA	C2-C1-O2A-CGA
22	c	512	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	CAA-CBA-CGA-O1A
26	Y	101	LMG	O9-C10-C11-C12
27	a	410	SQD	O49-C7-C8-C9
29	c	515	DGD	O1B-C1B-C2B-C3B
29	c	515	DGD	C1G-C2G-C3G-O3G
22	b	601	CLA	C2C-C3C-CAC-CBC
31	I	102	STE	C7-C8-C9-C10
22	b	601	CLA	CAA-CBA-CGA-O1A
22	B	605	CLA	C10-C11-C12-C13
22	c	503	CLA	C8-C10-C11-C12
22	c	512	CLA	C5-C6-C7-C8
28	D	411	LHG	C2-C3-O3-P
31	B	625	STE	C2-C3-C4-C5
28	d	409	LHG	C32-C33-C34-C35
22	c	507	CLA	O1A-CGA-O2A-C1
31	b	626	STE	C15-C16-C17-C18
28	D	410	LHG	C4-O6-P-O5
28	L	102	LHG	C3-O3-P-O5
28	L	102	LHG	C4-O6-P-O5
28	d	408	LHG	C4-O6-P-O5
26	b	622	LMG	O10-C28-C29-C30
27	A	410	SQD	O49-C7-C8-C9
30	K	102	BCR	C23-C24-C25-C26
30	b	617	BCR	C23-C24-C25-C26
22	b	603	CLA	C16-C17-C18-C20
30	H	102	BCR	C10-C11-C12-C13
30	K	102	BCR	C10-C11-C12-C13
22	B	602	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
31	b	624	STE	C5-C6-C7-C8
22	C	506	CLA	C13-C15-C16-C17
26	Y	101	LMG	C30-C31-C32-C33
28	d	409	LHG	O10-C23-C24-C25
25	A	408	PL9	C21-C22-C23-C24
22	B	608	CLA	CAD-CBD-CGD-O1D
27	B	621	SQD	C5-C6-S-O9
28	b	623	LHG	O10-C23-O8-C6
28	a	411	LHG	O10-C23-C24-C25
28	b	623	LHG	O8-C23-C24-C25
22	B	602	CLA	C11-C10-C8-C9
22	B	612	CLA	C6-C7-C8-C9
22	c	505	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	a	404	PHO	C6-C7-C8-C9
28	d	408	LHG	C13-C14-C15-C16
31	B	623	STE	C9-C10-C11-C12
31	R	101	STE	O1-C1-C2-C3
31	j	101	STE	O1-C1-C2-C3
26	c	521	LMG	C16-C17-C18-C19
26	b	622	LMG	O7-C10-C11-C12
26	b	622	LMG	O8-C28-C29-C30
29	C	517	DGD	O1G-C1A-C2A-C3A
29	c	515	DGD	O2G-C1B-C2B-C3B
31	C	520	STE	C15-C16-C17-C18
26	c	520	LMG	C38-C39-C40-C41
26	A	409	LMG	C40-C41-C42-C43
31	d	411	STE	C11-C10-C9-C8
22	A	402	CLA	C12-C13-C15-C16
22	A	405	CLA	C2-C3-C5-C6
22	B	608	CLA	C11-C12-C13-C15
22	B	612	CLA	C6-C7-C8-C10
22	B	613	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	H	101	CLA	C3A-C2A-CAA-CBA
22	a	405	CLA	C12-C13-C15-C16
22	b	612	CLA	C11-C10-C8-C7
22	c	504	CLA	C11-C10-C8-C7
22	c	505	CLA	C12-C13-C15-C16
22	c	508	CLA	C11-C12-C13-C15
22	c	511	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C10-C8-C7
25	a	409	PL9	C23-C24-C26-C27
28	D	411	LHG	O10-C23-C24-C25
28	a	411	LHG	O9-C7-C8-C9
22	H	101	CLA	CAA-CBA-CGA-O2A
22	c	510	CLA	CAA-CBA-CGA-O2A
27	A	410	SQD	O47-C7-C8-C9
30	B	616	BCR	C11-C12-C13-C14
29	h	101	DGD	O1A-C1A-C2A-C3A
27	L	101	SQD	C15-C16-C17-C18
22	b	613	CLA	CAA-CBA-CGA-O2A
22	B	615	CLA	C4C-C3C-CAC-CBC
31	R	101	STE	O2-C1-C2-C3
27	L	101	SQD	C10-C11-C12-C13
22	b	614	CLA	CAA-CBA-CGA-O2A

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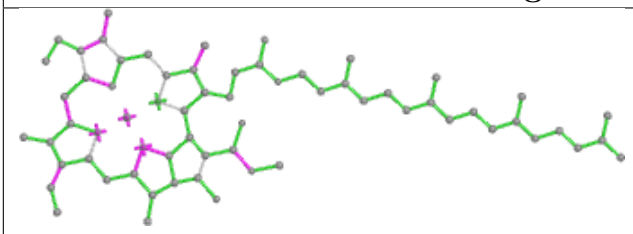
Mol	Chain	Res	Type	Atoms
27	B	621	SQD	O47-C7-C8-C9
25	d	407	PL9	C37-C38-C39-C40
31	j	101	STE	O2-C1-C2-C3
27	B	621	SQD	C26-C27-C28-C29
22	C	509	CLA	C5-C6-C7-C8
26	c	518	LMG	C29-C28-O8-C9
22	D	404	CLA	C4C-C3C-CAC-CBC
22	b	608	CLA	C4C-C3C-CAC-CBC
28	b	623	LHG	C25-C26-C27-C28
22	H	101	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	CAA-CBA-CGA-O2A
22	c	505	CLA	CAA-CBA-CGA-O2A
22	C	509	CLA	C8-C10-C11-C12

There are no ring outliers.

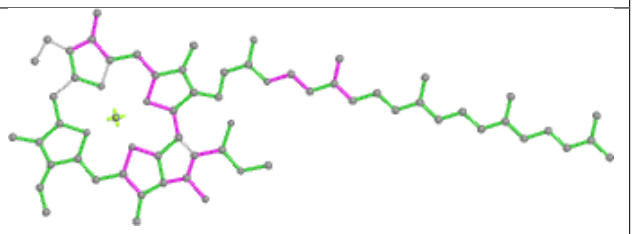
No monomer is involved in short contacts.

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

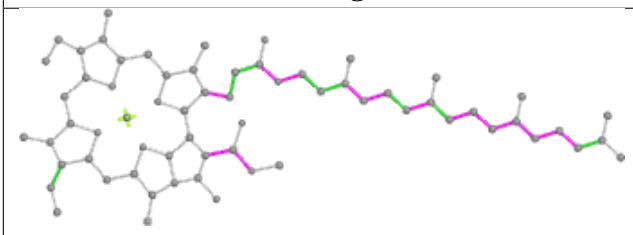
Ligand CLA C 506



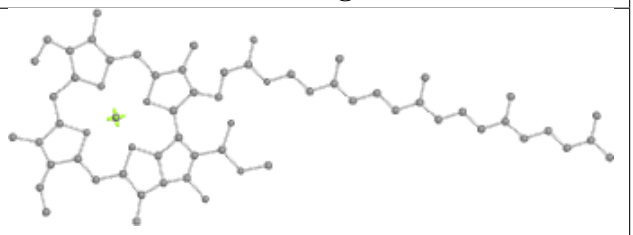
Bond lengths



Bond angles

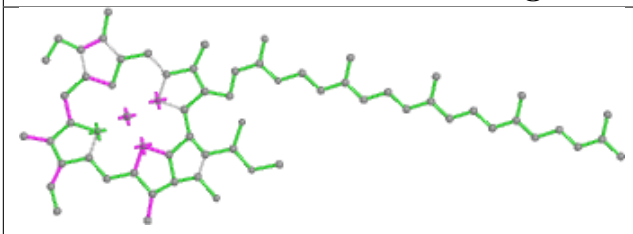


Torsions



Rings

Ligand CLA C 501



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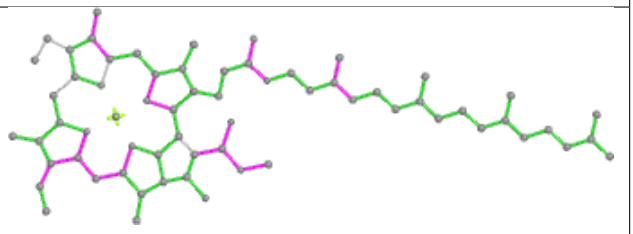

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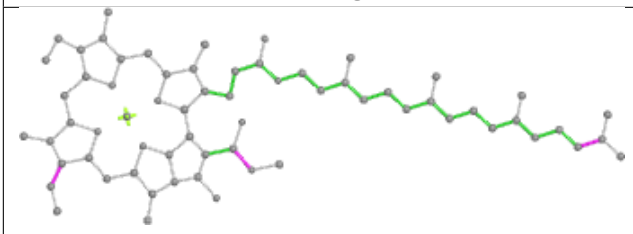

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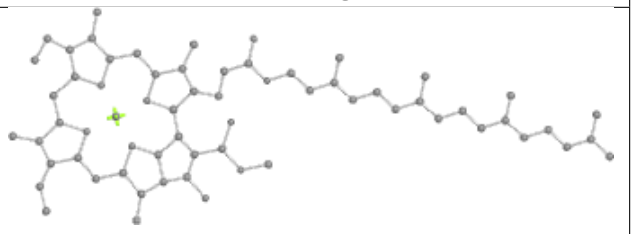
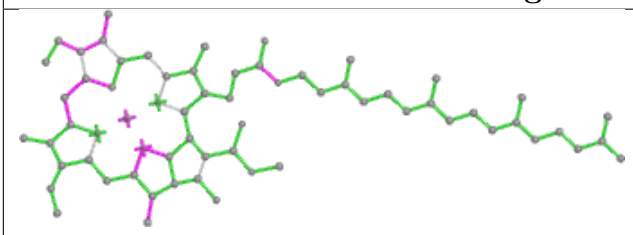


Rings

Ligand CLA B 614



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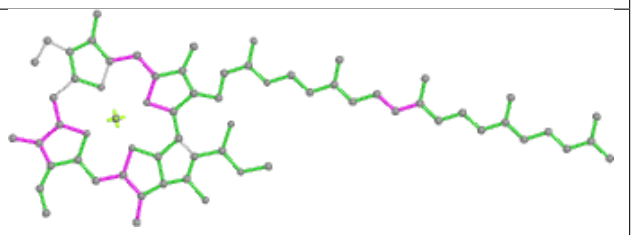
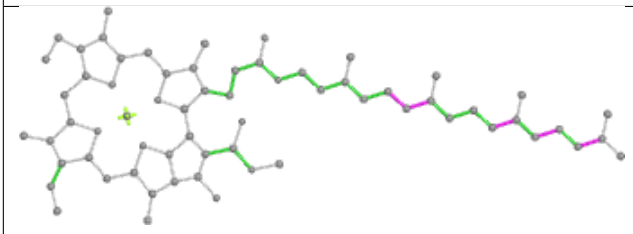
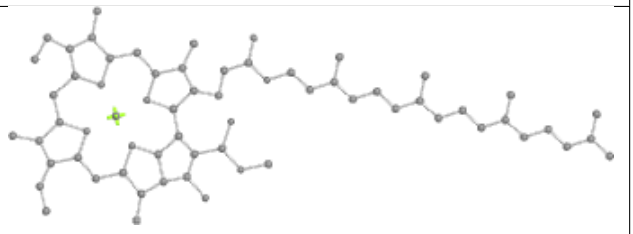


Bond angles



Torsions



Rings

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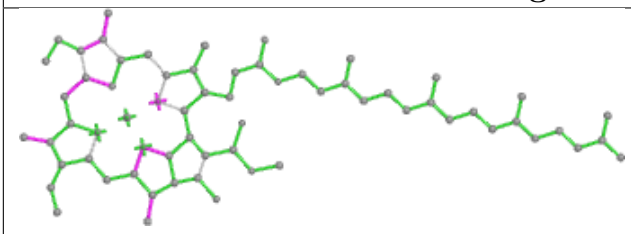

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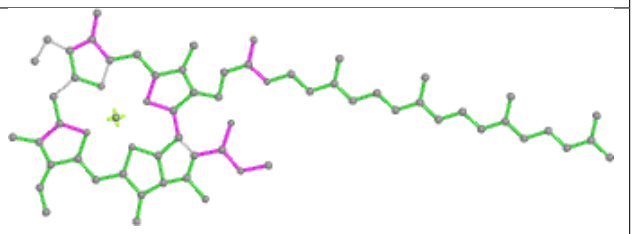

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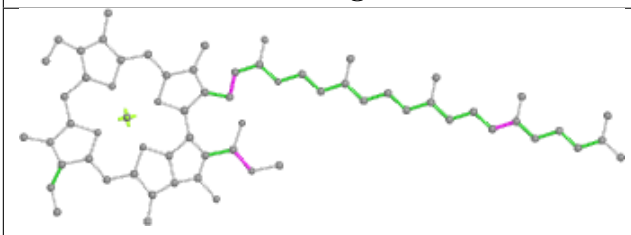

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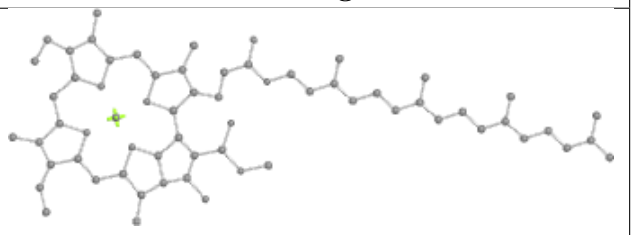
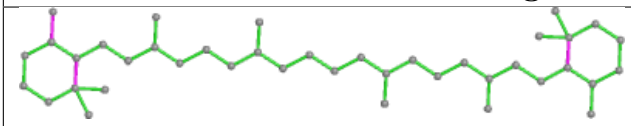


Rings

Ligand BCR B 616



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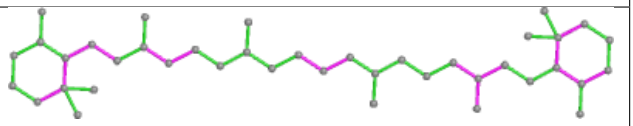

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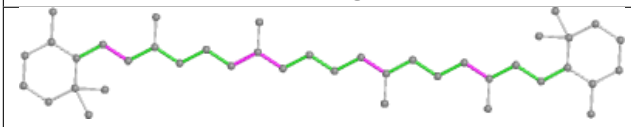
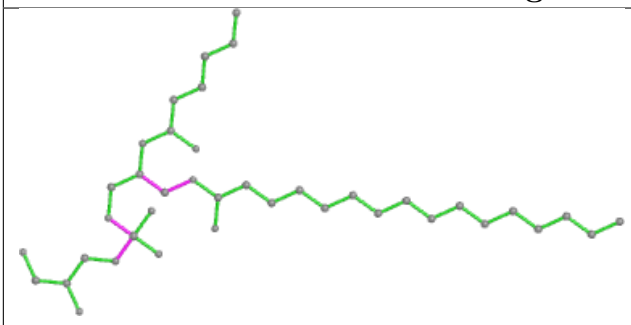


Torsions

Rings

Ligand LHG d 409



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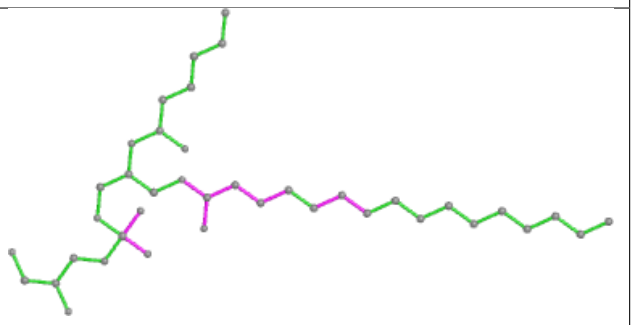

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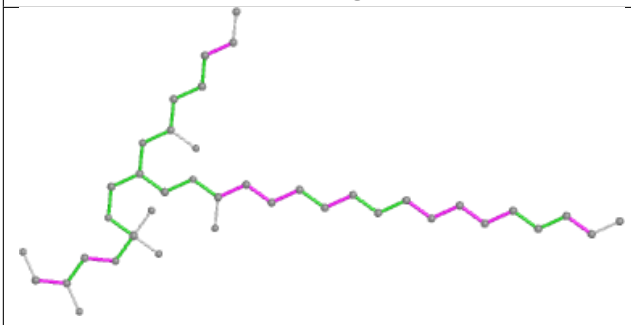

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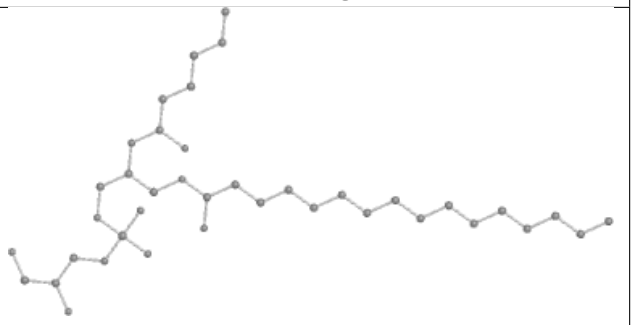
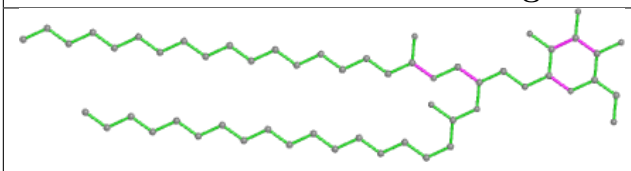


Rings

Ligand LMG b 622



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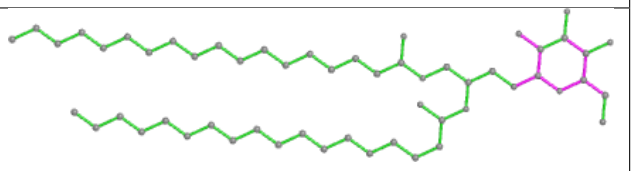

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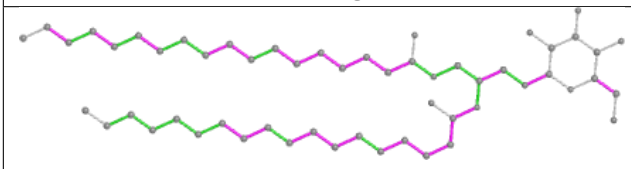

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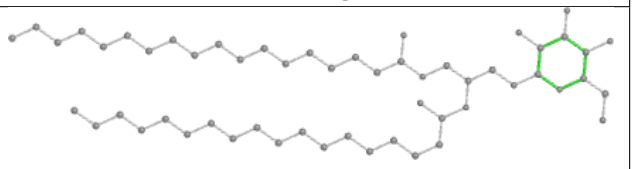
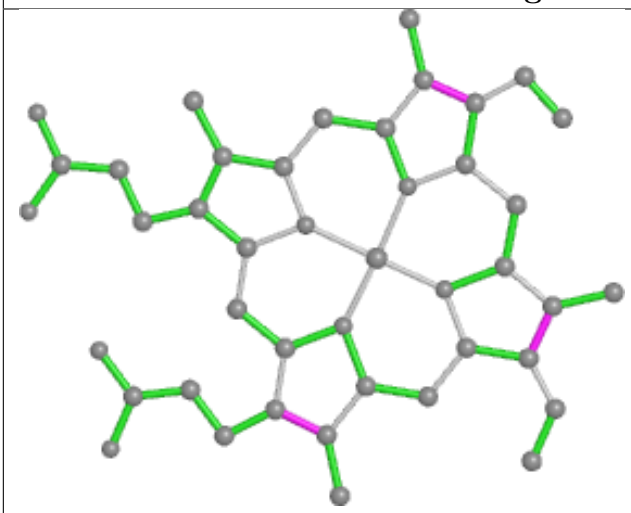


Rings

Ligand HEC F 101



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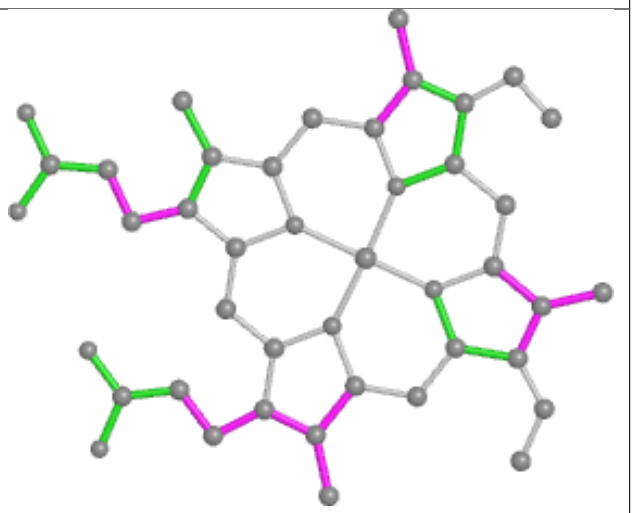

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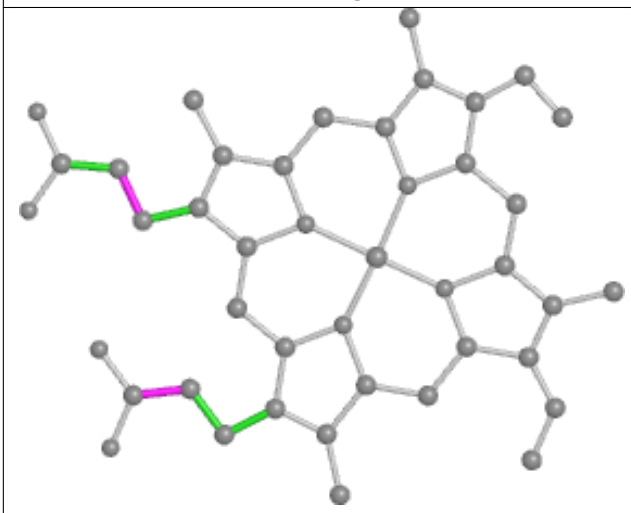

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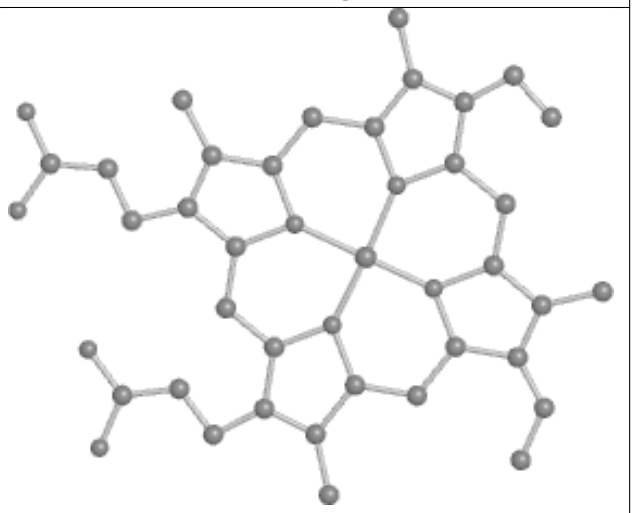
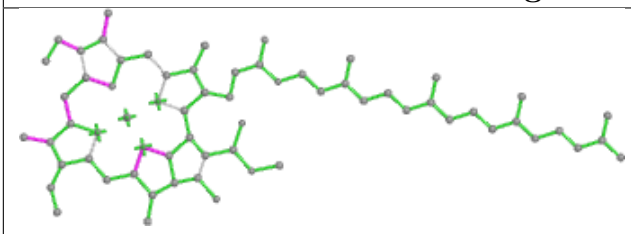


Rings

Ligand CLA C 505



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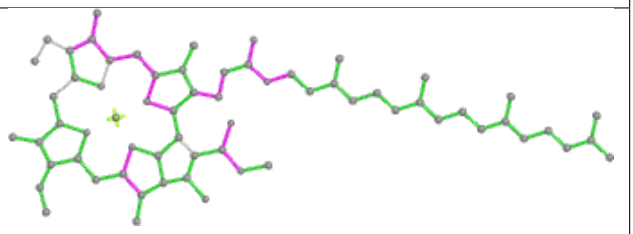

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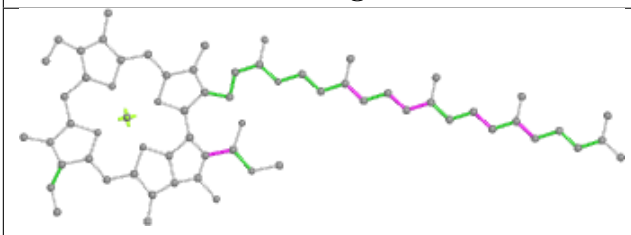

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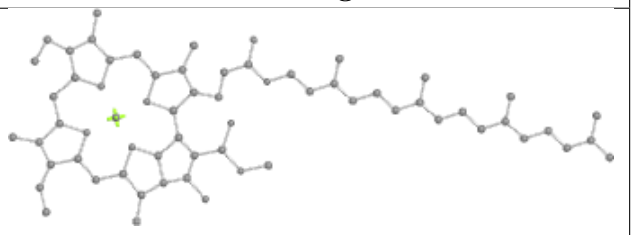
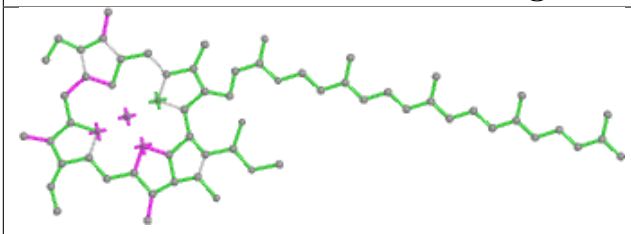


Rings

Ligand CLA a 405



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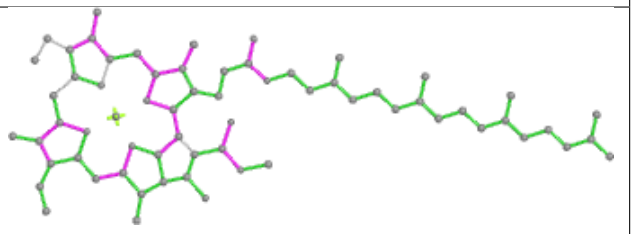

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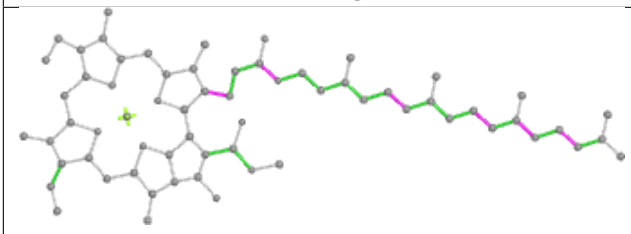

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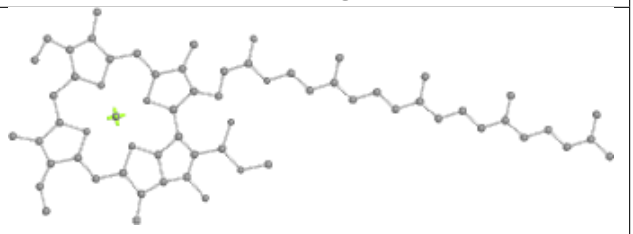

Rings

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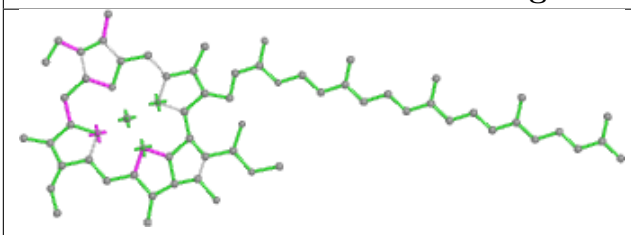

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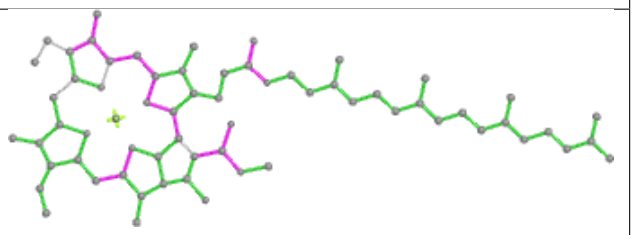

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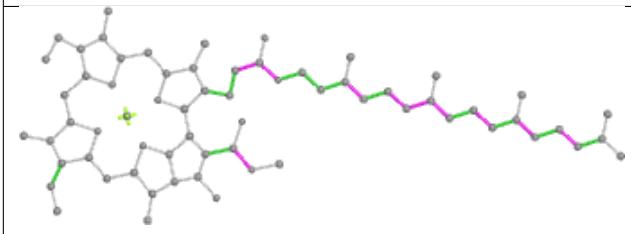

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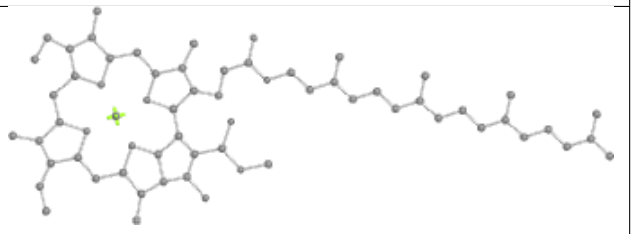
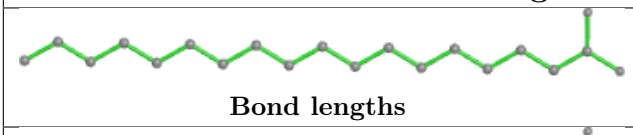


Rings

Ligand STE b 621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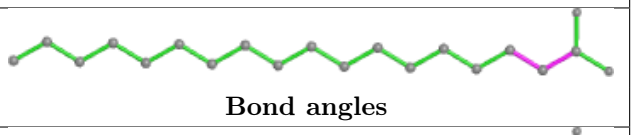
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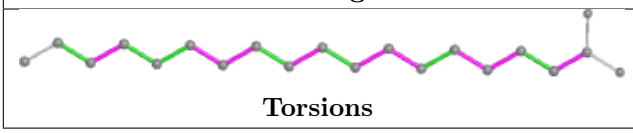
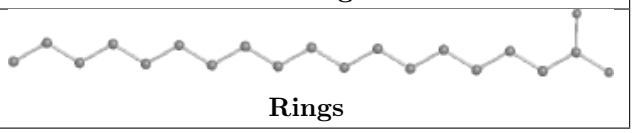
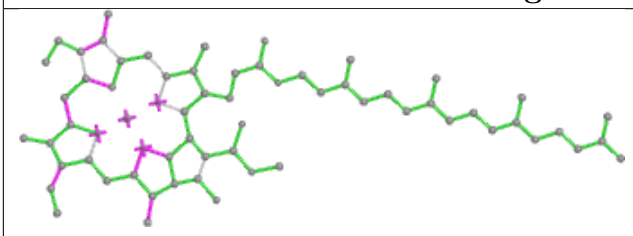
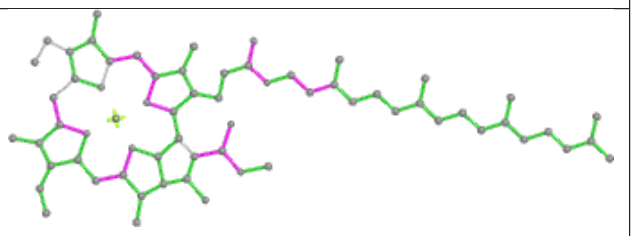
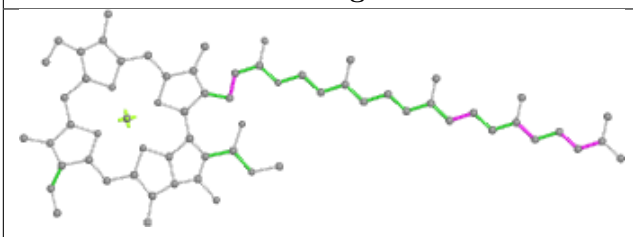

Torsions


Rings

Ligand CLA B 609


Bond lengths


Bond angles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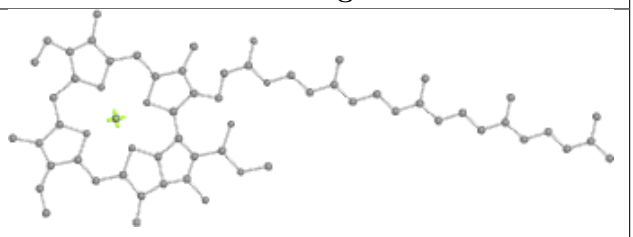
Rings

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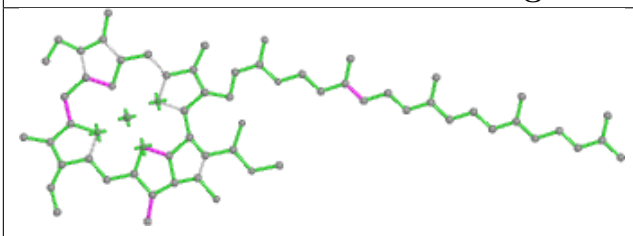
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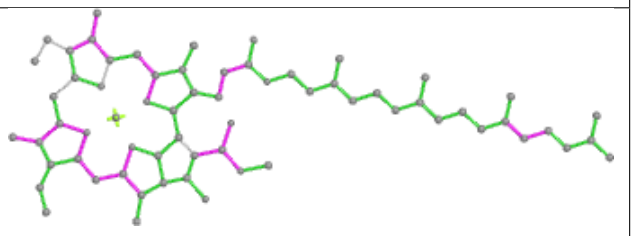
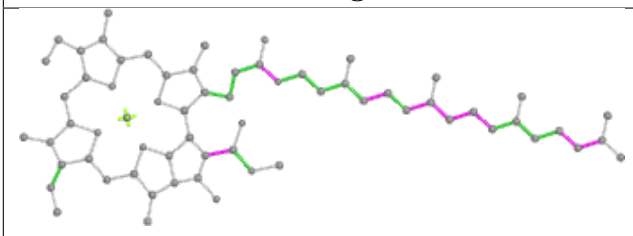
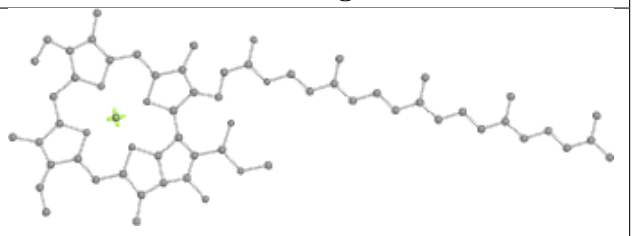
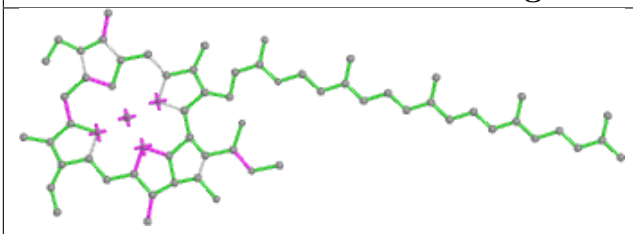

Bond angles


Torsions


Rings

Ligand CLA C 509



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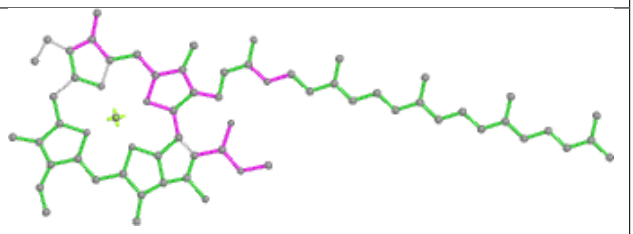
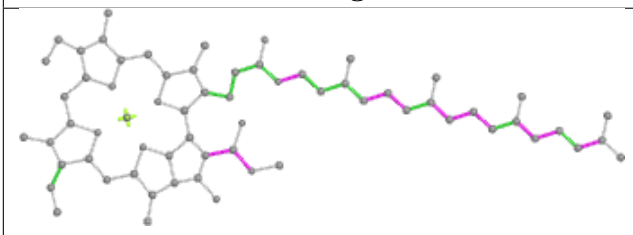


Bond angles



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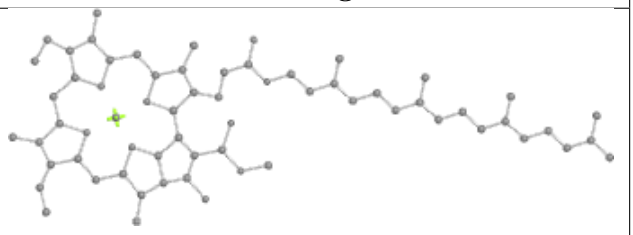
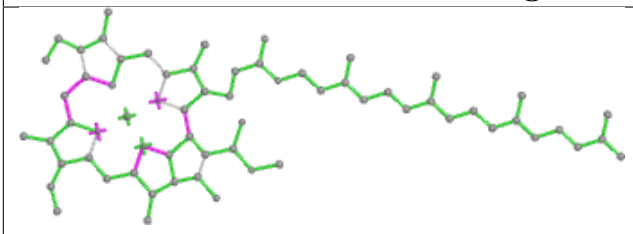


Rings

Ligand CLA D 403



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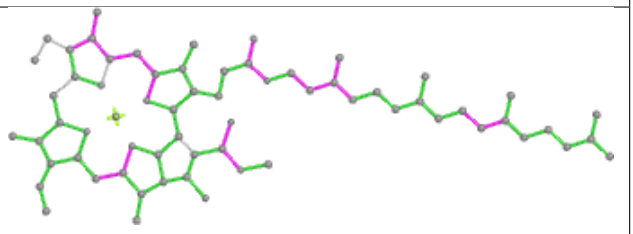
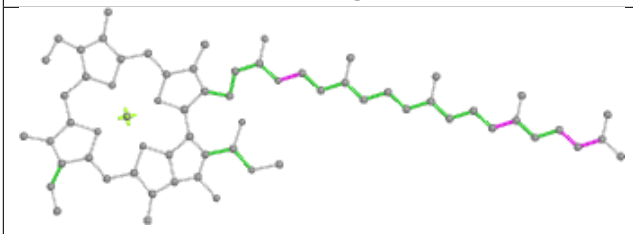


Bond angles



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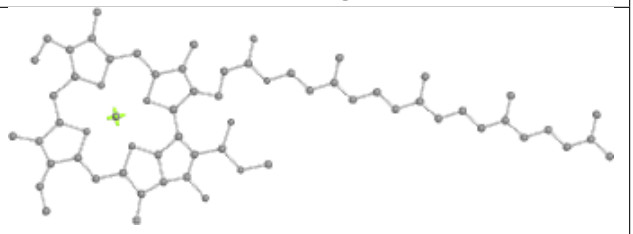
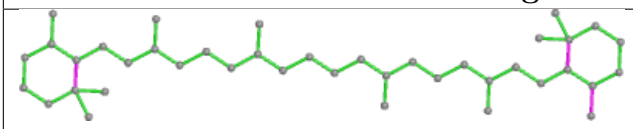


Rings

Ligand BCR D 406



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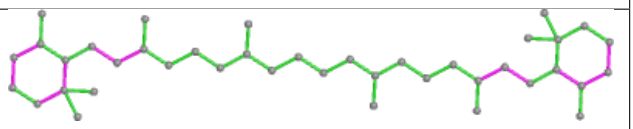
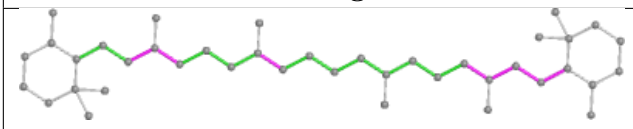


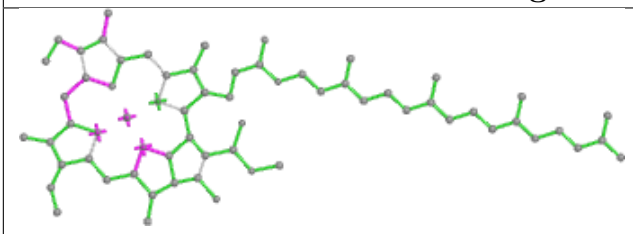
Bond angles



Torsions

Rings

Ligand CLA c 509



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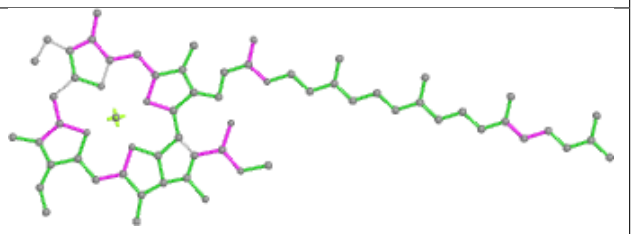

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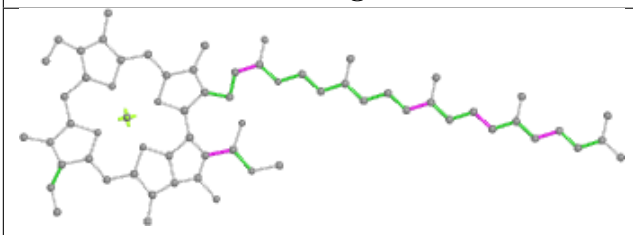

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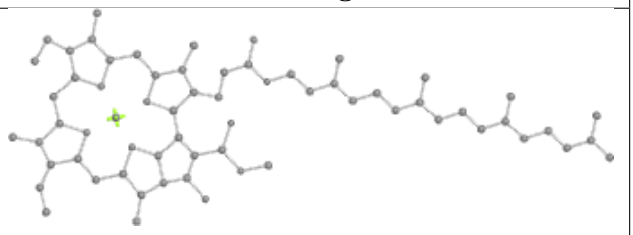
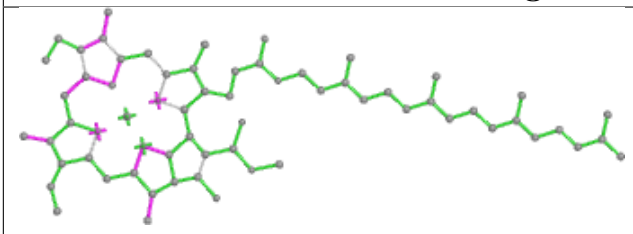


Rings

Ligand CLA C 511



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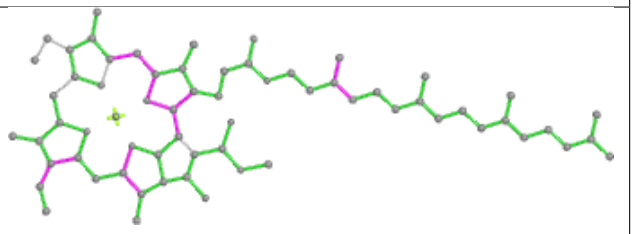

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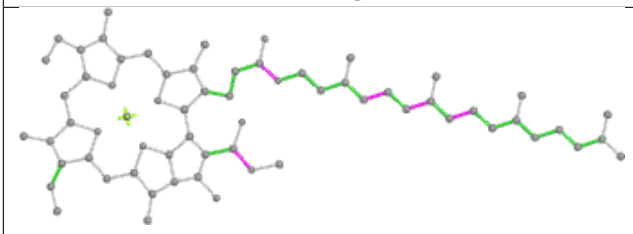

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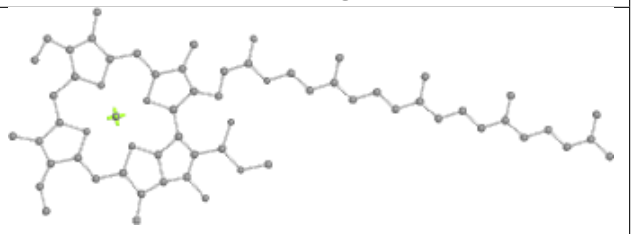
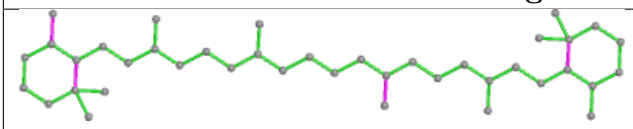


Rings

Ligand BCR b 618



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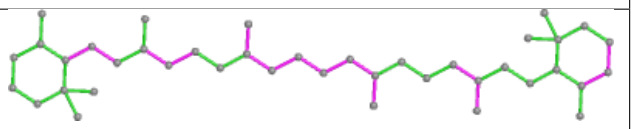

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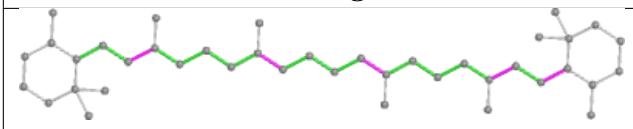
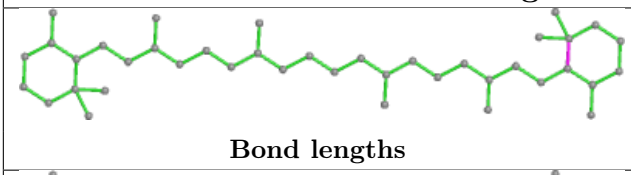


Torsions

Rings

Ligand BCR H 102



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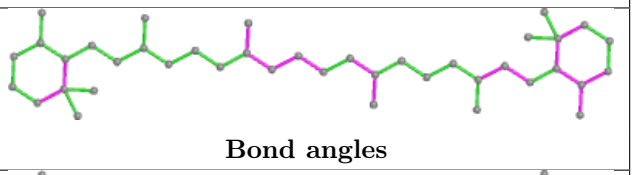

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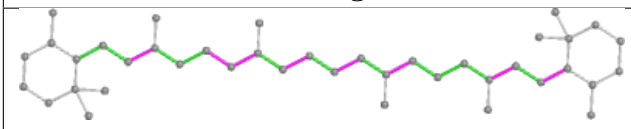

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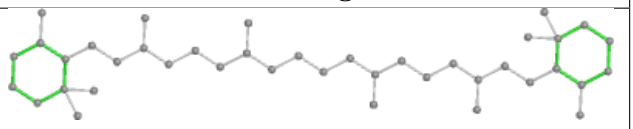
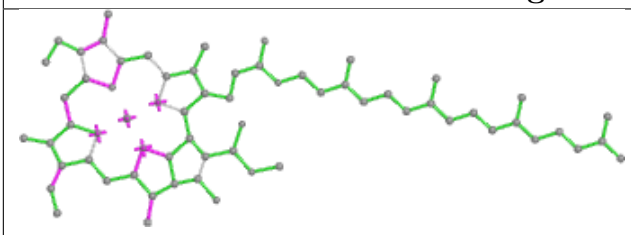


Rings

Ligand CLA b 615



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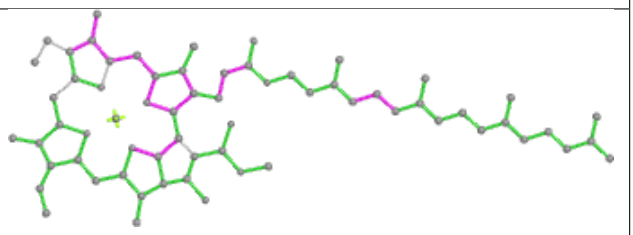
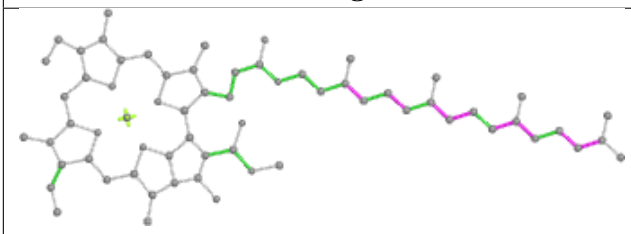


Bond angles



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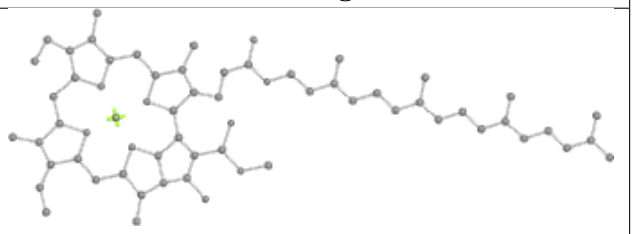
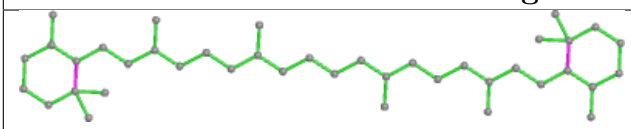


Rings

Ligand BCR K 101



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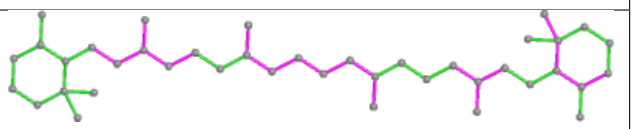
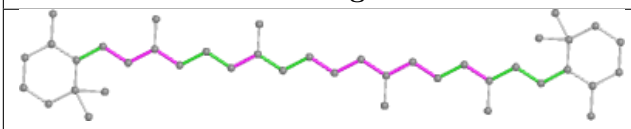


Bond angles



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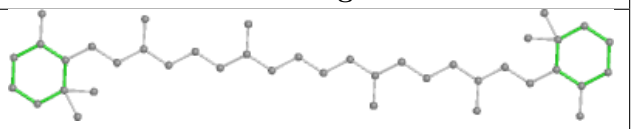
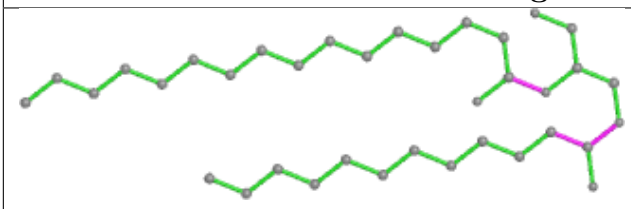


Rings

Ligand SQD t 102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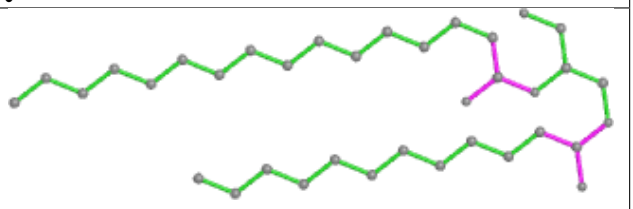
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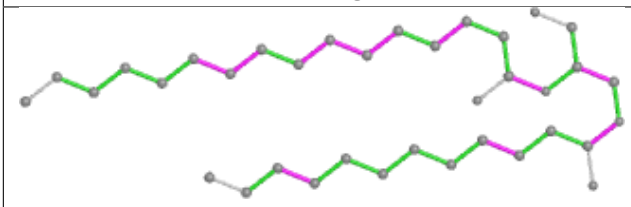
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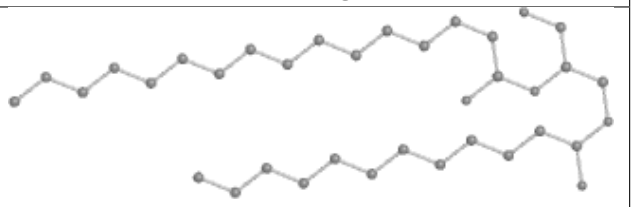
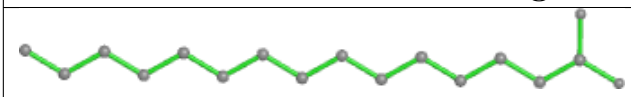

Rings

Ligand STE d 411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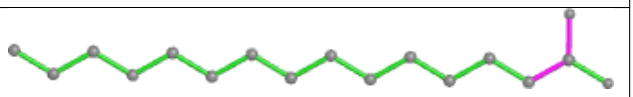
Bond angles

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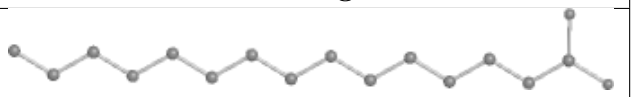
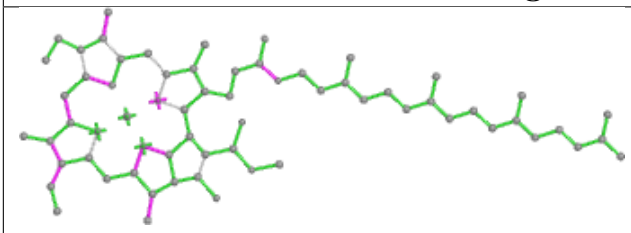

Rings

Ligand CLA C 510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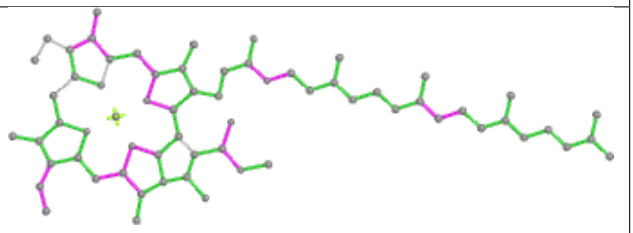
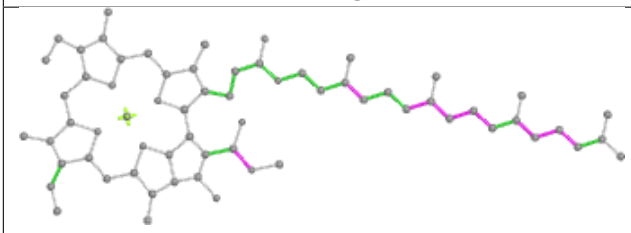

Bond angles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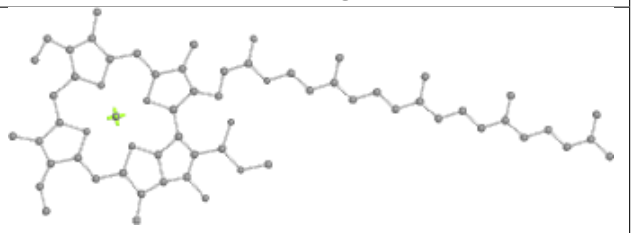
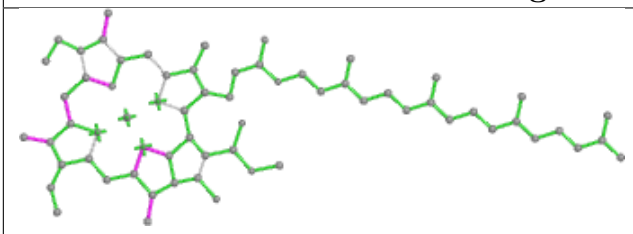
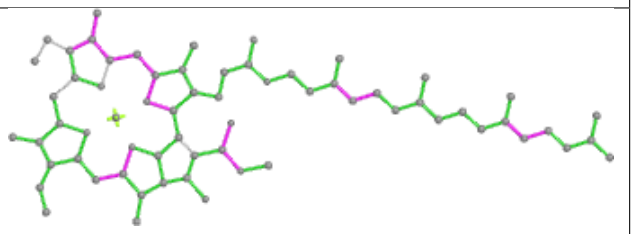

Rings

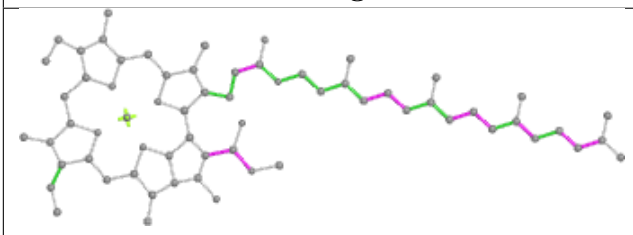
Ligand CLA c 510



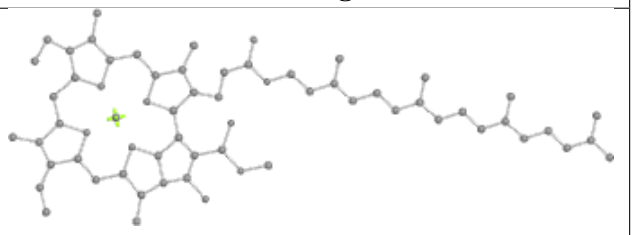
Bond lengths



Bond angles

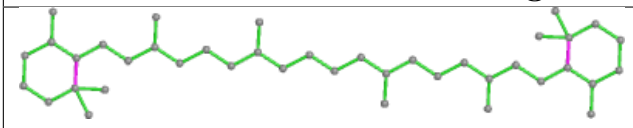


Torsions

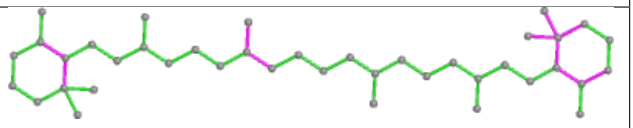


Rings

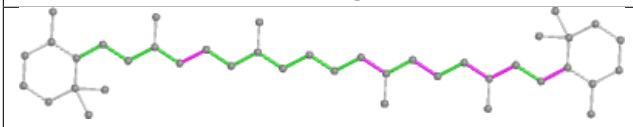
Ligand BCR k 103



Bond lengths



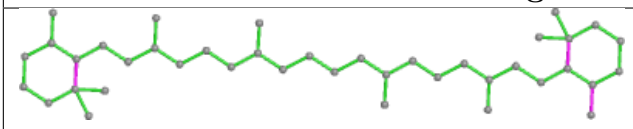
Bond angles



Torsions

Rings

Ligand BCR a 406



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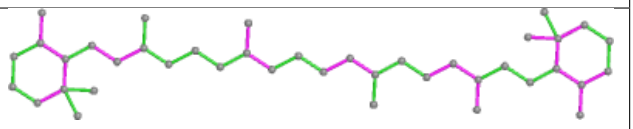
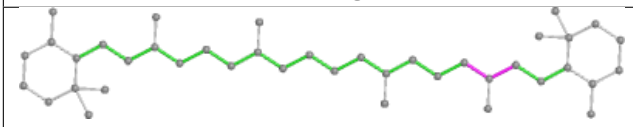


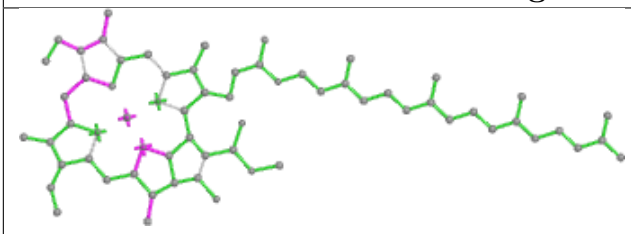
Bond angles



Torsions

Rings

Ligand CLA a 403



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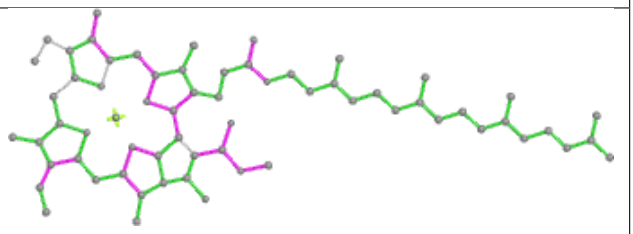
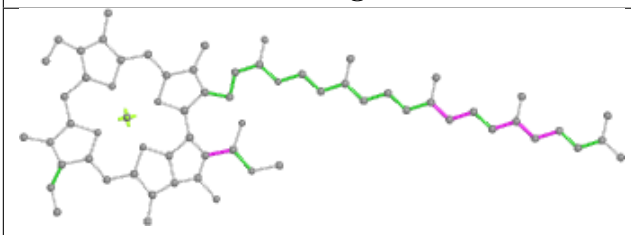
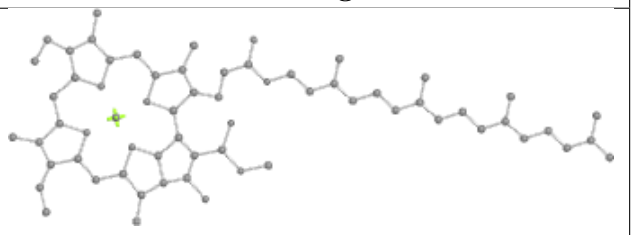


Bond angles

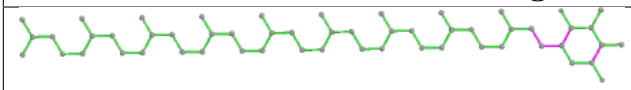


Torsions



Rings

Ligand PL9 A 408



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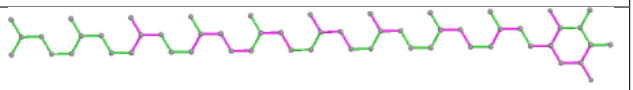
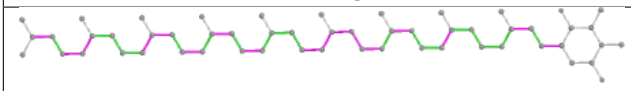
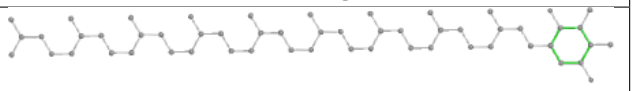


Bond angles

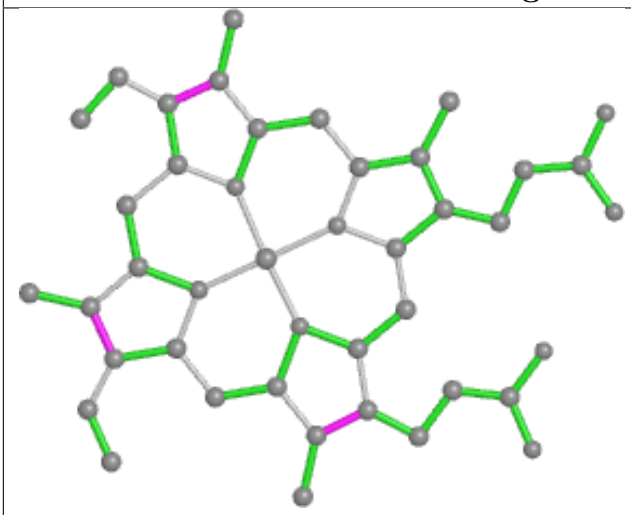


Torsions

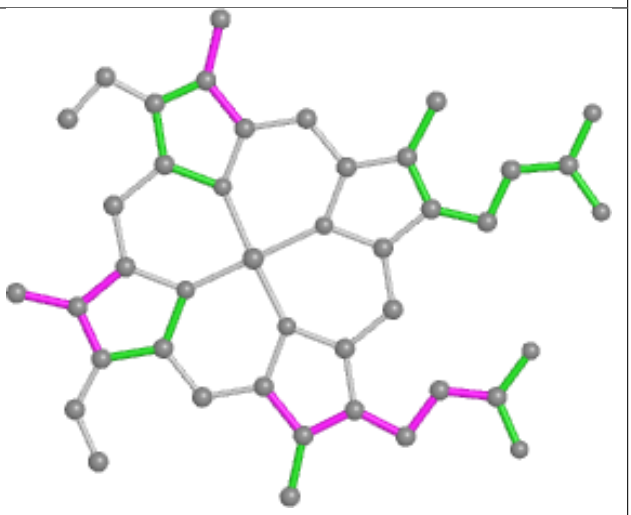


Rings

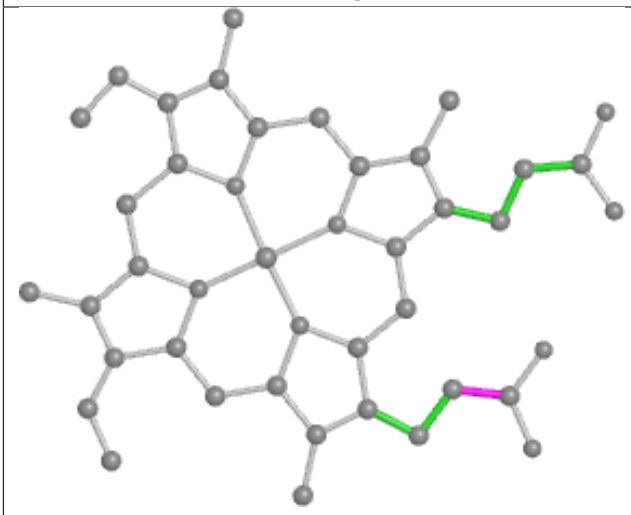
Ligand HEC V 201



Bond lengths



Bond angles



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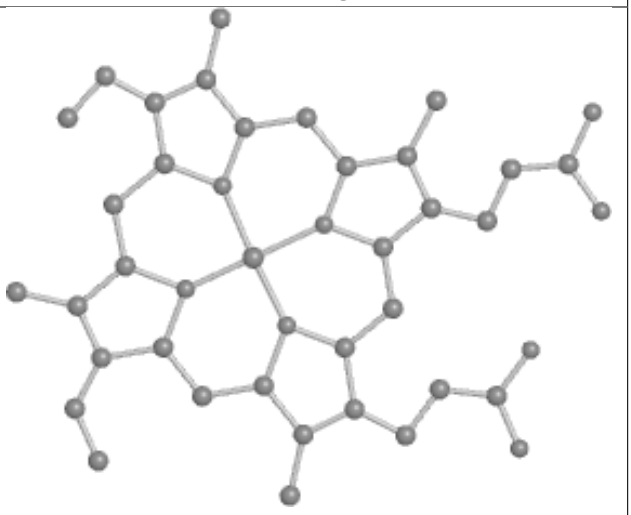
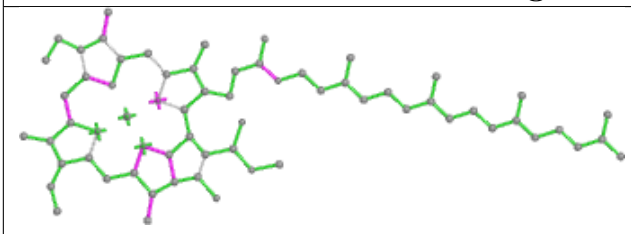


Rings

Ligand CLA b 601



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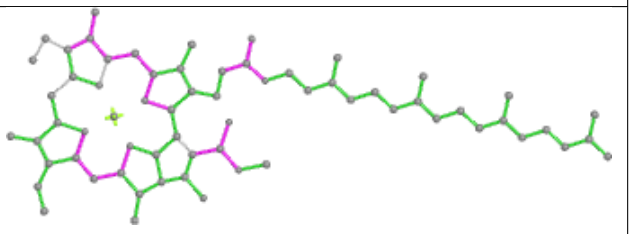
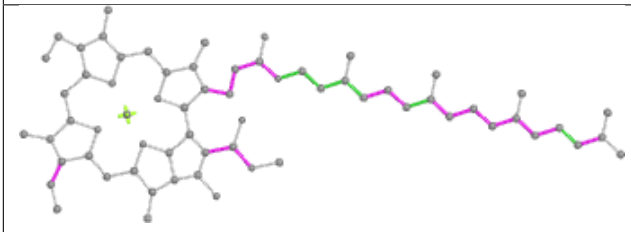
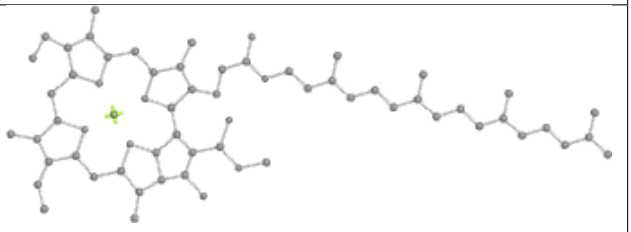


Bond angles

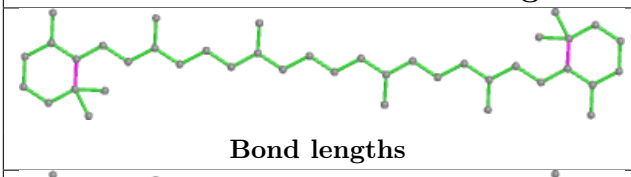


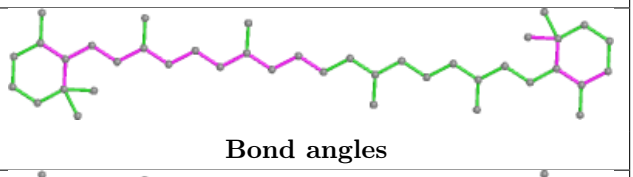
Torsions

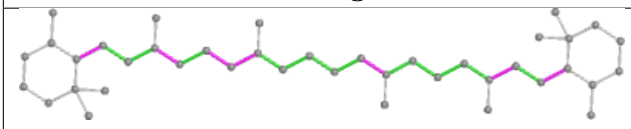


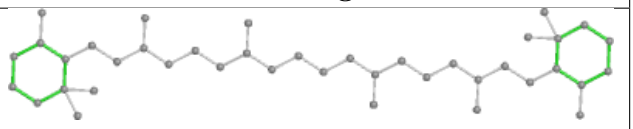
Rings

Ligand BCR K 102

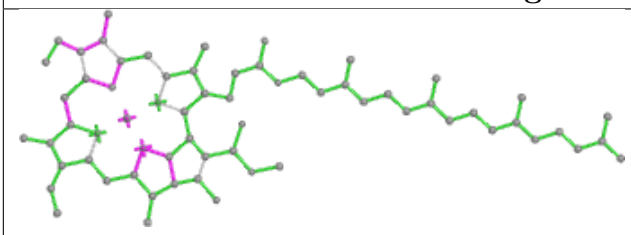

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA C 507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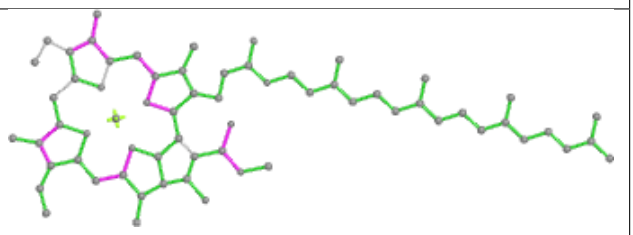
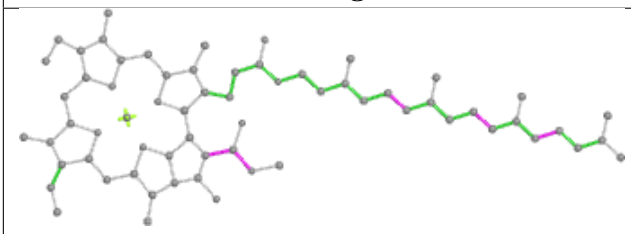
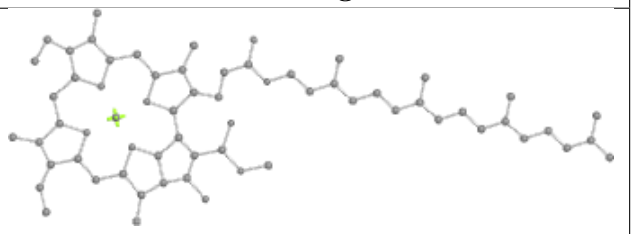

Bond angles

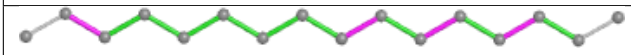

Torsions

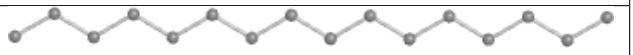

Rings

Ligand STE C 520

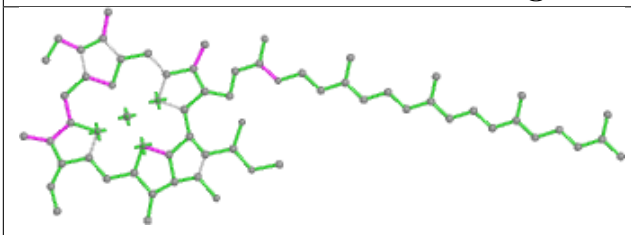
Bond lengths

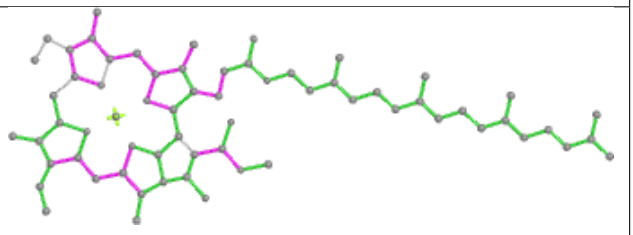
Bond angles

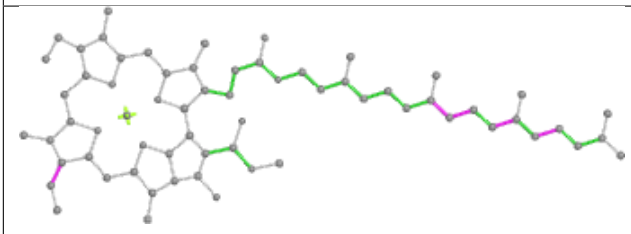

Torsions


Rings

Ligand CLA b 608


Bond lengths


Bond angles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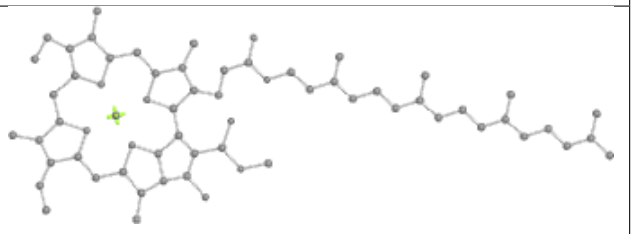
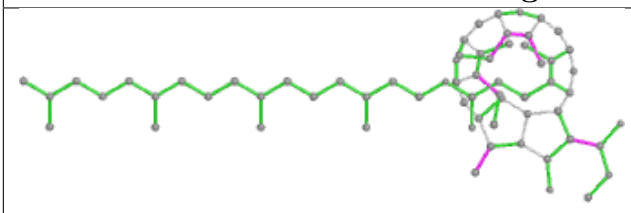

Rings

Ligand PHO D 401



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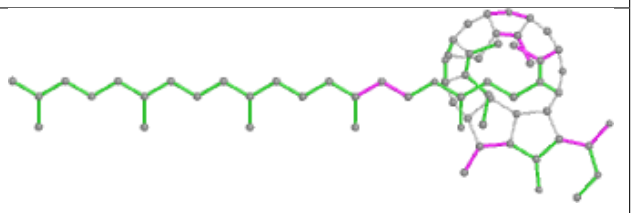
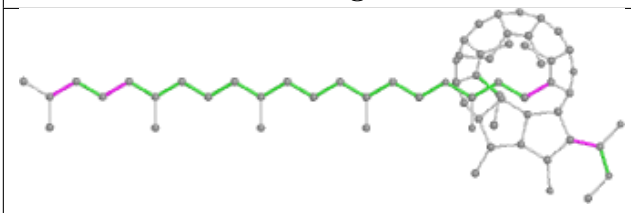
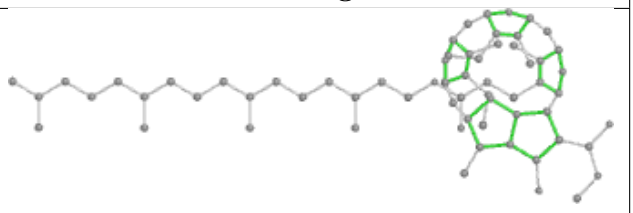


Bond angles

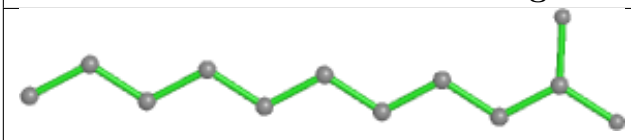


Torsions



Rings

Ligand STE L 103



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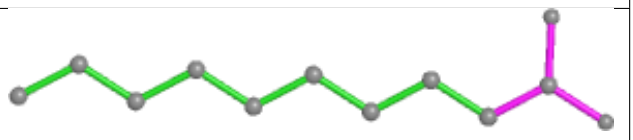
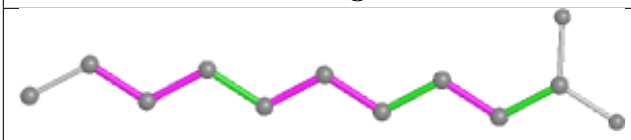
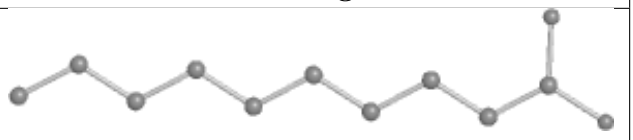


Bond angles

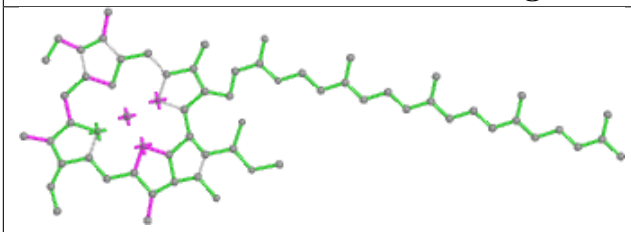


Torsions

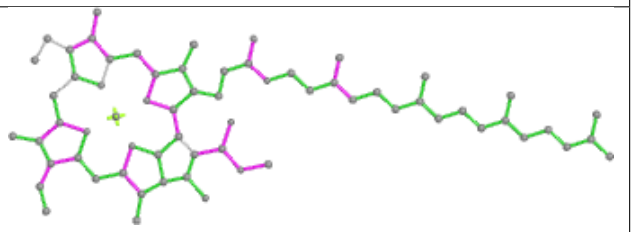


Rings

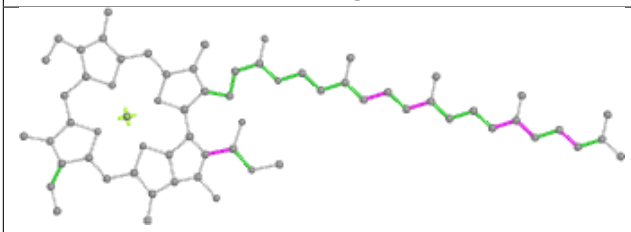
Ligand CLA A 403



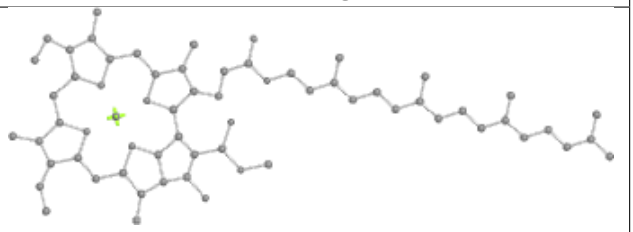
Bond lengths



Bond angles

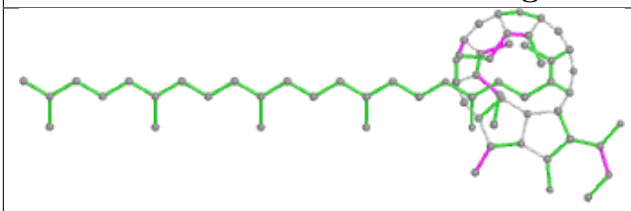


Torsions

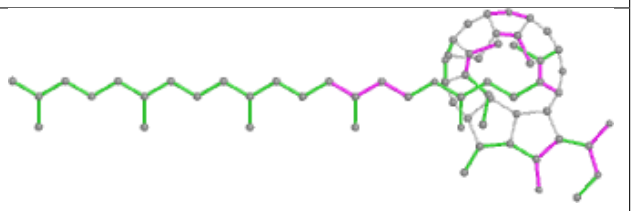


Rings

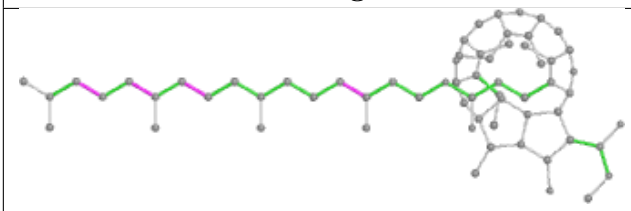
Ligand PHO A 404



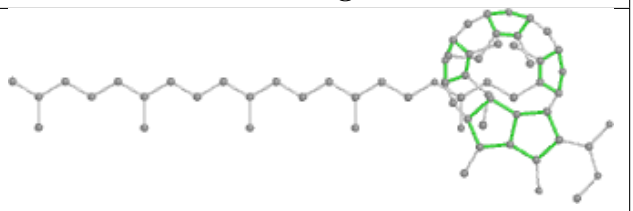
Bond lengths



Bond angles

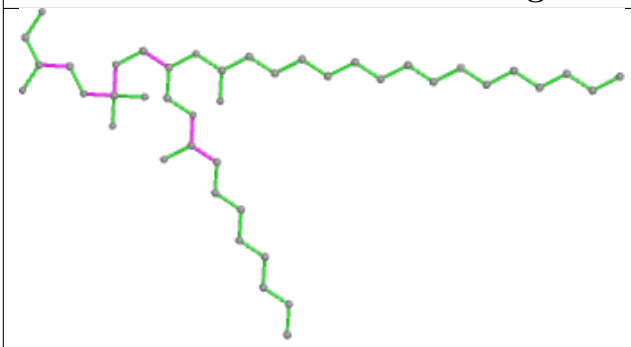


Torsions

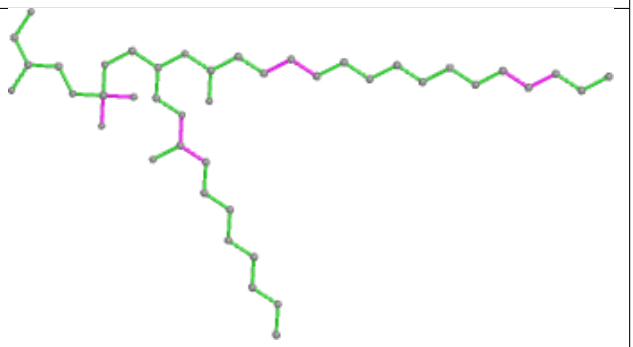


Rings

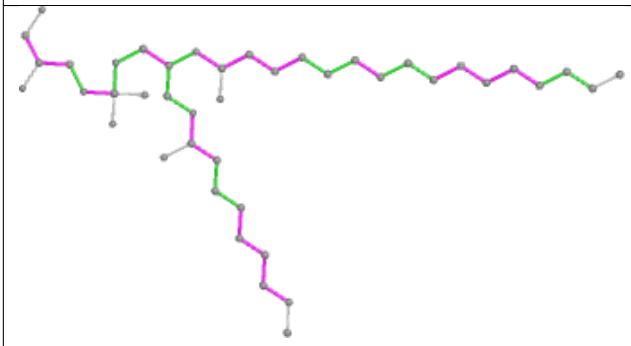
Ligand LHG a 411



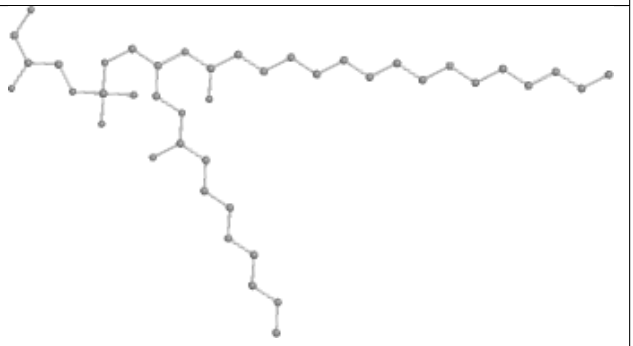
Bond lengths



Bond angles

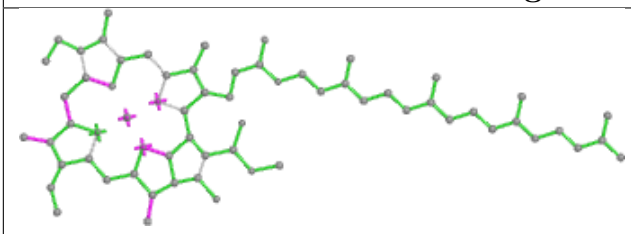


Torsions

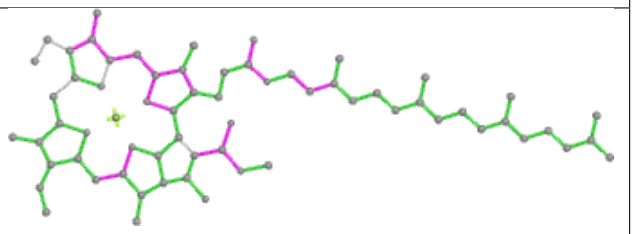


Rings

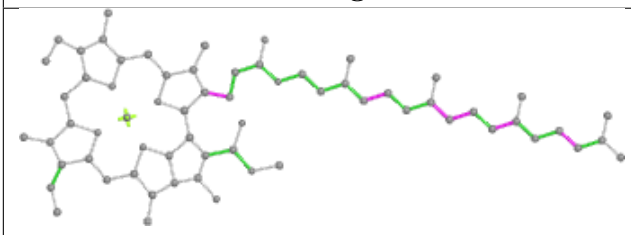
Ligand CLA C 512



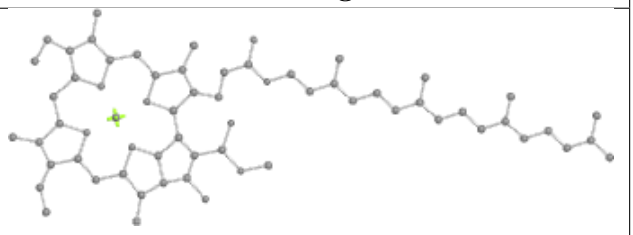
Bond lengths



Bond angles



Torsions



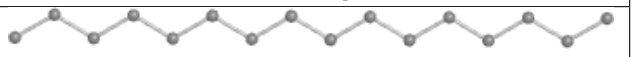
Rings

Ligand STE B 624

Bond lengths

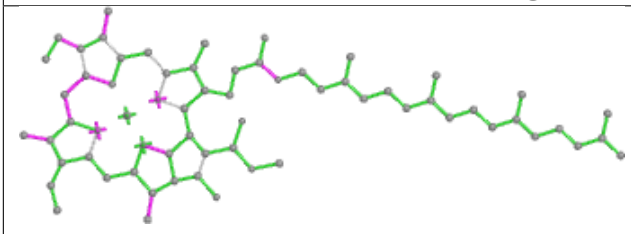
Bond angles

Torsions

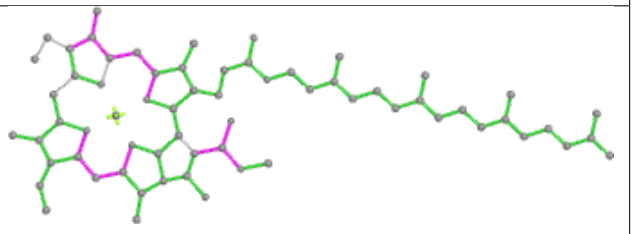


Rings

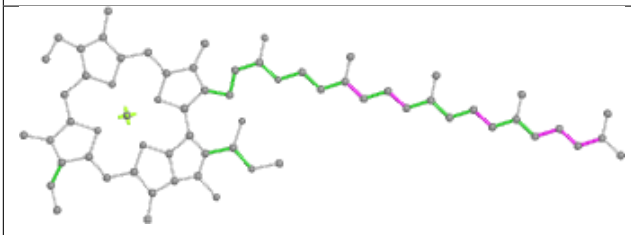
Ligand CLA B 607



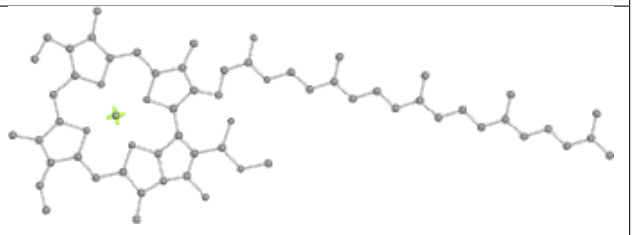
Bond lengths



Bond angles

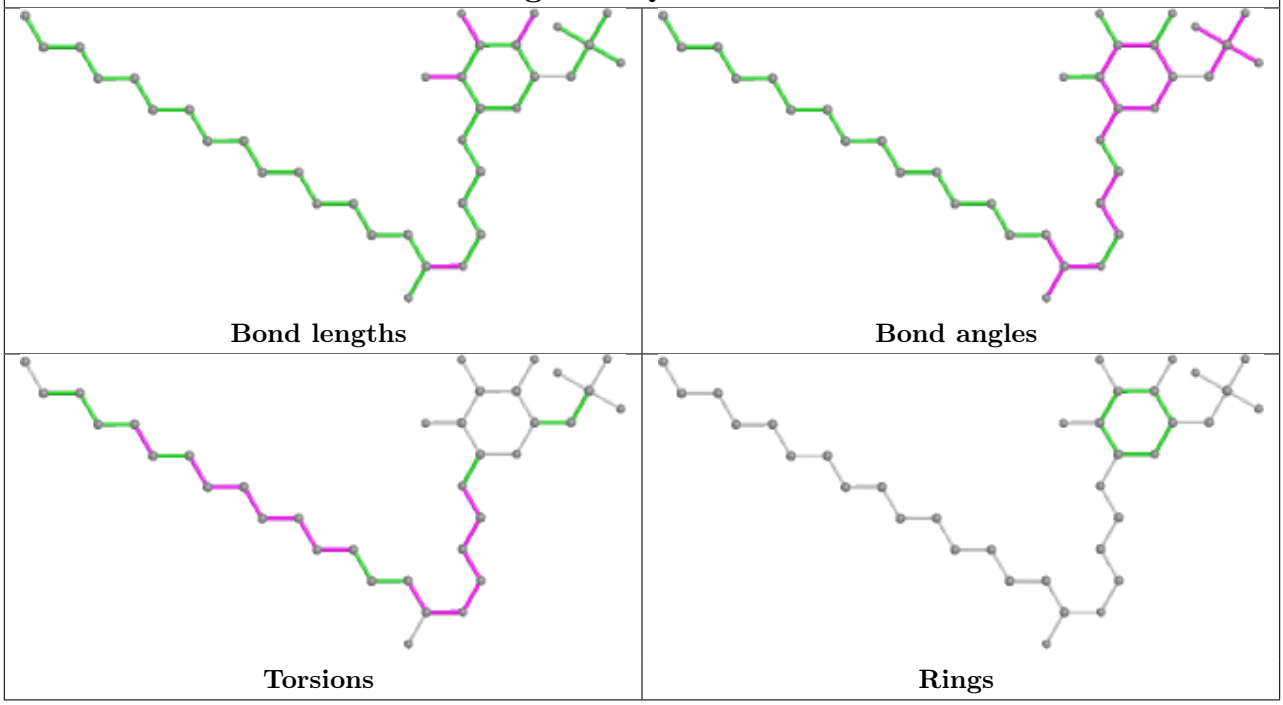


Torsions

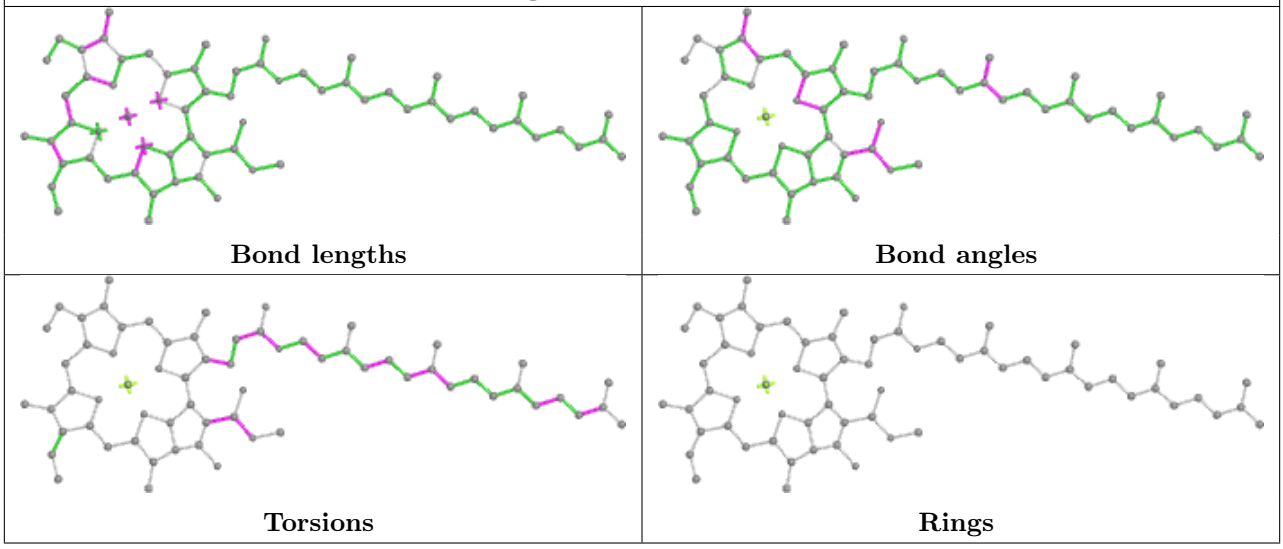


Rings

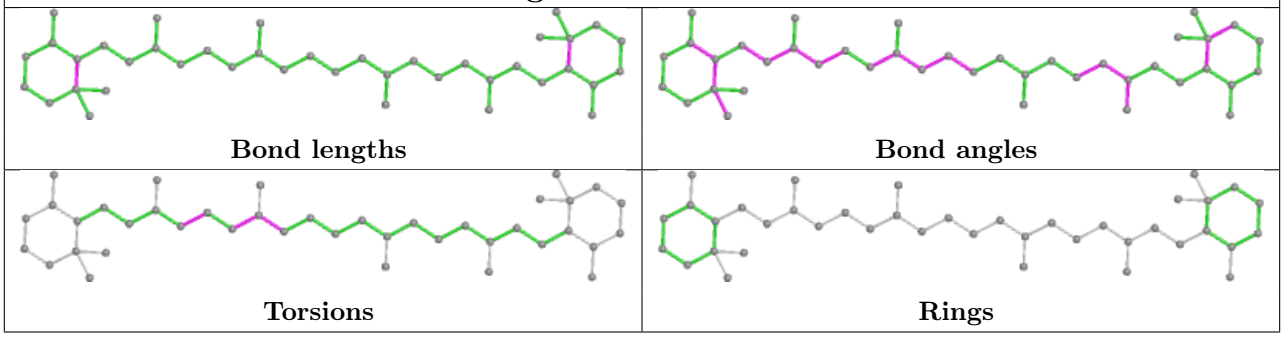
Ligand SQD D 409



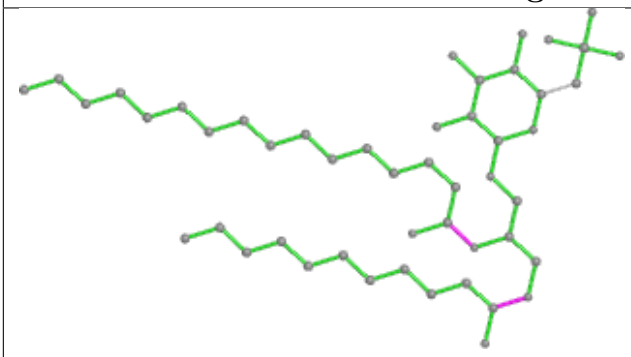
Ligand CLA H 101



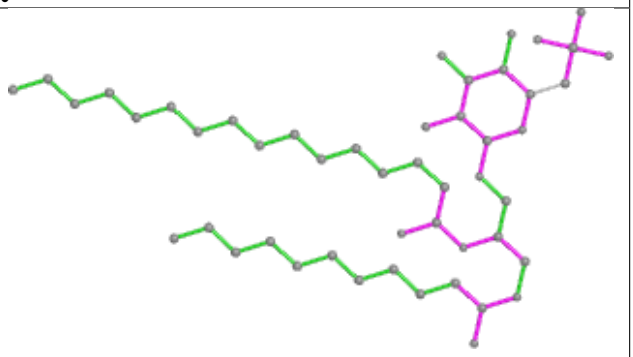
Ligand BCR b 619



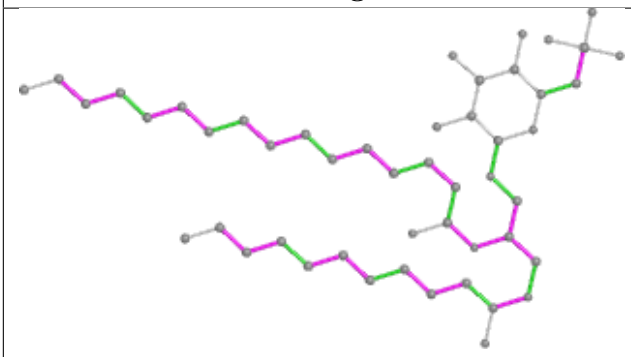
Ligand SQD L 101



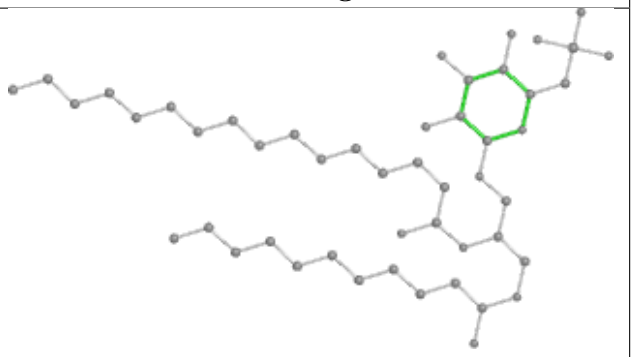
Bond lengths



Bond angles

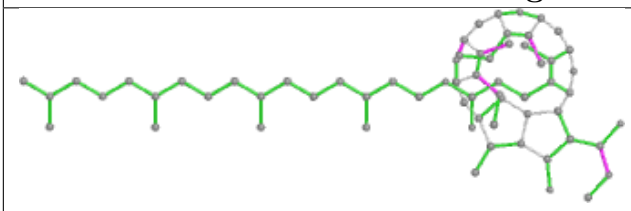


Torsions

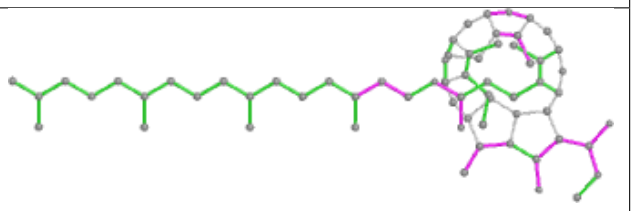


Rings

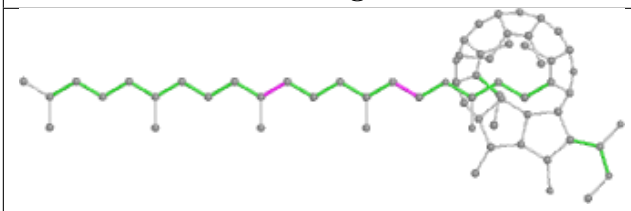
Ligand PHO a 404



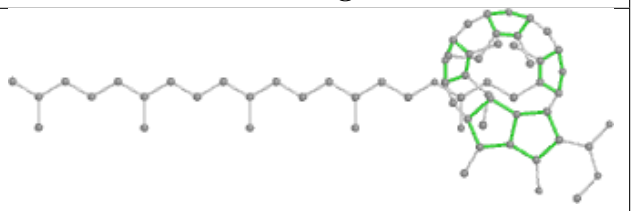
Bond lengths



Bond angles

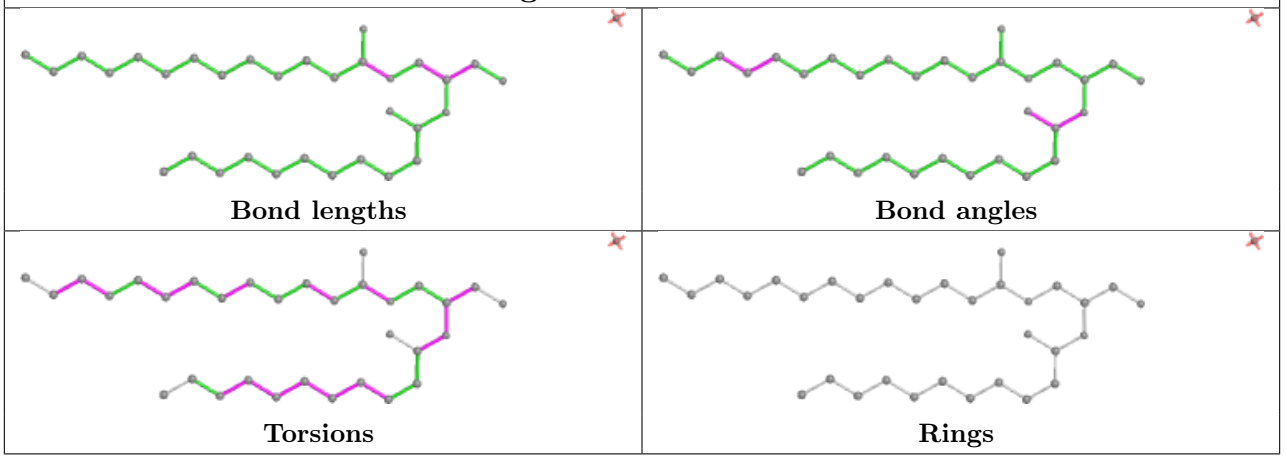


Torsions

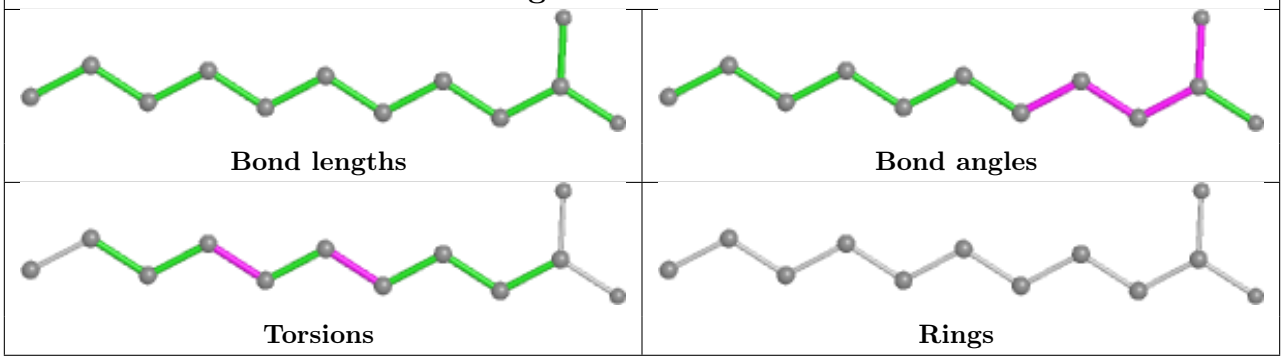


Rings

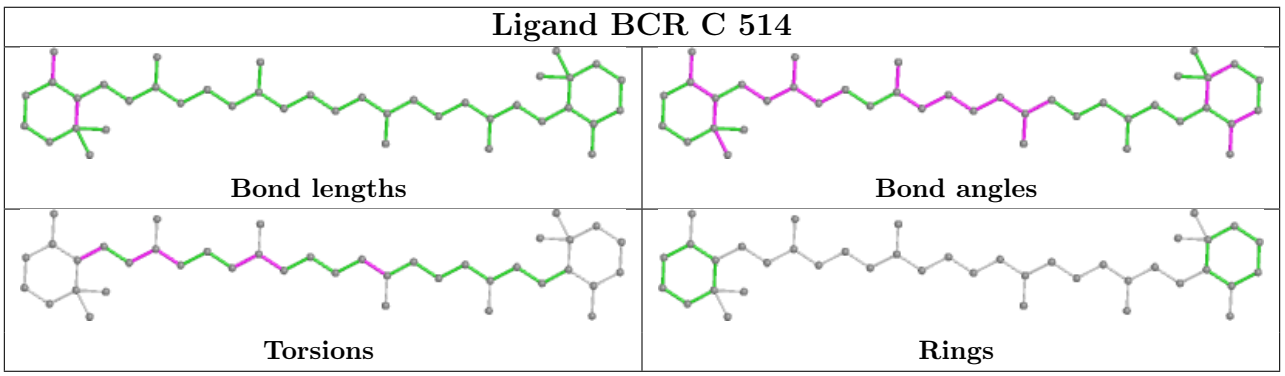
Ligand LMG D 412



Ligand STE C 521



Ligand BCR C 514



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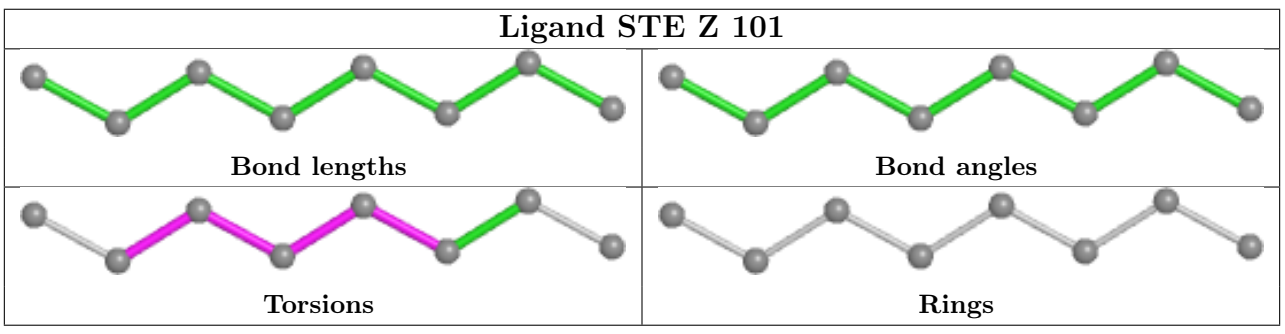

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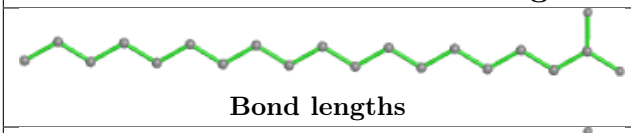
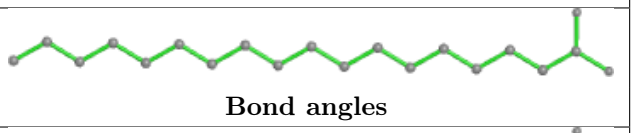
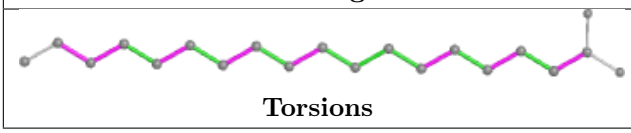
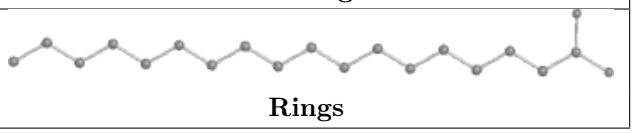
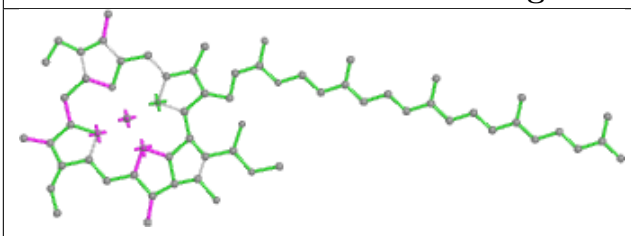

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA b 612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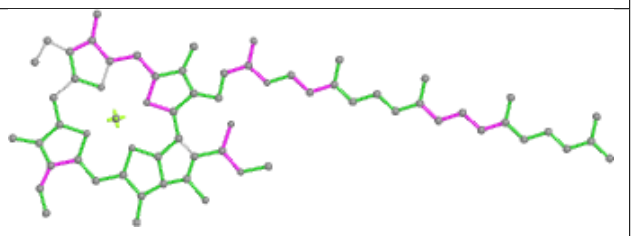
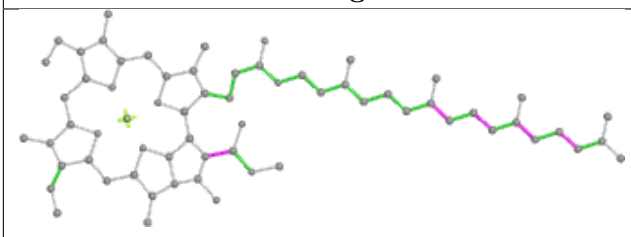
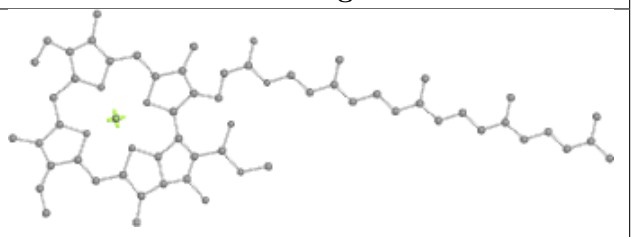
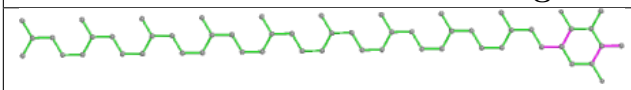

Bond angles


Torsions


Rings

Ligand PL9 a 409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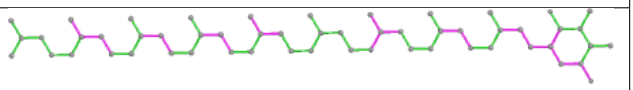
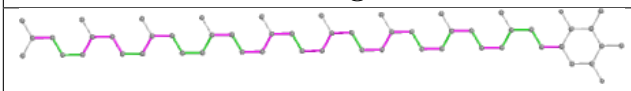

Bond angles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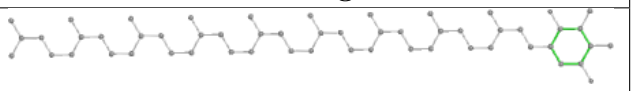
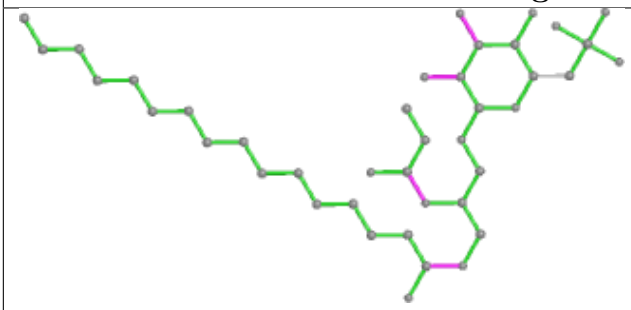

Rings

Ligand SQD f 102



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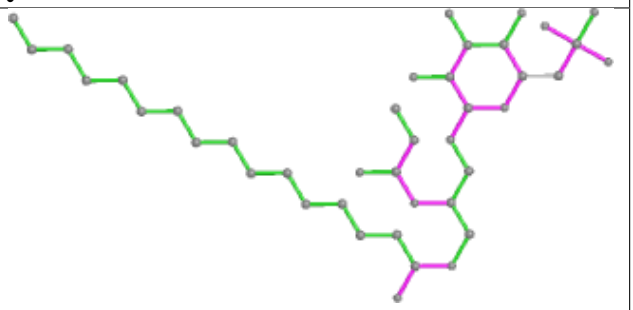
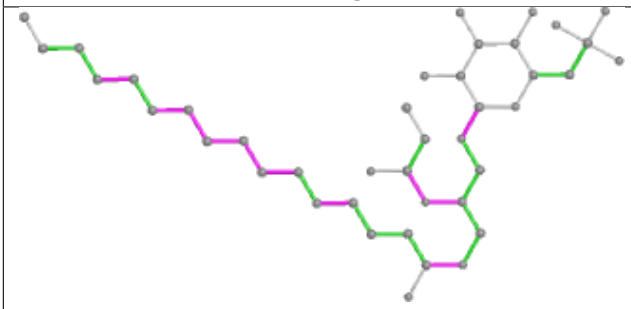


Bond angles



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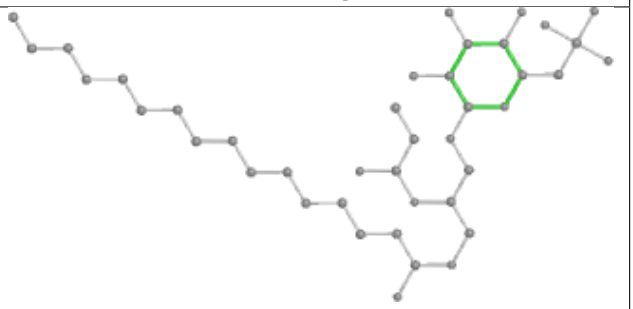
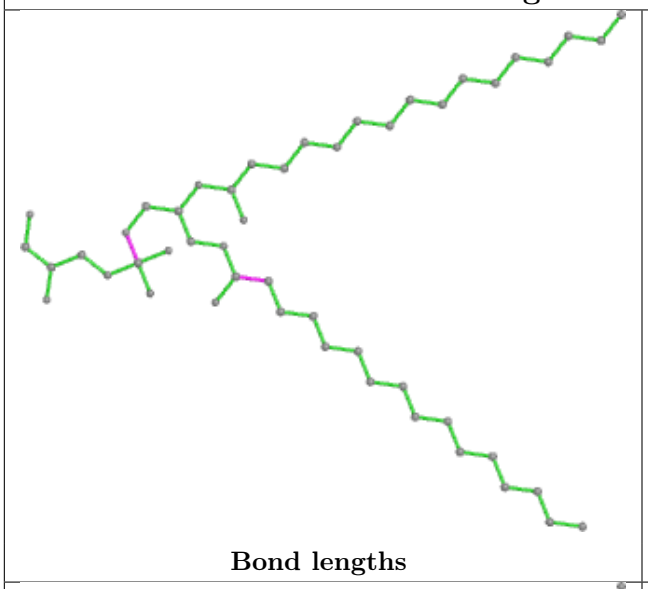


Rings

Ligand LHG A 411



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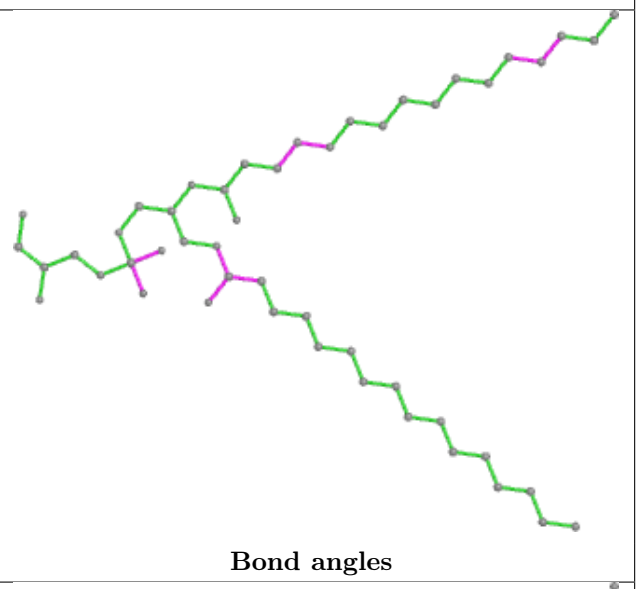
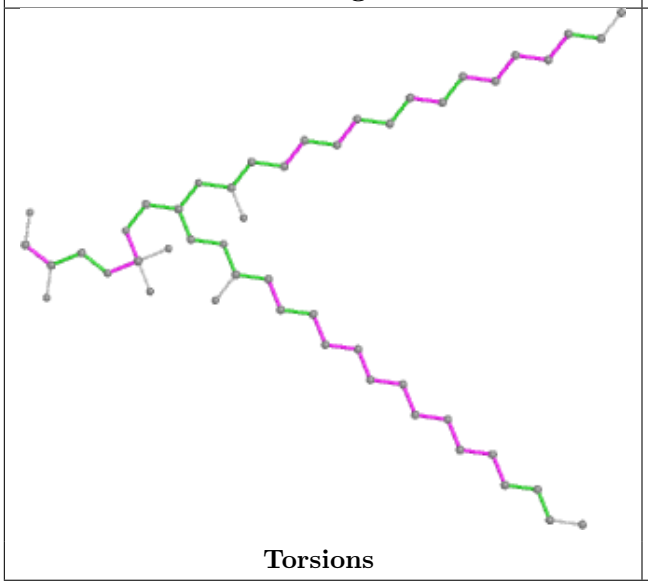
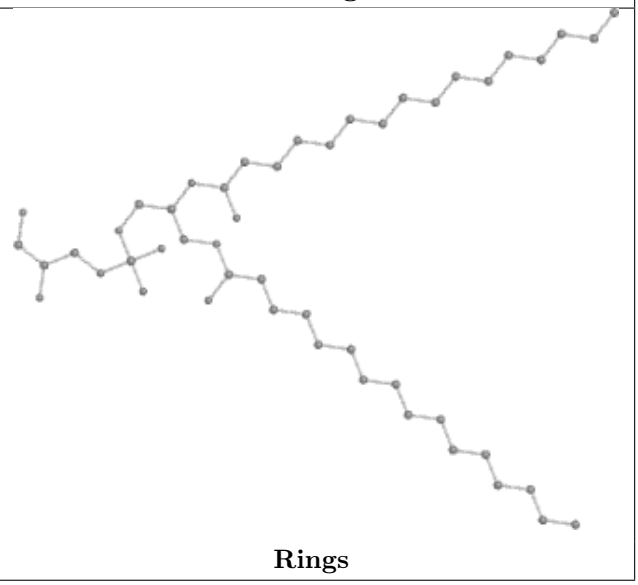


Bond angles

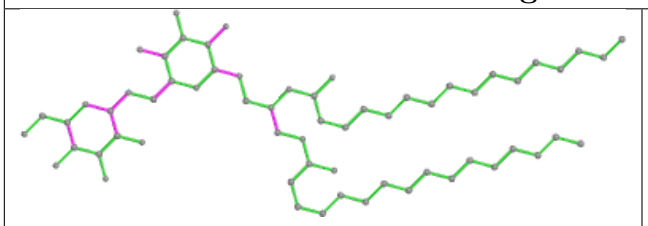


Torsions

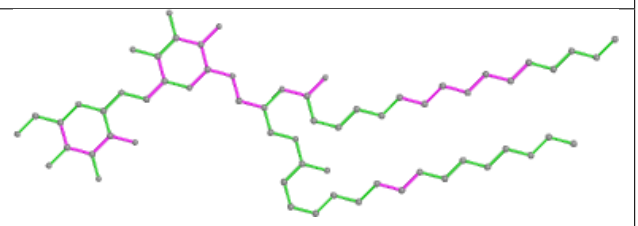


Rings

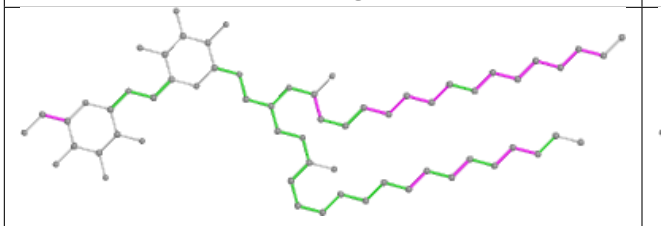
Ligand DGD H 103



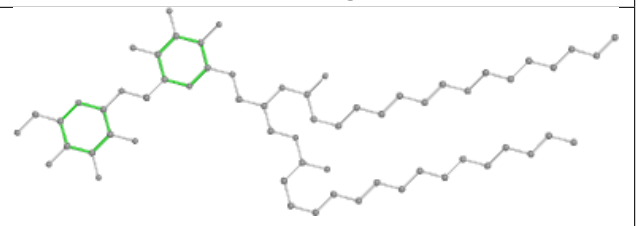
Bond lengths



Bond angles

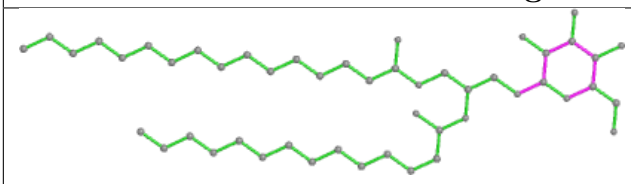


Torsions



Rings

Ligand LMG c 521



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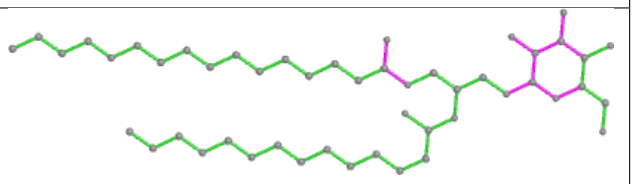
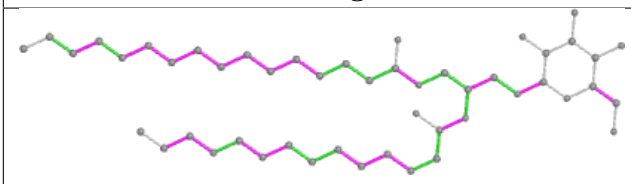
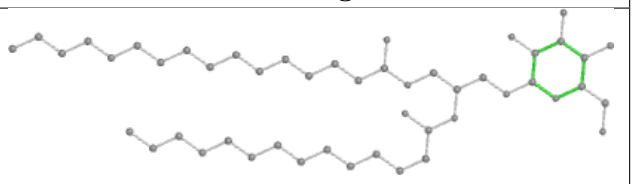


Bond angles

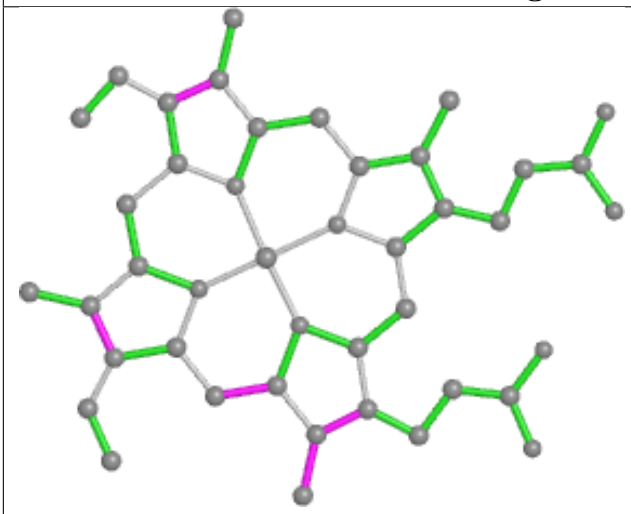


Torsions

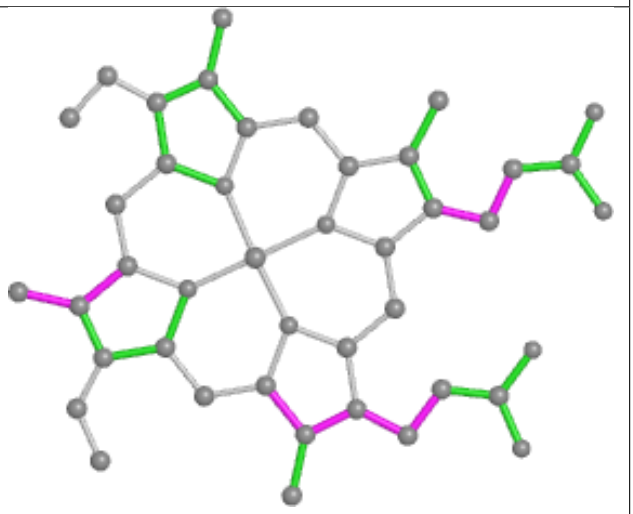


Rings

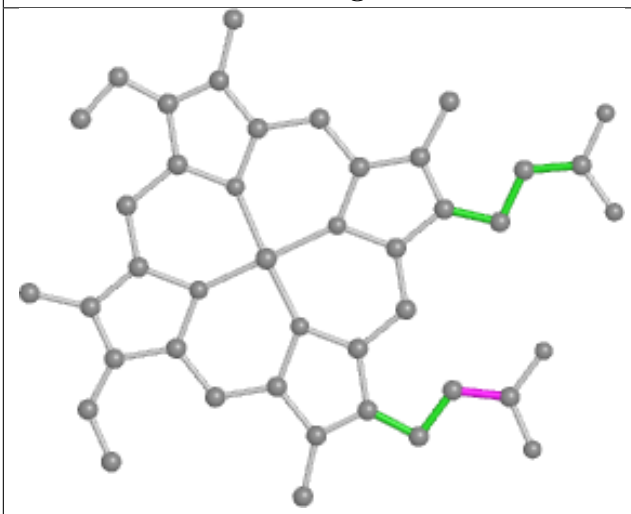
Ligand HEC v 201



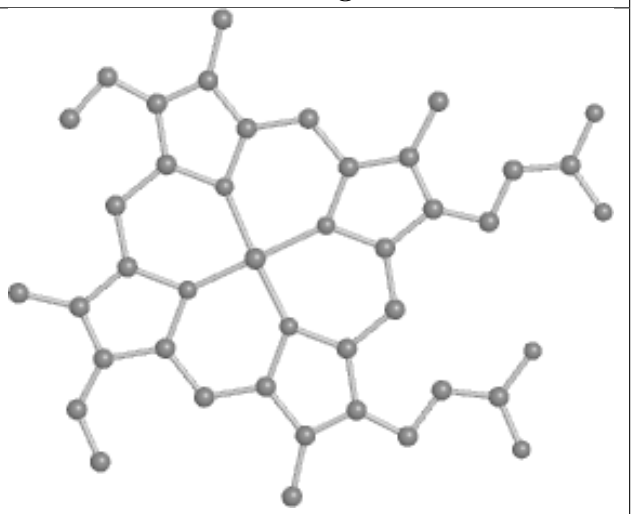
Bond lengths



Bond angles

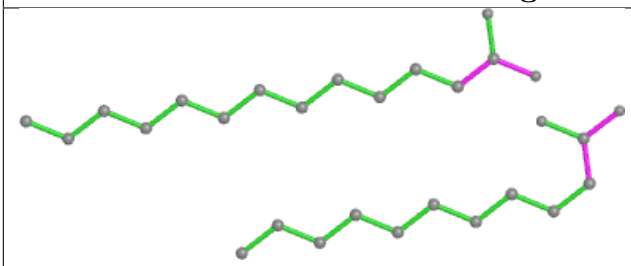


Torsions

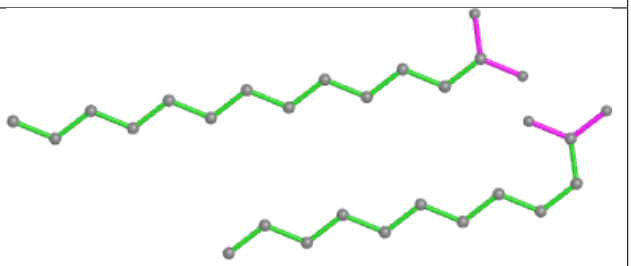


Rings

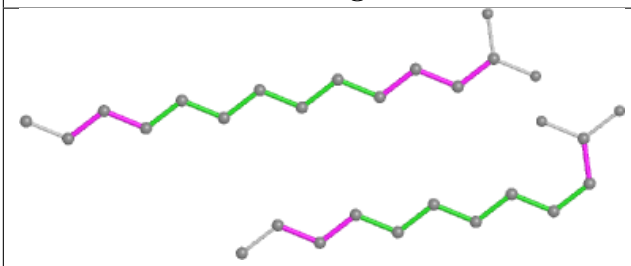
Ligand LMG B 620



Bond lengths



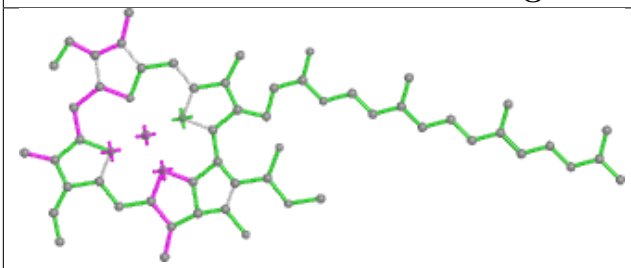
Bond angles



Torsions

Rings

Ligand CLA B 615



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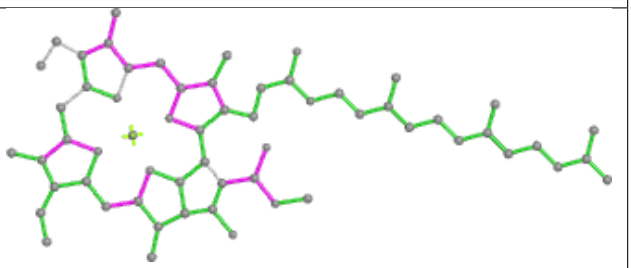
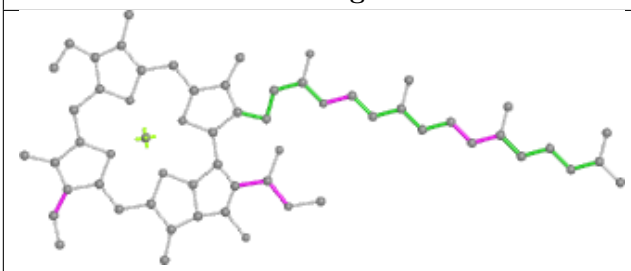


Bond angles



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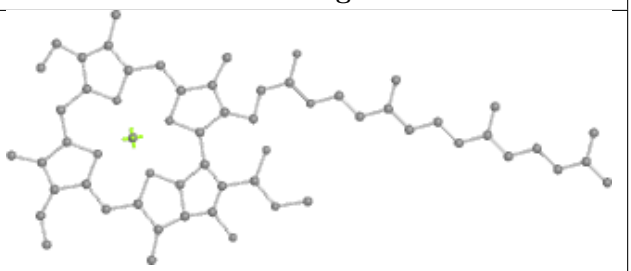
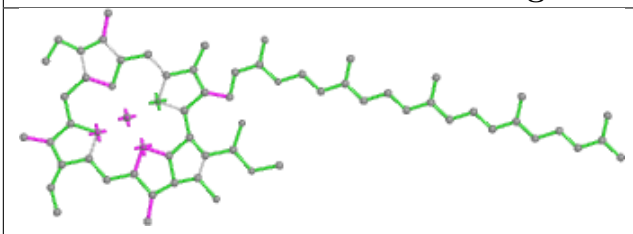


Rings

Ligand CLA b 613



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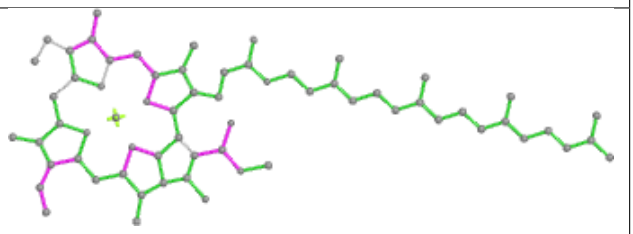
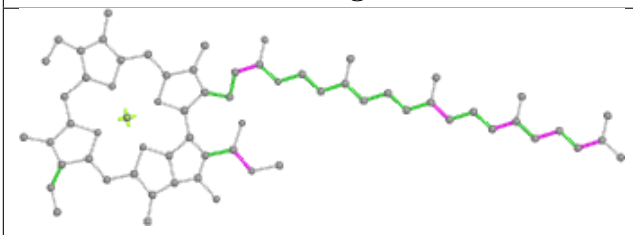
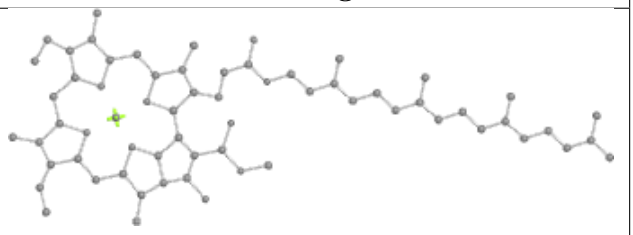


Bond angles

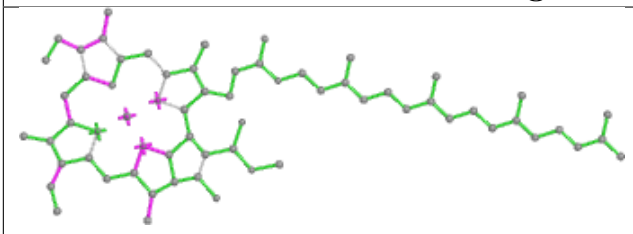


Torsions



Rings

Ligand CLA b 602



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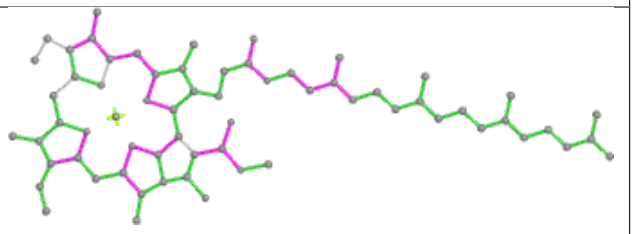
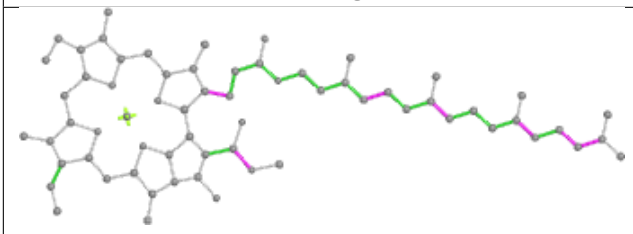


Bond angles



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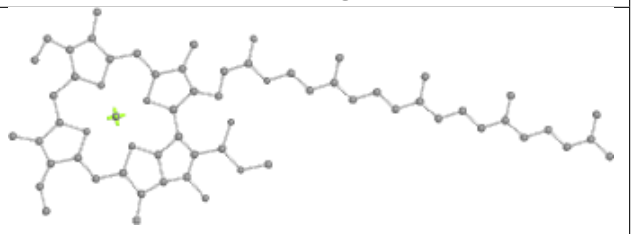
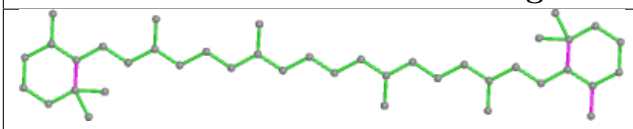


Rings

Ligand BCR k 102



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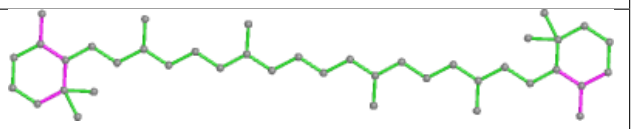
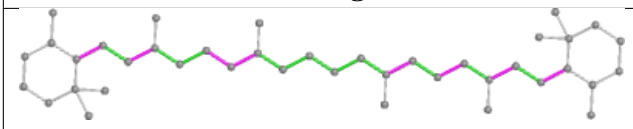
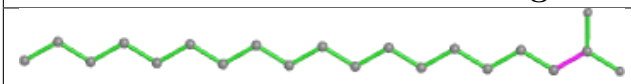
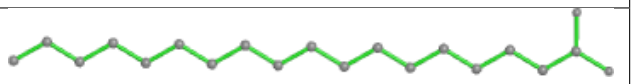
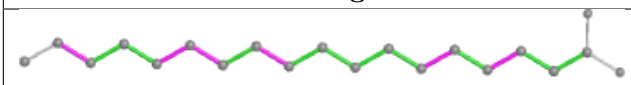
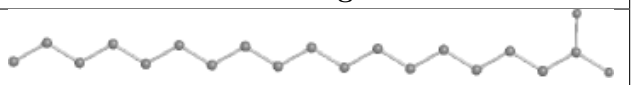


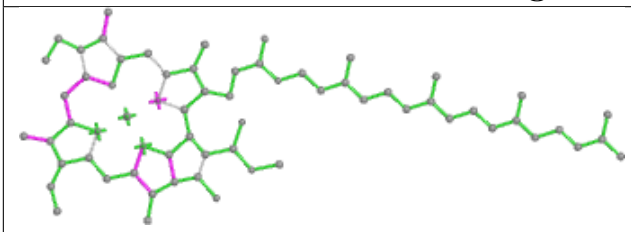
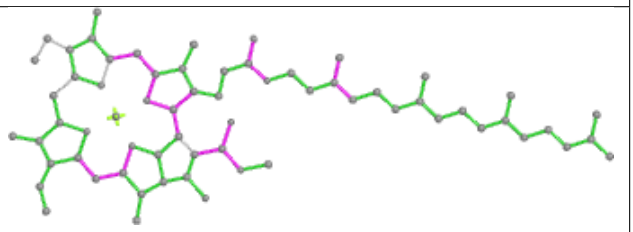
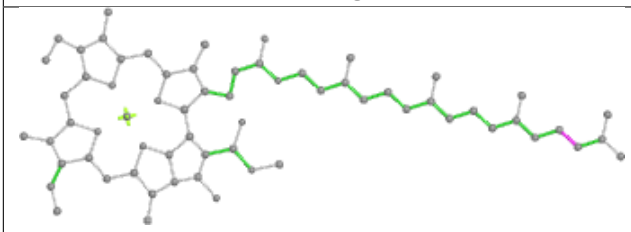
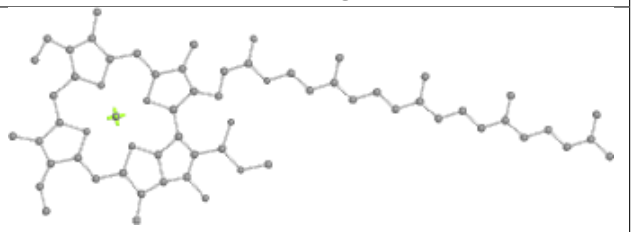
Bond angles

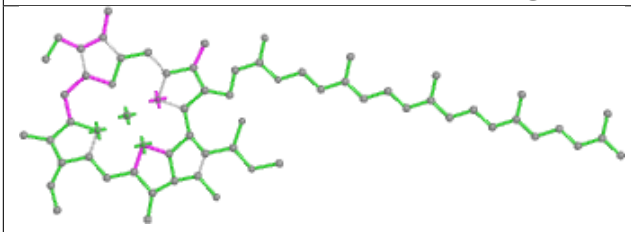
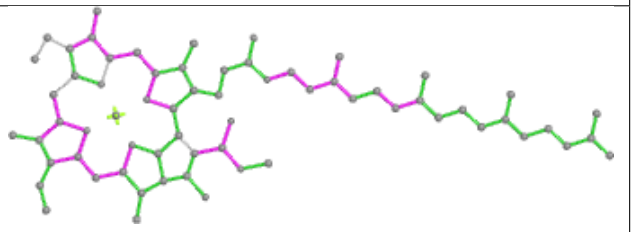
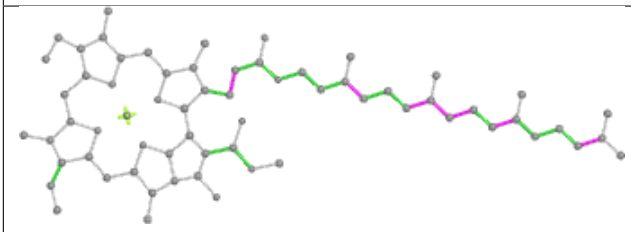
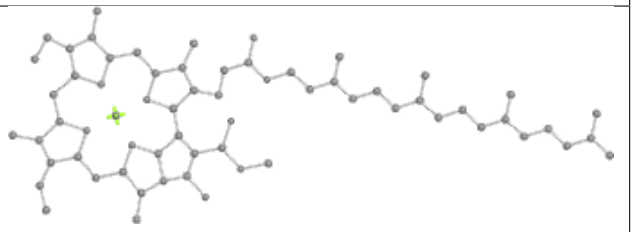


Torsions

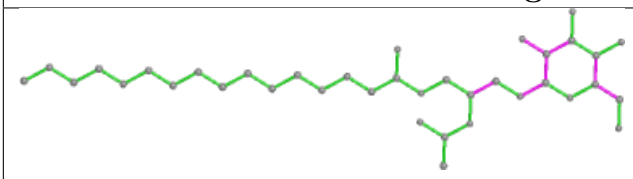
Rings

Ligand STE b 629	
 Bond lengths	 Bond angles
 Torsions	 Rings

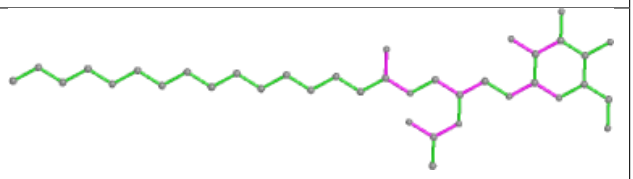
Ligand CLA a 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

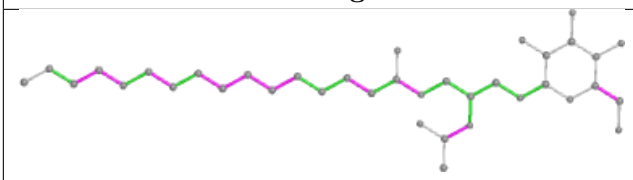
Ligand LMG c 518



Bond lengths



Bond angles



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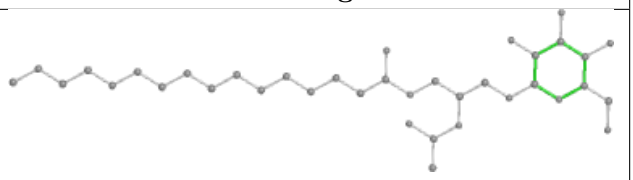
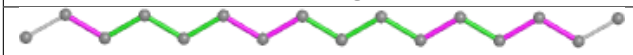


Rings

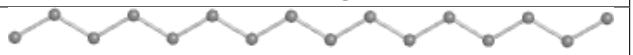
Ligand STE b 620

Bond lengths

Bond angles

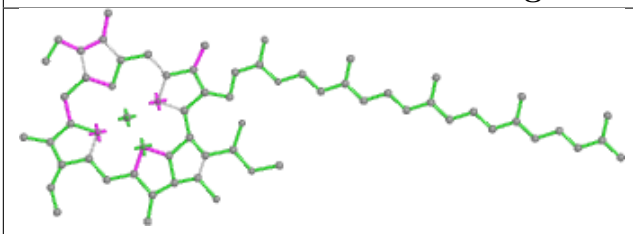


Torsions

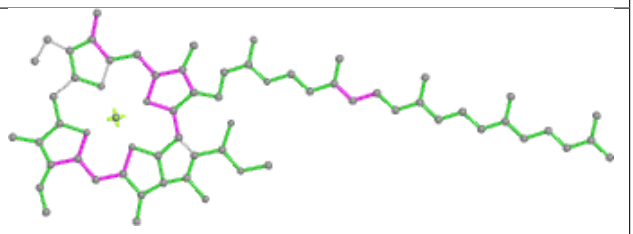


Rings

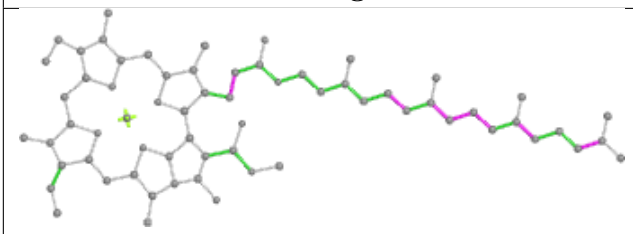
Ligand CLA B 605



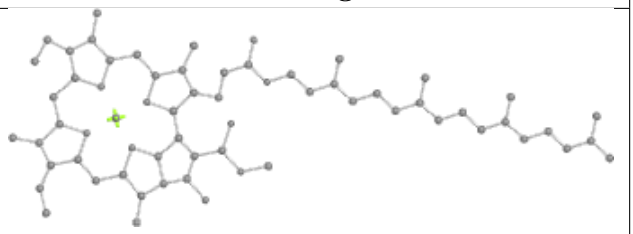
Bond lengths



Bond angles

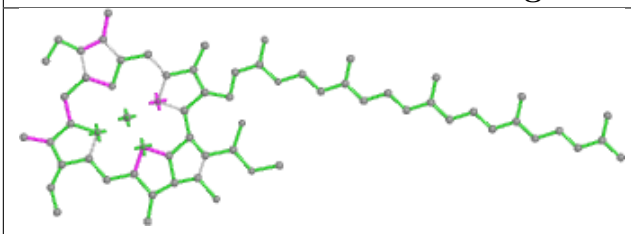


Torsions

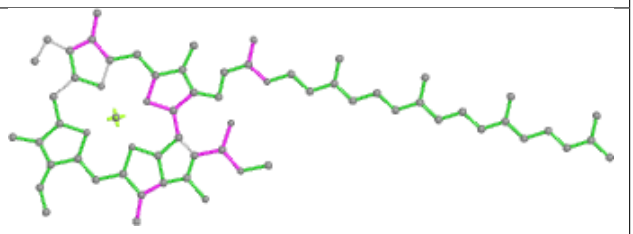


Rings

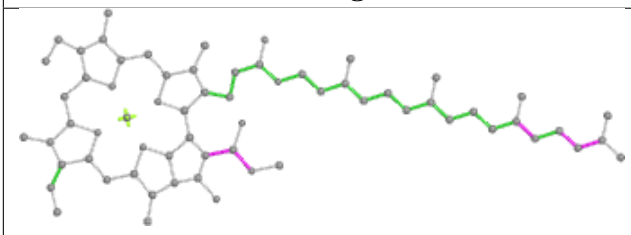
Ligand CLA C 502



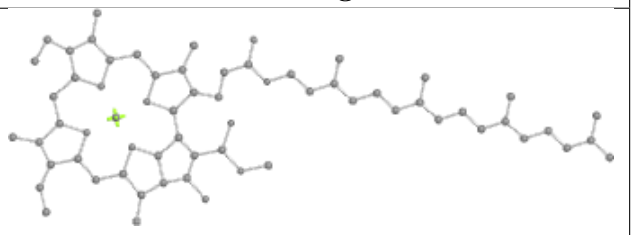
Bond lengths



Bond angles

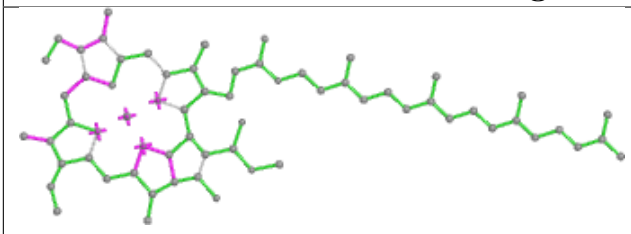


Torsions

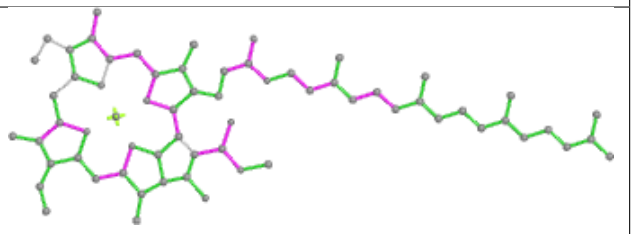


Rings

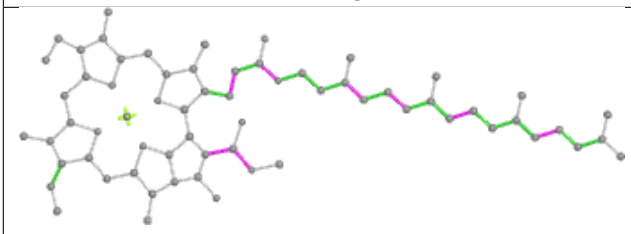
Ligand CLA c 507



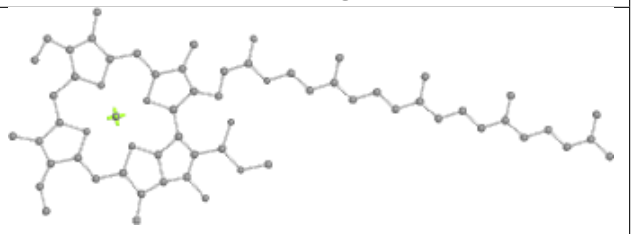
Bond lengths



Bond angles

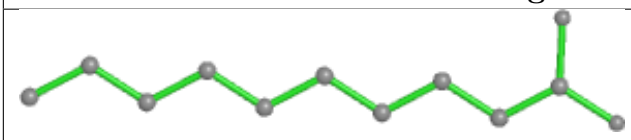


Torsions

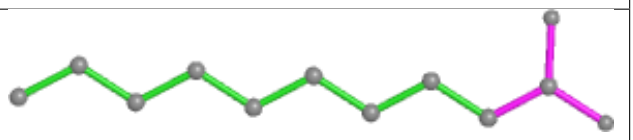


Rings

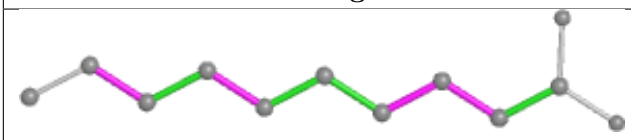
Ligand STE B 625



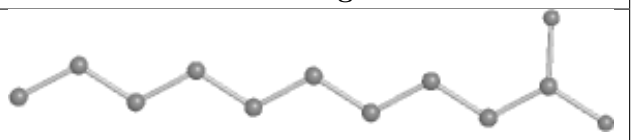
Bond lengths



Bond angles

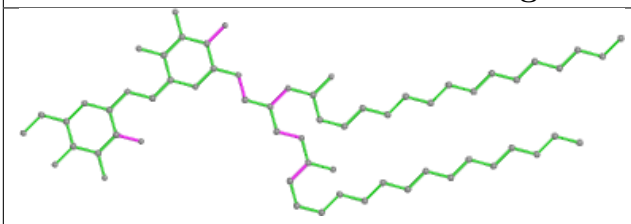


Torsions

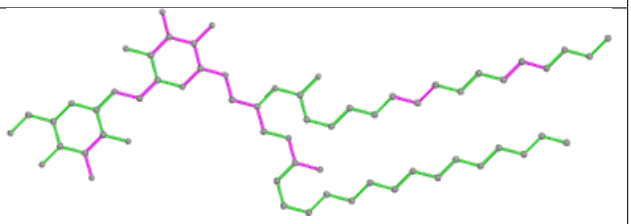


Rings

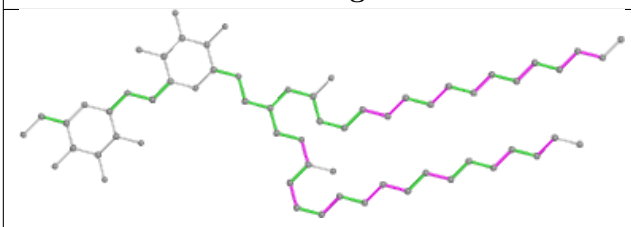
Ligand DGD C 518



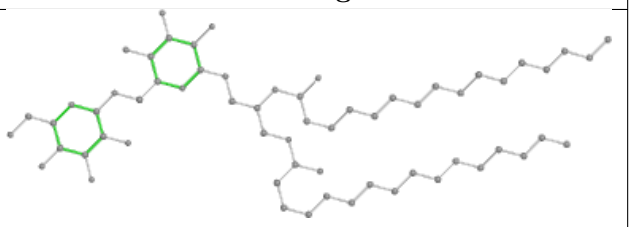
Bond lengths



Bond angles

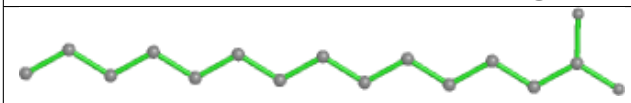


Torsions



Rings

Ligand STE b 624



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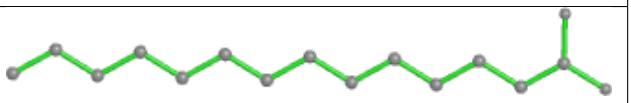
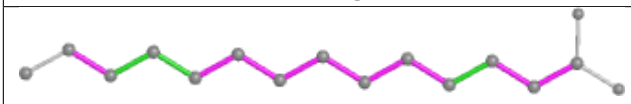


Bond angles



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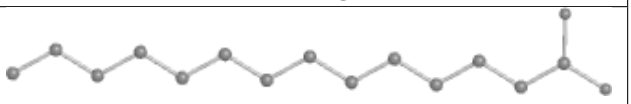
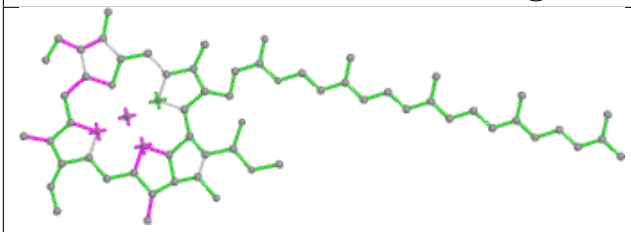


Rings

Ligand CLA b 610



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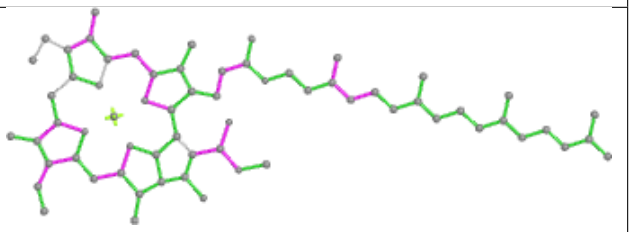
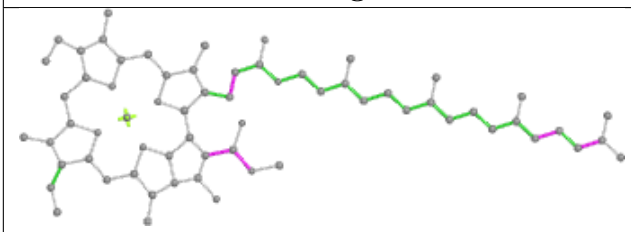


Bond angles



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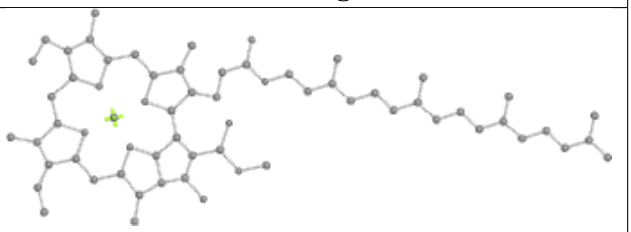
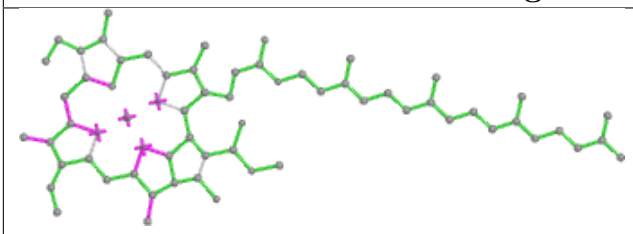


Rings

Ligand CLA B 611



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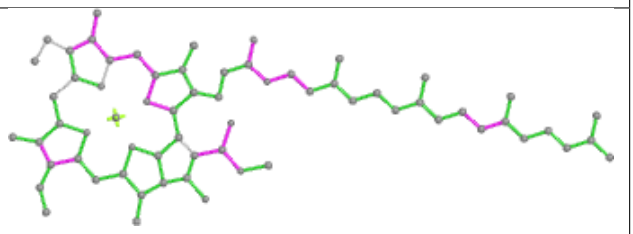
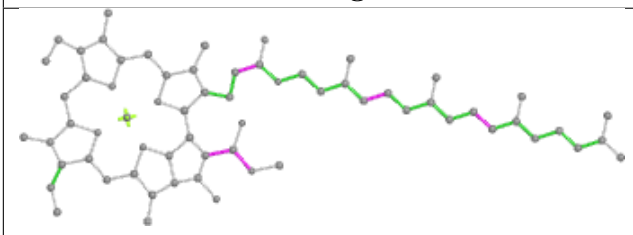


Bond angles



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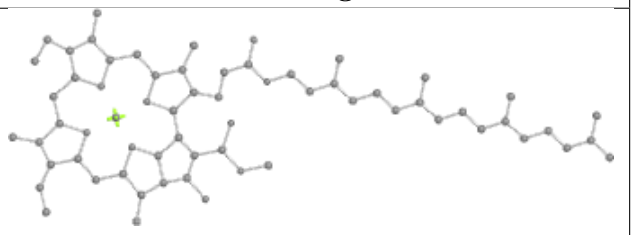
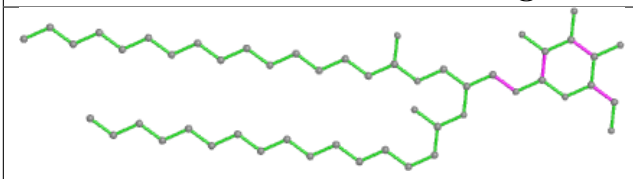


Rings

Ligand LMG m 101



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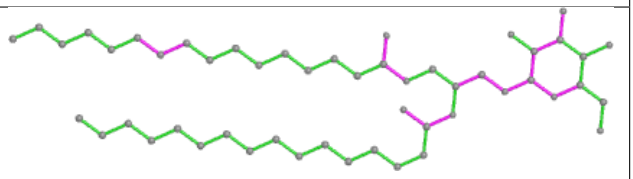
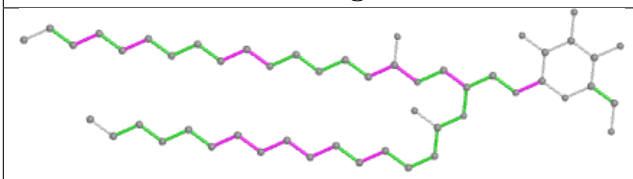


Bond angles



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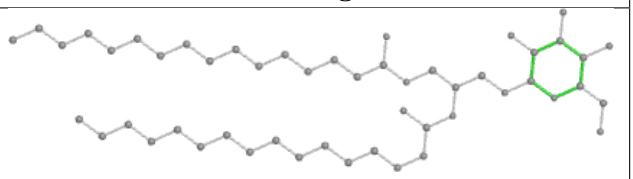
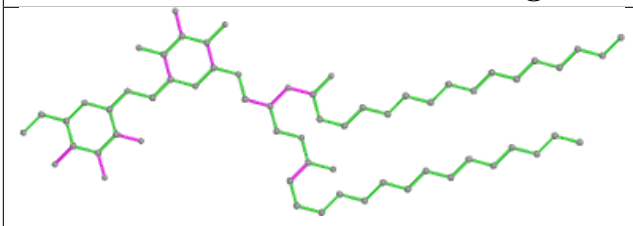


Rings

Ligand DGD c 517



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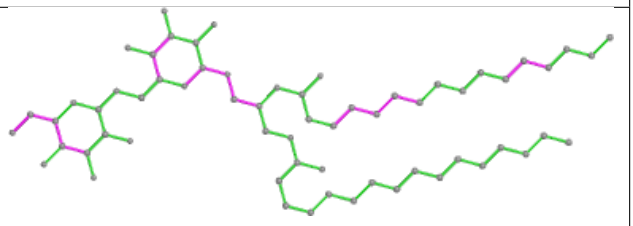
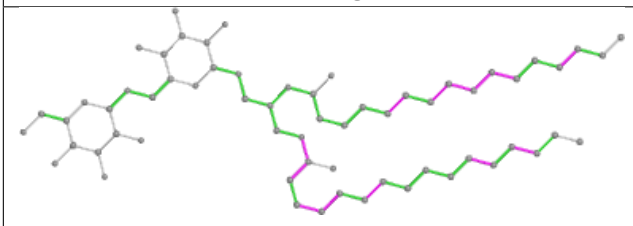


Bond angles



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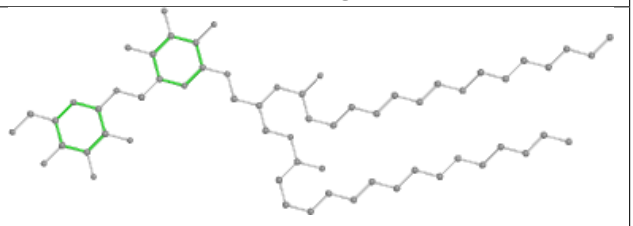
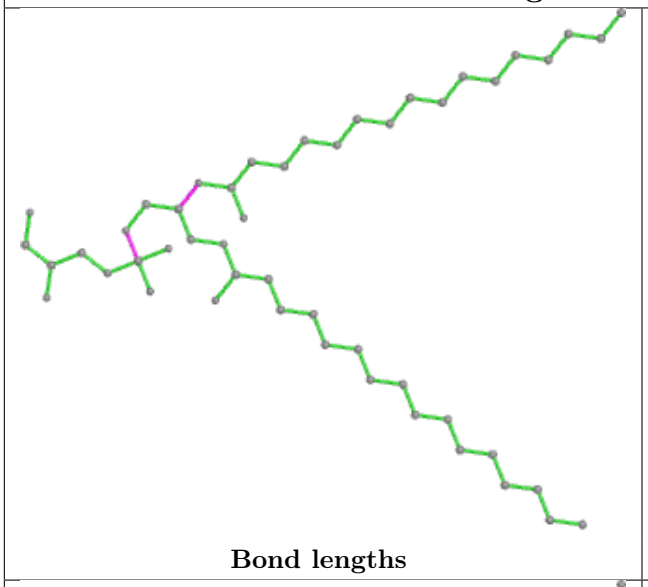


Rings

Ligand LHG L 102



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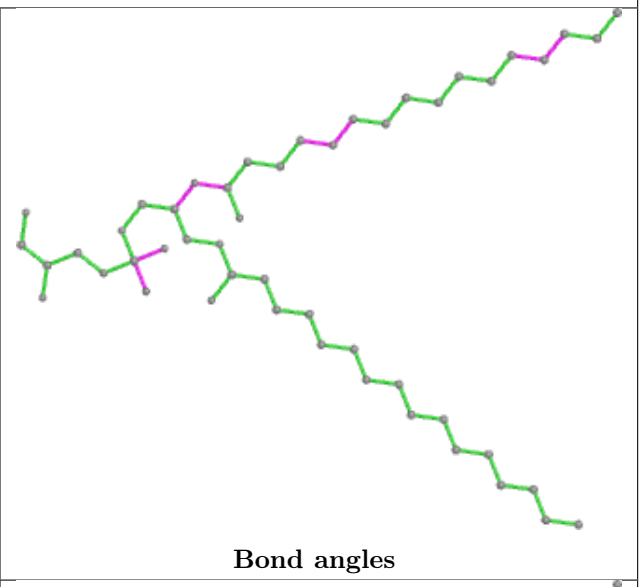
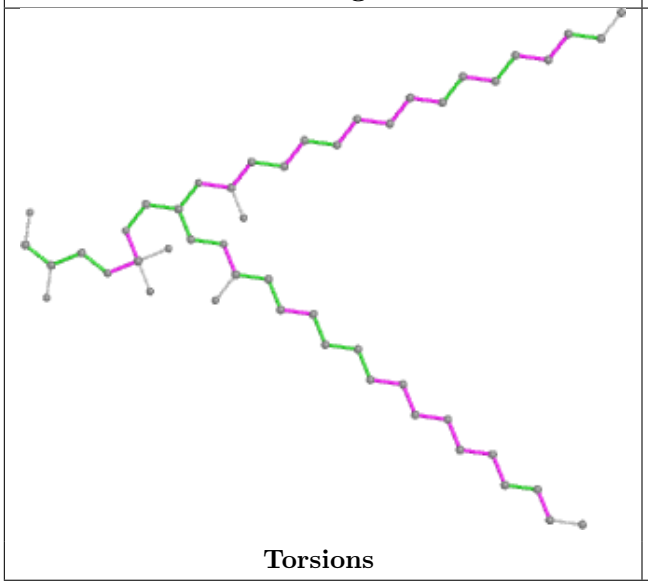


Bond angles



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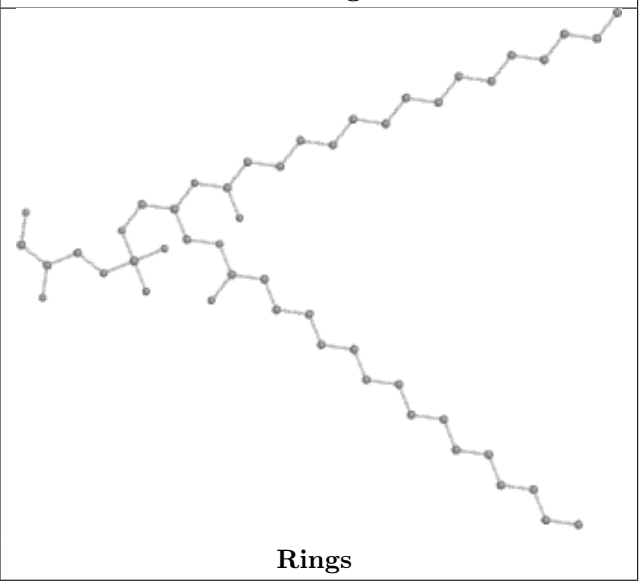
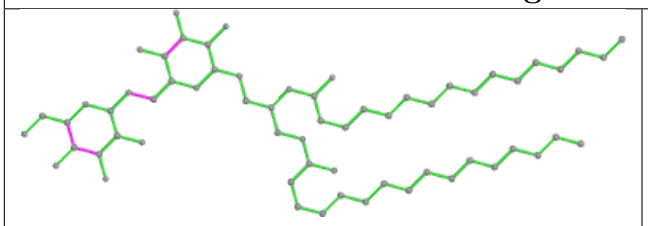


Rings

Ligand DGD h 101



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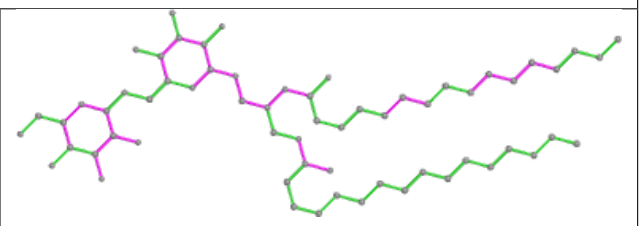
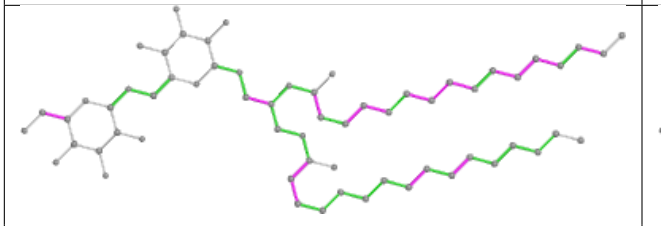


Bond angles



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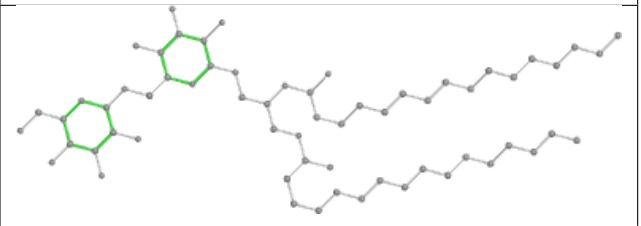
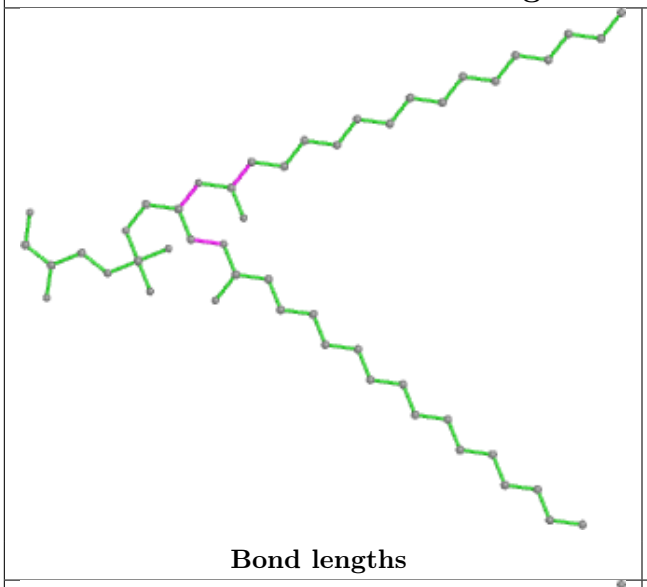


Rings

Ligand LHG D 410



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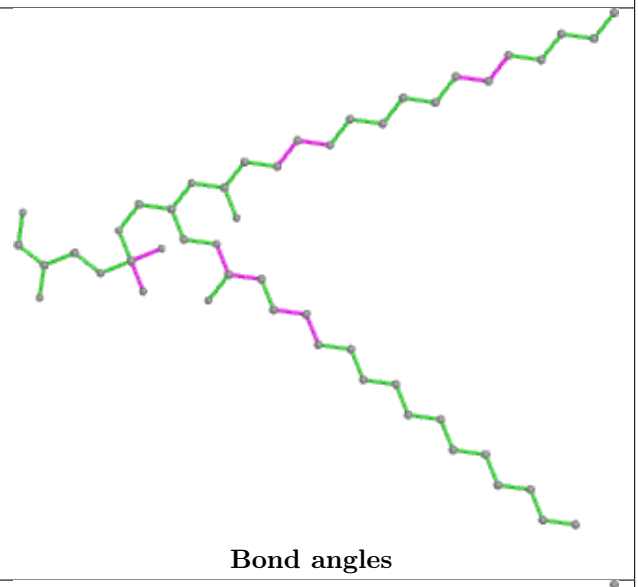
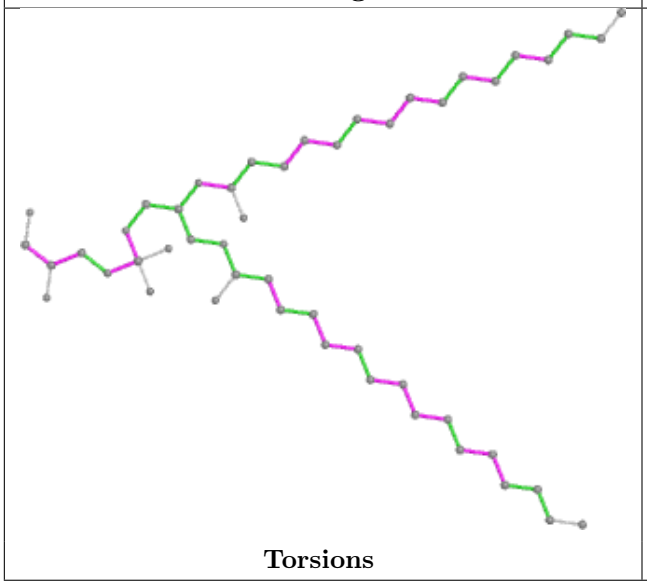


Bond angles



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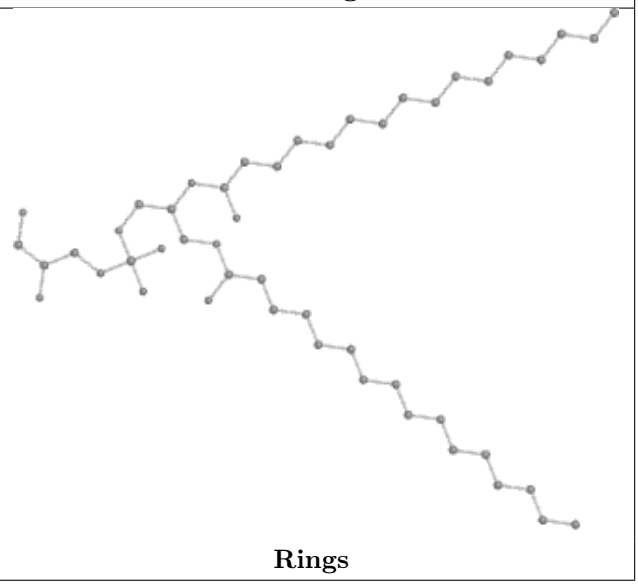
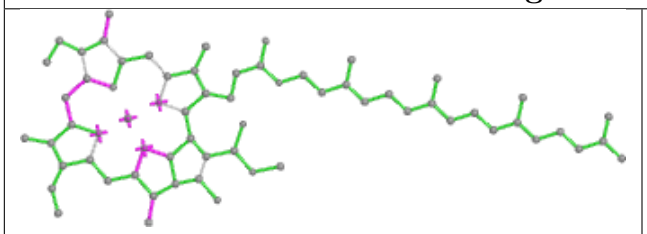


Rings

Ligand CLA B 610



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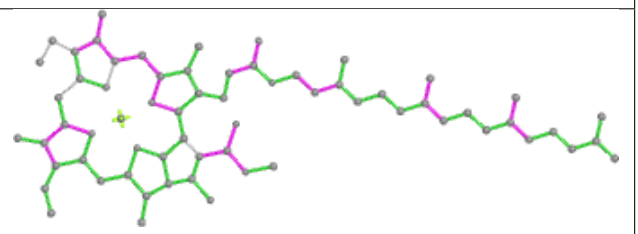
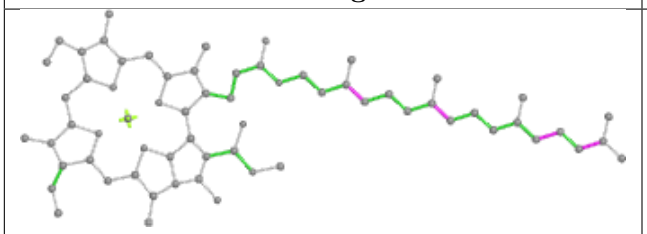


Bond angles



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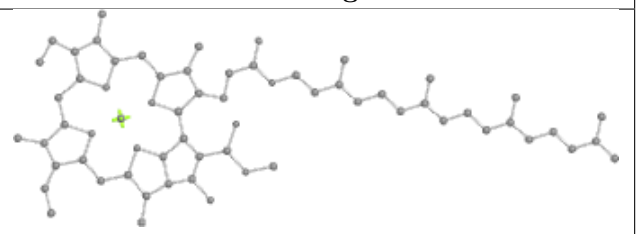
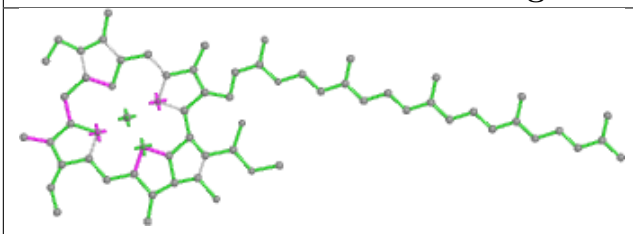


Rings

Ligand CLA b 604



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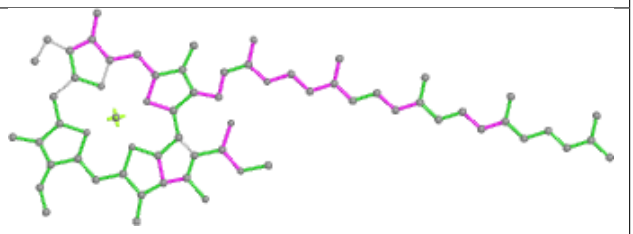

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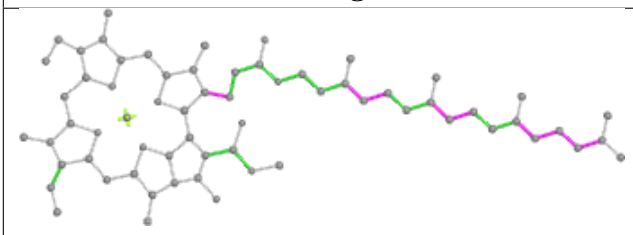

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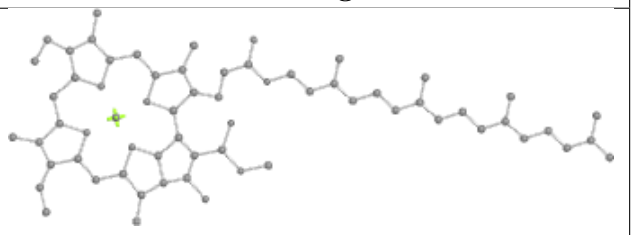
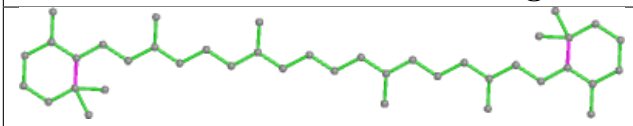


Rings

Ligand BCR d 406



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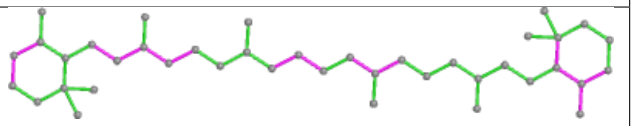
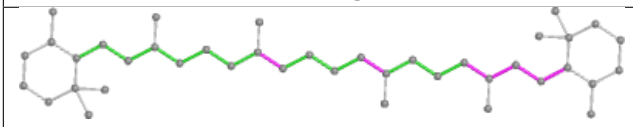


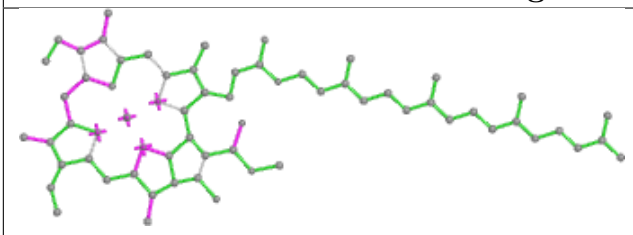
Bond angles



Torsions

Rings

Ligand CLA d 405



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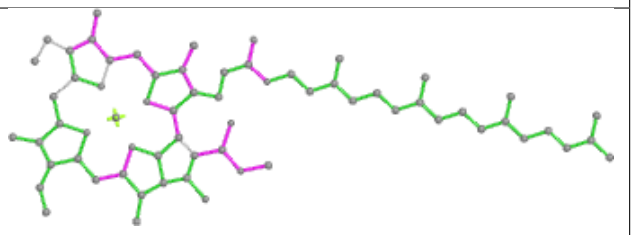
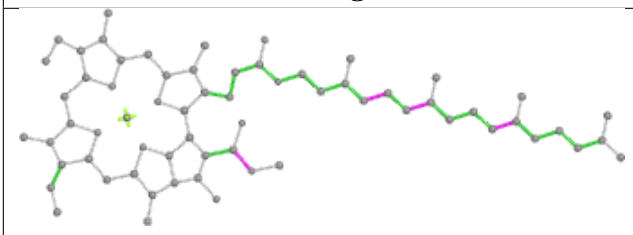
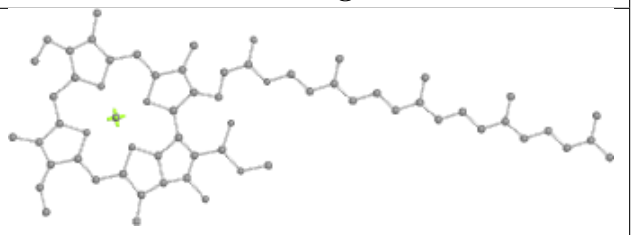


Bond angles

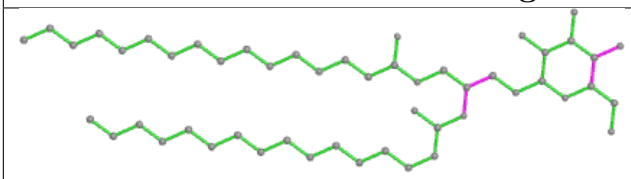


Torsions



Rings

Ligand LMG D 408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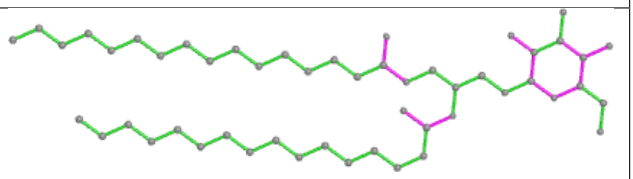
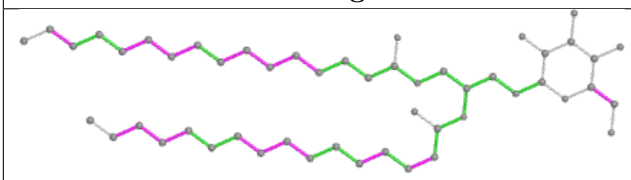
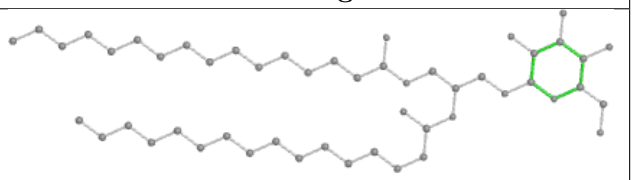
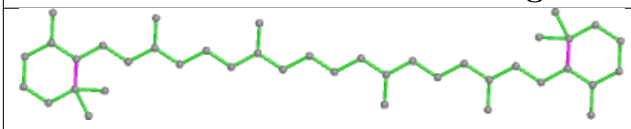
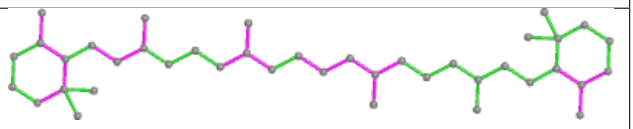

Bond angles

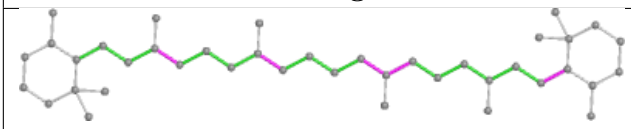

Torsions


Rings

Ligand BCR x 101


Bond lengths


Bond angles

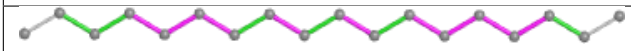

Torsions

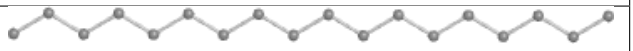
Rings

Ligand STE M 104

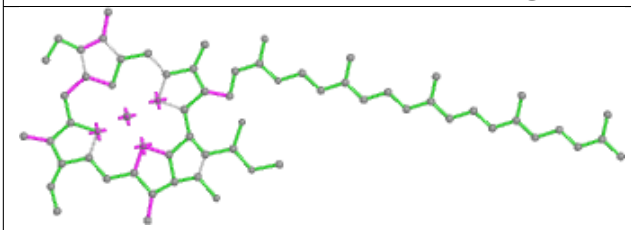
Bond lengths

Bond angles


Torsions


Rings

Ligand CLA D 405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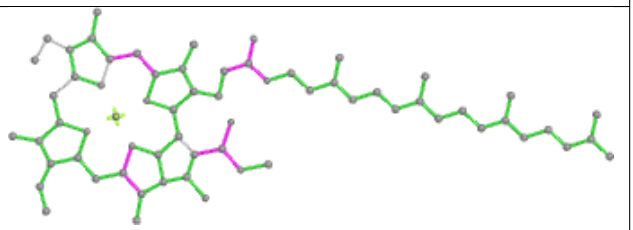
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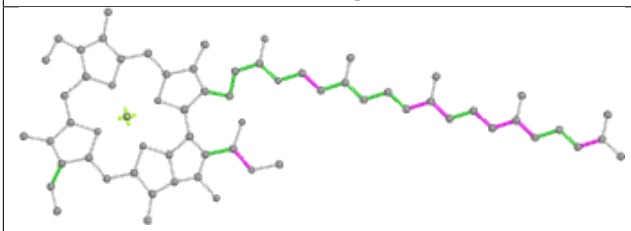
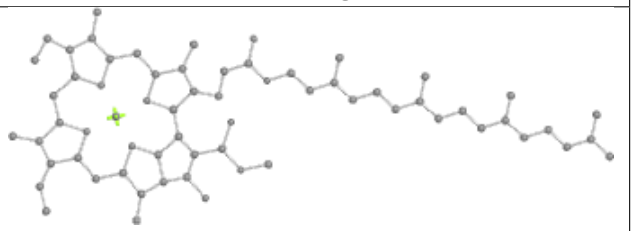
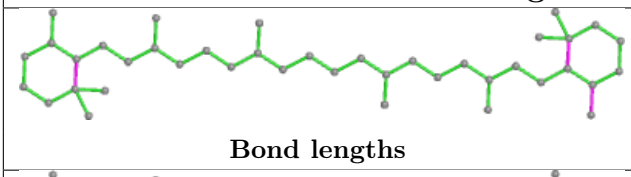

Torsions


Rings

Ligand BCR c 514



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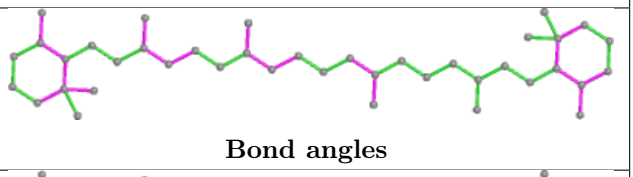
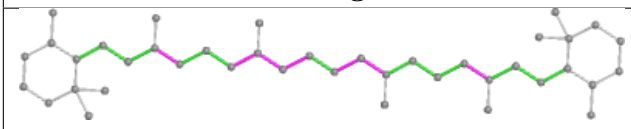


Bond angles



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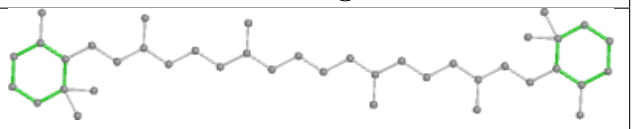
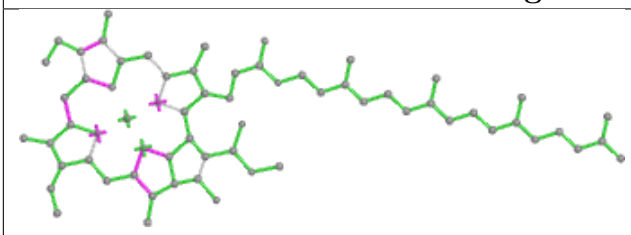
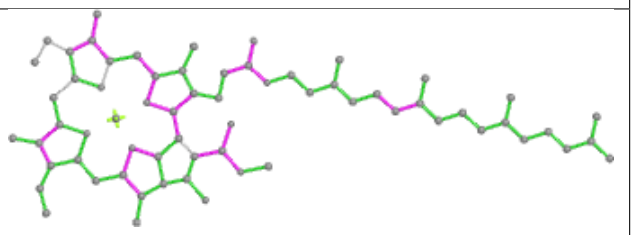


Rings

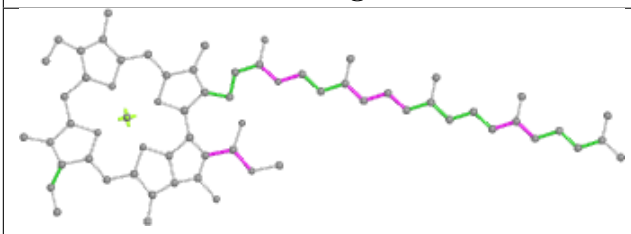
Ligand CLA B 603



Bond lengths



Bond angles



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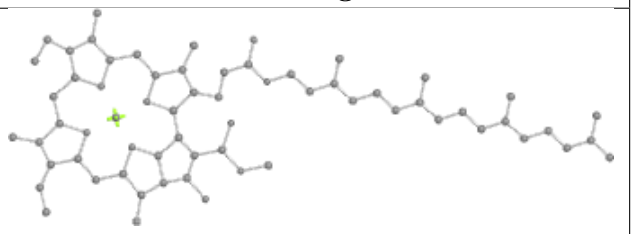
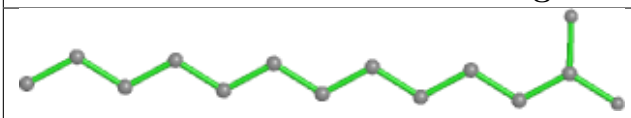


Rings

Ligand STE t 103



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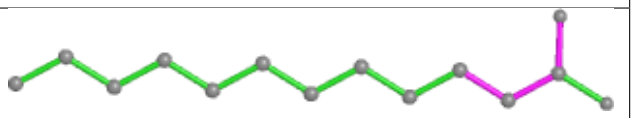
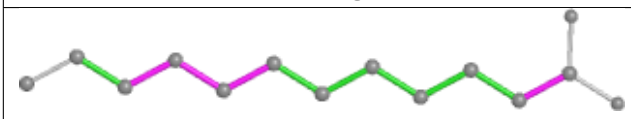


Bond angles



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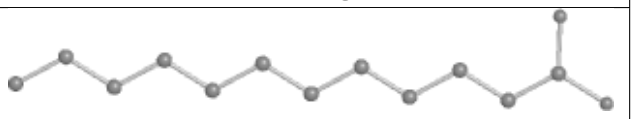
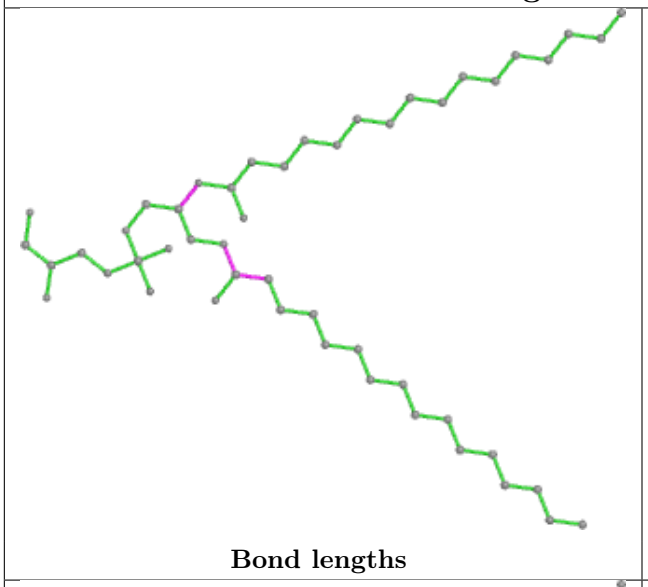


Rings

Ligand LHG D 413



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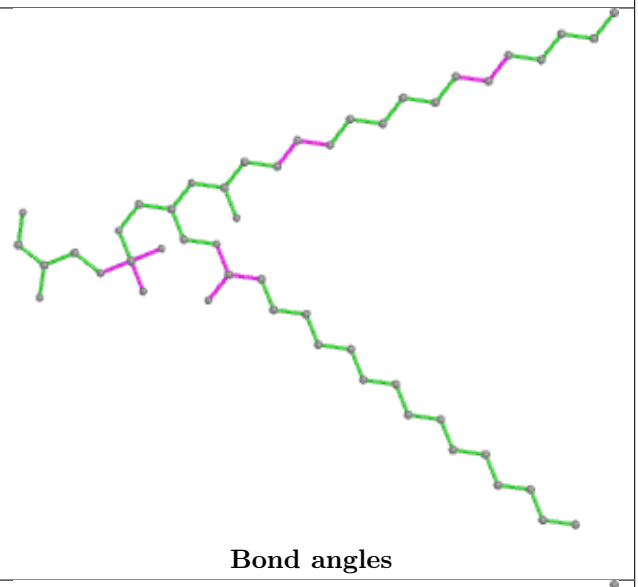
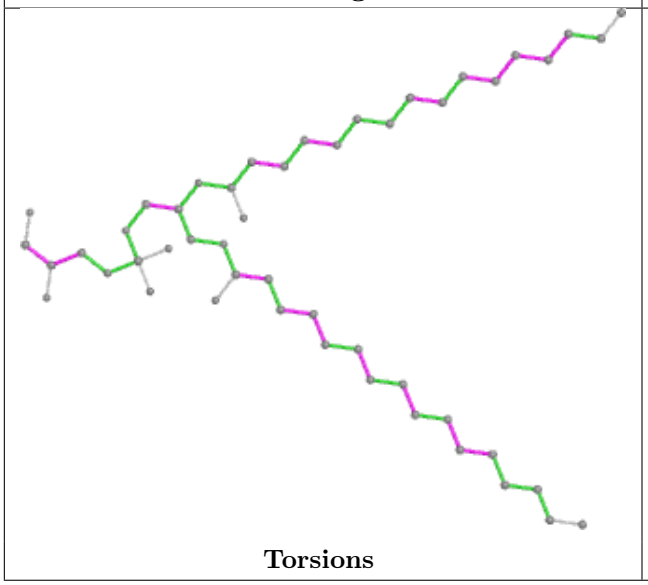


Bond angles



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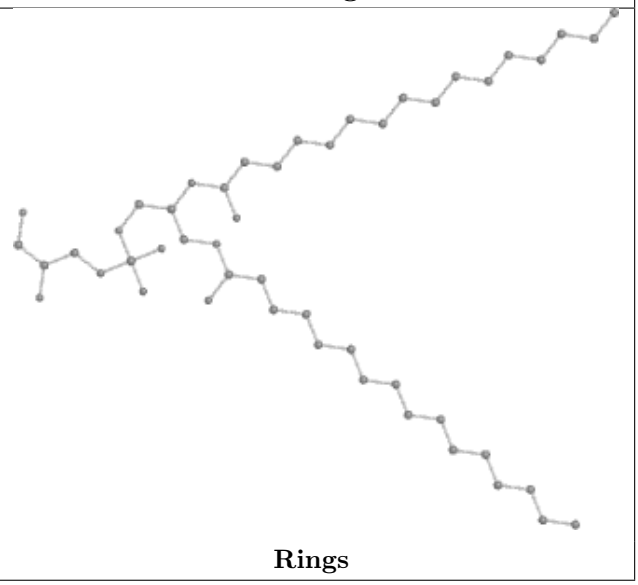
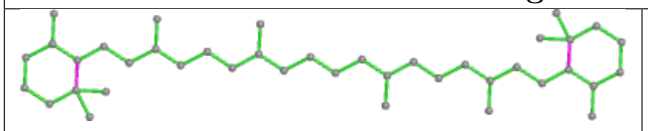


Rings

Ligand BCR b 617



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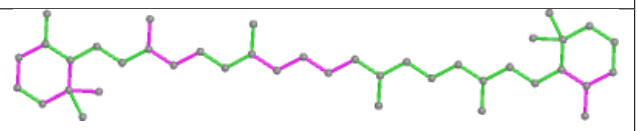
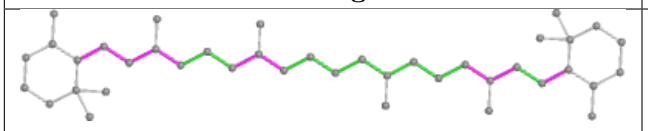


Bond angles



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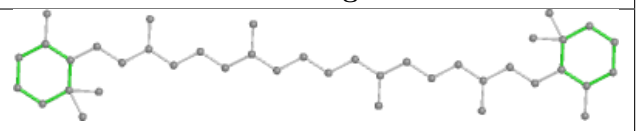
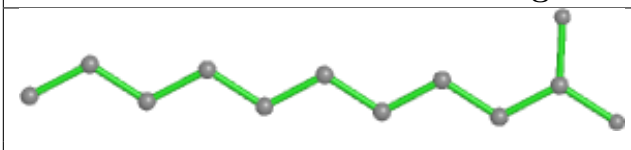


Rings

Ligand STE a 412



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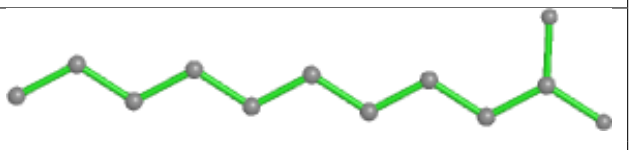
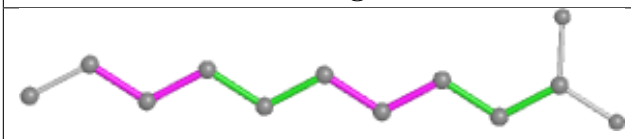


Bond angles



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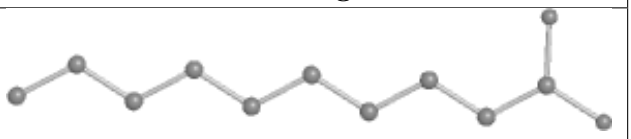
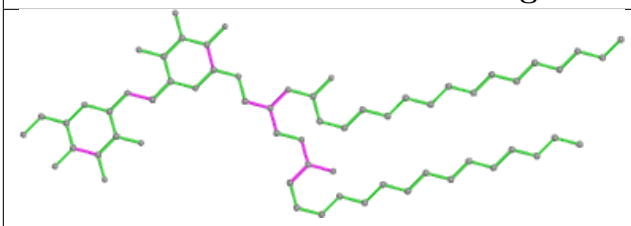


Rings

Ligand DGD C 516



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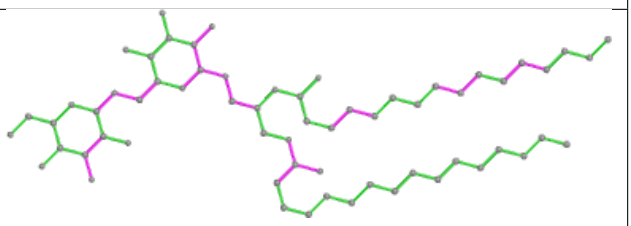
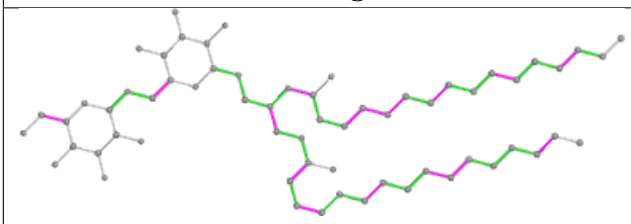
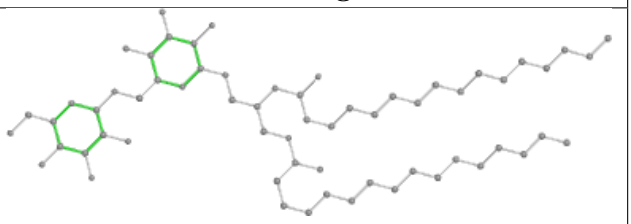


Bond angles

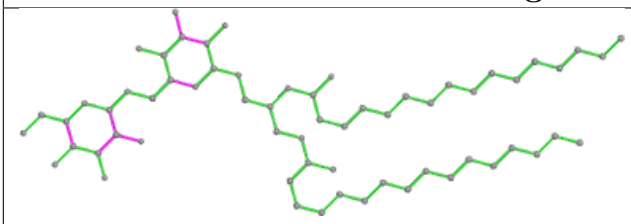


Torsions



Rings

Ligand DGD c 516



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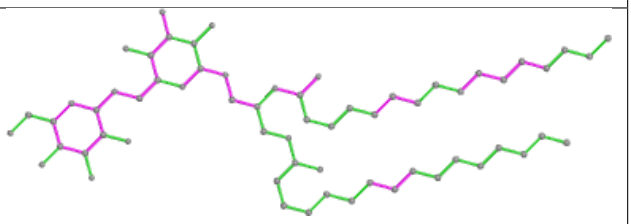
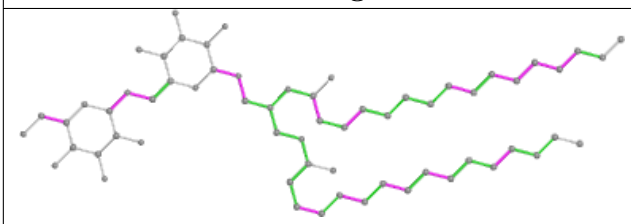
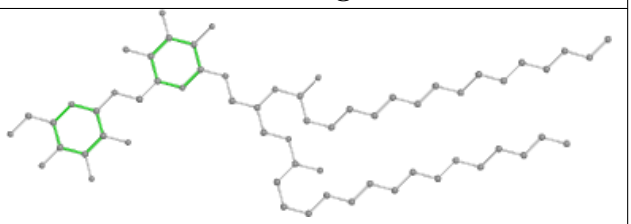


Bond angles

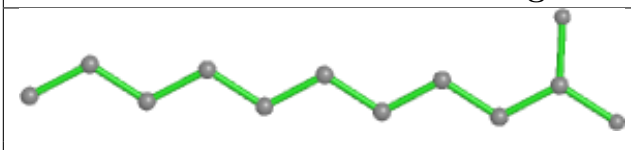


Torsions



Rings

Ligand STE B 622



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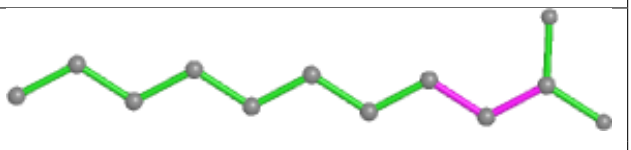
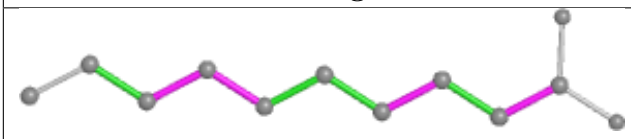
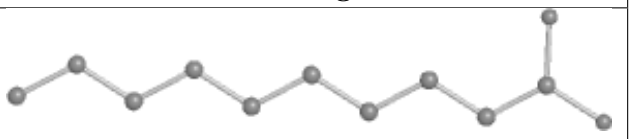


Bond angles

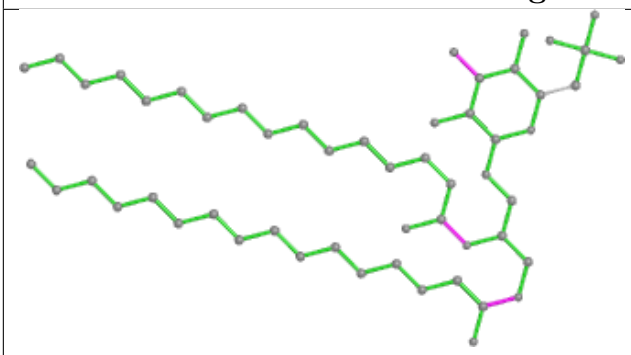


Torsions



Rings

Ligand SQD a 410



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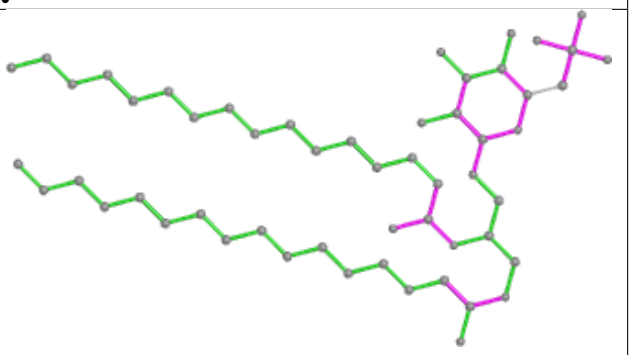
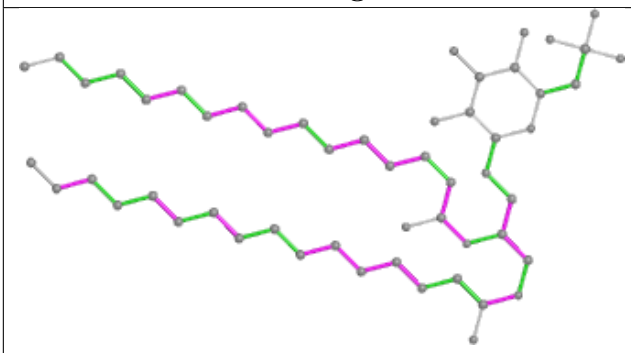


Bond angles



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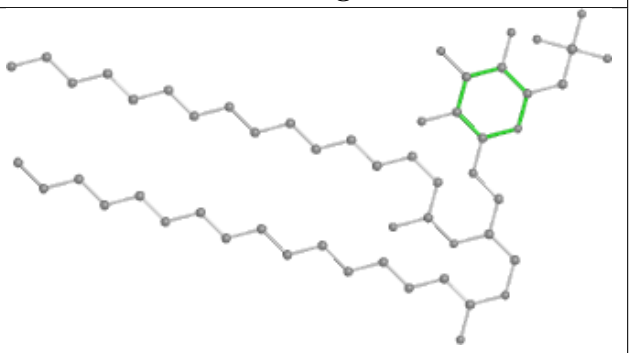
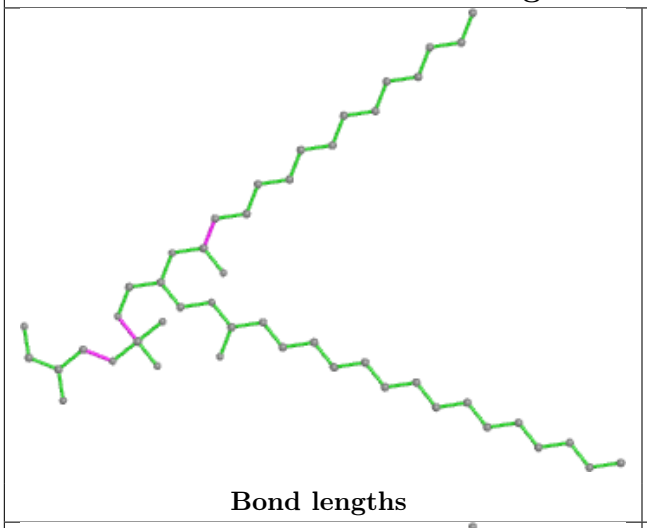
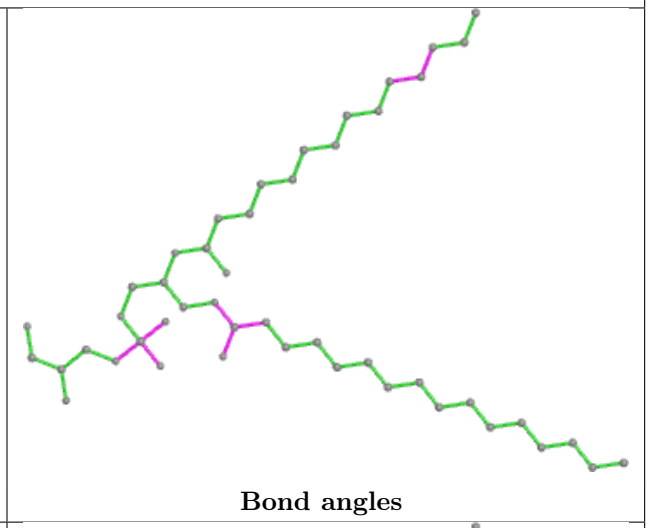


Rings

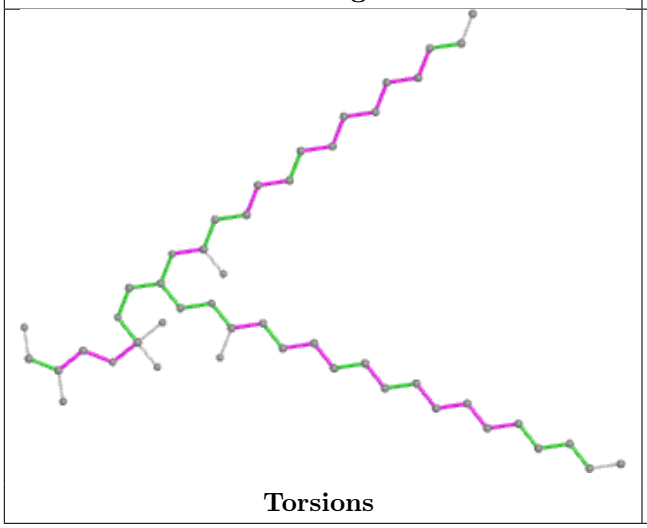
Ligand LHG D 411



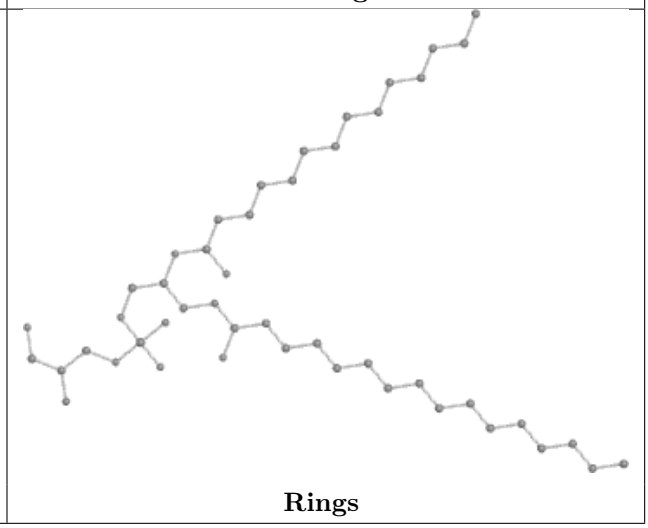
Bond lengths



Bond angles

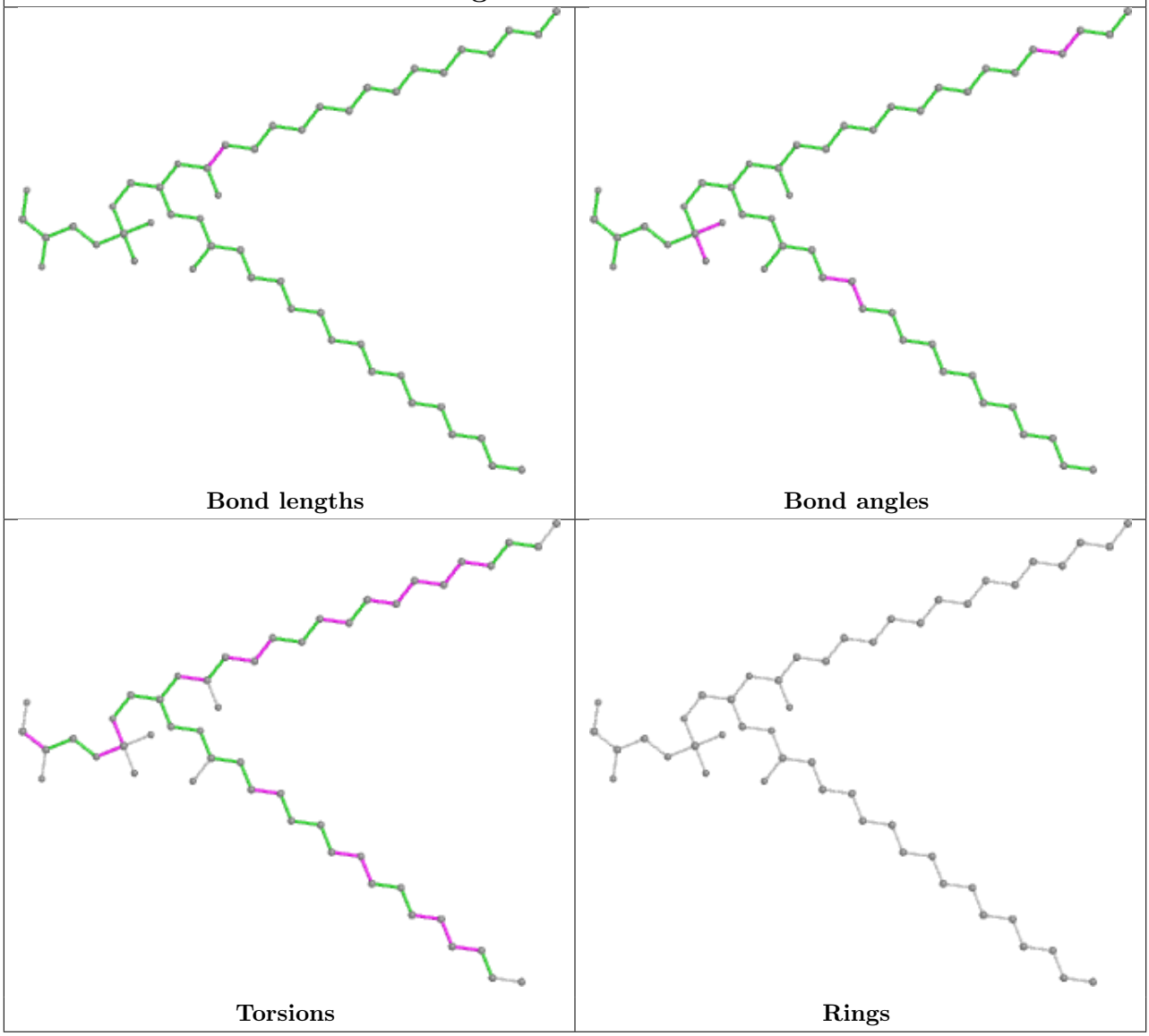


Torsions

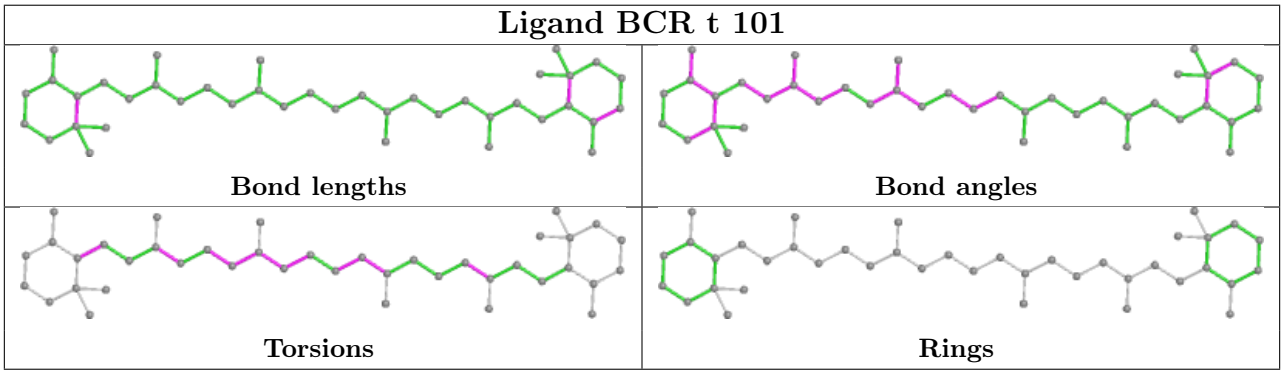


Rings

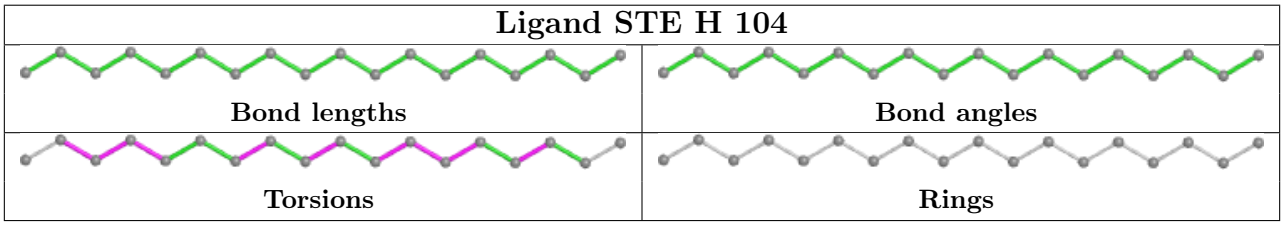
Ligand LHG d 408



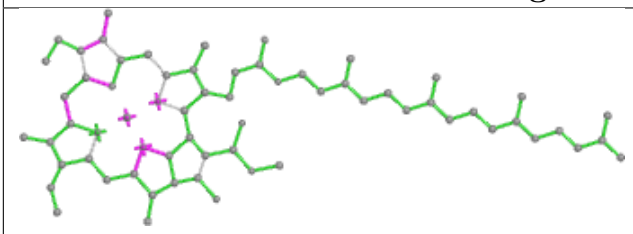
Ligand BCR t 101



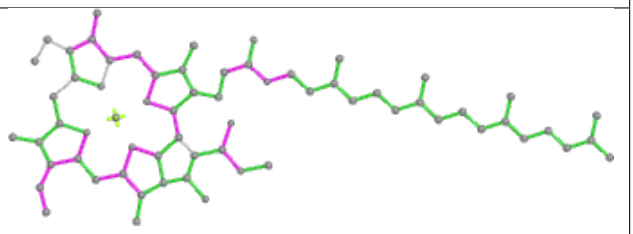
Ligand STE H 104



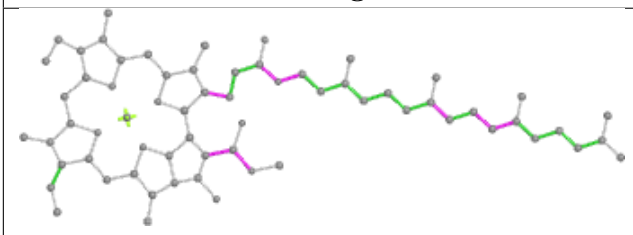
Ligand CLA c 506



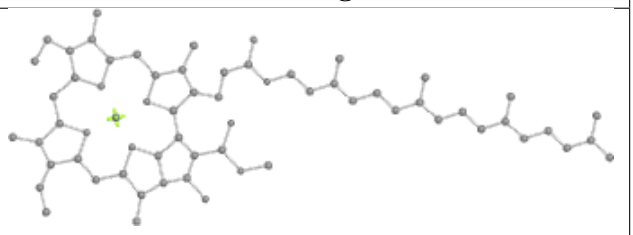
Bond lengths



Bond angles

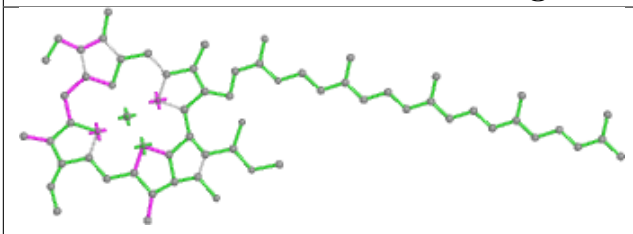


Torsions



Rings

Ligand CLA c 502



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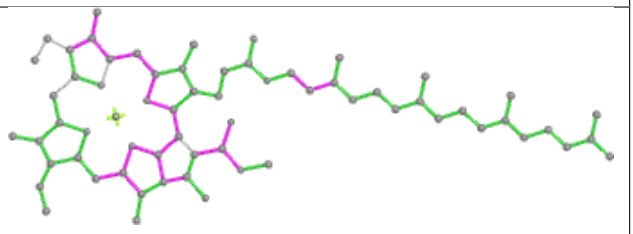
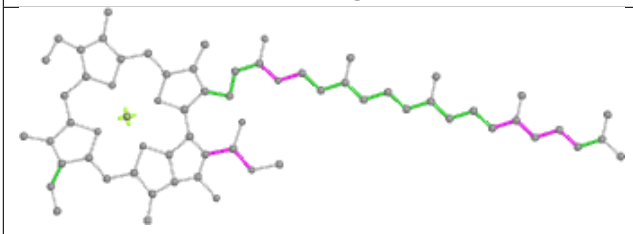
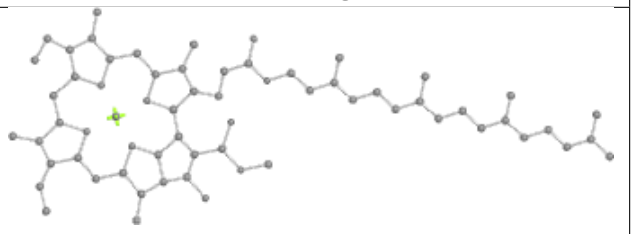


Bond angles

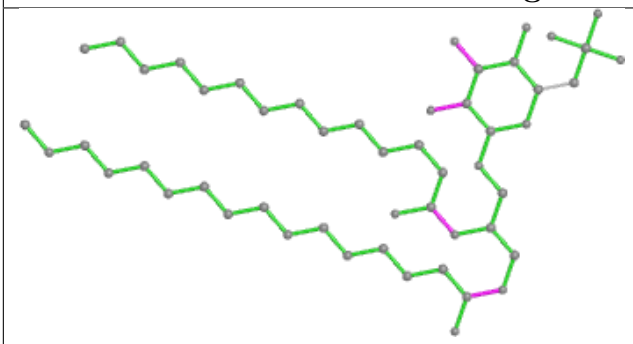


Torsions



Rings

Ligand SQD A 410



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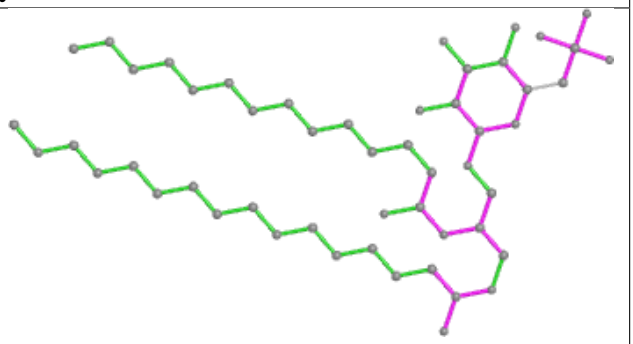
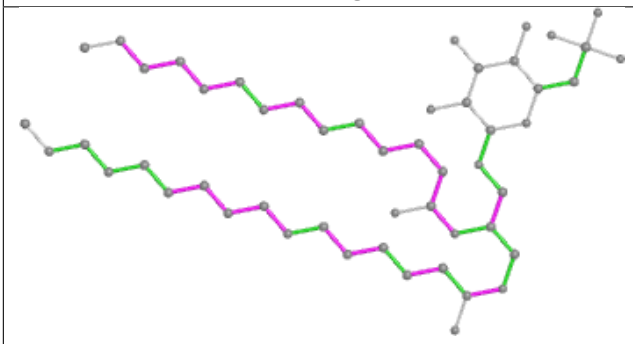


Bond angles



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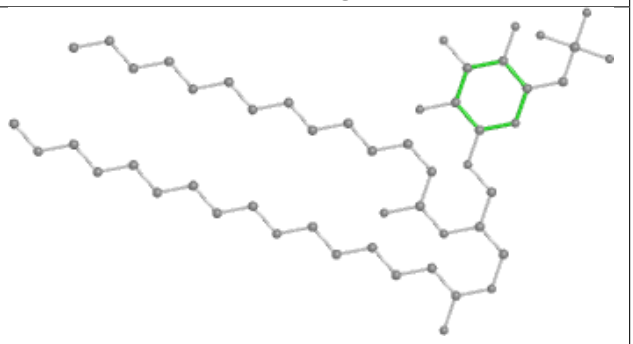
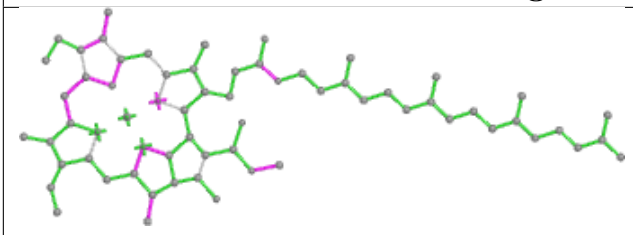


Rings

Ligand CLA b 606



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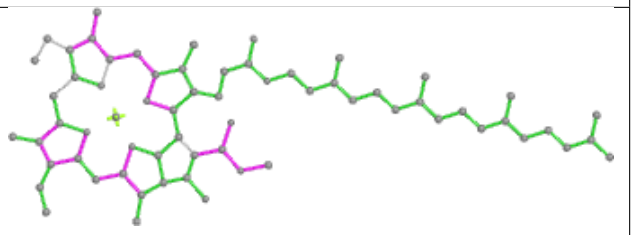
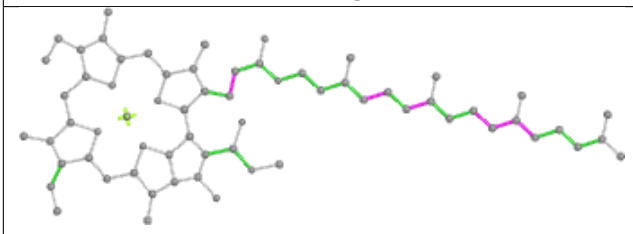


Bond angles



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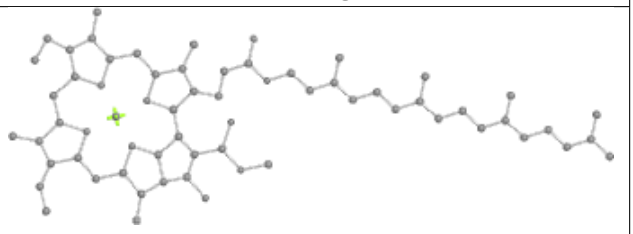
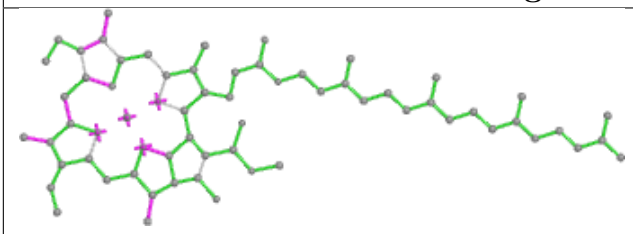


Rings

Ligand CLA C 508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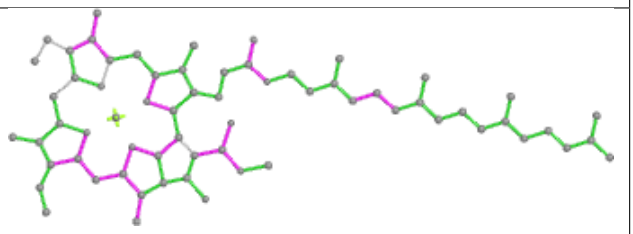
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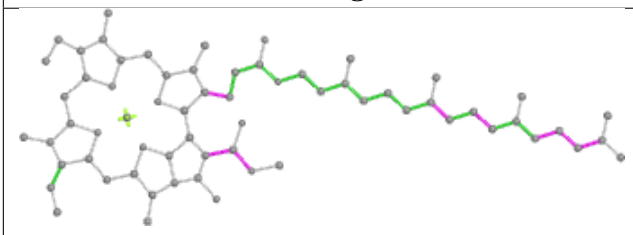
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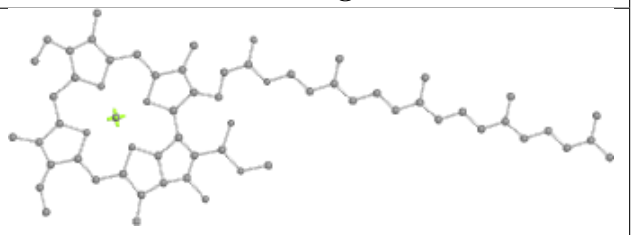
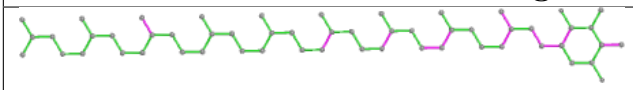

Rings

Ligand PL9 d 407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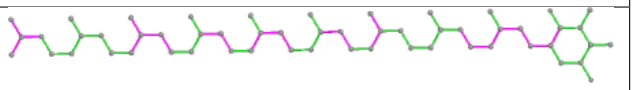
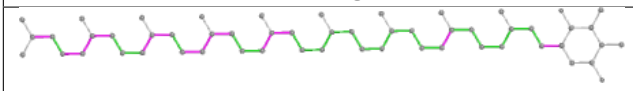

Bond angles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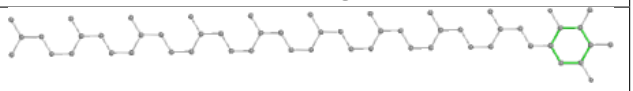
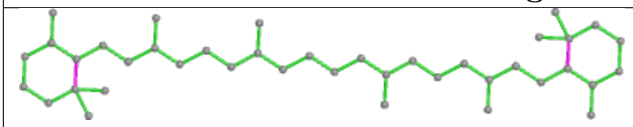

Rings

Ligand BCR k 101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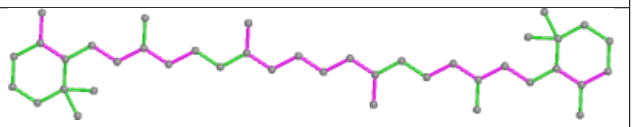
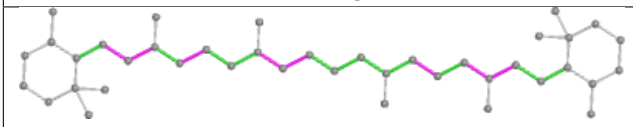

Bond angles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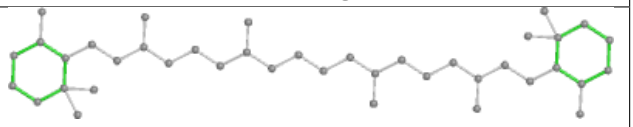
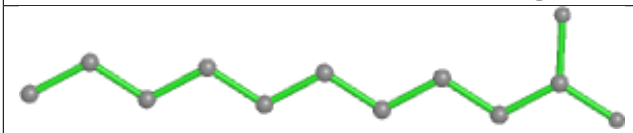

Rings

Ligand STE k 104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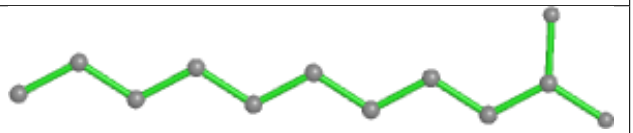
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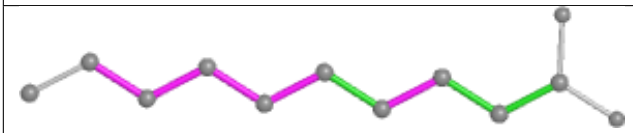
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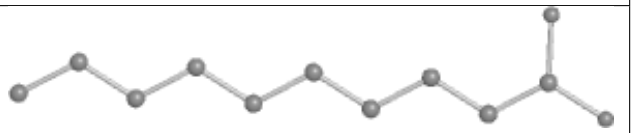
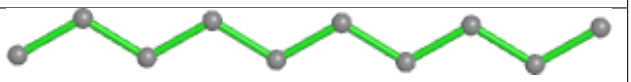
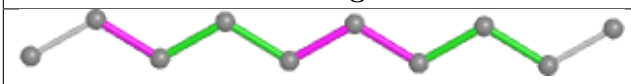

Rings

Ligand STE t 104

Bond lengths



Bond angles



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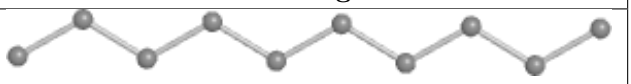
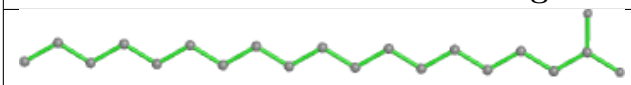


Rings

Ligand STE x 102



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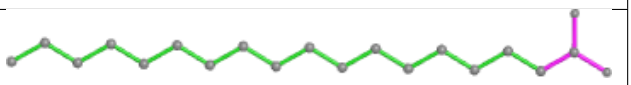

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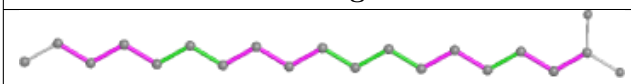

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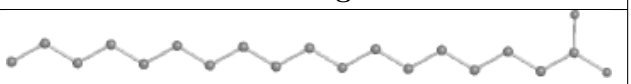
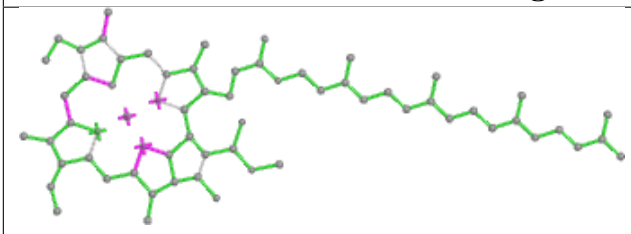


Rings

Ligand CLA c 511



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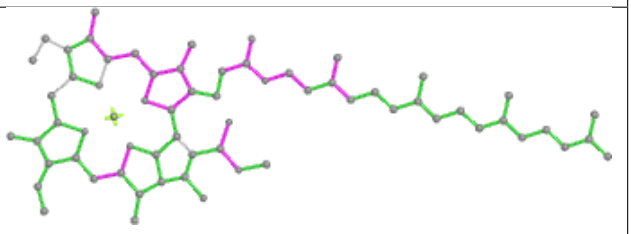

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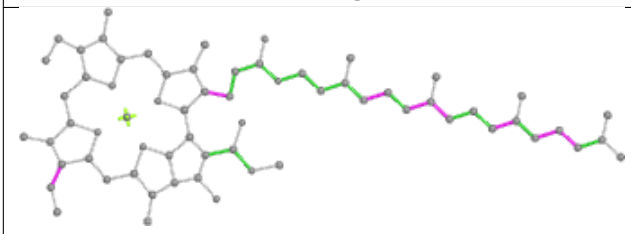

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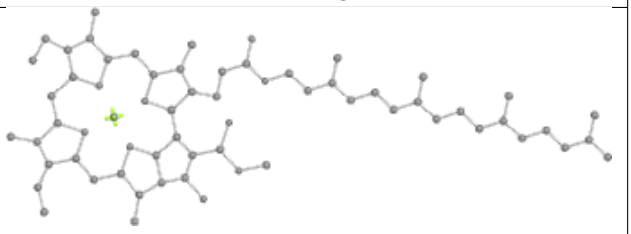
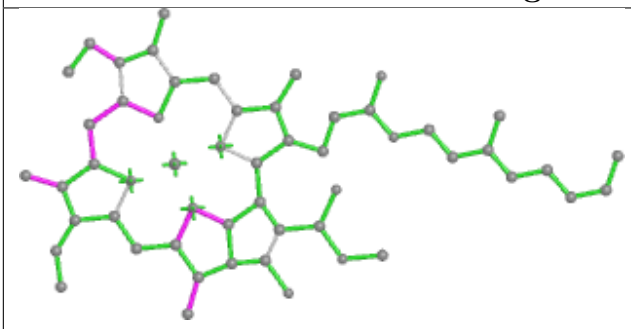


Rings

Ligand CLA A 405



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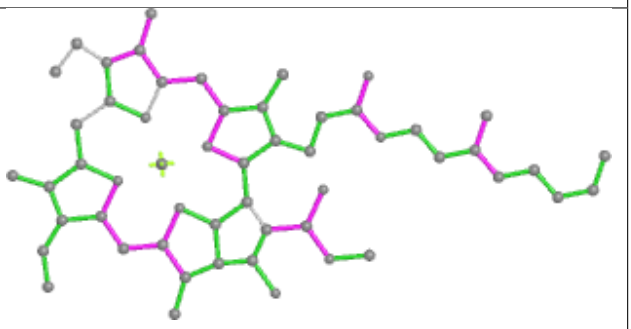
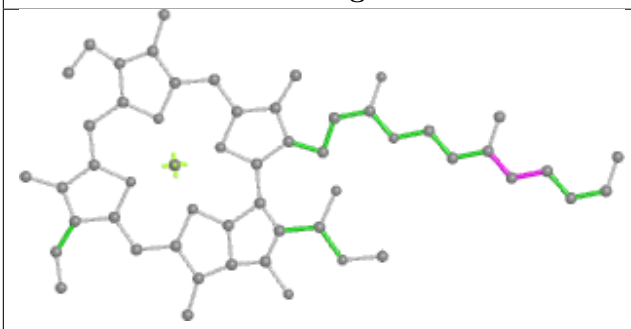


Bond angles



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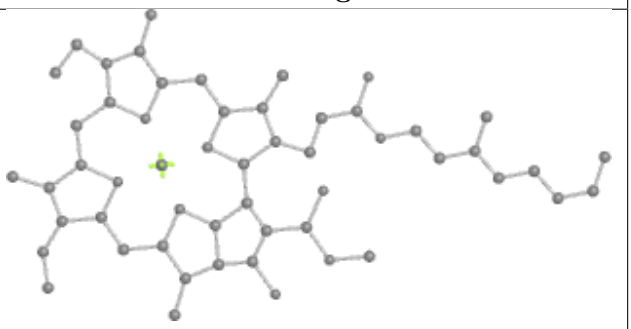
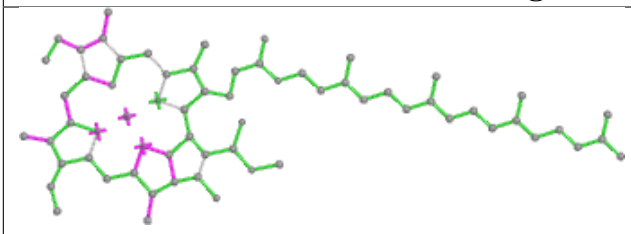


Rings

Ligand CLA b 609



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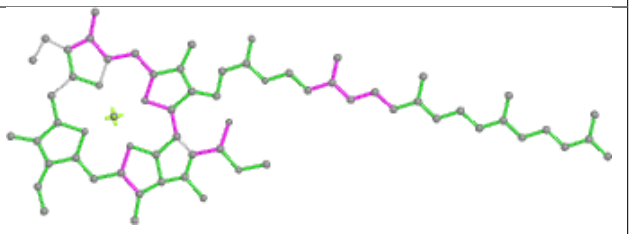
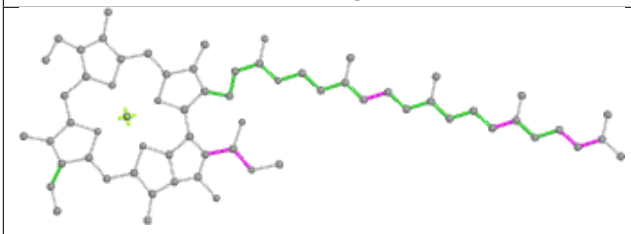
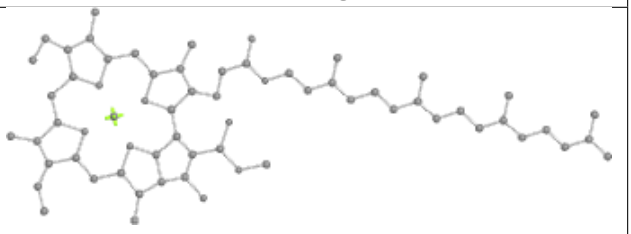


Bond angles

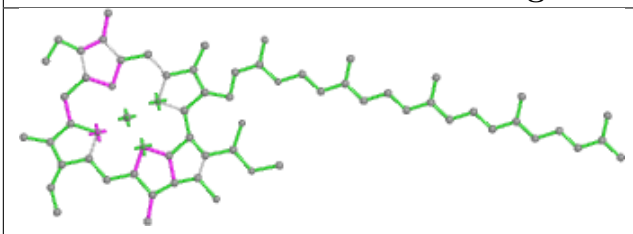


Torsions



Rings

Ligand CLA d 403



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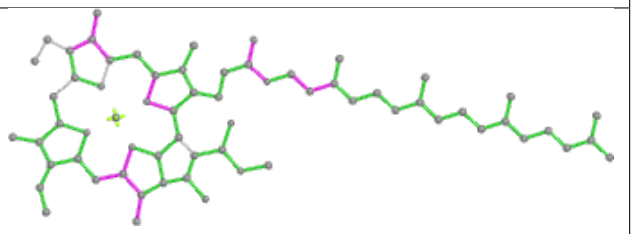
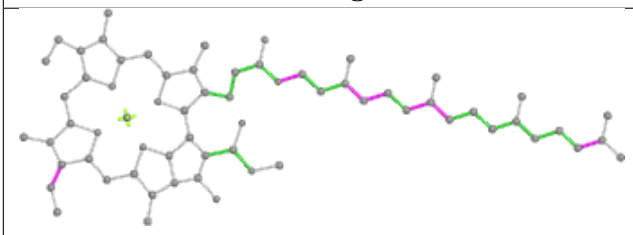


Bond angles



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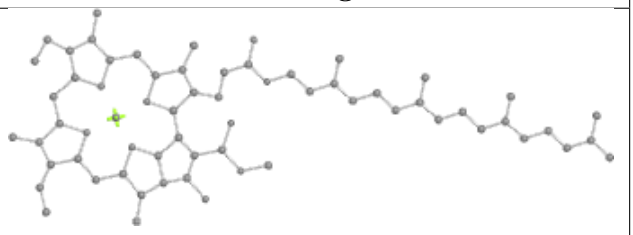
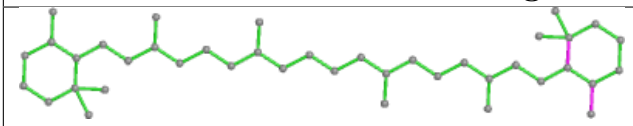
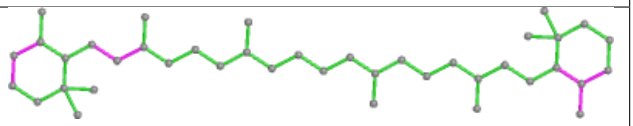


Rings

Ligand BCR T 101



Bond lengths



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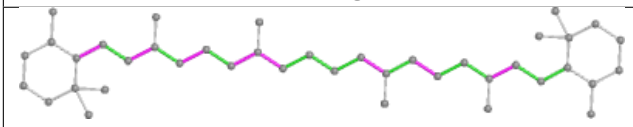
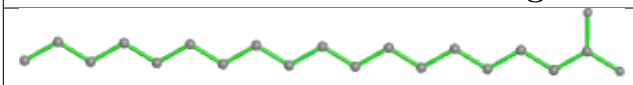


Torsions

Rings

Ligand STE X 101



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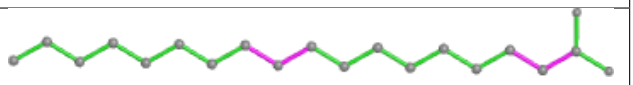

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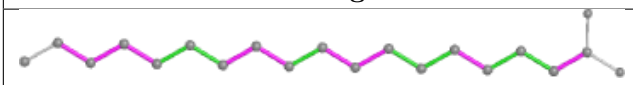
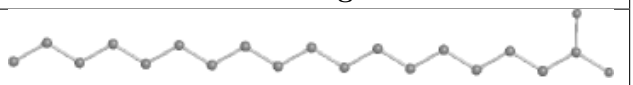
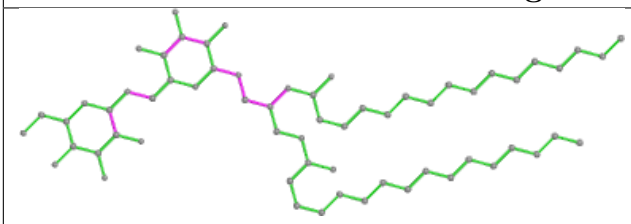


Torsions



Rings

Ligand DGD c 515



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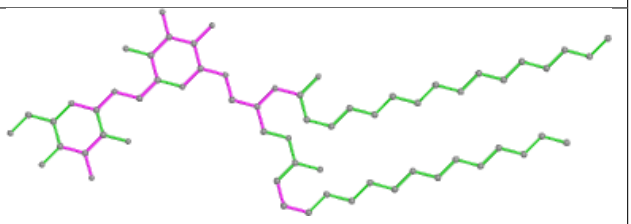

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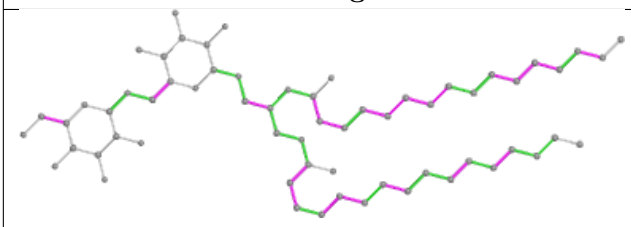

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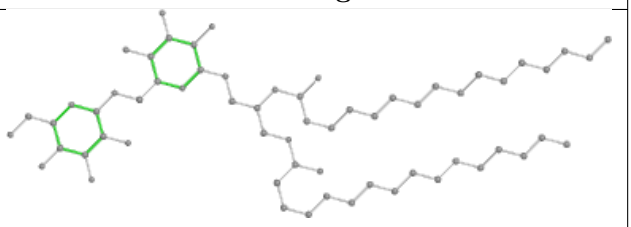
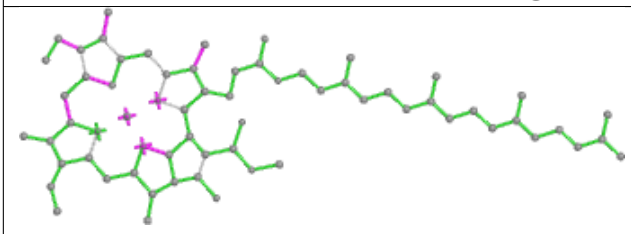


Rings

Ligand CLA d 404



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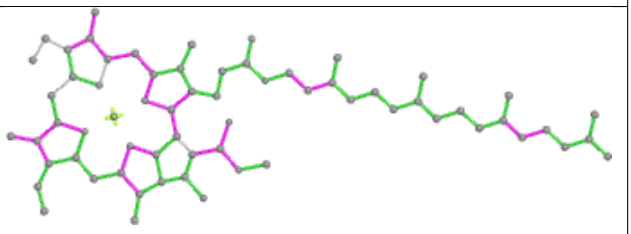
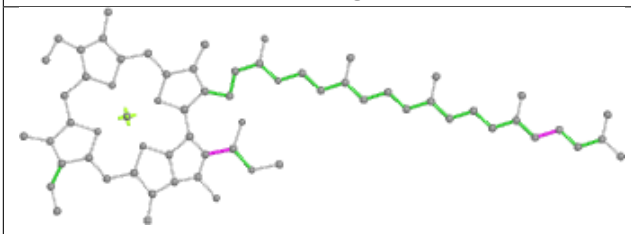
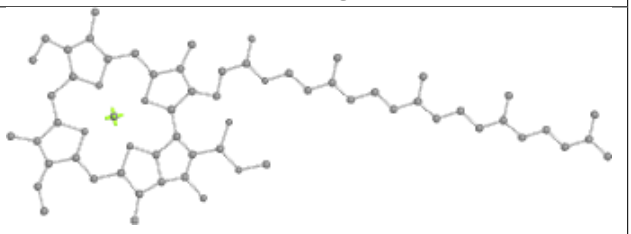


Bond angles

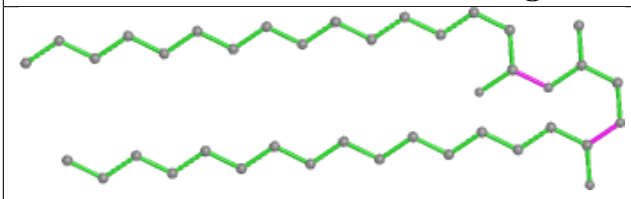


Torsions



Rings

Ligand SQD A 412



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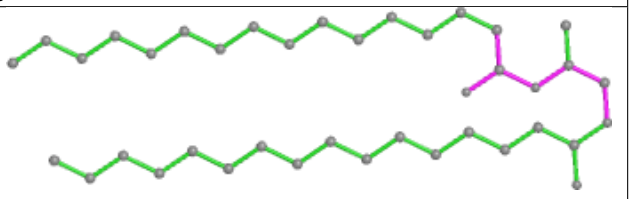

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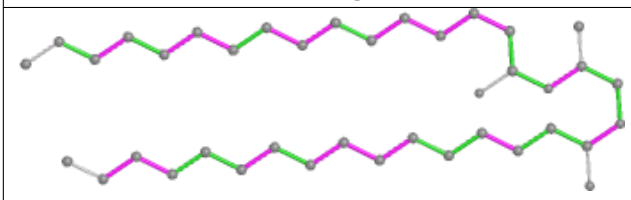

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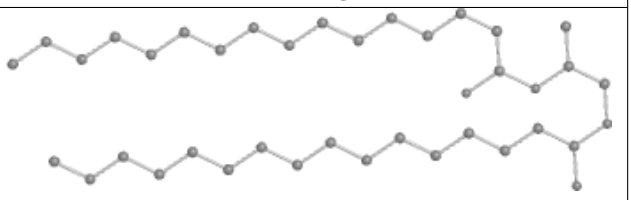
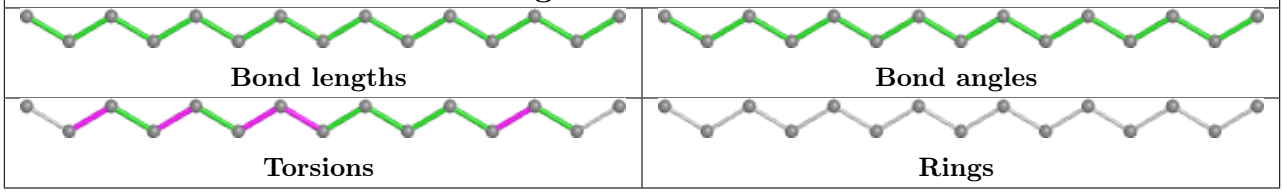
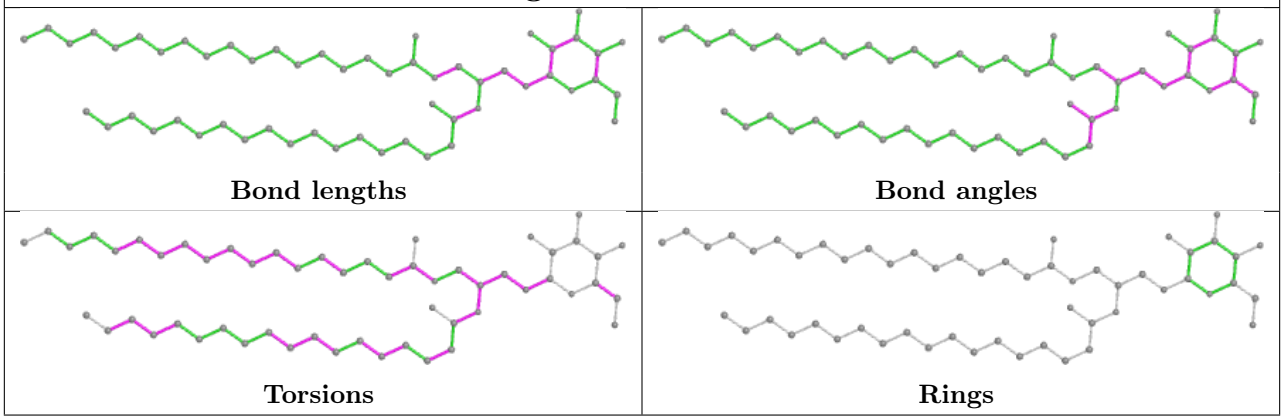


Rings

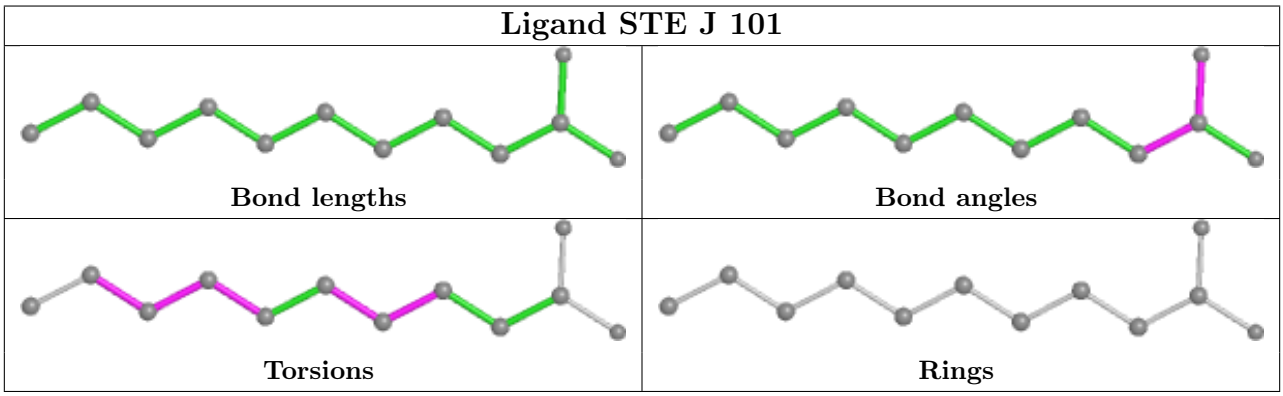
Ligand STE I 102



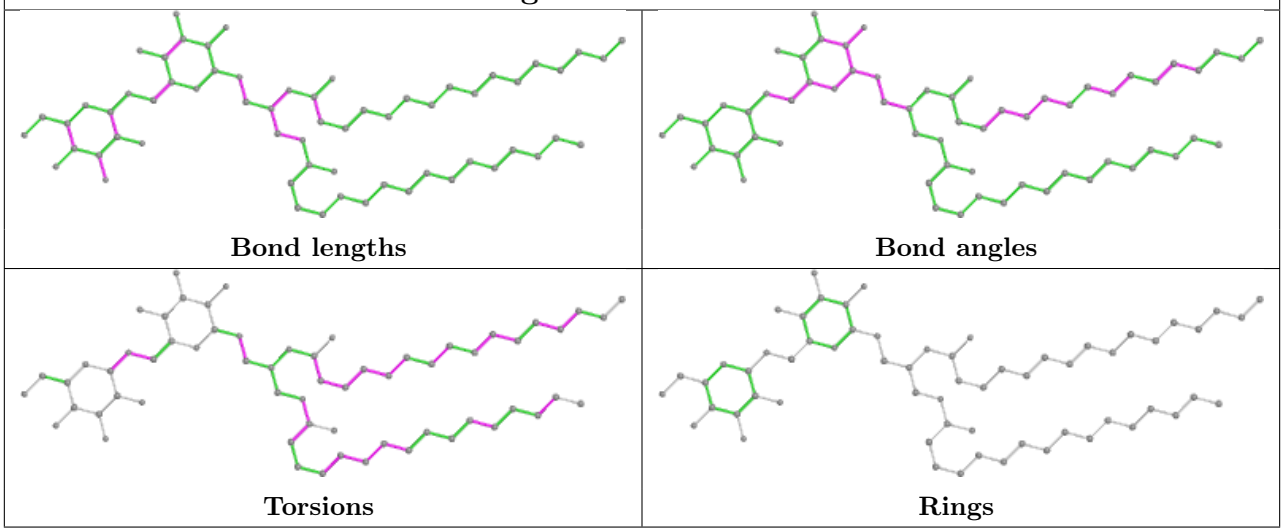
Ligand LMG a 414



Ligand STE J 101



Ligand DGD C 517



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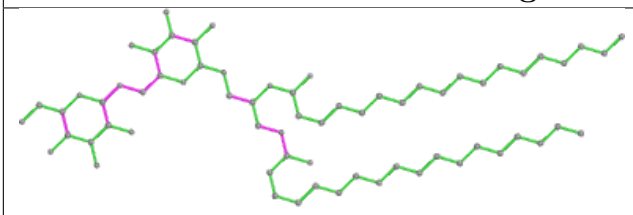

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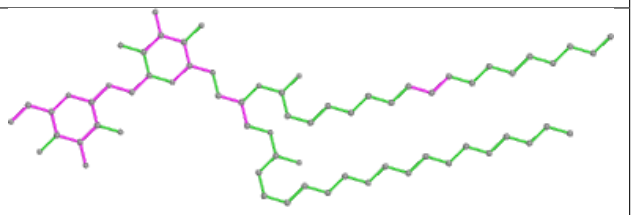
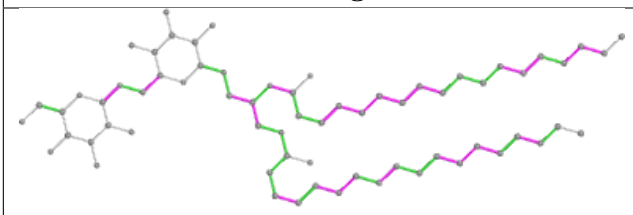
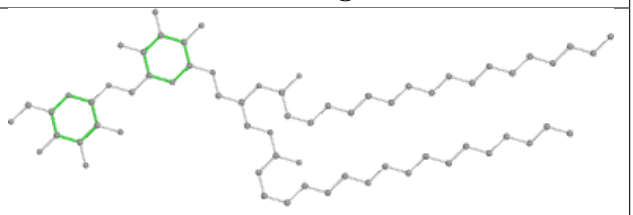


Bond angles

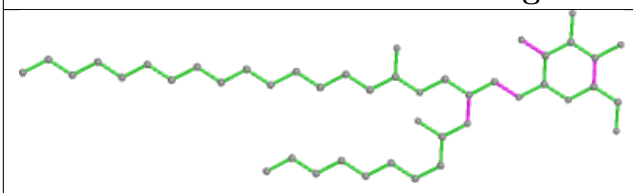


Torsions



Rings

Ligand LMG d 410



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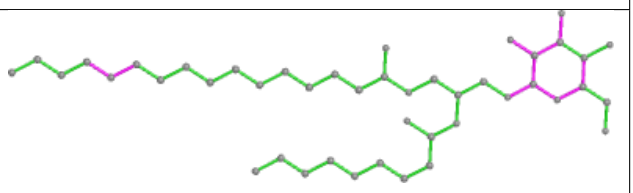

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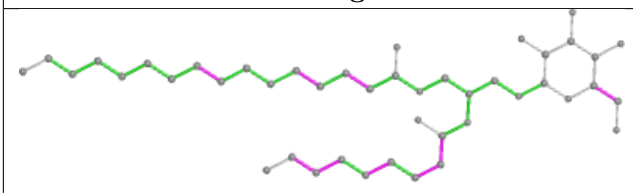

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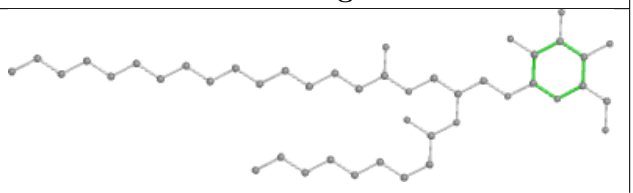
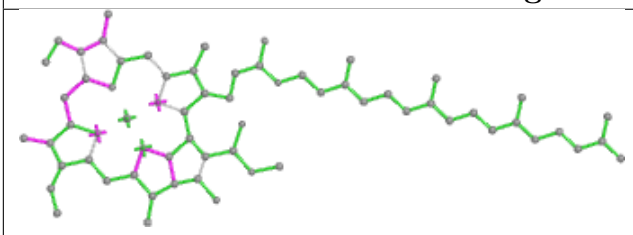


Rings

Ligand CLA B 606



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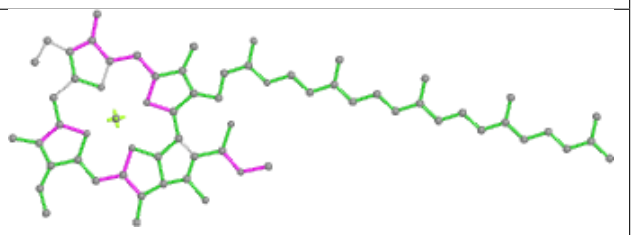
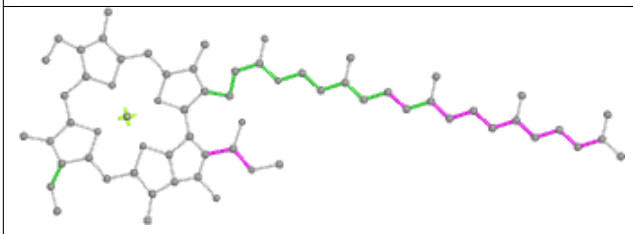


Bond angles



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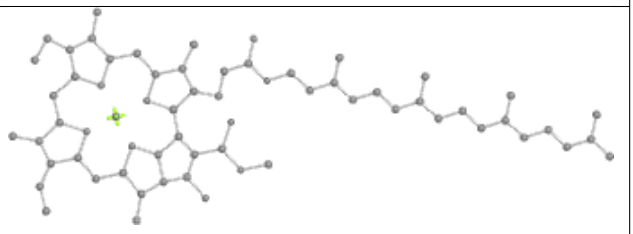
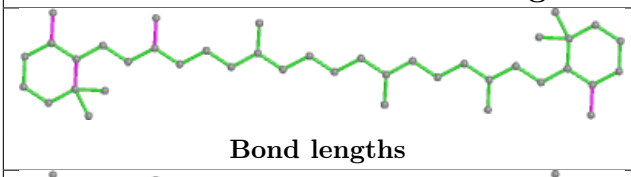


Rings

Ligand BCR I 101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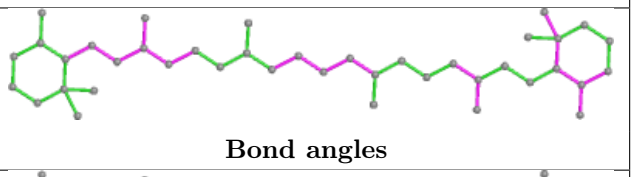
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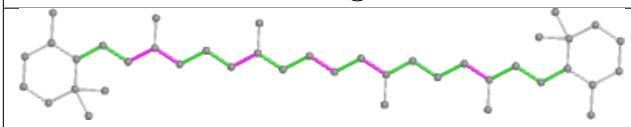
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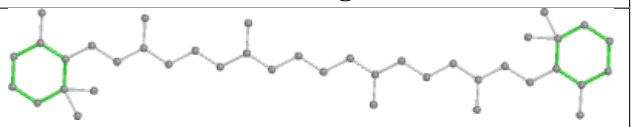
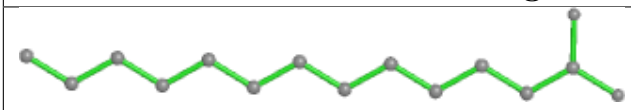

Rings

Ligand STE M 102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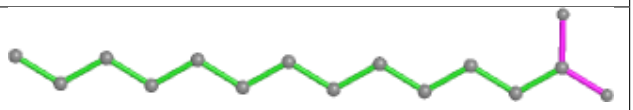
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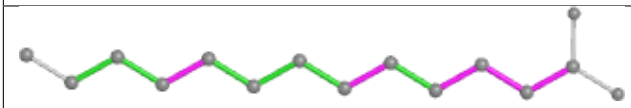
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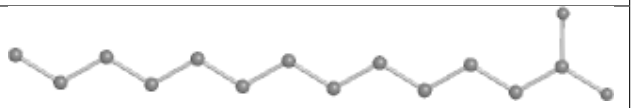
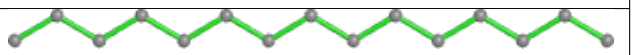

Rings

Ligand STE a 413

Bond lengths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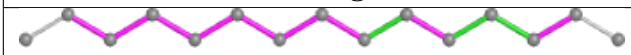
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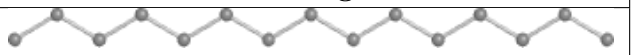
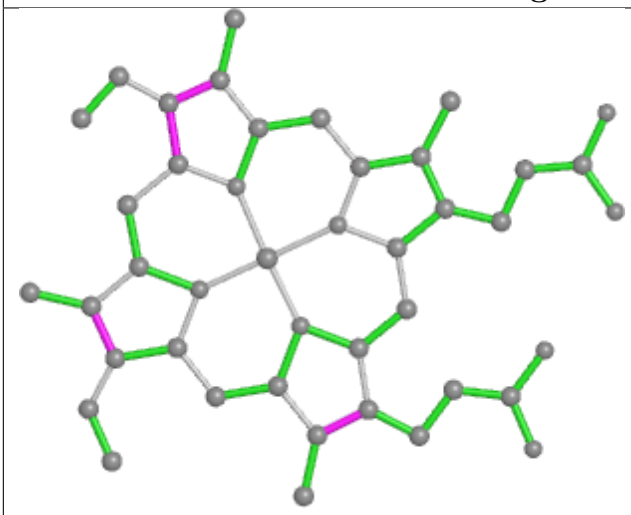

Rings

Ligand HEC f 101



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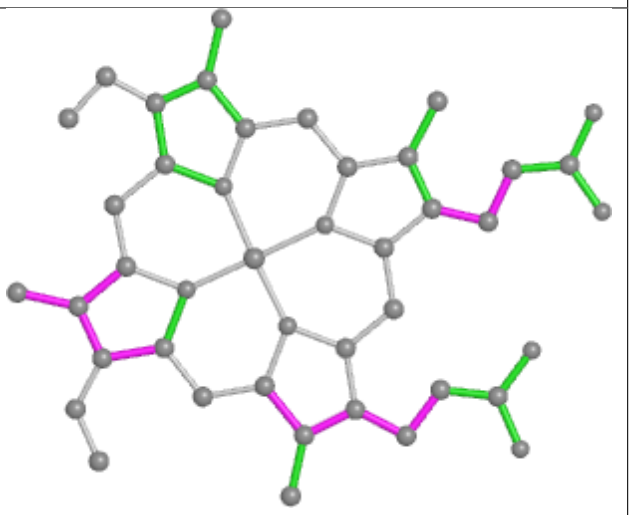
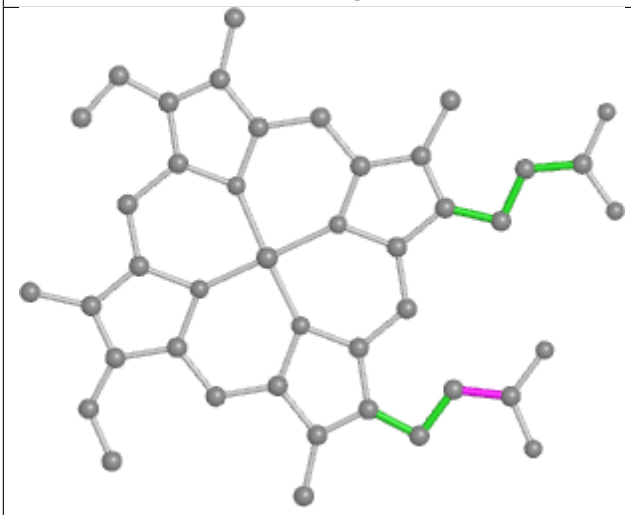


Bond angles



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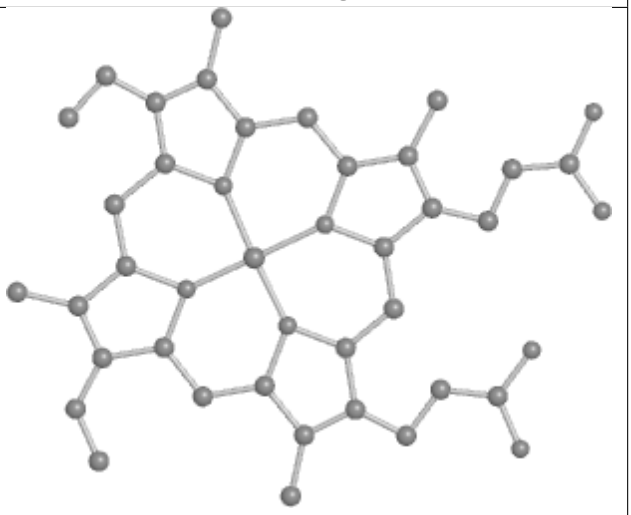
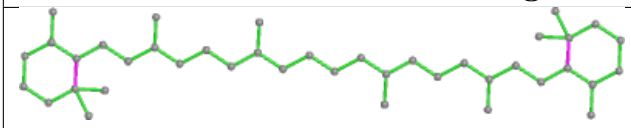


Rings

Ligand BCR B 618



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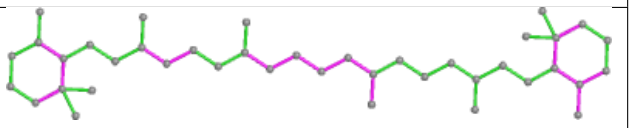
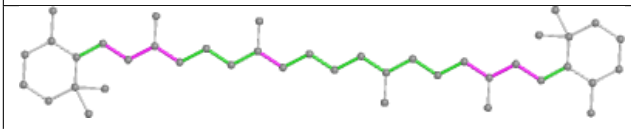


Bond angles



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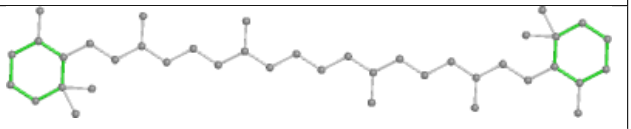
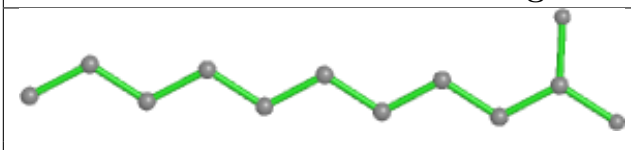


Rings

Ligand STE R 101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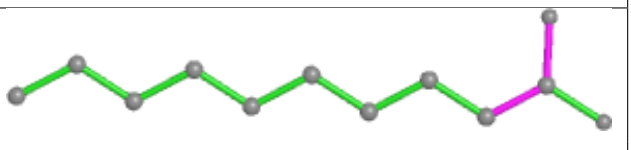
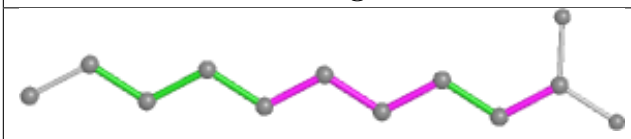
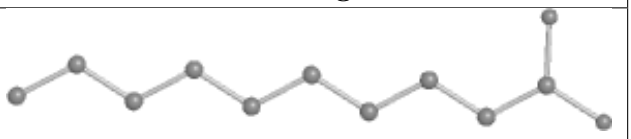
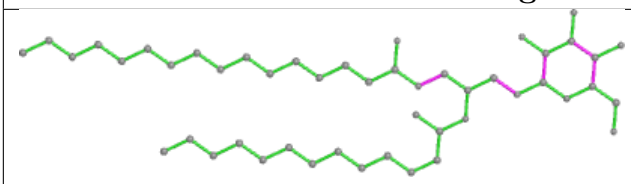
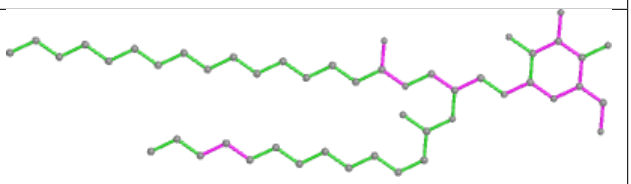

Bond angles


Torsions


Rings

Ligand LMG A 409


Bond lengths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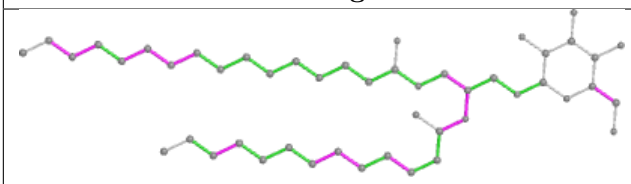
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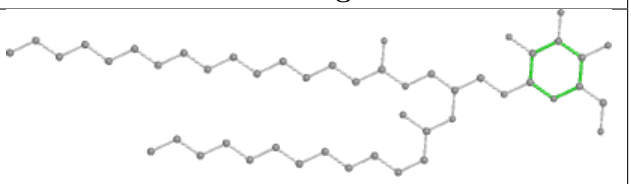
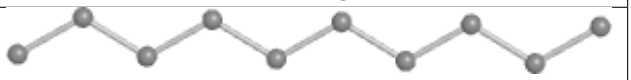

Rings

Ligand STE b 627

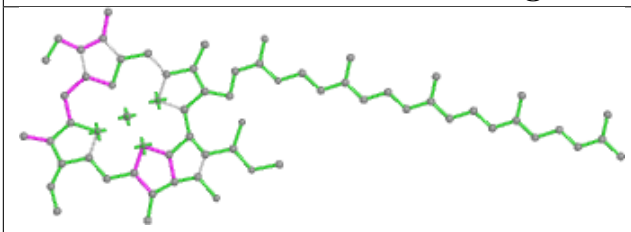
Bond lengths

Bond angles

Torsions


Rings

Ligand CLA C 513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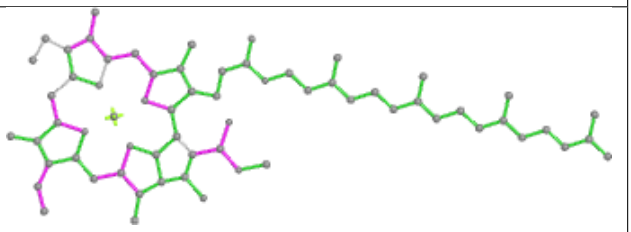
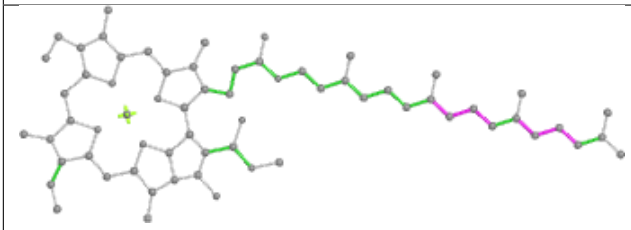
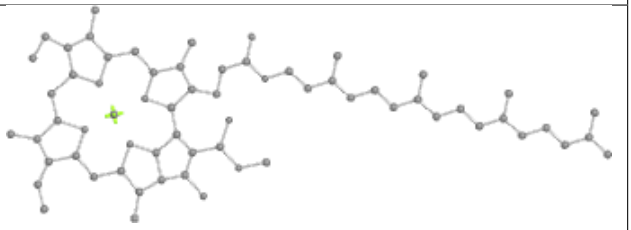
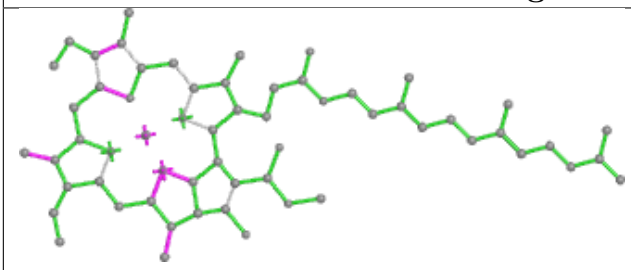

Bond angles

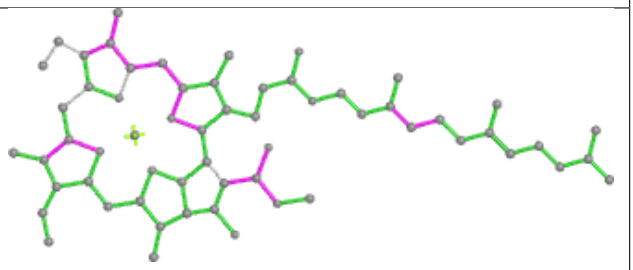

Torsions


Rings

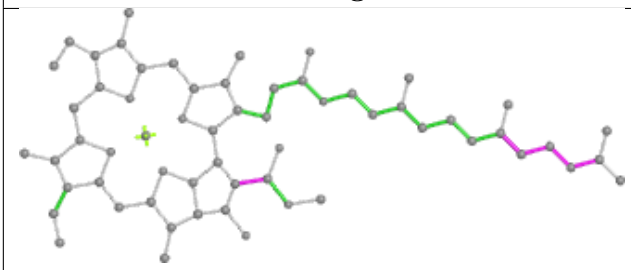
Ligand CLA b 616



Bond lengths



Bond angles



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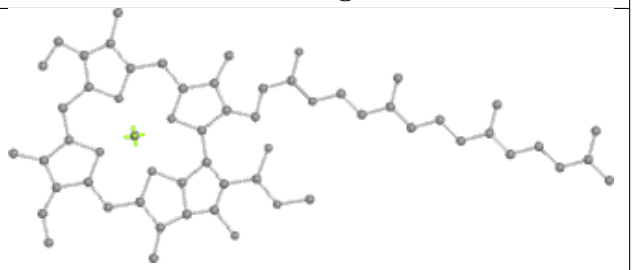
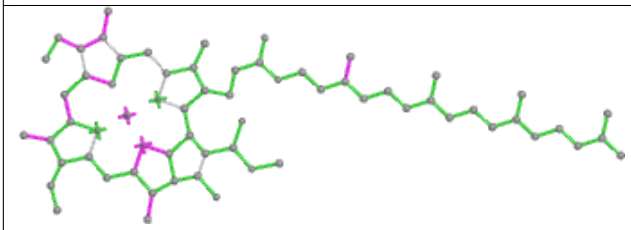


Rings

Ligand CLA B 612



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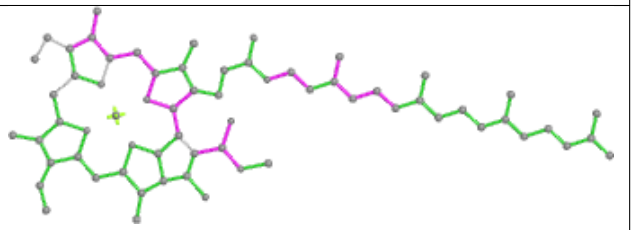
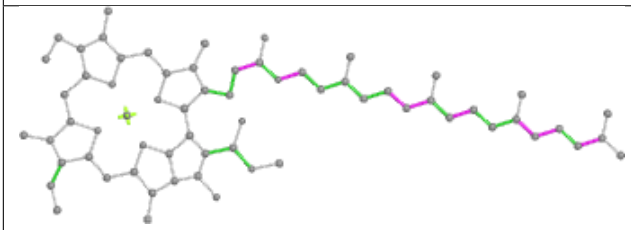


Bond angles



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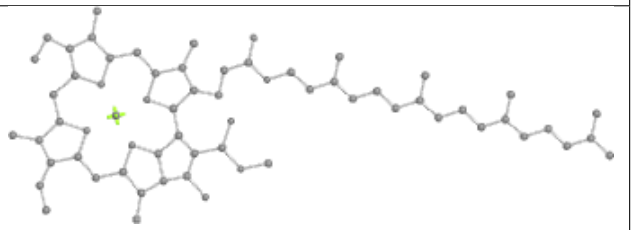
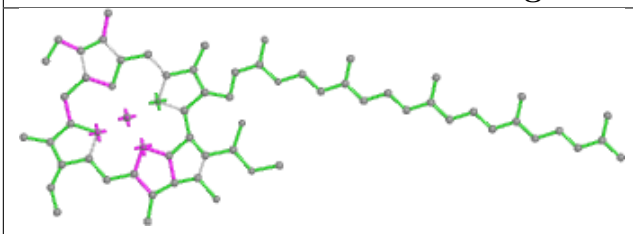


Rings

Ligand CLA C 503



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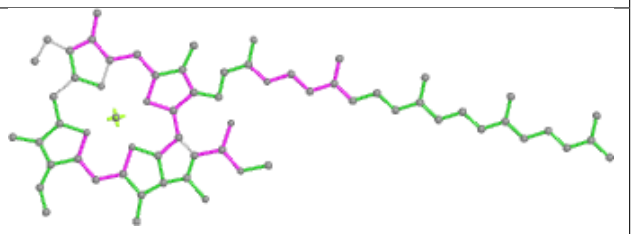

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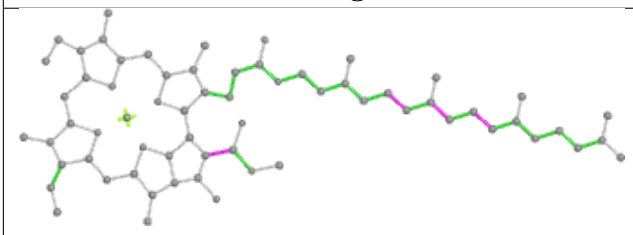

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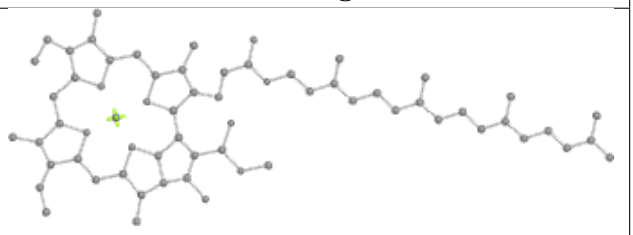
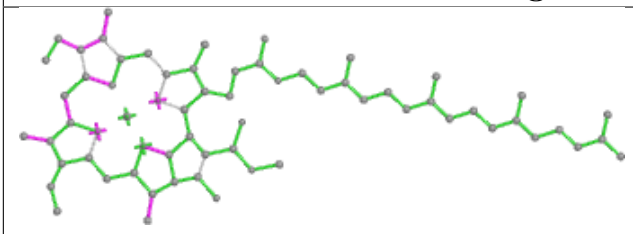


Rings

Ligand CLA b 603



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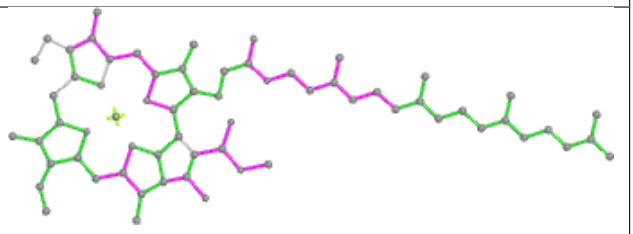
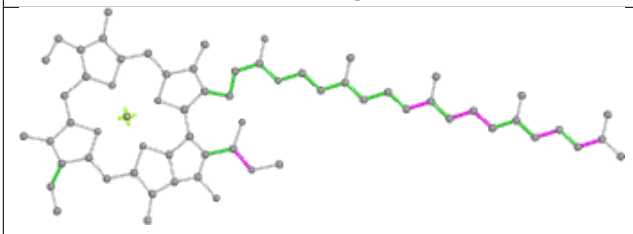


Bond angles



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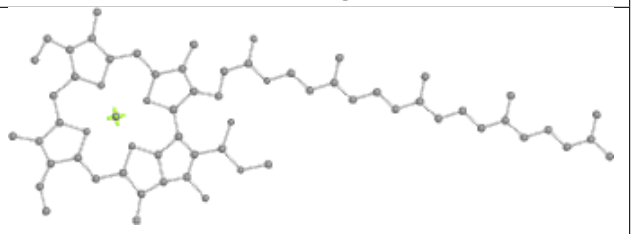
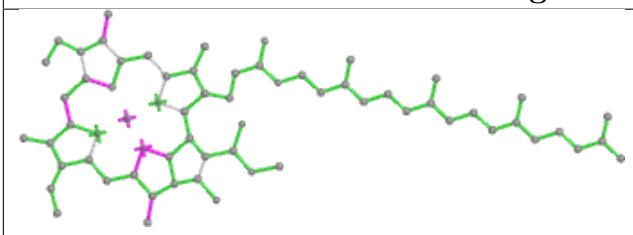


Rings

Ligand CLA c 513



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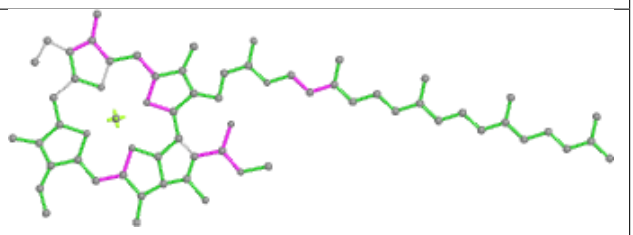
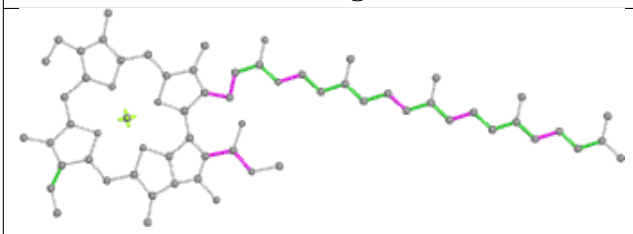


Bond angles



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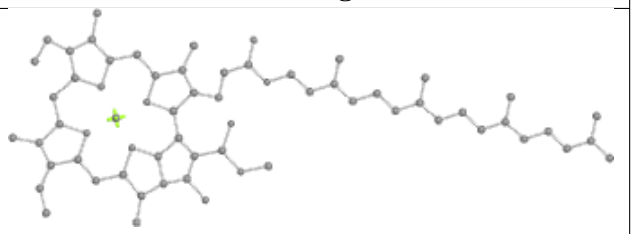
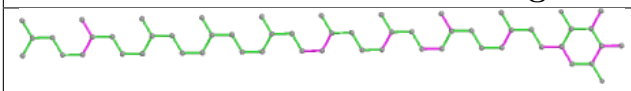


Rings

Ligand PL9 D 407



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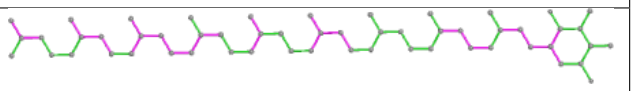
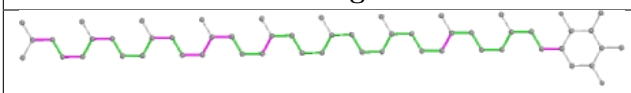


Bond angles



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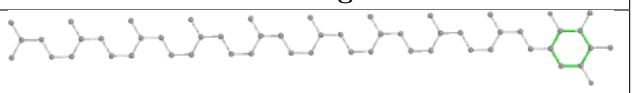
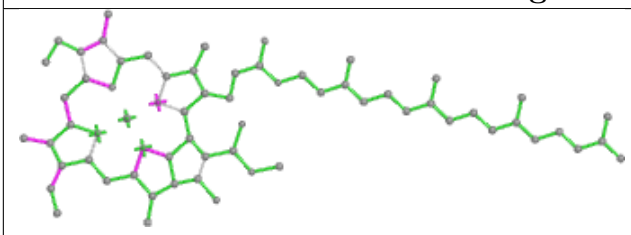


Rings

Ligand CLA c 503



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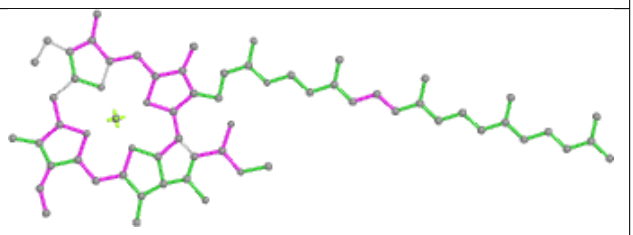
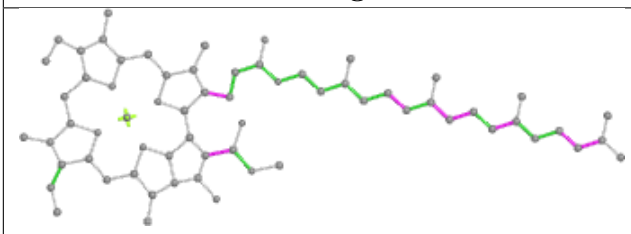


Bond angles



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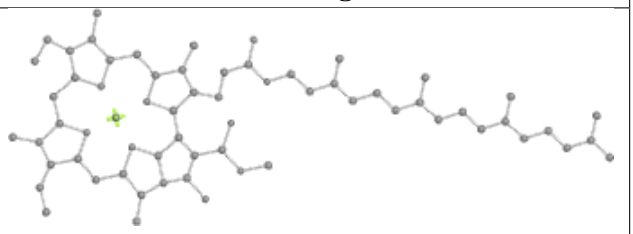
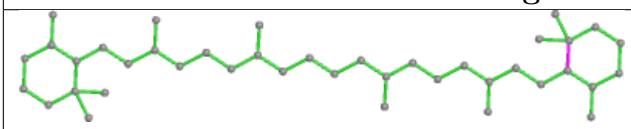


Rings

Ligand BCR B 617



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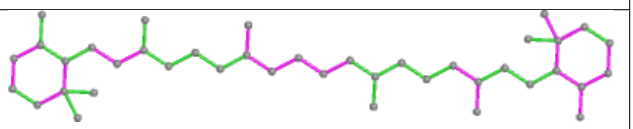
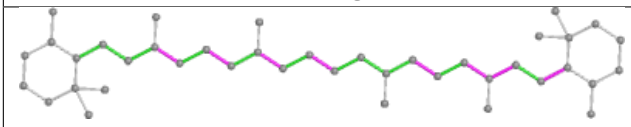


Bond angles



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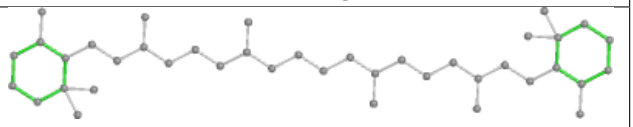
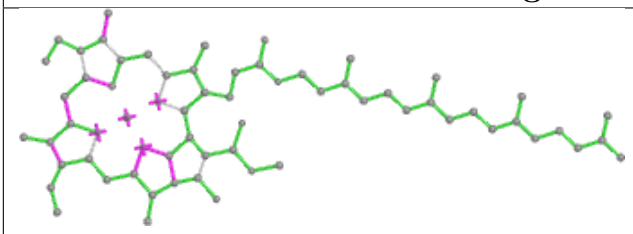


Rings

Ligand CLA D 404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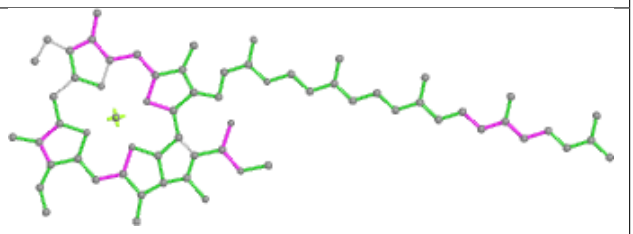
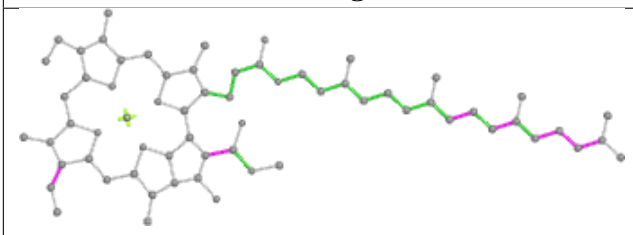

Bond angles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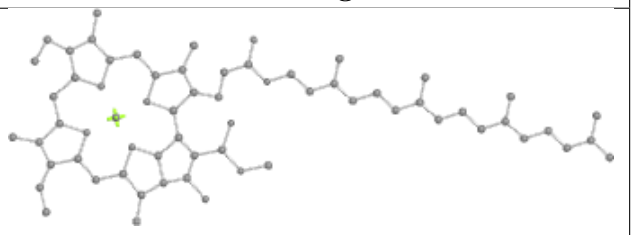
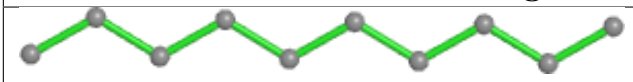

Rings

Ligand STE M 103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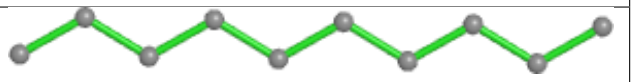
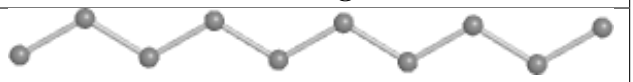

Bond angles

Torsions

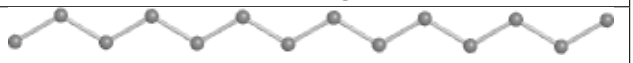

Rings

Ligand STE b 628

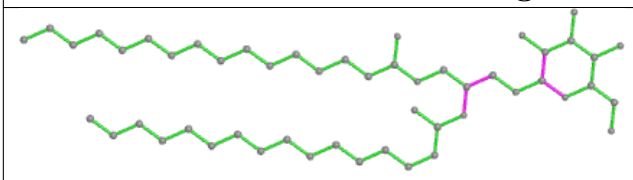
Bond lengths

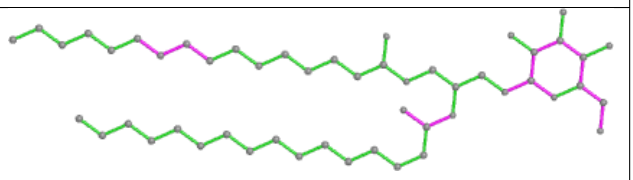
Bond angles

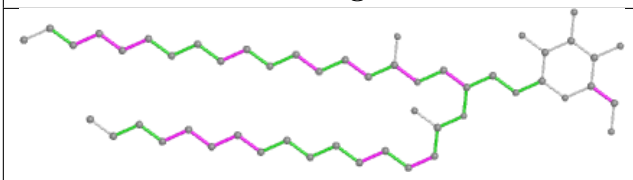
Torsions


Rings

Ligand LMG M 101


Bond lengths


Bond angles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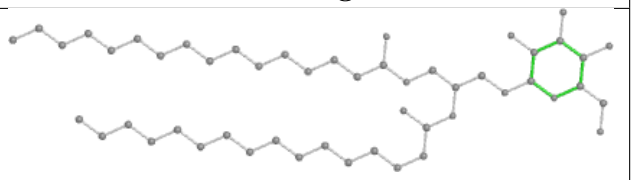
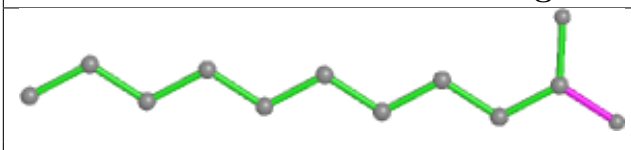
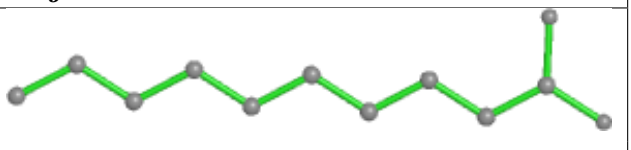

Rings

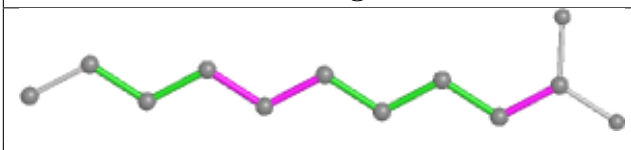
Ligand STE j 101



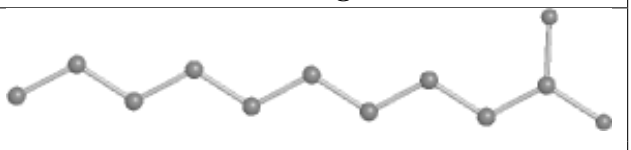
Bond lengths



Bond angles

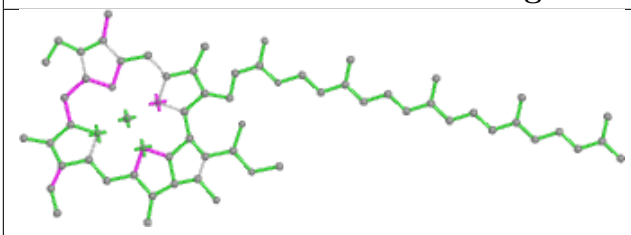


Torsions

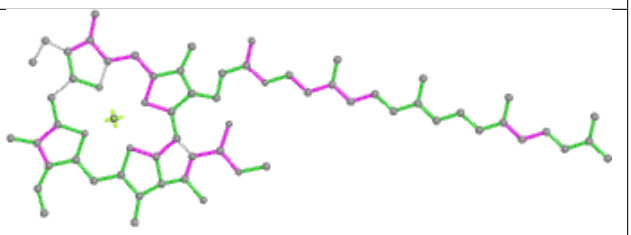


Rings

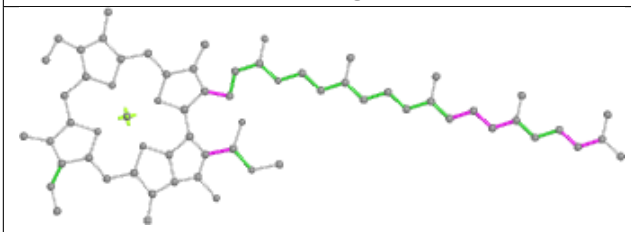
Ligand CLA B 601



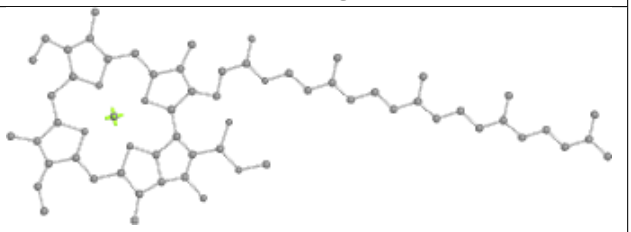
Bond lengths



Bond angles

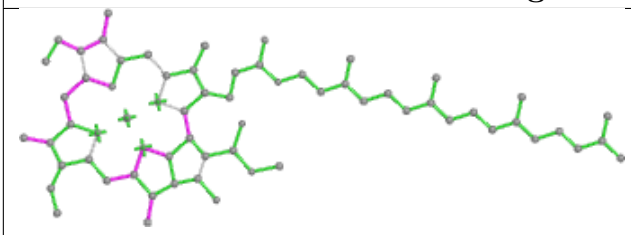


Torsions

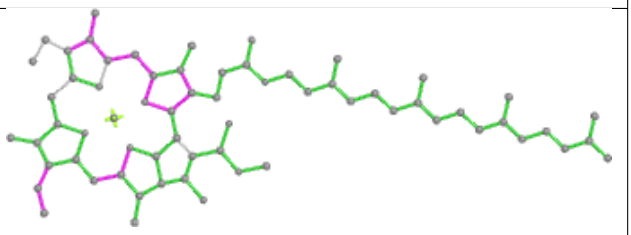


Rings

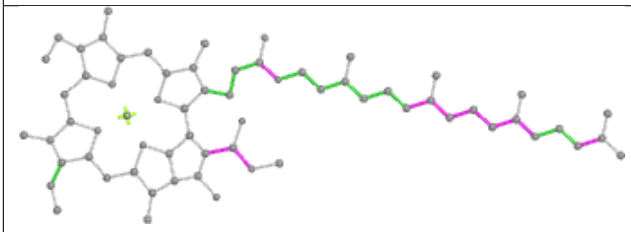
Ligand CLA b 607



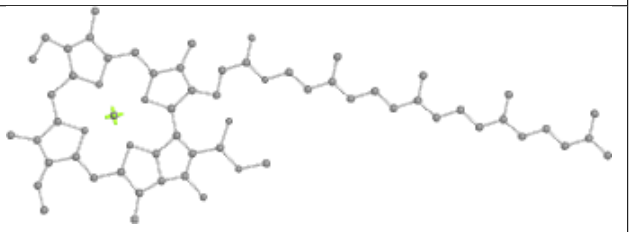
Bond lengths



Bond angles

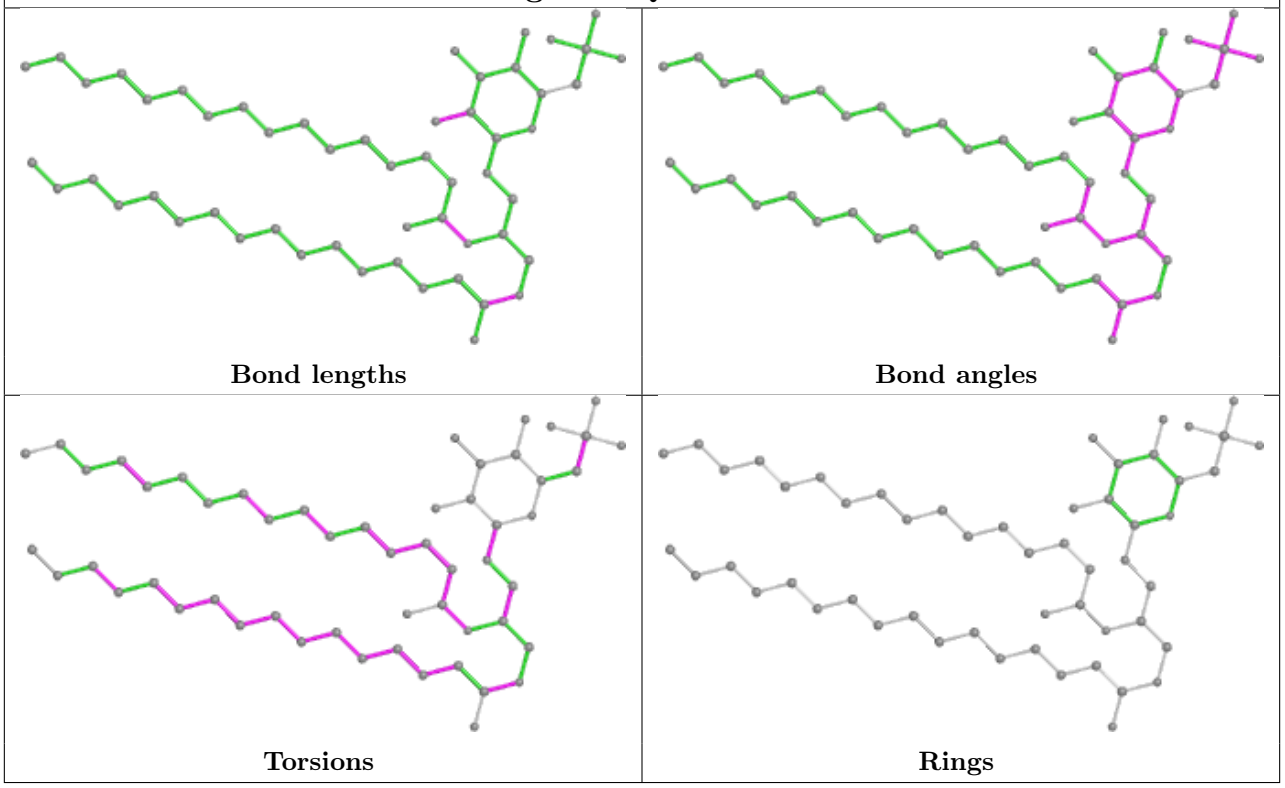


Torsions

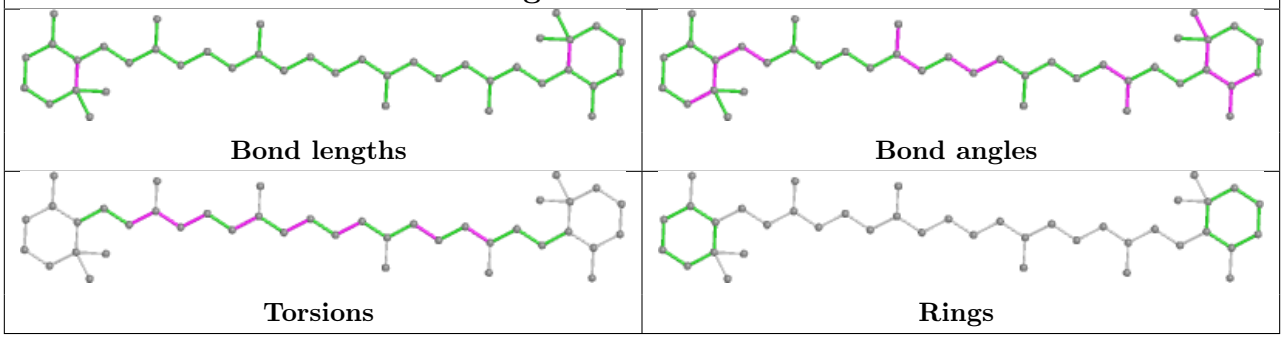


Rings

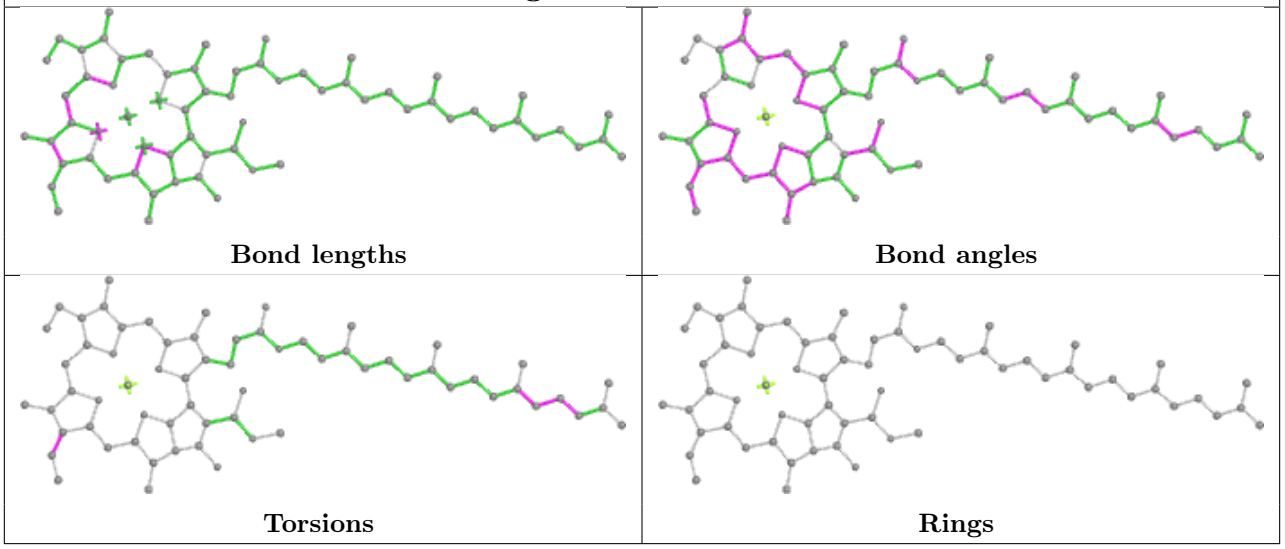
Ligand SQD B 621



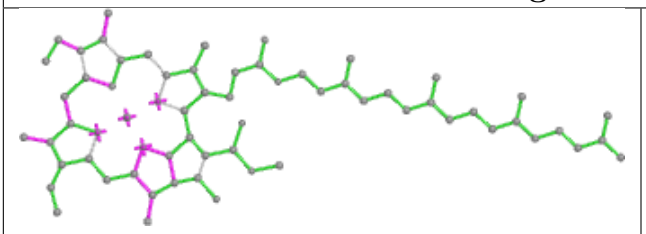
Ligand BCR C 515



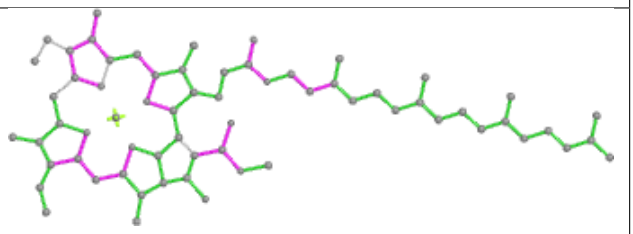
Ligand CLA A 402



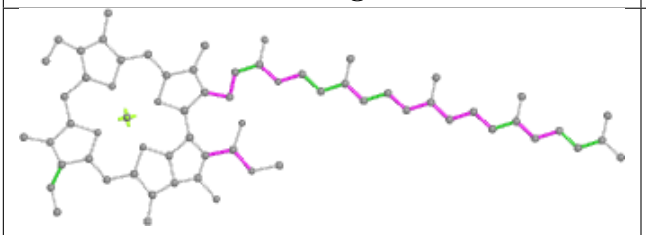
Ligand CLA c 512



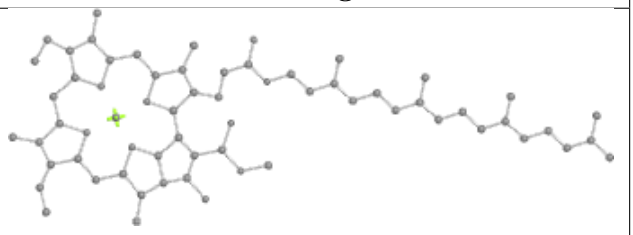
Bond lengths



Bond angles

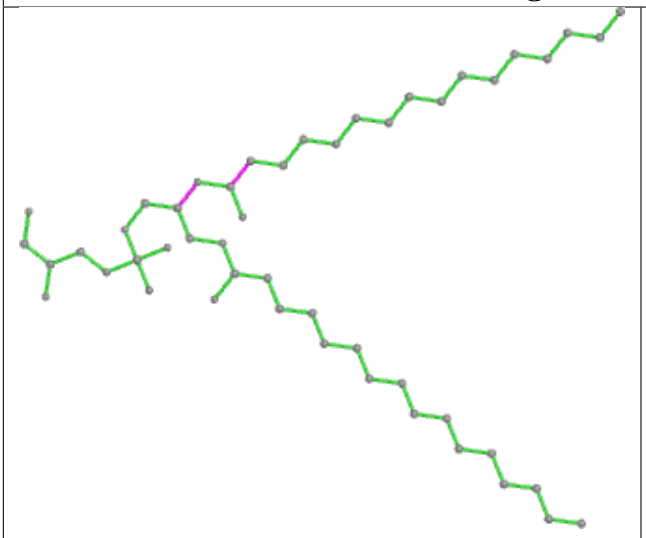


Torsions

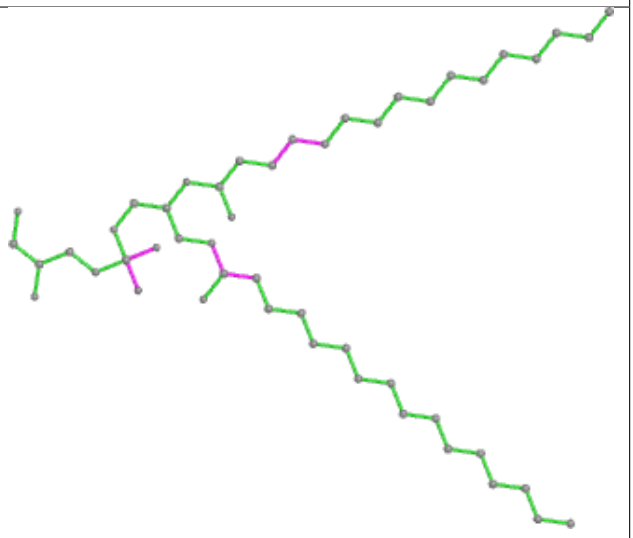


Rings

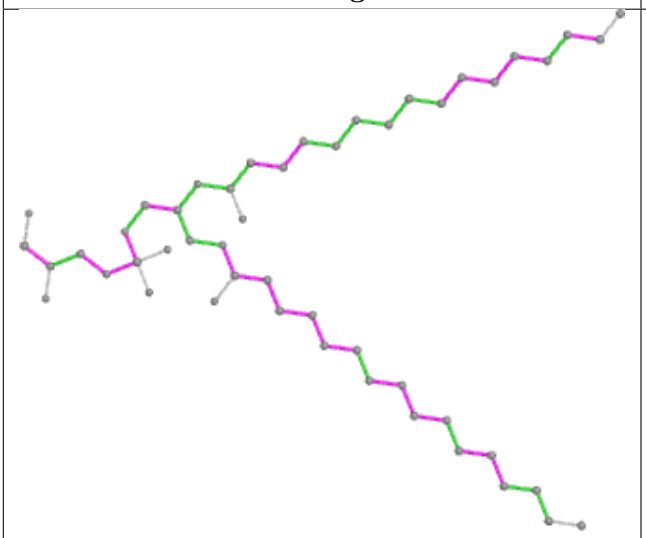
Ligand LHG b 623



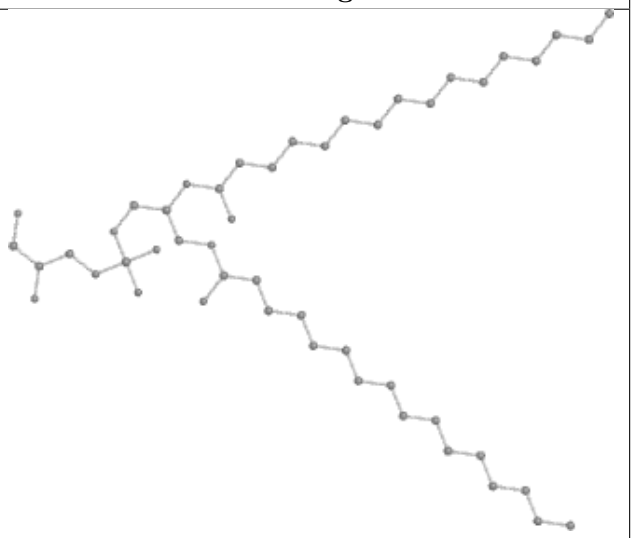
Bond lengths



Bond angles

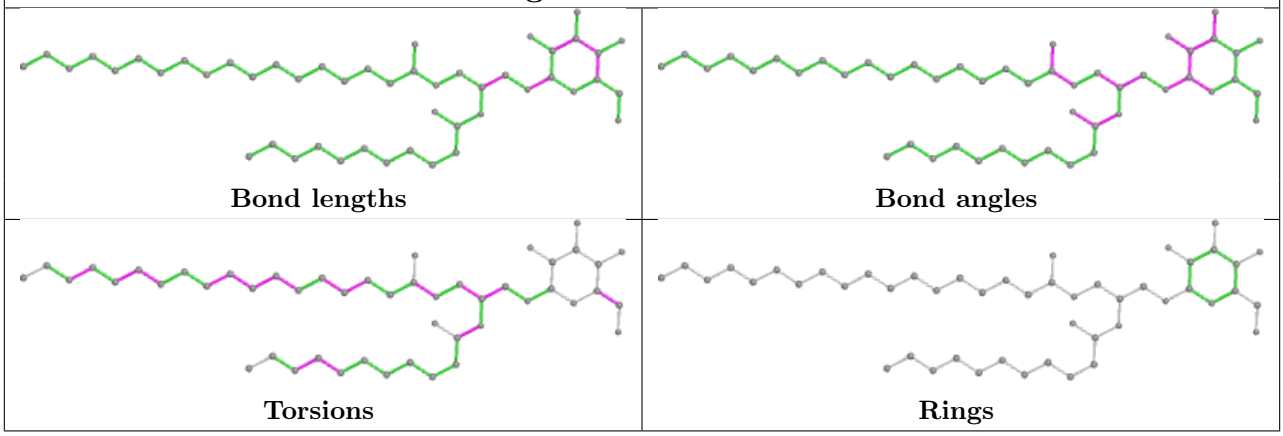


Torsions

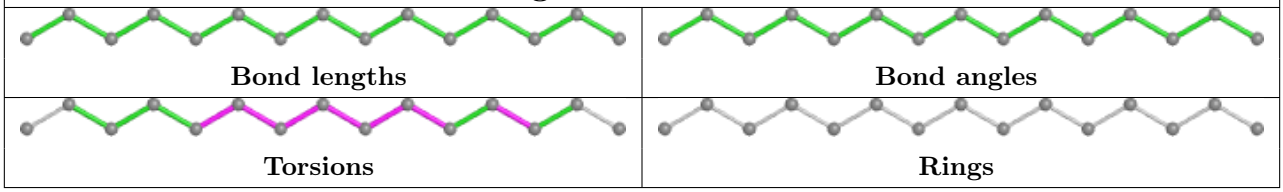


Rings

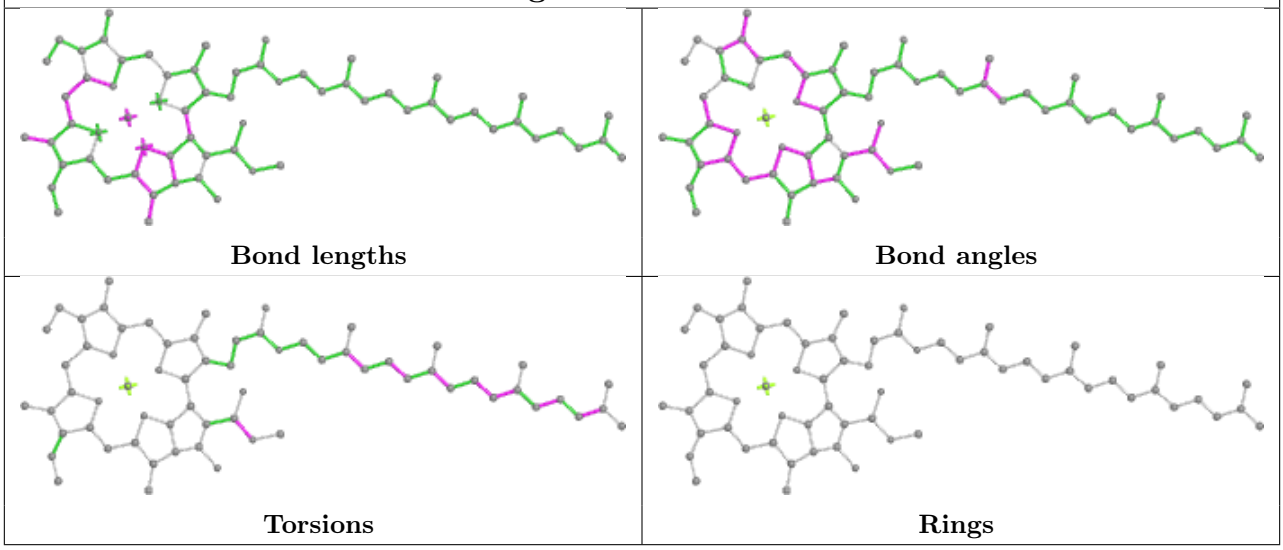
Ligand LMG c 520



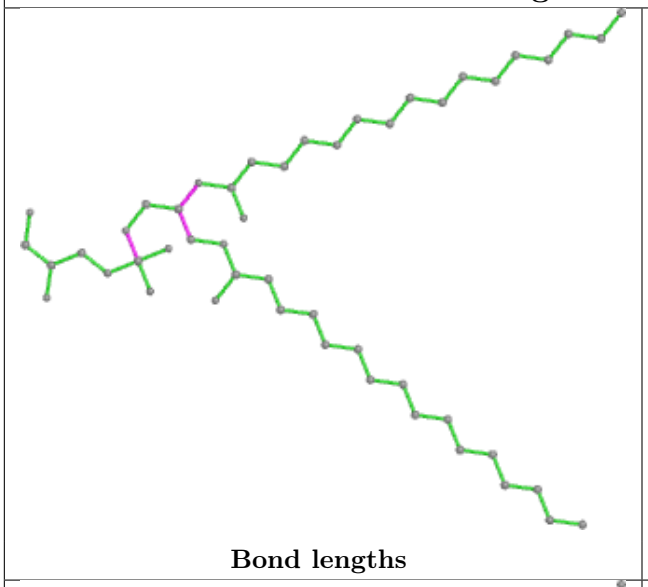
Ligand STE b 625



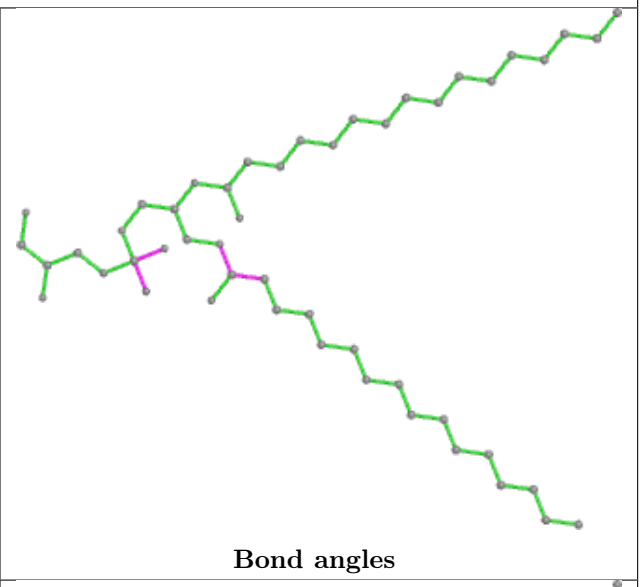
Ligand CLA b 605



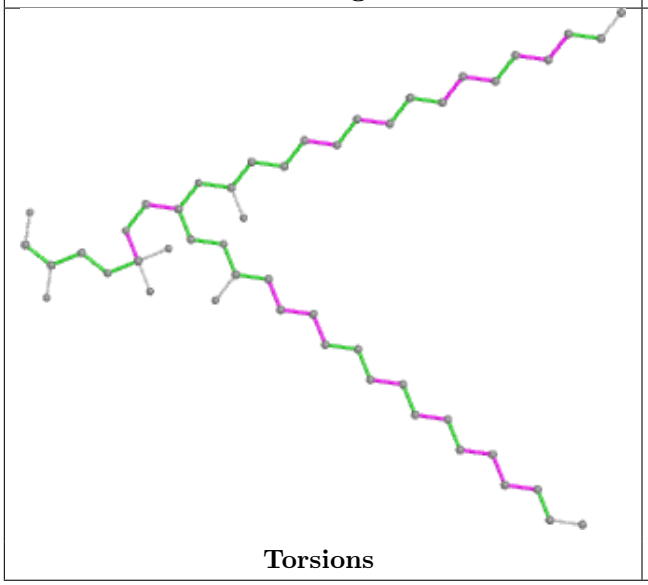
Ligand LHG l 101



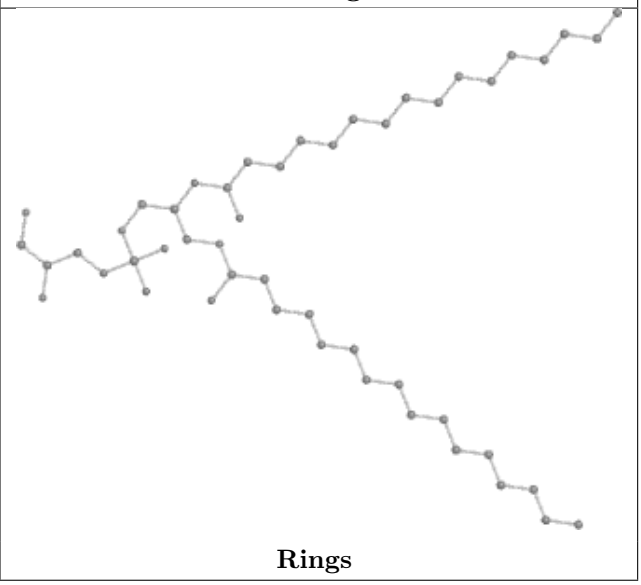
Bond lengths



Bond angles

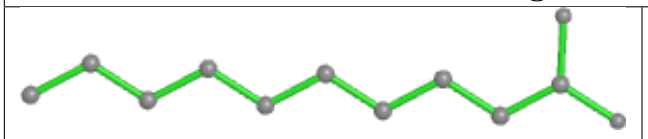


Torsions

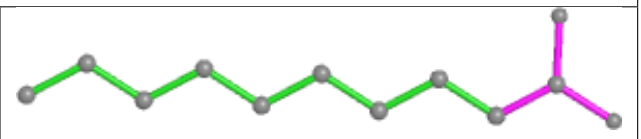


Rings

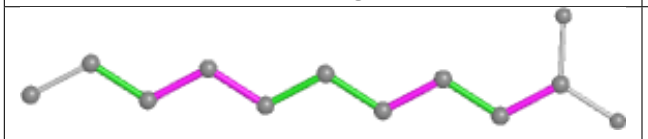
Ligand STE C 519



Bond lengths



Bond angles



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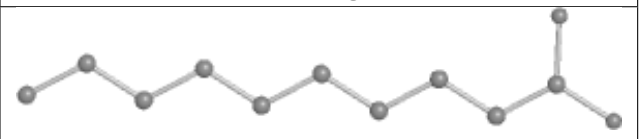
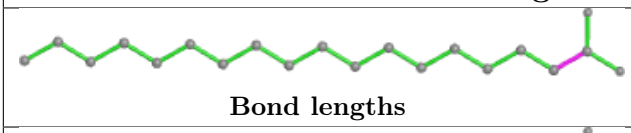


Rings

Ligand STE c 519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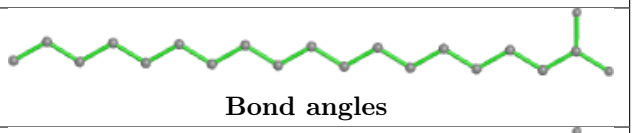
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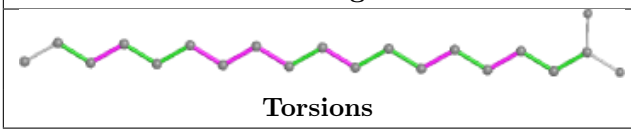
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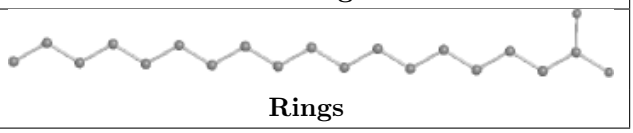
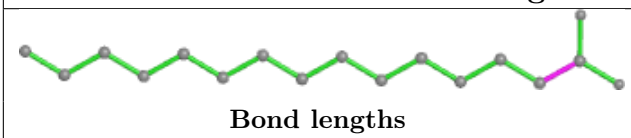

Rings

Ligand STE B 619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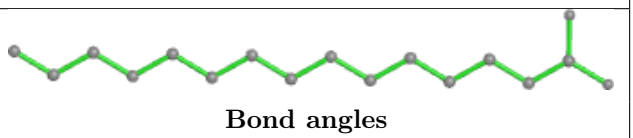
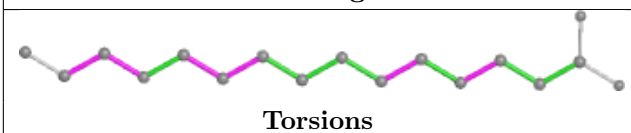

Bond angles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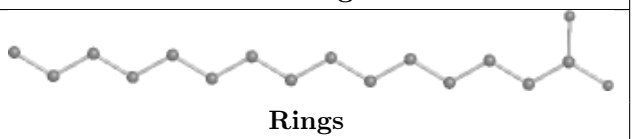
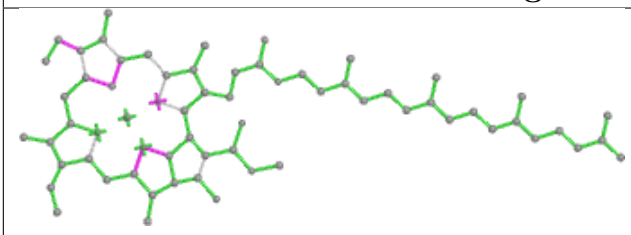

Rings

Ligand CLA B 613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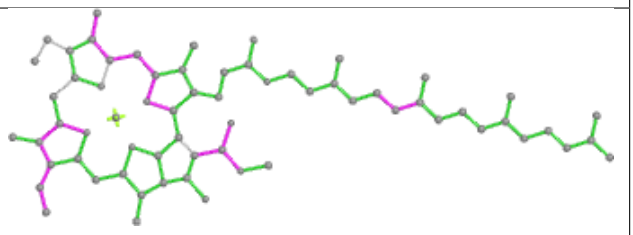
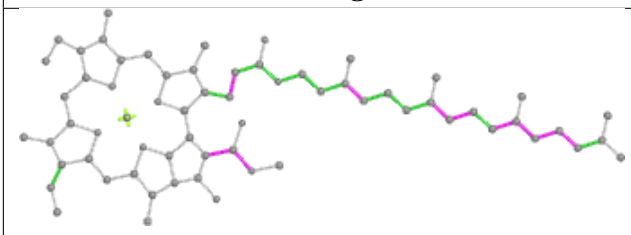
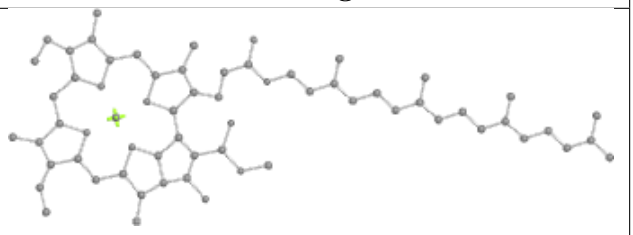
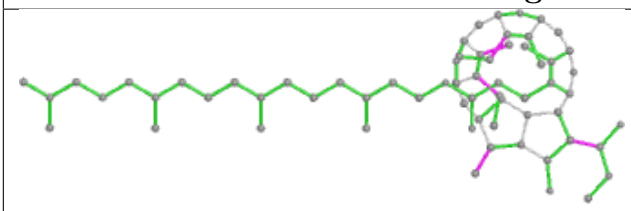

Bond angles


Torsions


Rings

Ligand PHO d 401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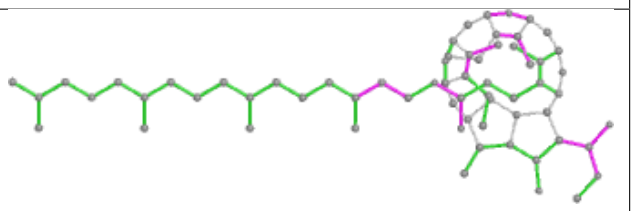
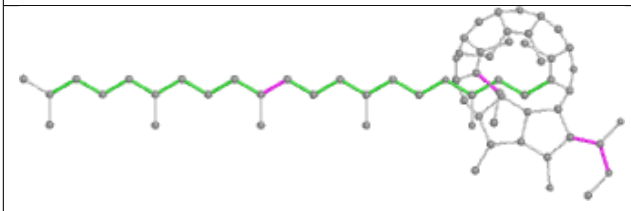
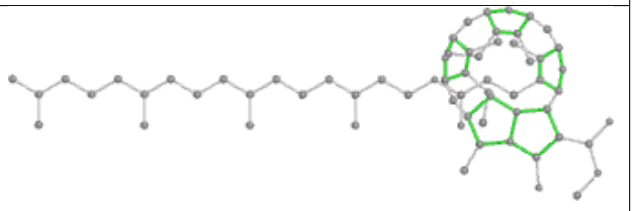
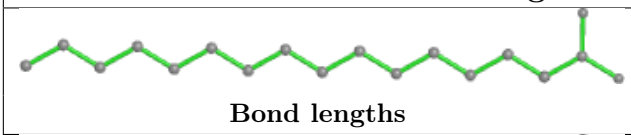

Bond angles


Torsions


Rings

Ligand STE B 623



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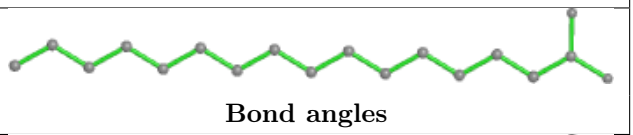
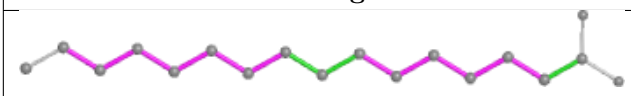


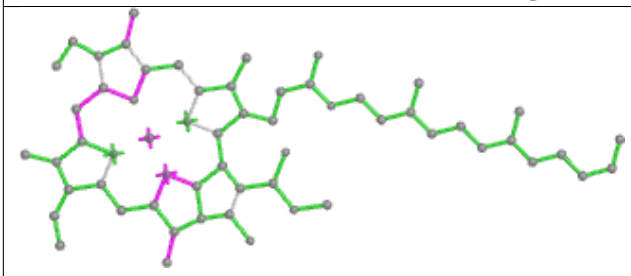
Bond angles



Torsions

Rings

Ligand CLA C 504



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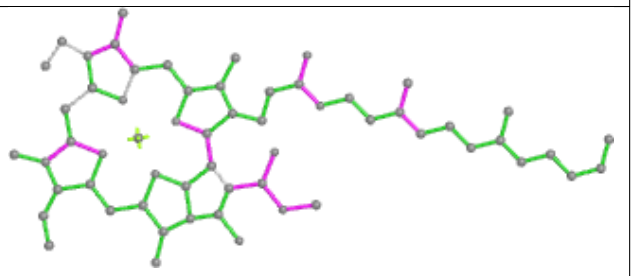
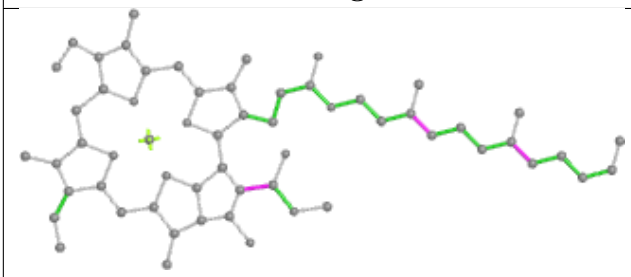
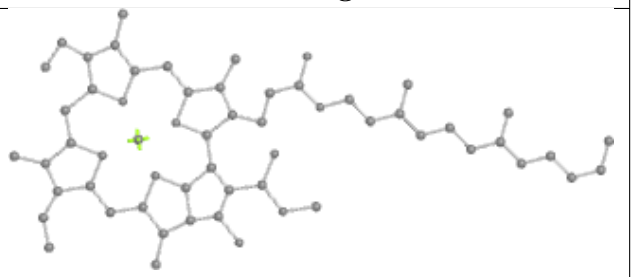


Bond angles

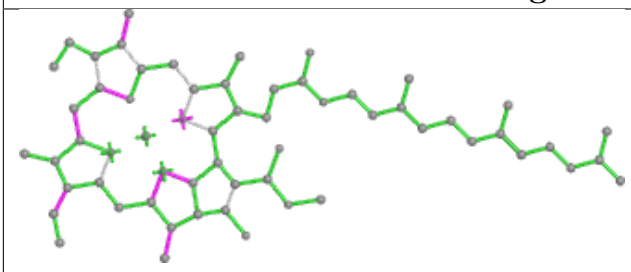


Torsions

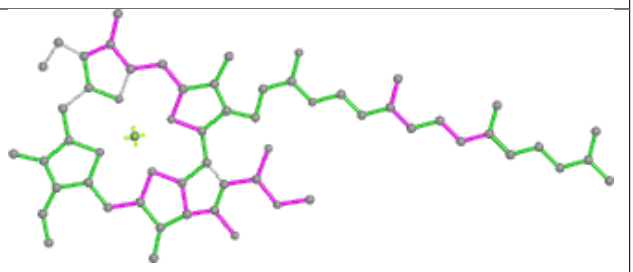


Rings

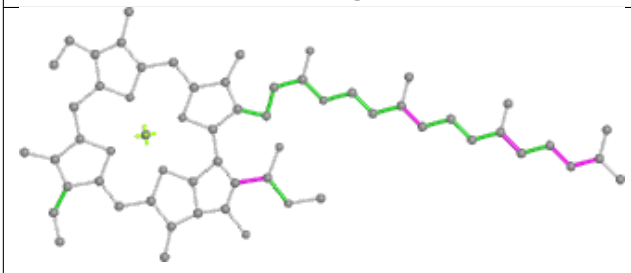
Ligand CLA c 504



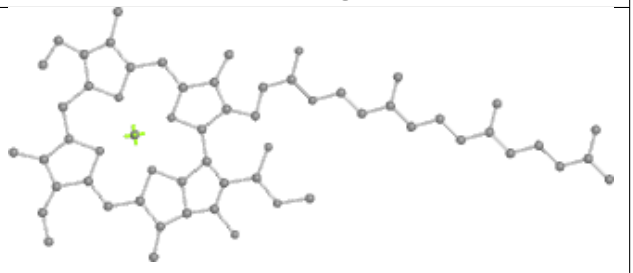
Bond lengths



Bond angles

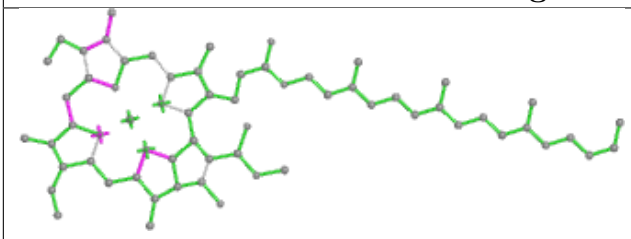


Torsions

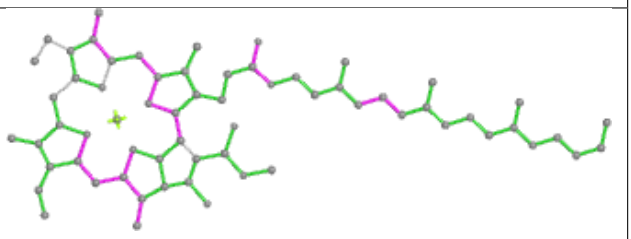


Rings

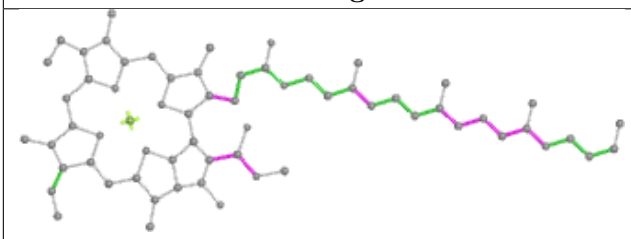
Ligand CLA c 508



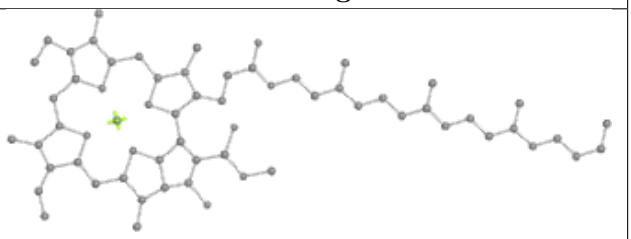
Bond lengths



Bond angles

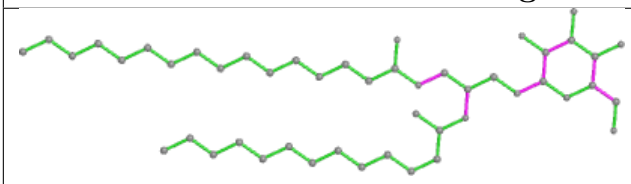


Torsions

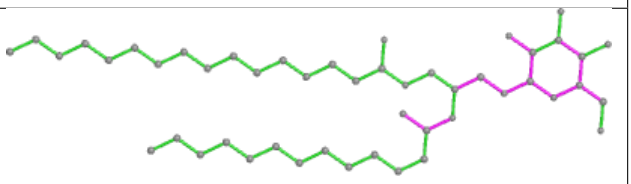


Rings

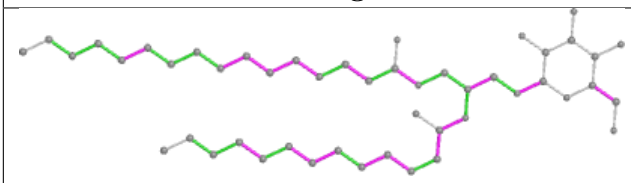
Ligand LMG Y 101



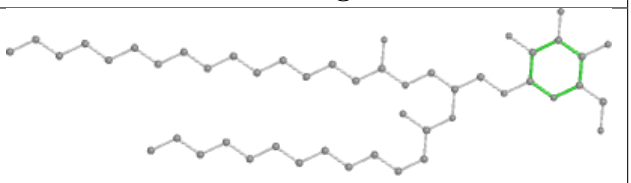
Bond lengths



Bond angles

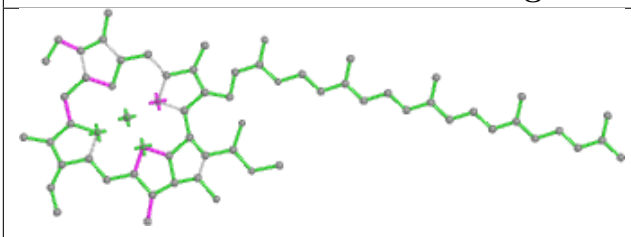


Torsions

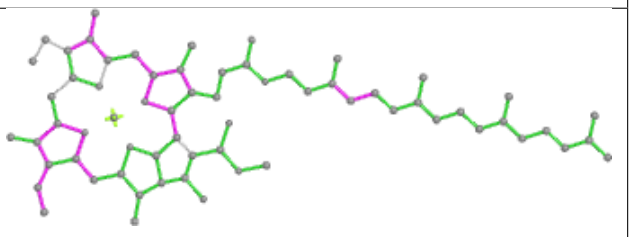


Rings

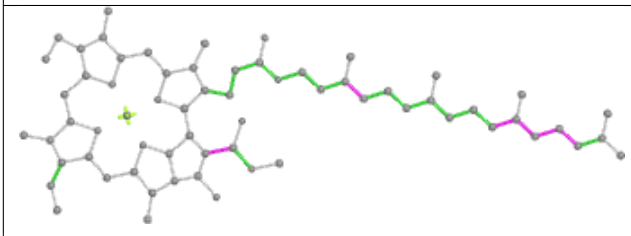
Ligand CLA B 608



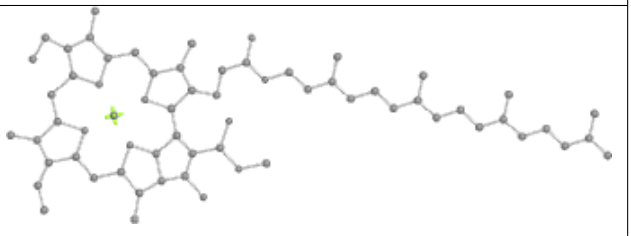
Bond lengths



Bond angles

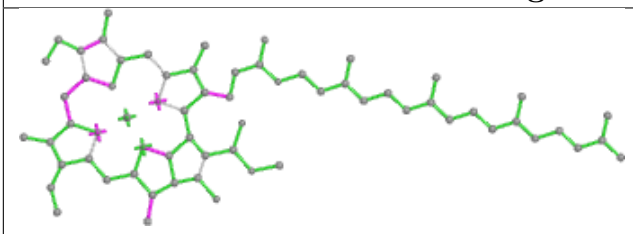


Torsions

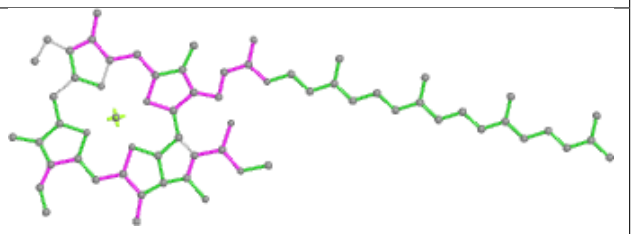


Rings

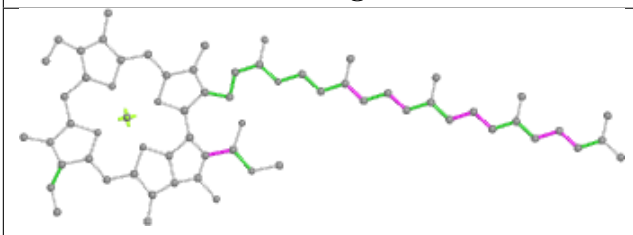
Ligand CLA b 611



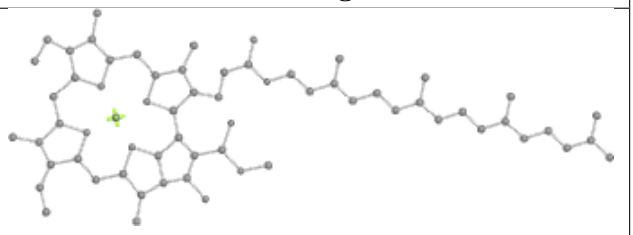
Bond lengths



Bond angles

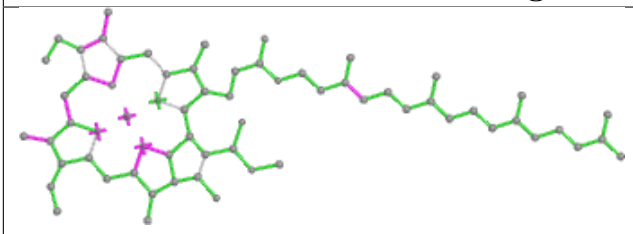


Torsions

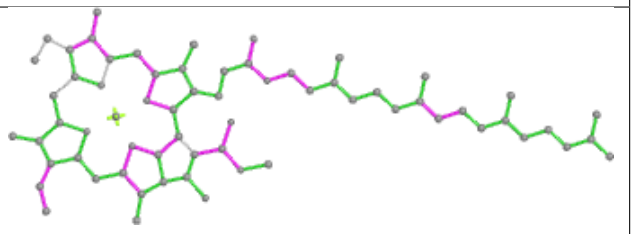


Rings

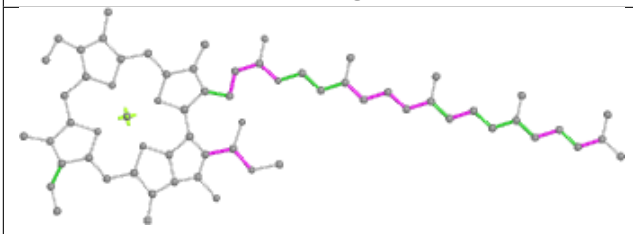
Ligand CLA b 614



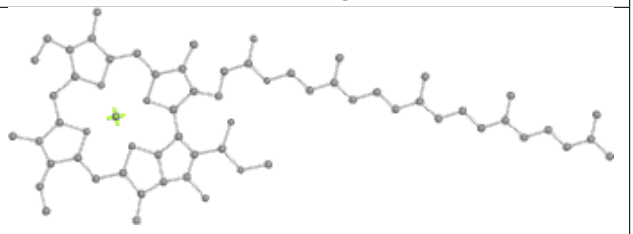
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.37	5 (1%) 73 78	26, 34, 53, 79	0
1	a	334/344 (97%)	-0.42	1 (0%) 94 95	27, 36, 63, 80	0
2	B	505/506 (99%)	-0.37	6 (1%) 79 82	27, 38, 68, 94	0
2	b	505/506 (99%)	-0.19	16 (3%) 47 53	29, 42, 75, 105	0
3	C	442/461 (95%)	-0.27	10 (2%) 60 66	29, 41, 59, 85	0
3	c	451/461 (97%)	-0.19	11 (2%) 59 65	31, 45, 67, 103	0
4	D	341/352 (96%)	-0.36	1 (0%) 94 95	27, 36, 54, 84	0
4	d	341/352 (96%)	-0.25	1 (0%) 94 95	27, 39, 63, 84	0
5	E	82/84 (97%)	-0.11	3 (3%) 41 47	38, 57, 76, 81	0
5	e	82/84 (97%)	0.18	8 (9%) 7 9	44, 66, 84, 88	0
6	F	34/45 (75%)	-0.49	0 100 100	40, 49, 66, 82	0
6	f	34/45 (75%)	-0.27	1 (2%) 51 57	46, 54, 79, 96	0
7	H	65/66 (98%)	-0.09	1 (1%) 73 78	36, 46, 65, 72	0
7	h	63/66 (95%)	0.23	6 (9%) 8 10	45, 56, 67, 76	0
8	I	35/38 (92%)	-0.28	1 (2%) 51 57	36, 45, 74, 84	0
8	i	35/38 (92%)	-0.09	3 (8%) 10 13	34, 46, 76, 88	0
9	J	36/40 (90%)	-0.10	3 (8%) 11 14	40, 54, 80, 89	0
9	j	36/40 (90%)	0.14	4 (11%) 5 7	44, 58, 93, 106	0
10	K	37/46 (80%)	0.09	3 (8%) 12 15	47, 58, 72, 76	0
10	k	37/46 (80%)	-0.07	0 100 100	53, 61, 77, 83	0
11	L	37/37 (100%)	-0.41	0 100 100	30, 34, 68, 78	0
11	l	36/37 (97%)	-0.34	3 (8%) 11 14	29, 36, 78, 85	0
12	M	32/36 (88%)	-0.00	1 (3%) 49 54	34, 39, 69, 76	0
12	m	31/36 (86%)	-0.05	0 100 100	32, 39, 59, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.05	12 (4%) 29 35	32, 47, 87, 132	0
13	o	244/272 (89%)	-0.21	12 (4%) 29 35	28, 46, 83, 132	0
14	R	34/41 (82%)	1.47	11 (32%) 0 0	67, 76, 92, 100	0
14	r	31/41 (75%)	3.37	25 (80%) 0 0	83, 99, 116, 127	0
15	T	29/30 (96%)	-0.48	1 (3%) 45 50	31, 36, 67, 87	0
15	t	29/30 (96%)	-0.37	2 (6%) 16 21	32, 36, 85, 92	0
16	U	97/134 (72%)	-0.20	2 (2%) 63 69	35, 49, 74, 97	0
16	u	97/134 (72%)	-0.45	0 100 100	37, 46, 64, 79	0
17	V	137/163 (84%)	-0.53	0 100 100	31, 46, 60, 84	0
17	v	137/163 (84%)	-0.22	2 (1%) 73 78	36, 52, 76, 87	0
18	X	38/41 (92%)	0.06	2 (5%) 26 31	46, 56, 77, 87	0
18	x	39/41 (95%)	0.15	4 (10%) 6 8	53, 62, 92, 107	0
19	Y	27/46 (58%)	1.15	10 (37%) 0 0	60, 79, 96, 101	0
19	y	30/46 (65%)	0.55	2 (6%) 17 22	67, 79, 92, 104	0
20	Z	62/62 (100%)	0.74	14 (22%) 0 1	59, 73, 116, 128	0
20	z	62/62 (100%)	0.77	10 (16%) 1 2	62, 79, 114, 123	0
All	All	5302/5688 (93%)	-0.18	197 (3%) 41 47	26, 43, 79, 132	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	9.2
14	r	14	LEU	7.1
14	r	28	VAL	6.4
20	z	33	TRP	6.3
14	r	10	LEU	6.2
20	Z	62	VAL	6.2
20	Z	1	MET	6.1
1	A	13	LEU	6.1
14	r	9	LEU	5.8
13	o	3	GLN	5.8
14	r	3	TRP	5.6
18	X	2	THR	5.4
13	O	4	THR	5.3
13	O	60	ARG	5.3
14	R	3	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
14	r	25	PRO	4.9
13	O	3	GLN	4.9
3	c	143	TYR	4.9
7	h	21	VAL	4.8
5	e	79	PHE	4.8
14	r	29	LYS	4.7
18	x	40	SER	4.7
14	r	6	LEU	4.6
14	r	13	LEU	4.6
13	o	4	THR	4.6
13	O	56	PRO	4.6
3	c	23	ALA	4.5
13	o	57	LYS	4.5
2	b	127	ARG	4.5
2	b	495	PHE	4.5
2	b	486	LEU	4.3
13	o	62	GLU	4.2
9	j	7	ARG	4.1
14	R	6	LEU	4.1
9	j	8	ILE	4.1
20	Z	35	ARG	4.0
14	r	5	VAL	4.0
6	f	12	SER	3.9
1	A	11	ALA	3.9
2	b	502	VAL	3.8
13	o	56	PRO	3.8
13	o	59	LYS	3.8
3	c	146	PHE	3.7
13	o	60	ARG	3.7
19	Y	40	ALA	3.7
9	j	5	GLY	3.7
5	E	79	PHE	3.6
3	C	143	TYR	3.6
13	o	61	GLN	3.5
2	b	505	ARG	3.5
19	Y	20	ALA	3.5
8	i	36	ASP	3.5
13	O	62	GLU	3.5
13	O	59	LYS	3.4
14	r	23	ILE	3.4
14	R	21	ARG	3.4
19	y	43	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
14	r	27	ALA	3.4
20	Z	61	VAL	3.4
14	r	26	TYR	3.4
14	r	8	VAL	3.3
2	B	295	GLY	3.3
20	z	3	ILE	3.3
9	J	5	GLY	3.3
13	O	63	ALA	3.2
14	r	24	LEU	3.2
19	Y	43	ARG	3.2
2	b	494	GLY	3.2
20	z	30	PRO	3.2
20	z	36	SER	3.1
20	Z	33	TRP	3.1
14	r	19	ALA	3.1
14	r	4	ARG	3.1
5	E	3	GLY	3.1
19	y	19	ILE	3.1
18	x	38	GLN	3.0
19	Y	42	ARG	3.0
12	M	33	GLN	3.0
14	R	2	ASP	3.0
2	b	496	TYR	3.0
5	e	82	GLN	3.0
14	r	31	VAL	2.9
14	r	18	TRP	2.9
14	R	25	PRO	2.9
19	Y	37	PHE	2.9
5	e	61	ARG	2.9
14	R	32	GLN	2.9
19	Y	25	ILE	2.8
11	l	7	ARG	2.8
13	O	61	GLN	2.8
18	x	2	THR	2.8
20	z	35	ARG	2.8
20	z	1	MET	2.8
14	r	21	ARG	2.8
20	Z	3	ILE	2.8
20	Z	41	PHE	2.8
9	J	7	ARG	2.8
20	Z	42	LEU	2.7
13	O	32	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
20	z	31	GLN	2.7
13	o	246	ALA	2.7
20	Z	7	LEU	2.7
14	r	2	ASP	2.7
3	c	24	THR	2.7
20	Z	38	GLN	2.6
3	C	62	PHE	2.6
13	O	246	ALA	2.6
7	h	10	ILE	2.6
18	X	3	ILE	2.6
9	j	6	GLY	2.6
3	C	57	ALA	2.6
20	z	41	PHE	2.6
19	Y	21	GLN	2.6
8	i	35	LYS	2.5
2	b	374	ASN	2.5
3	C	146	PHE	2.5
20	z	60	PHE	2.5
20	Z	34	ASP	2.5
2	b	295	GLY	2.5
20	Z	32	ASP	2.5
14	R	26	TYR	2.4
2	b	489	GLU	2.4
7	h	6	TRP	2.4
15	t	29	ILE	2.4
2	B	127	ARG	2.4
3	c	262	ARG	2.4
13	O	5	LEU	2.4
1	A	15	GLU	2.4
19	Y	45	ASN	2.4
3	C	60	ILE	2.4
9	J	6	GLY	2.4
2	B	293	ALA	2.4
3	c	147	PHE	2.4
7	h	20	LYS	2.3
2	B	486	LEU	2.3
4	D	227	GLU	2.3
4	d	227[A]	GLU	2.3
19	Y	46	LEU	2.3
5	e	60	GLN	2.3
3	c	55	ALA	2.3
14	r	16	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	b	289	GLN	2.3
3	C	119	LEU	2.3
1	A	12	ASN	2.3
20	z	59	PHE	2.3
10	K	17	ILE	2.3
2	b	128	THR	2.2
3	C	61	VAL	2.2
14	R	28	VAL	2.2
10	K	12	PRO	2.2
11	l	2	GLU	2.2
13	O	54	GLU	2.2
8	i	34	ARG	2.2
3	c	25	ASN	2.2
14	r	12	VAL	2.2
5	E	84	LYS	2.2
10	K	10	LYS	2.2
3	C	65	GLY	2.2
15	T	30	THR	2.2
18	x	34	ILE	2.2
5	e	74	GLN	2.2
3	C	122	SER	2.2
20	Z	60	PHE	2.2
16	U	8	GLU	2.2
20	Z	31	GLN	2.2
2	b	490	GLN	2.2
1	a	11	ALA	2.2
2	b	503	THR	2.2
15	t	28	ARG	2.2
7	H	6	TRP	2.2
5	e	71	GLU	2.2
8	I	34	ARG	2.1
14	r	32	GLN	2.1
19	Y	41	VAL	2.1
11	l	3	PRO	2.1
3	c	261	ARG	2.1
2	b	218	LEU	2.1
5	e	17	VAL	2.1
3	c	142	GLU	2.1
17	v	21	LEU	2.1
14	R	30	GLN	2.1
1	A	16	ARG	2.1
2	B	502	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
7	h	18	TYR	2.1
14	R	10	LEU	2.1
13	o	207	ARG	2.1
2	b	219	VAL	2.1
14	r	7	VAL	2.0
5	e	84	LYS	2.0
3	C	275	SER	2.0
13	o	63	ALA	2.0
14	R	29	LYS	2.0
17	v	17	LYS	2.0
16	U	67	LEU	2.0
2	B	289	GLN	2.0
7	h	56	ASP	2.0
3	c	57	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	FME	T	1	10/11	0.94	0.11	30,62,79,79	0
15	FME	t	1	10/11	0.94	0.10	33,54,70,73	0
12	FME	m	1	10/11	0.95	0.14	46,57,89,91	0
8	FME	I	1	10/11	0.96	0.20	46,62,75,90	0
12	FME	M	1	10/11	0.97	0.13	44,61,78,87	0
8	FME	i	1	10/11	0.97	0.15	45,59,72,78	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	STE	B	623	18/20	0.76	0.22	54,72,94,94	0
31	STE	b	626	20/20	0.76	0.24	43,74,97,100	0
31	STE	c	519	20/20	0.77	0.25	43,66,97,102	0
31	STE	x	102	20/20	0.78	0.22	51,68,91,94	0
28	LHG	a	411	42/49	0.79	0.27	66,95,118,141	0
31	STE	B	624	16/20	0.79	0.29	43,71,87,89	0
31	STE	a	412	12/20	0.79	0.42	46,79,97,98	0
31	STE	k	104	12/20	0.81	0.23	56,73,85,89	0
31	STE	b	628	14/20	0.81	0.39	57,77,110,110	0
26	LMG	D	412	33/55	0.82	0.20	36,63,101,106	0
30	BCR	H	102	40/40	0.82	0.17	35,51,67,75	0
26	LMG	c	520	48/55	0.83	0.24	35,83,112,118	0
31	STE	B	625	12/20	0.83	0.40	47,69,89,93	0
31	STE	R	101	12/20	0.83	0.29	59,80,103,104	0
22	CLA	C	512	65/65	0.84	0.19	40,61,96,105	0
31	STE	M	104	18/20	0.84	0.19	38,53,75,86	0
30	BCR	x	101	40/40	0.84	0.16	40,59,76,81	0
22	CLA	c	512	65/65	0.85	0.18	44,62,97,112	0
28	LHG	A	411	49/49	0.85	0.22	50,86,108,119	0
22	CLA	b	601	65/65	0.85	0.18	51,74,102,106	0
31	STE	b	624	16/20	0.85	0.17	53,74,88,95	0
31	STE	b	625	15/20	0.85	0.21	52,68,93,94	0
26	LMG	a	414	55/55	0.85	0.17	40,67,93,105	0
31	STE	I	102	15/20	0.85	0.17	40,58,82,84	0
31	STE	b	629	20/20	0.85	0.18	40,71,89,93	0
31	STE	J	101	12/20	0.85	0.17	51,71,80,81	0
31	STE	L	103	12/20	0.85	0.19	49,66,79,86	0
31	STE	M	103	10/20	0.85	0.16	35,56,69,69	0
27	SQD	A	412	39/54	0.86	0.20	47,69,107,111	0
31	STE	b	621	20/20	0.86	0.26	44,63,85,87	0
26	LMG	b	622	55/55	0.86	0.27	48,80,110,117	0
31	STE	B	619	17/20	0.86	0.18	37,58,76,80	0
25	PL9	a	409	55/55	0.86	0.23	42,77,102,105	0
31	STE	H	104	18/20	0.87	0.30	49,76,90,93	0
27	SQD	t	102	36/54	0.87	0.16	31,69,96,103	0
31	STE	a	413	15/20	0.87	0.17	35,65,81,92	0
25	PL9	A	408	55/55	0.88	0.22	34,70,94,98	0
22	CLA	C	513	65/65	0.88	0.20	43,65,107,118	0
29	DGD	A	413	66/66	0.88	0.14	41,65,89,95	0
22	CLA	H	101	65/65	0.88	0.17	36,70,99,108	0
30	BCR	K	102	40/40	0.88	0.14	37,57,74,74	0
27	SQD	L	101	49/54	0.88	0.16	40,66,106,121	0
31	STE	t	104	10/20	0.88	0.28	45,59,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	c	513	65/65	0.88	0.21	44,80,112,121	0
22	CLA	c	502	65/65	0.89	0.17	30,49,69,76	0
27	SQD	B	621	54/54	0.89	0.17	40,67,93,104	0
26	LMG	M	101	51/55	0.89	0.14	37,56,84,88	0
31	STE	C	519	12/20	0.89	0.14	41,55,68,73	0
31	STE	C	520	16/20	0.89	0.16	43,63,75,79	0
27	SQD	f	102	41/54	0.89	0.18	61,87,110,127	0
26	LMG	Y	101	48/55	0.89	0.18	54,76,95,104	0
26	LMG	c	521	49/55	0.89	0.15	32,66,98,113	0
22	CLA	a	405	65/65	0.90	0.16	20,44,90,104	0
26	LMG	c	518	37/55	0.90	0.18	49,72,93,98	0
22	CLA	c	508	64/65	0.90	0.17	36,56,98,124	0
26	LMG	A	409	48/55	0.90	0.17	36,63,86,104	0
30	BCR	d	406	40/40	0.90	0.13	30,58,103,111	0
31	STE	X	101	20/20	0.90	0.17	40,60,81,91	0
30	BCR	k	102	40/40	0.90	0.14	46,67,84,86	0
30	BCR	k	103	40/40	0.90	0.20	45,63,78,85	0
26	LMG	B	620	28/55	0.90	0.16	35,52,67,71	0
31	STE	b	627	10/20	0.91	0.29	45,58,65,68	0
31	STE	C	521	12/20	0.91	0.10	37,48,59,64	0
31	STE	b	620	16/20	0.91	0.22	42,55,83,100	0
30	BCR	k	101	40/40	0.91	0.16	48,67,82,91	0
31	STE	d	411	17/20	0.91	0.14	49,65,73,79	0
26	LMG	m	101	51/55	0.91	0.15	40,61,86,96	0
31	STE	B	622	12/20	0.91	0.09	36,57,72,72	0
26	LMG	D	408	51/55	0.91	0.20	34,66,92,114	0
26	LMG	d	410	44/55	0.92	0.15	41,61,90,108	0
22	CLA	b	616	60/65	0.92	0.15	31,48,93,99	0
22	CLA	D	405	65/65	0.92	0.15	26,50,132,139	0
22	CLA	d	405	65/65	0.92	0.15	32,56,101,116	0
31	STE	Z	101	8/20	0.92	0.14	38,65,78,78	0
27	SQD	D	409	36/54	0.92	0.17	50,78,97,114	0
29	DGD	c	517	62/66	0.92	0.17	36,64,94,109	0
31	STE	j	101	12/20	0.92	0.14	50,63,72,76	0
30	BCR	C	514	40/40	0.92	0.14	30,47,58,76	0
31	STE	t	103	14/20	0.92	0.14	41,59,67,71	0
22	CLA	B	605	65/65	0.92	0.13	29,45,82,98	0
30	BCR	K	101	40/40	0.92	0.13	45,63,82,83	0
22	CLA	c	510	65/65	0.93	0.15	36,51,66,92	0
22	CLA	c	511	65/65	0.93	0.16	41,62,80,90	0
22	CLA	B	615	60/65	0.93	0.15	23,43,96,105	0
29	DGD	c	516	62/66	0.93	0.14	36,61,97,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	502	65/65	0.93	0.14	29,48,70,79	0
30	BCR	B	618	40/40	0.93	0.12	24,48,68,80	0
22	CLA	C	507	65/65	0.93	0.15	25,46,67,73	0
22	CLA	C	508	65/65	0.93	0.13	29,48,112,124	0
22	CLA	b	609	65/65	0.93	0.14	31,54,74,77	0
22	CLA	b	615	65/65	0.93	0.14	27,47,67,74	0
22	CLA	C	509	65/65	0.93	0.18	31,51,68,77	0
31	STE	M	102	15/20	0.93	0.13	37,54,63,69	0
22	CLA	B	601	65/65	0.93	0.17	26,42,63,67	0
22	CLA	c	506	65/65	0.93	0.14	34,56,106,111	0
27	SQD	a	410	54/54	0.93	0.16	44,70,104,112	0
22	CLA	B	614	65/65	0.93	0.13	26,42,69,86	0
22	CLA	c	509	65/65	0.93	0.20	32,54,74,84	0
30	BCR	B	616	40/40	0.94	0.12	30,46,69,72	0
30	BCR	B	617	40/40	0.94	0.11	29,44,57,64	0
22	CLA	C	506	65/65	0.94	0.13	28,50,90,108	0
25	PL9	D	407	55/55	0.94	0.11	26,39,57,63	0
30	BCR	C	515	40/40	0.94	0.17	42,60,73,75	0
30	BCR	D	406	40/40	0.94	0.11	35,50,88,108	0
22	CLA	c	503	65/65	0.94	0.16	34,50,62,68	0
22	CLA	c	504	60/65	0.94	0.12	36,51,85,99	0
22	CLA	c	505	65/65	0.94	0.17	30,47,73,77	0
30	BCR	b	617	40/40	0.94	0.12	34,48,64,67	0
30	BCR	b	619	40/40	0.94	0.12	24,55,73,87	0
30	BCR	c	514	40/40	0.94	0.14	35,51,69,74	0
22	CLA	b	602	65/65	0.94	0.16	31,48,68,71	0
22	CLA	c	507	65/65	0.94	0.14	31,50,65,78	0
22	CLA	b	606	65/65	0.94	0.12	29,47,83,90	0
22	CLA	B	613	65/65	0.94	0.16	26,45,87,104	0
22	CLA	b	611	65/65	0.94	0.14	25,41,55,66	0
22	CLA	b	613	65/65	0.94	0.16	21,41,83,97	0
22	CLA	b	614	65/65	0.94	0.14	26,43,87,93	0
29	DGD	C	516	62/66	0.94	0.14	28,48,85,107	0
29	DGD	C	517	62/66	0.94	0.14	30,57,112,139	0
29	DGD	C	518	62/66	0.94	0.13	33,57,77,94	0
29	DGD	H	103	62/66	0.94	0.11	34,51,67,75	0
22	CLA	a	403	65/65	0.94	0.15	29,47,106,117	0
22	CLA	B	603	65/65	0.94	0.14	25,40,97,105	0
29	DGD	h	101	62/66	0.94	0.14	35,53,70,78	0
22	CLA	D	403	65/65	0.95	0.12	22,36,53,65	0
22	CLA	D	404	65/65	0.95	0.12	22,35,57,66	0
22	CLA	c	501	65/65	0.95	0.14	30,50,65,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	503	65/65	0.95	0.14	31,49,59,63	0
22	CLA	C	504	59/65	0.95	0.13	30,49,95,100	0
22	CLA	a	402	65/65	0.95	0.12	24,36,51,59	0
22	CLA	C	505	65/65	0.95	0.16	27,47,75,82	0
22	CLA	B	611	65/65	0.95	0.16	22,37,50,60	0
22	CLA	B	612	65/65	0.95	0.15	21,40,75,84	0
22	CLA	B	602	65/65	0.95	0.16	23,38,67,75	0
22	CLA	b	604	65/65	0.95	0.14	24,45,87,105	0
22	CLA	b	605	65/65	0.95	0.14	24,39,59,63	0
27	SQD	A	410	52/54	0.95	0.16	39,68,101,103	0
22	CLA	A	405	54/65	0.95	0.12	22,36,72,78	0
30	BCR	T	101	40/40	0.95	0.09	30,46,61,66	0
30	BCR	a	406	40/40	0.95	0.11	24,38,59,64	0
22	CLA	b	608	65/65	0.95	0.14	30,48,73,79	0
30	BCR	b	618	40/40	0.95	0.11	29,44,61,68	0
22	CLA	C	510	65/65	0.95	0.15	30,50,68,81	0
22	CLA	d	403	65/65	0.95	0.14	25,41,70,83	0
22	CLA	d	404	65/65	0.95	0.12	22,37,47,53	0
22	CLA	b	610	65/65	0.95	0.18	28,43,58,69	0
23	PHO	a	404	64/64	0.95	0.14	24,37,46,47	0
22	CLA	C	511	65/65	0.95	0.13	34,59,80,85	0
22	CLA	b	612	65/65	0.95	0.17	27,40,54,58	0
28	LHG	b	623	49/49	0.95	0.15	38,58,85,104	0
28	LHG	d	409	39/49	0.95	0.12	37,55,73,83	0
22	CLA	A	403	65/65	0.95	0.15	23,42,94,109	0
25	PL9	d	407	55/55	0.95	0.11	25,40,54,60	0
22	CLA	B	608	65/65	0.95	0.12	27,43,60,65	0
22	CLA	C	501	65/65	0.96	0.12	25,43,59,65	0
22	CLA	b	607	65/65	0.96	0.12	26,42,86,96	0
22	CLA	A	402	65/65	0.96	0.11	19,33,52,62	0
28	LHG	l	101	49/49	0.96	0.12	34,50,65,71	0
30	BCR	I	101	40/40	0.96	0.09	22,40,52,54	0
23	PHO	A	404	64/64	0.96	0.12	15,35,45,47	0
23	PHO	D	401	64/64	0.96	0.12	26,39,51,54	0
22	CLA	B	607	65/65	0.96	0.13	27,43,71,75	0
23	PHO	d	401	64/64	0.96	0.12	25,43,55,67	0
22	CLA	B	604	65/65	0.96	0.14	21,38,53,63	0
29	DGD	c	515	62/66	0.96	0.11	31,49,85,92	0
22	CLA	b	603	65/65	0.96	0.15	26,43,82,91	0
22	CLA	B	609	65/65	0.96	0.14	25,39,49,58	0
22	CLA	B	610	65/65	0.96	0.15	19,38,54,62	0
28	LHG	D	410	49/49	0.96	0.11	31,47,58,65	0

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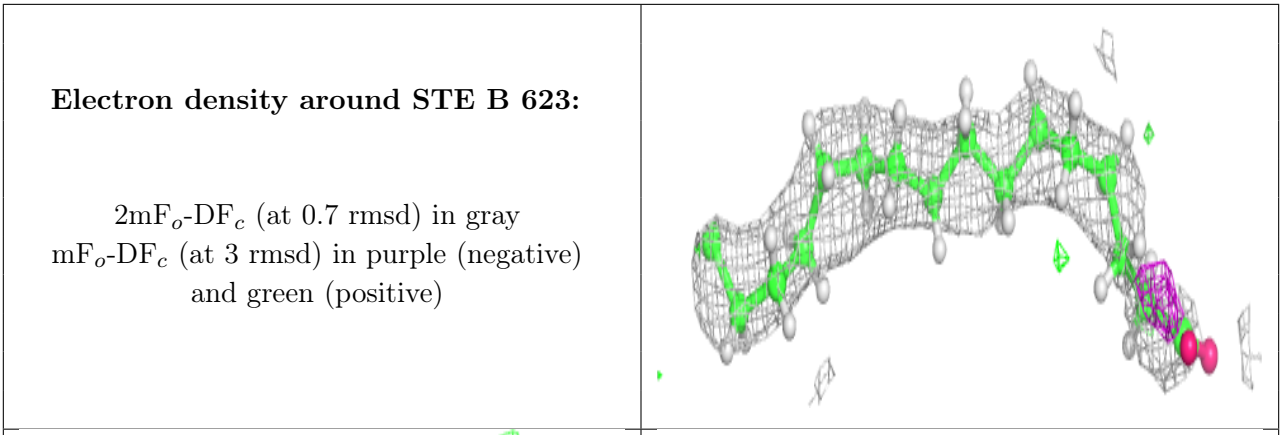
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	LHG	D	411	47/49	0.96	0.13	27,54,84,95	0
28	LHG	D	413	49/49	0.96	0.12	32,48,80,93	0
30	BCR	t	101	40/40	0.96	0.09	28,44,55,63	0
33	BCT	d	402	4/4	0.96	0.17	35,40,52,62	0
34	HEC	F	101	43/43	0.96	0.12	37,54,73,76	0
34	HEC	f	101	43/43	0.96	0.14	44,62,87,99	0
35	NA	V	202	1/1	0.96	0.22	61,61,61,61	0
28	LHG	L	102	49/49	0.97	0.10	30,47,67,80	0
24	CL	A	407	1/1	0.97	0.06	39,39,39,39	0
34	HEC	V	201	43/43	0.97	0.13	25,39,48,49	0
22	CLA	B	606	65/65	0.97	0.12	18,39,81,92	0
34	HEC	v	201	43/43	0.97	0.12	31,42,53,61	0
28	LHG	d	408	49/49	0.97	0.11	28,48,60,65	0
33	BCT	D	402	4/4	0.98	0.18	28,35,46,55	0
24	CL	a	407	1/1	0.99	0.07	34,34,34,34	0
24	CL	a	408	1/1	0.99	0.04	35,35,35,35	0
24	CL	A	406	1/1	0.99	0.09	35,35,35,35	0
32	OEX	C	522	10/10	0.99	0.14	26,33,37,38	0
32	OEX	a	415	10/10	0.99	0.13	26,34,36,40	0
21	FE2	A	401	1/1	0.99	0.10	32,32,32,32	0
21	FE2	a	401	1/1	1.00	0.07	36,36,36,36	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.

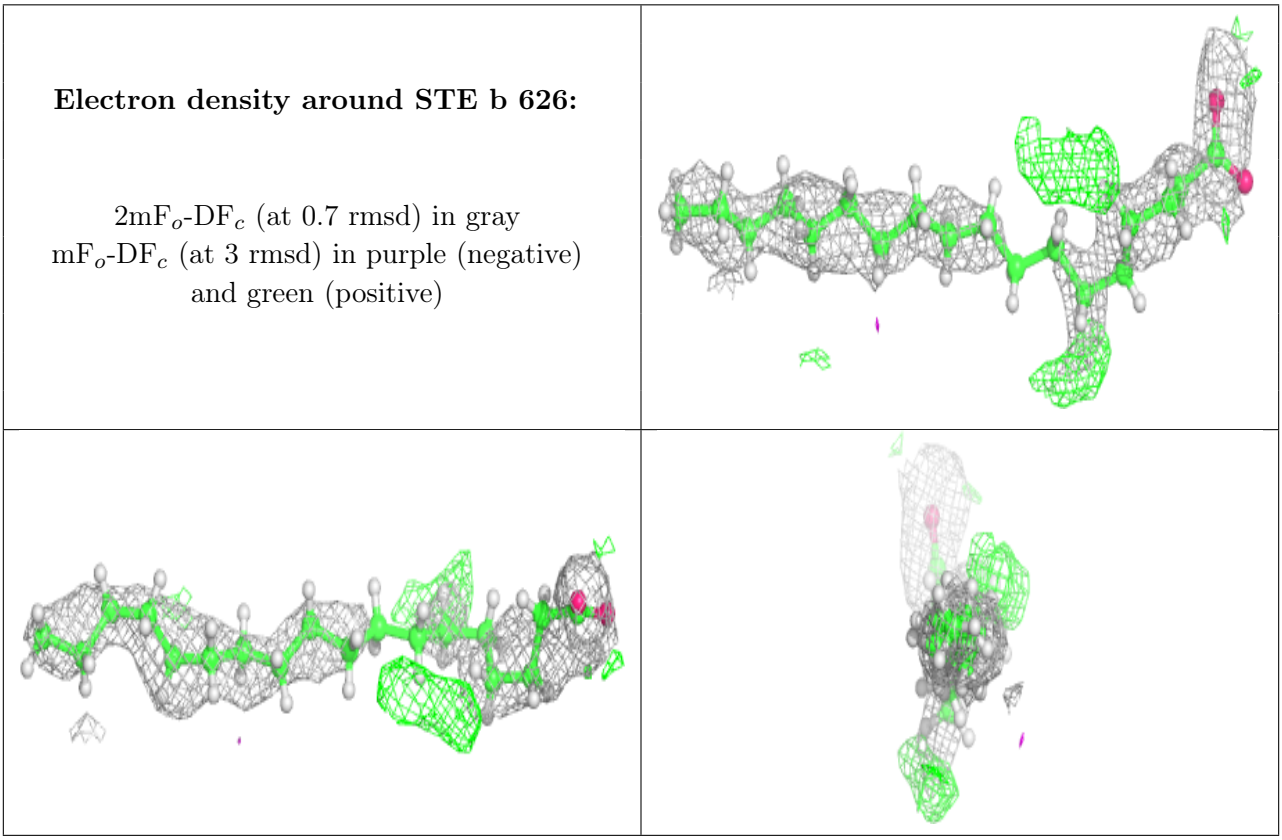
Electron density around STE B 623:

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



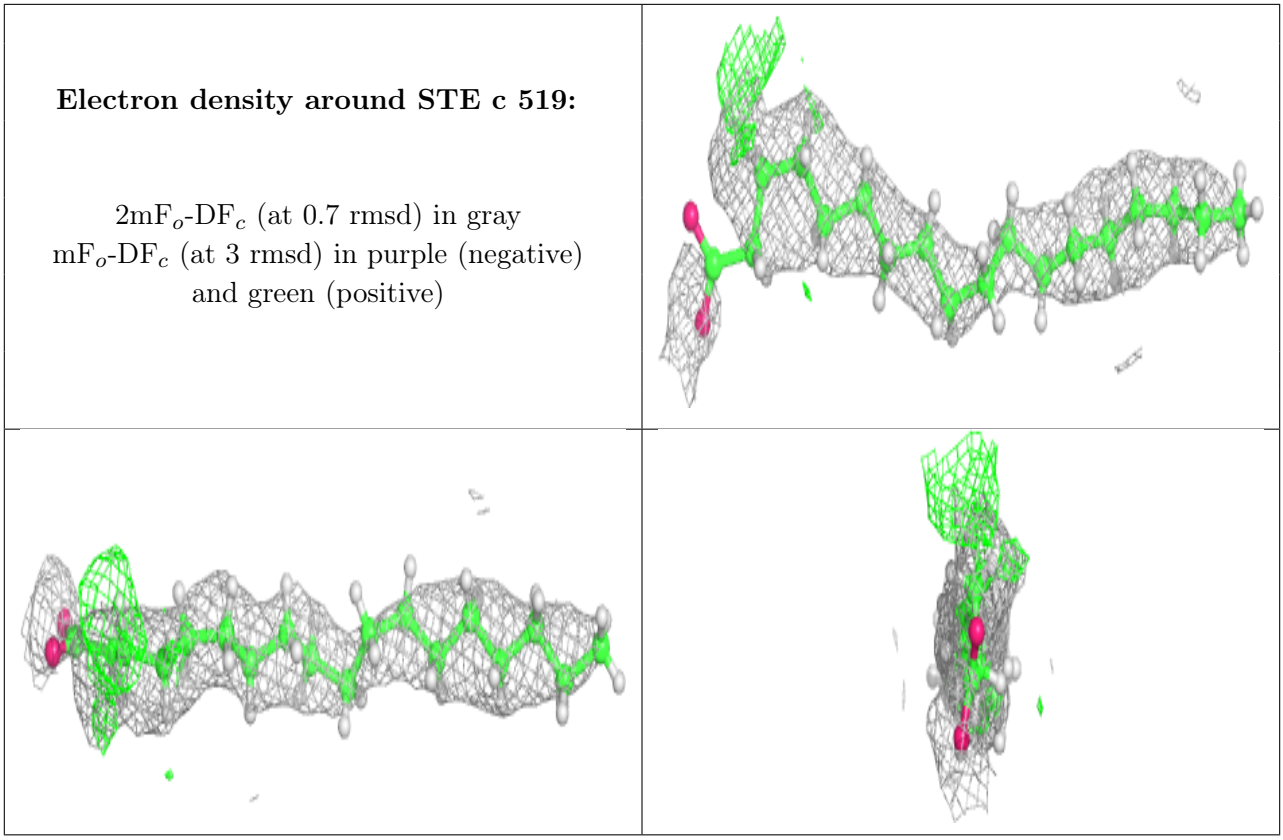
Electron density around STE b 626:

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



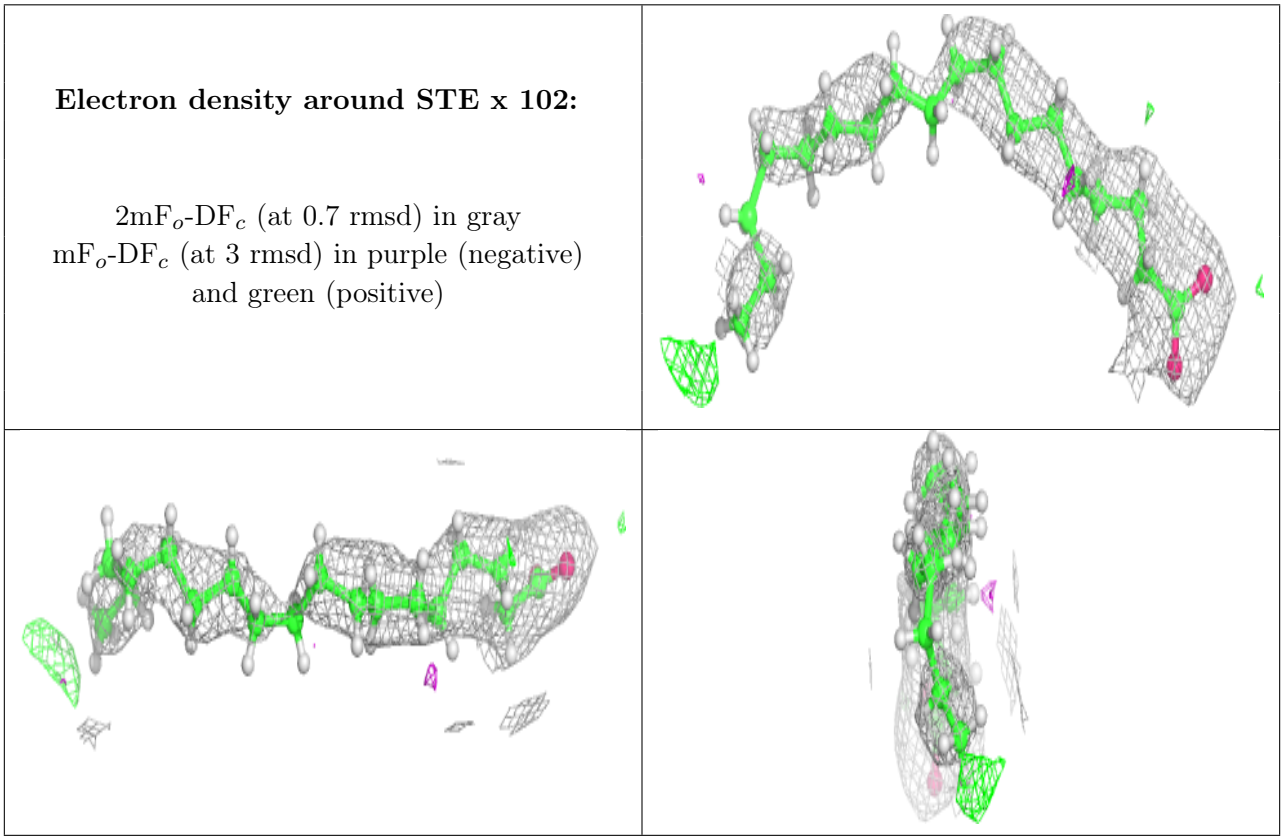
Electron density around STE c 519:

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



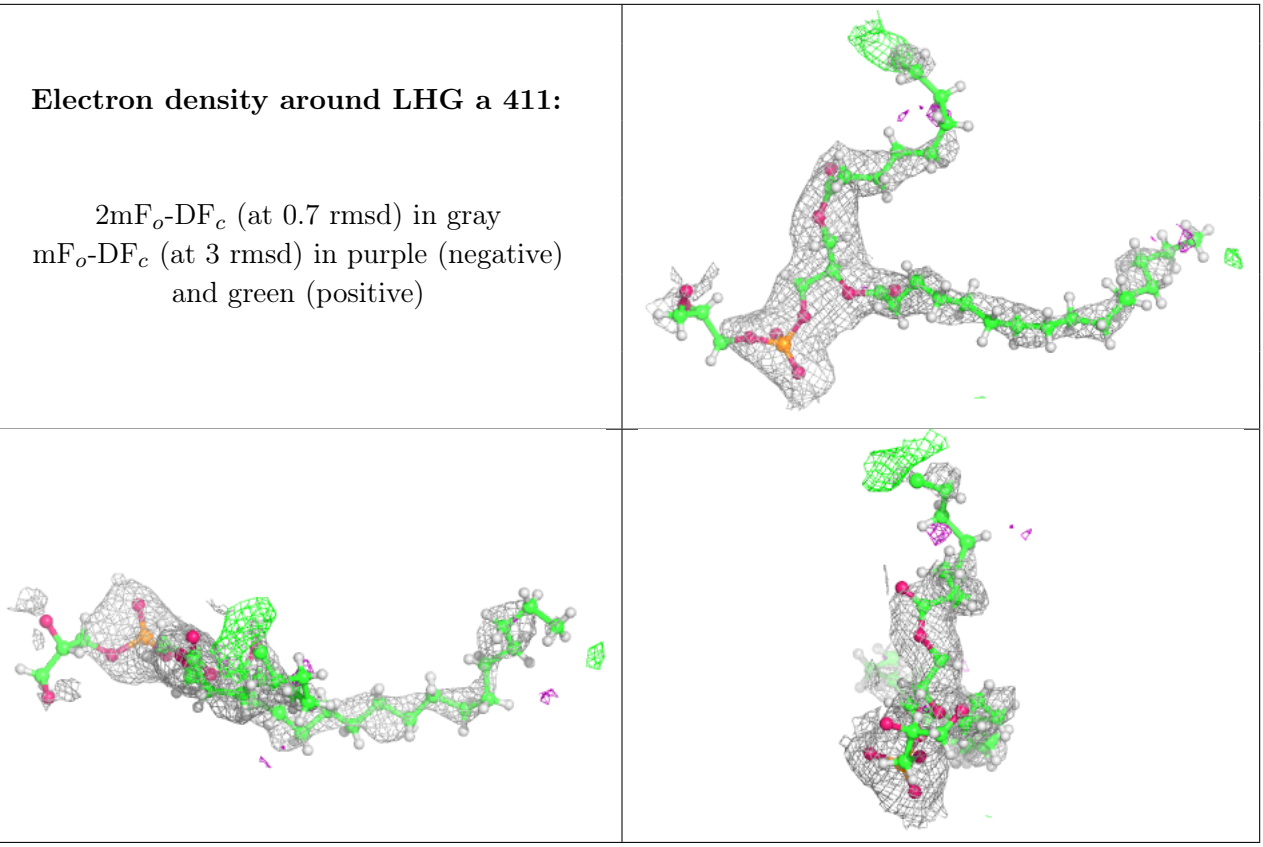
Electron density around STE x 102:

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



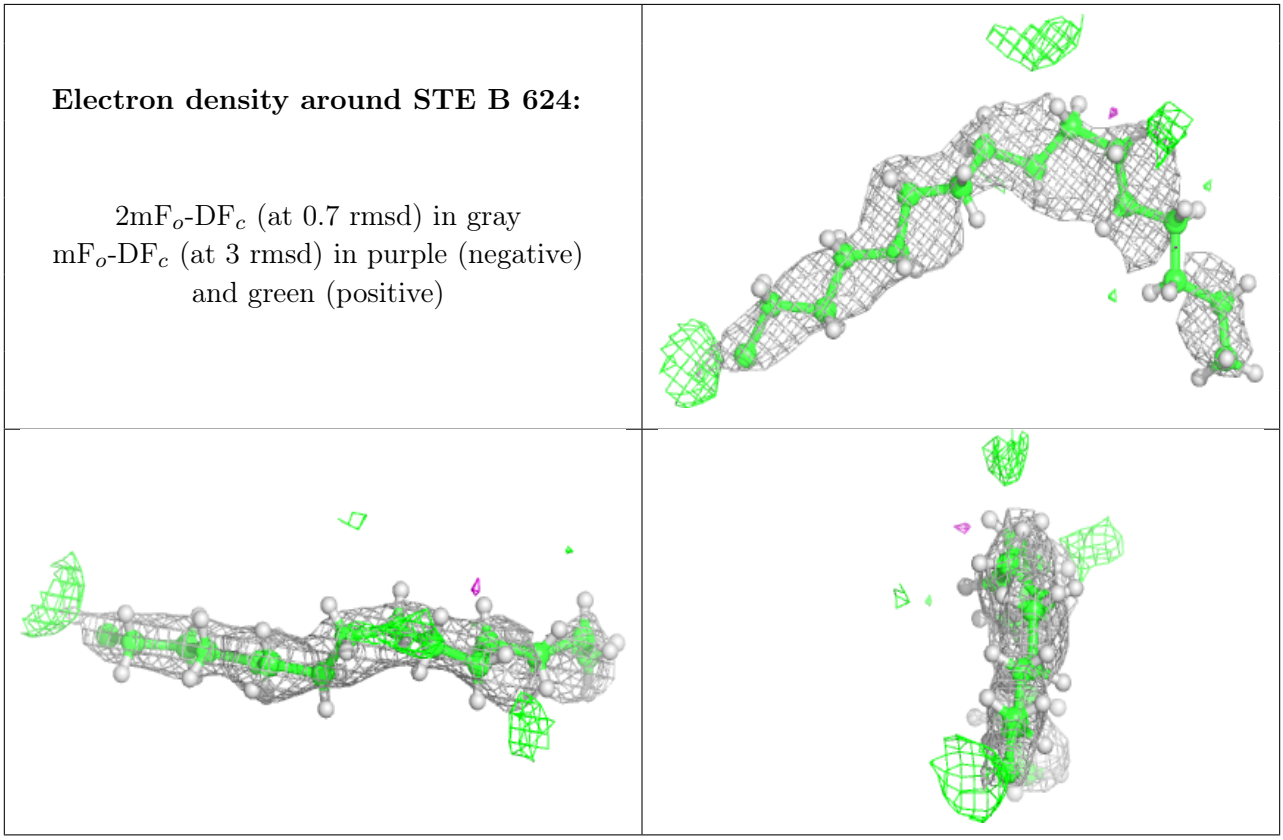
Electron density around LHG a 411:

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



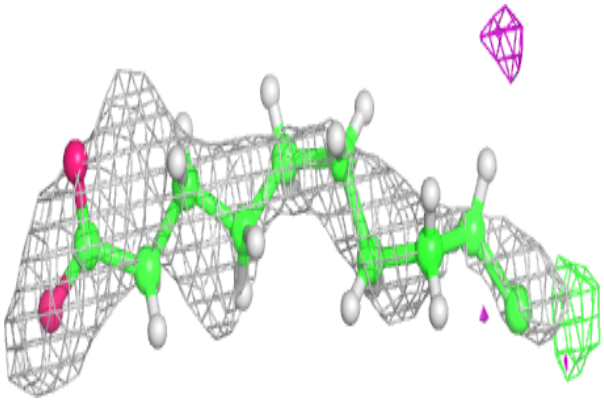
Electron density around STE B 624:

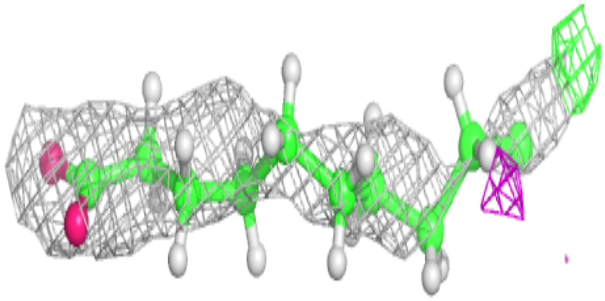
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

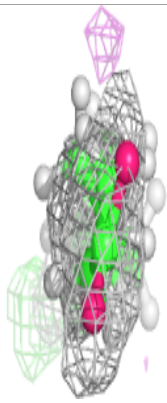


Electron density around STE a 412:

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

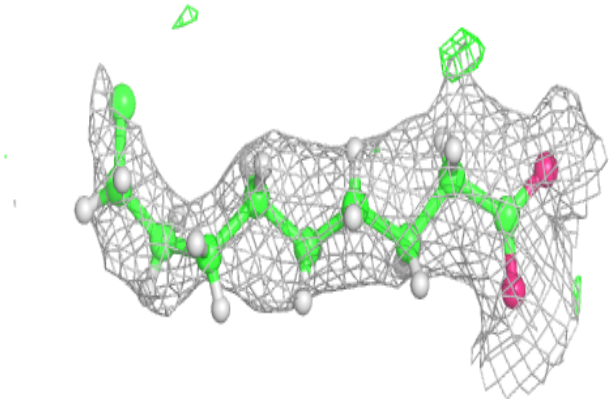


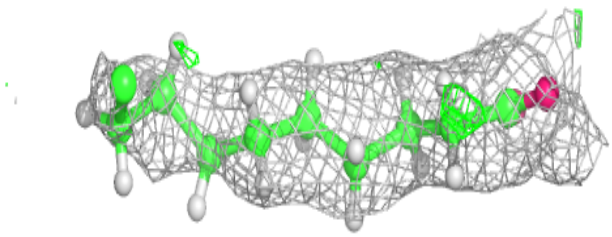


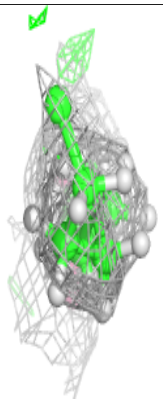


Electron density around STE k 104:

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

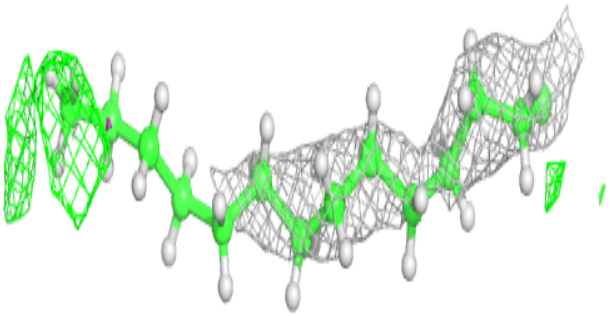


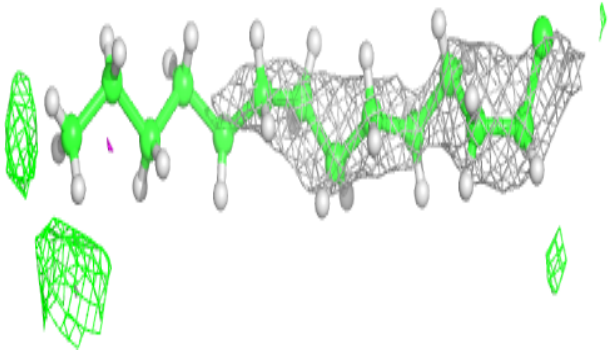


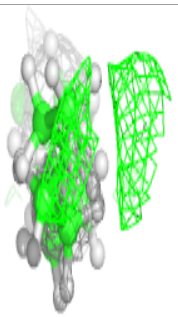


Electron density around STE b 628:

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

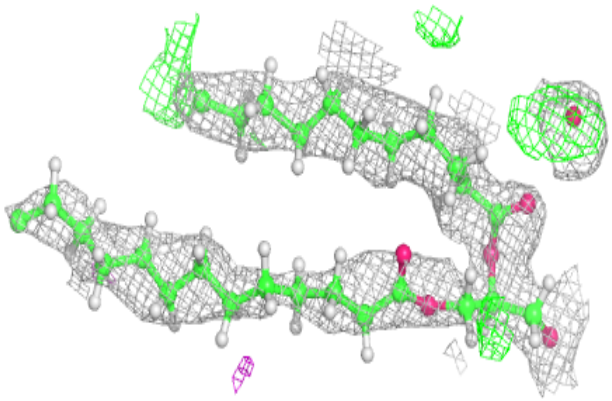


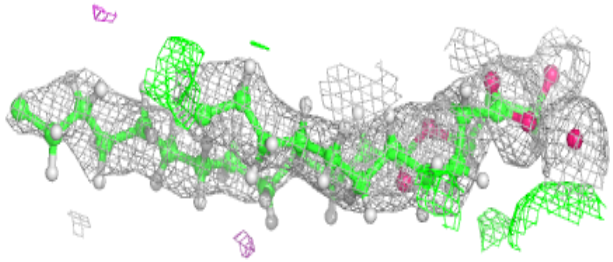


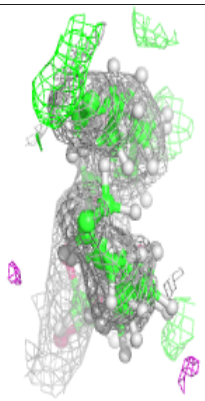


Electron density around LMG D 412:

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

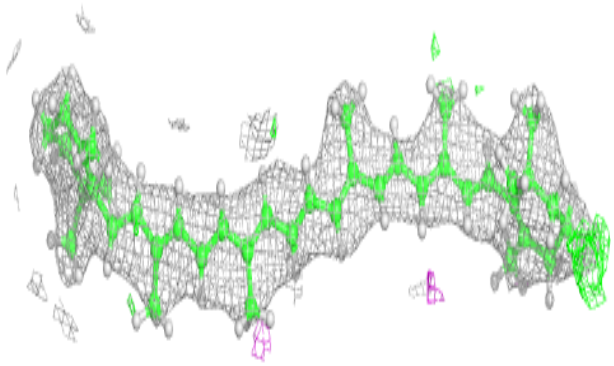


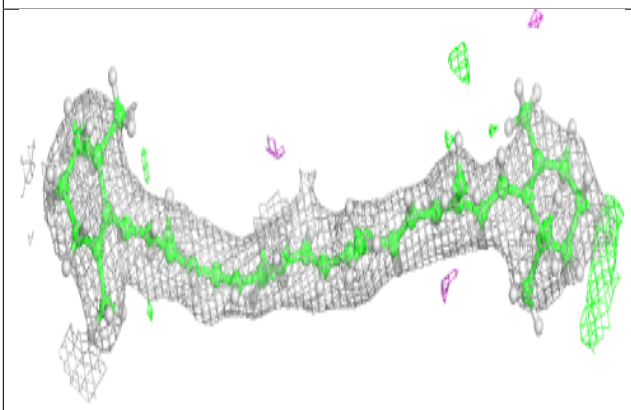


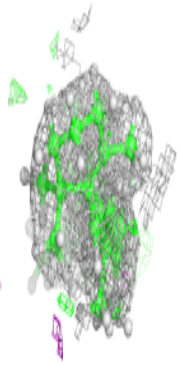


Electron density around BCR H 102:

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

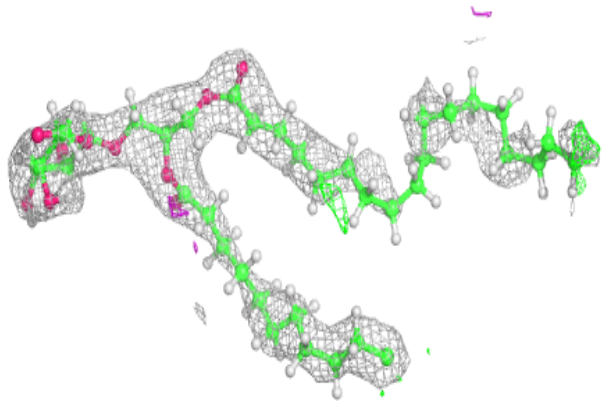


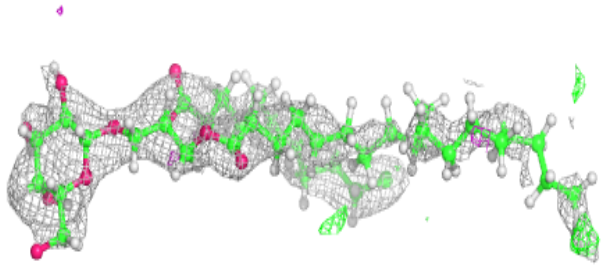


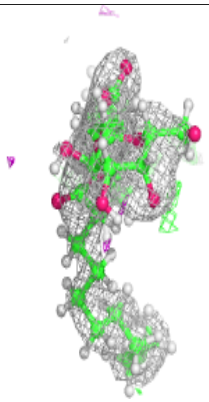


Electron density around LMG c 520:

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

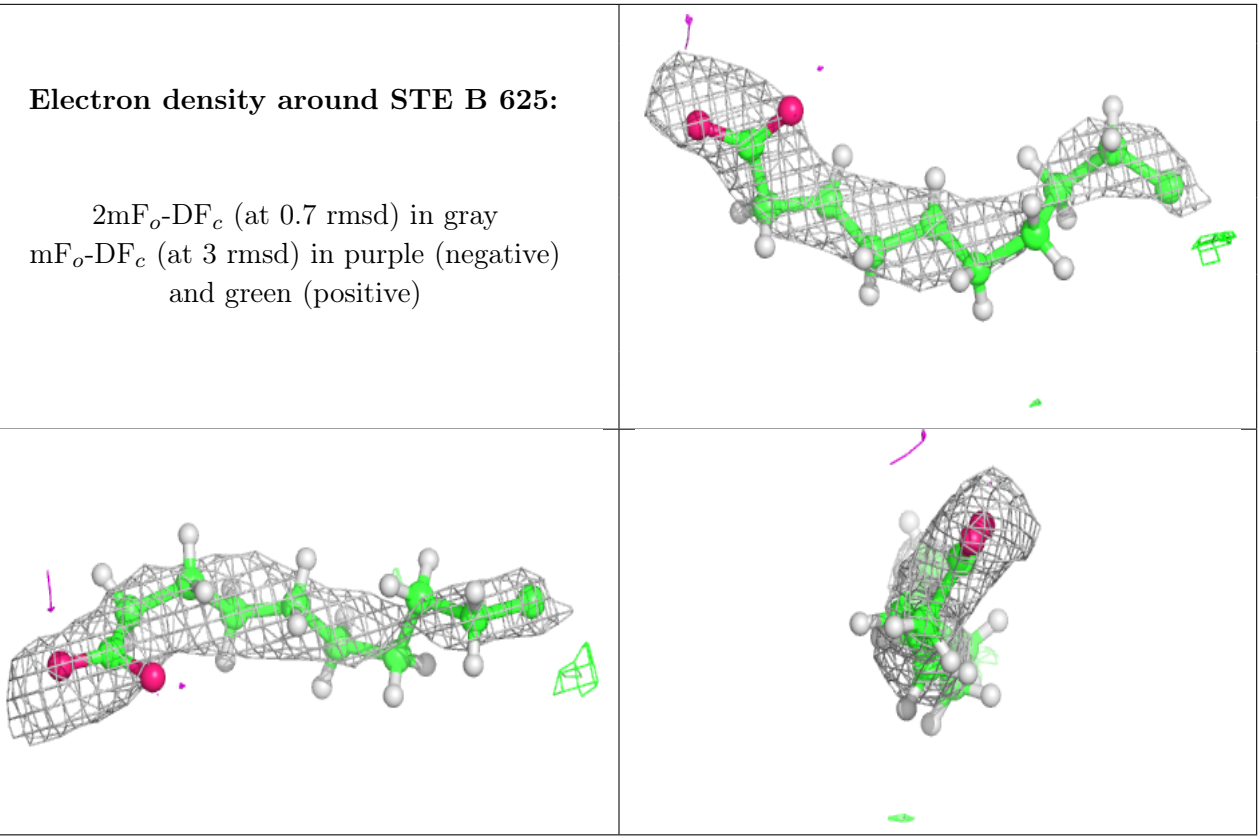






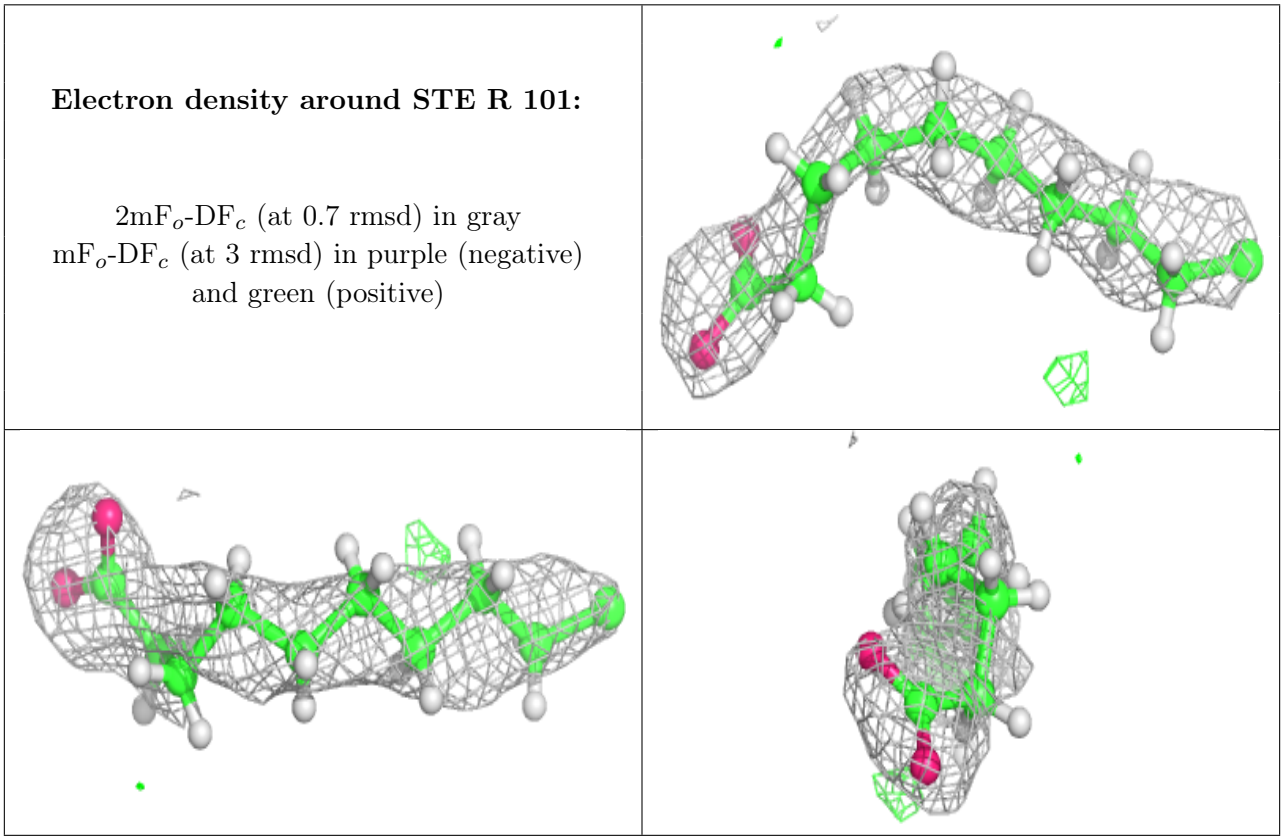
Electron density around STE B 625:

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



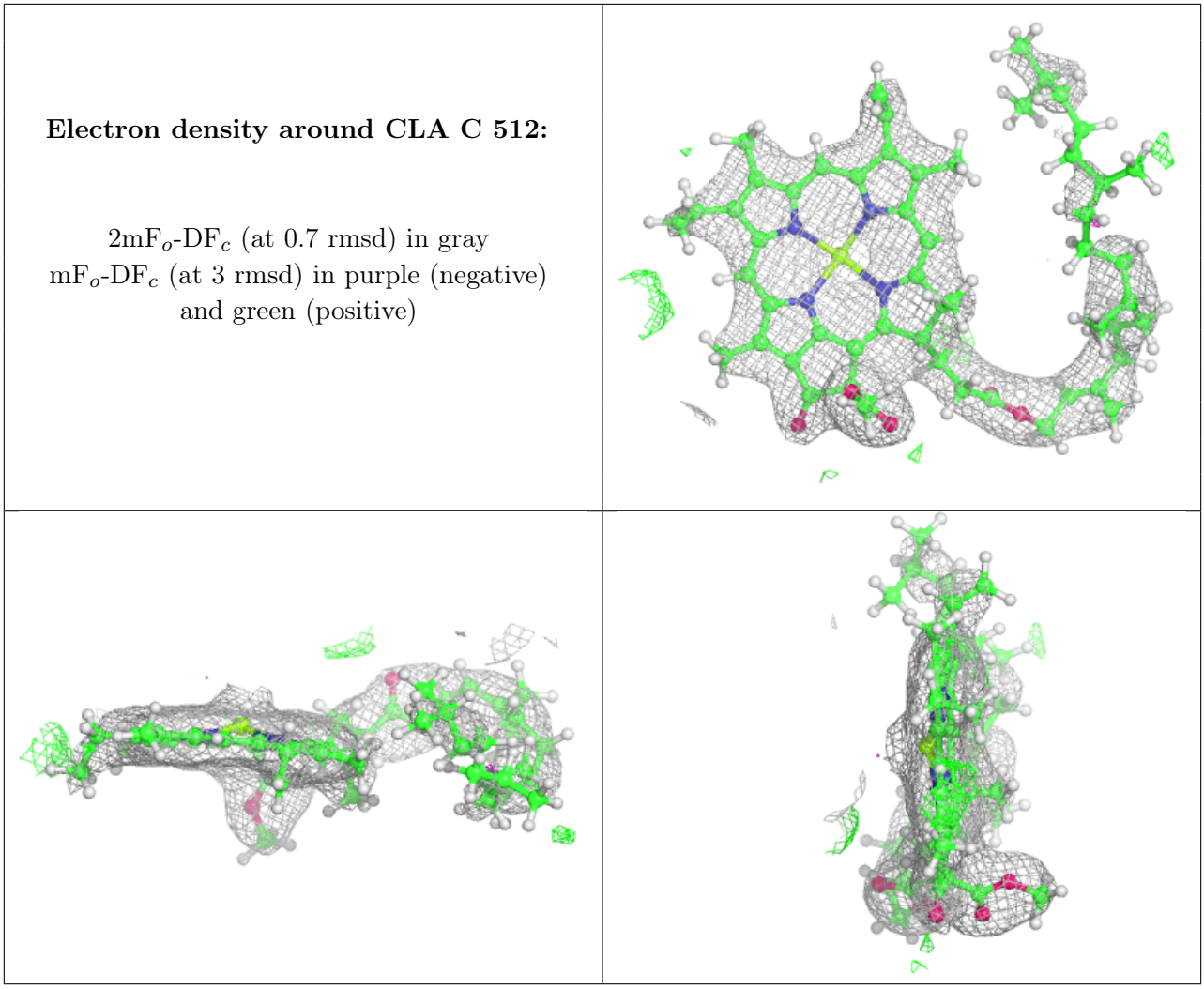
Electron density around STE R 101:

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



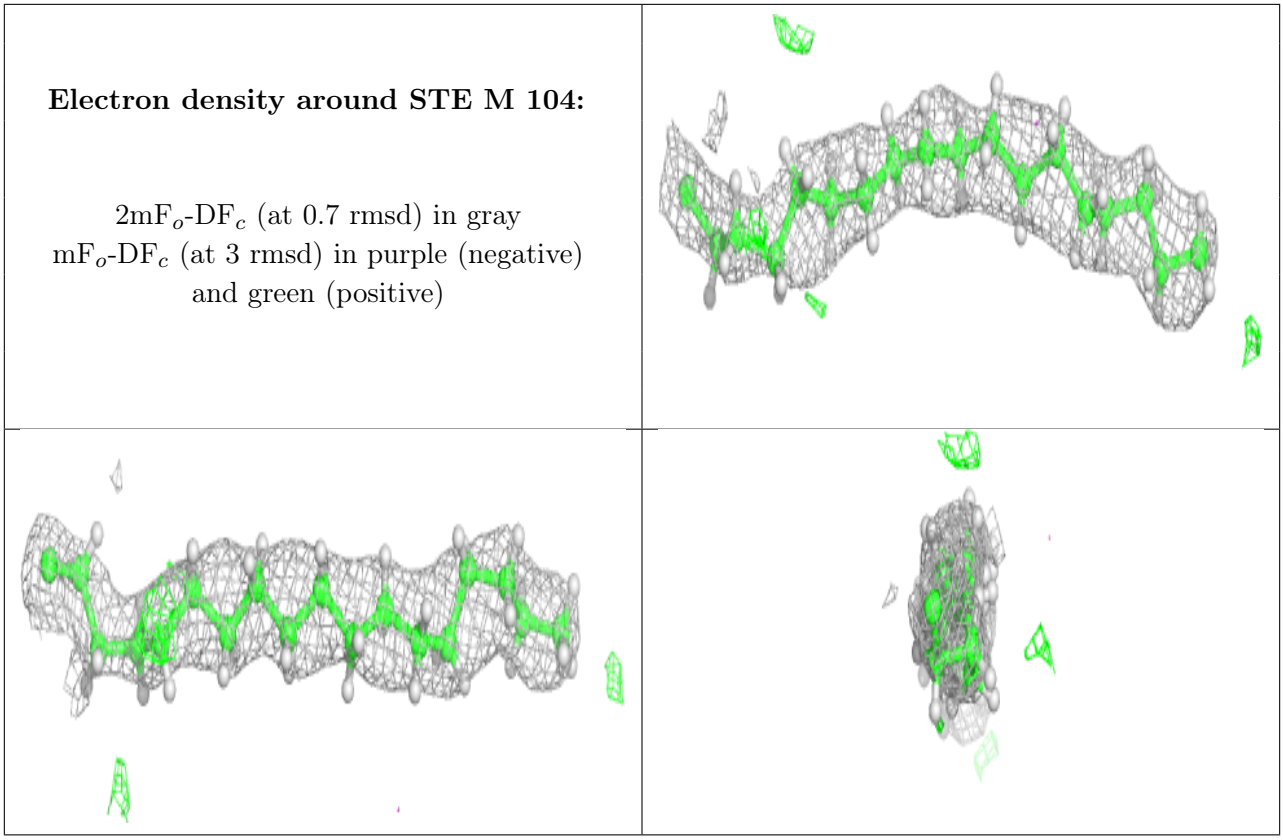
Electron density around CLA C 512:

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



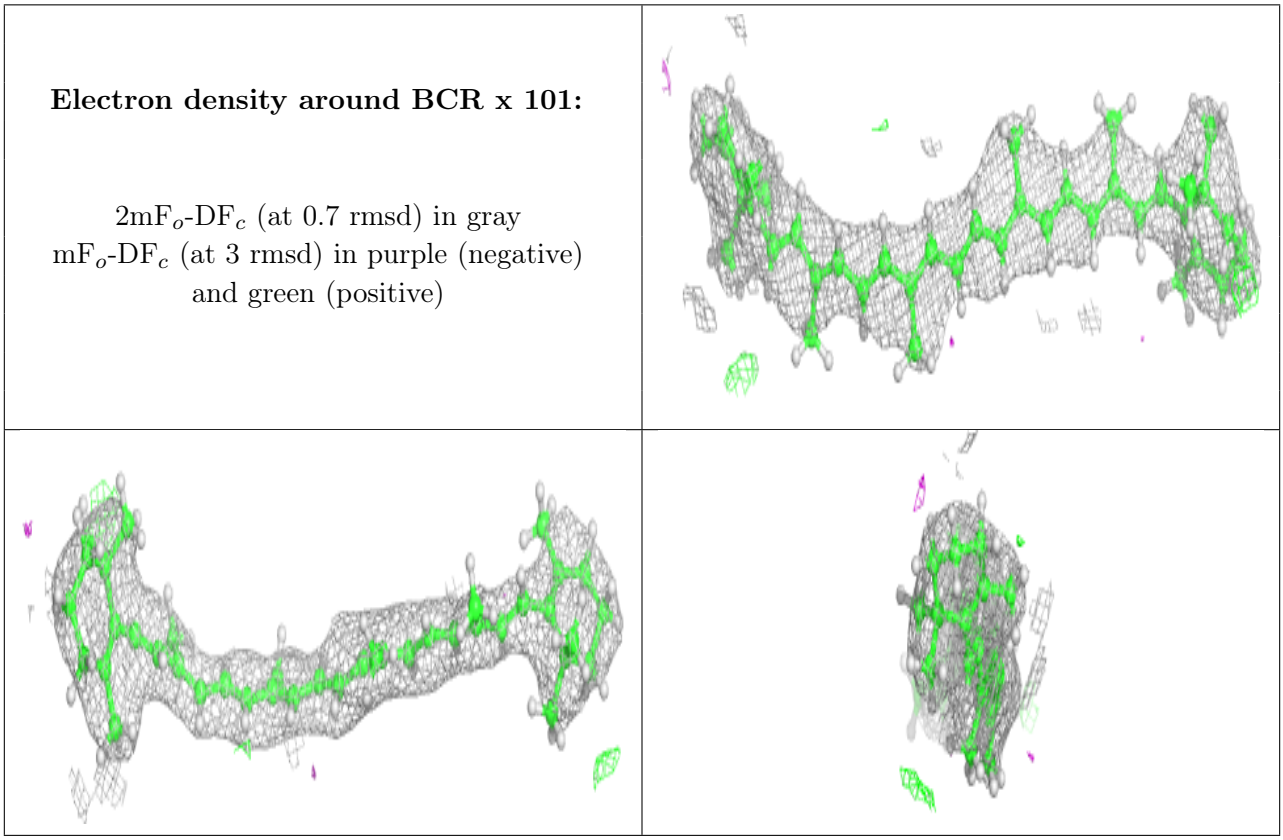
Electron density around STE M 104:

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



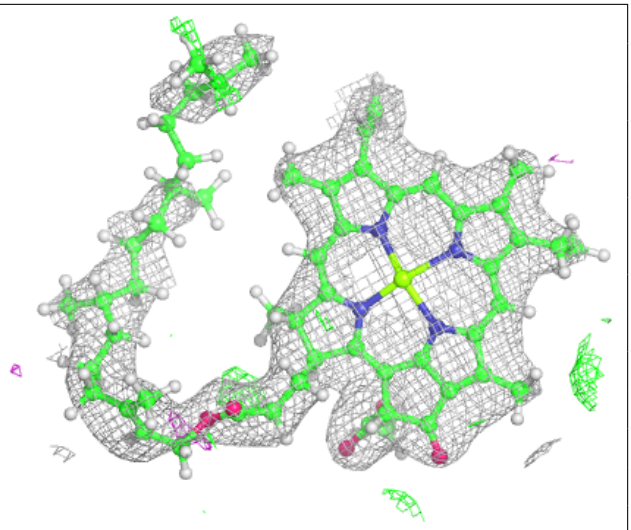
Electron density around BCR x 101:

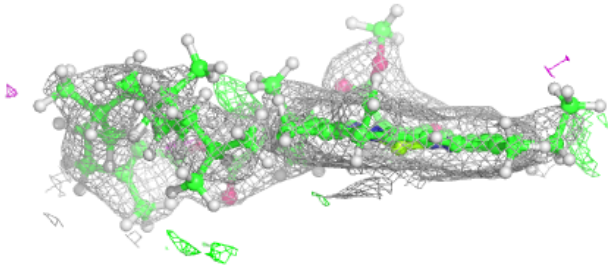
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

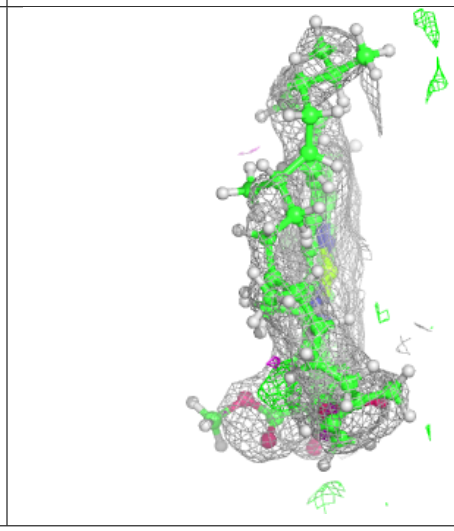


Electron density around CLA c 512:

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

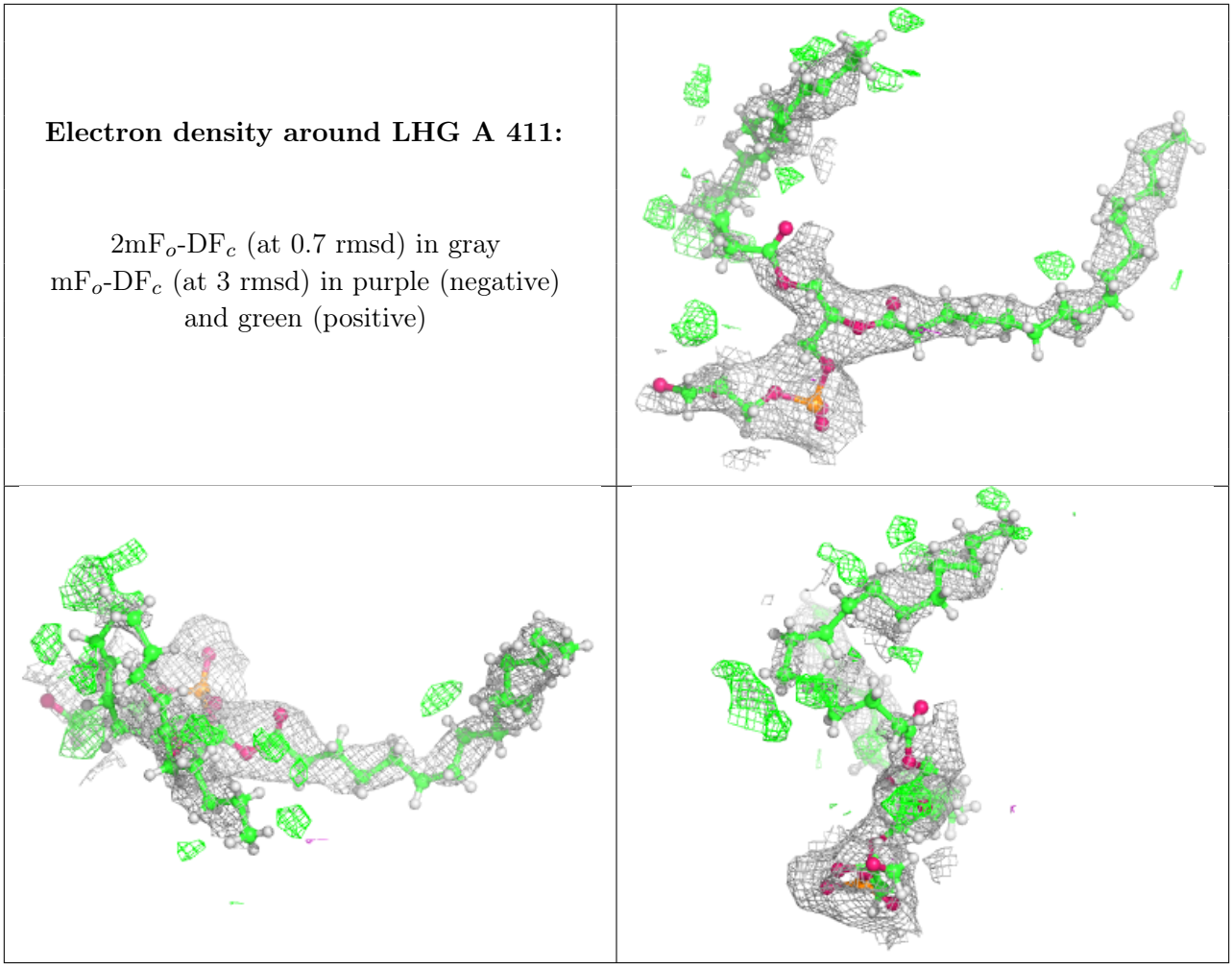






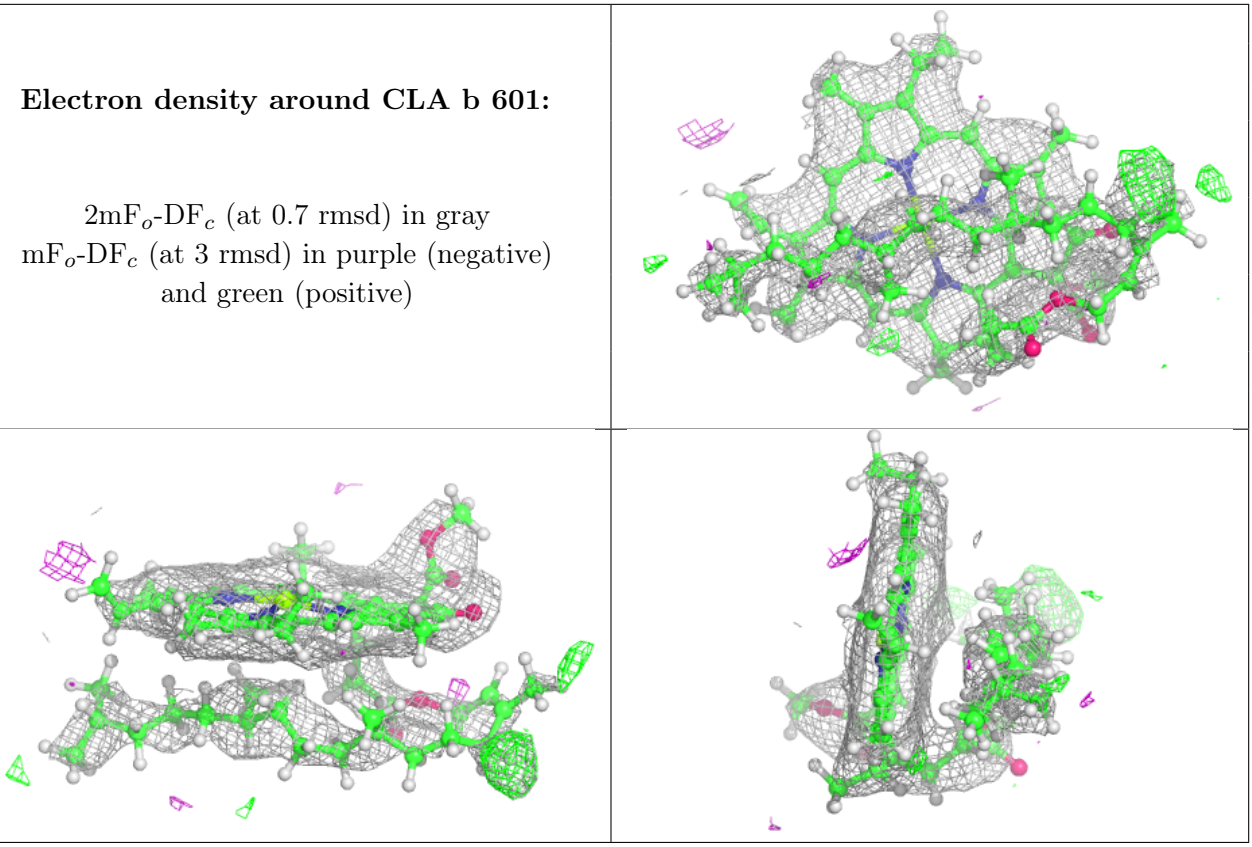
Electron density around LHG A 411:

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



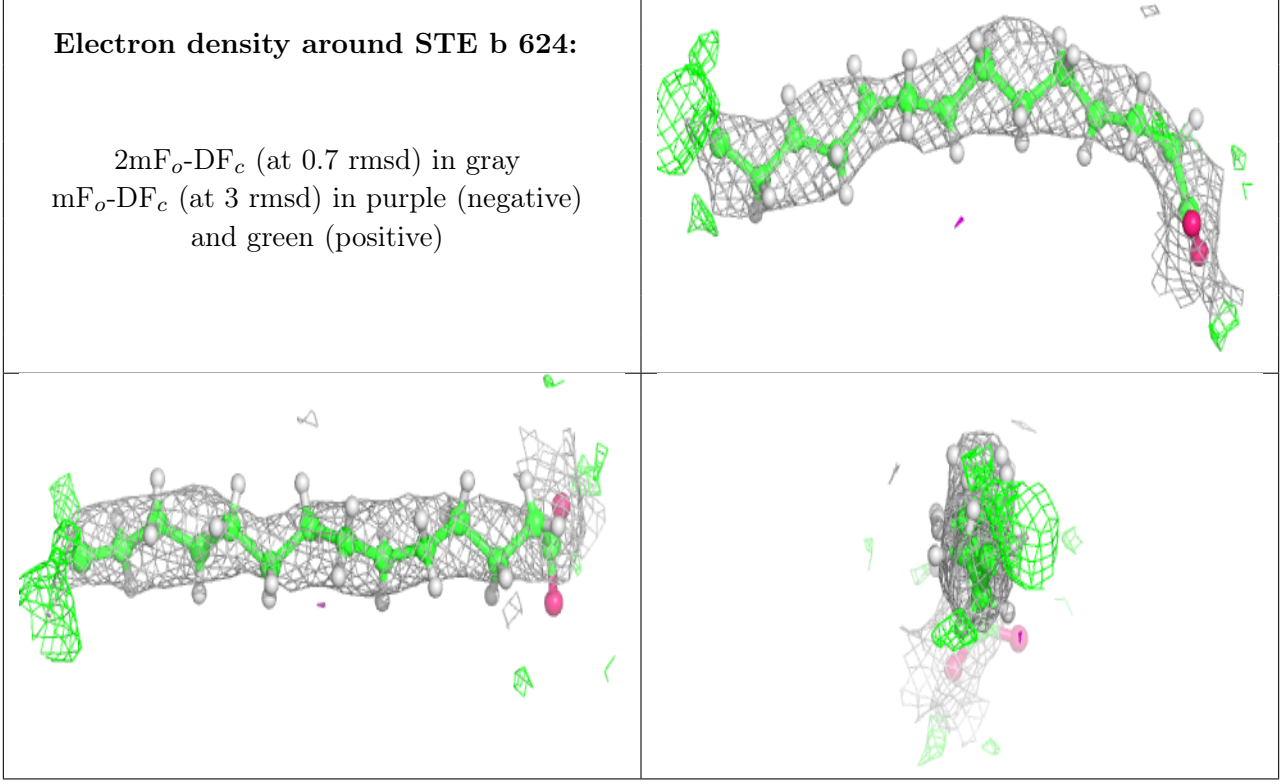
Electron density around CLA b 601:

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



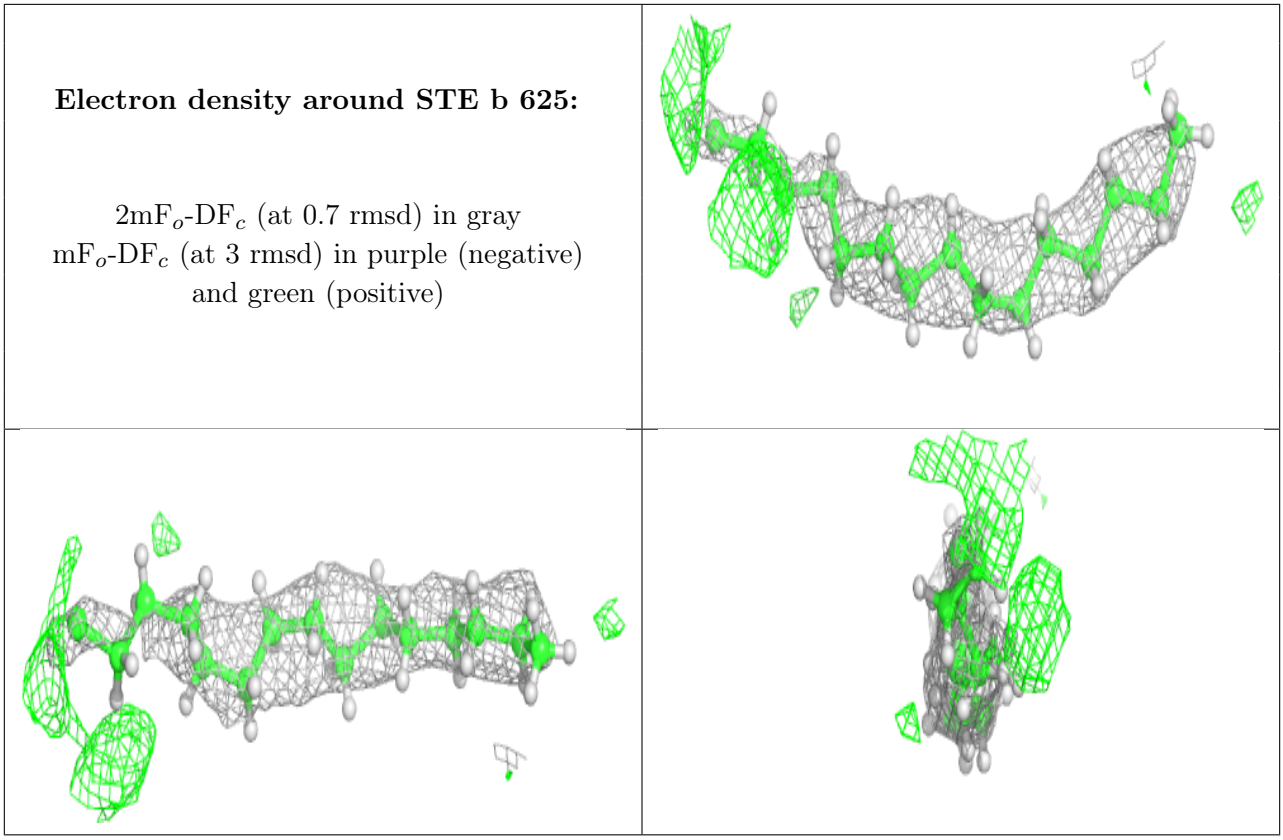
Electron density around STE b 624:

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



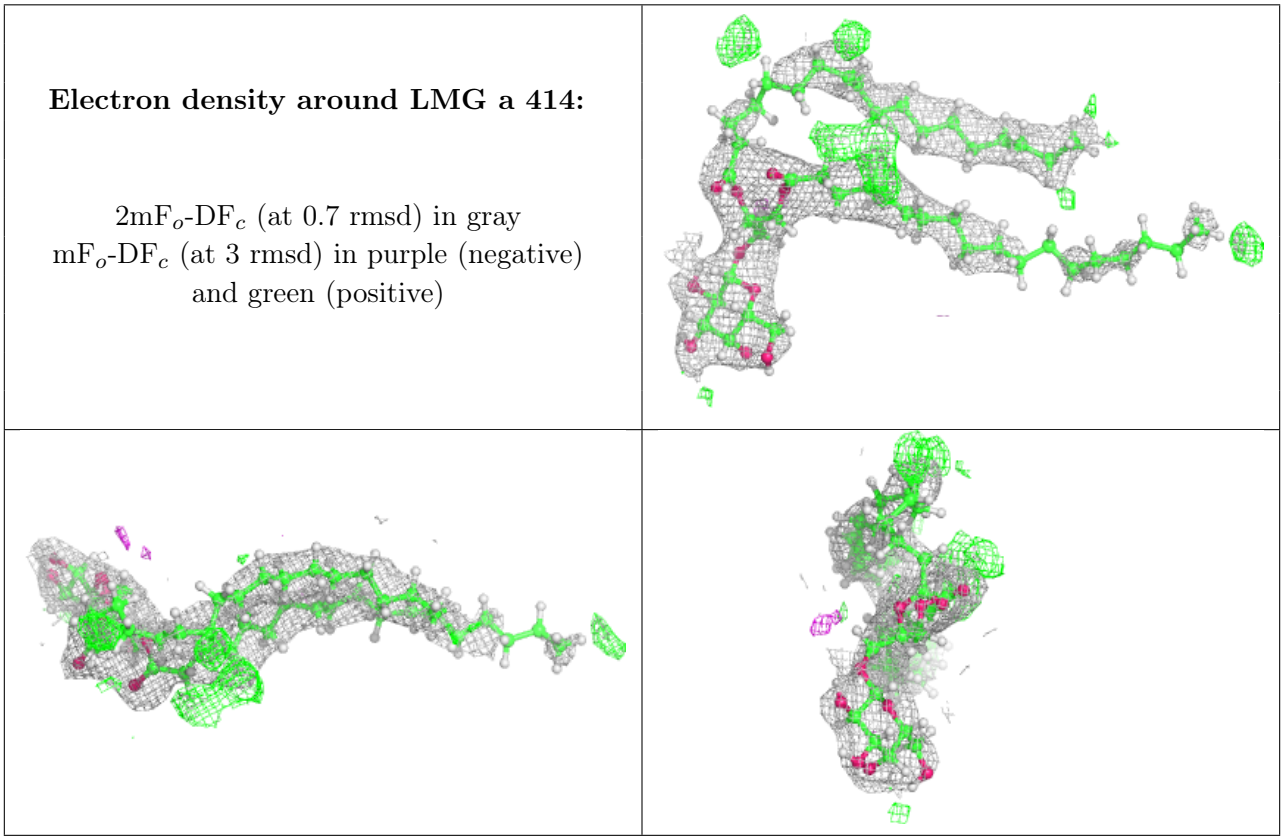
Electron density around STE b 625:

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



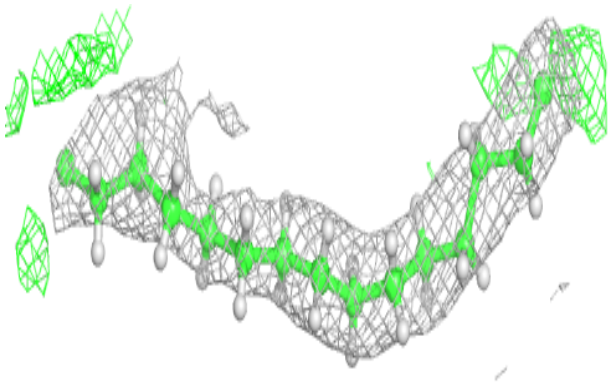
Electron density around LMG a 414:

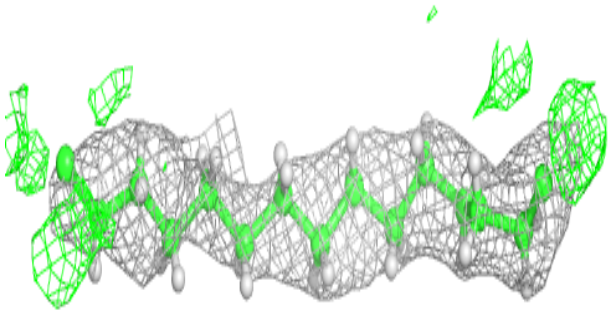
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

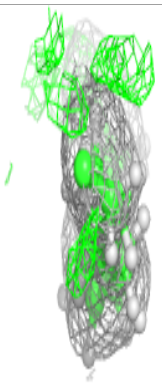


Electron density around STE I 102:

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

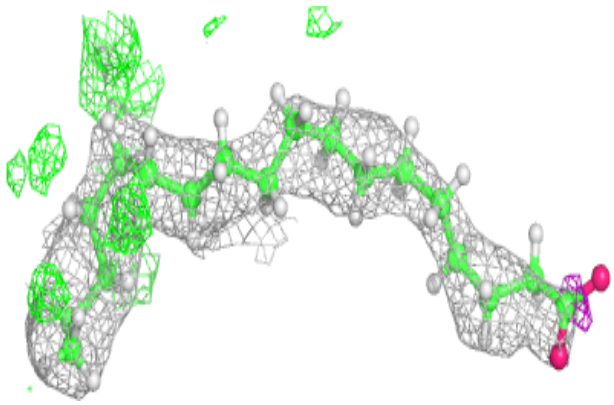


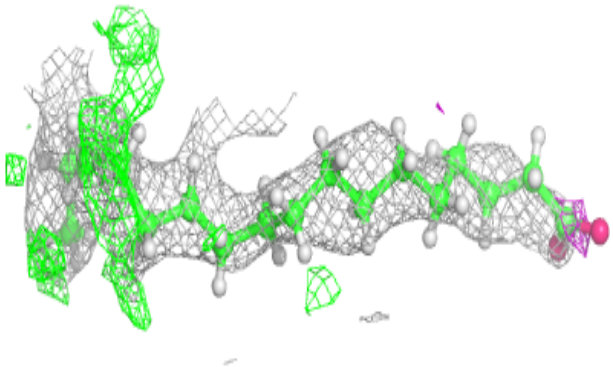


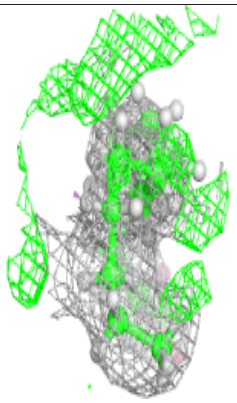


Electron density around STE b 629:

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

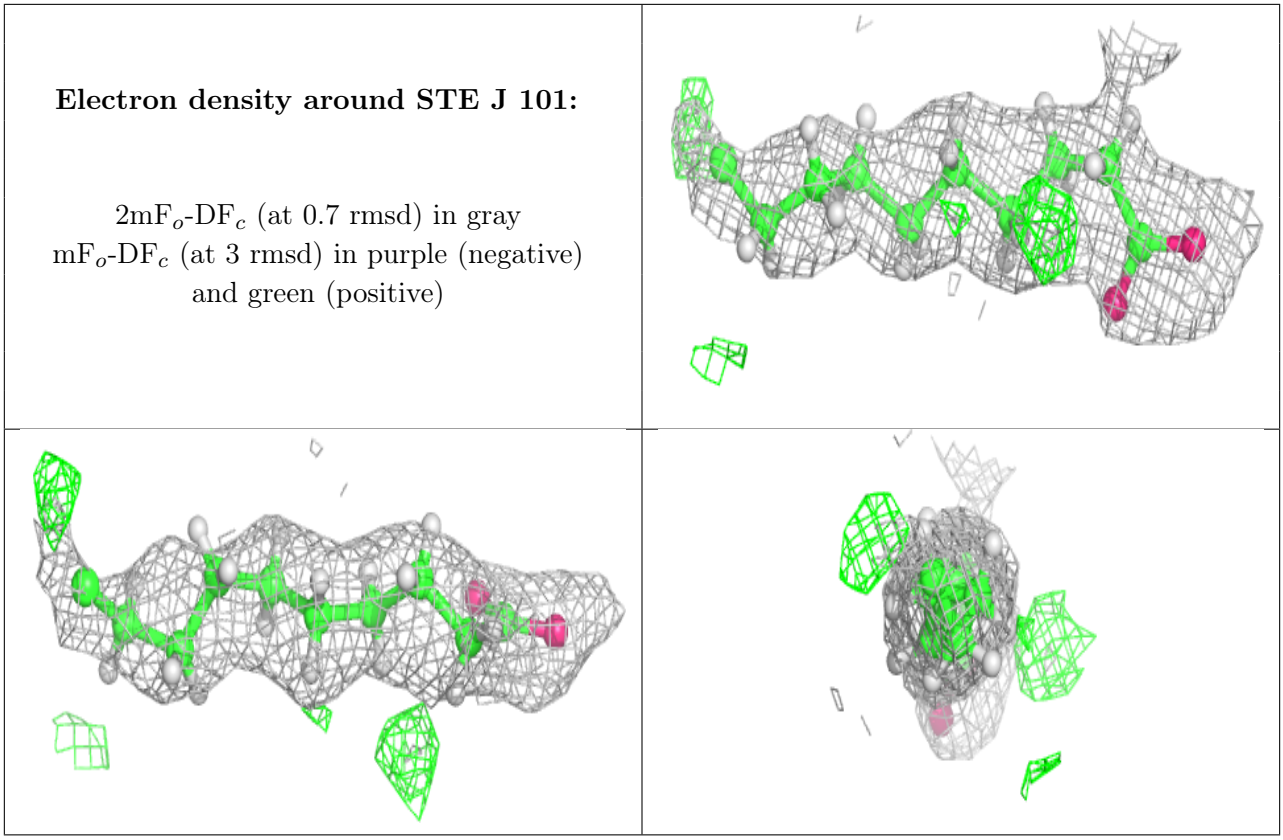






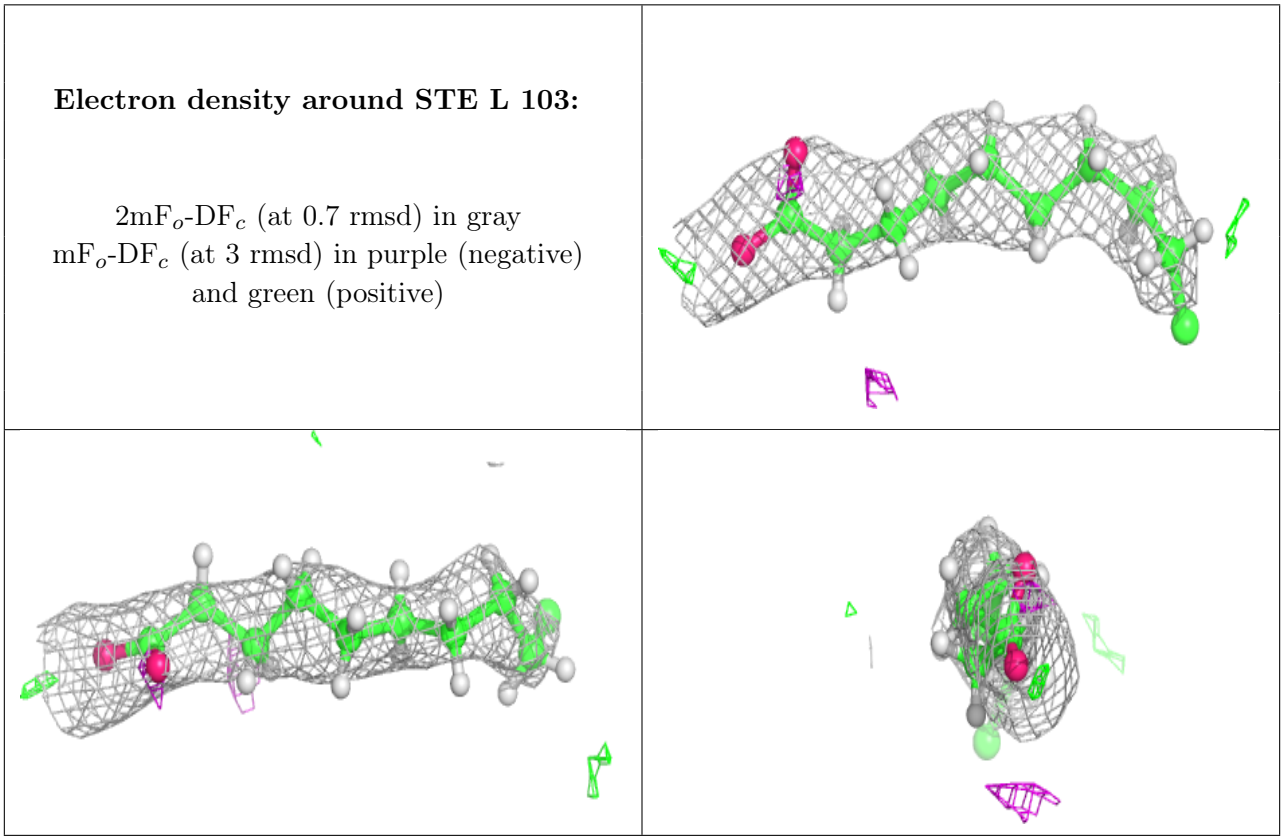
Electron density around STE J 101:

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



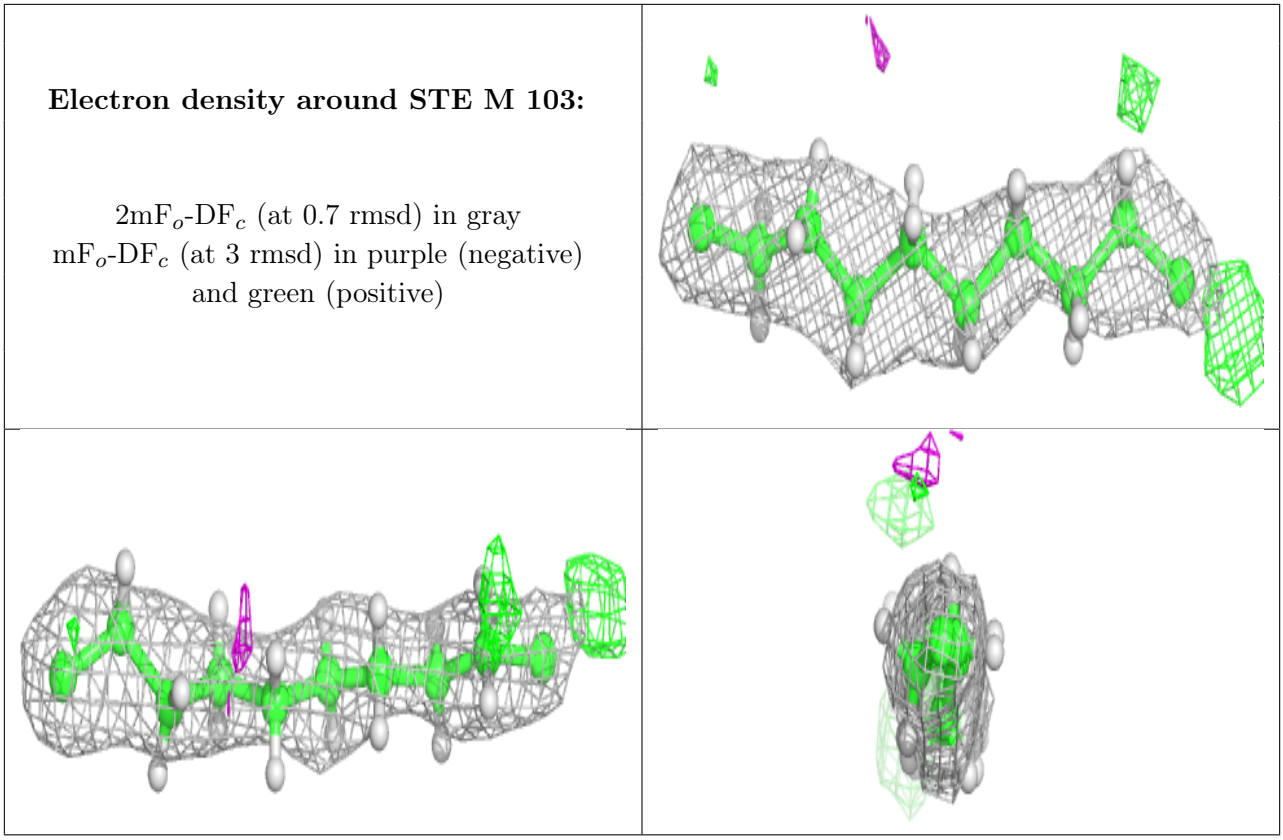
Electron density around STE L 103:

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



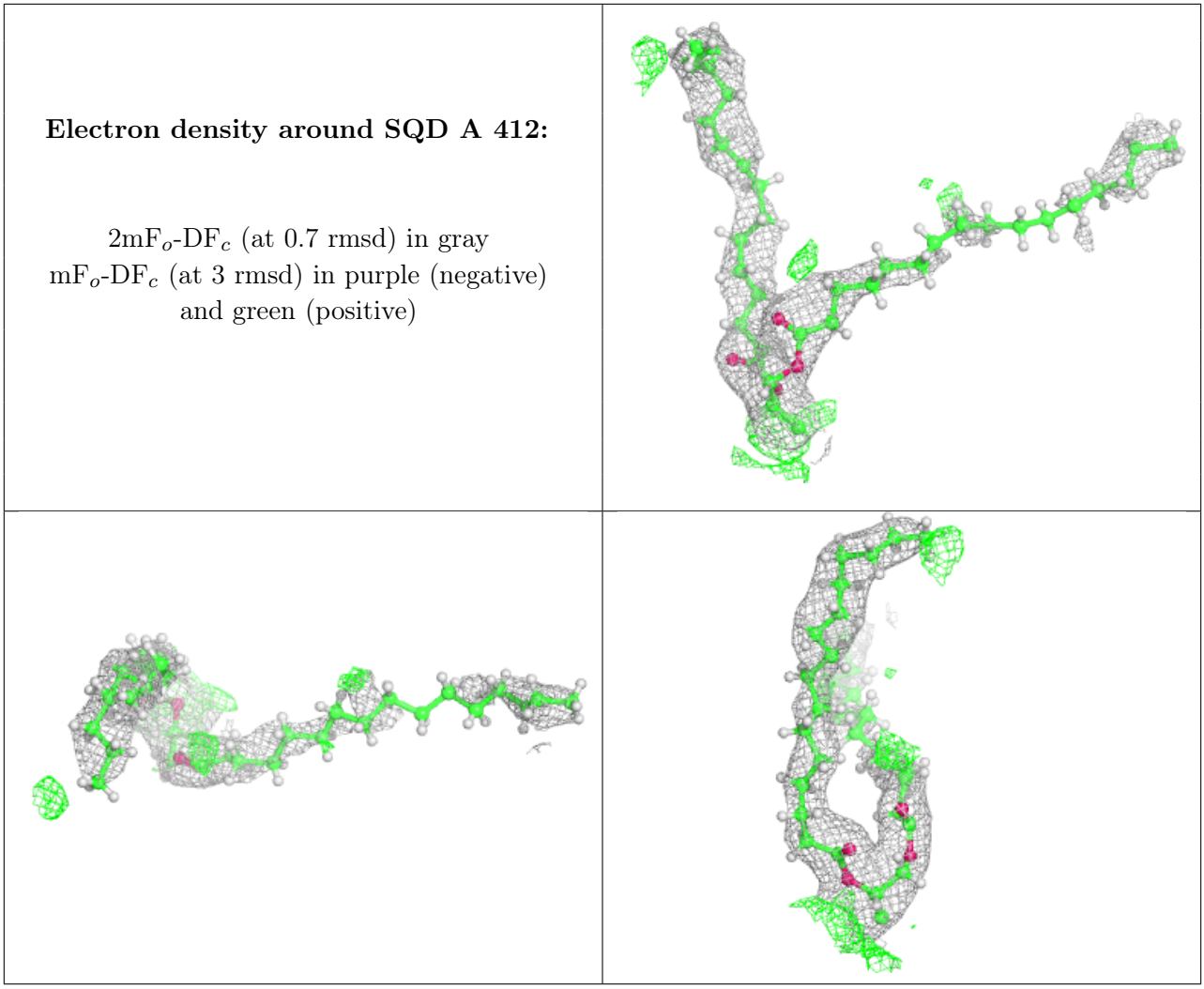
Electron density around STE M 103:

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



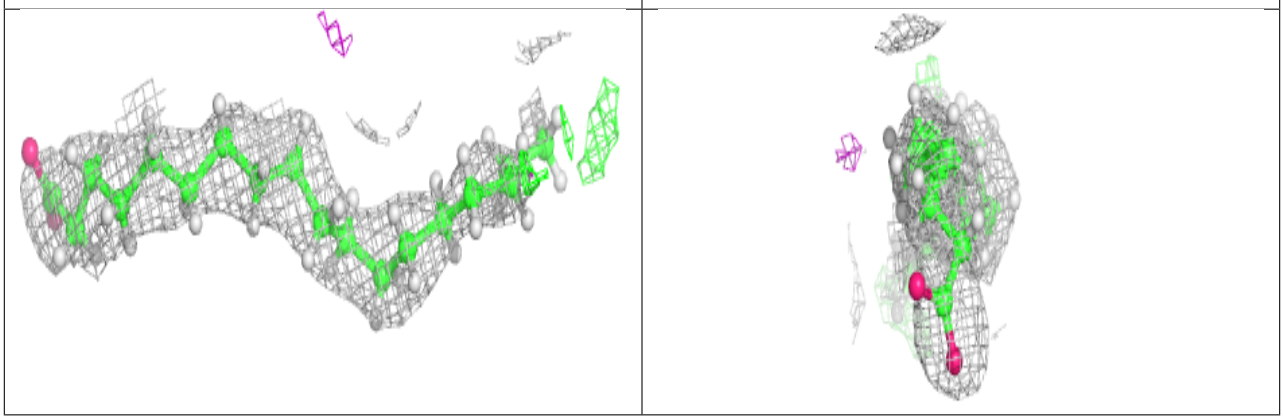
Electron density around SQD A 412:

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



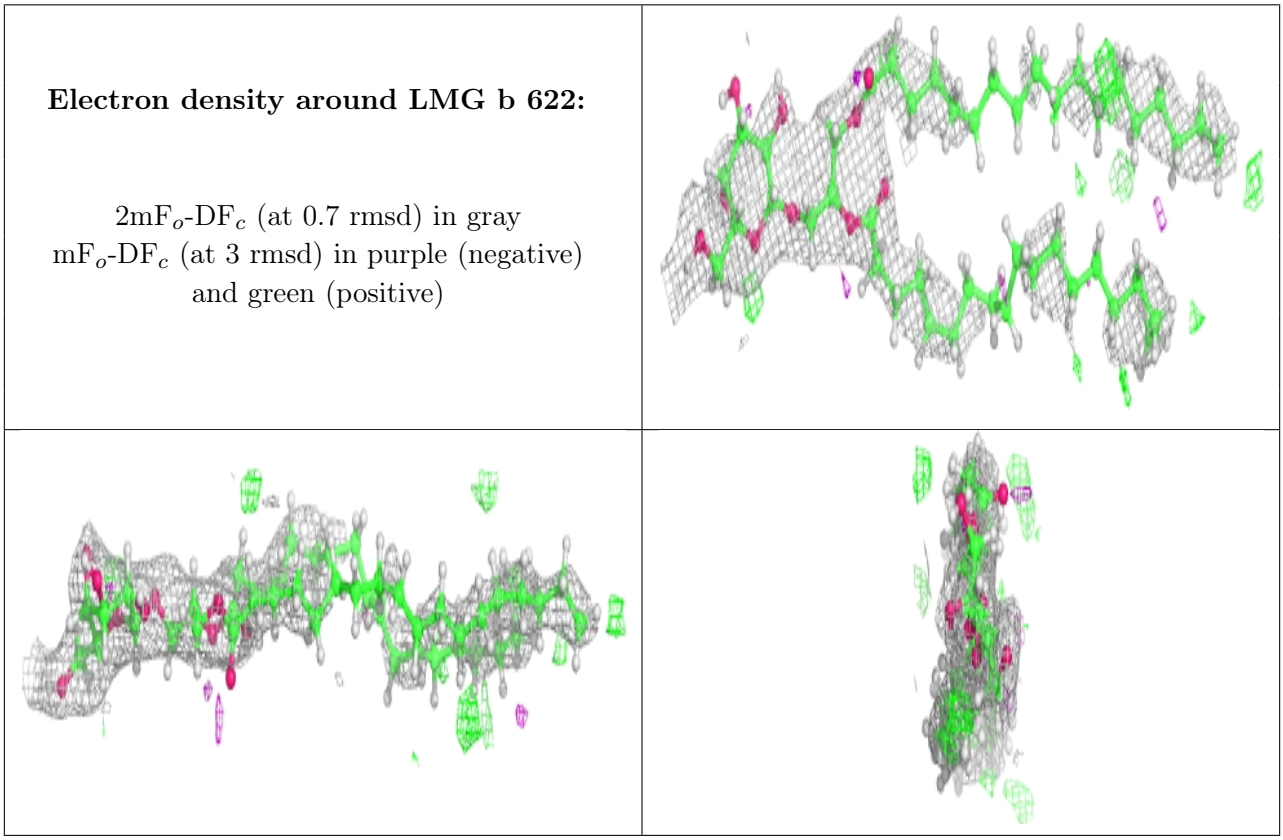
Electron density around STE b 621:

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



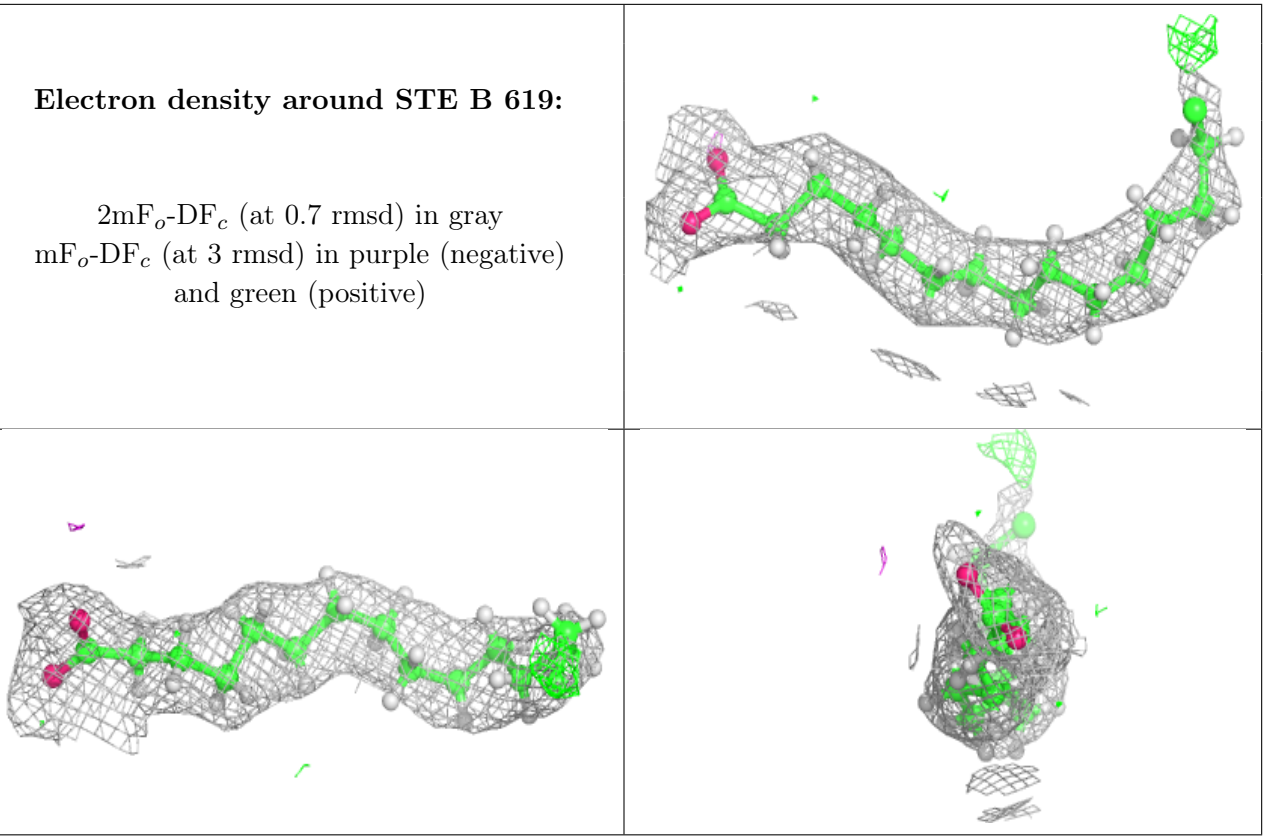
Electron density around LMG b 622:

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



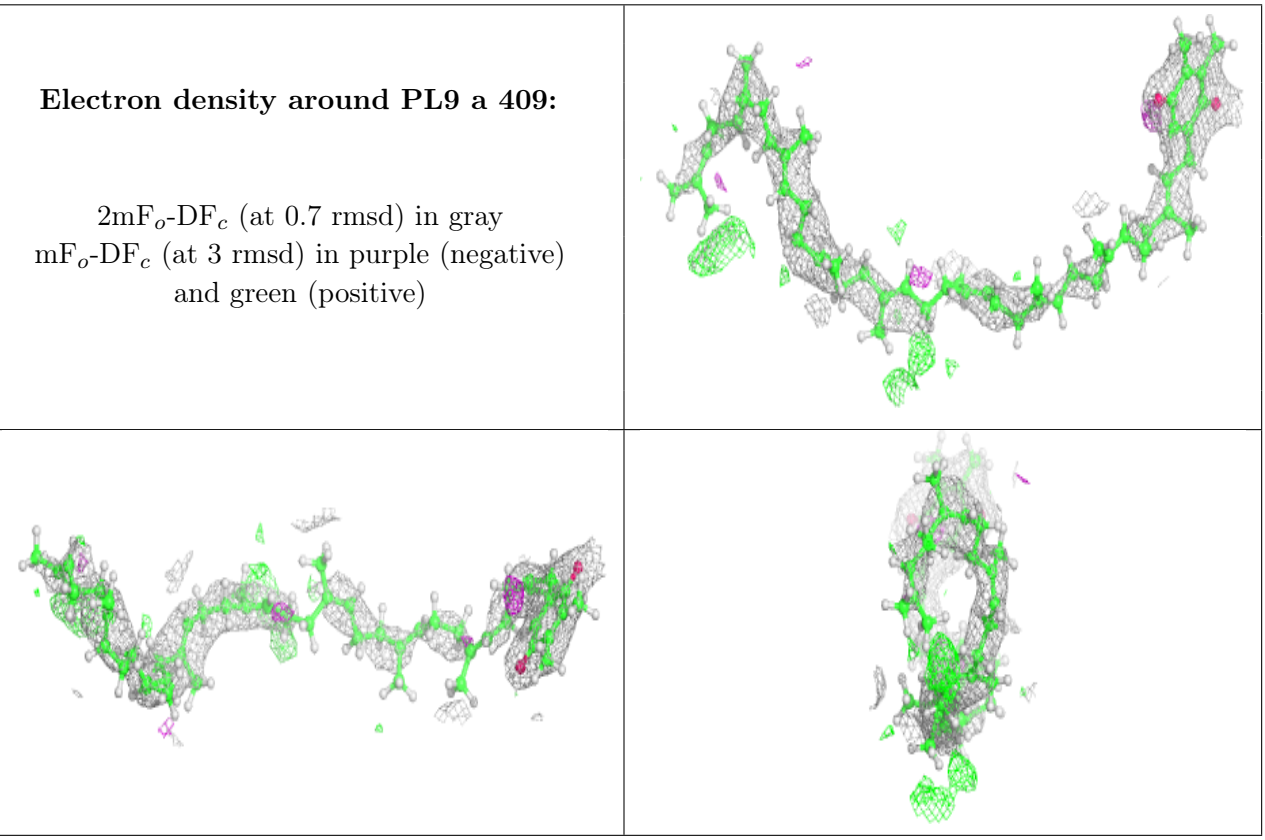
Electron density around STE B 619:

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



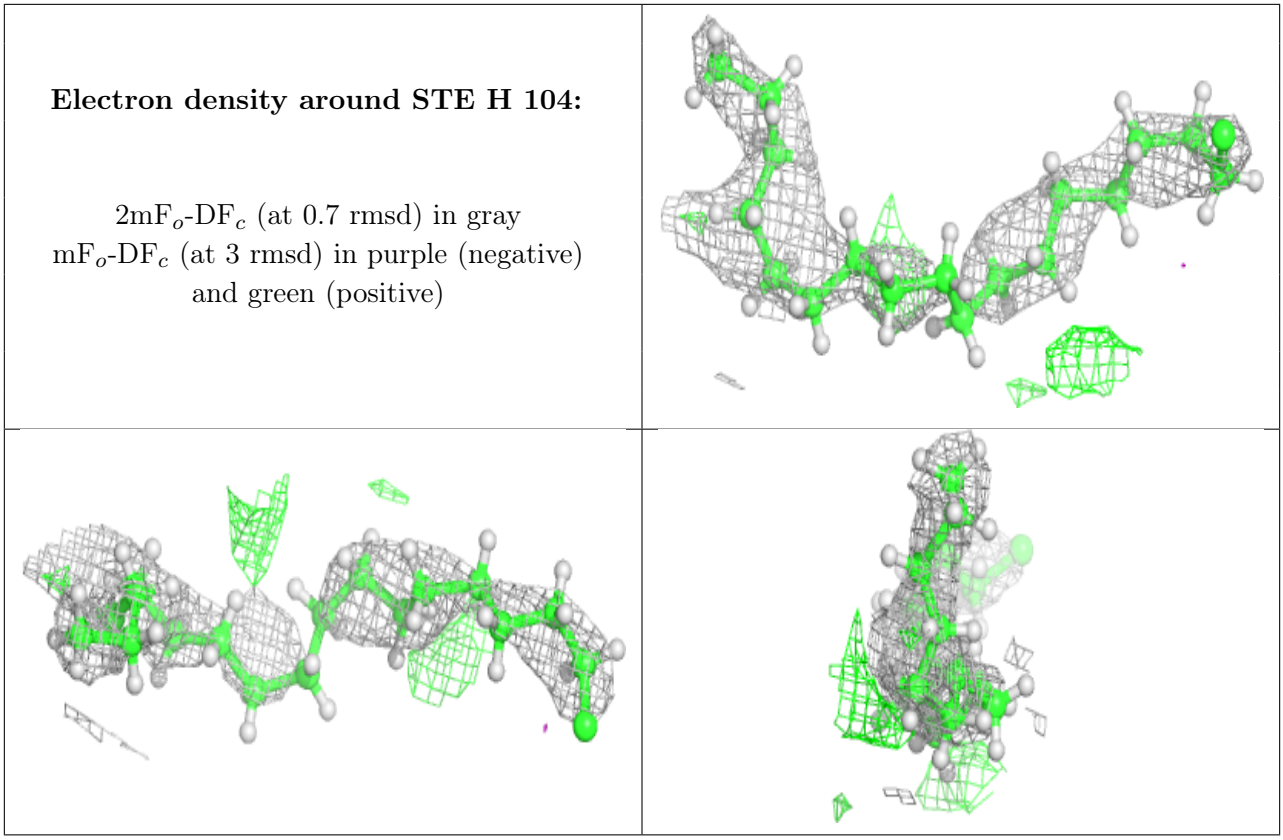
Electron density around PL9 a 409:

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



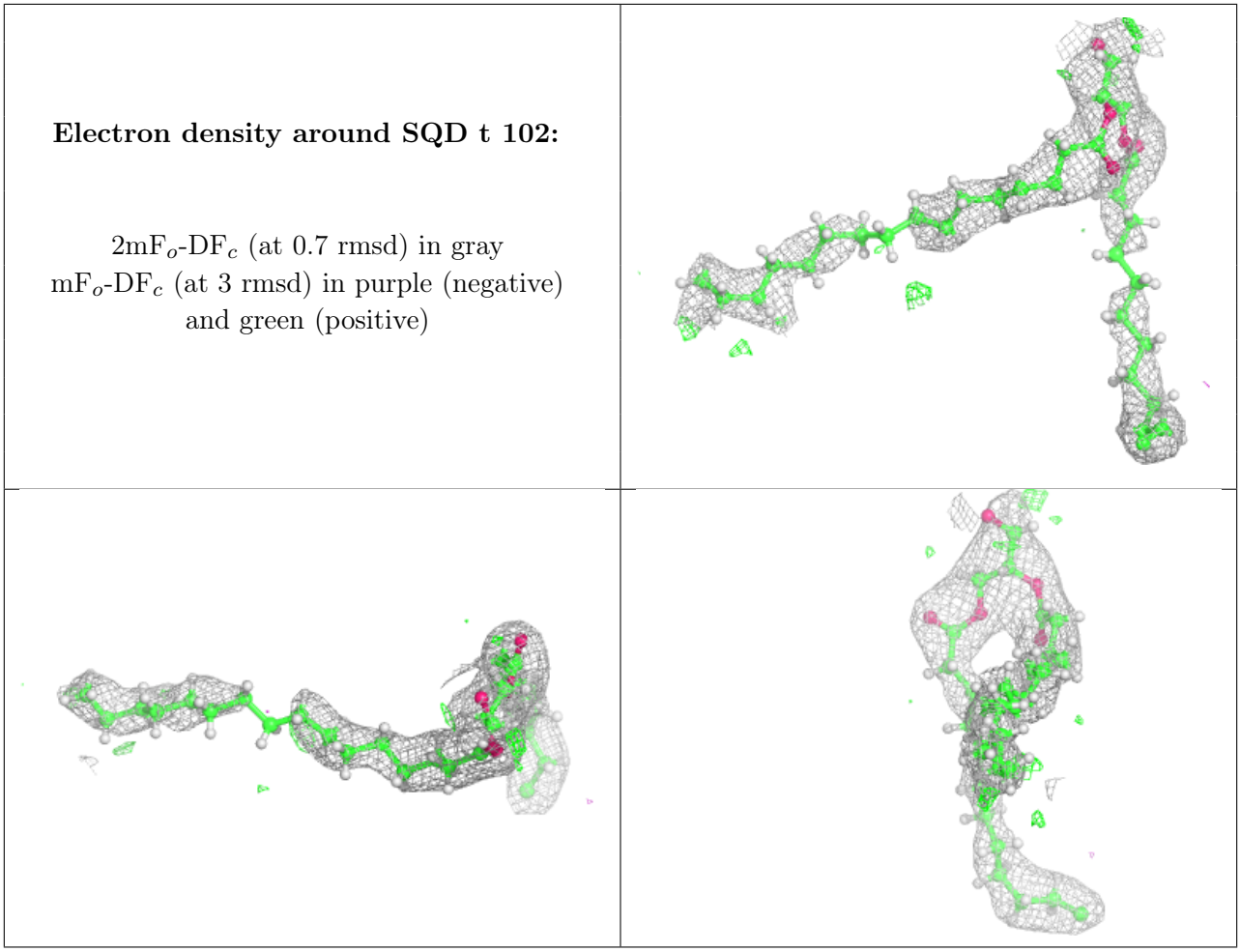
Electron density around STE H 104:

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



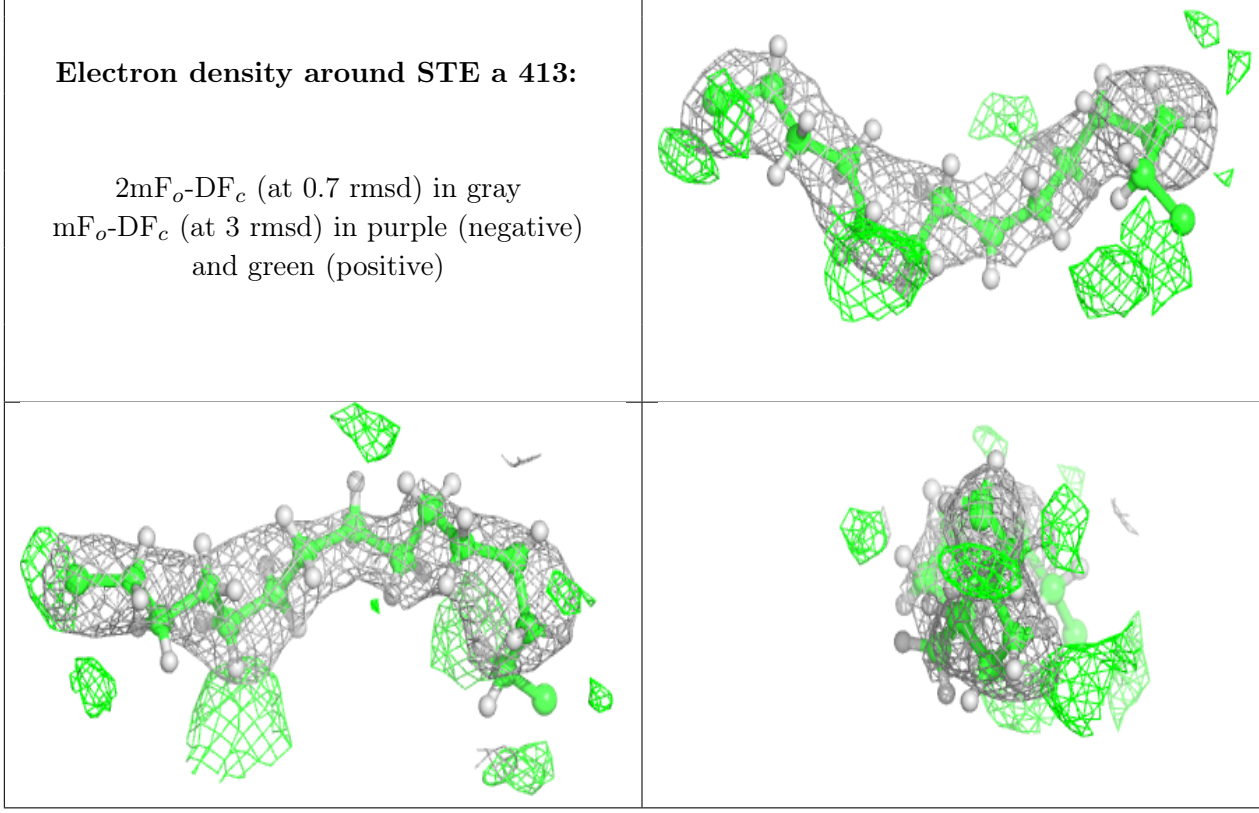
Electron density around SQD t 102:

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



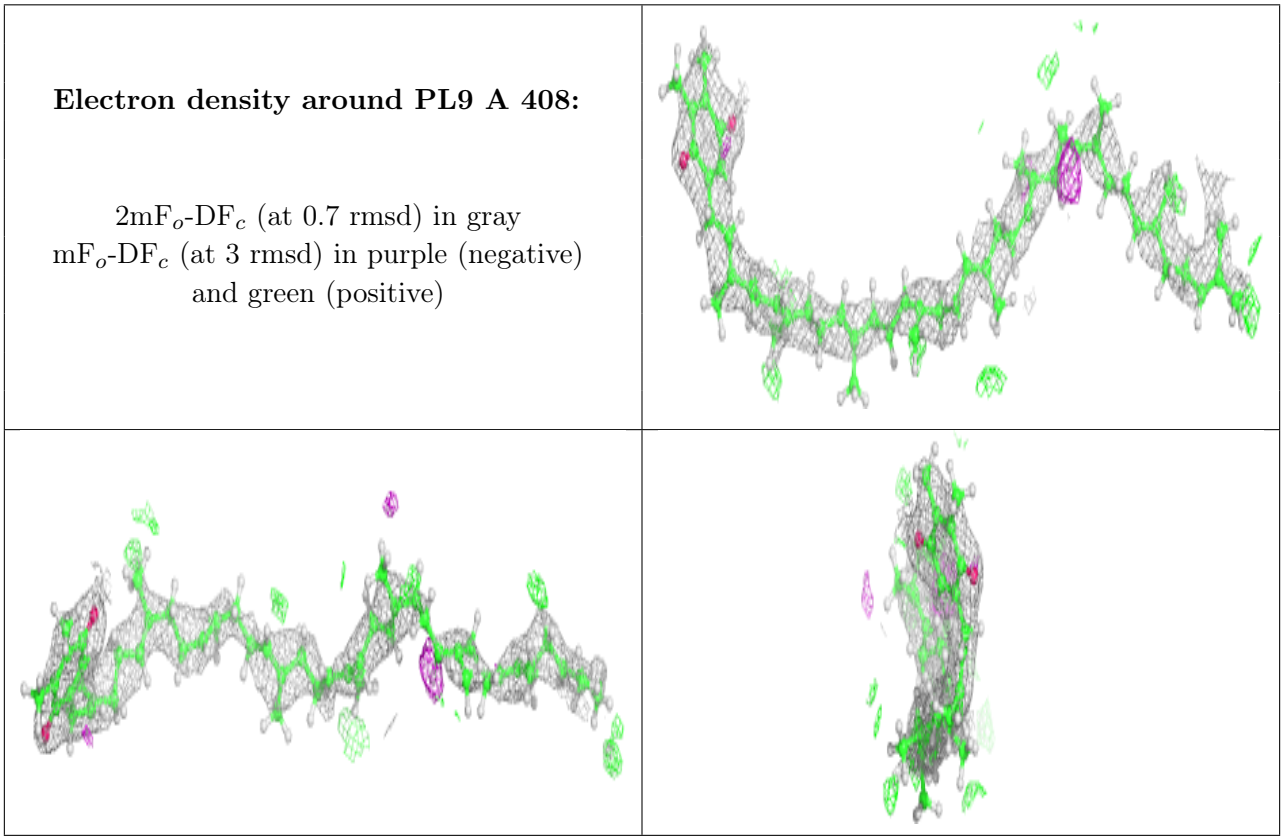
Electron density around STE a 413:

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



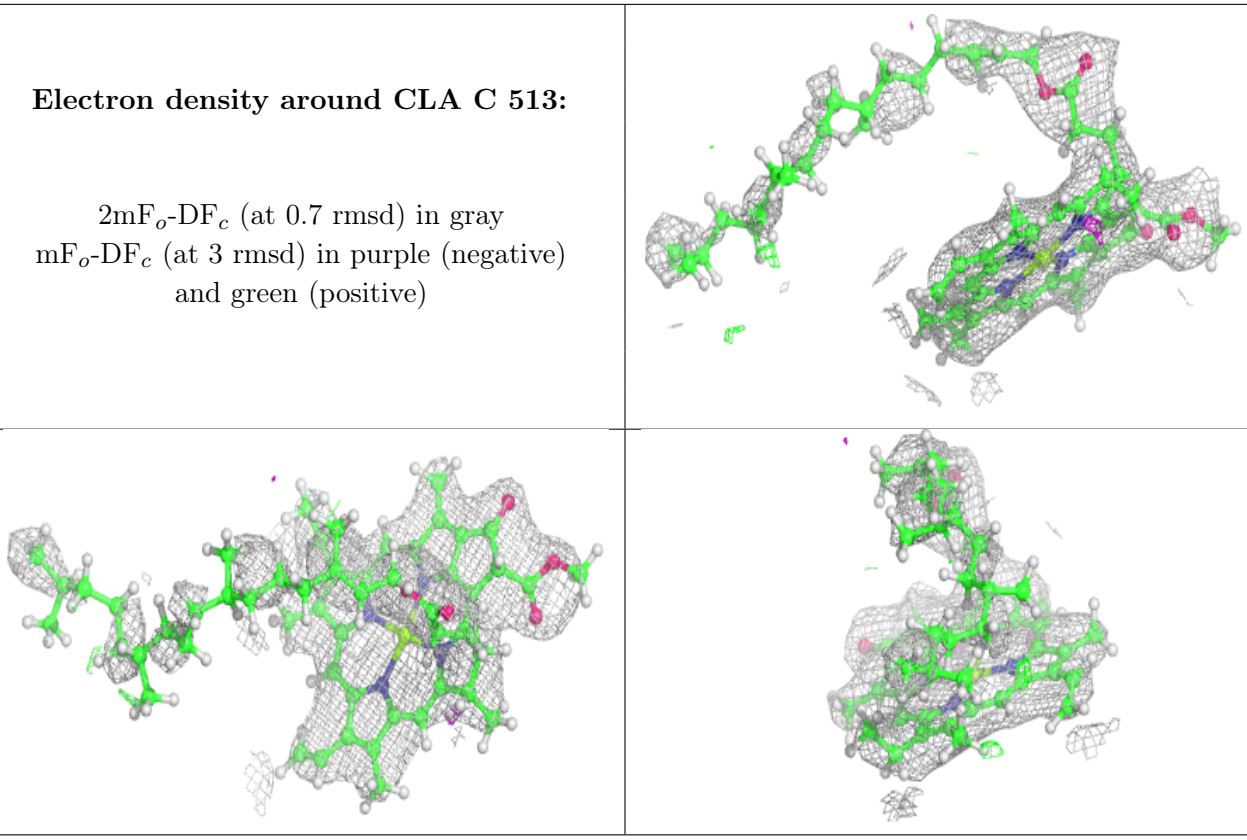
Electron density around PL9 A 408:

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



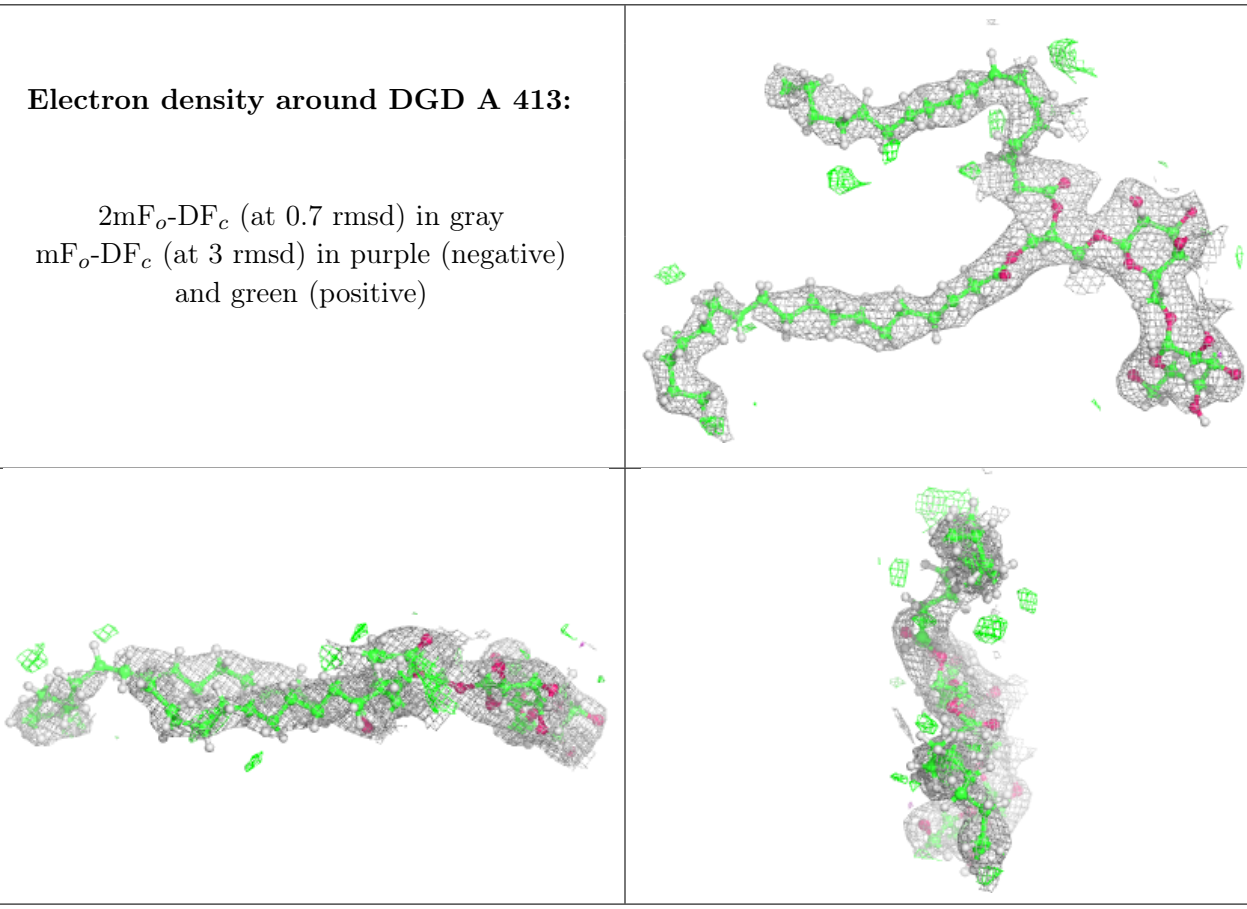
Electron density around CLA C 513:

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



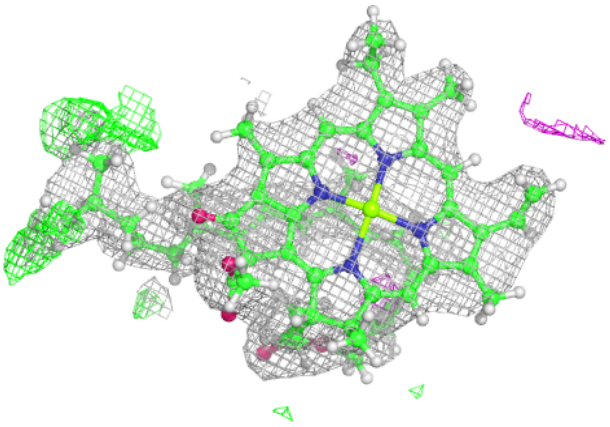
Electron density around DGD A 413:

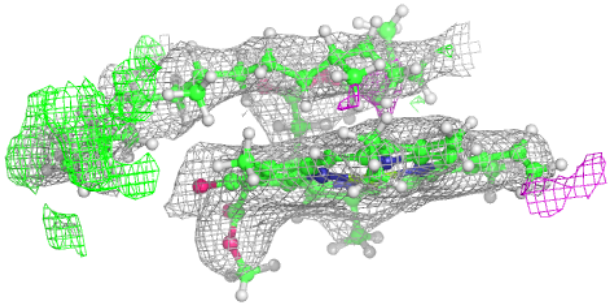
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

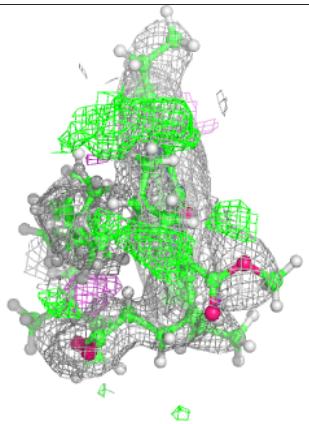


Electron density around CLA H 101:

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

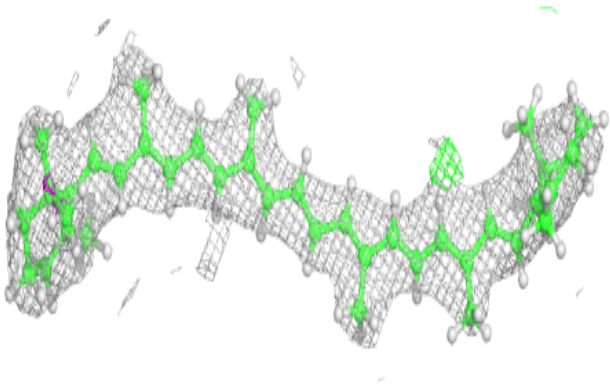


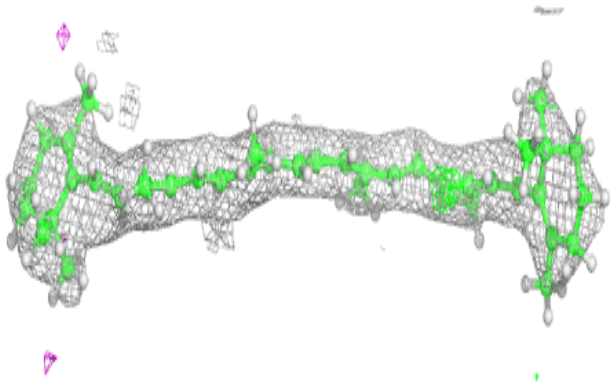


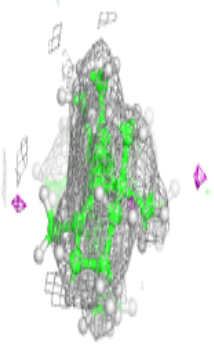


Electron density around BCR K 102:

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

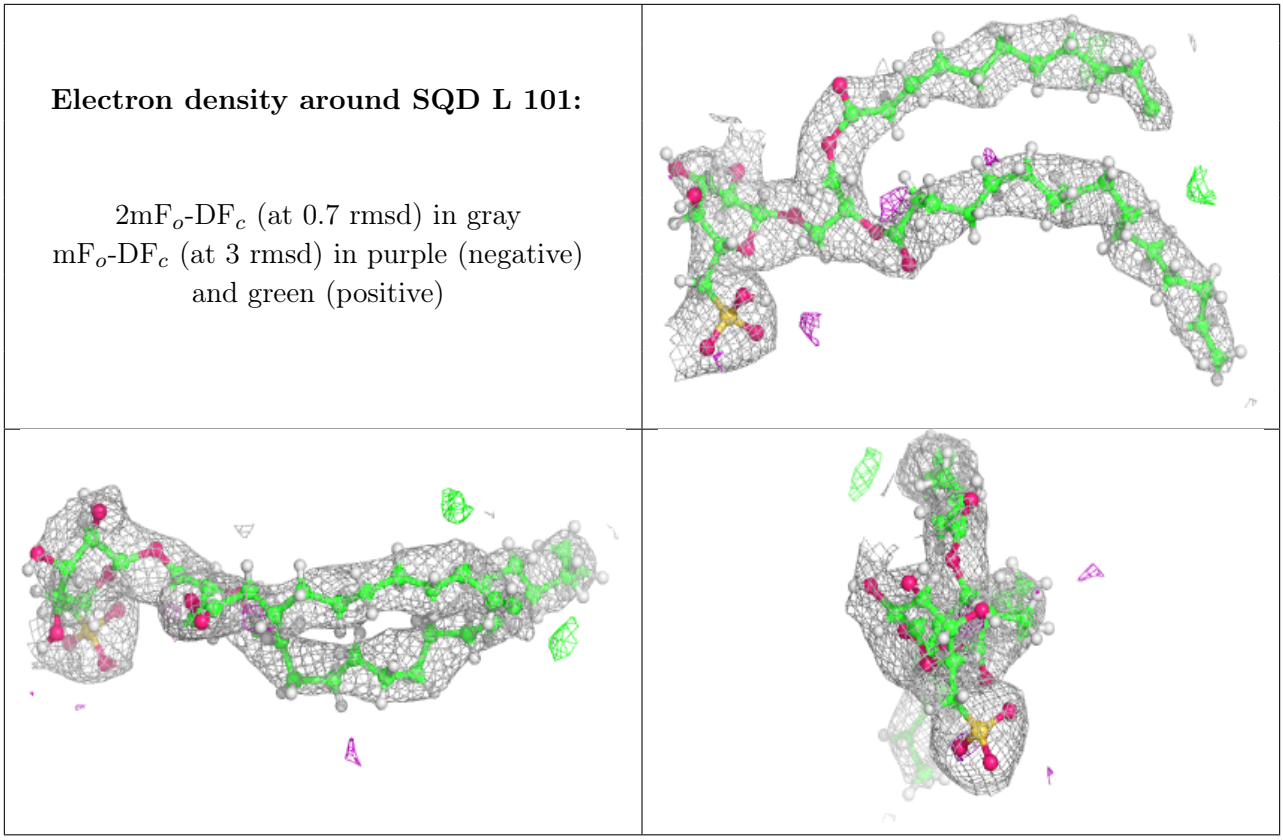






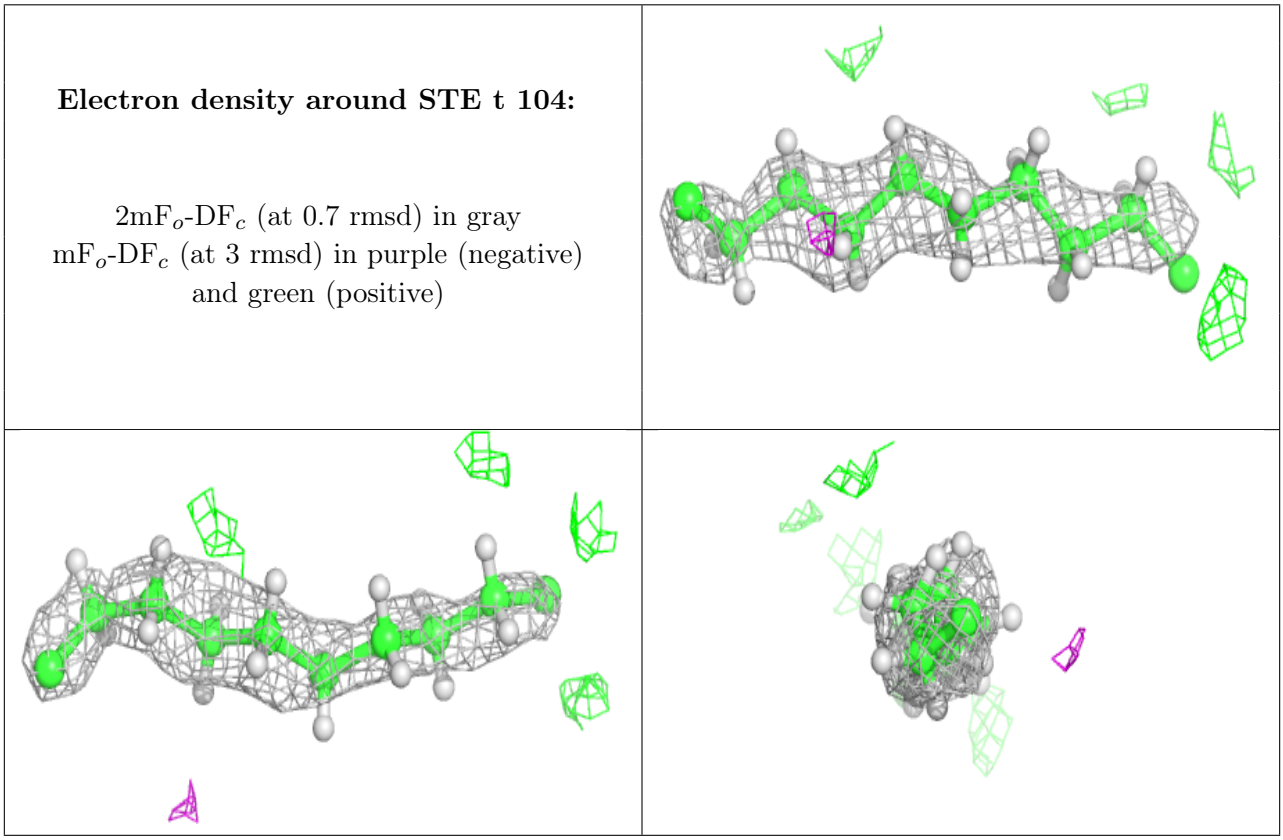
Electron density around SQD L 101:

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



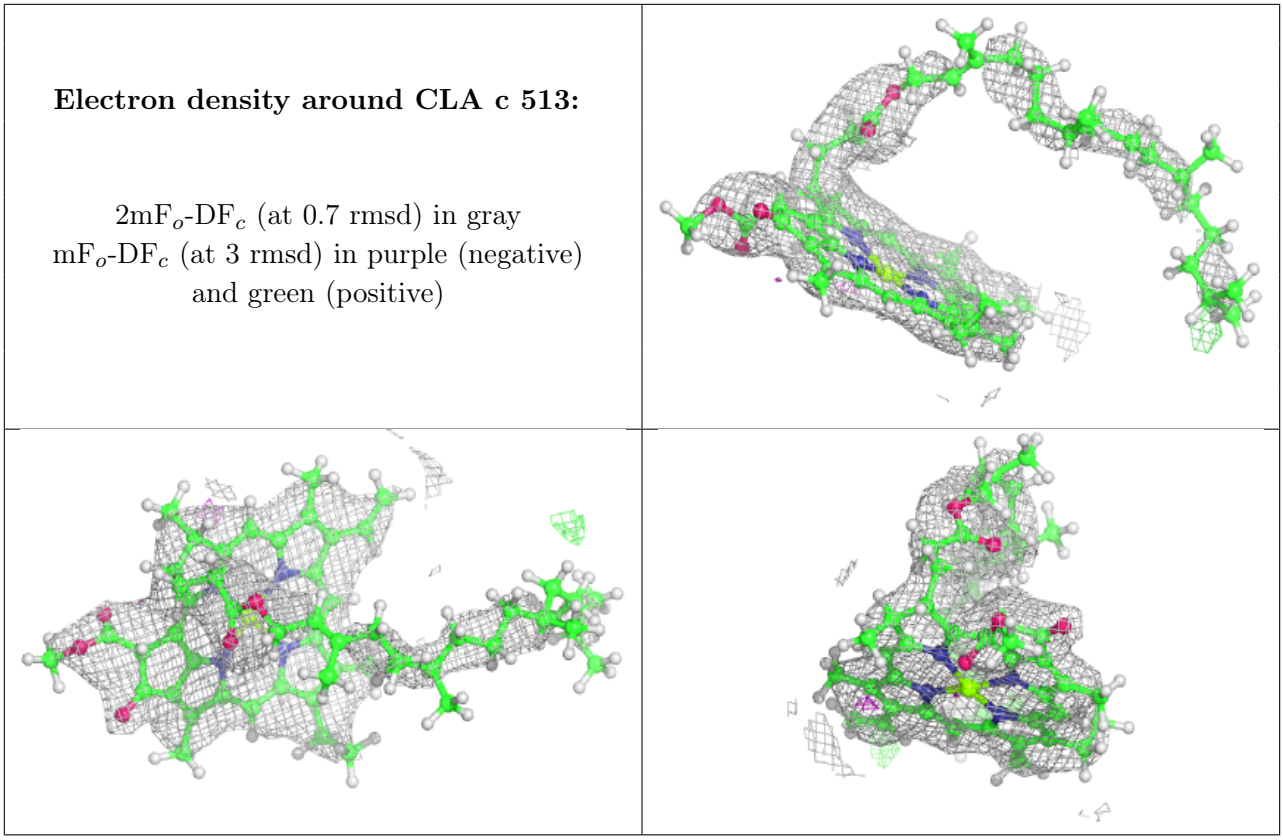
Electron density around STE t 104:

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



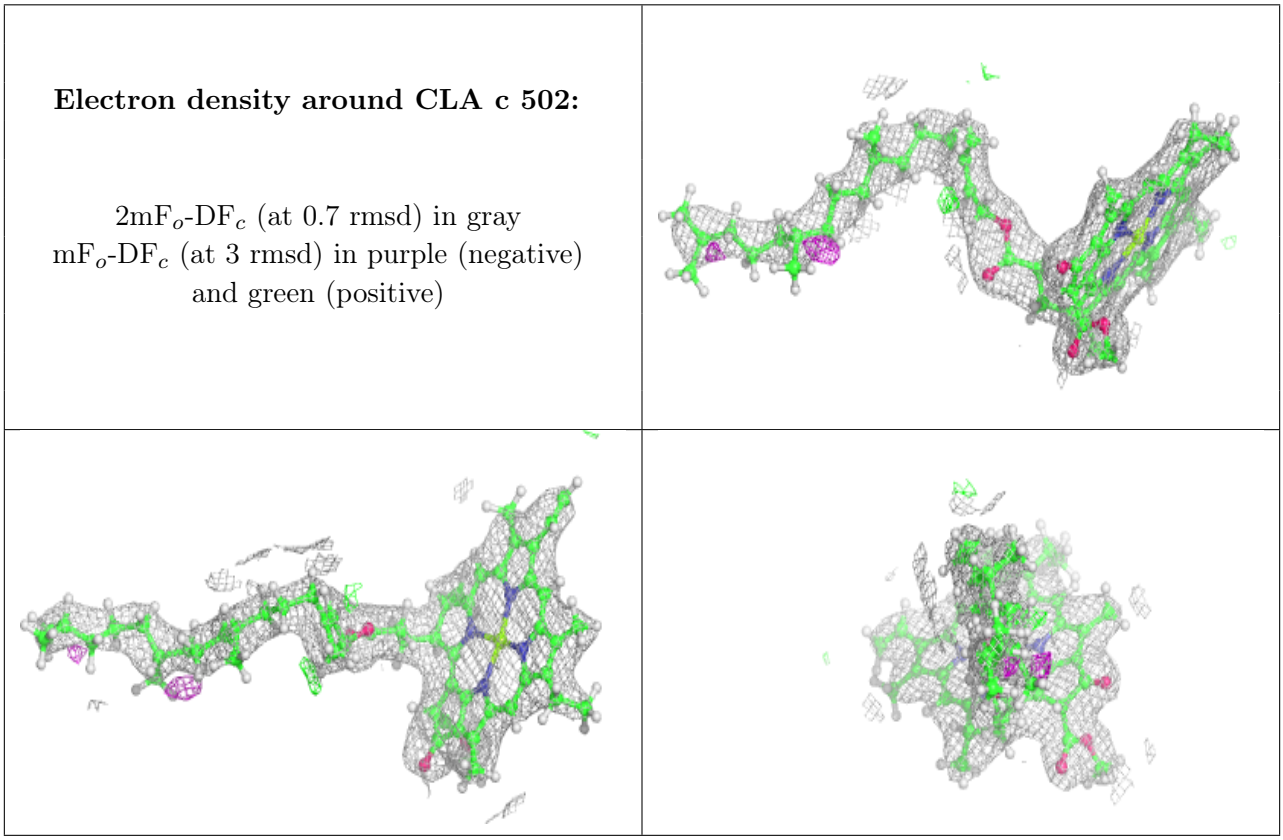
Electron density around CLA c 513:

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



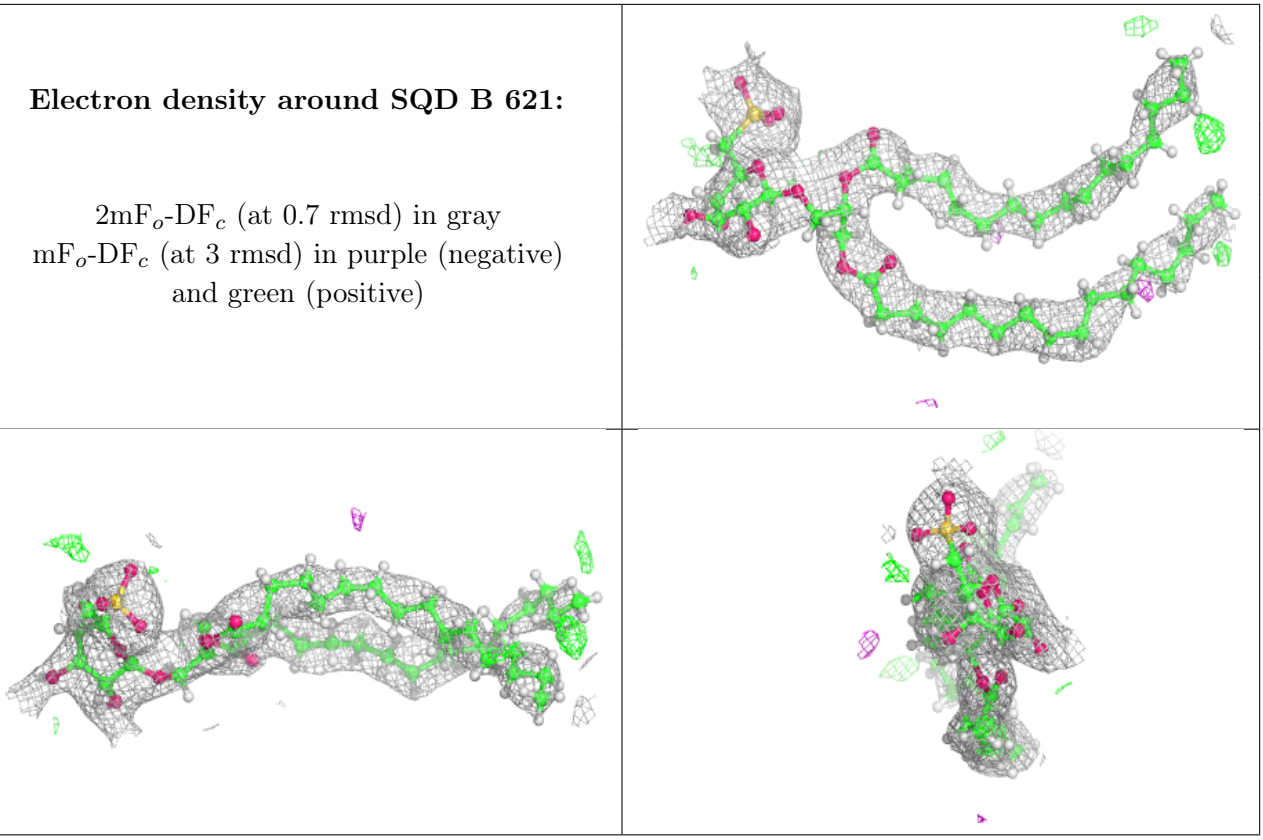
Electron density around CLA c 502:

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



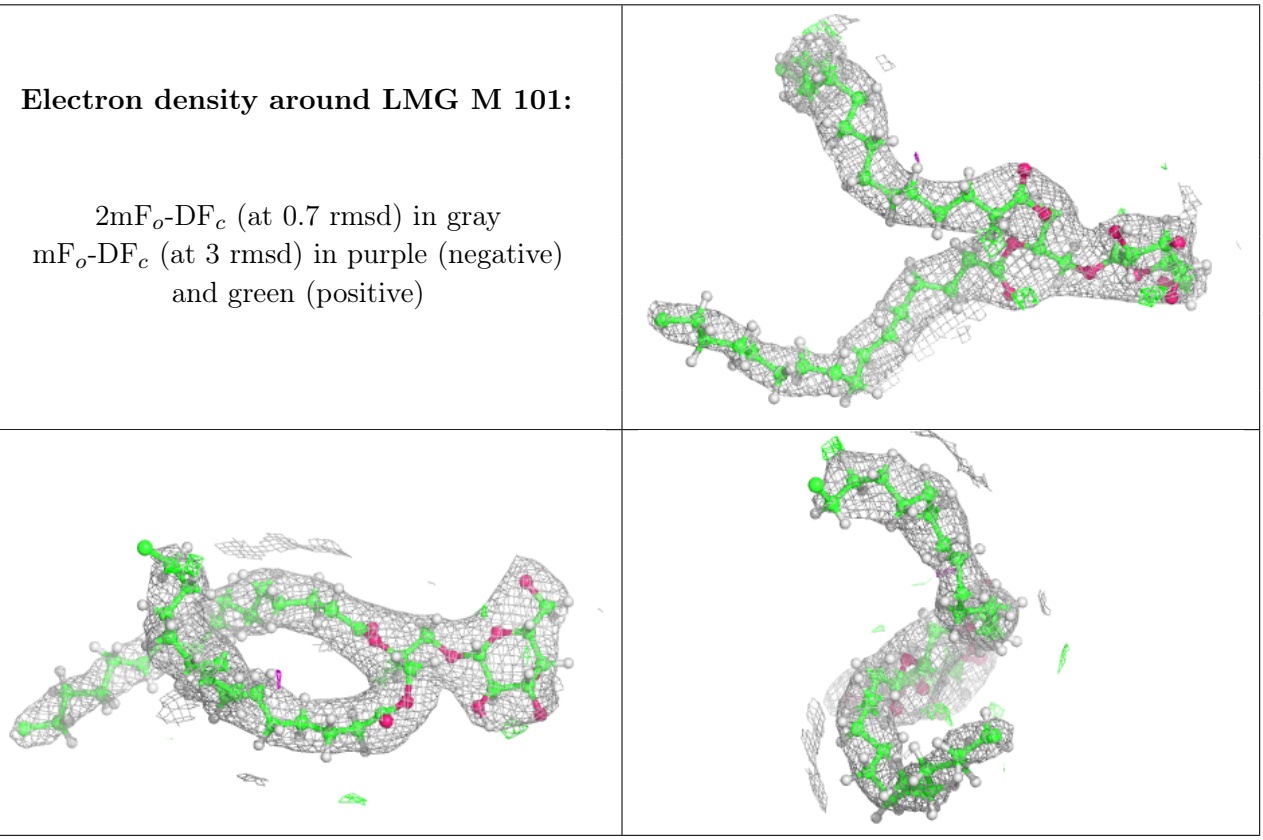
Electron density around SQD B 621:

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



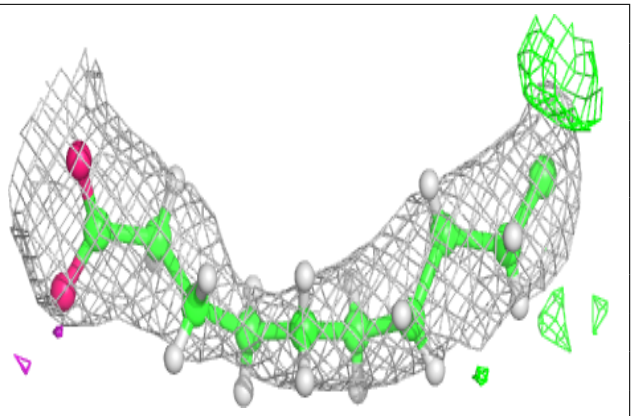
Electron density around LMG M 101:

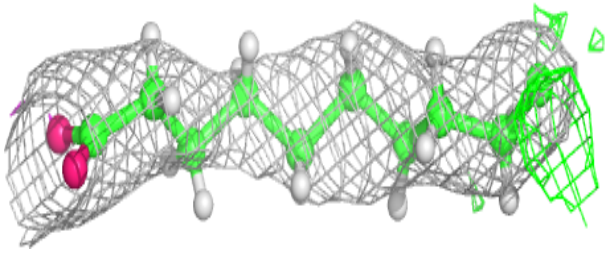
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

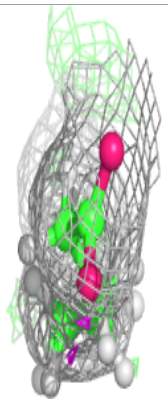


Electron density around STE C 519:

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

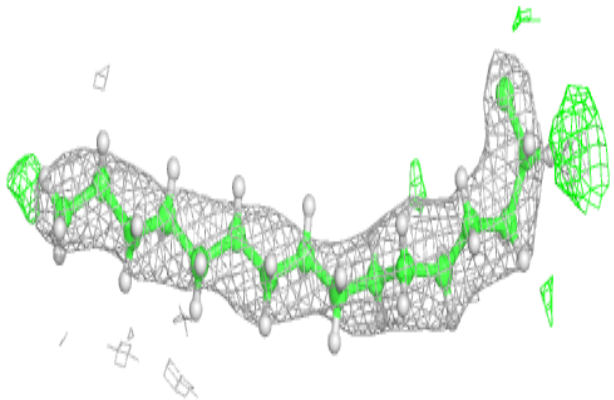


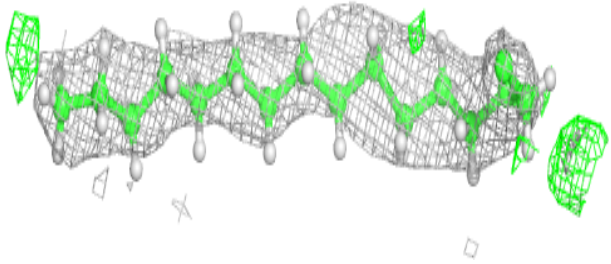


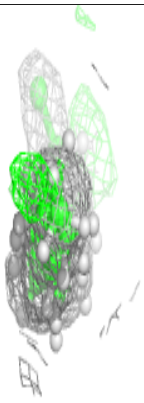


Electron density around STE C 520:

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

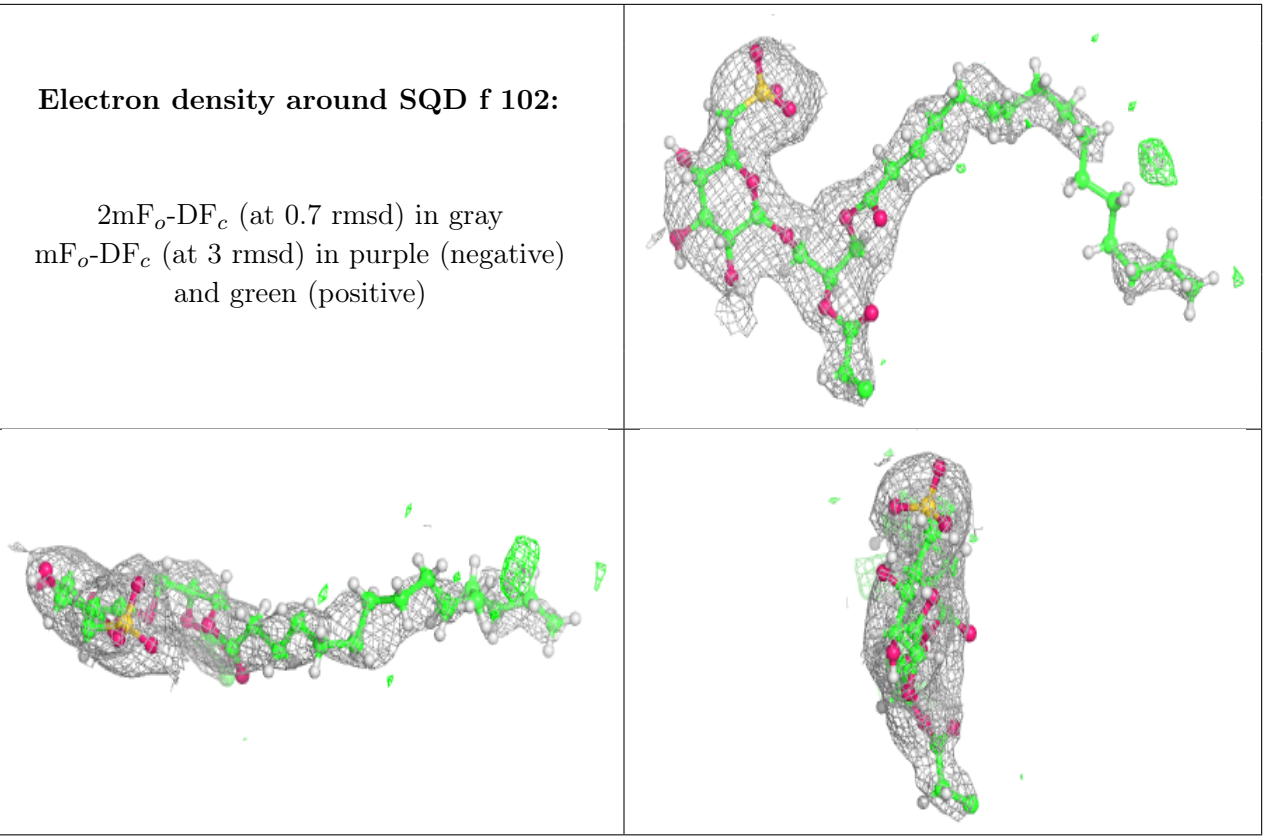






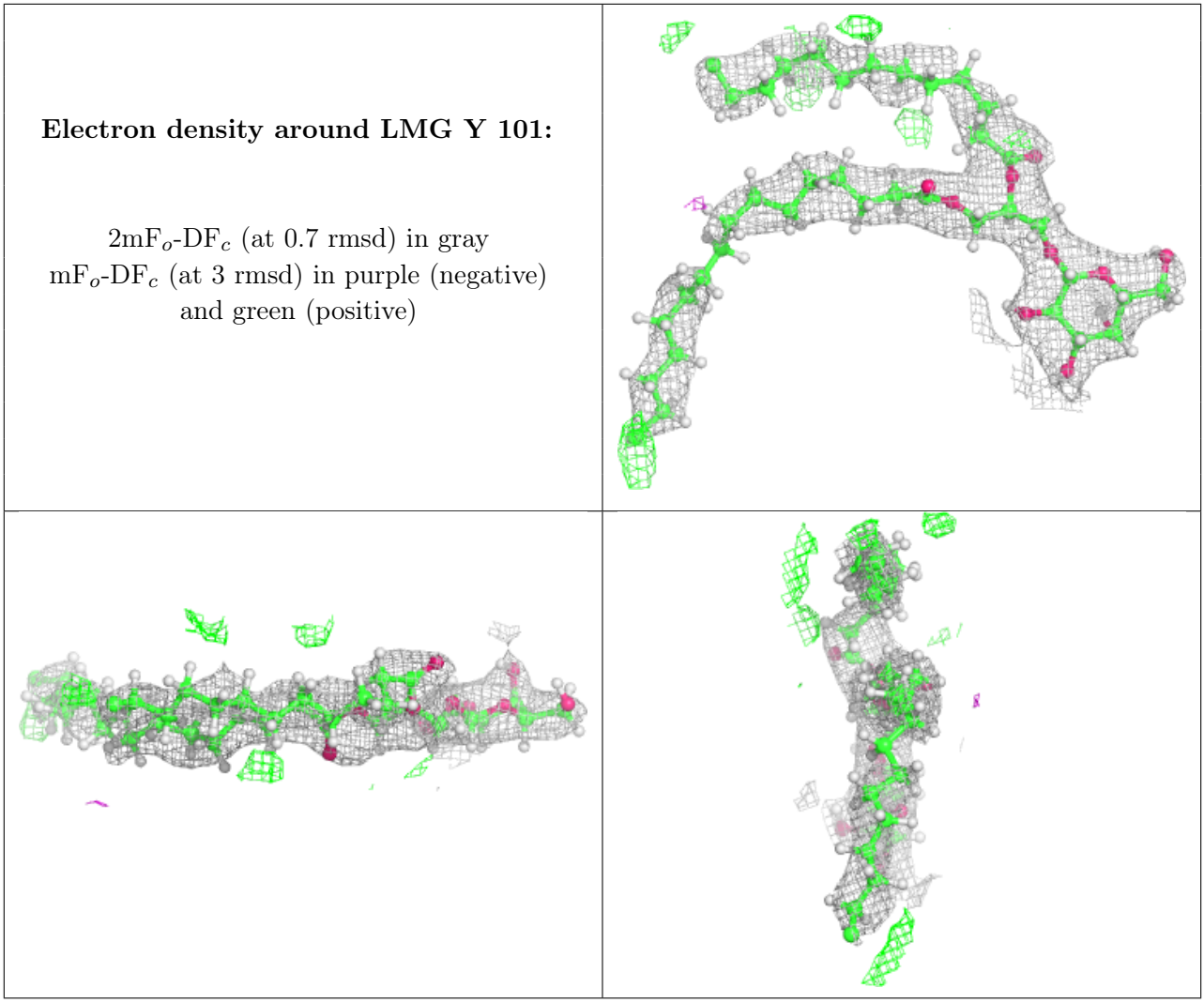
Electron density around SQD f 102:

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



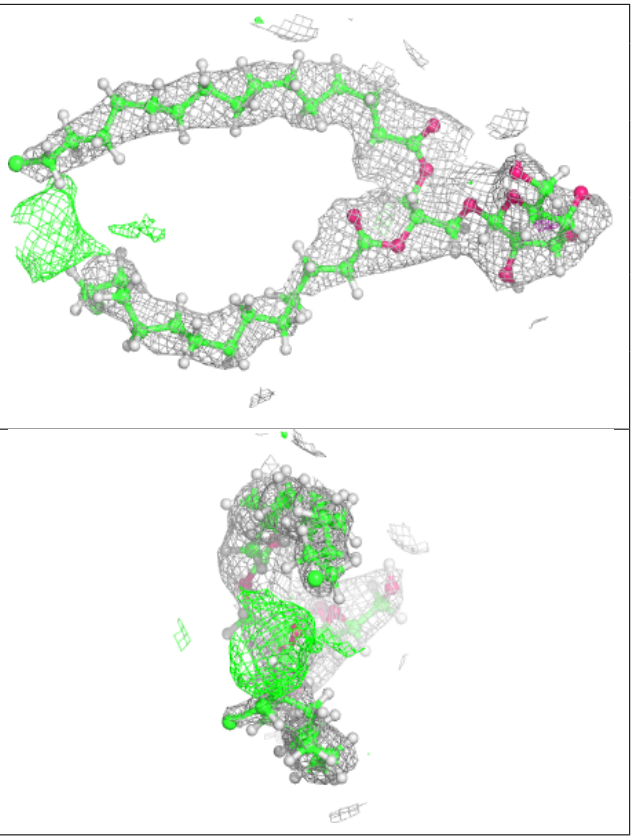
Electron density around LMG Y 101:

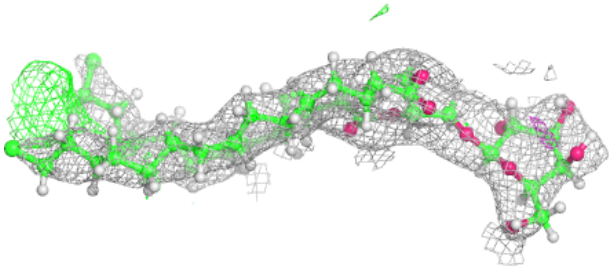
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG c 521:

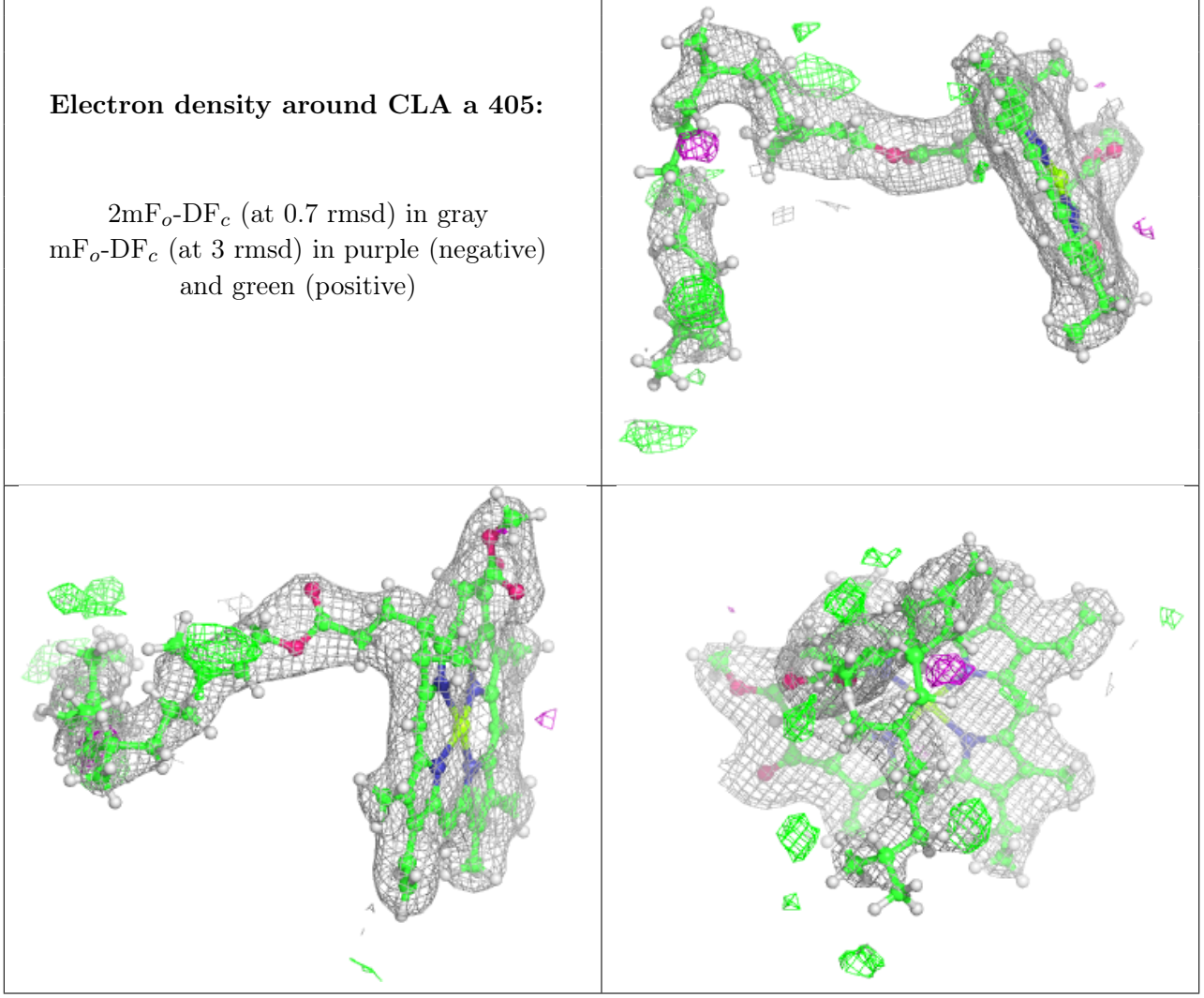
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





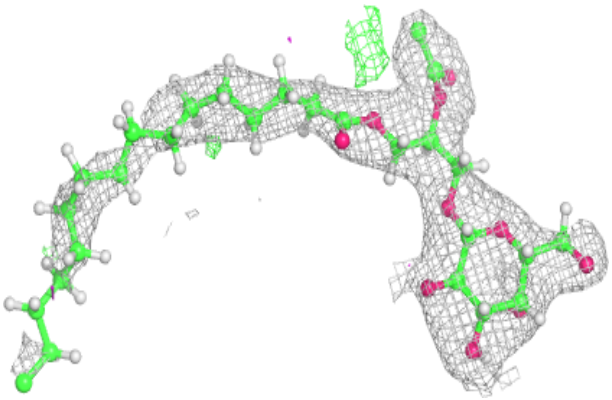
Electron density around CLA a 405:

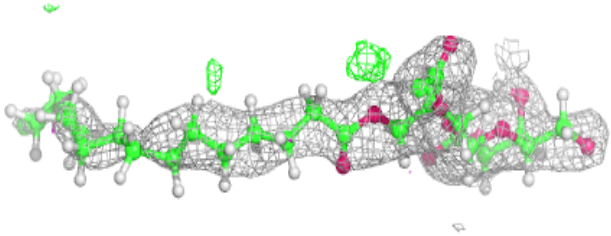
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG c 518:

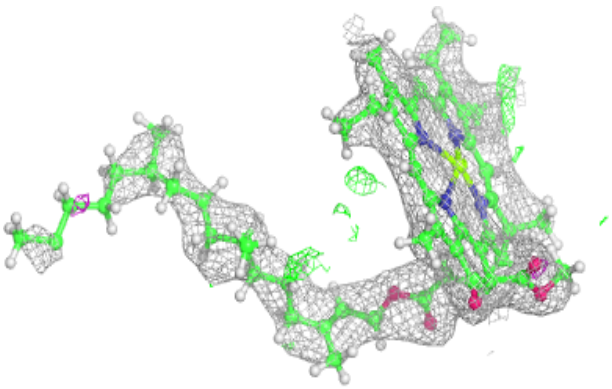
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

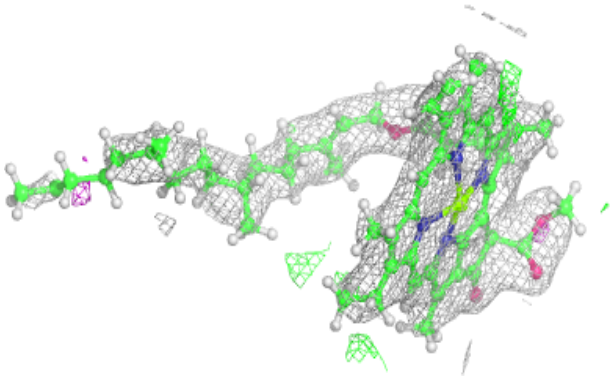


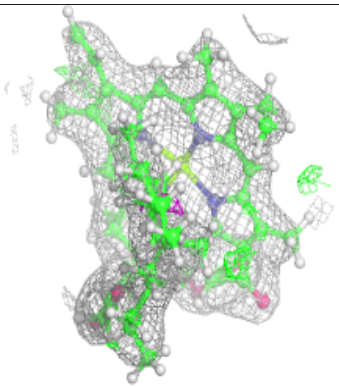


Electron density around CLA c 508:

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

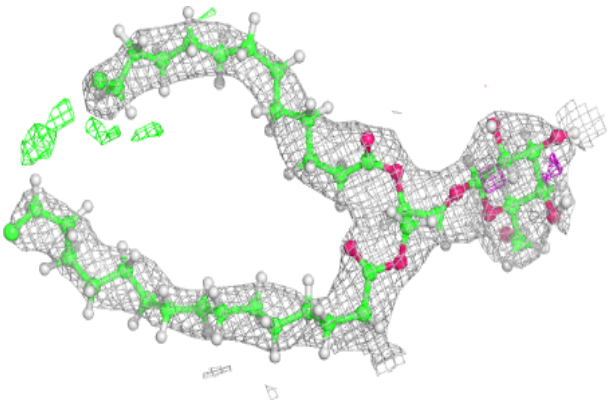


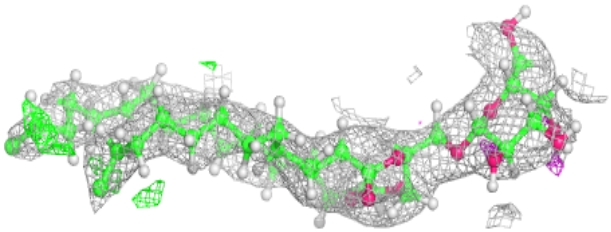


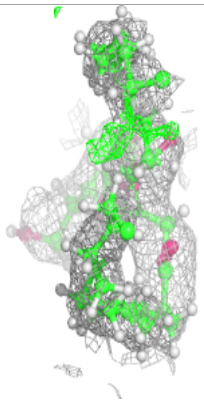


Electron density around LMG A 409:

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

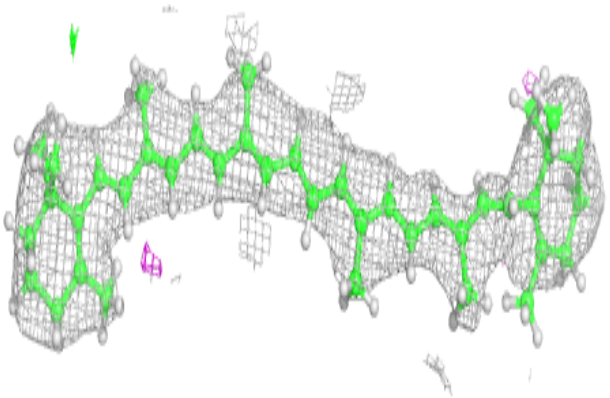


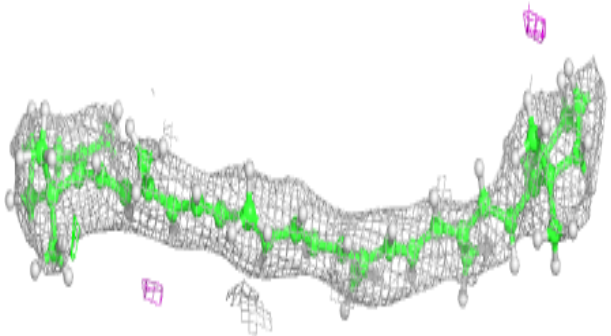


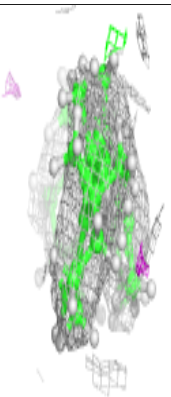


Electron density around BCR d 406:

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

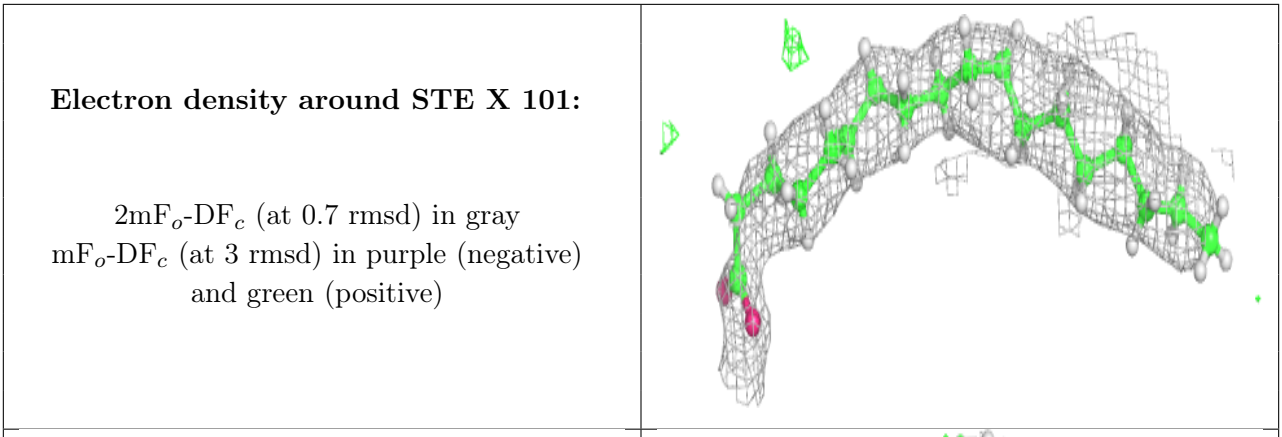






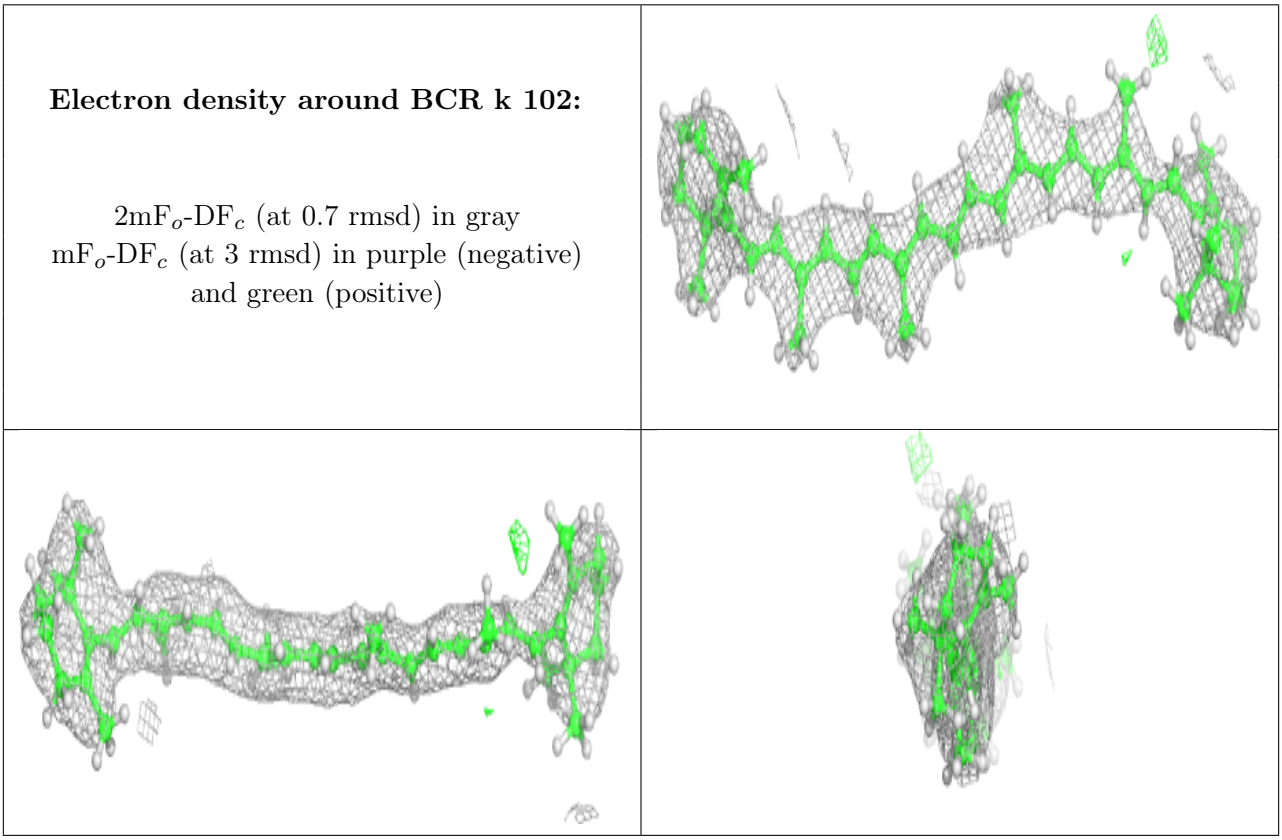
Electron density around STE X 101:

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



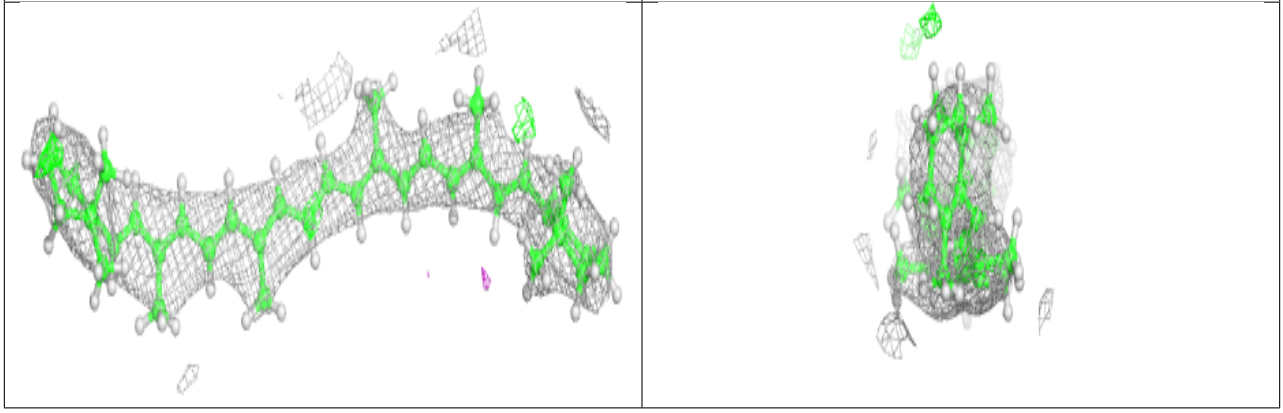
Electron density around BCR k 102:

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



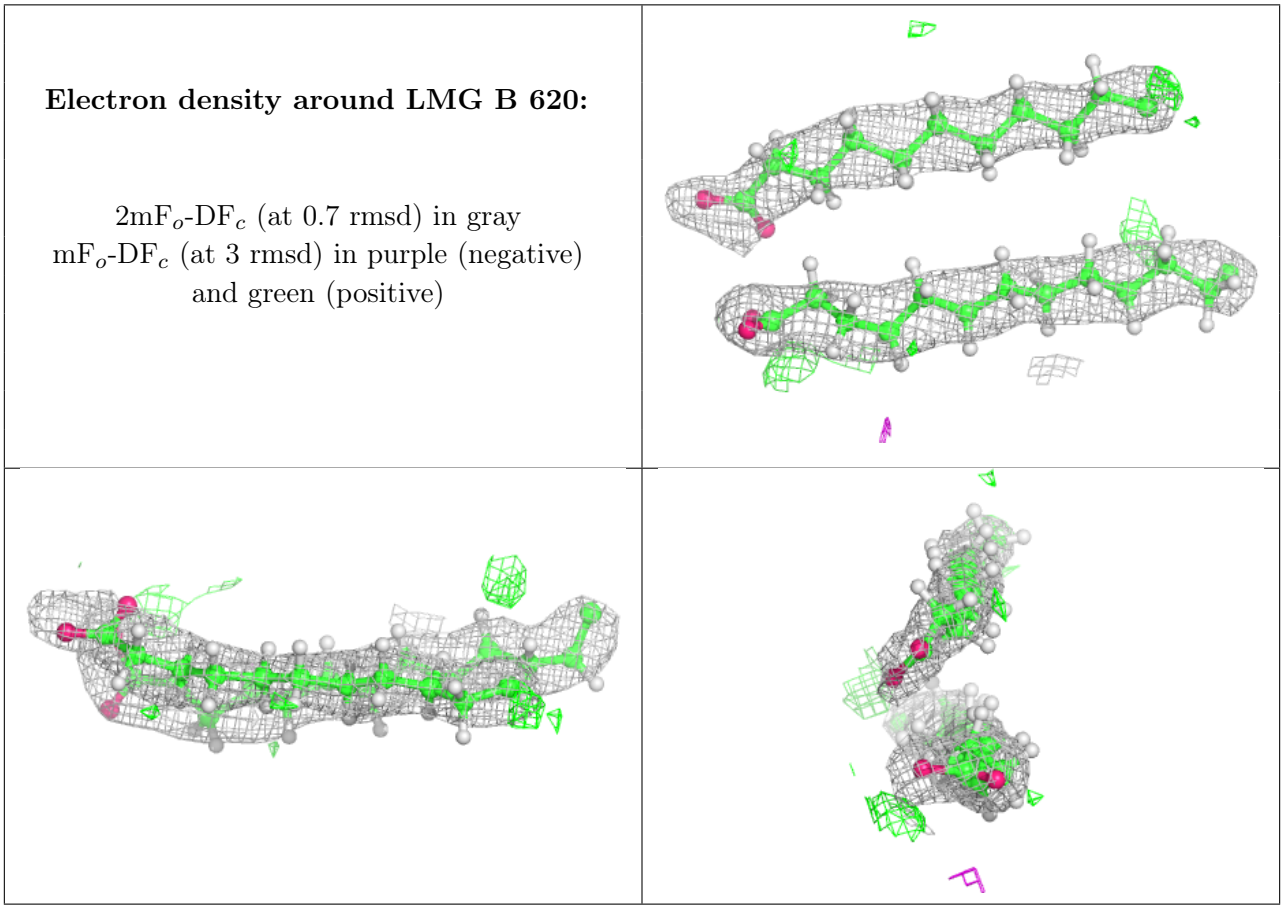
Electron density around BCR k 103:

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



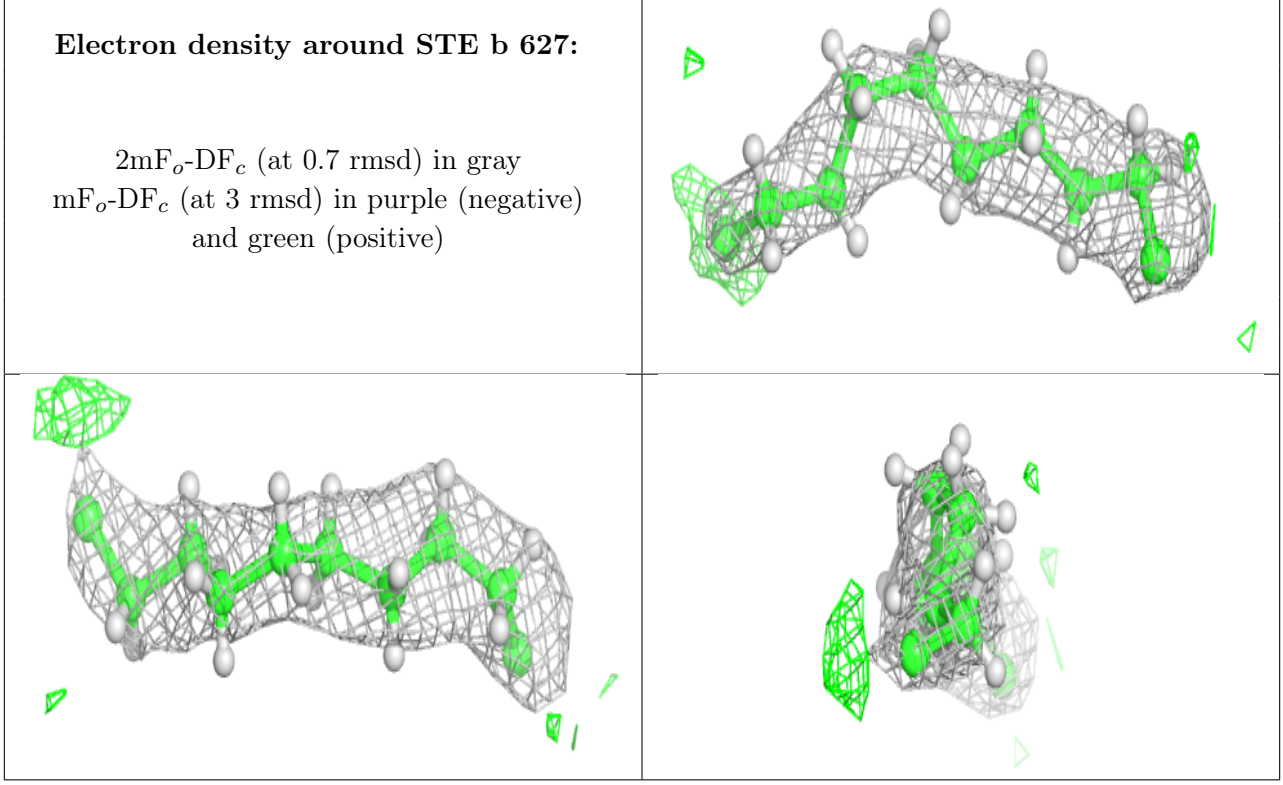
Electron density around LMG B 620:

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



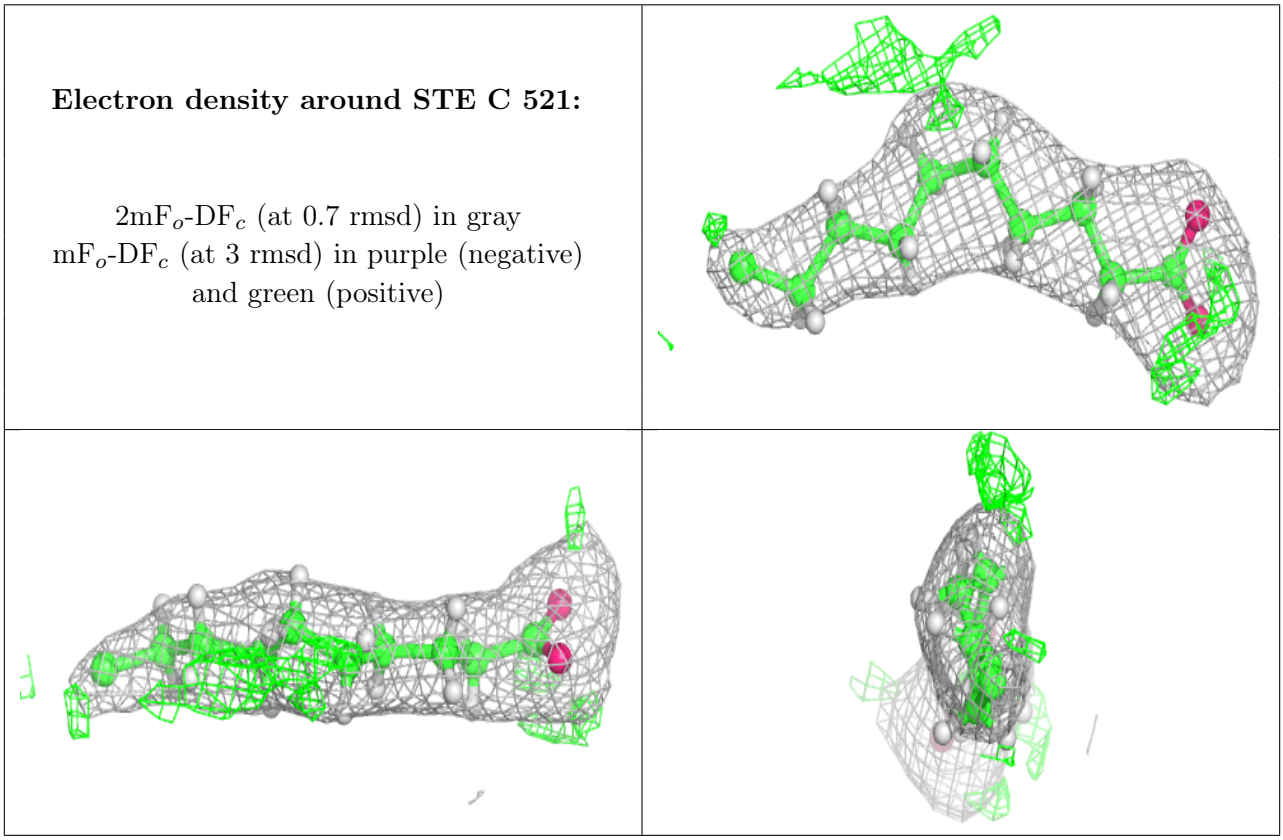
Electron density around STE b 627:

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



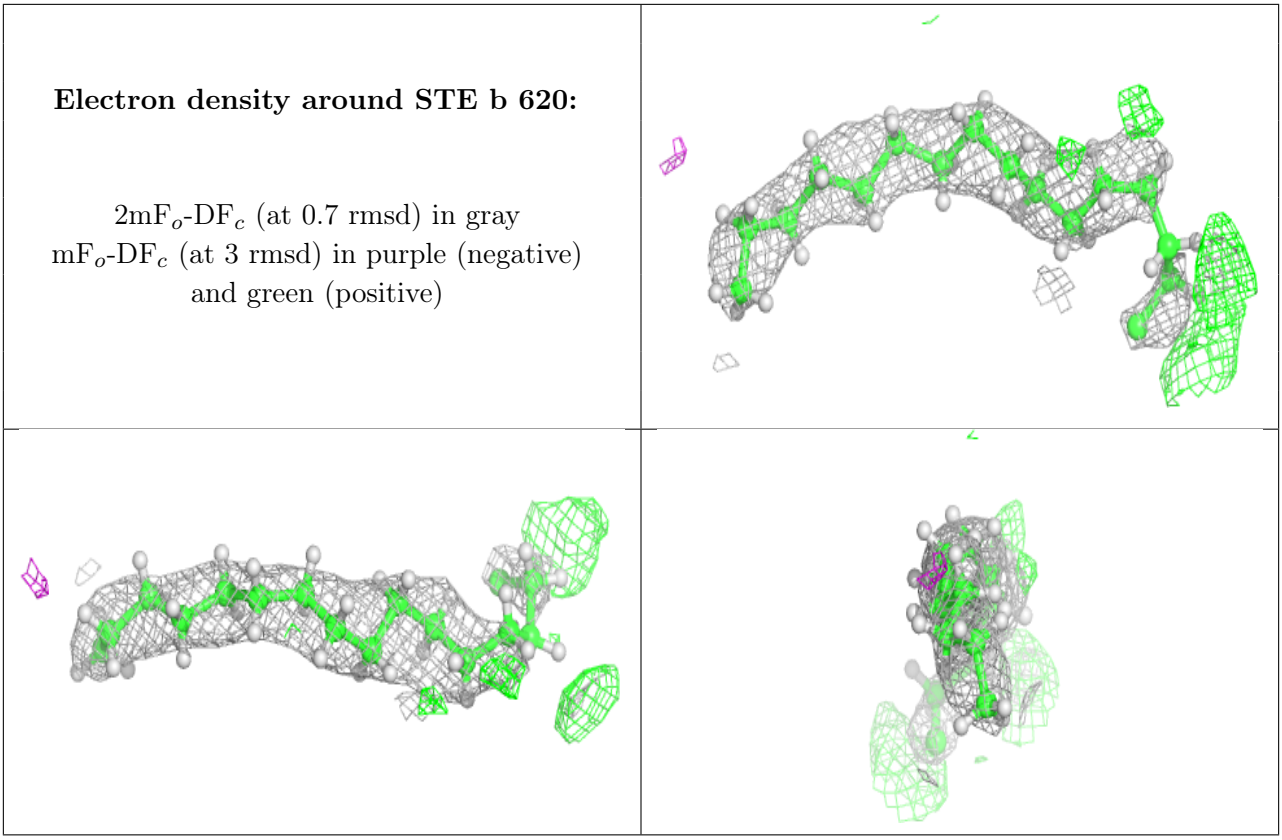
Electron density around STE C 521:

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



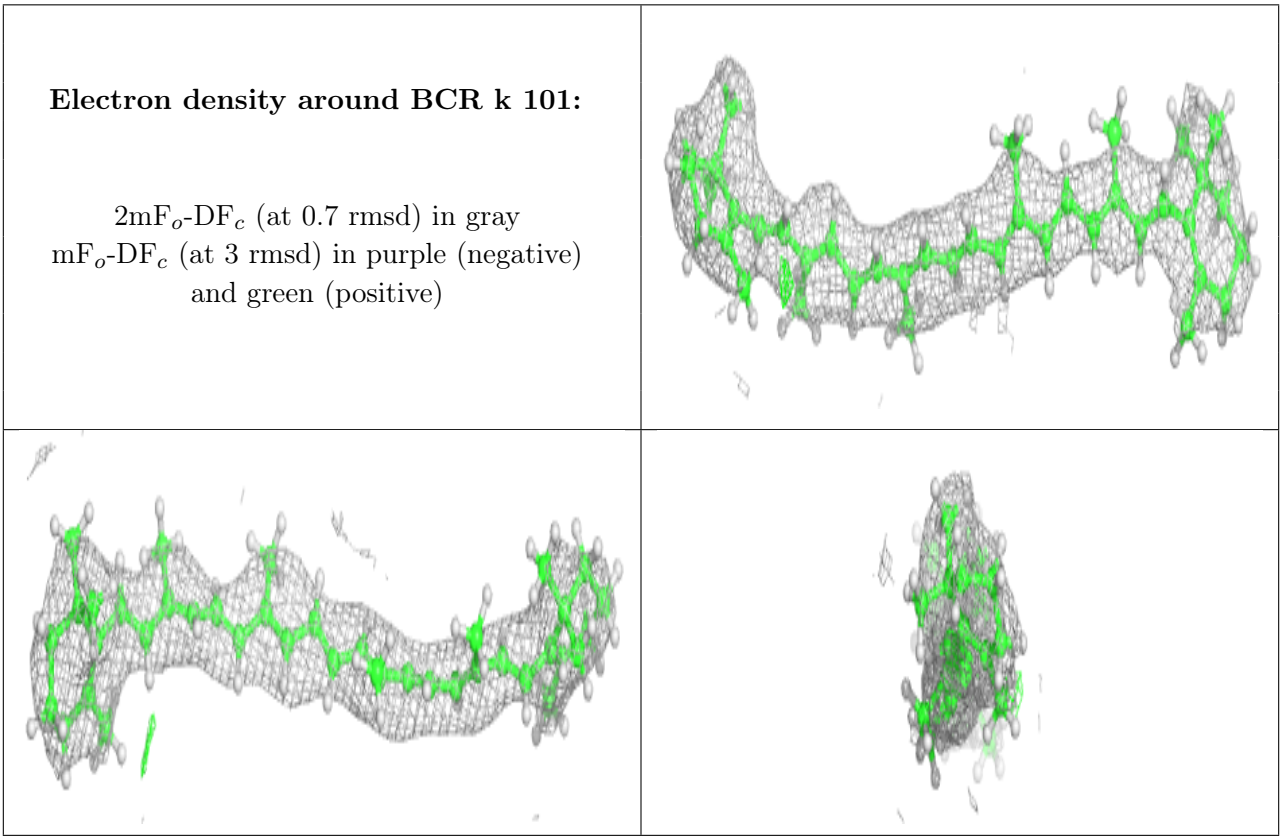
Electron density around STE b 620:

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



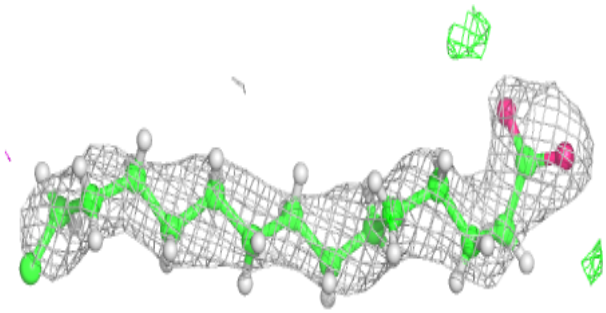
Electron density around BCR k 101:

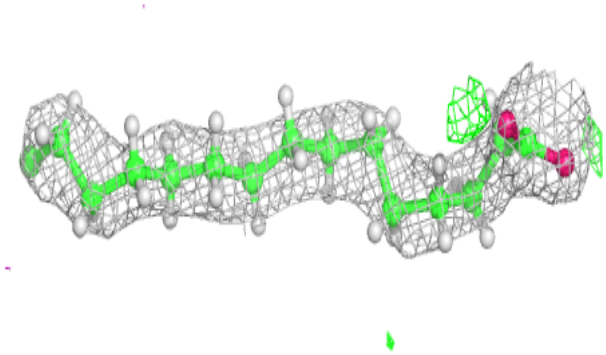
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

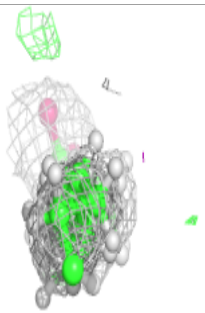


Electron density around STE d 411:

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

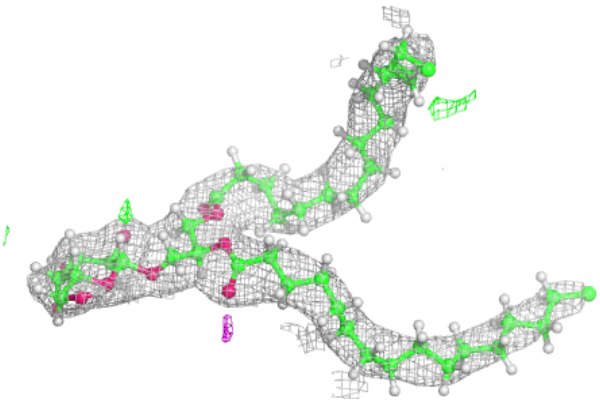


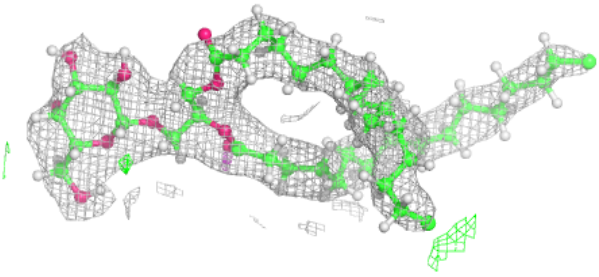


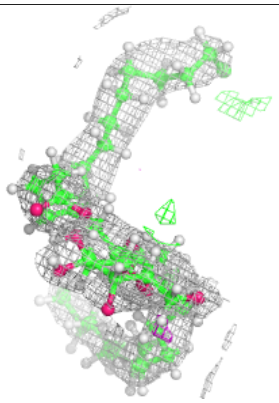


Electron density around LMG m 101:

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

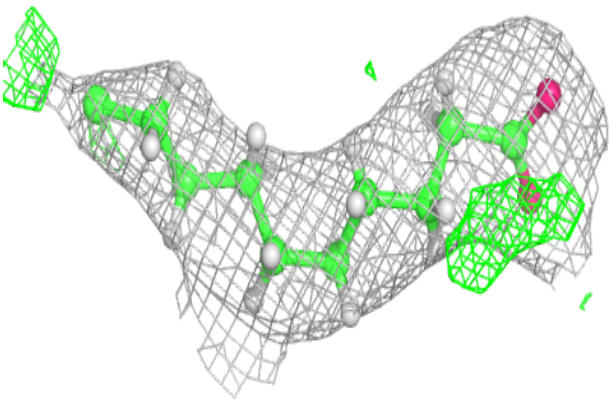


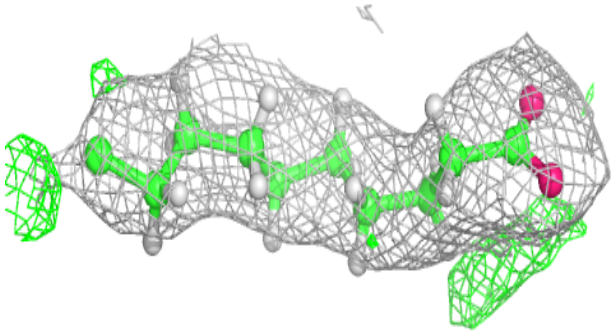


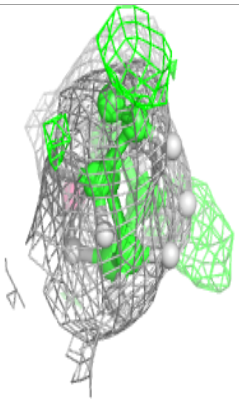


Electron density around STE B 622:

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

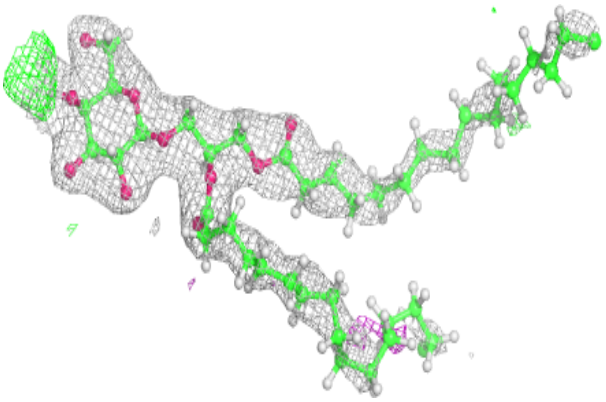


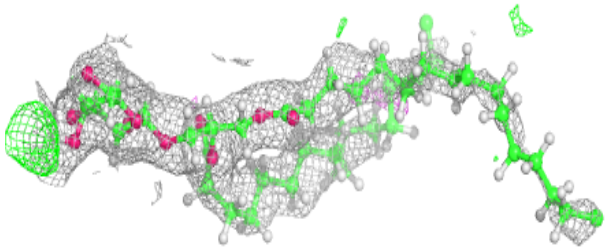


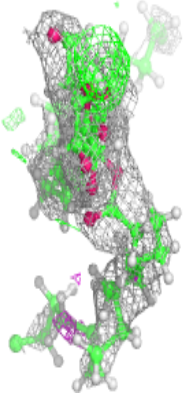


Electron density around LMG D 408:

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

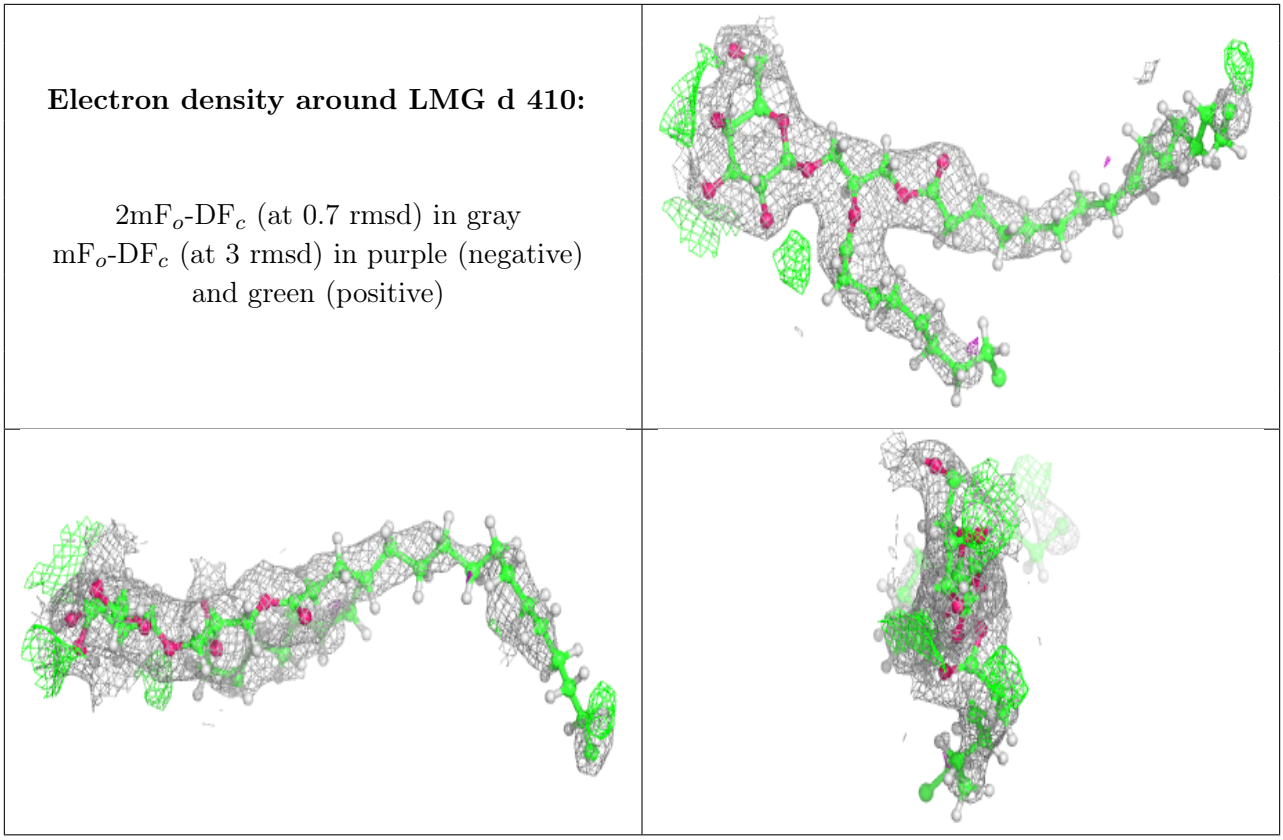






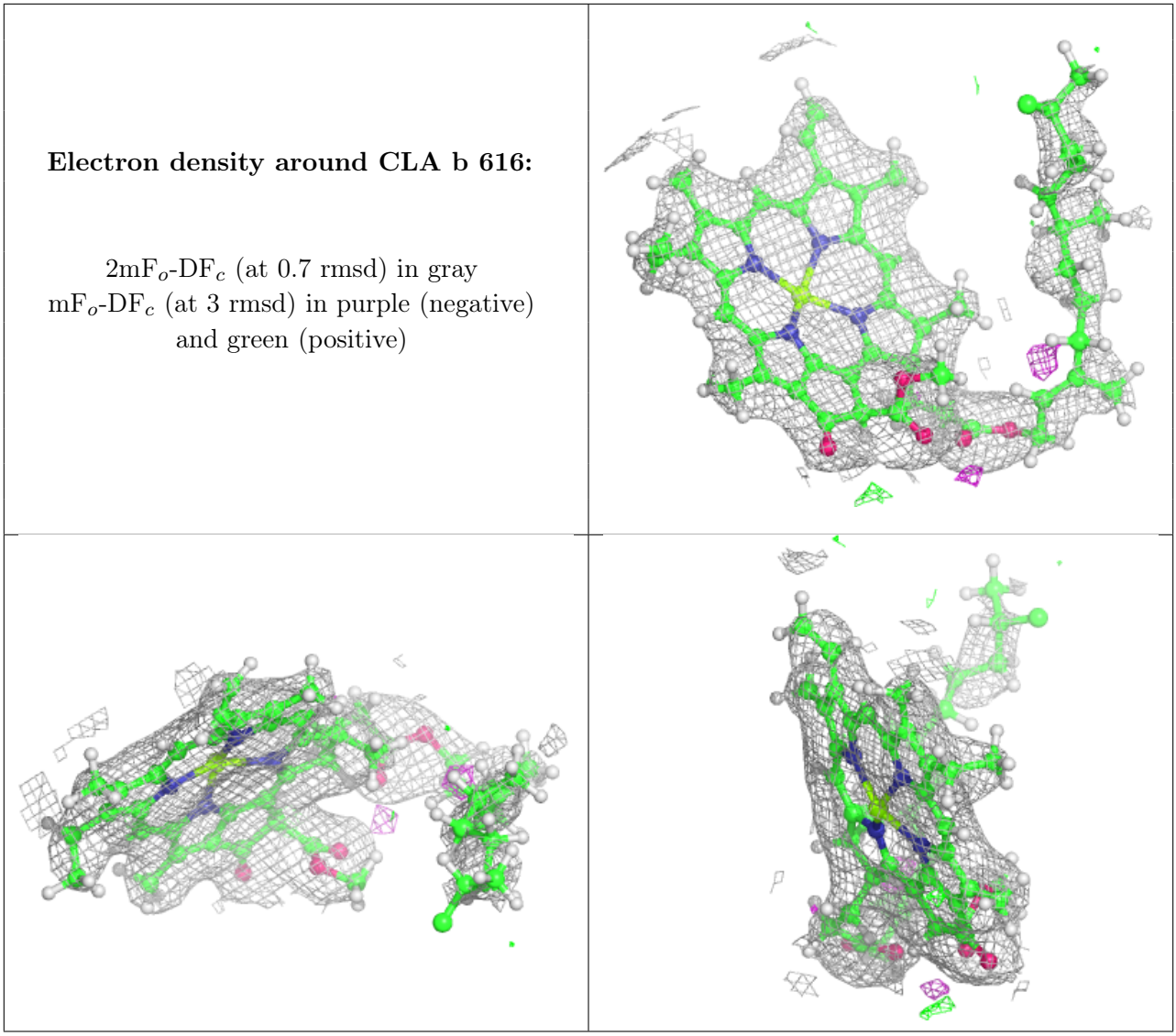
Electron density around LMG d 410:

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



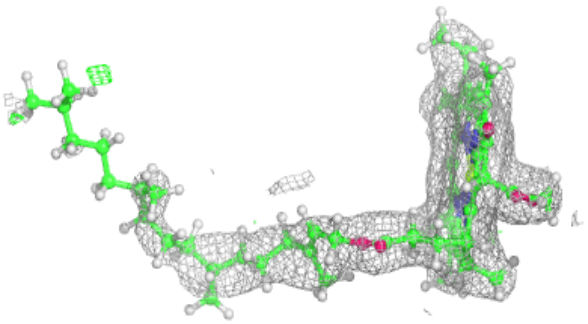
Electron density around CLA b 616:

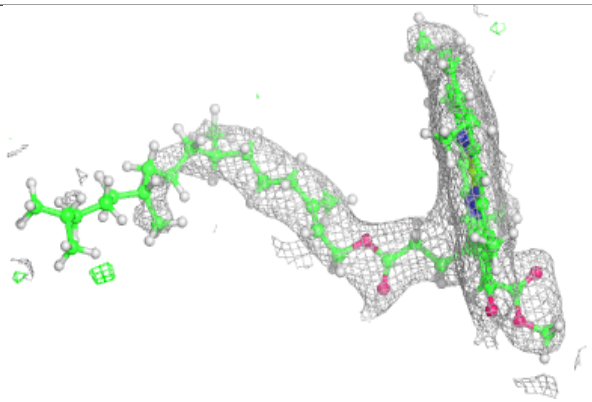
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

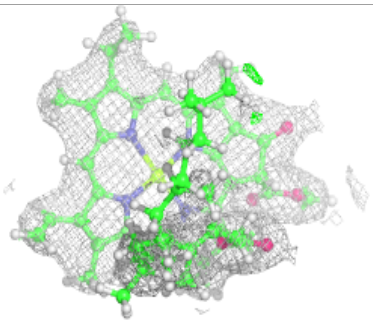


Electron density around CLA D 405:

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

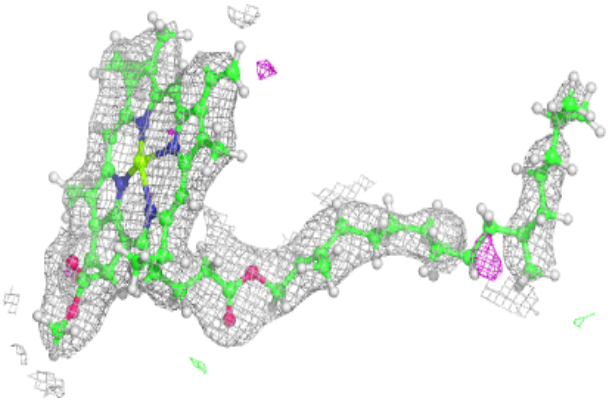


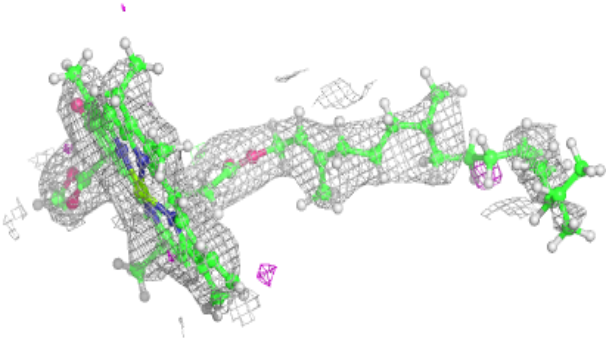


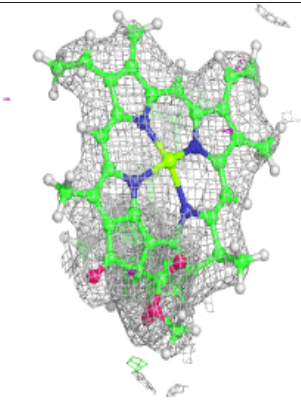


Electron density around CLA d 405:

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

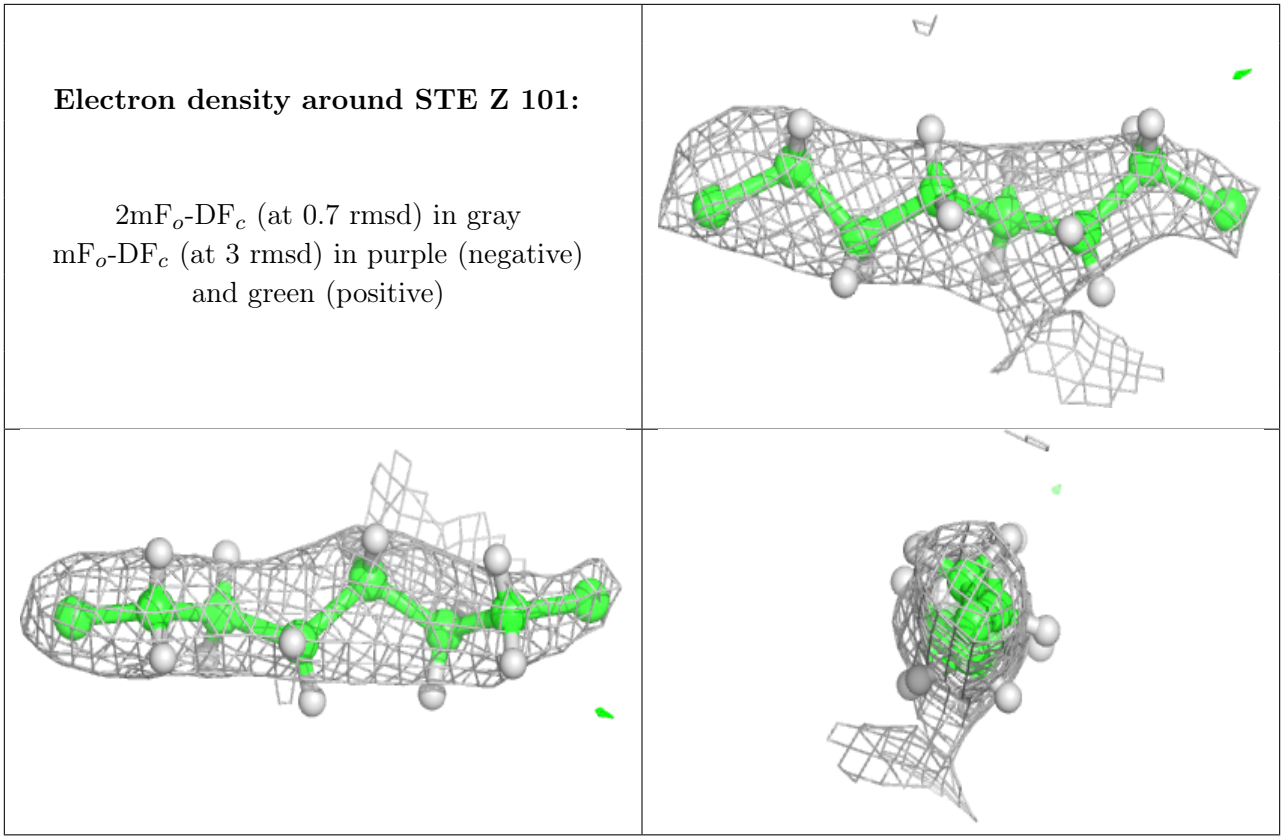






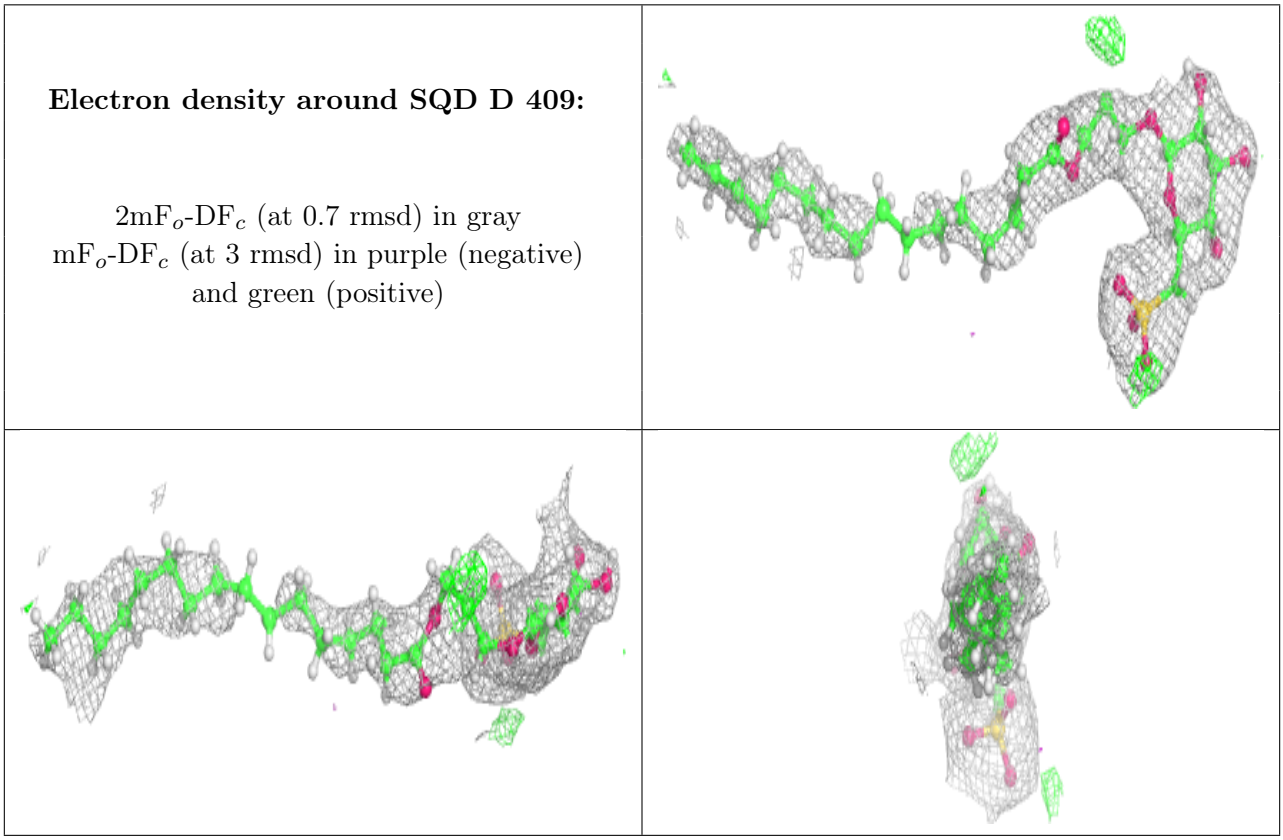
Electron density around STE Z 101:

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



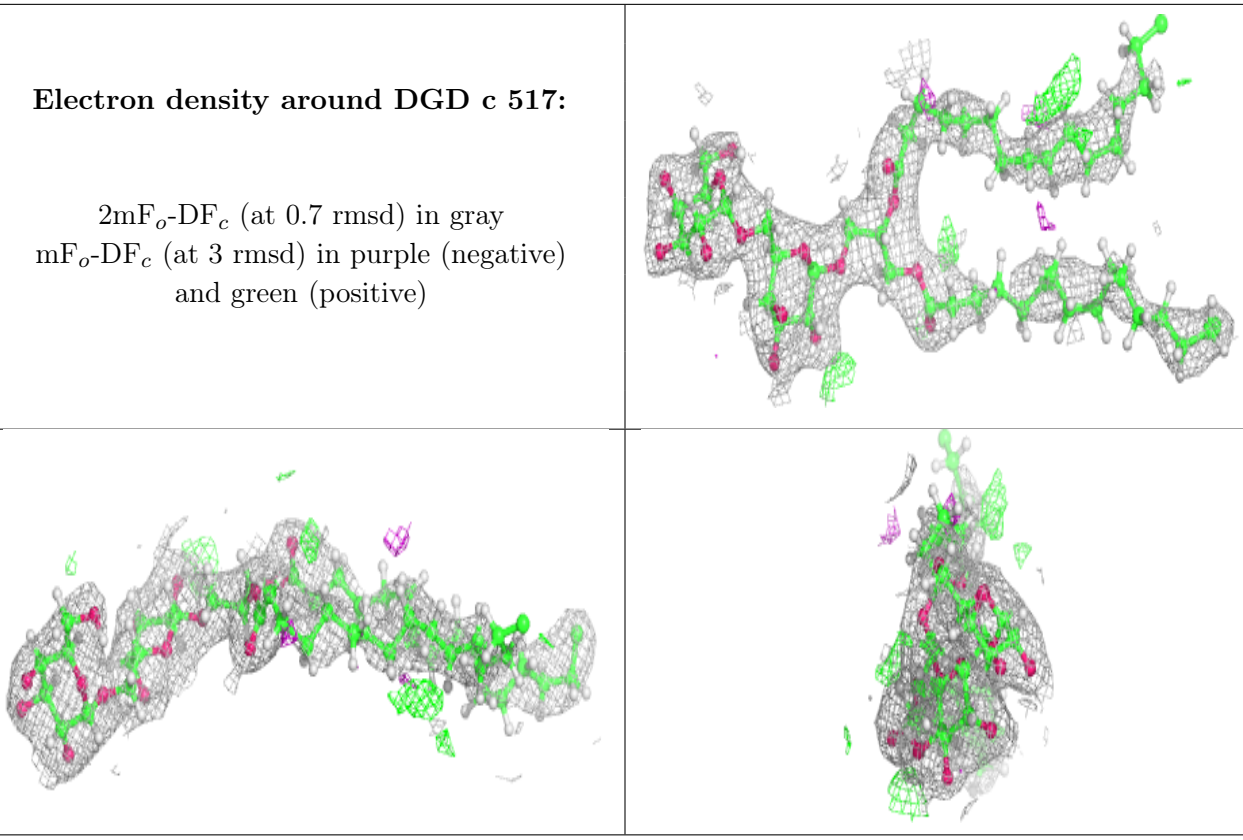
Electron density around SQD D 409:

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



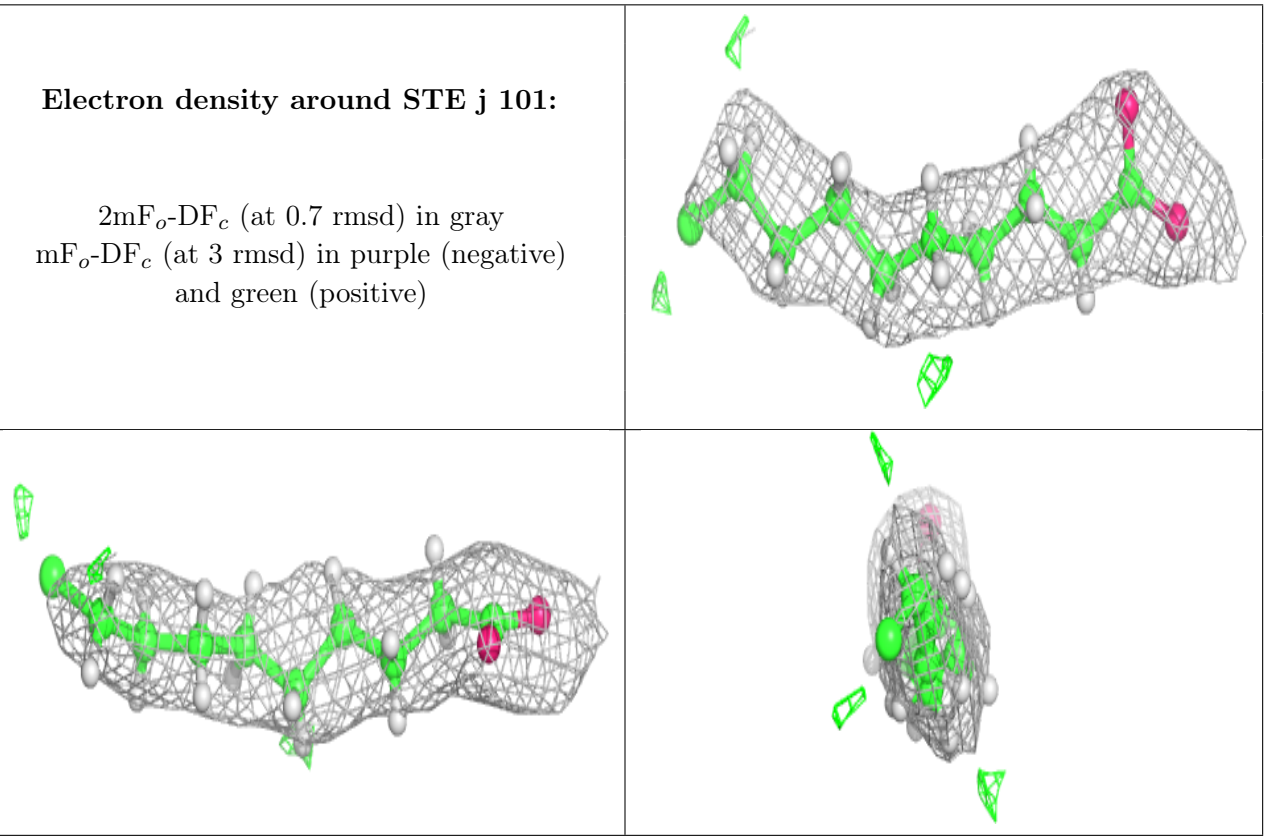
Electron density around DGD c 517:

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



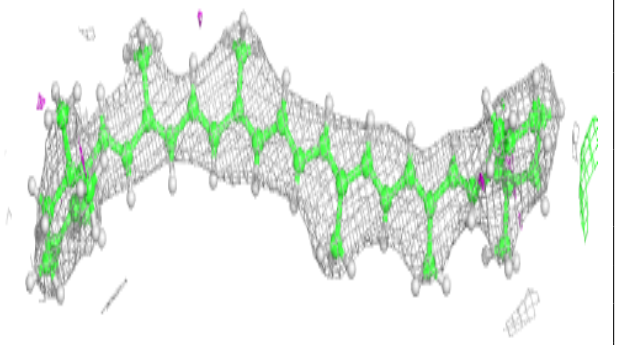
Electron density around STE j 101:

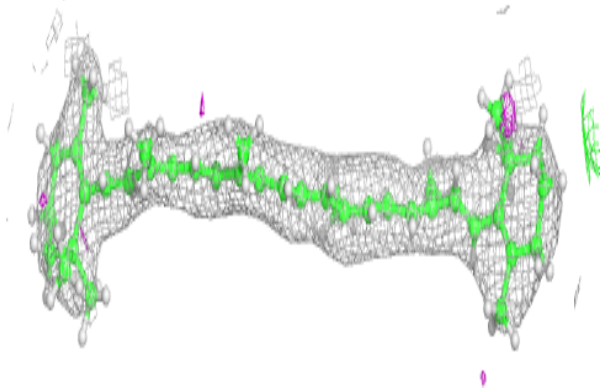
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

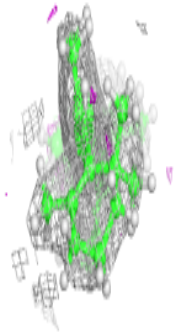


Electron density around BCR C 514:

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

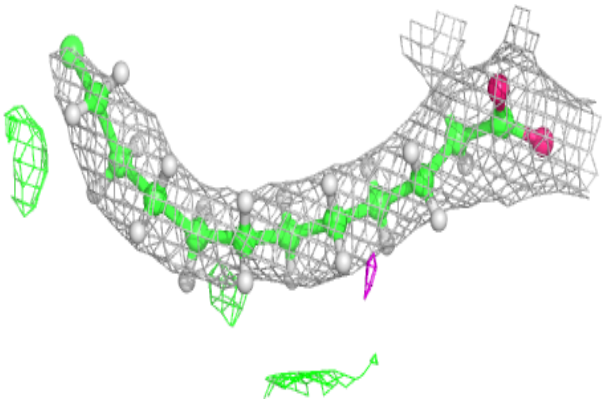


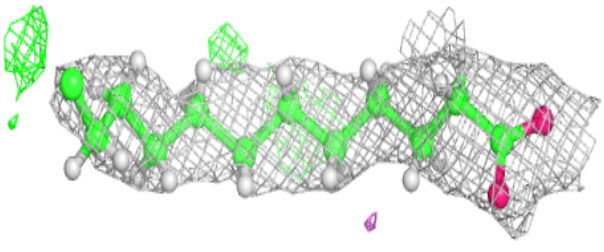


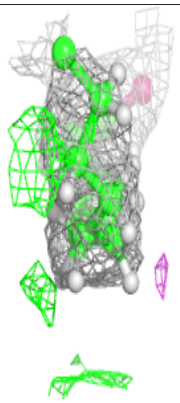


Electron density around STE t 103:

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

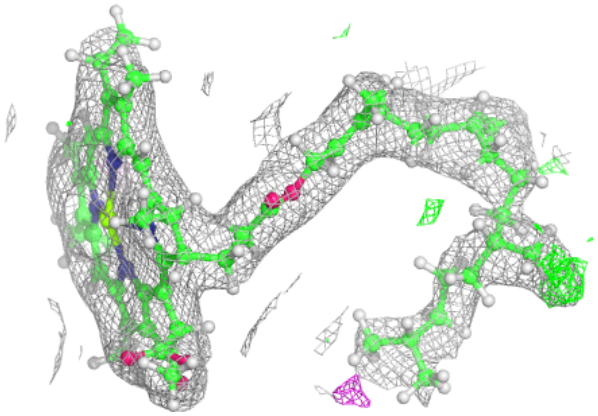


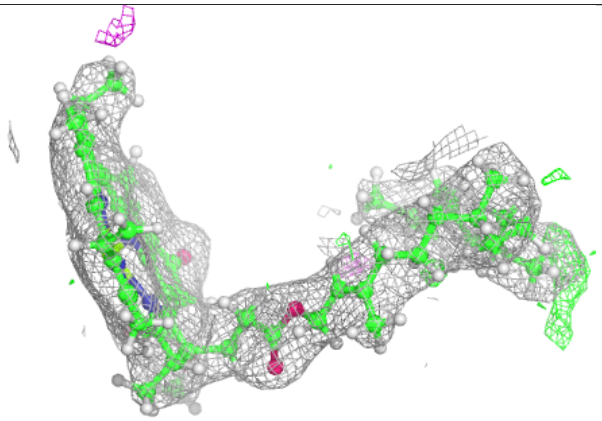


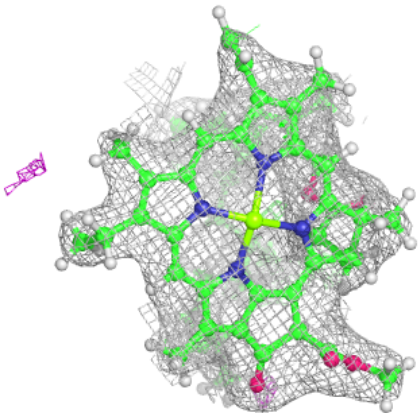


Electron density around CLA B 605:

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

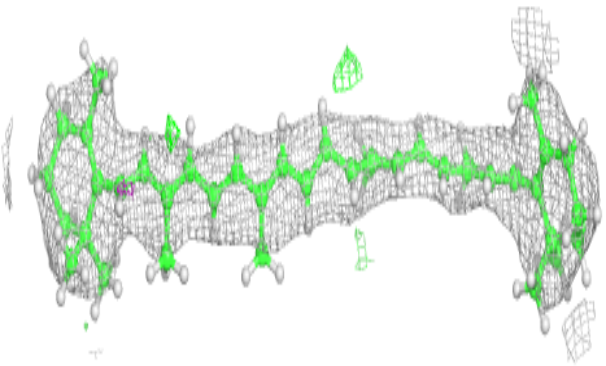


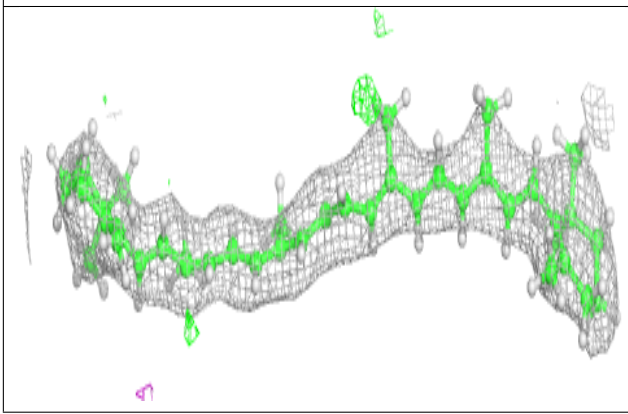


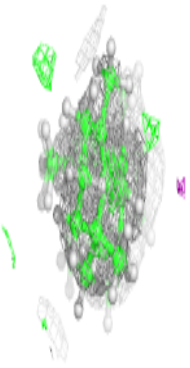


Electron density around BCR K 101:

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

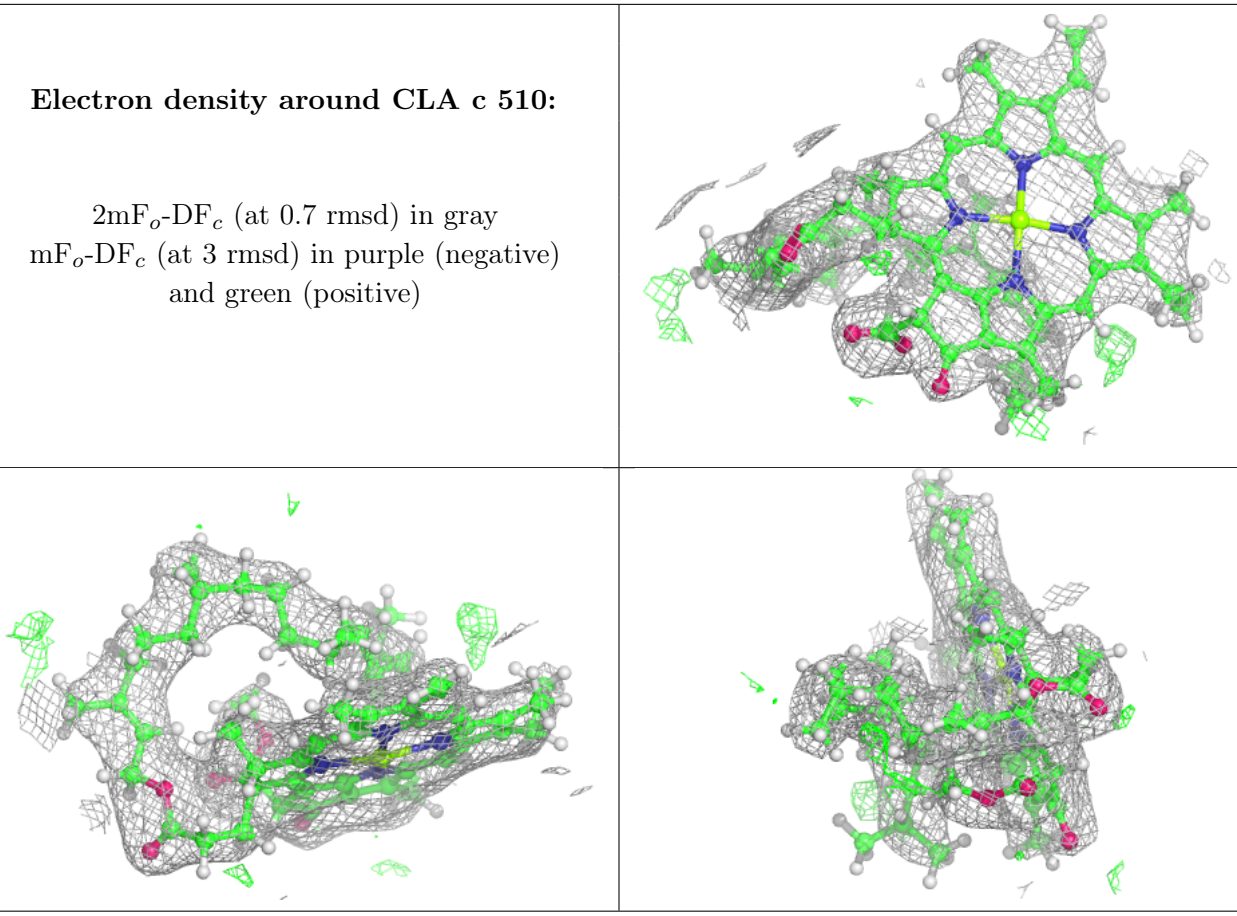






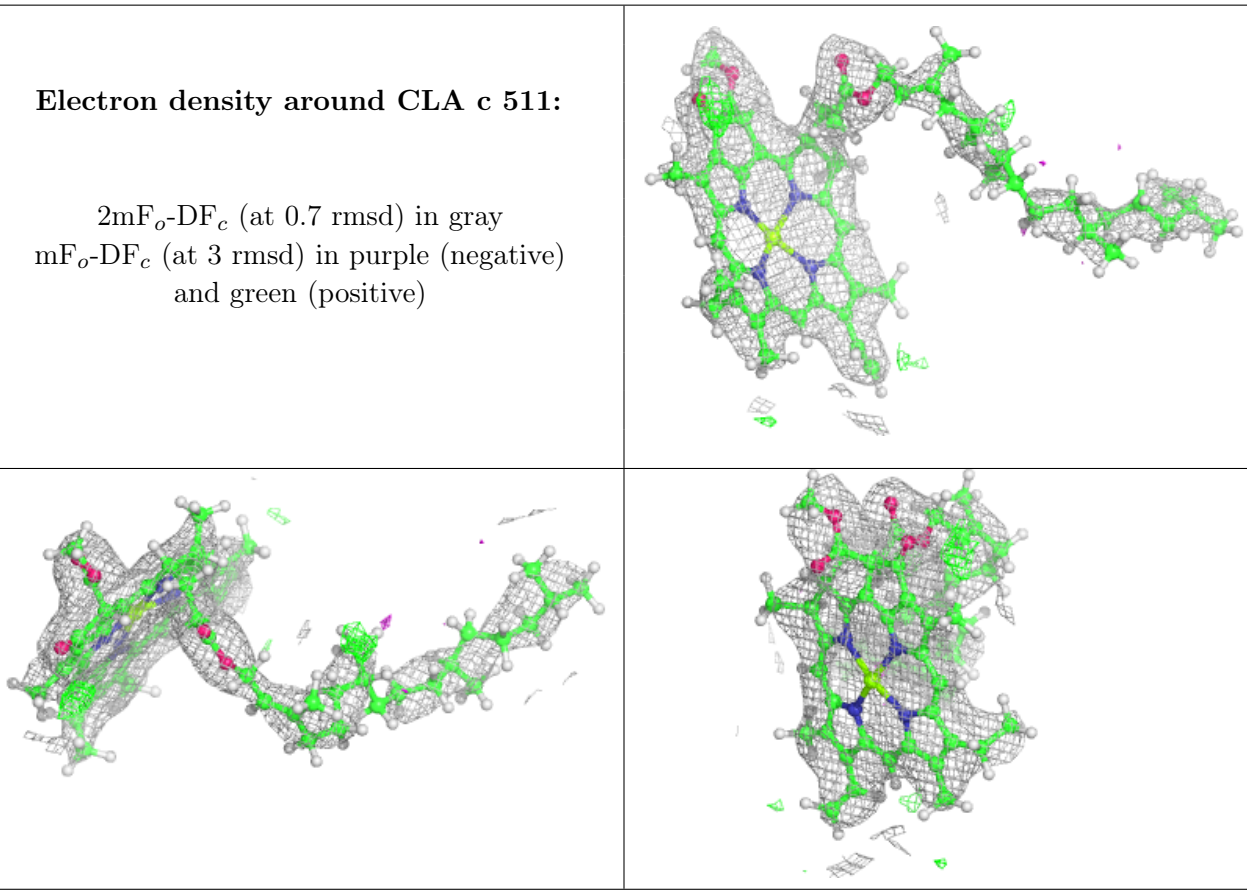
Electron density around CLA c 510:

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



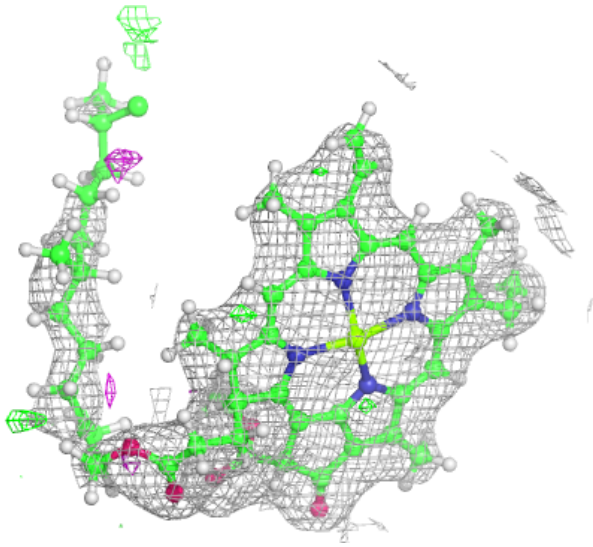
Electron density around CLA c 511:

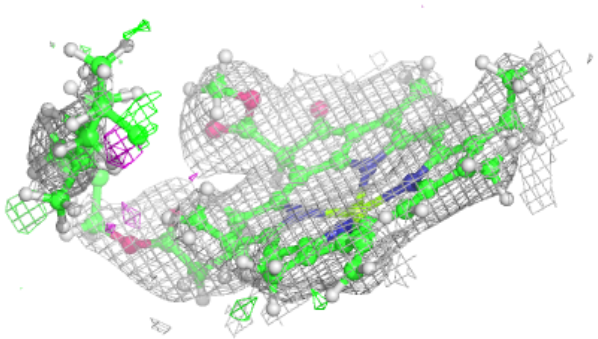
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

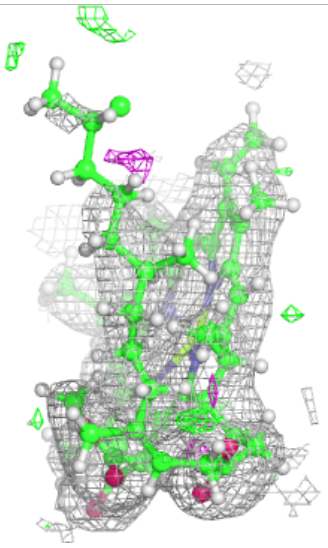


Electron density around CLA B 615:

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

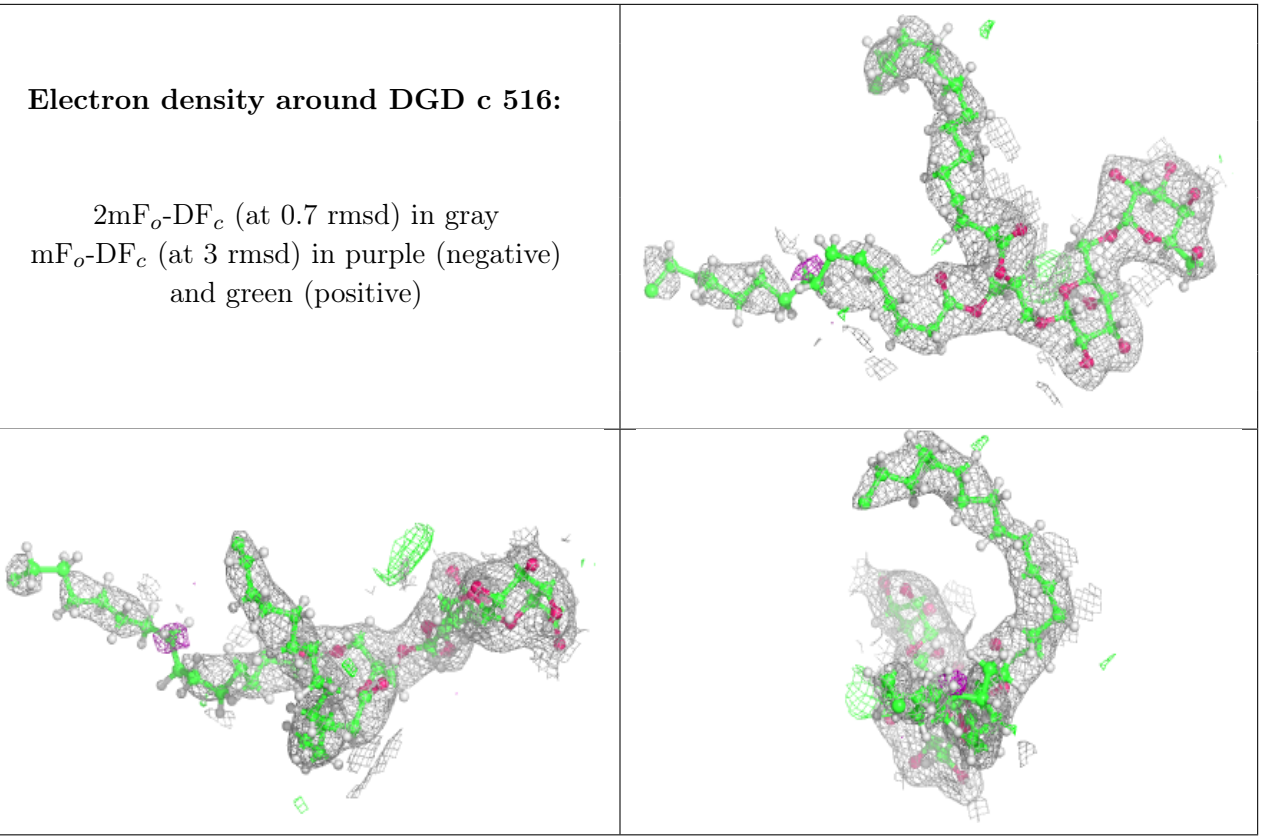






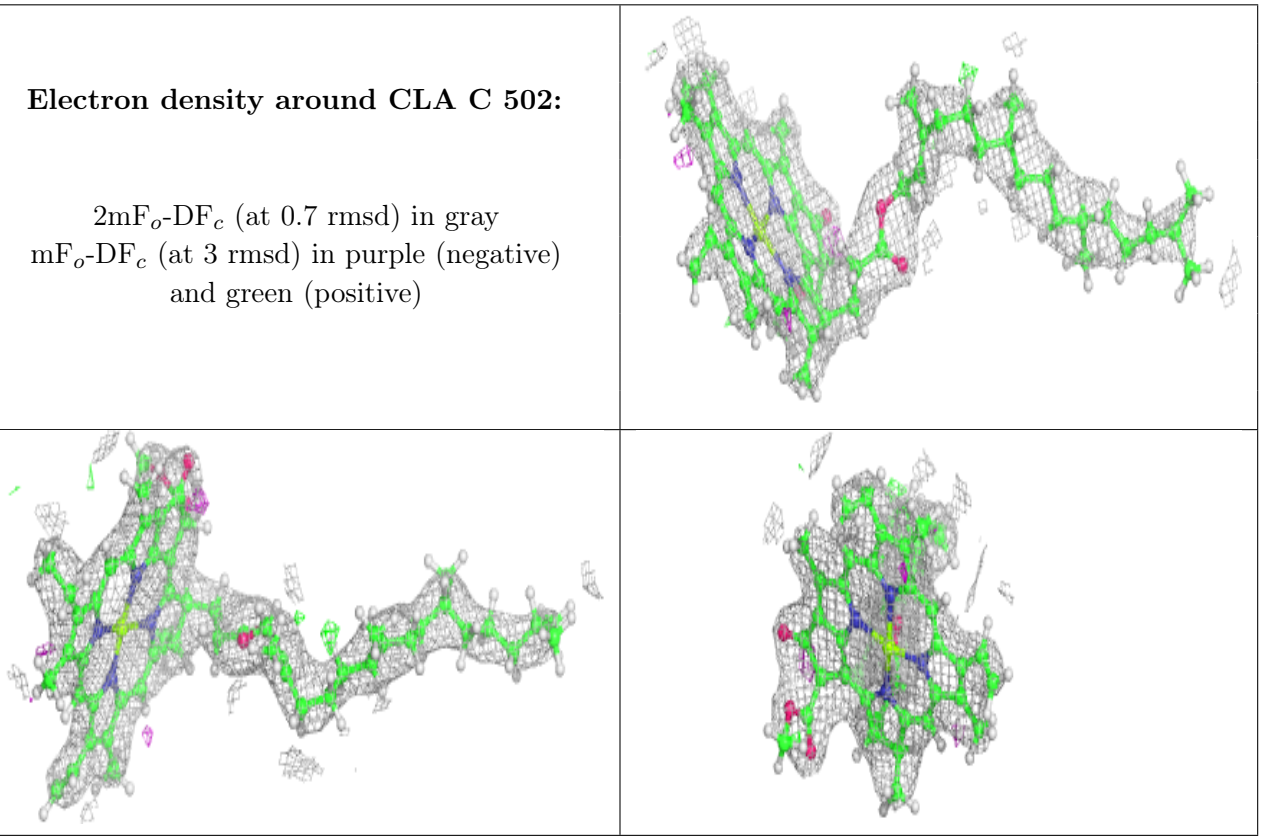
Electron density around DGD c 516:

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



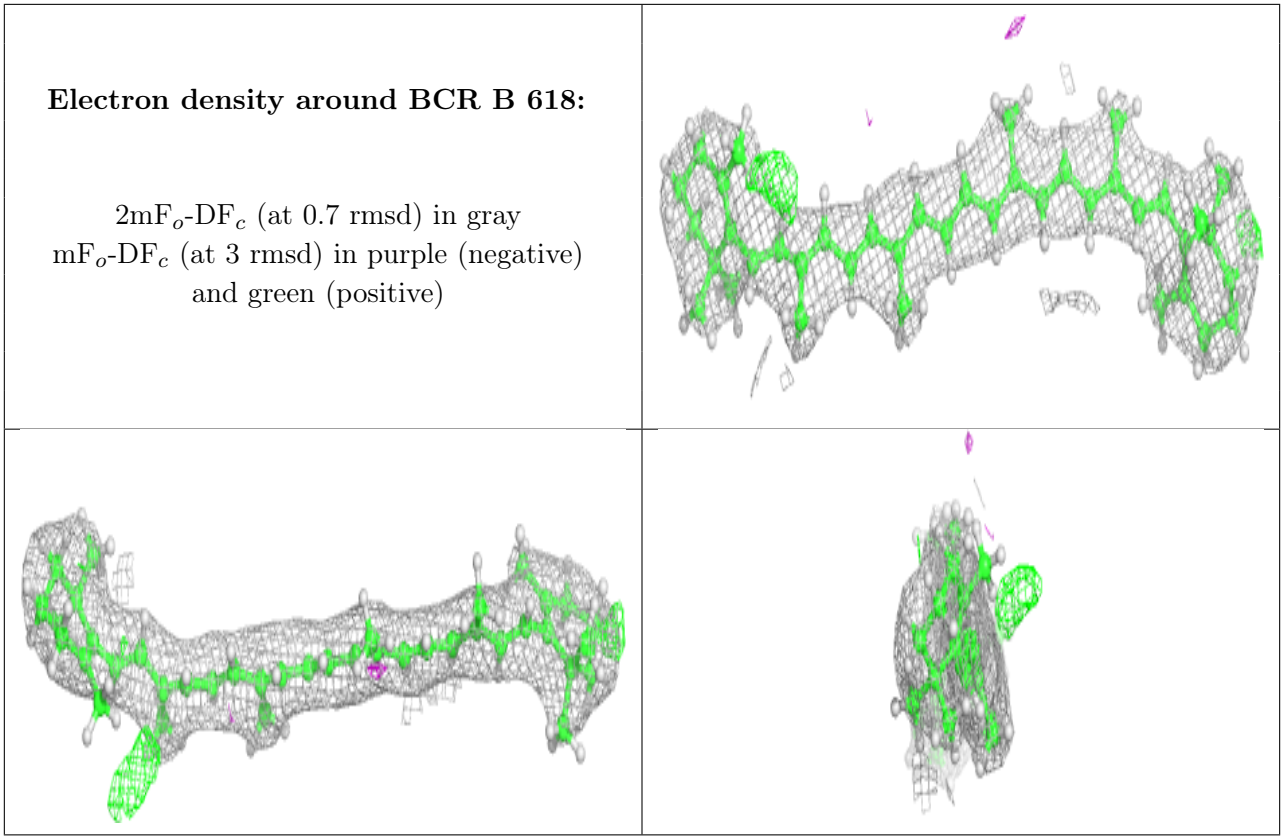
Electron density around CLA C 502:

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



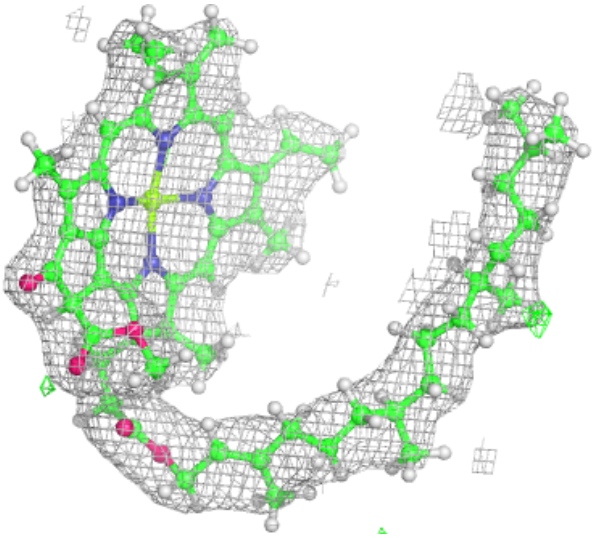
Electron density around BCR B 618:

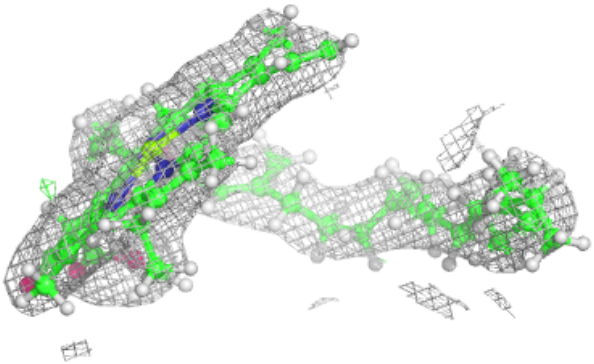
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

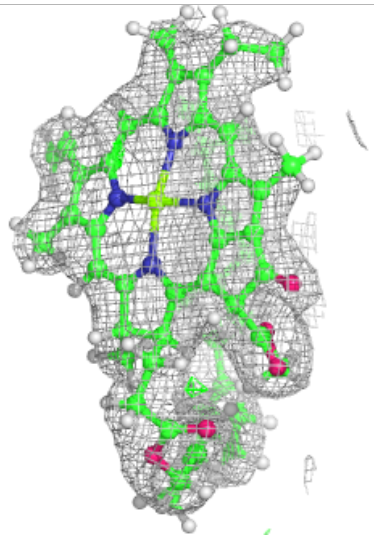


Electron density around CLA C 507:

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

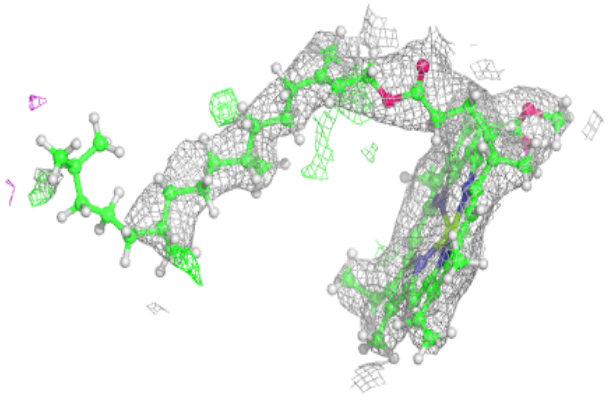


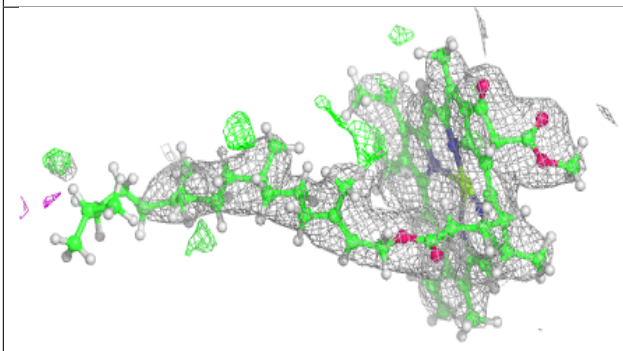


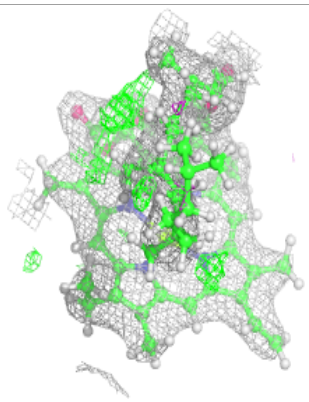


Electron density around CLA C 508:

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

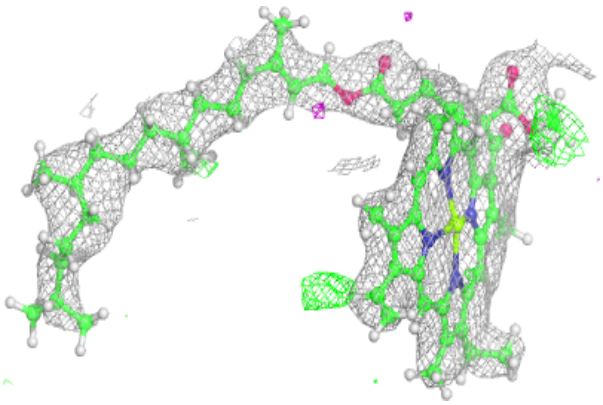


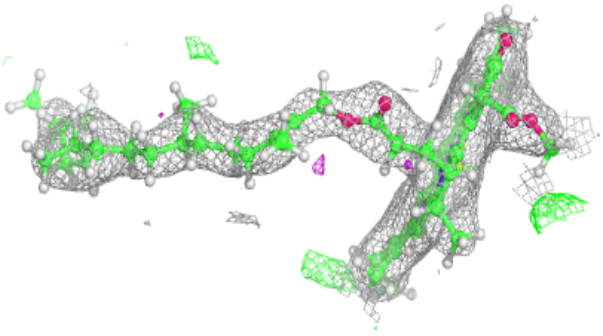


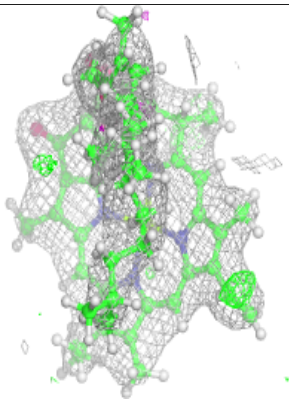


Electron density around CLA b 609:

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

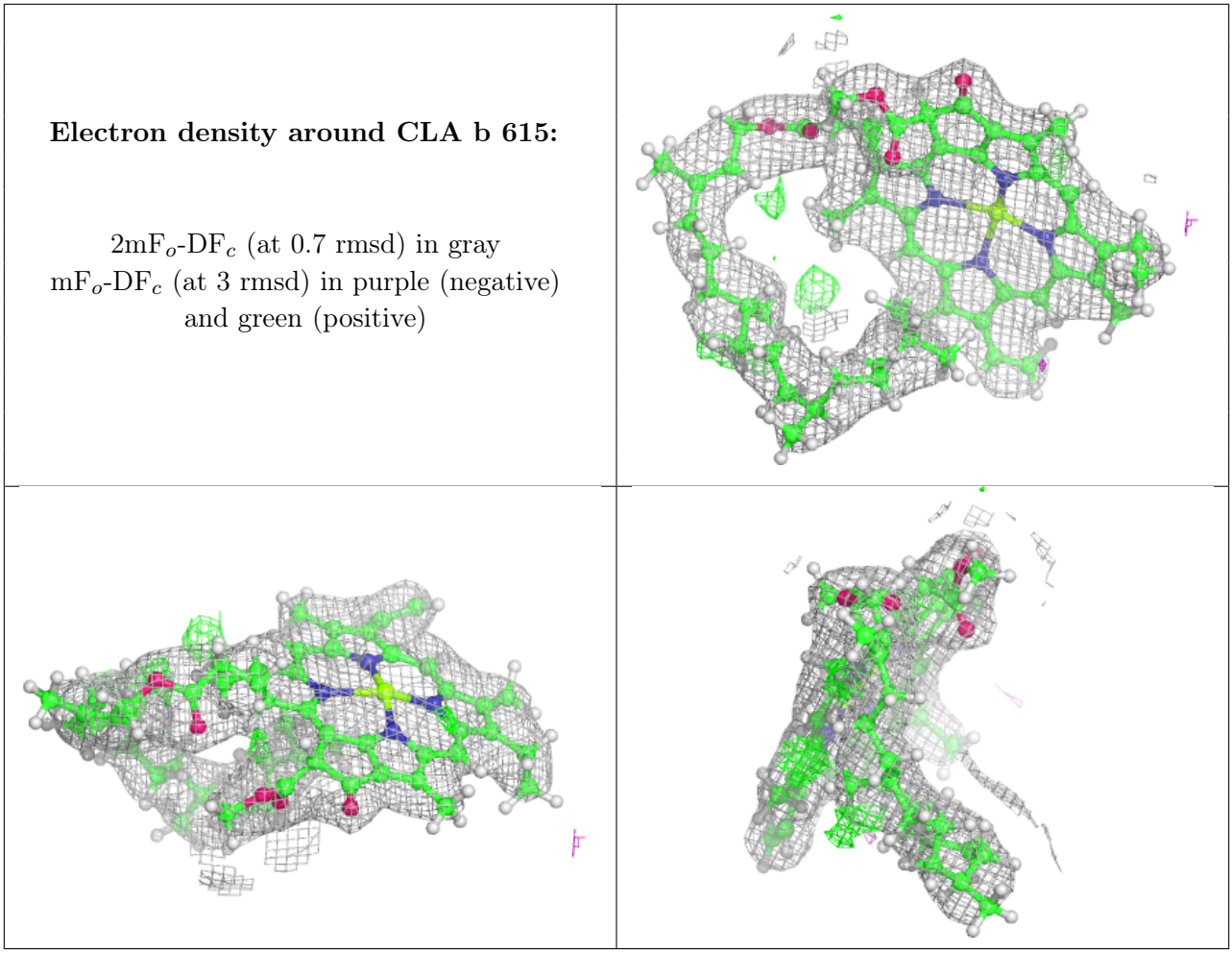






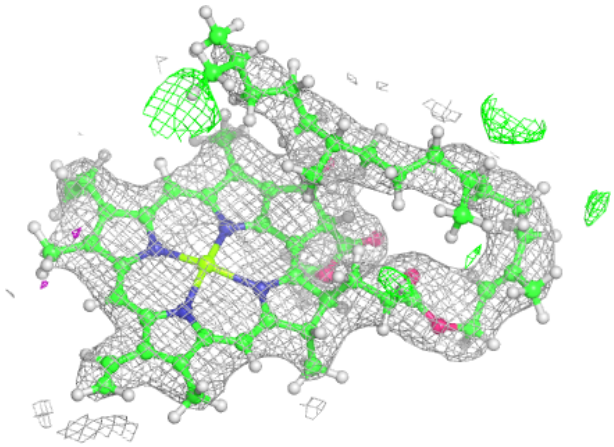
Electron density around CLA b 615:

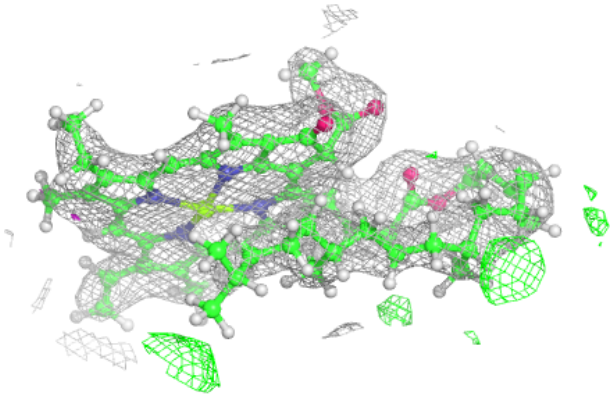
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

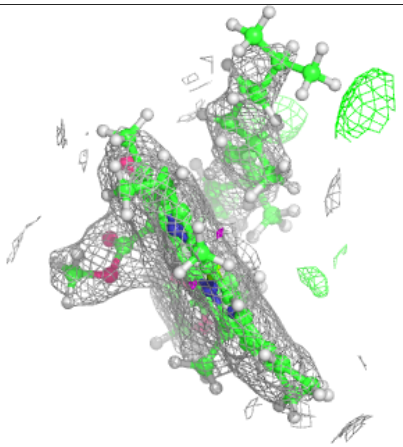


Electron density around CLA C 509:

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

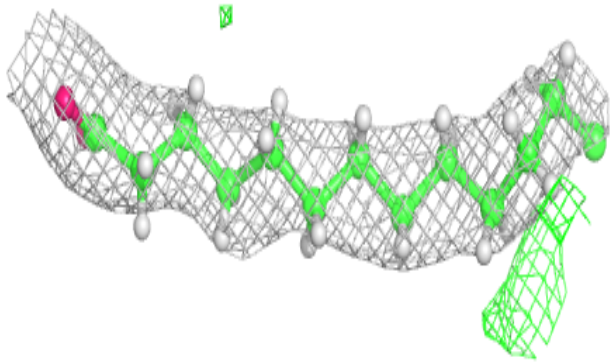


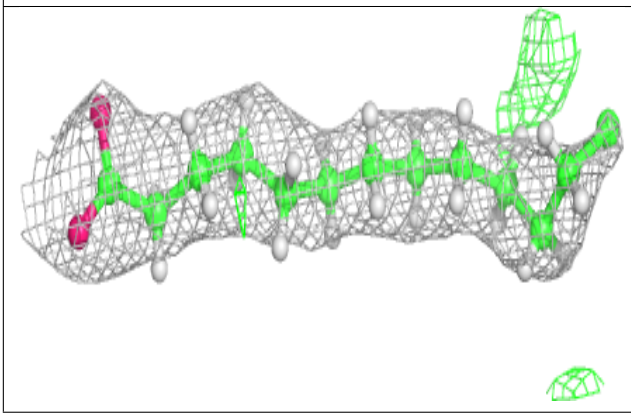


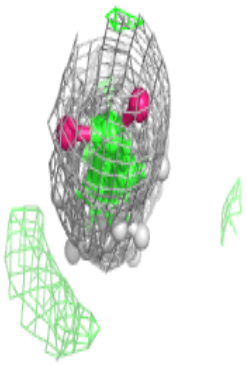


Electron density around STE M 102:

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

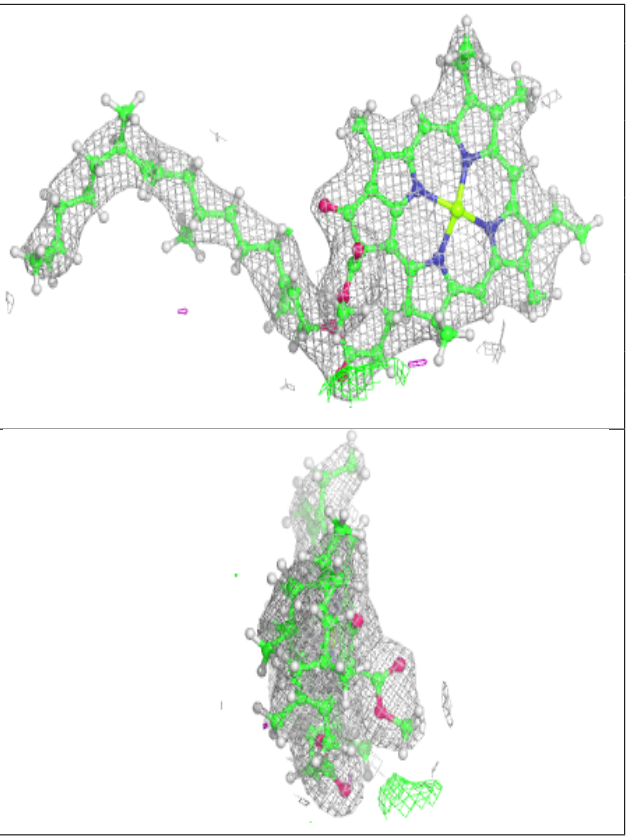


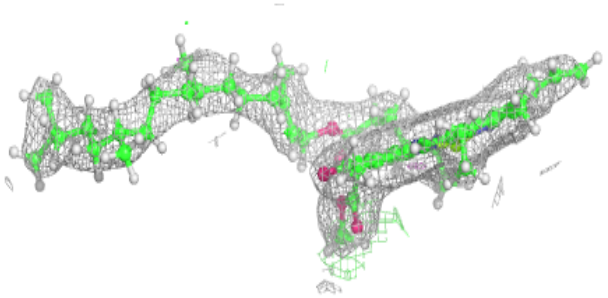




Electron density around CLA B 601:

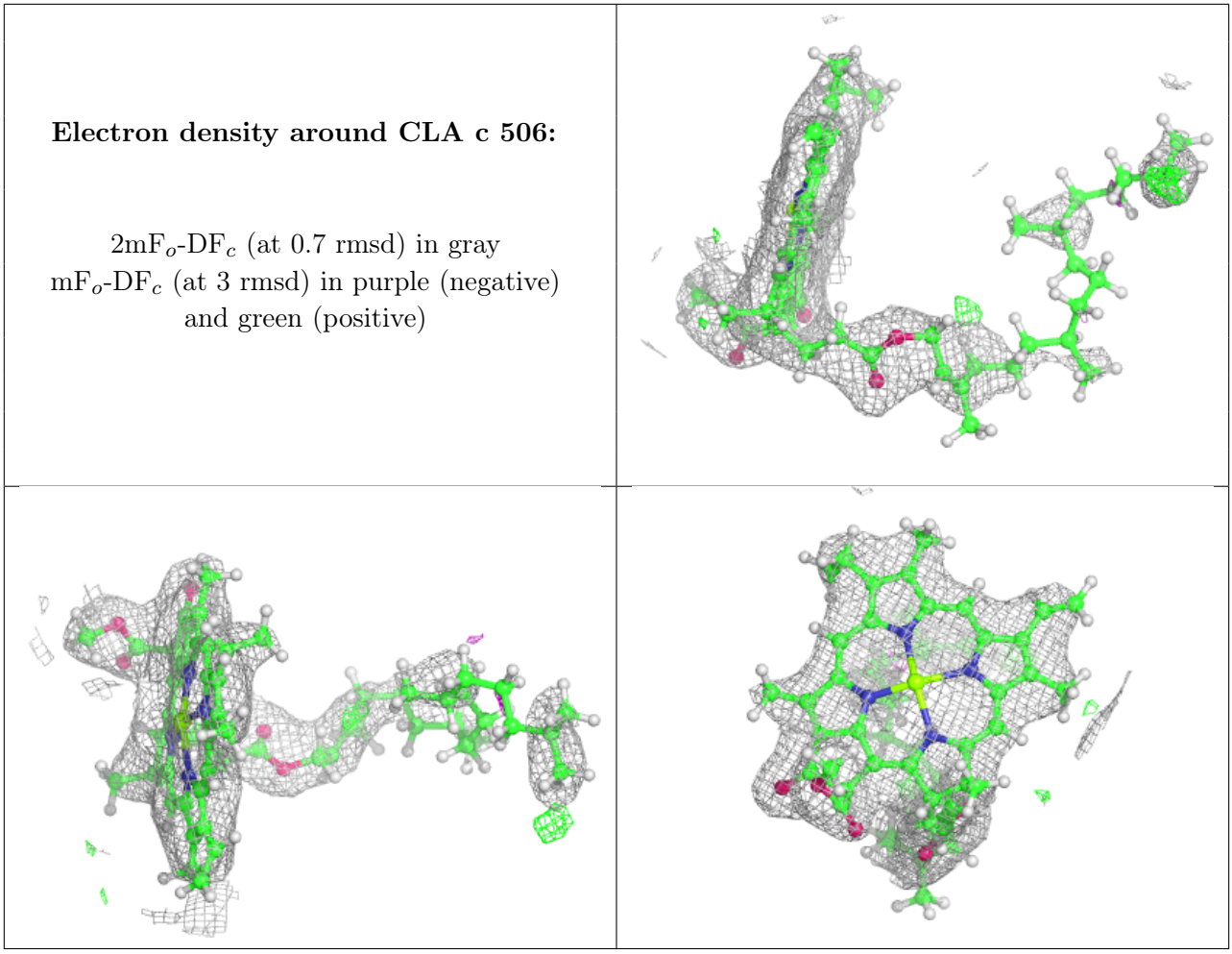
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





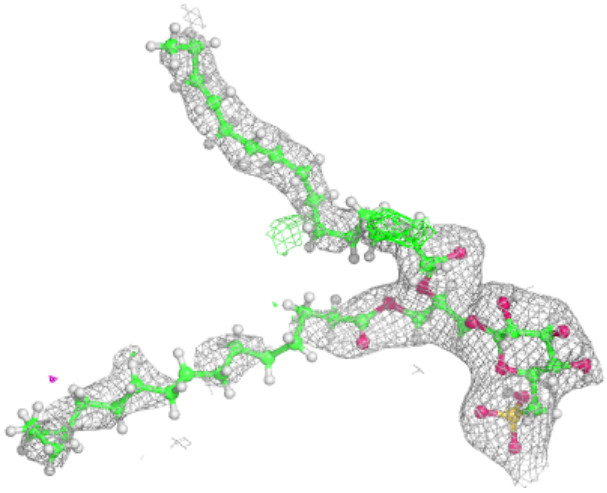
Electron density around CLA c 506:

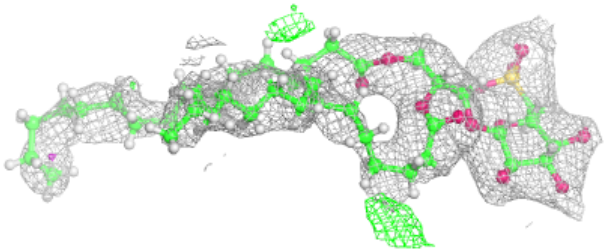
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

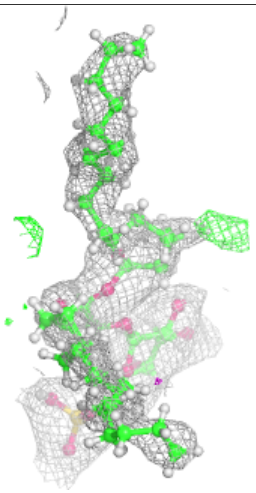


Electron density around SQD a 410:

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

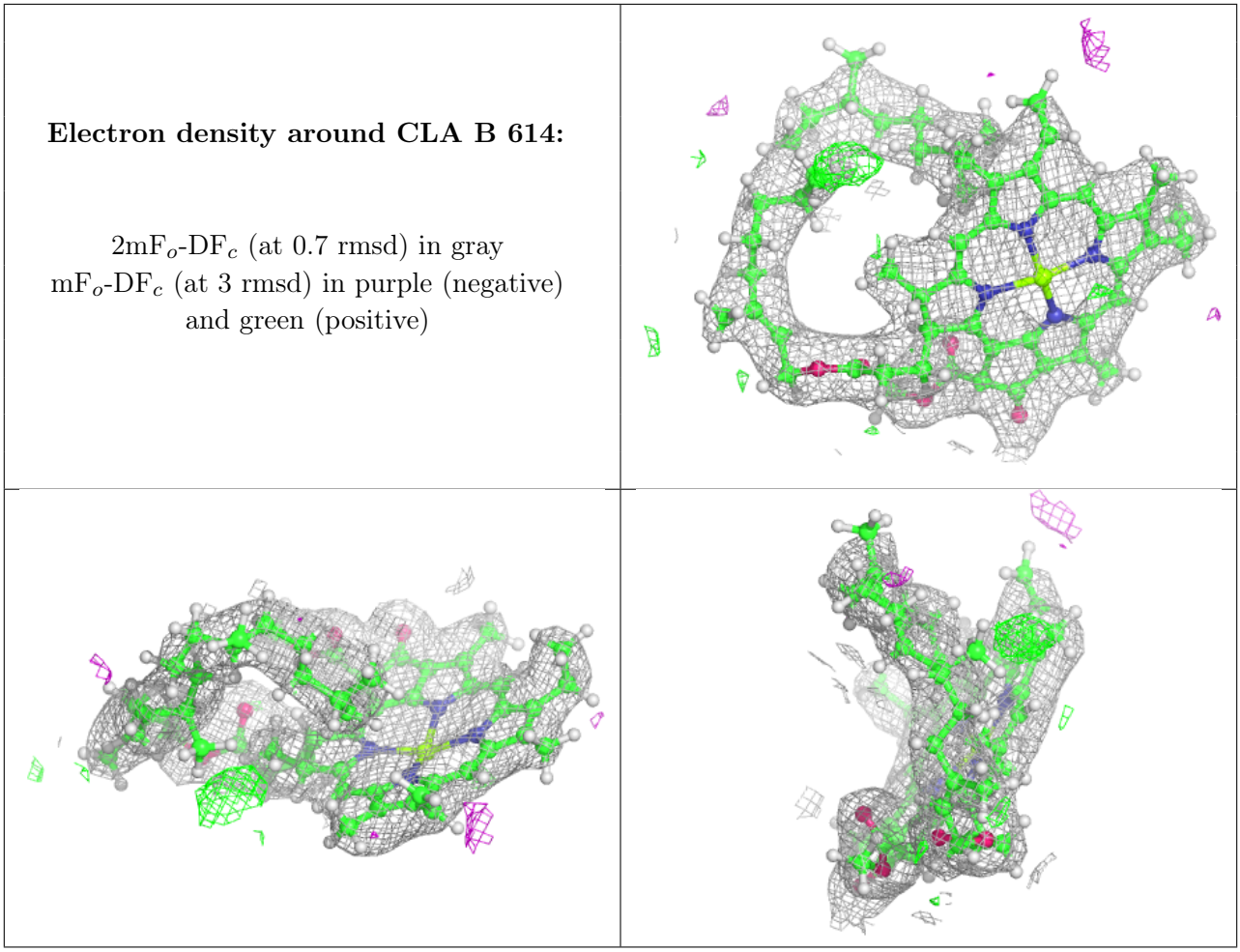






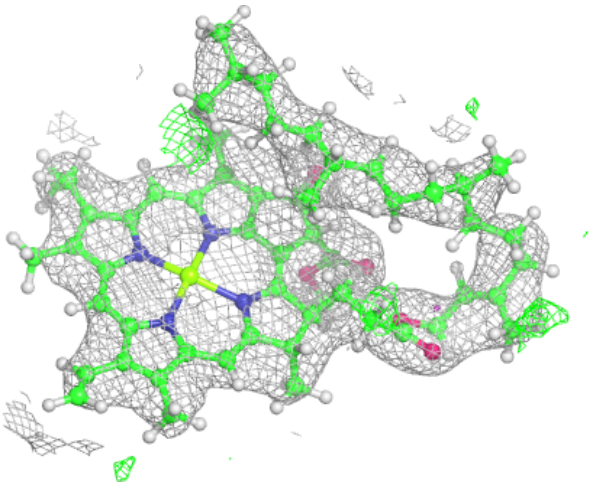
Electron density around CLA B 614:

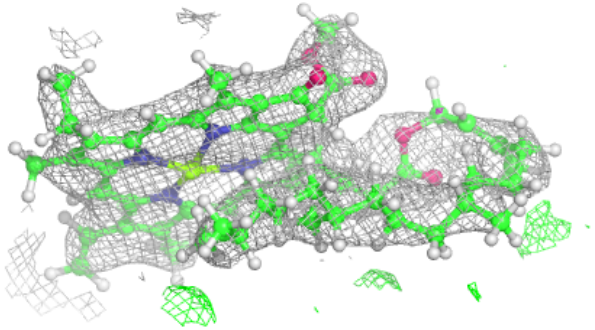
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

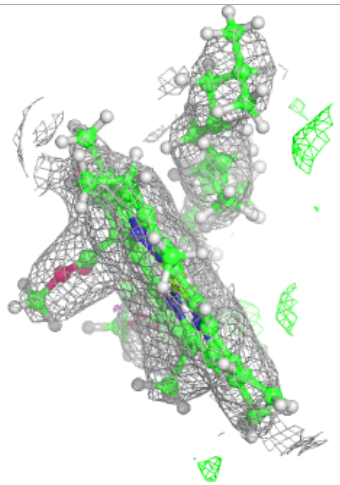


Electron density around CLA c 509:

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

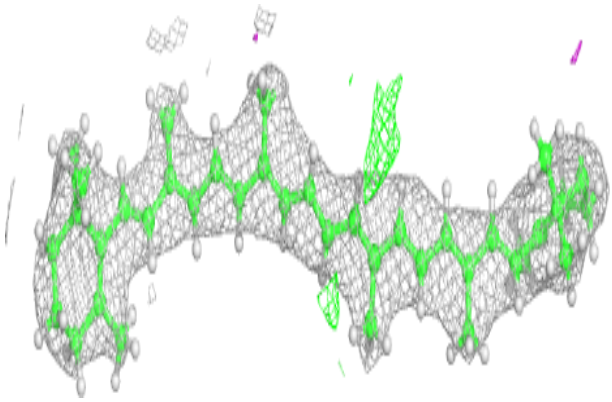


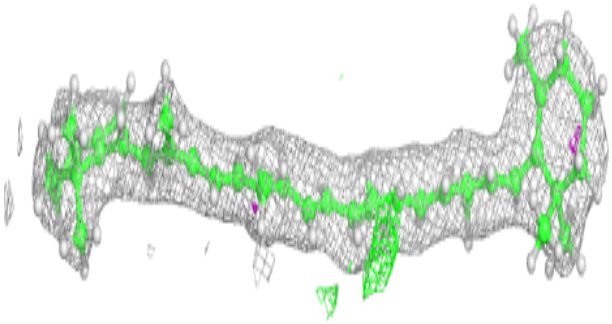


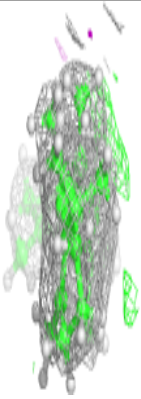


Electron density around BCR B 616:

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

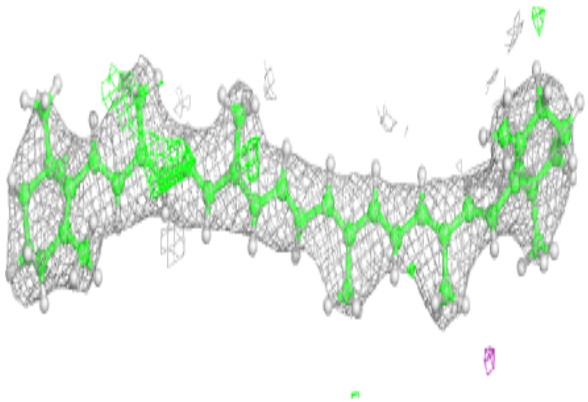


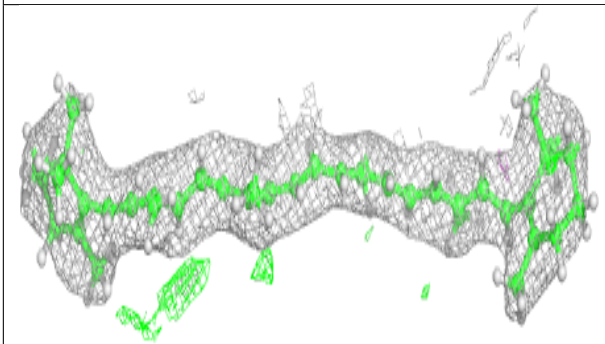


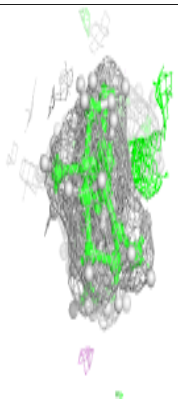


Electron density around BCR B 617:

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

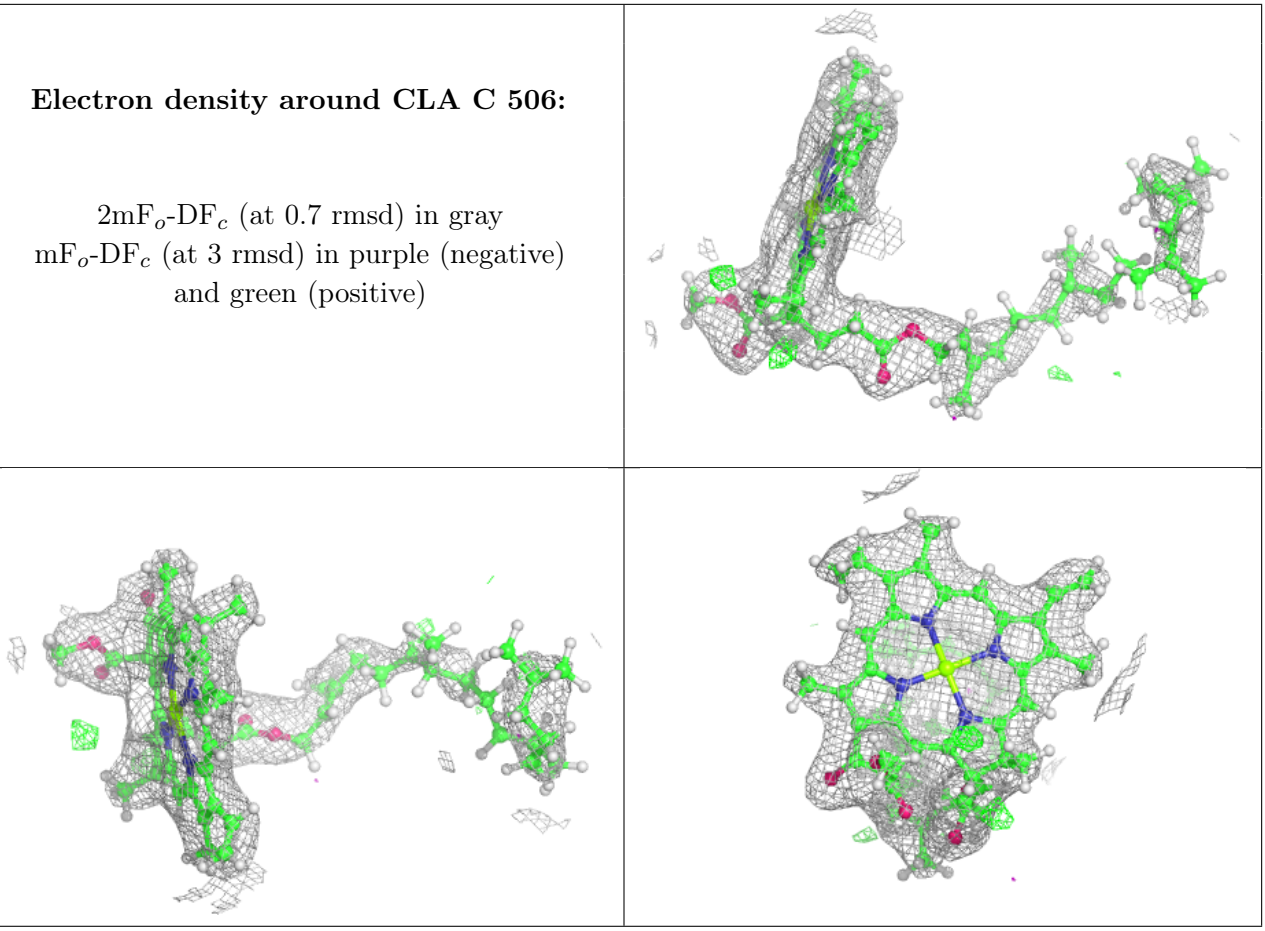






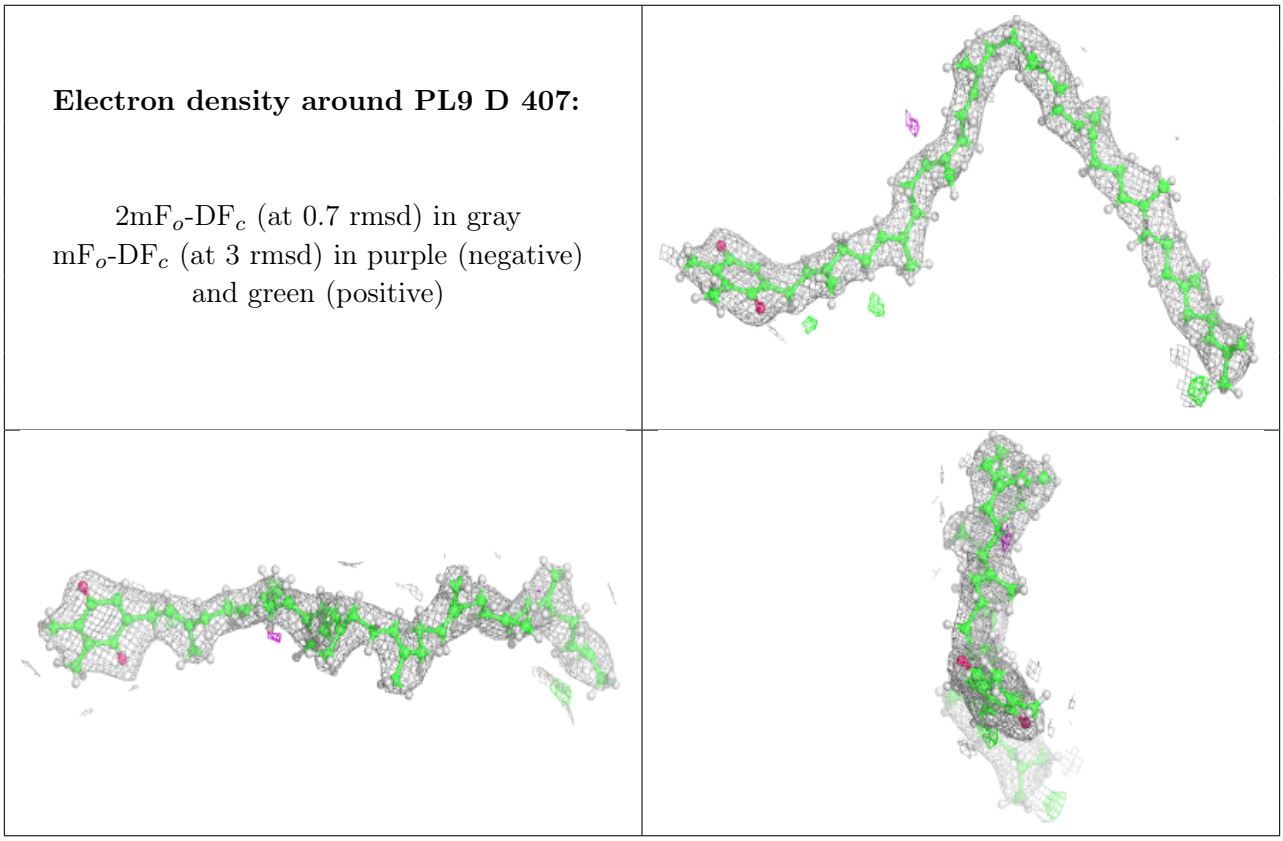
Electron density around CLA C 506:

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



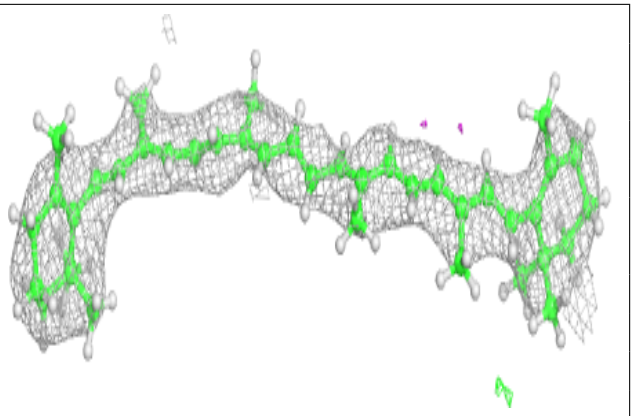
Electron density around PL9 D 407:

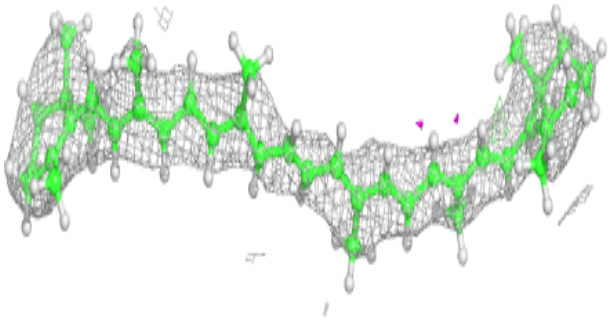
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

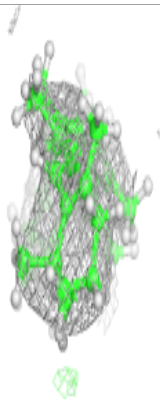


Electron density around BCR C 515:

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

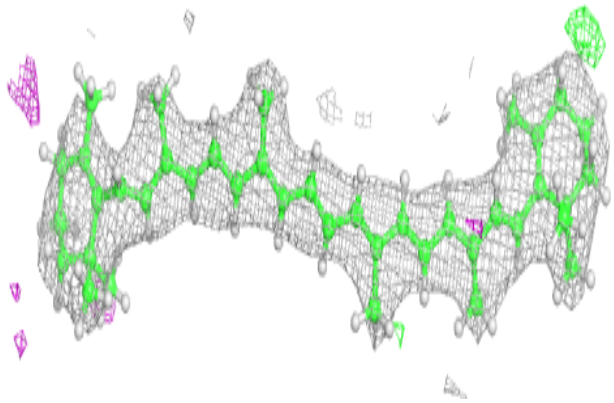


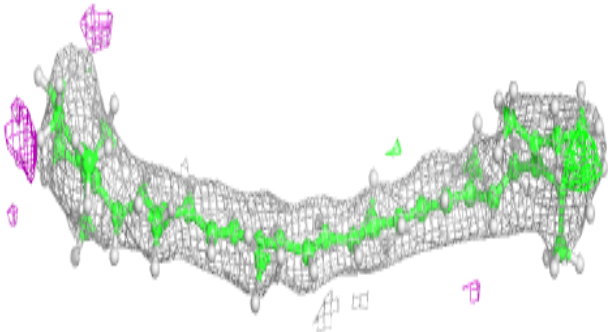


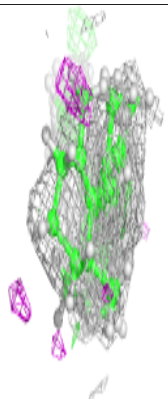


Electron density around BCR D 406:

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

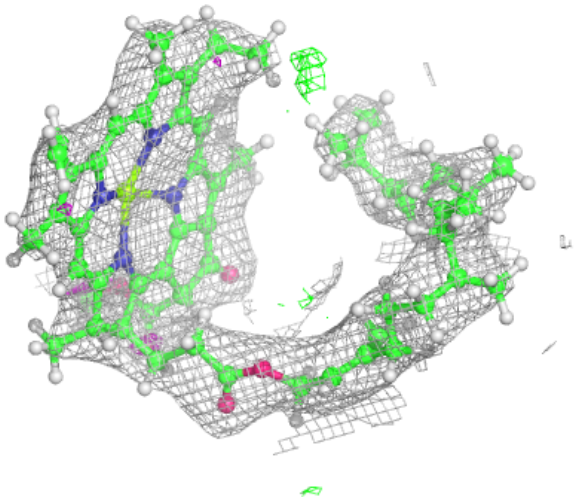


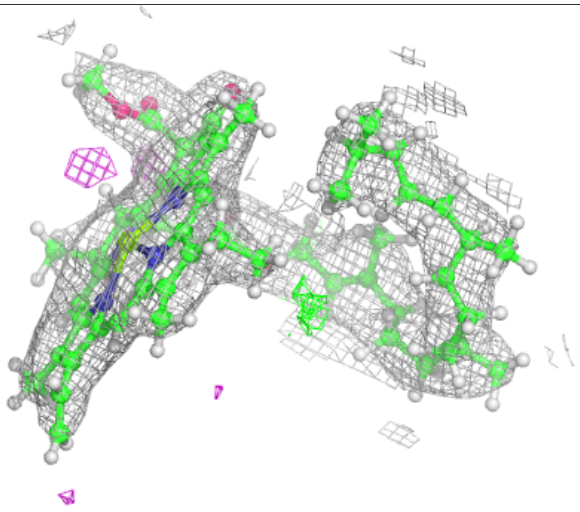


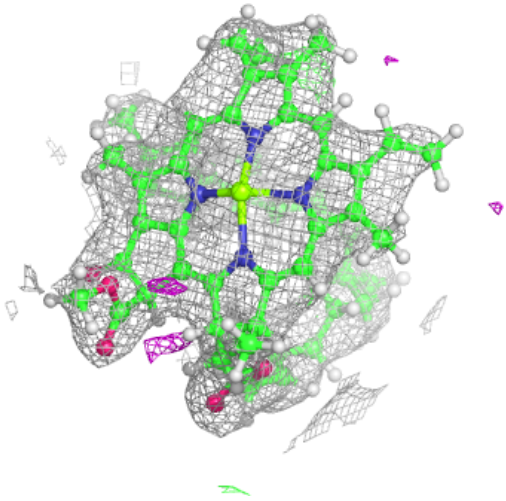


Electron density around CLA c 503:

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

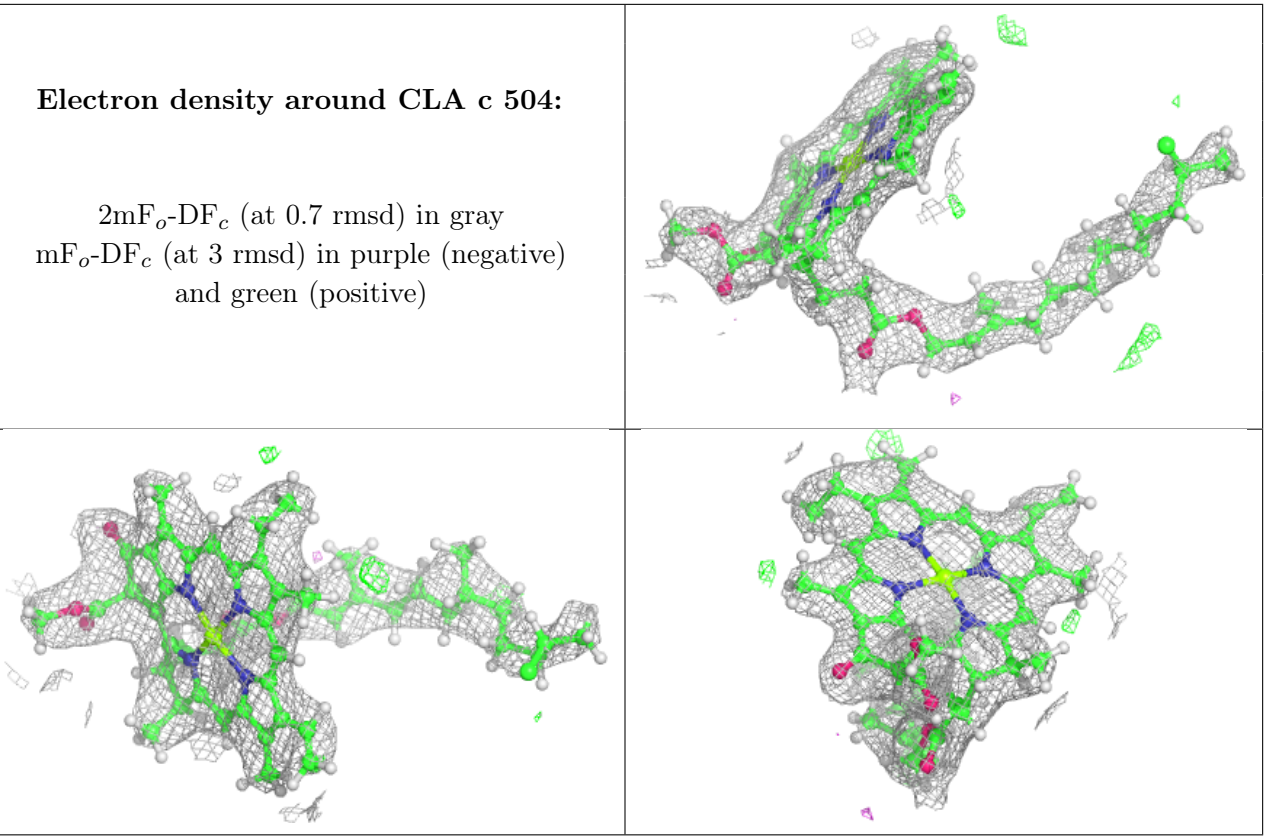






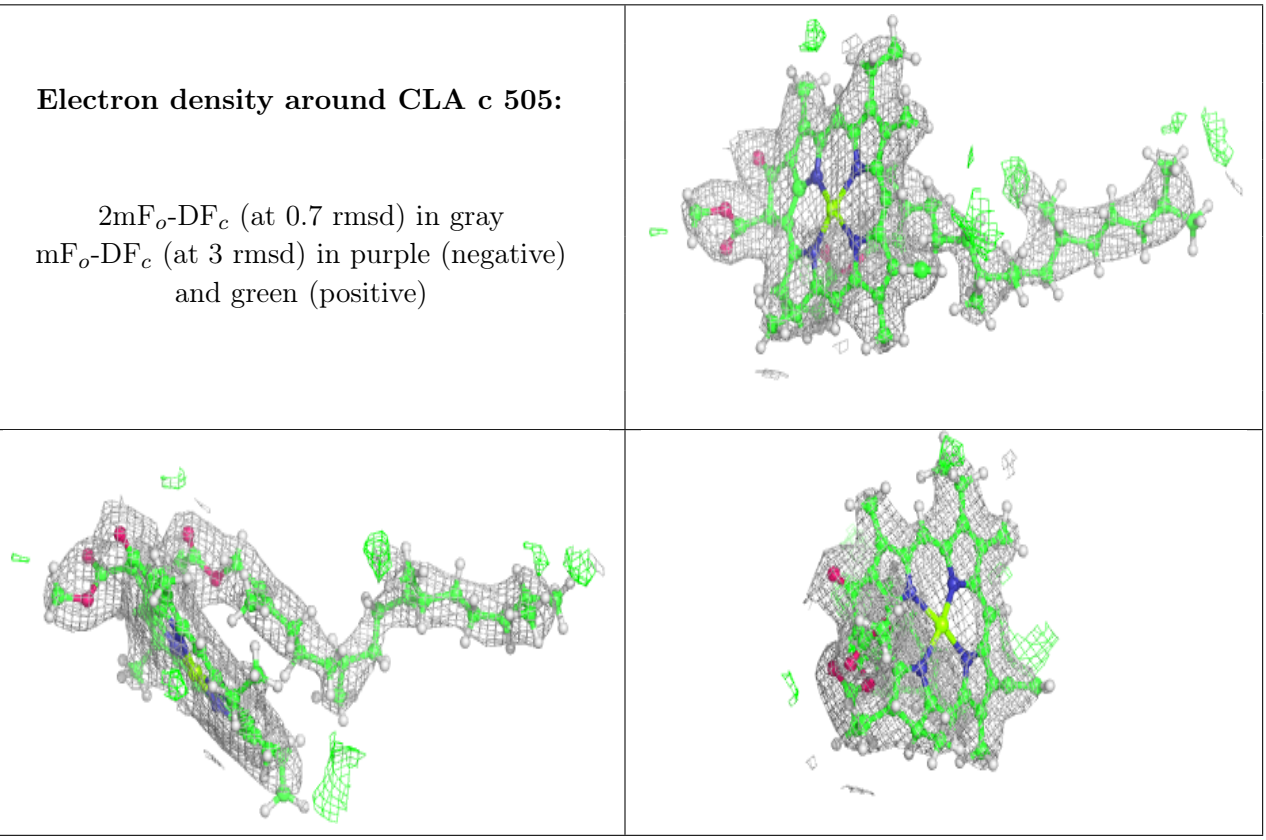
Electron density around CLA c 504:

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



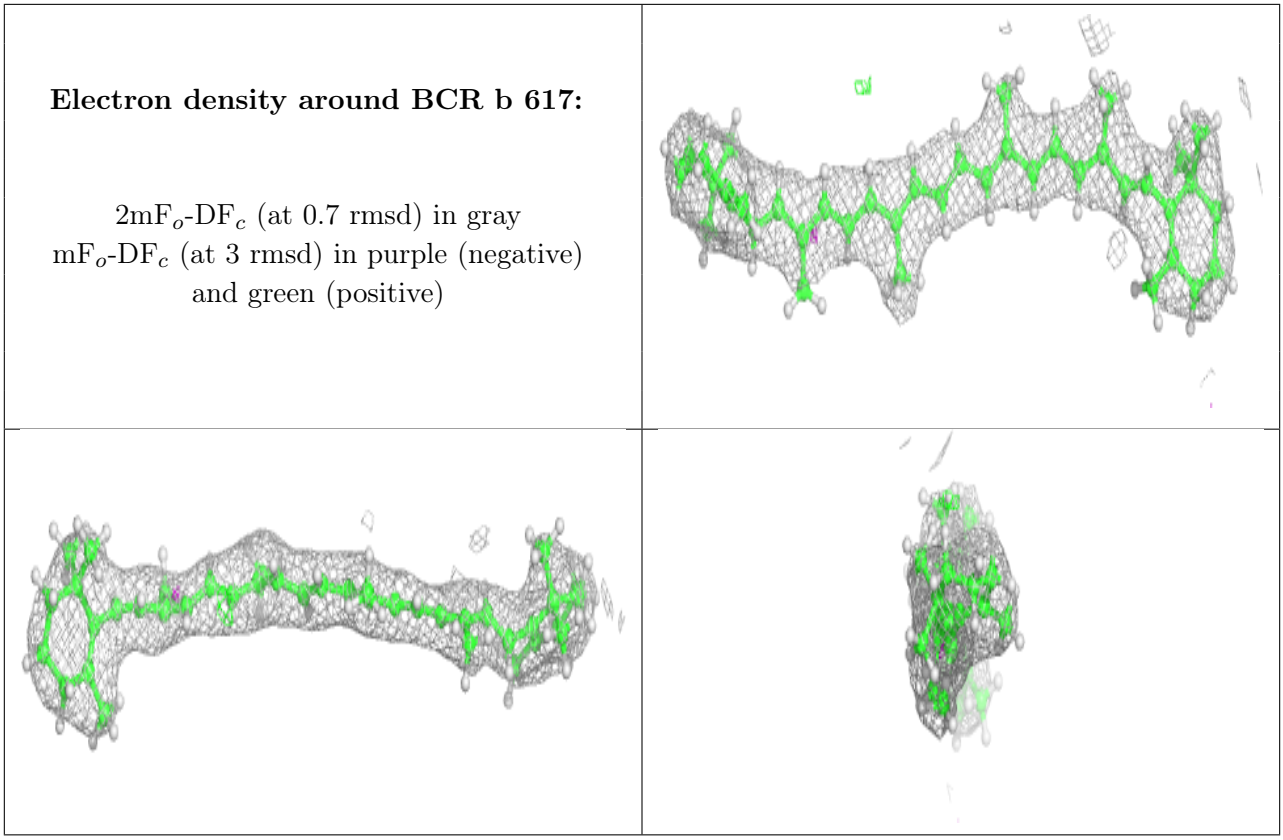
Electron density around CLA c 505:

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



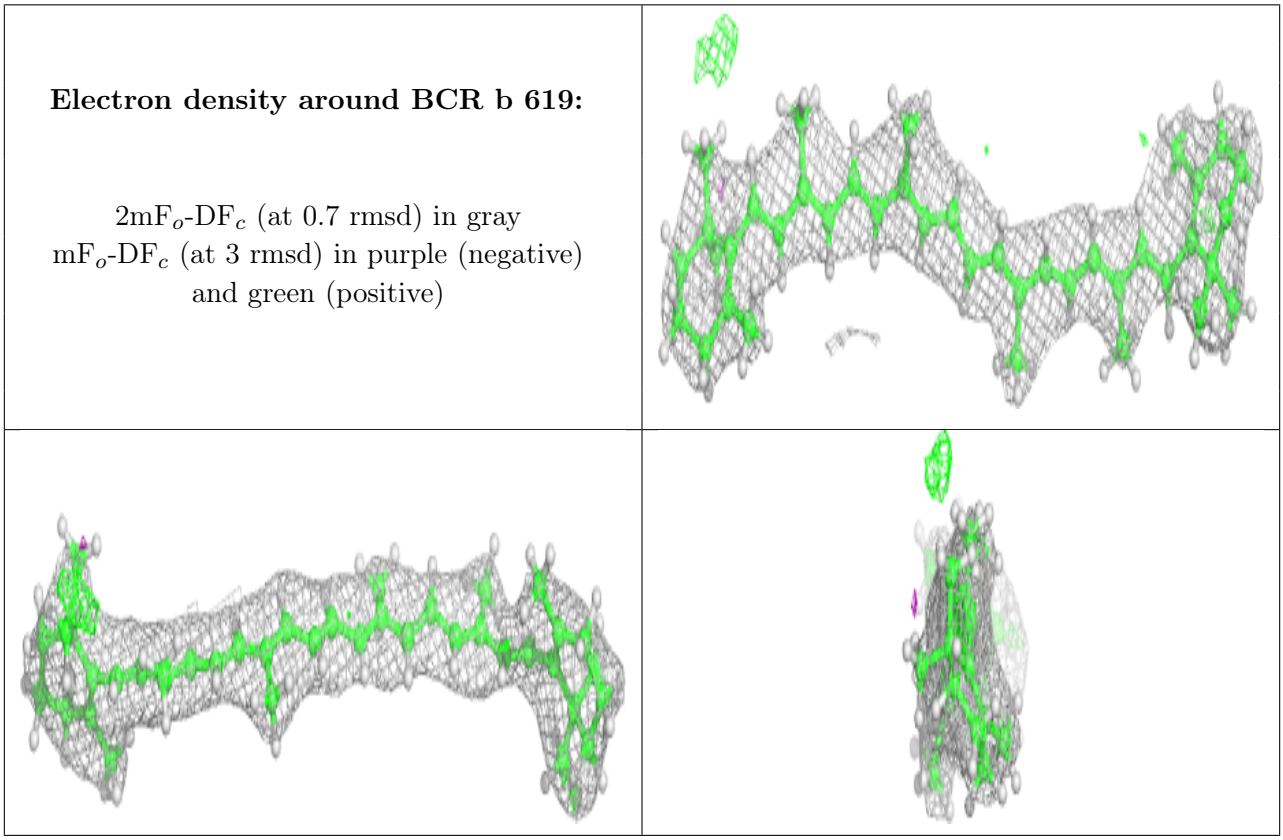
Electron density around BCR b 617:

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



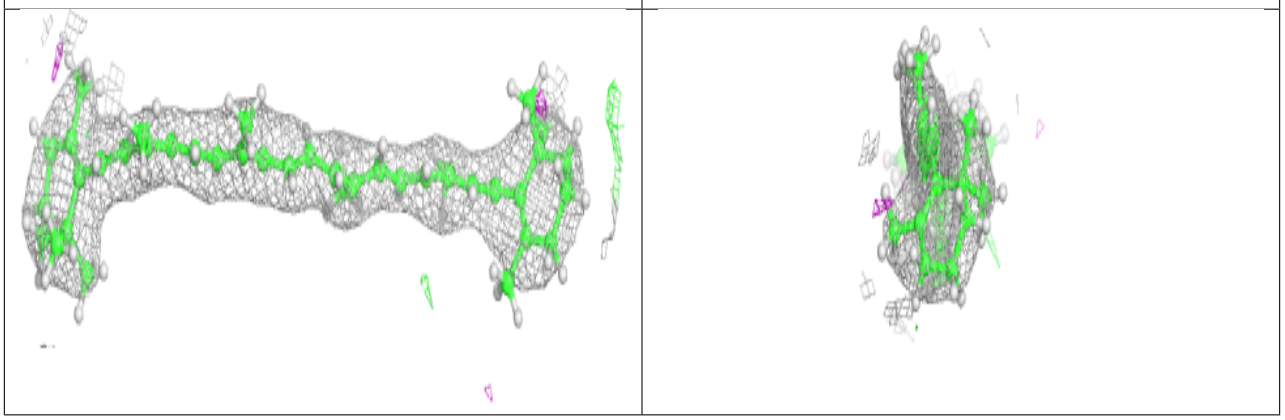
Electron density around BCR b 619:

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



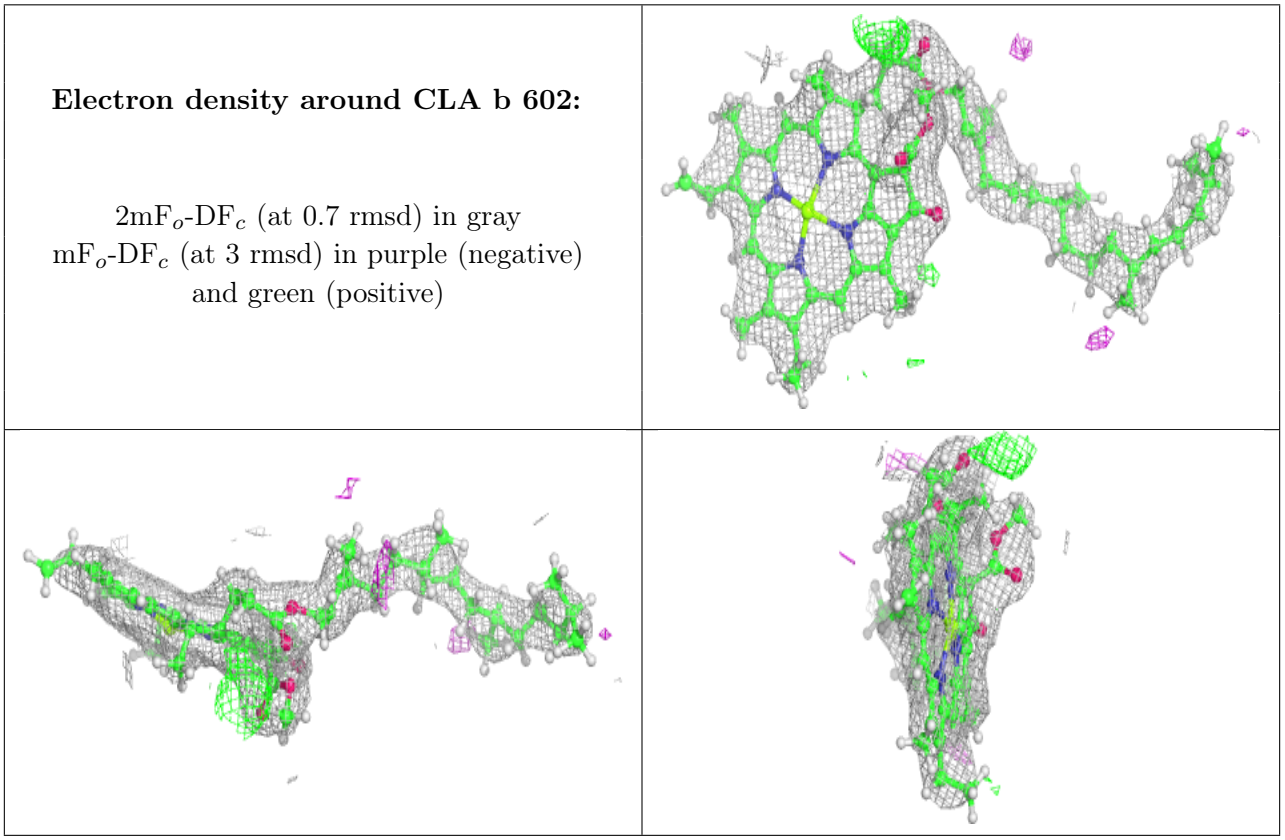
Electron density around BCR c 514:

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



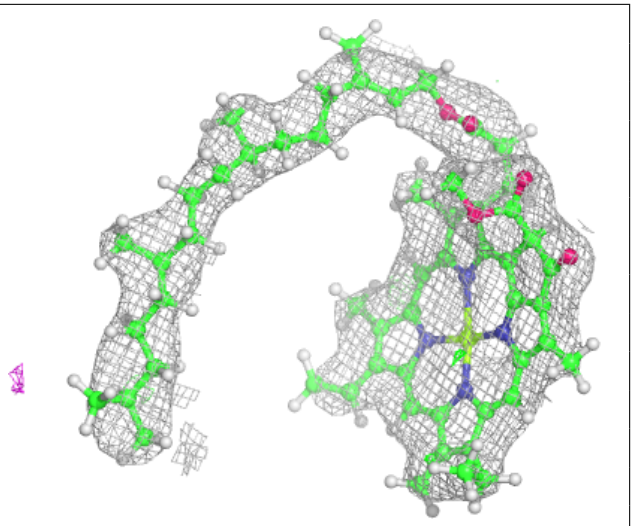
Electron density around CLA b 602:

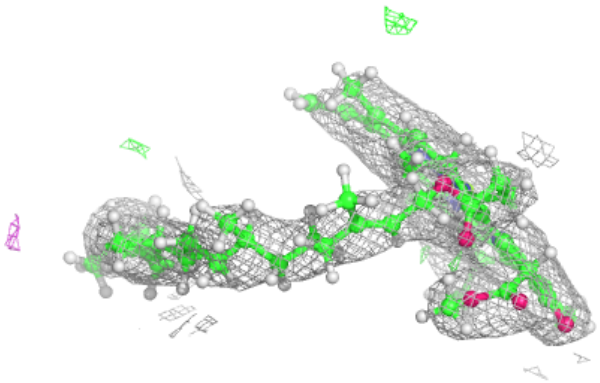
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

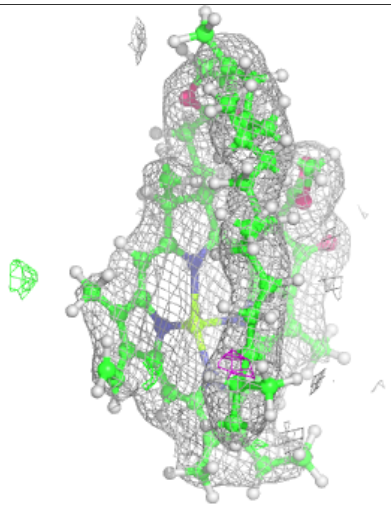


Electron density around CLA c 507:

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

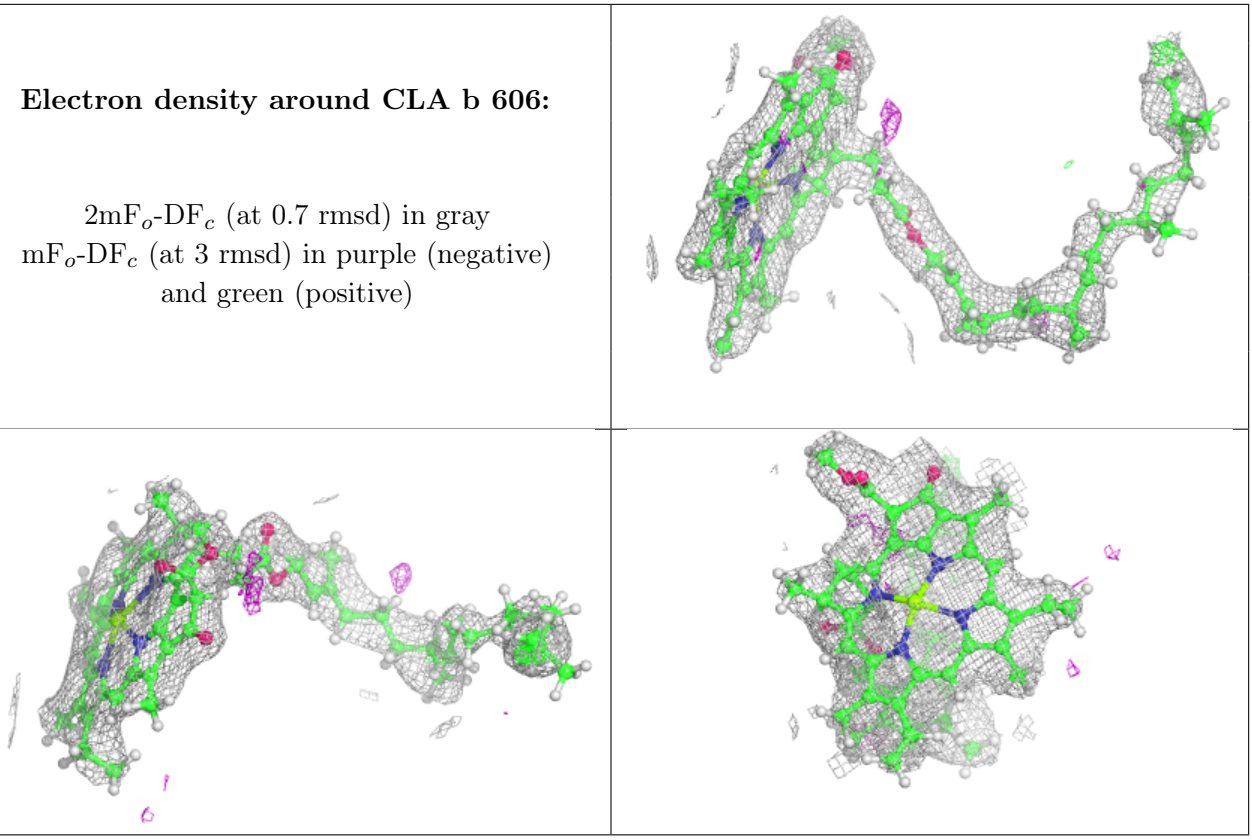






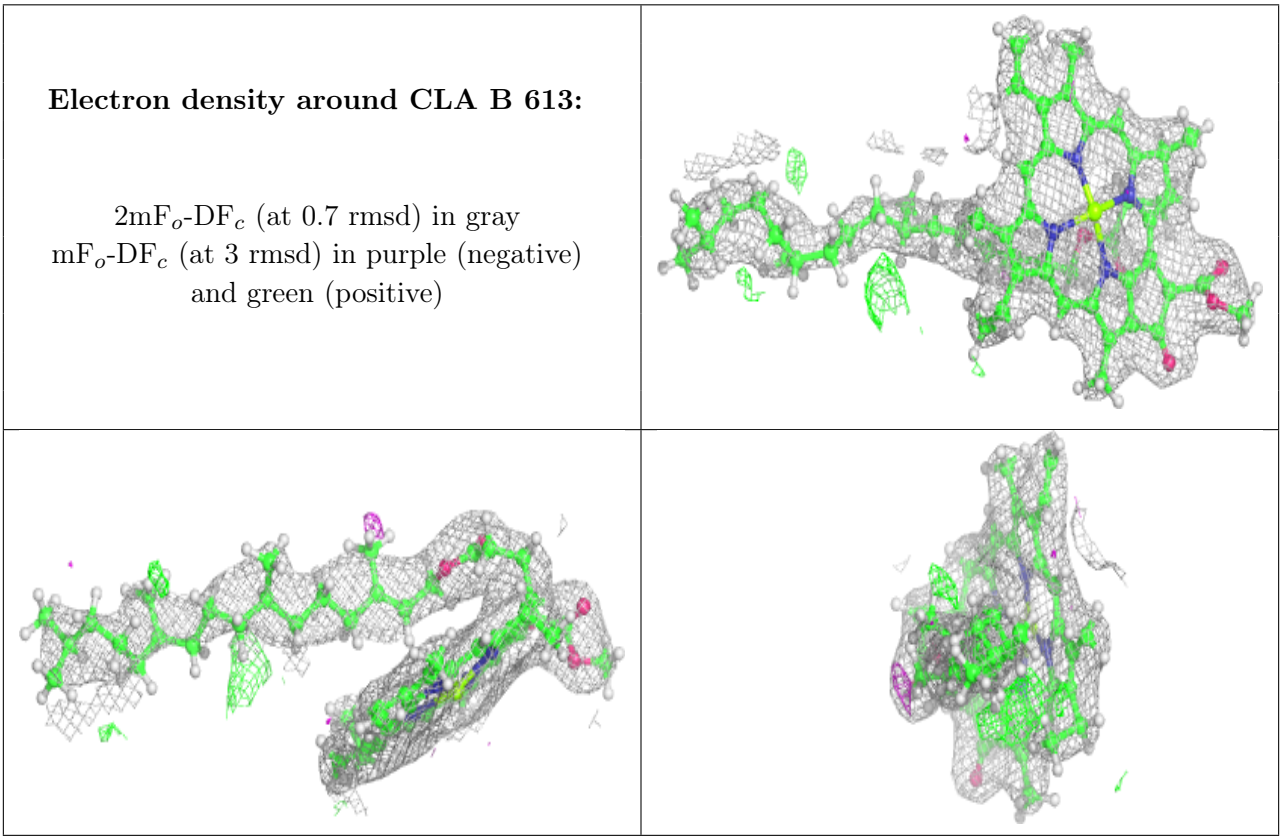
Electron density around CLA b 606:

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



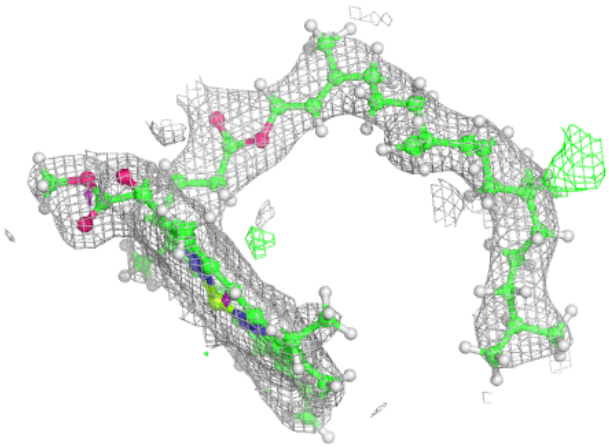
Electron density around CLA B 613:

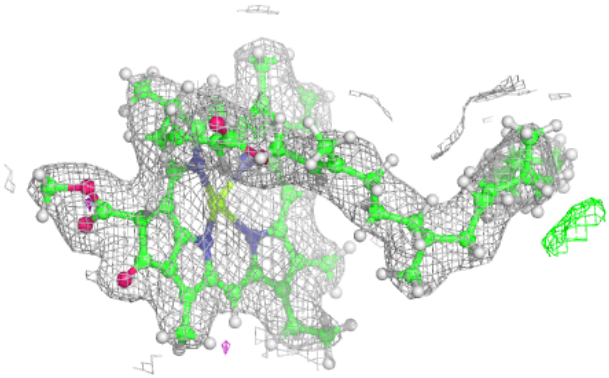
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

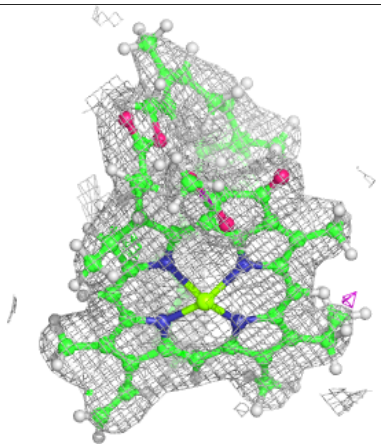


Electron density around CLA b 611:

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

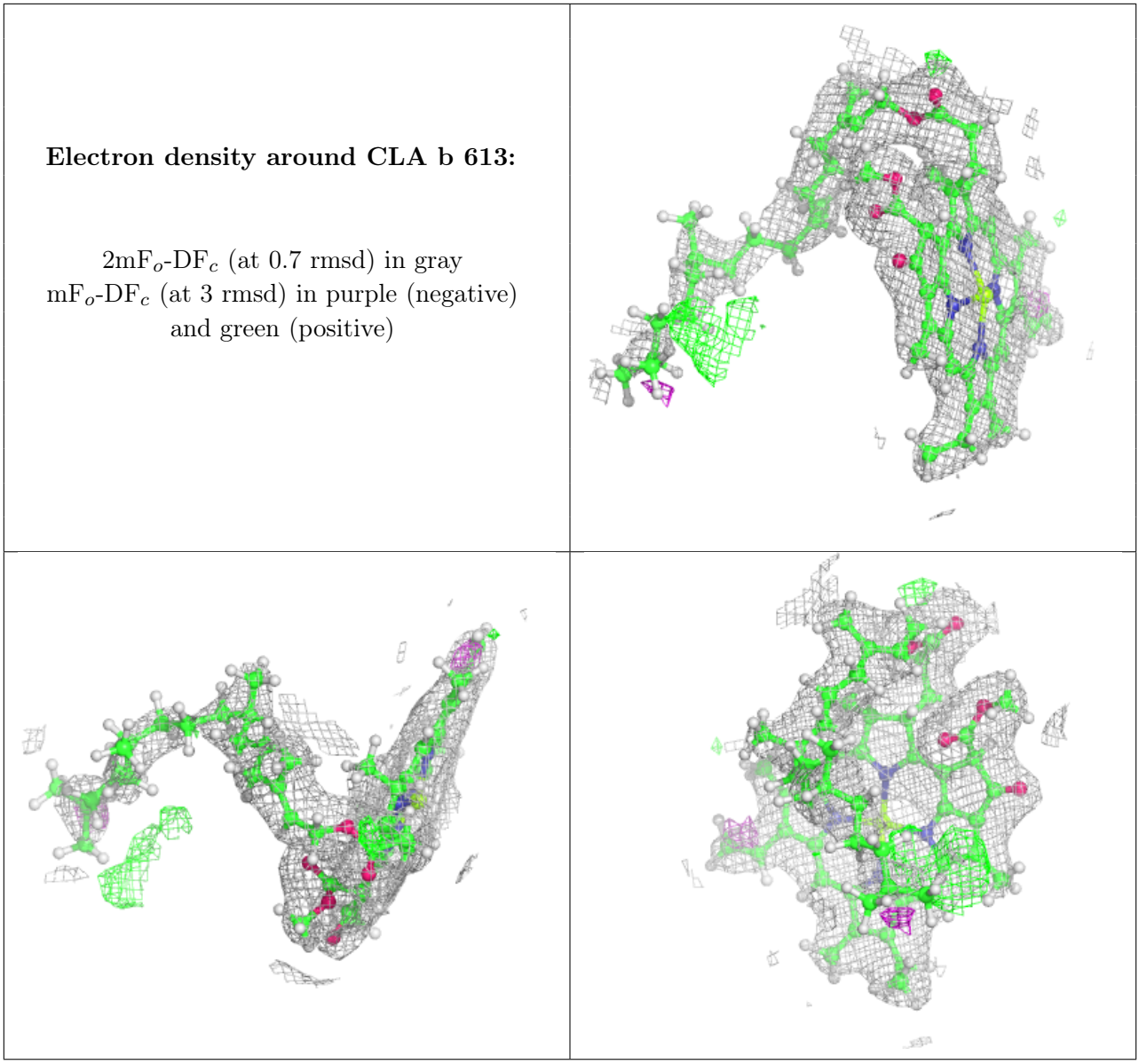






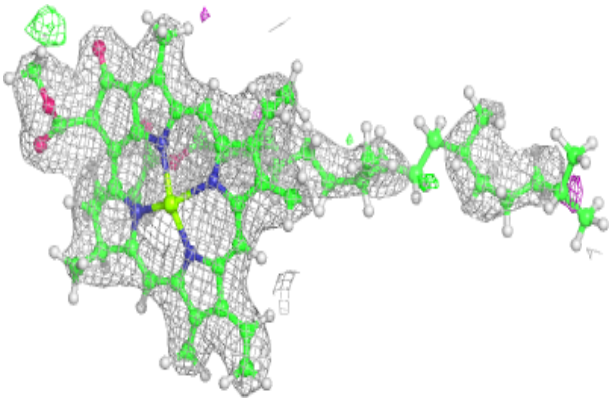
Electron density around CLA b 613:

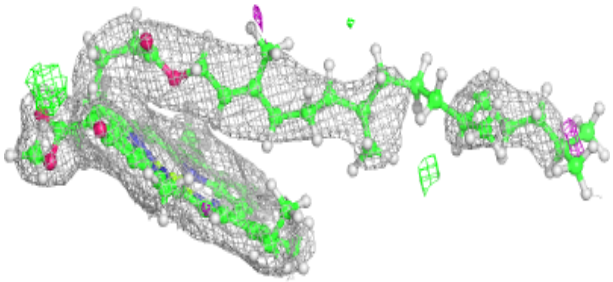
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

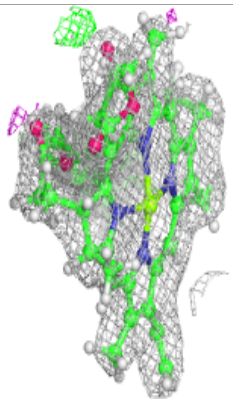


Electron density around CLA b 614:

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

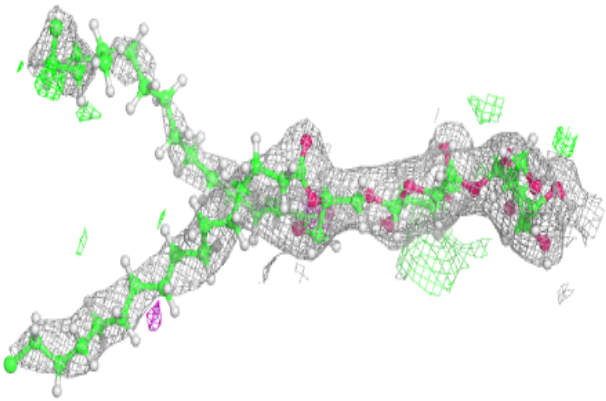


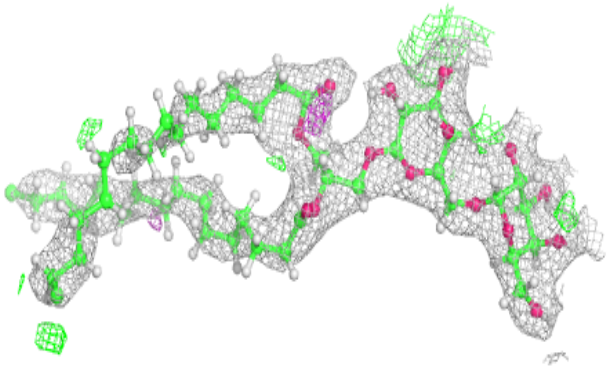


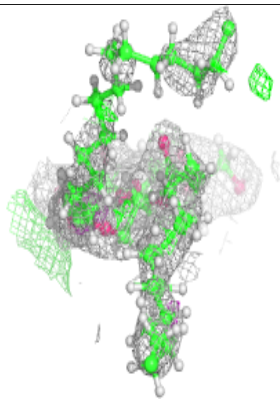


Electron density around DGD C 516:

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

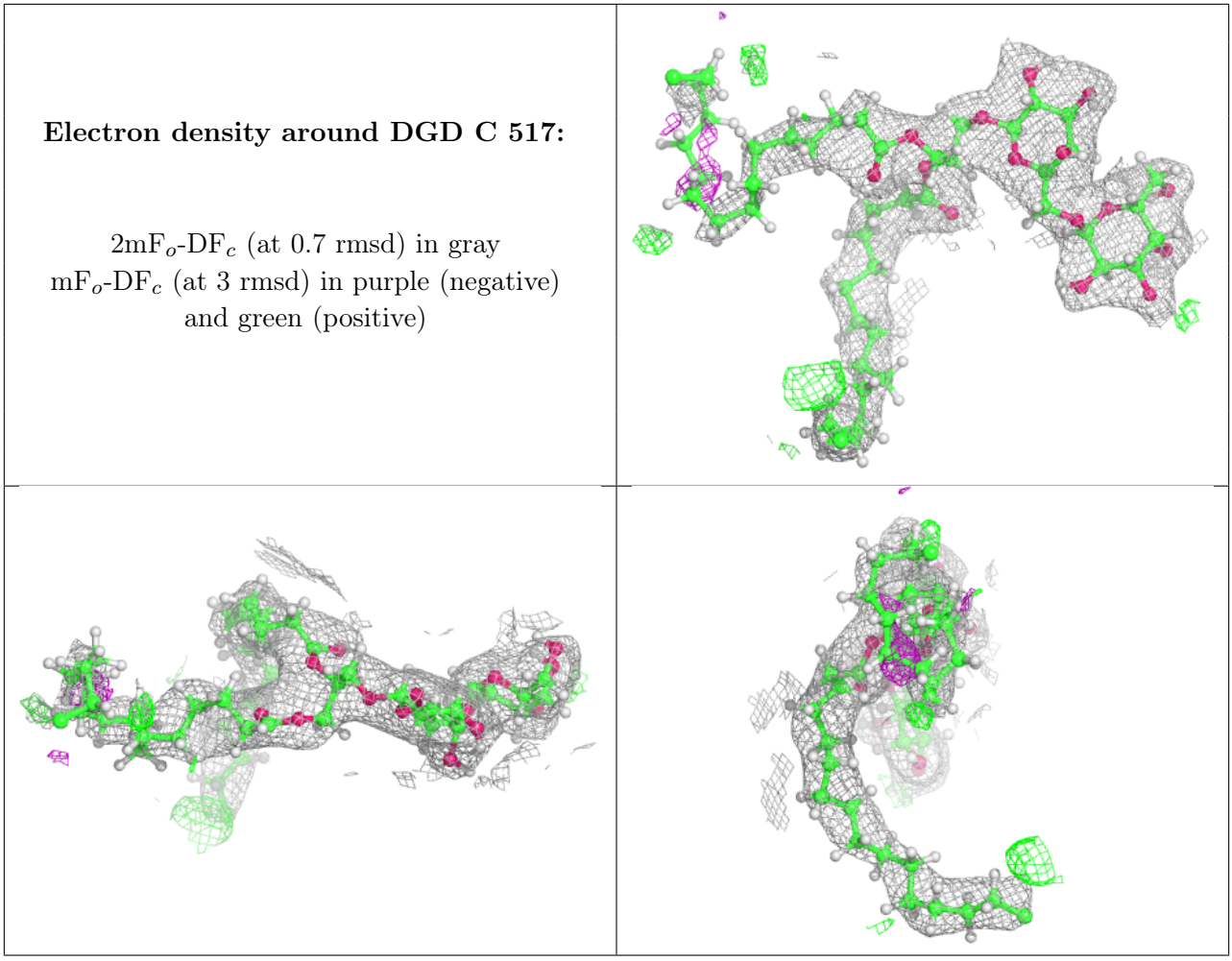






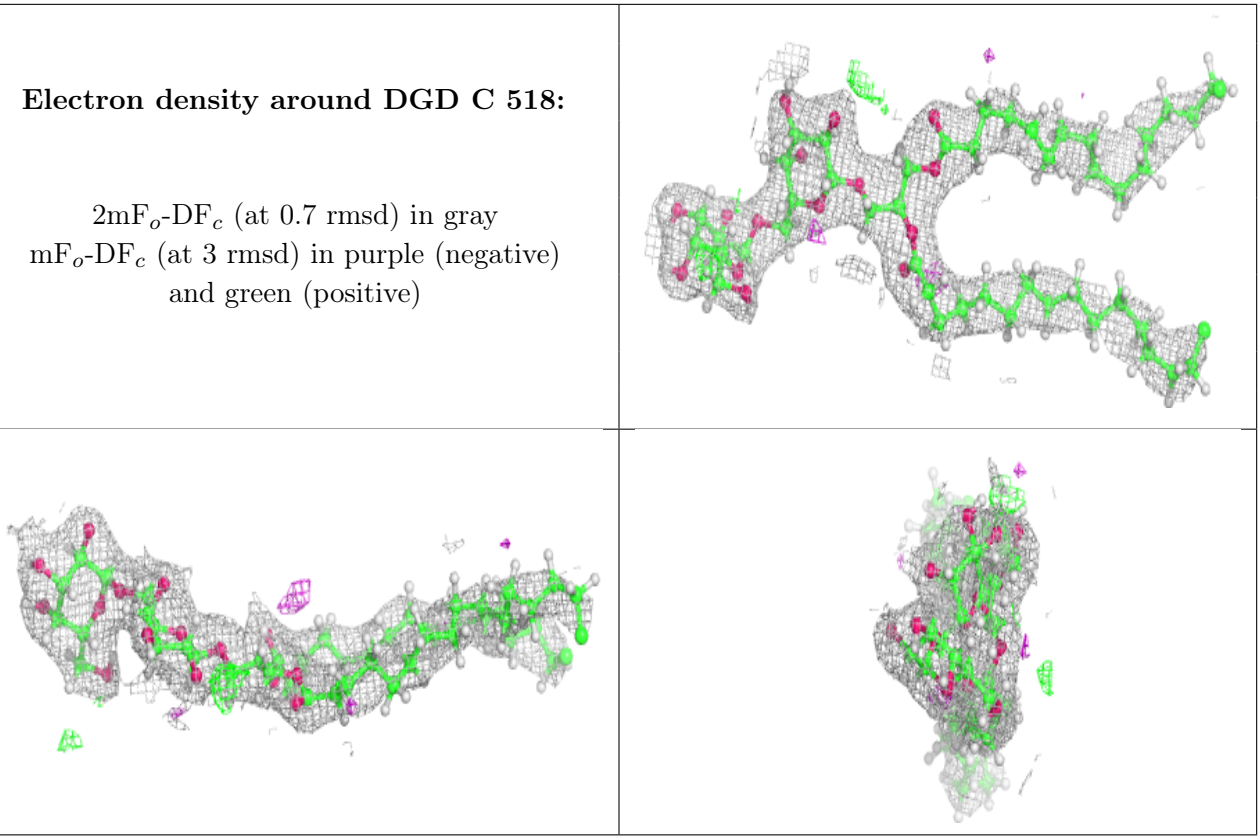
Electron density around DGD C 517:

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



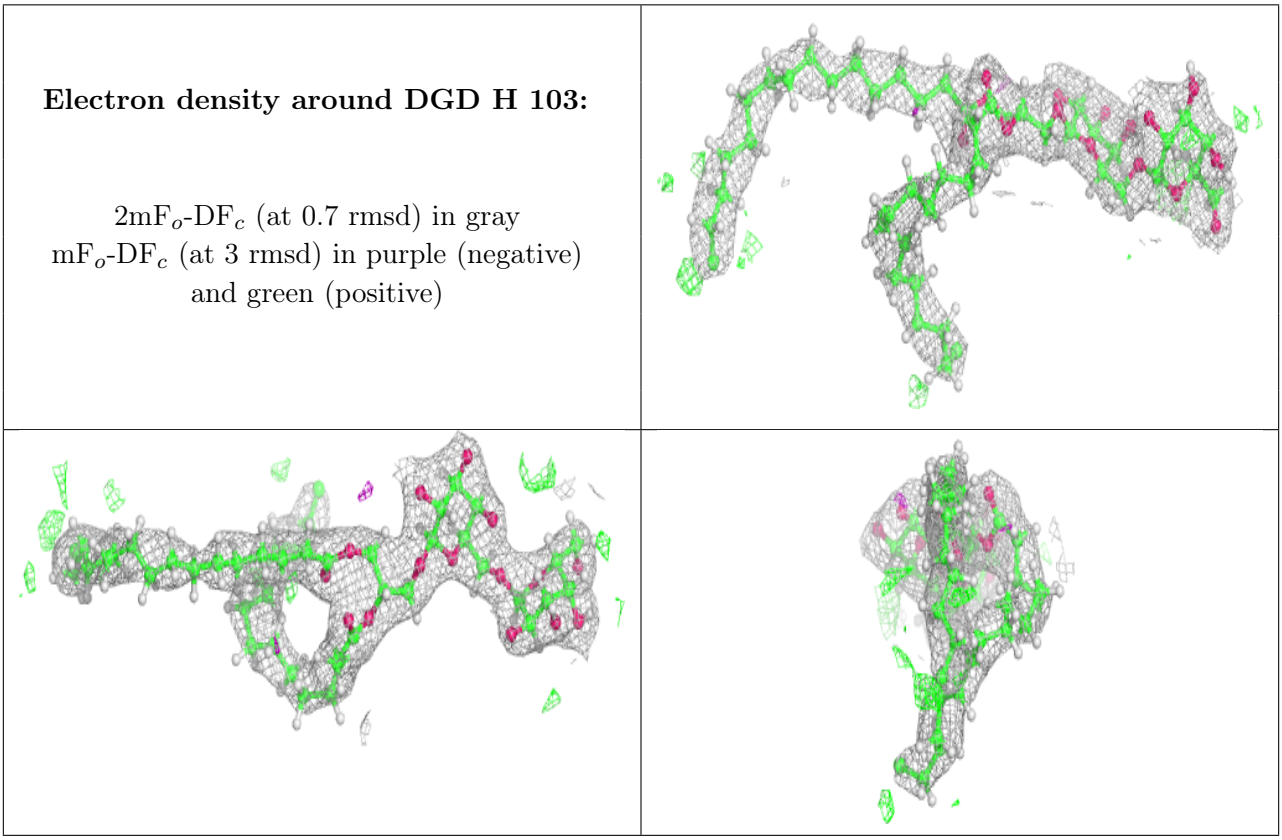
Electron density around DGD C 518:

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



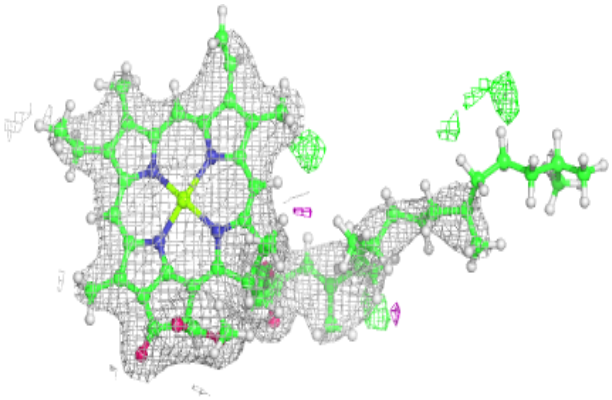
Electron density around DGD H 103:

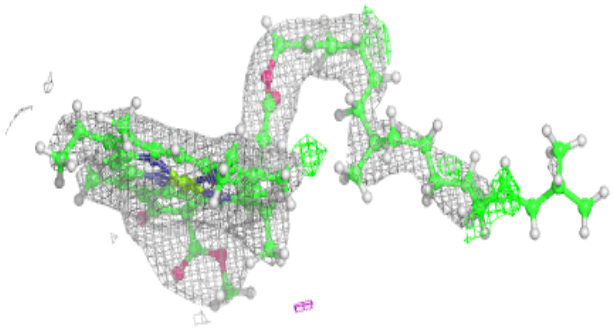
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

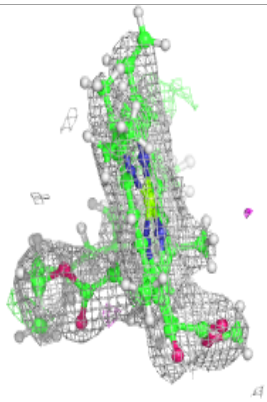


Electron density around CLA a 403:

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

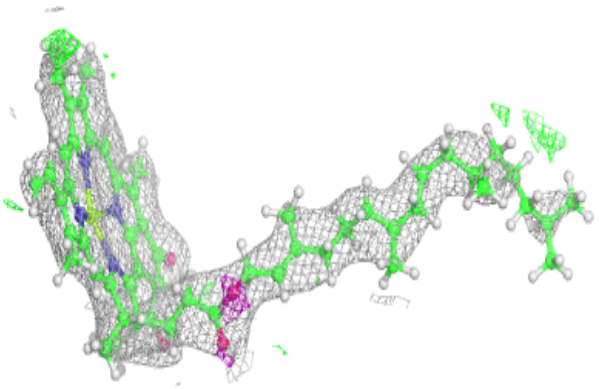


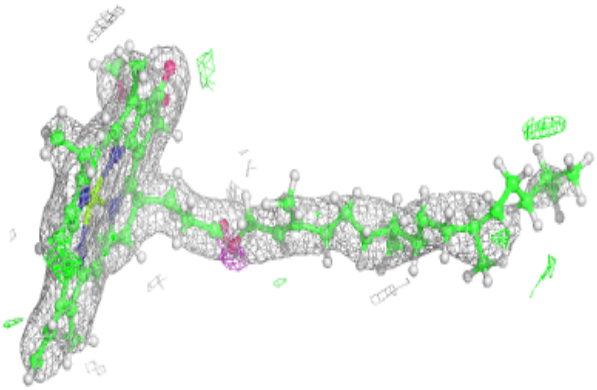


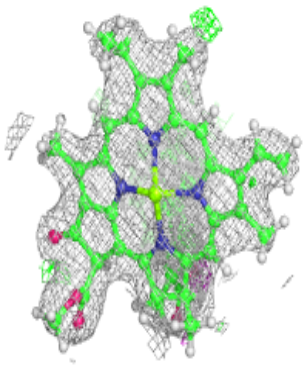


Electron density around CLA B 603:

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

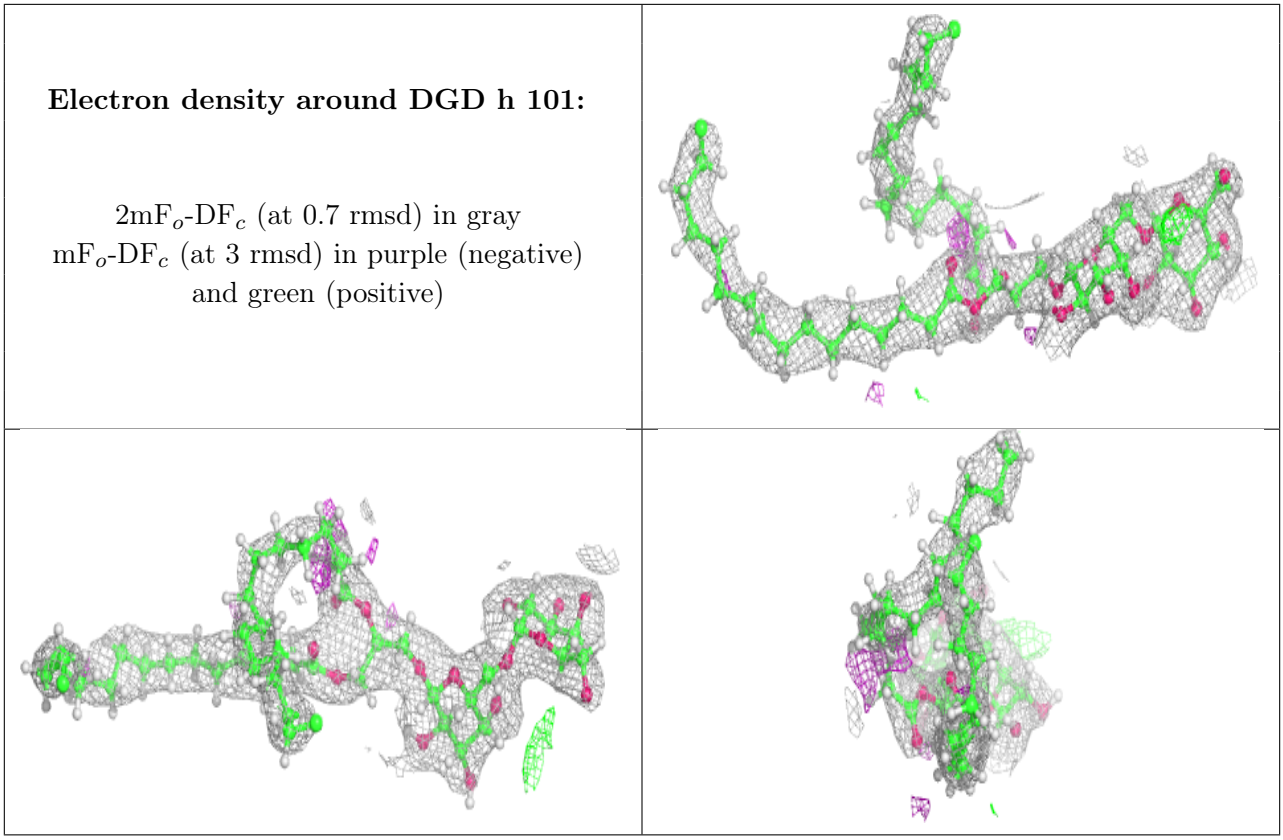






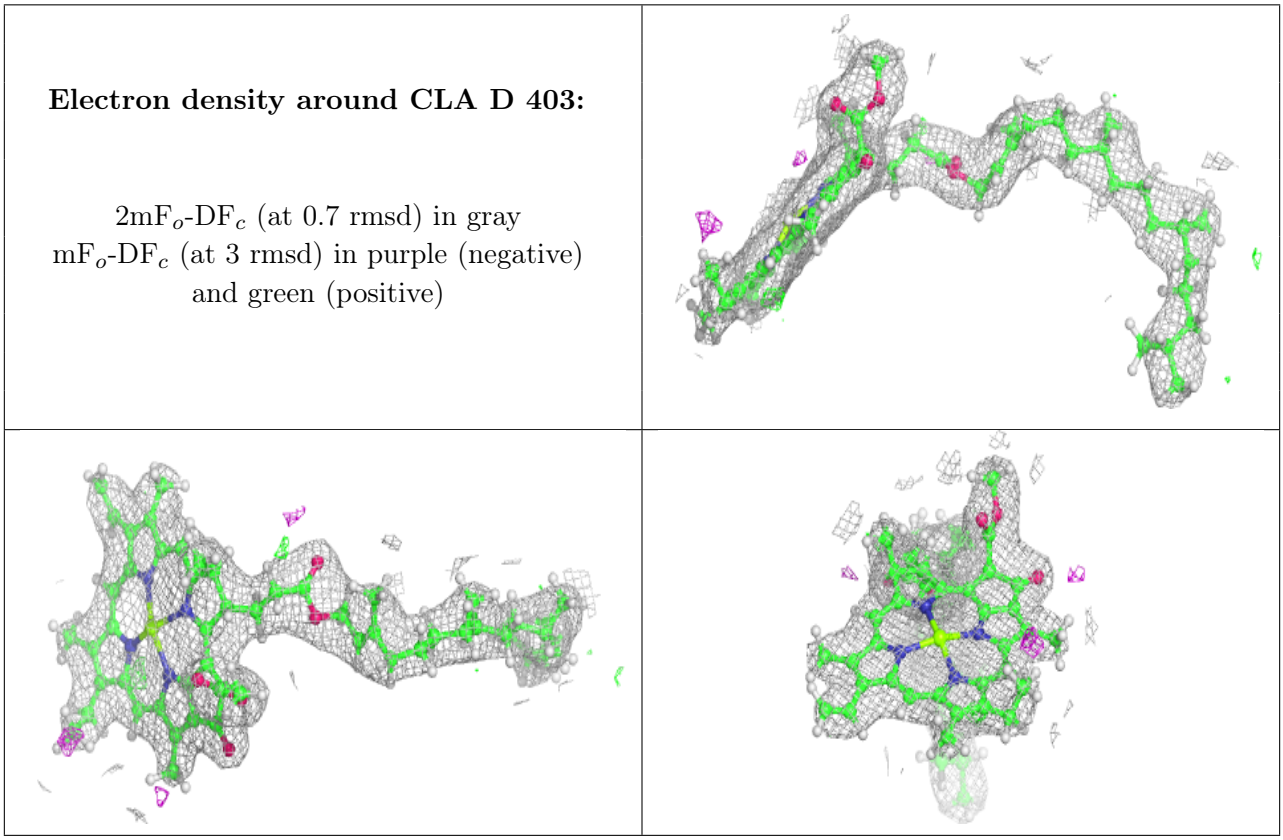
Electron density around DGD h 101:

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



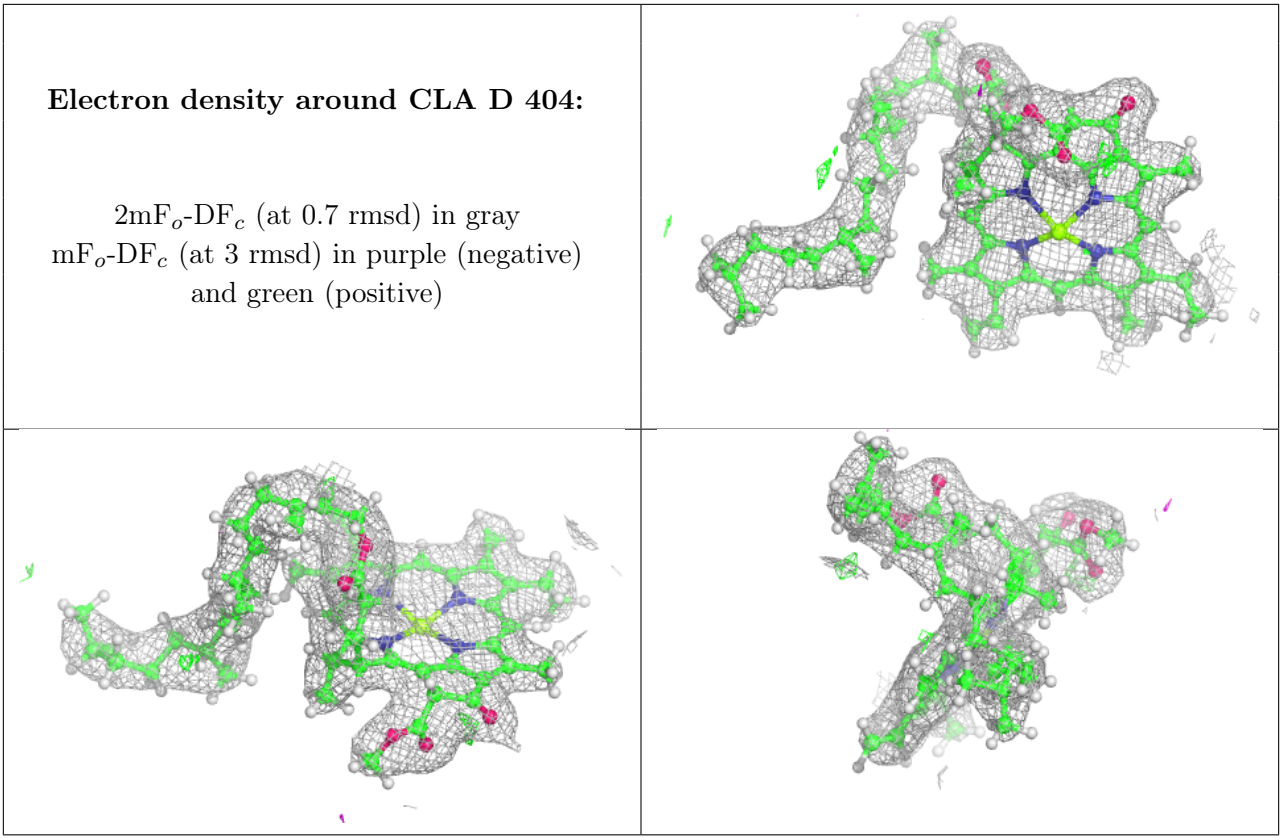
Electron density around CLA D 403:

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



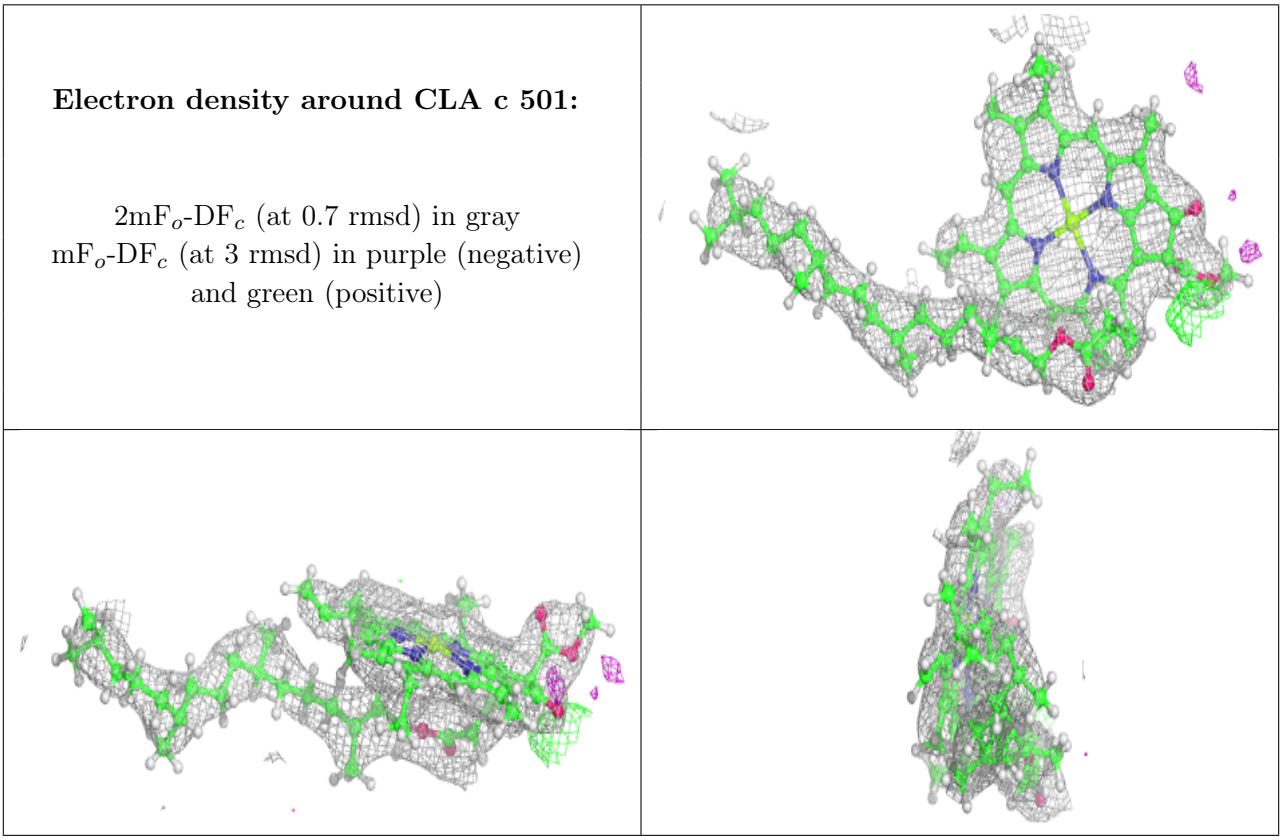
Electron density around CLA D 404:

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



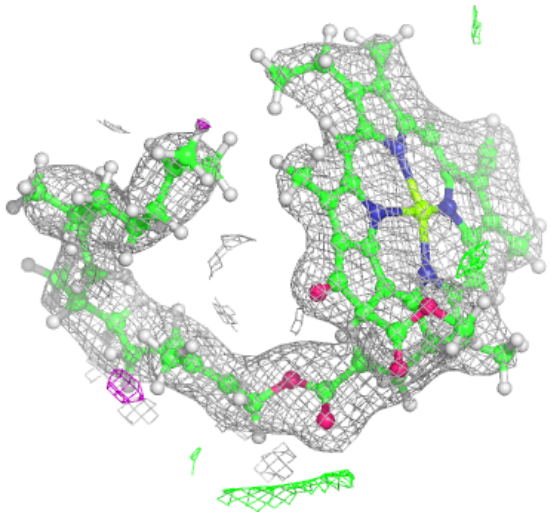
Electron density around CLA c 501:

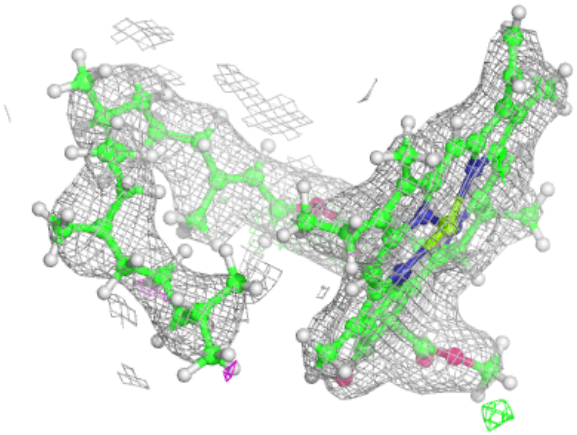
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

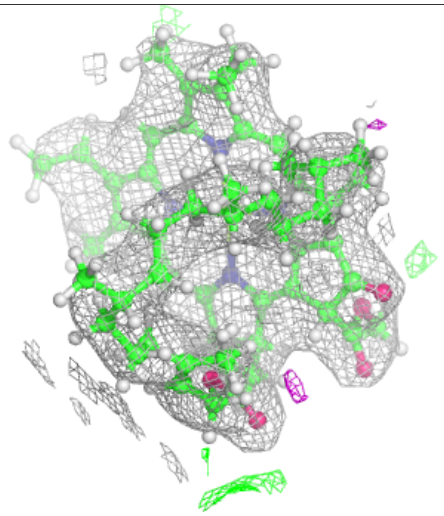


Electron density around CLA C 503:

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

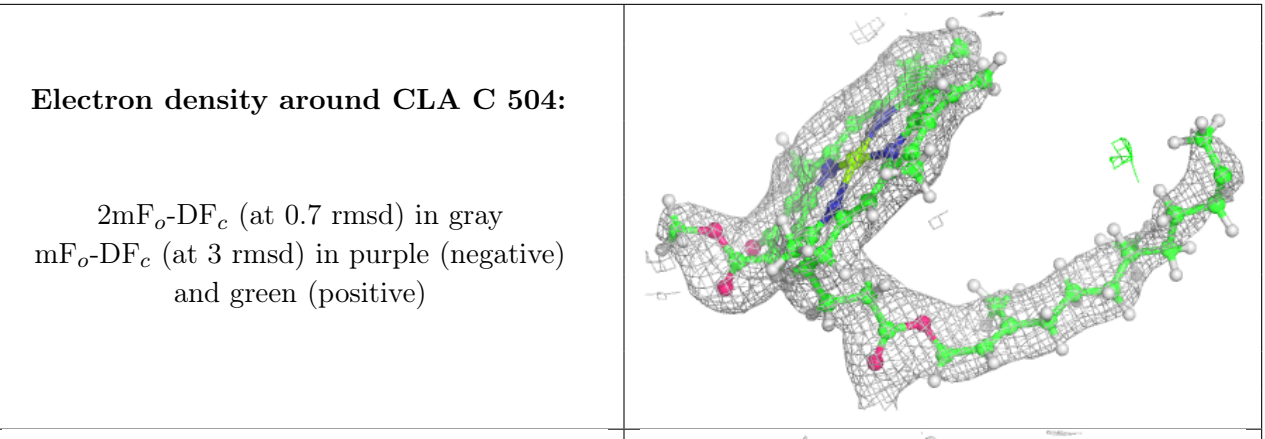






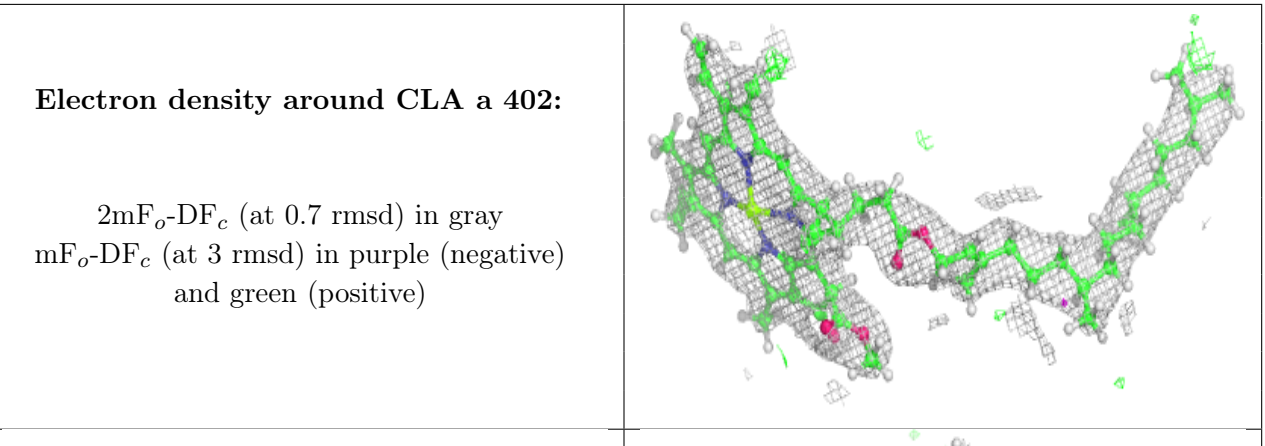
Electron density around CLA C 504:

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



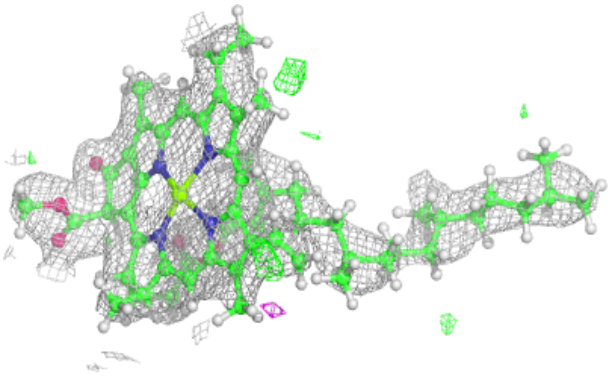
Electron density around CLA a 402:

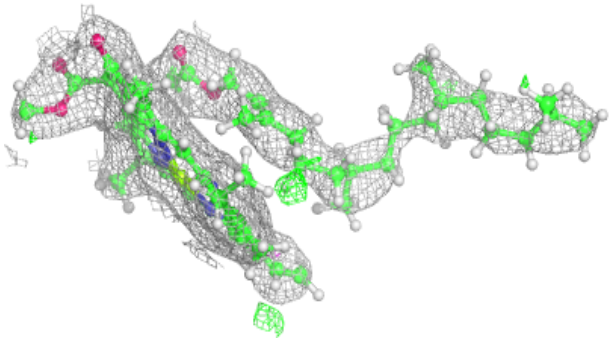
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

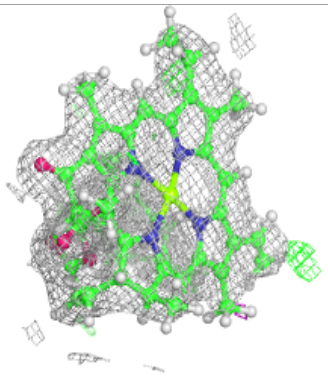


Electron density around CLA C 505:

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

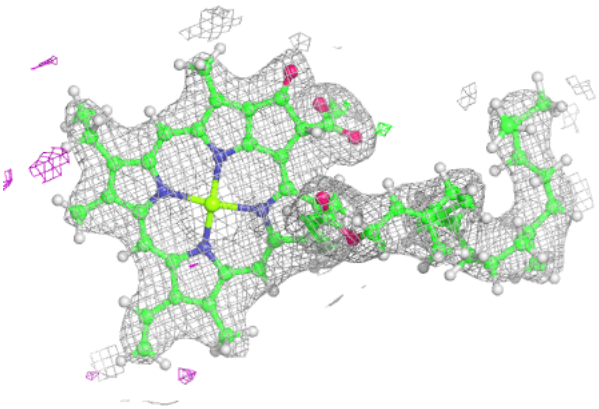


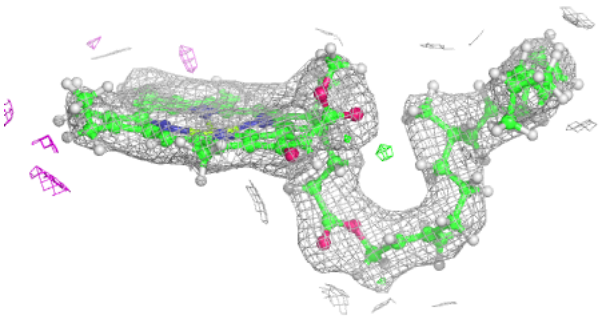


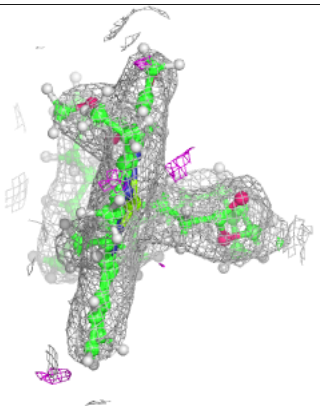


Electron density around CLA B 611:

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

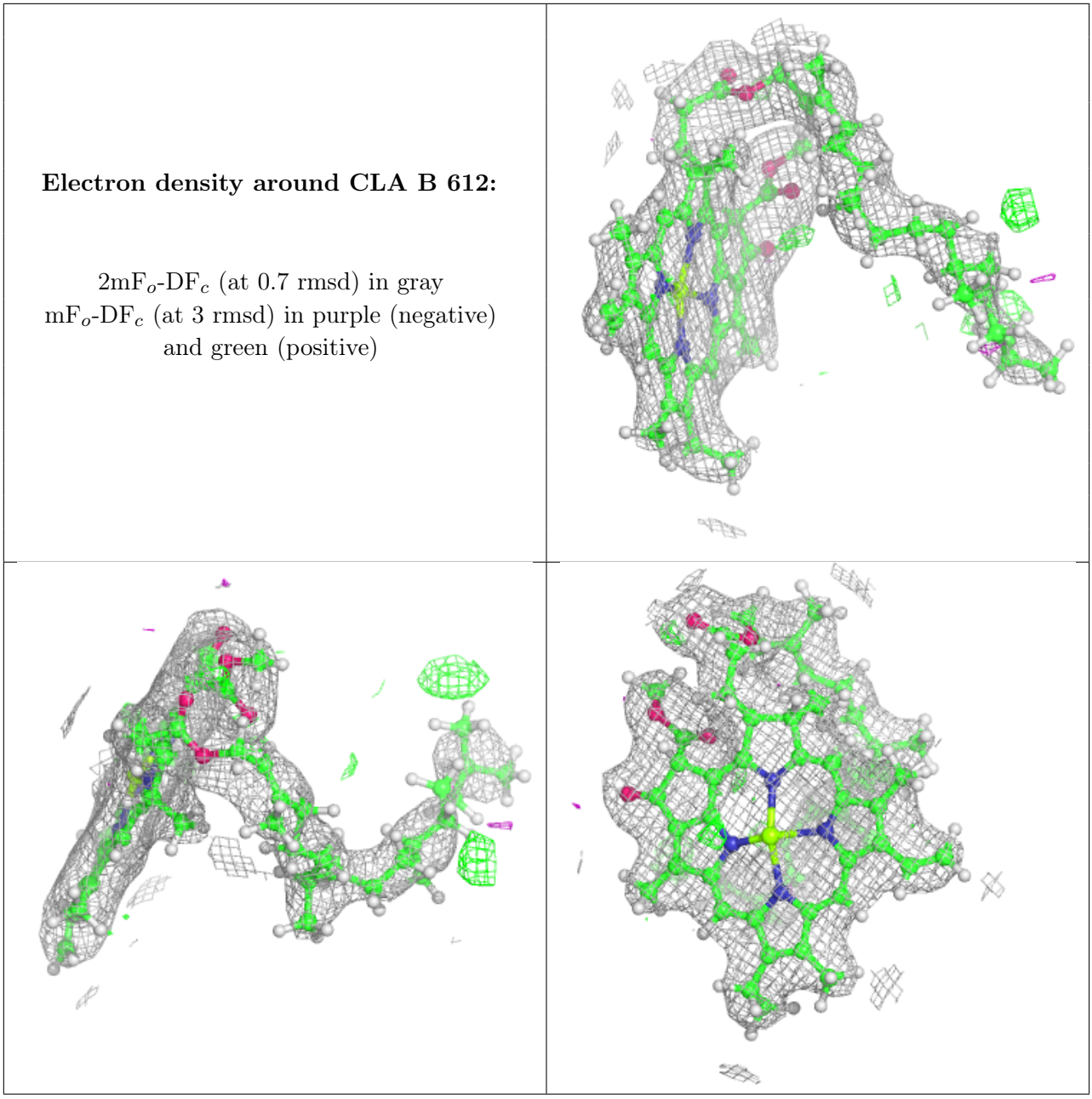






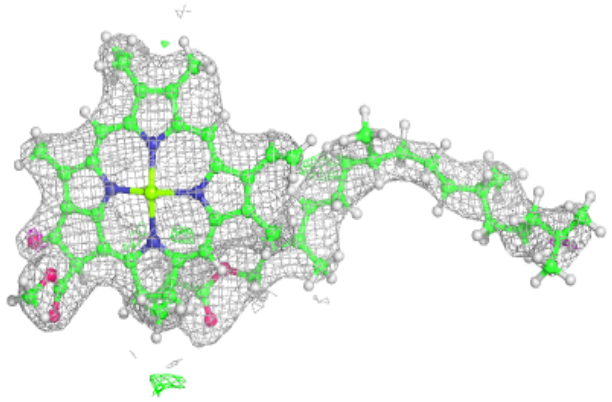
Electron density around CLA B 612:

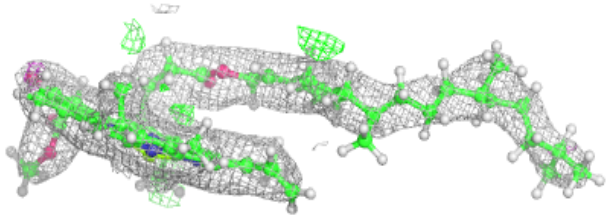
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

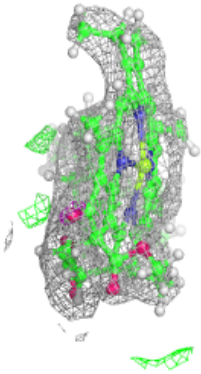


Electron density around CLA B 602:

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

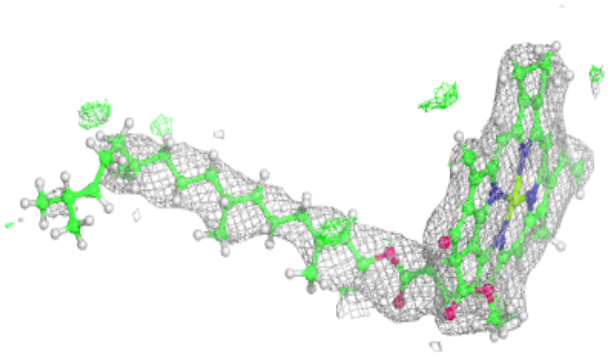


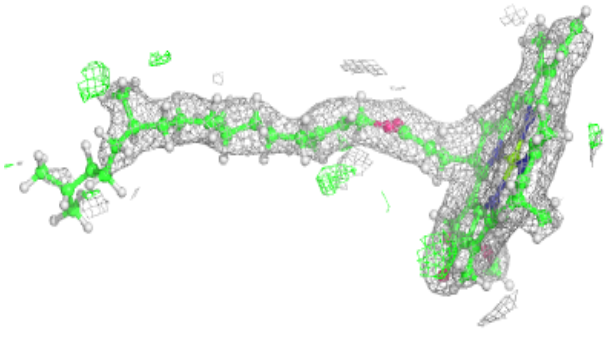


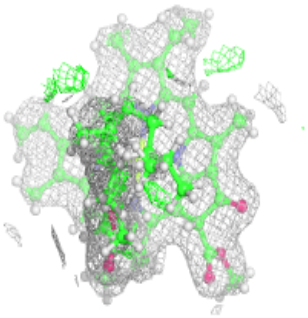


Electron density around CLA b 604:

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

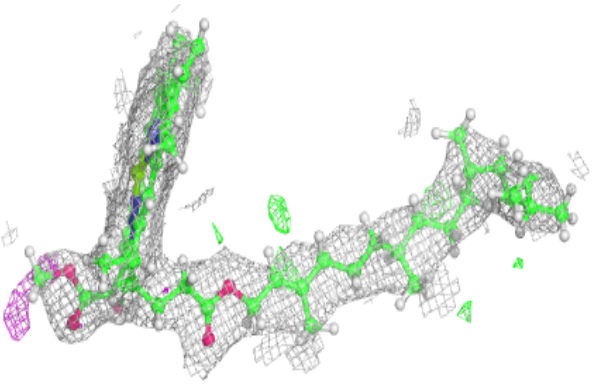


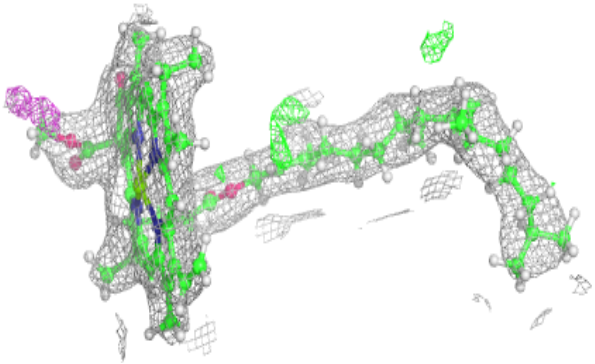


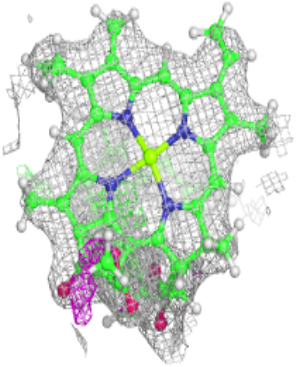


Electron density around CLA b 605:

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

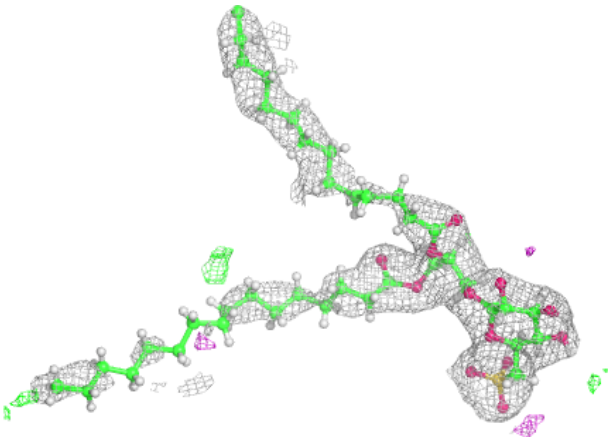


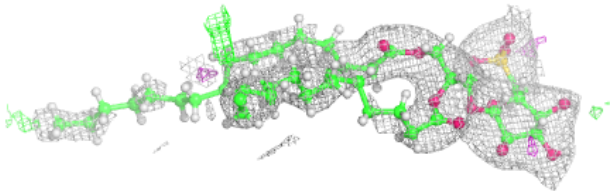


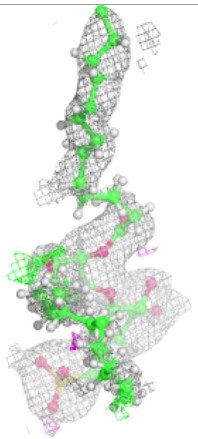


Electron density around SQD A 410:

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

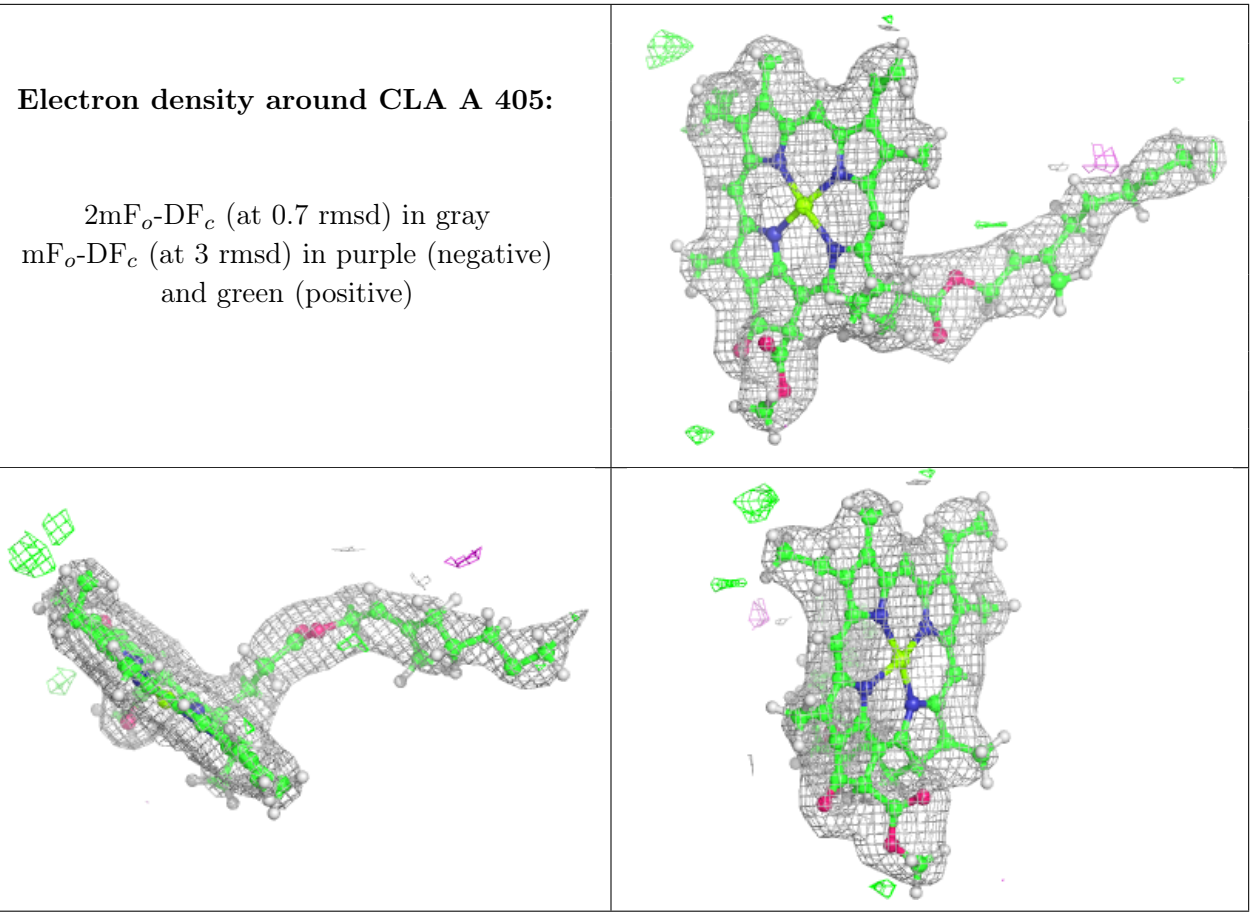






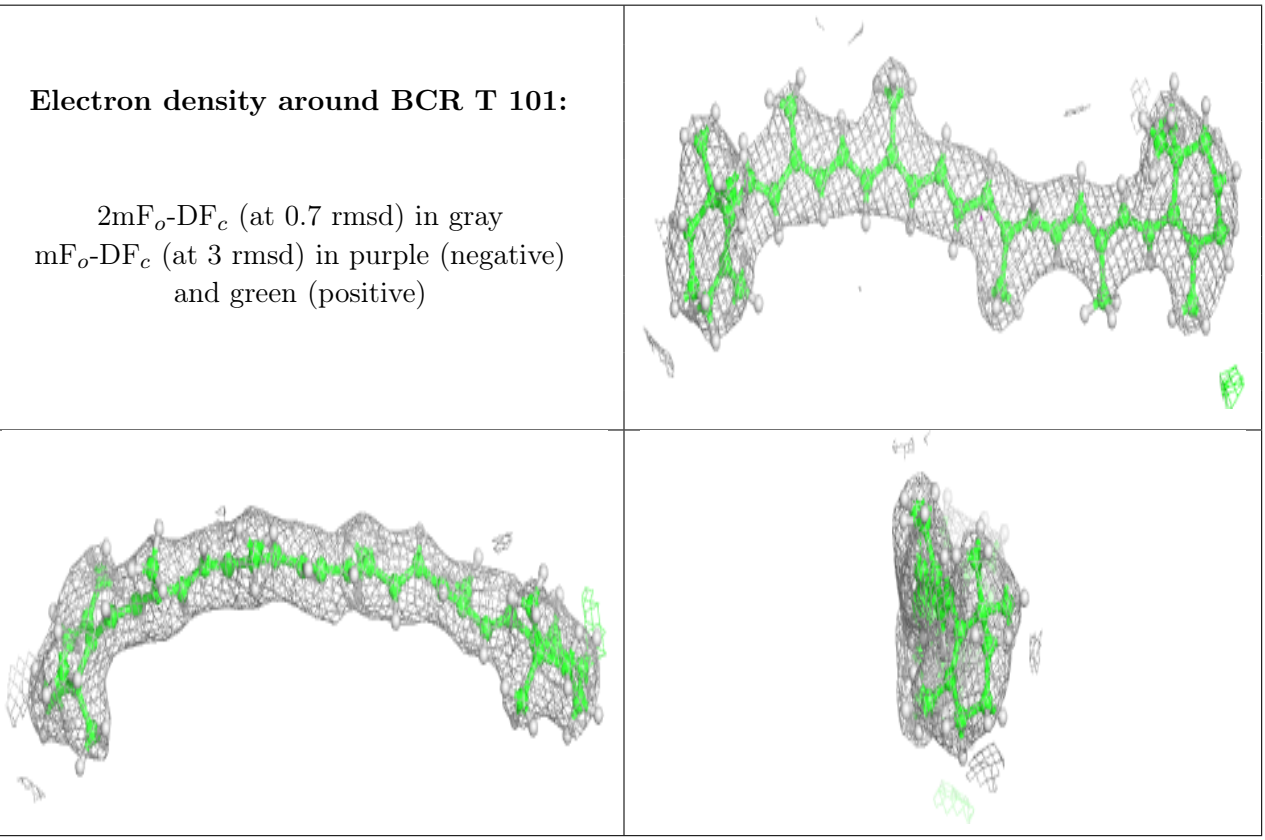
Electron density around CLA A 405:

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



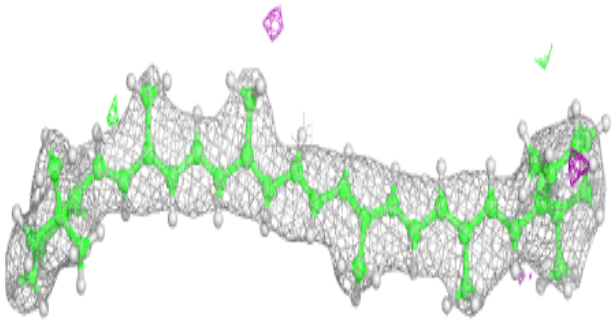
Electron density around BCR T 101:

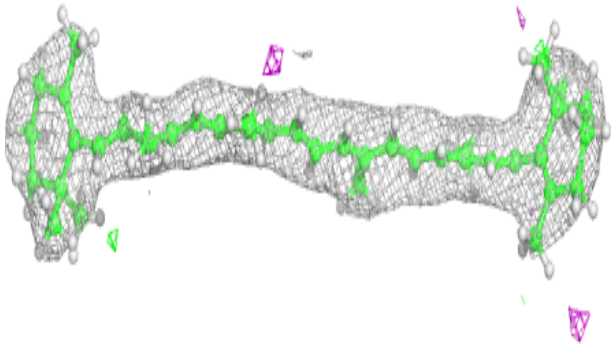
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

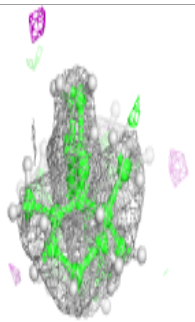


Electron density around BCR a 406:

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

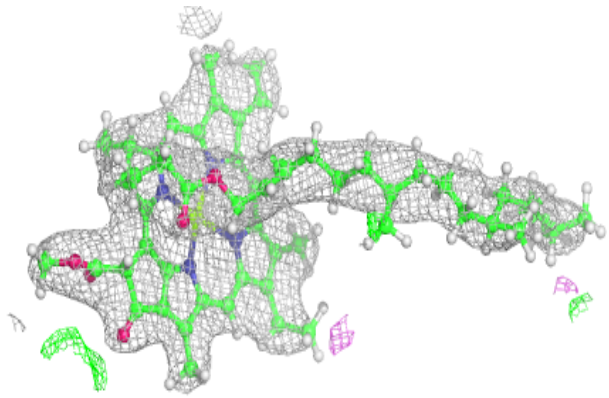


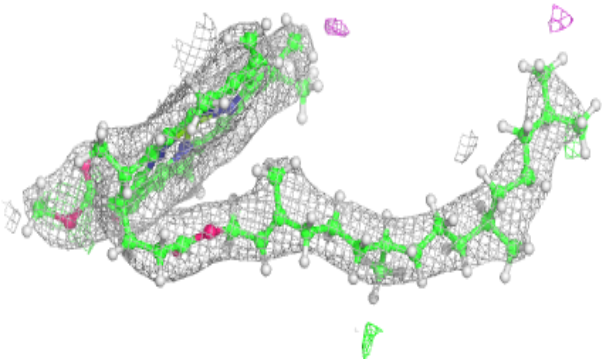


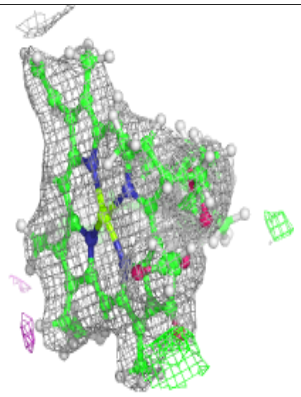


Electron density around CLA b 608:

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

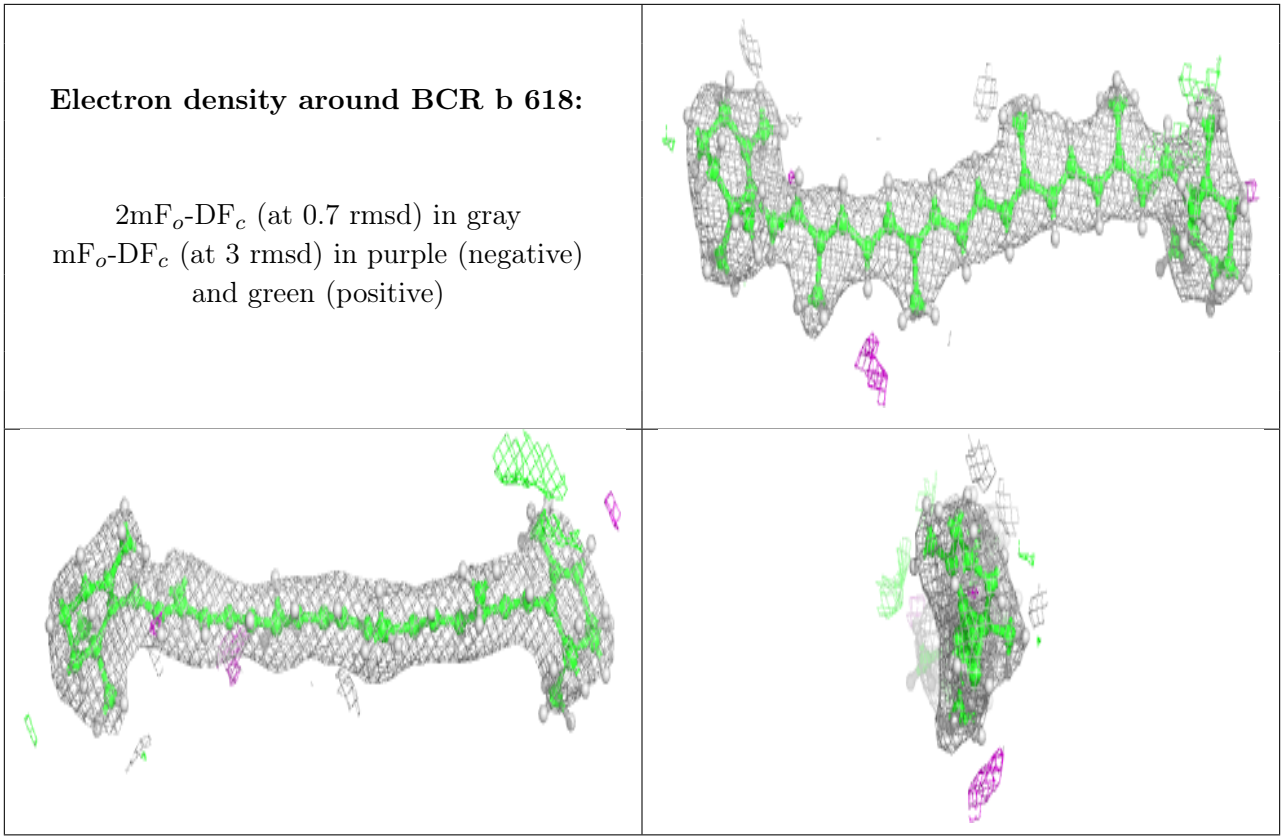






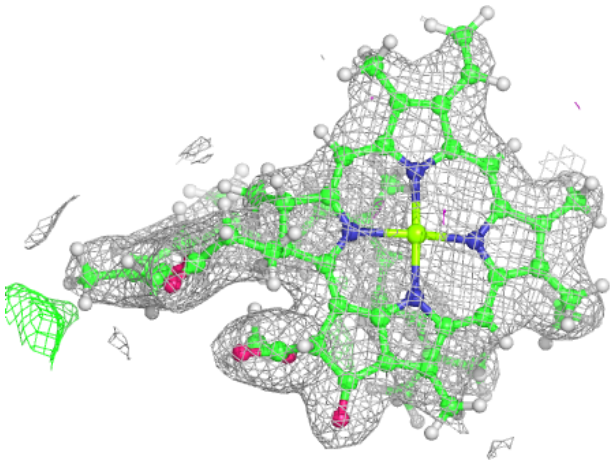
Electron density around BCR b 618:

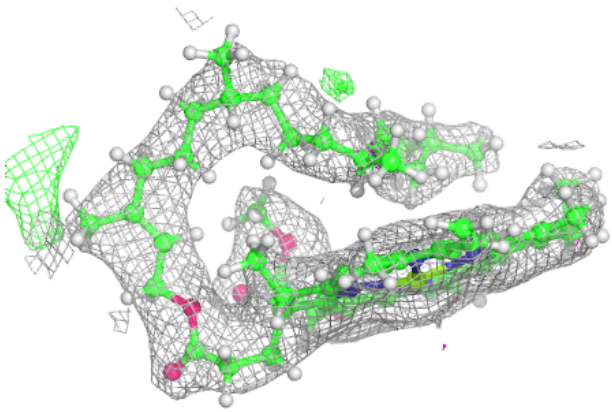
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

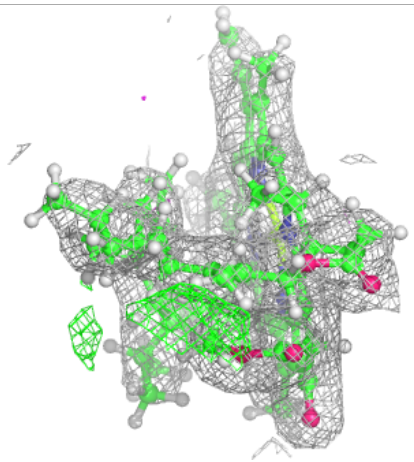


Electron density around CLA C 510:

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

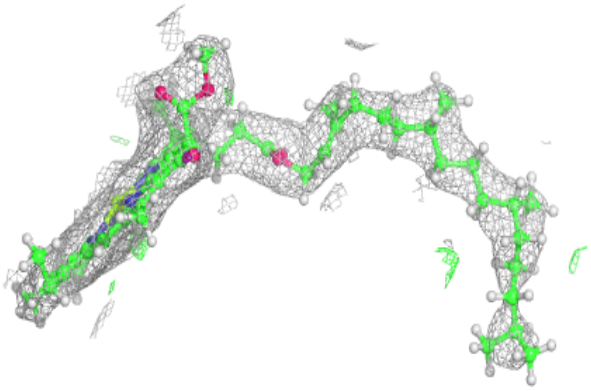


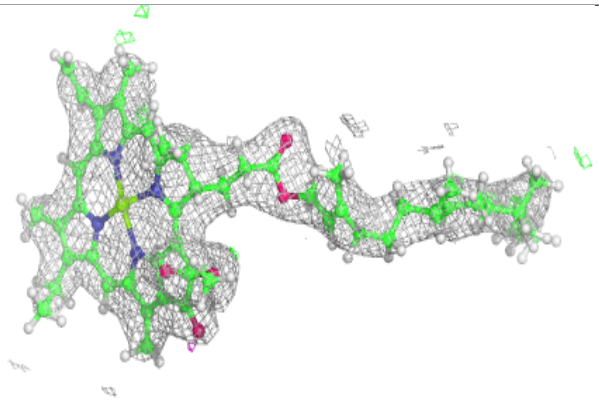


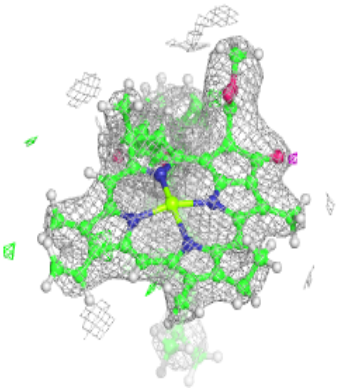


Electron density around CLA d 403:

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

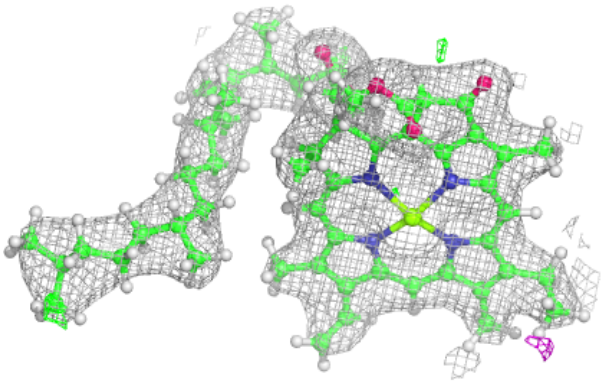


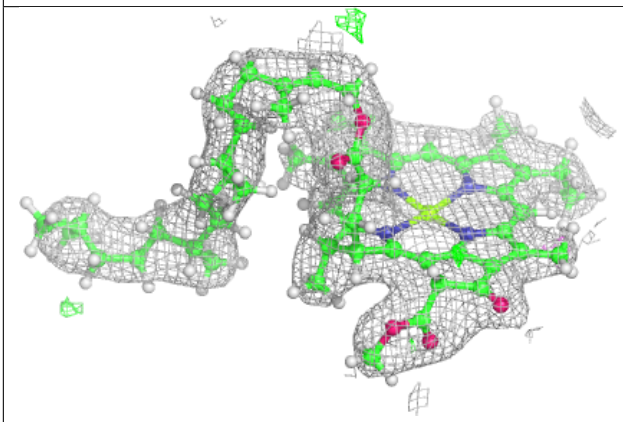


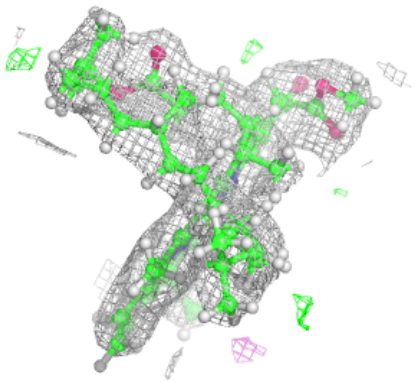


Electron density around CLA d 404:

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

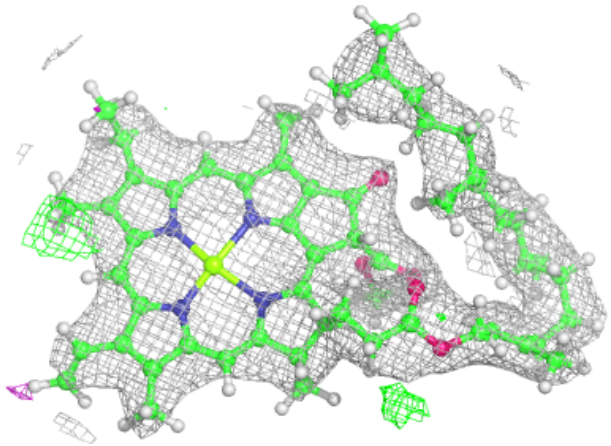


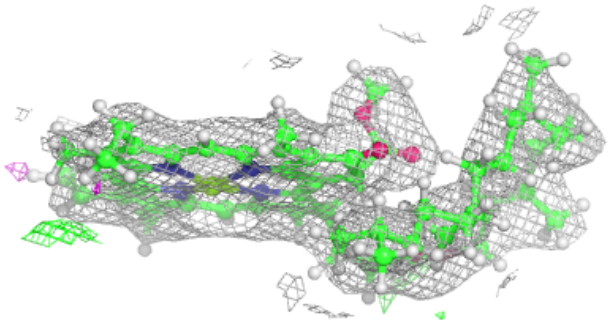


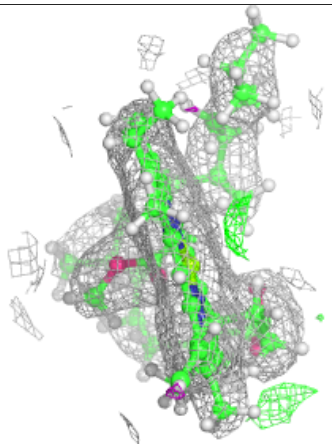


Electron density around CLA b 610:

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

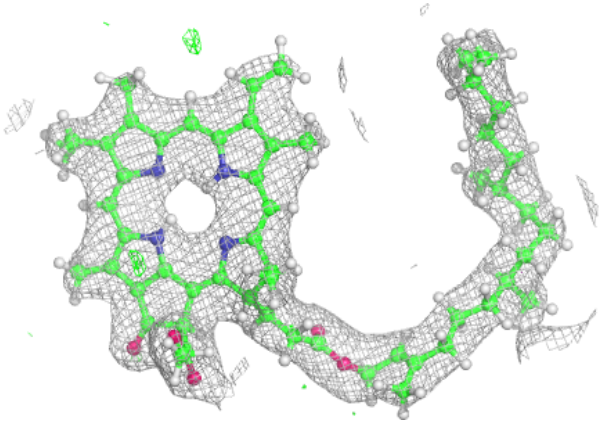


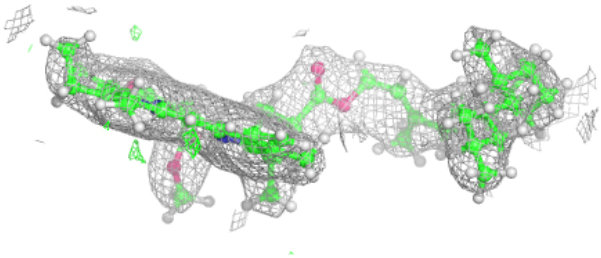


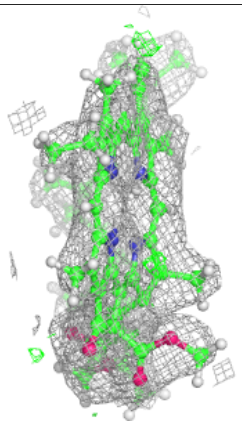


Electron density around PHO a 404:

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

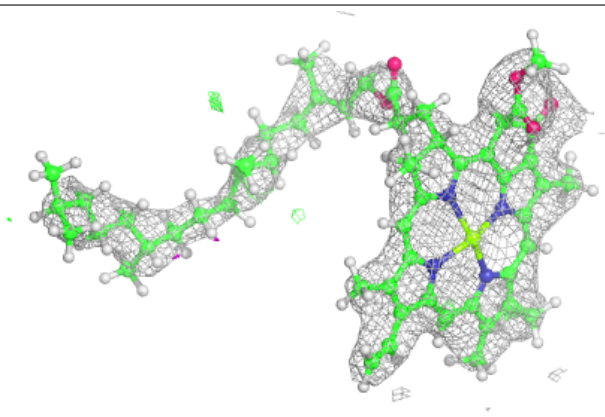


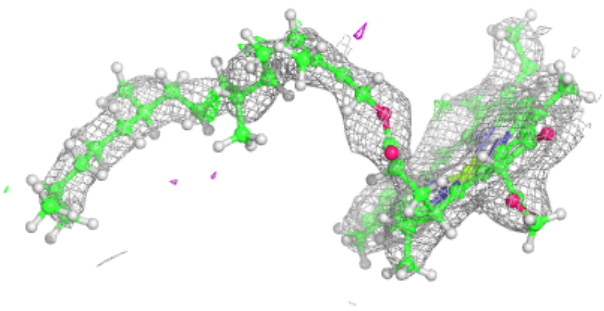


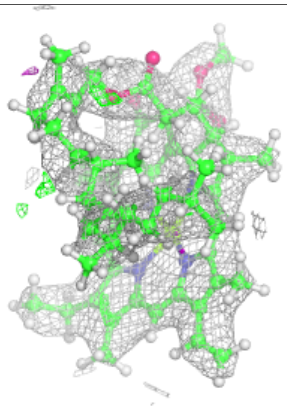


Electron density around CLA C 511:

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

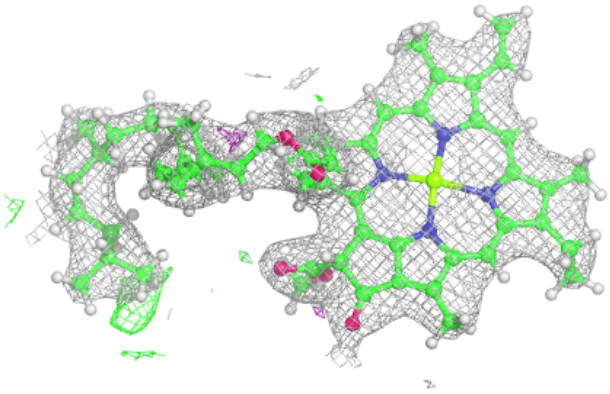


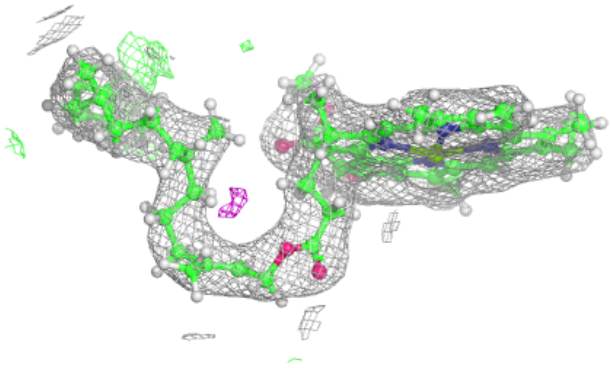


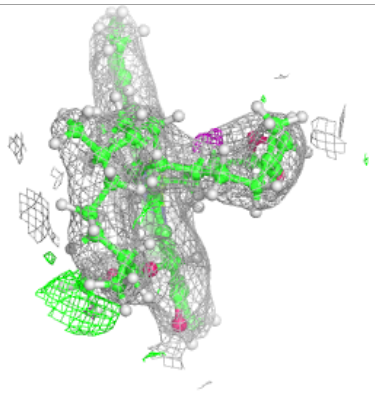


Electron density around CLA b 612:

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

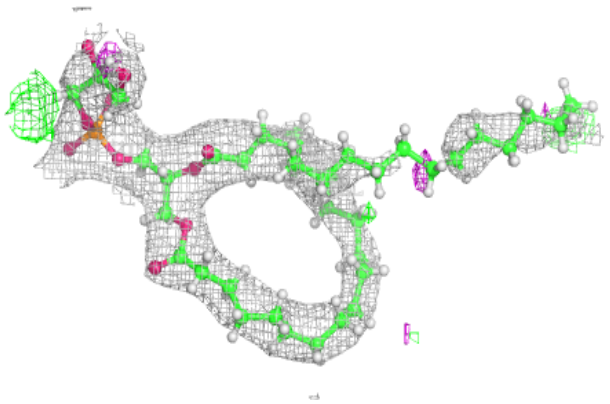


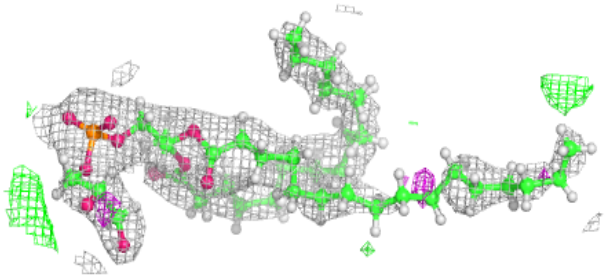


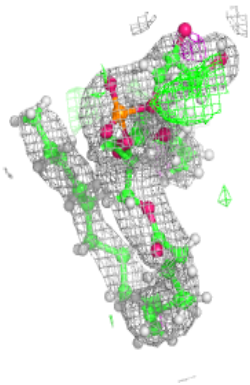


Electron density around LHG b 623:

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

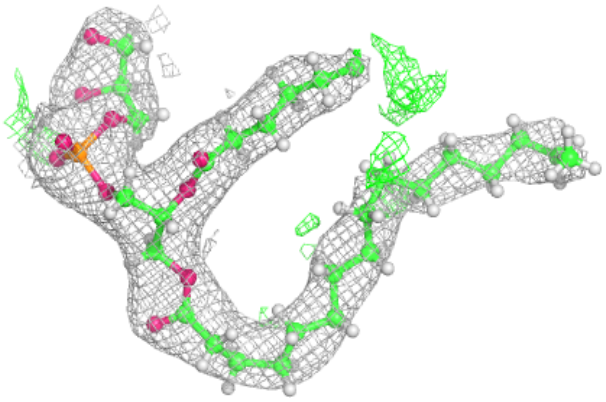


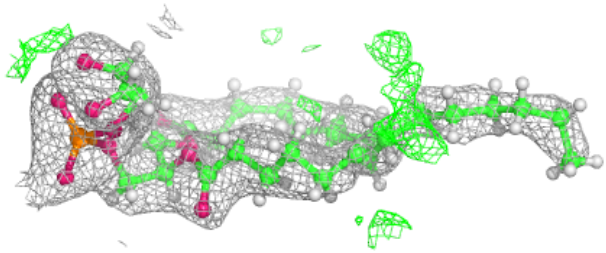


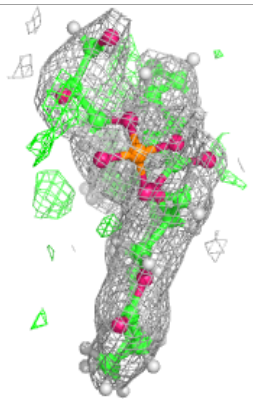


Electron density around LHG d 409:

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

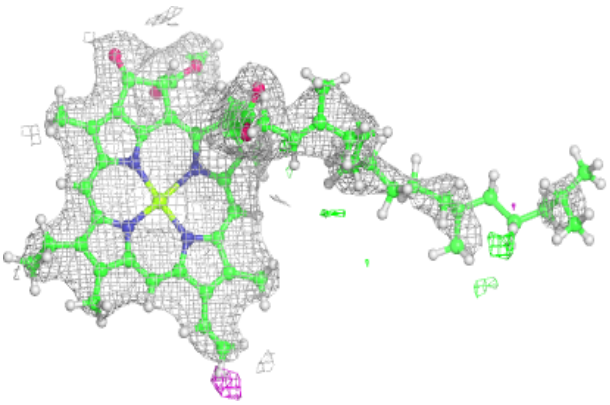


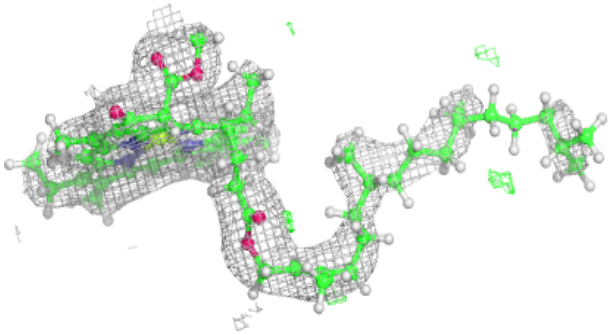


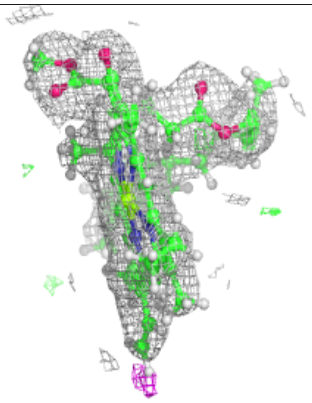


Electron density around CLA A 403:

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

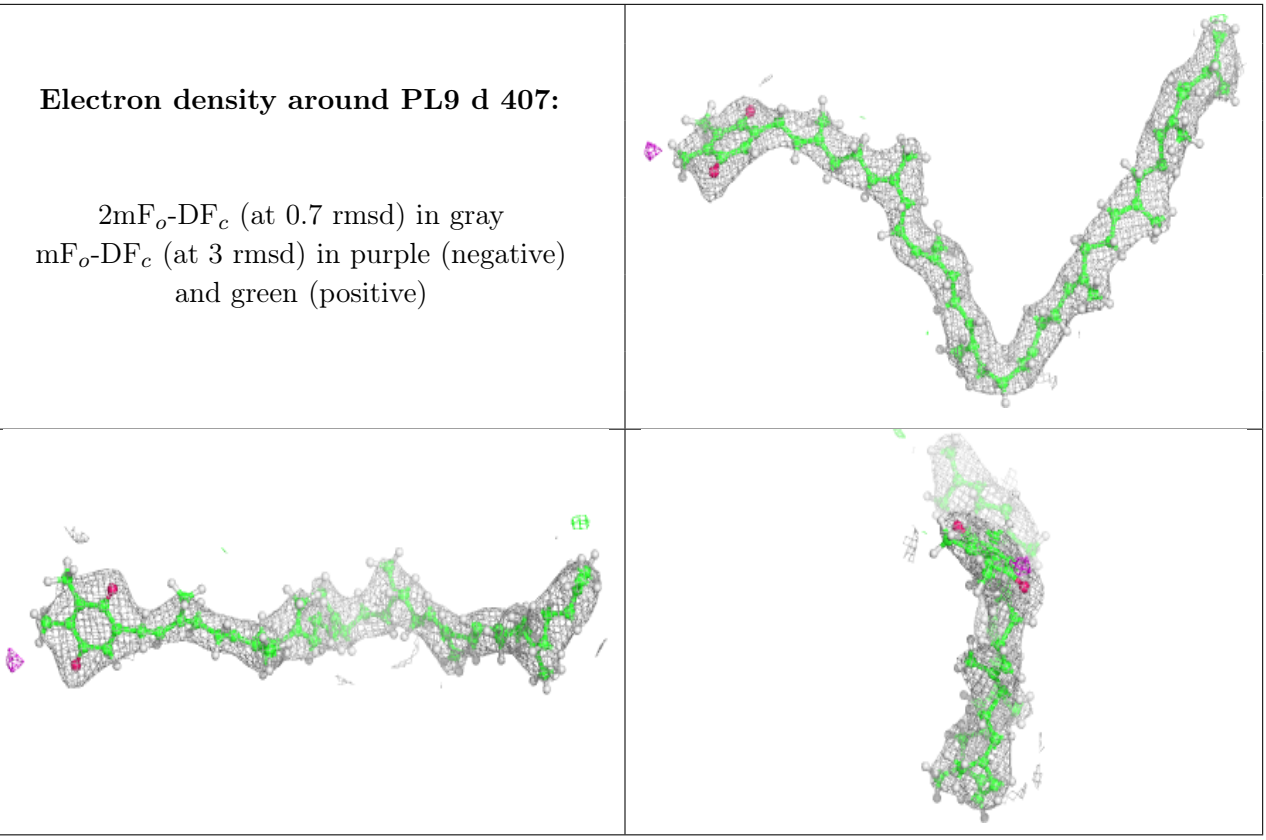






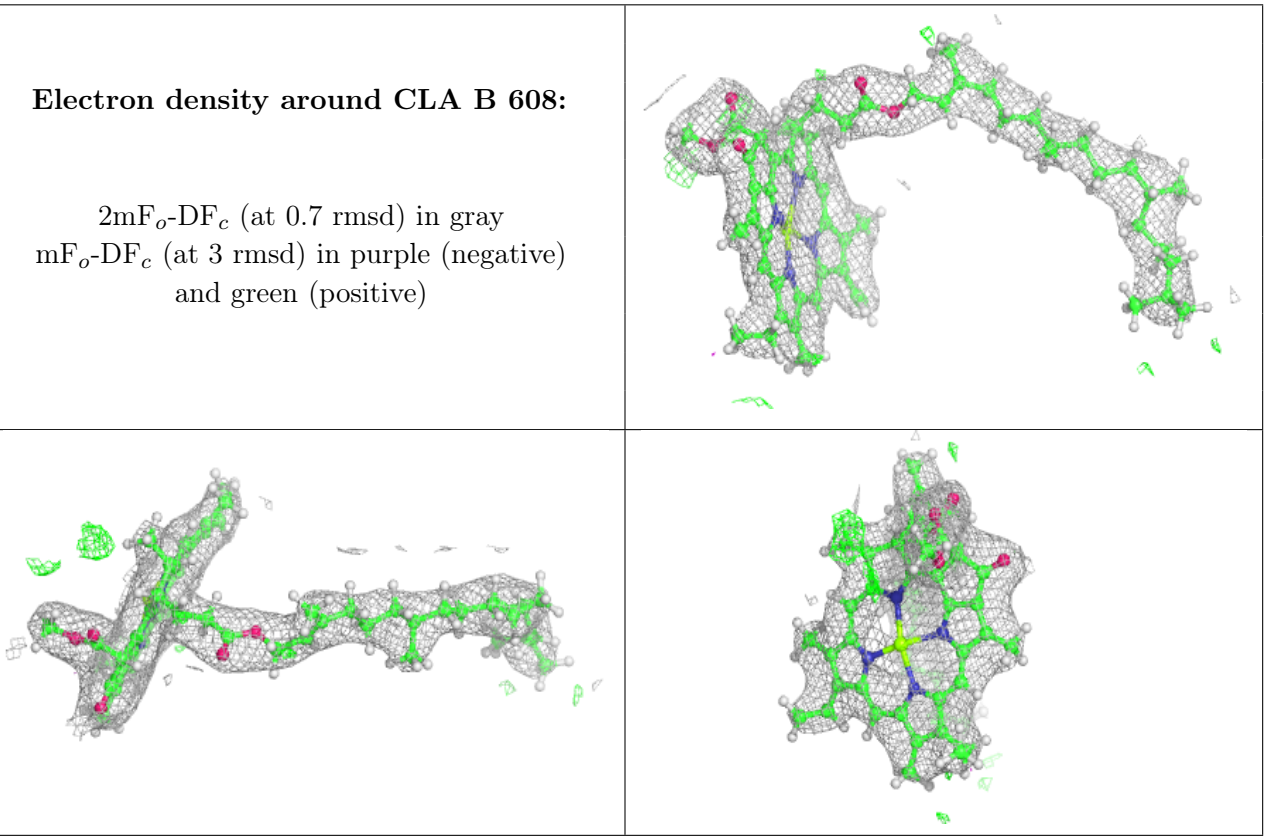
Electron density around PL9 d 407:

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



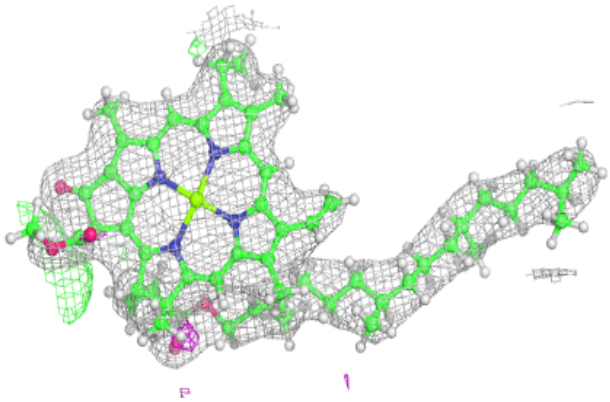
Electron density around CLA B 608:

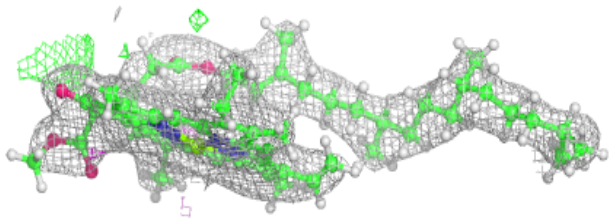
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

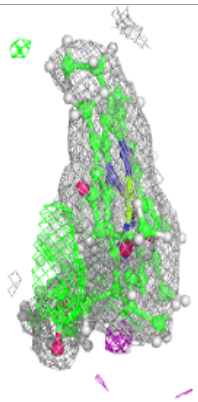


Electron density around CLA C 501:

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

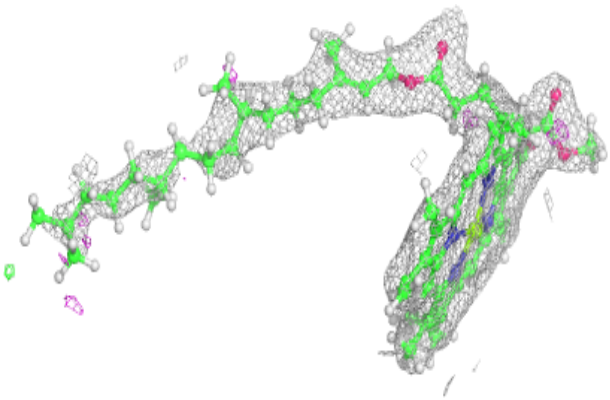


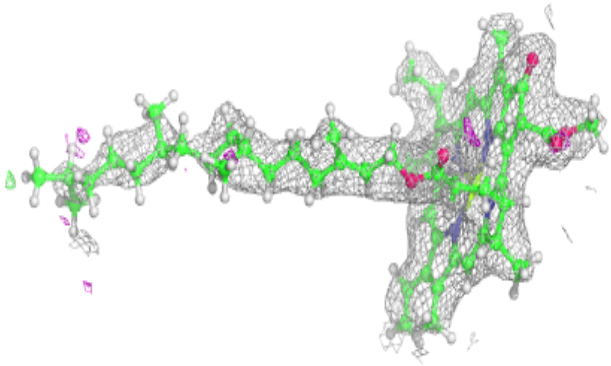


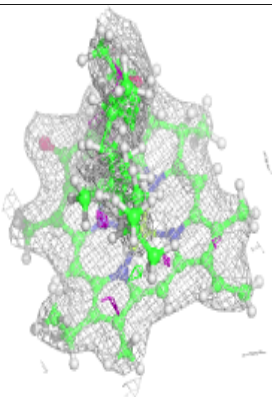


Electron density around CLA b 607:

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

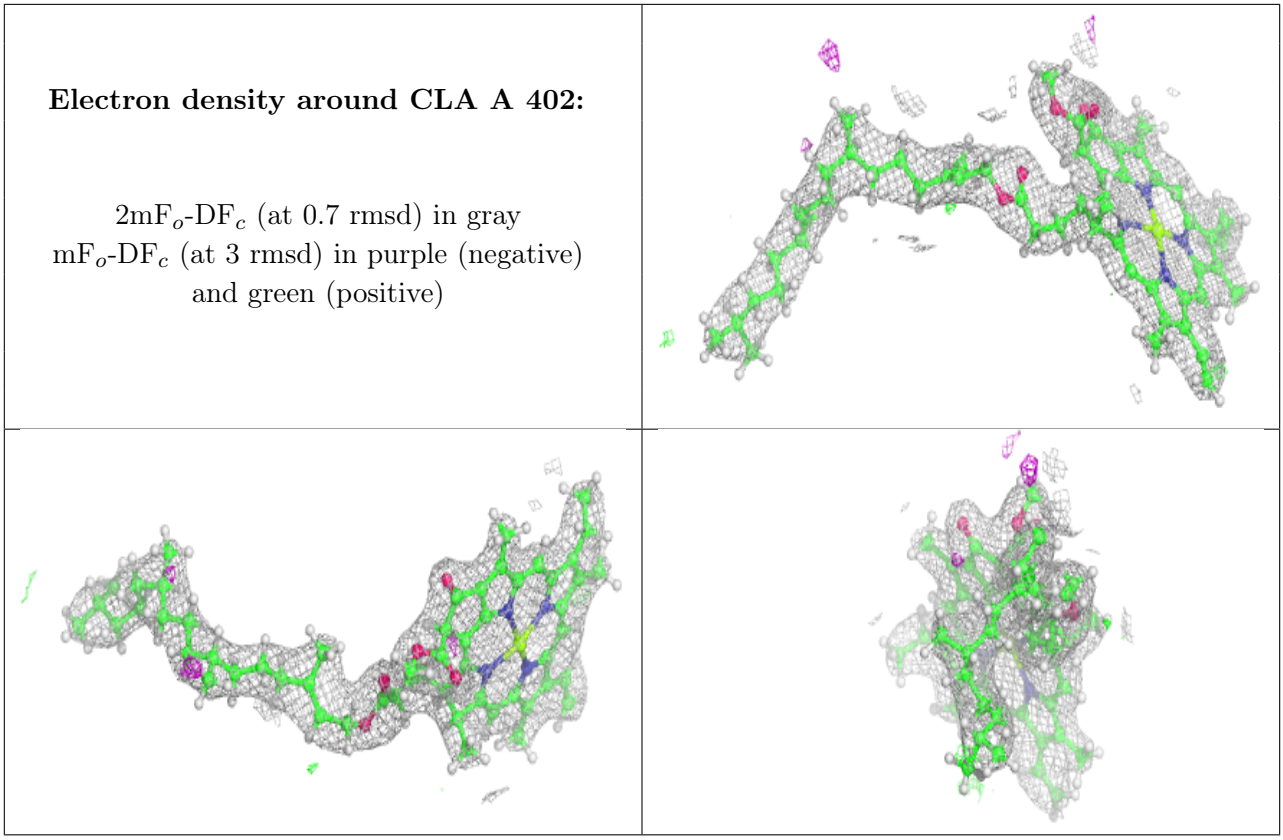






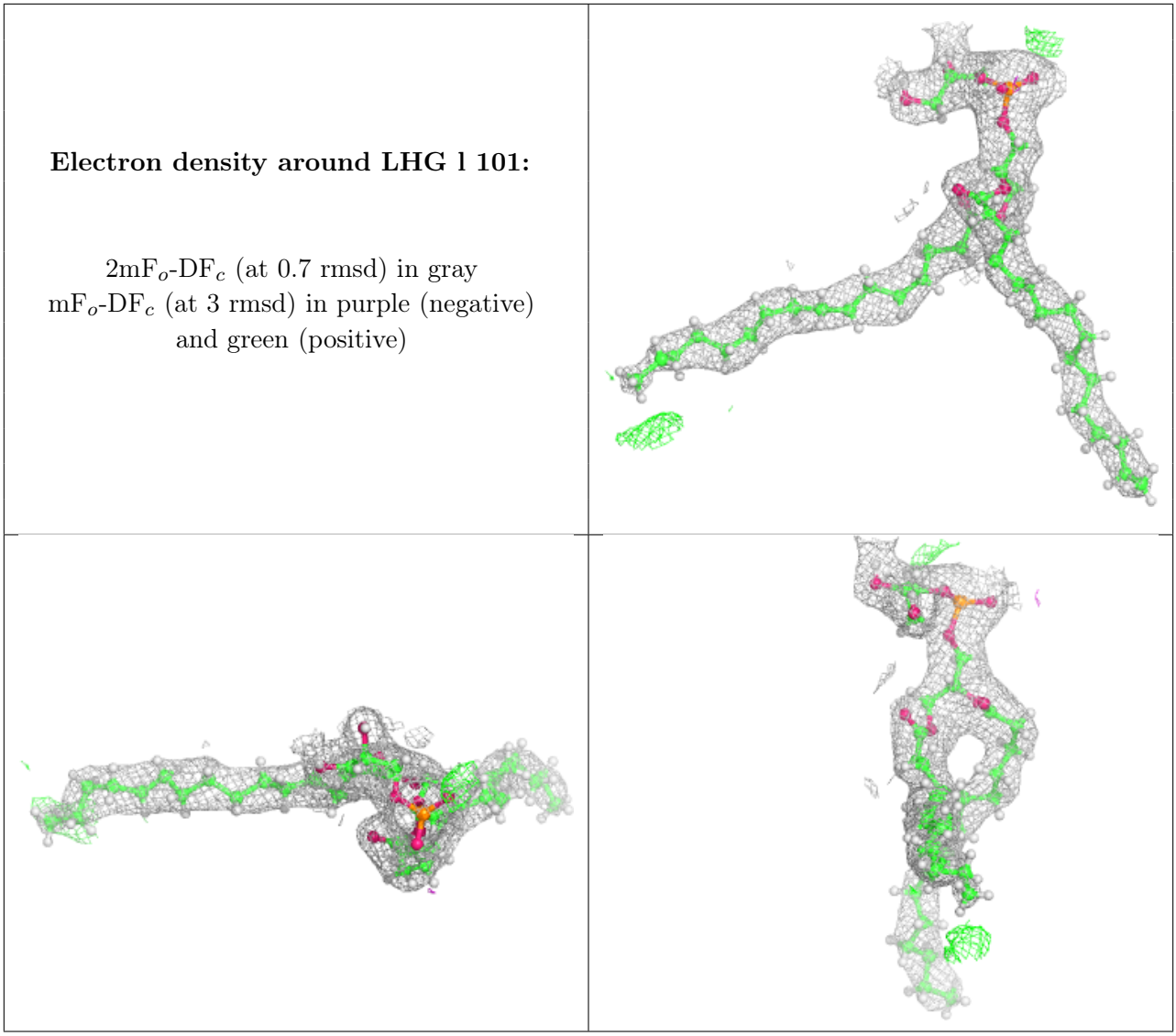
Electron density around CLA A 402:

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



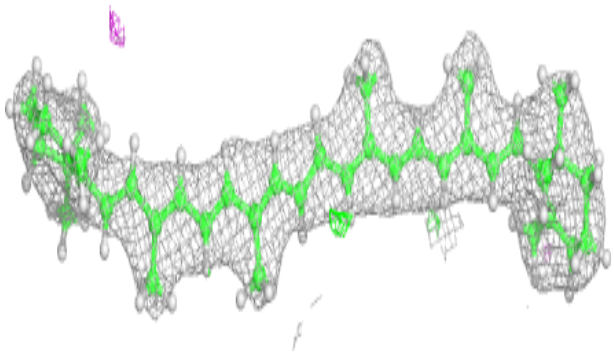
Electron density around LHG l 101:

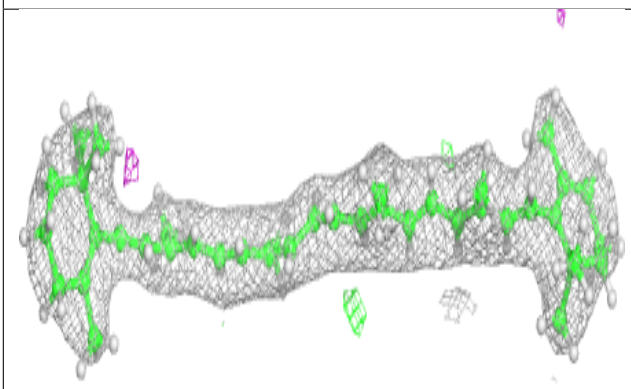
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

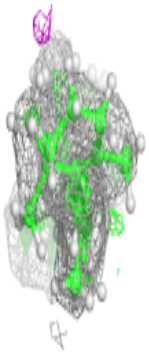


Electron density around BCR I 101:

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

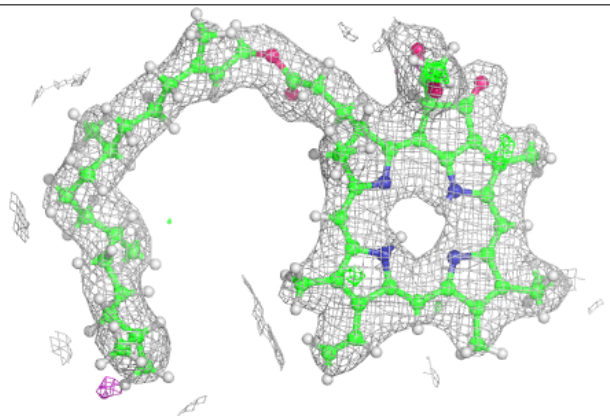


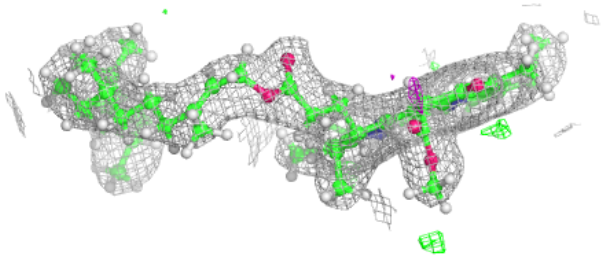


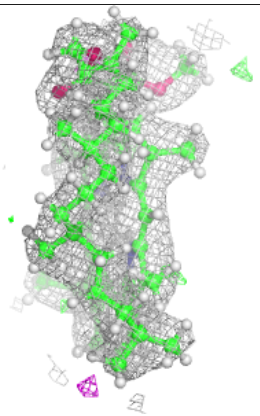


Electron density around PHO A 404:

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

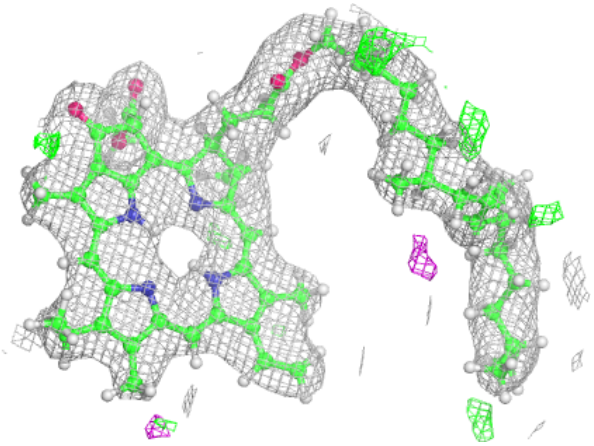


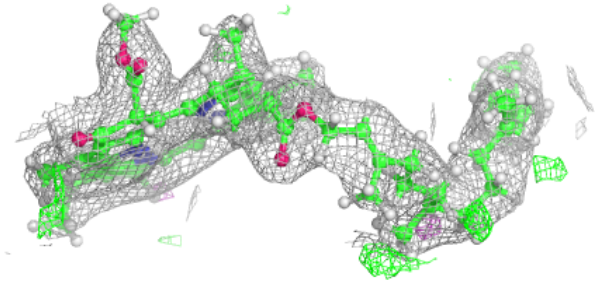


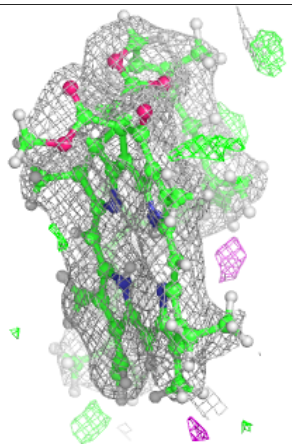


Electron density around PHO D 401:

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

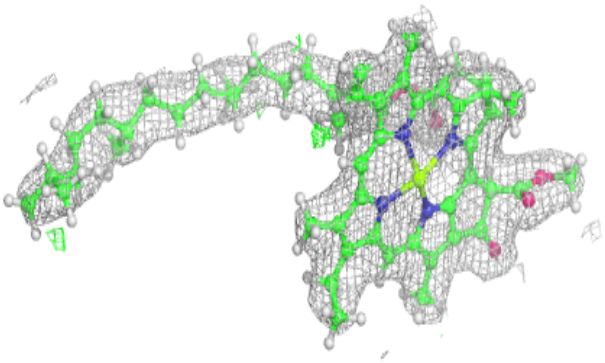


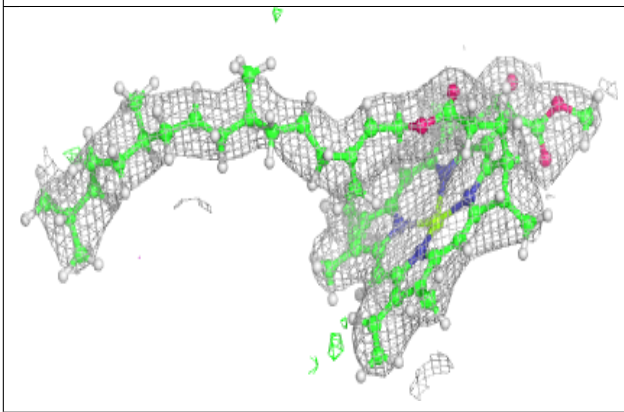


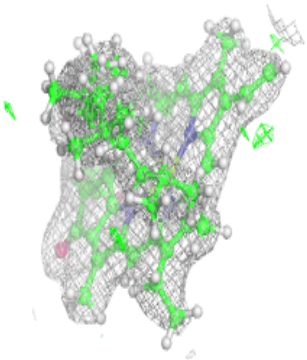


Electron density around CLA B 607:

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

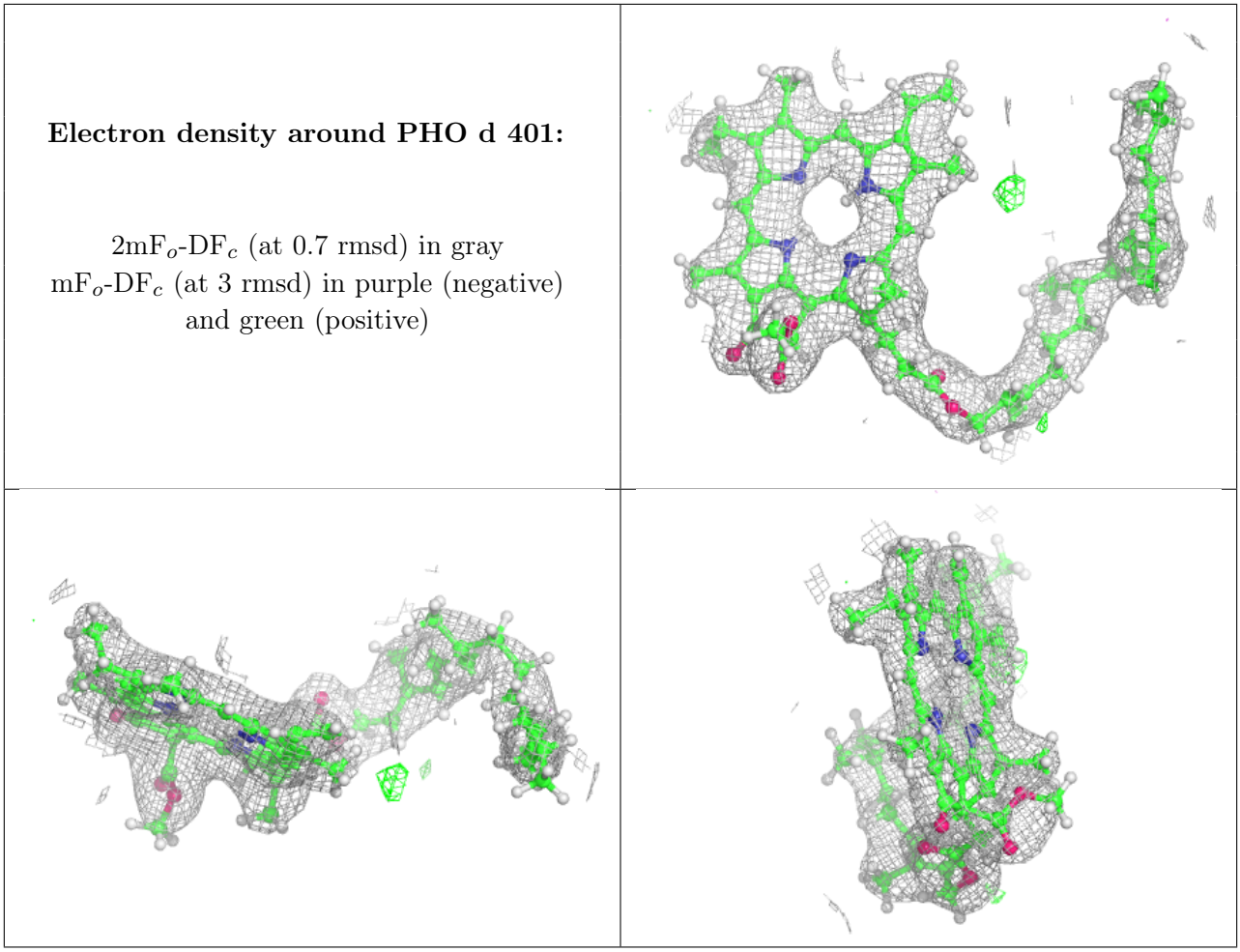






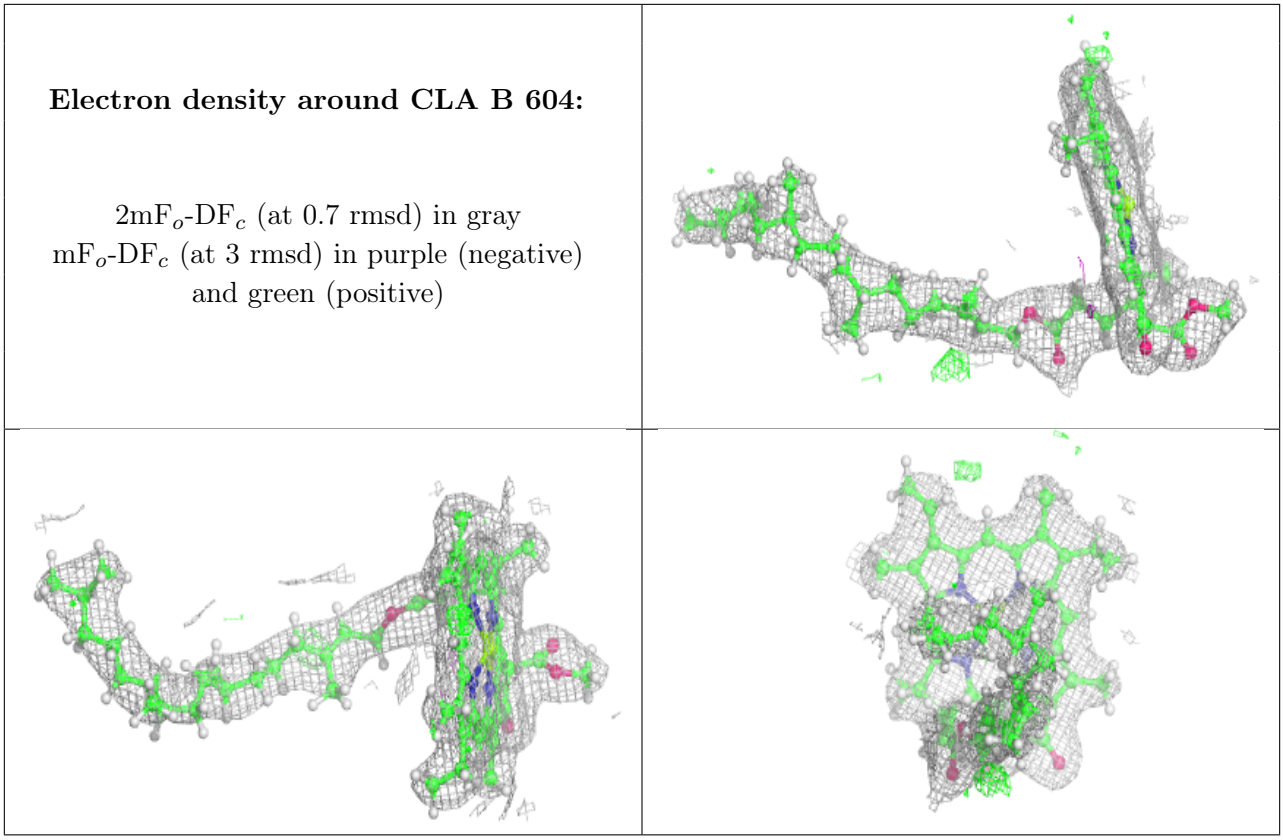
Electron density around PHO d 401:

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



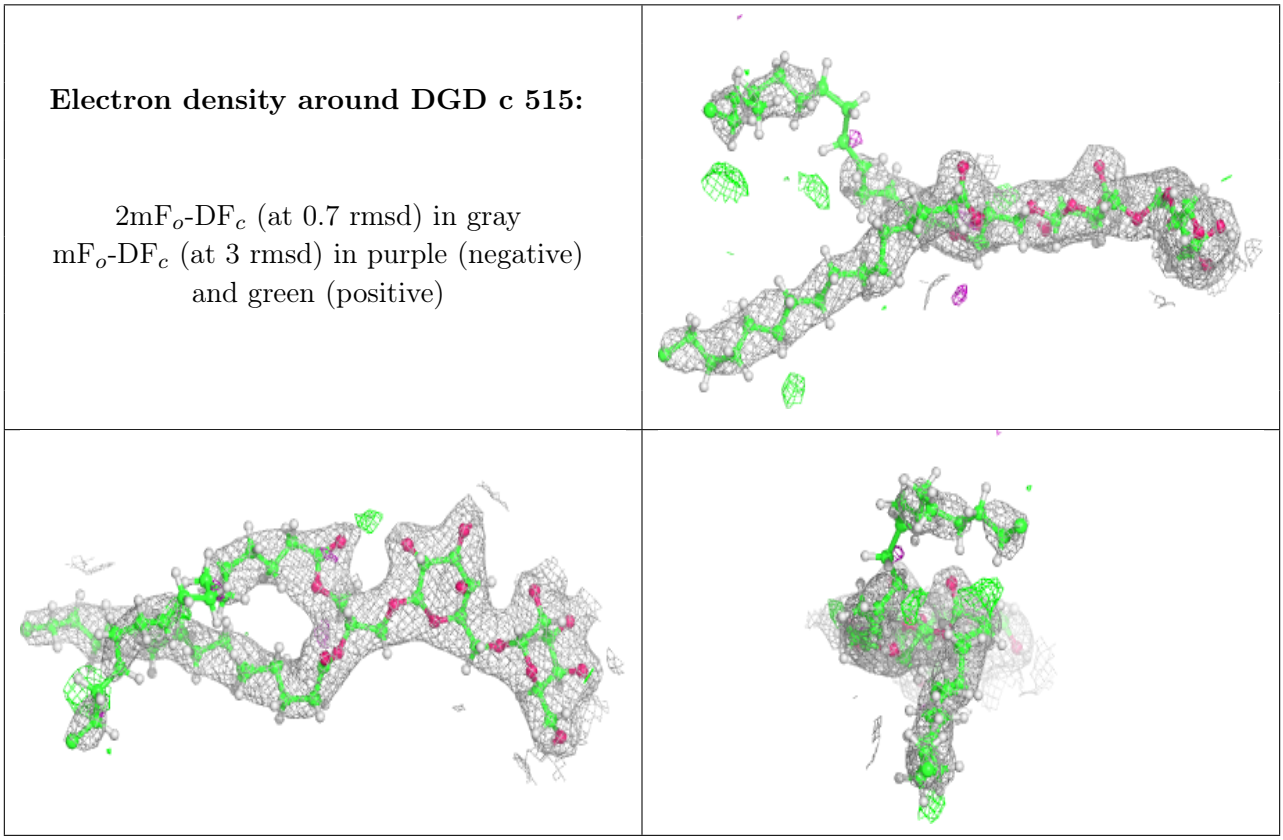
Electron density around CLA B 604:

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



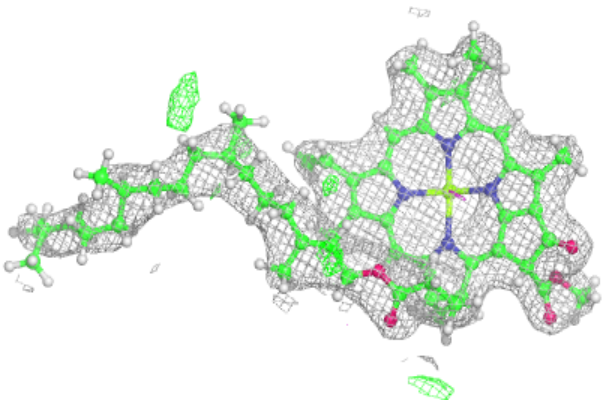
Electron density around DGD c 515:

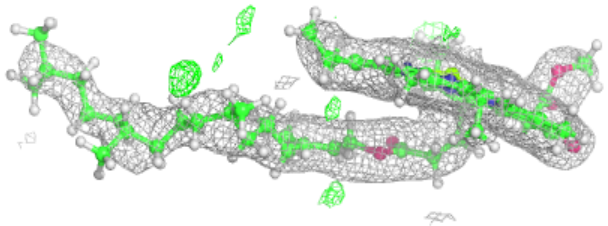
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

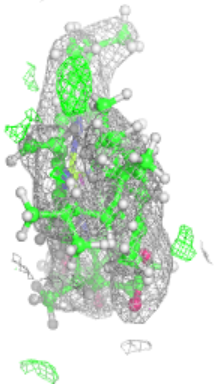


Electron density around CLA b 603:

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

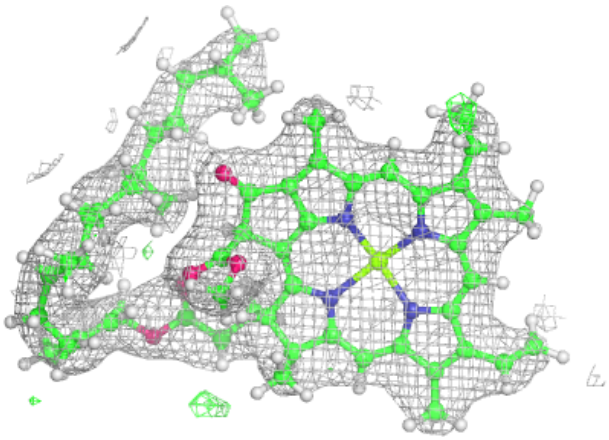


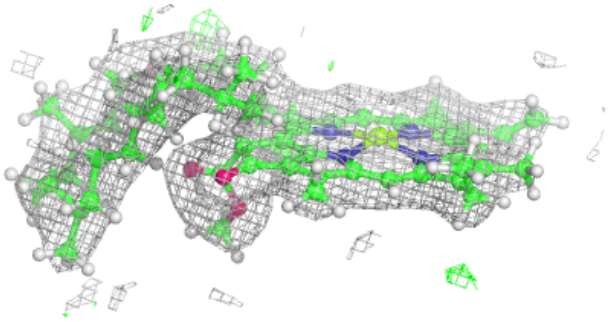


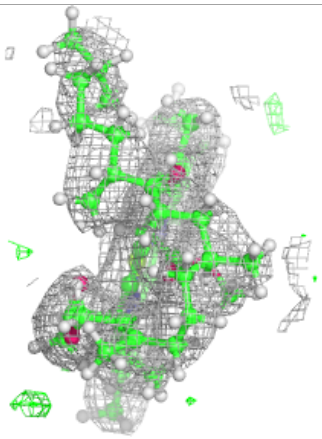


Electron density around CLA B 609:

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

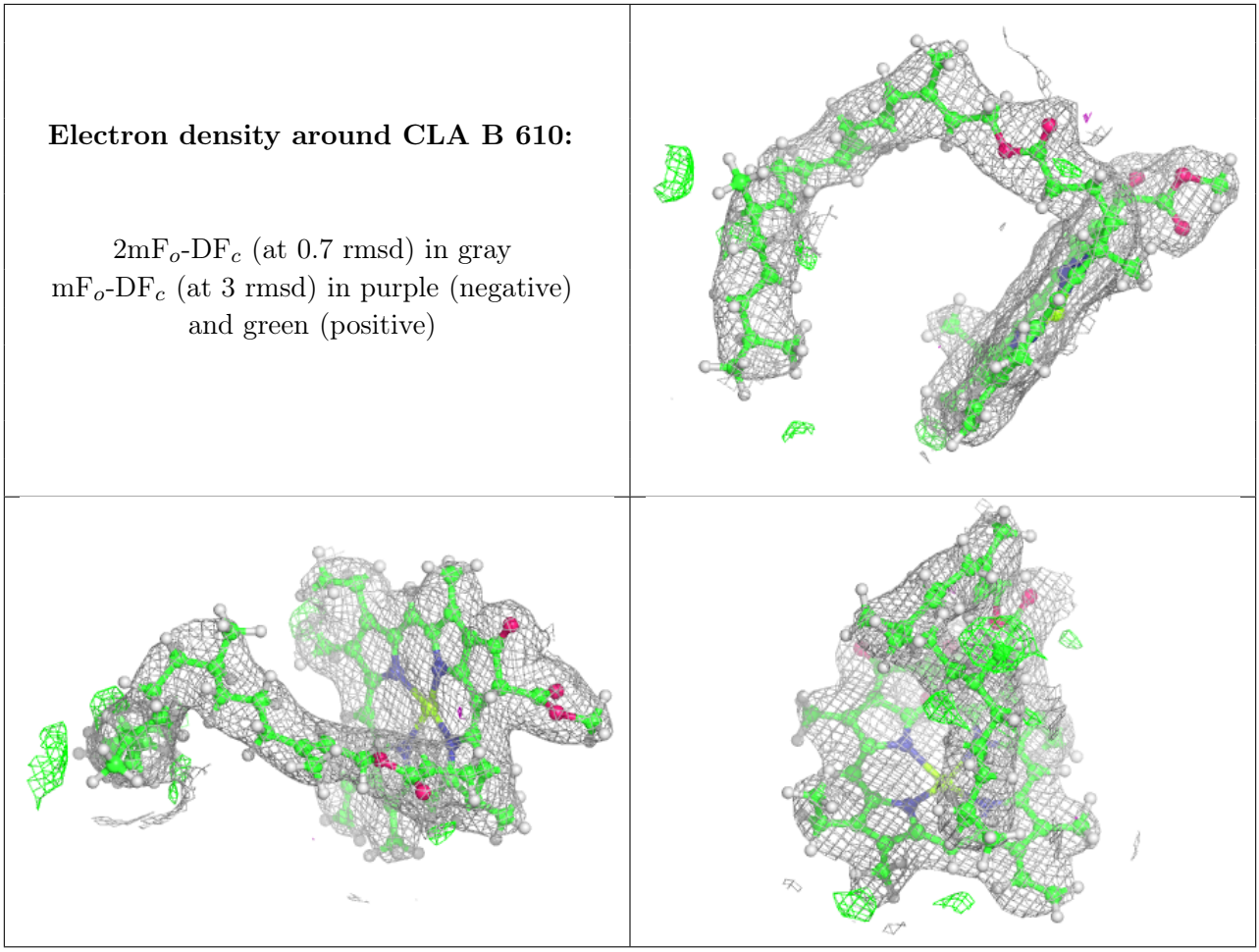






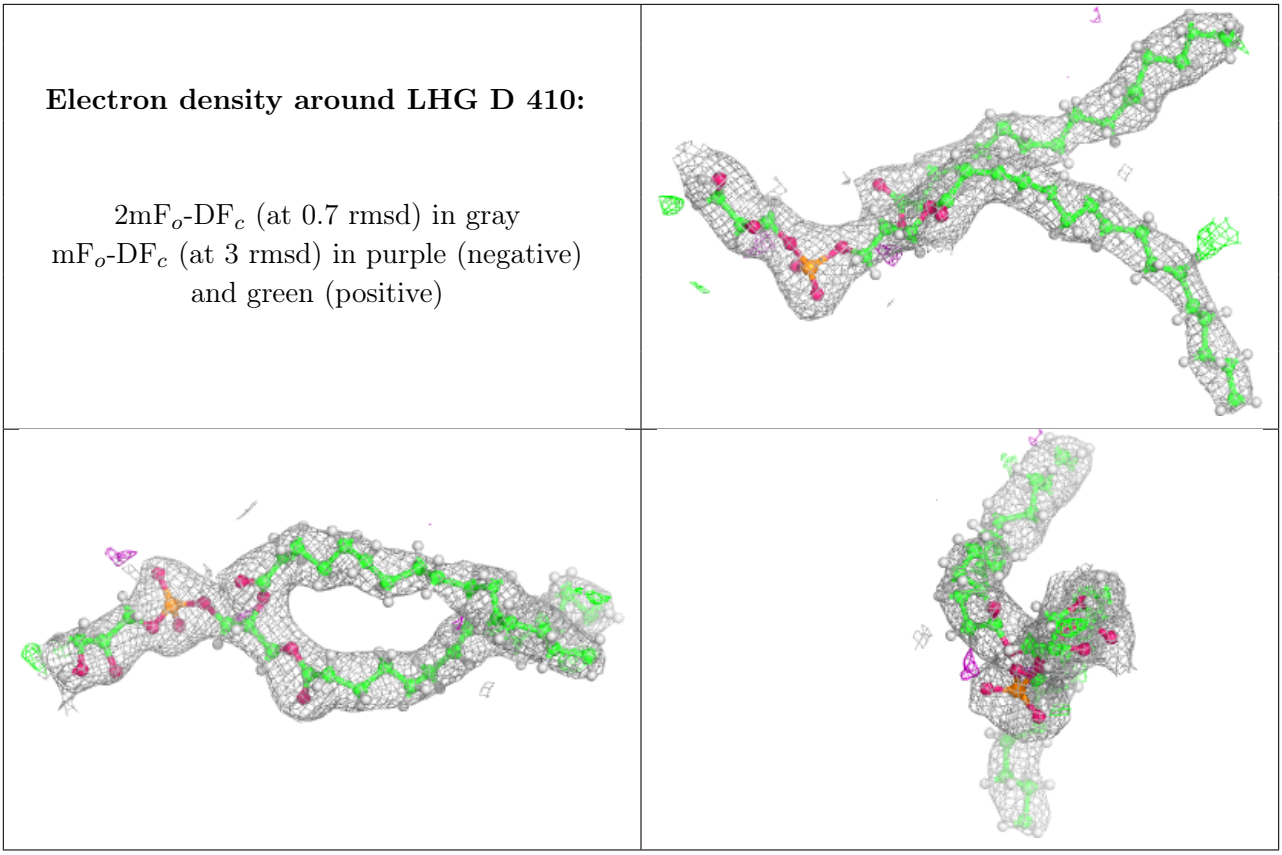
Electron density around CLA B 610:

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



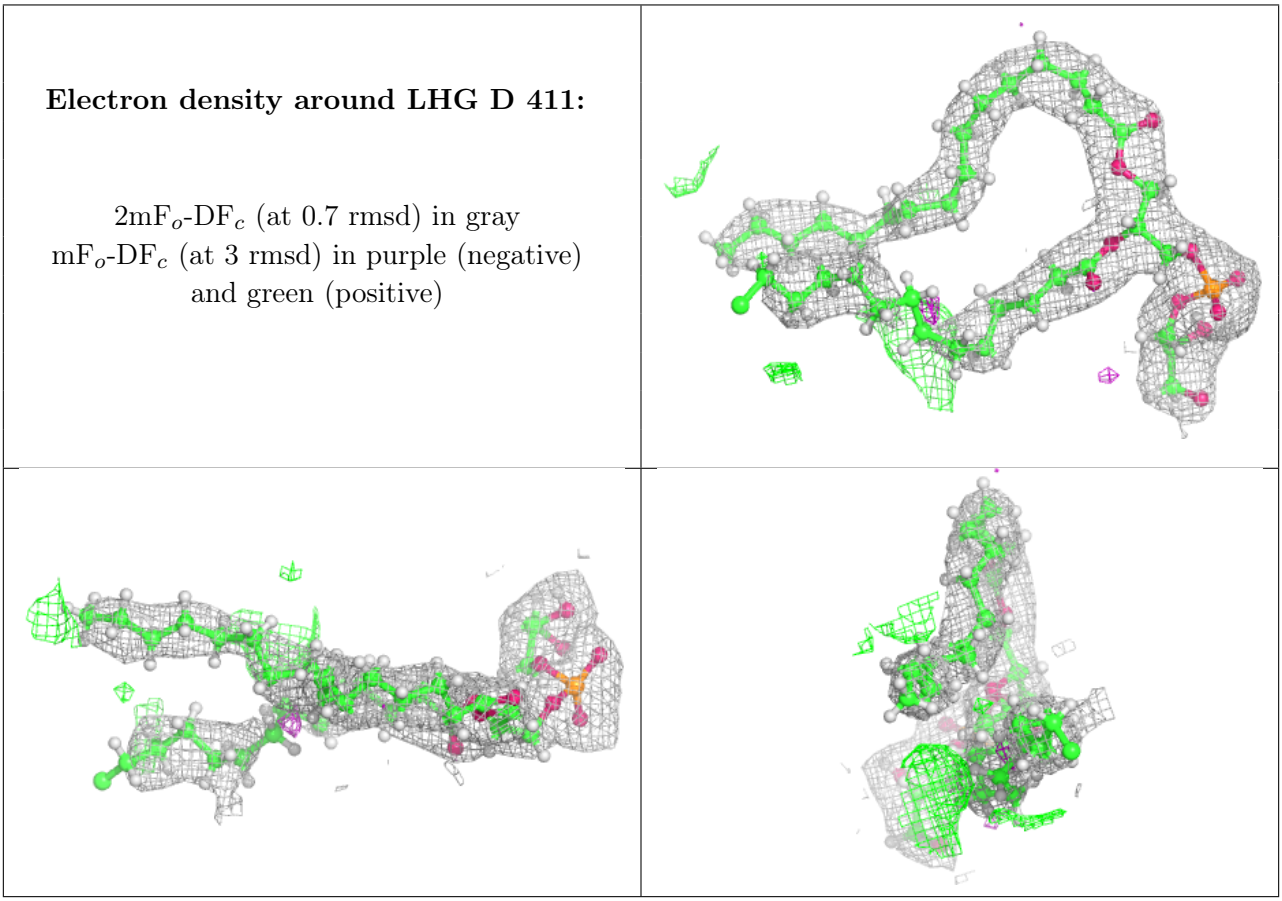
Electron density around LHG D 410:

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



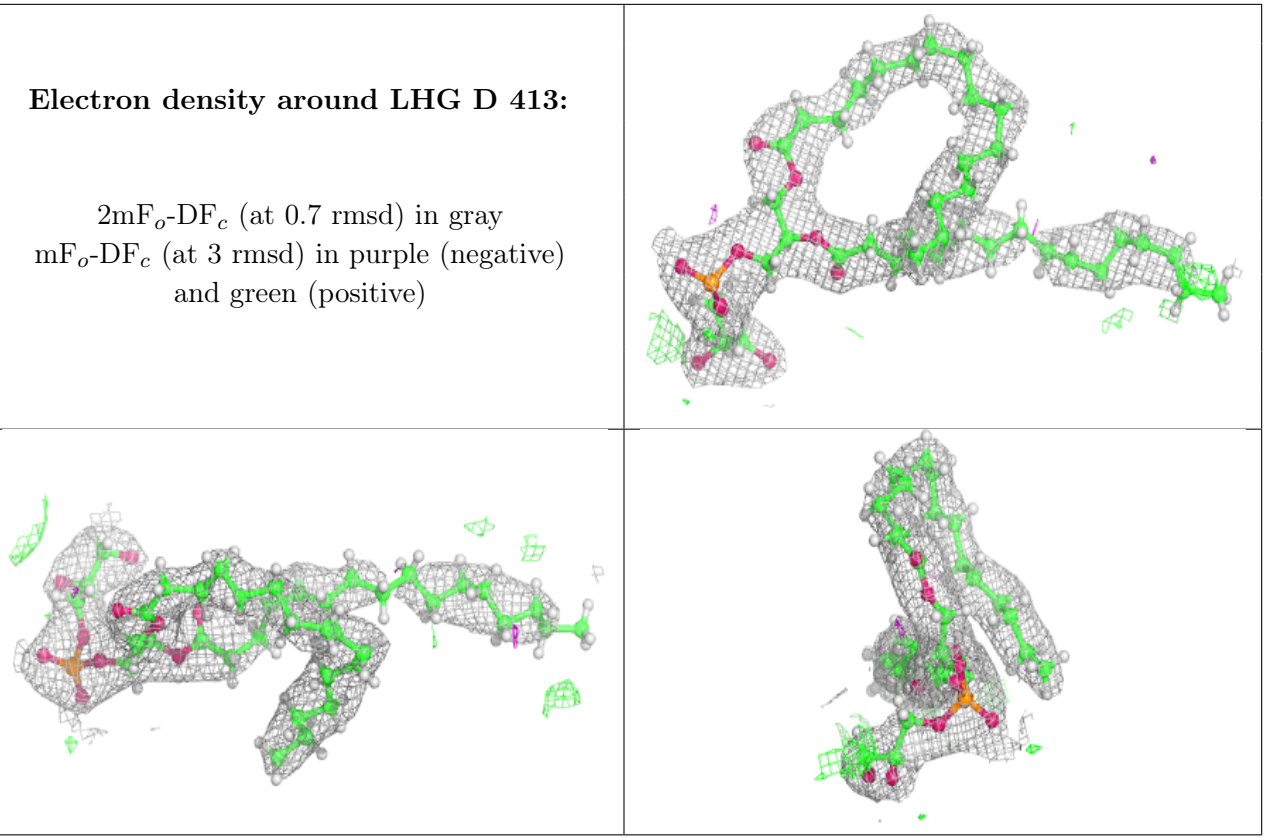
Electron density around LHG D 411:

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



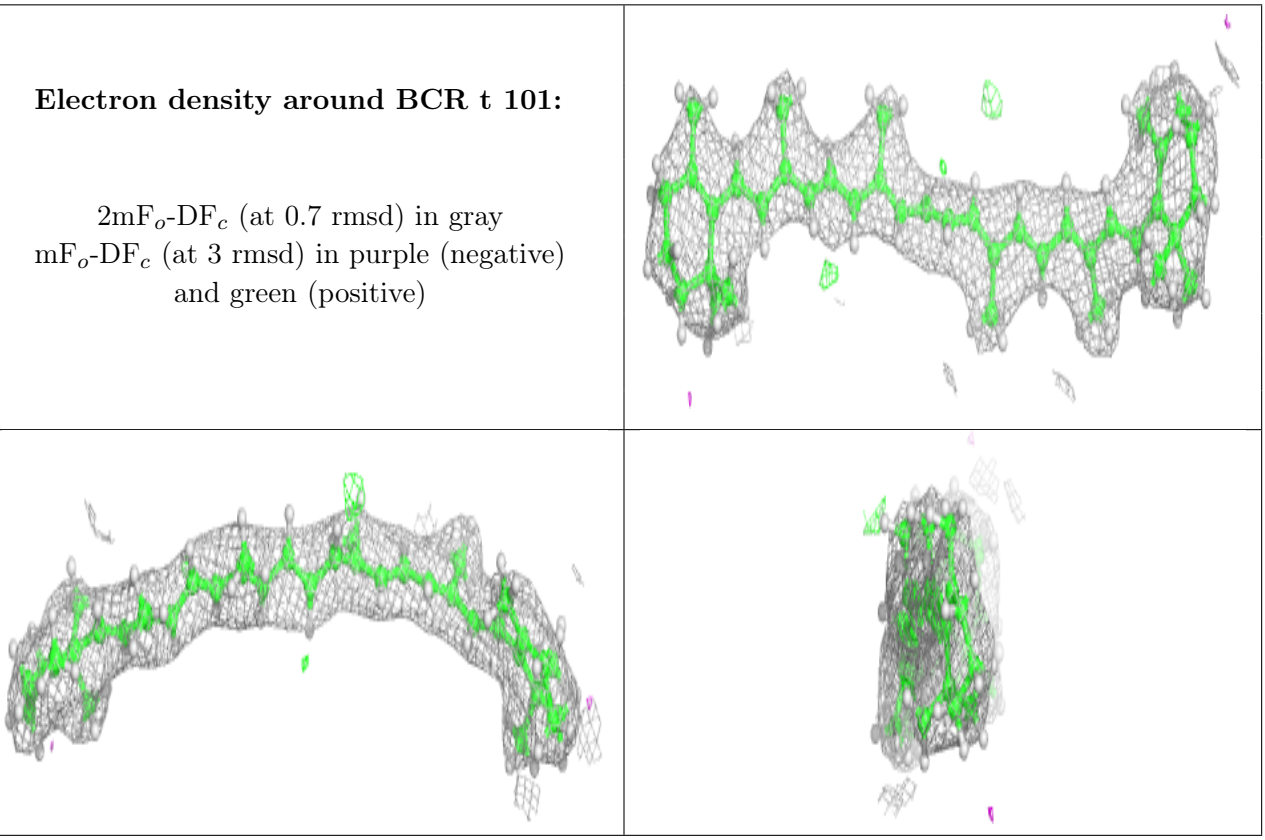
Electron density around LHG D 413:

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



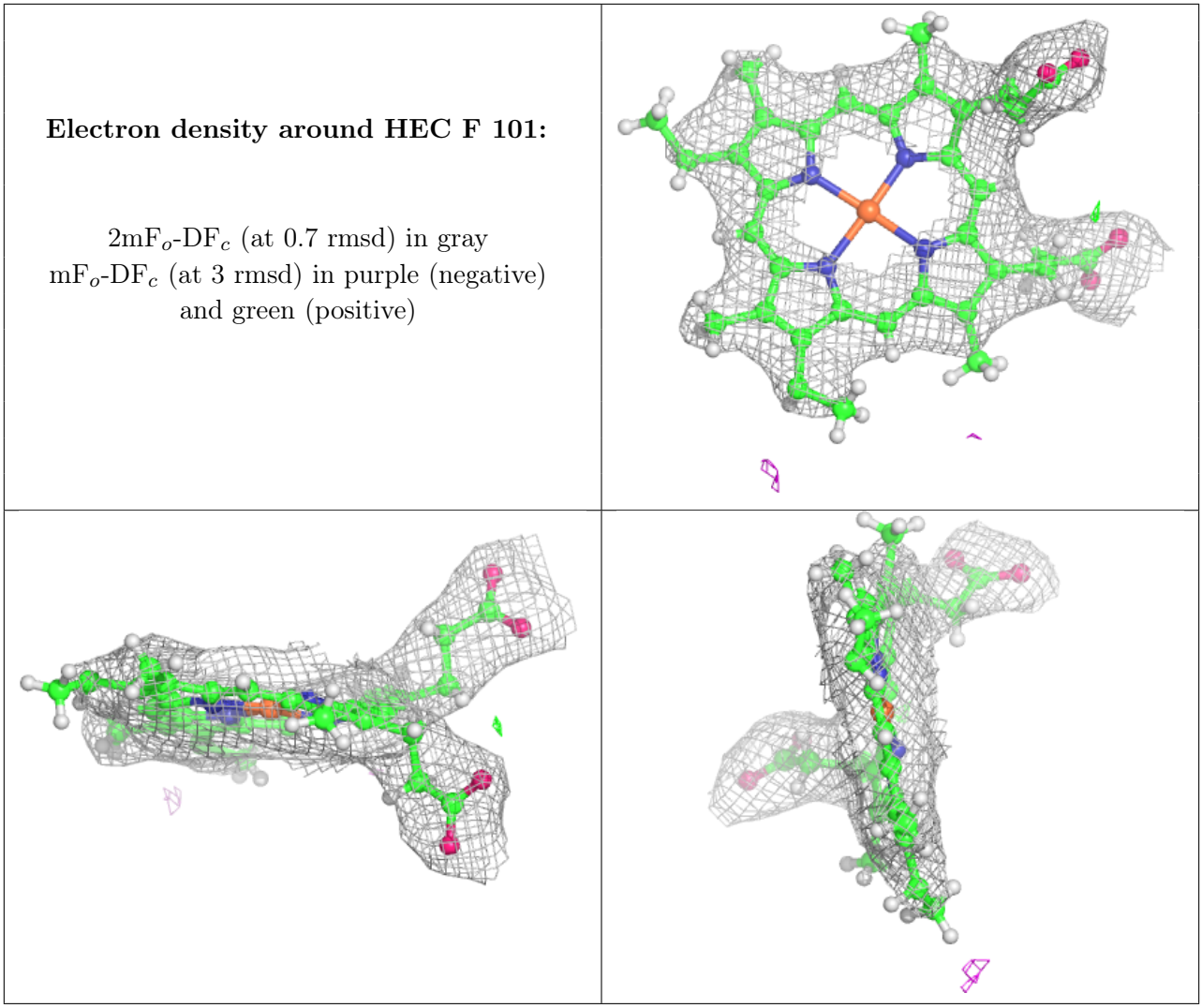
Electron density around BCR t 101:

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



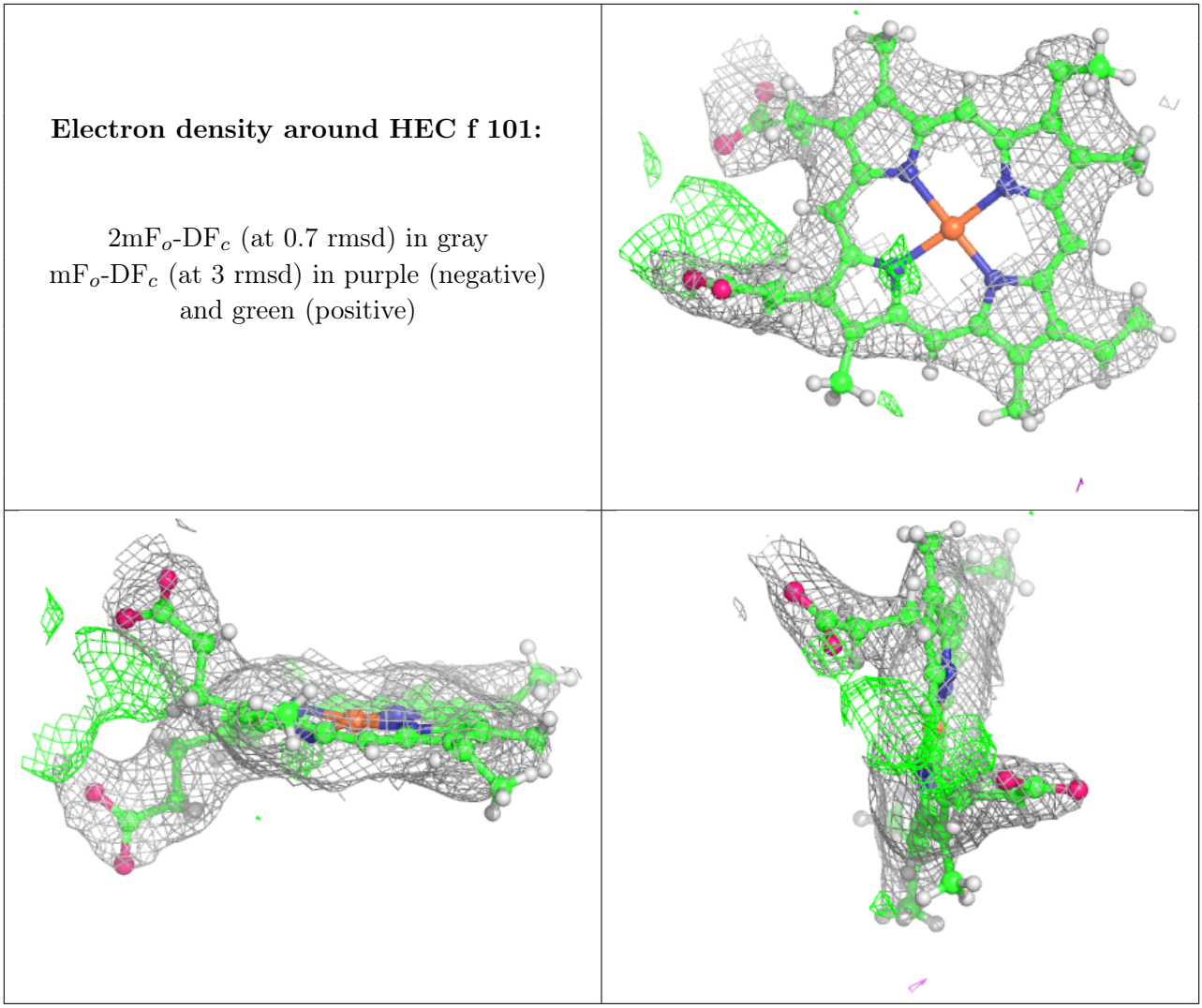
Electron density around HEC F 101:

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



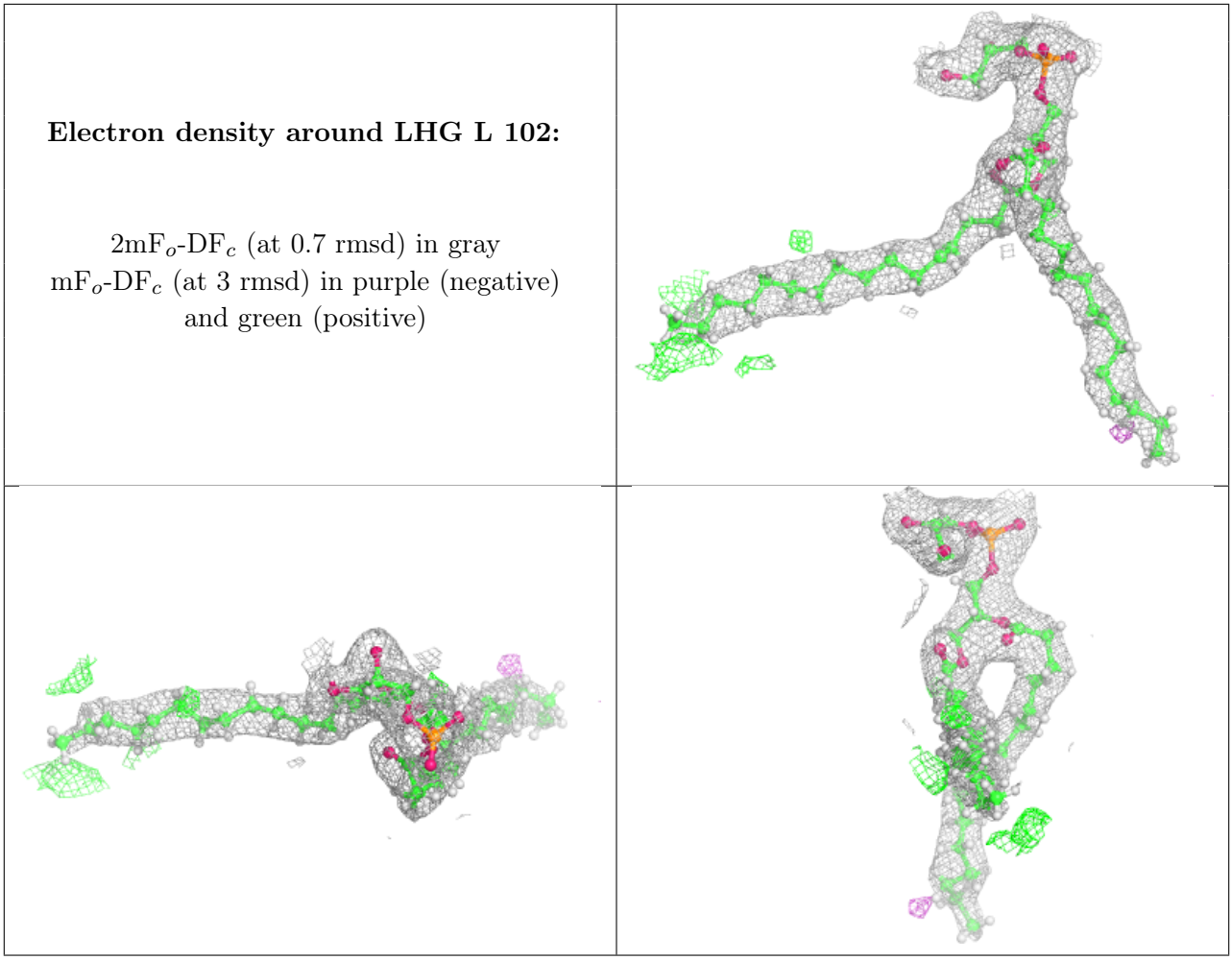
Electron density around HEC f 101:

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



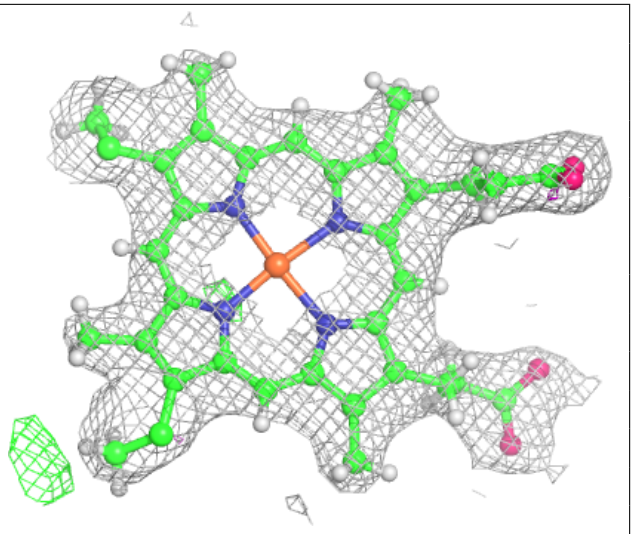
Electron density around LHG L 102:

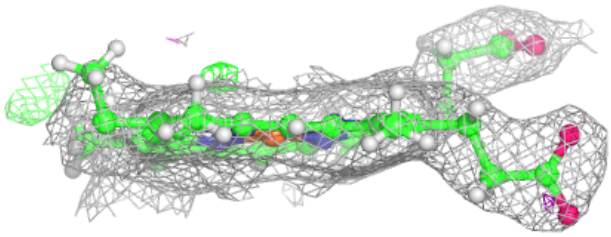
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC V 201:

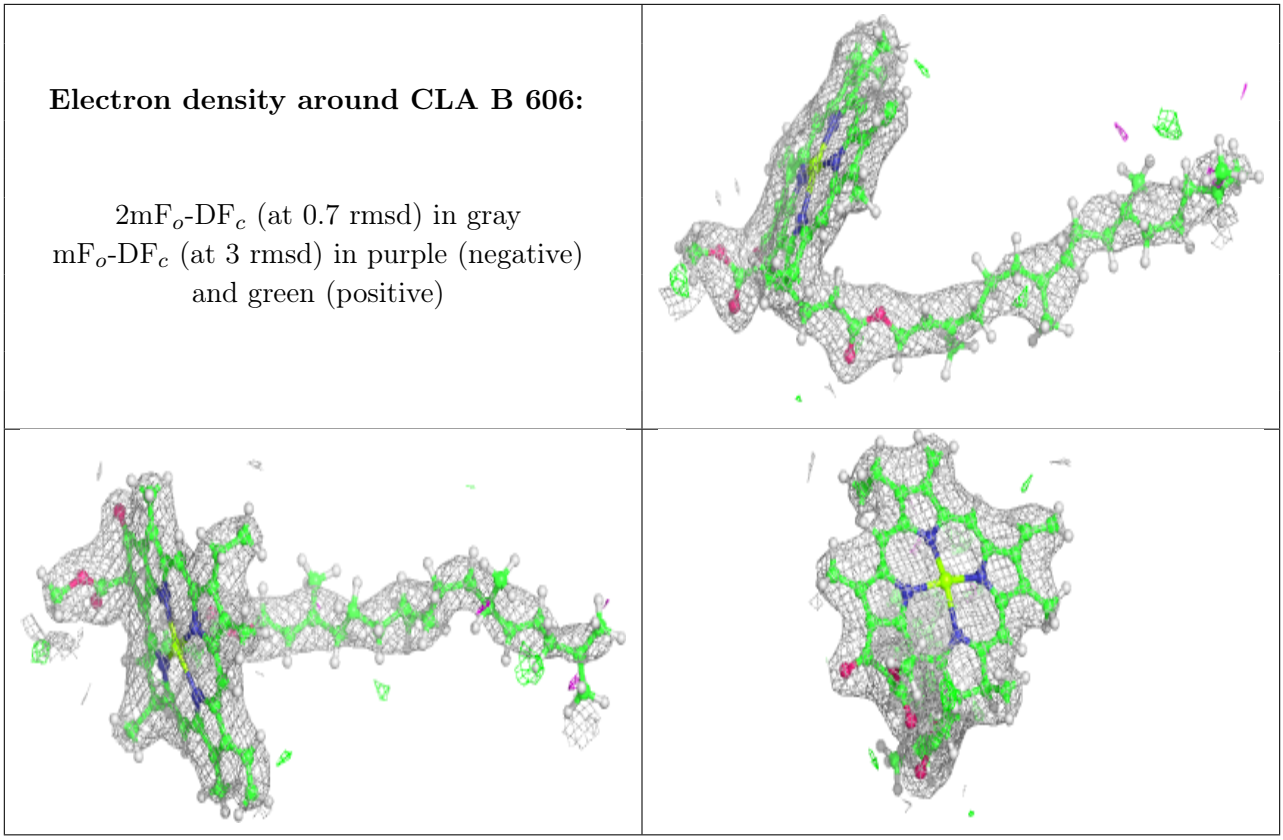
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





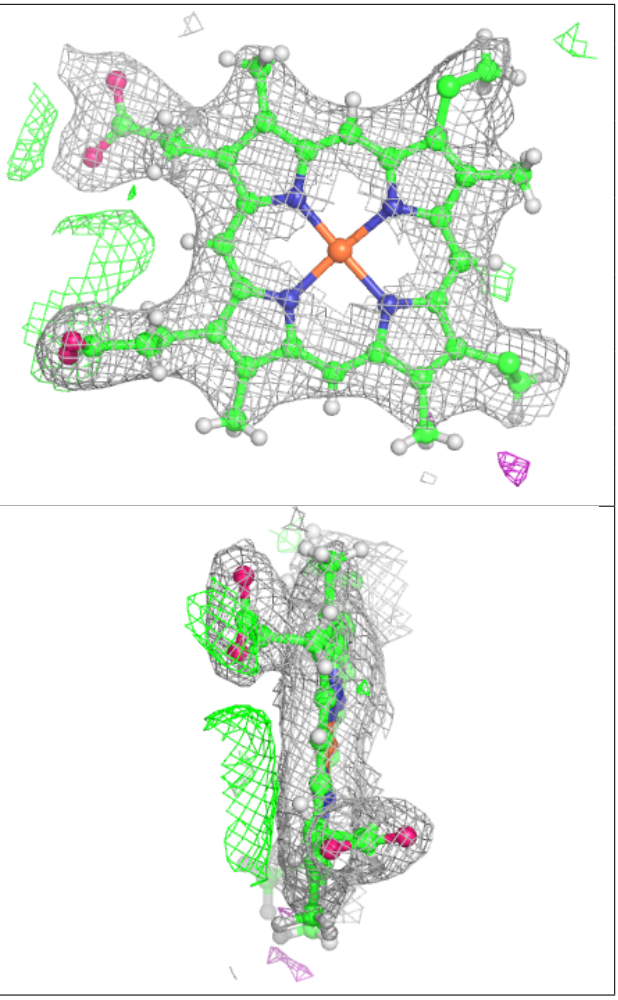
Electron density around CLA B 606:

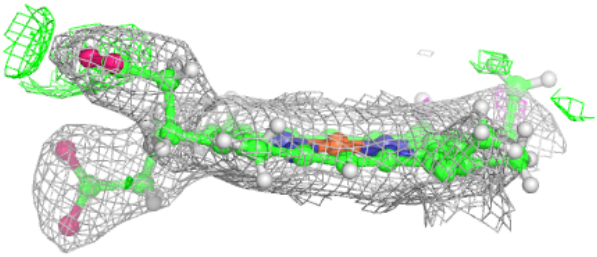
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC v 201:

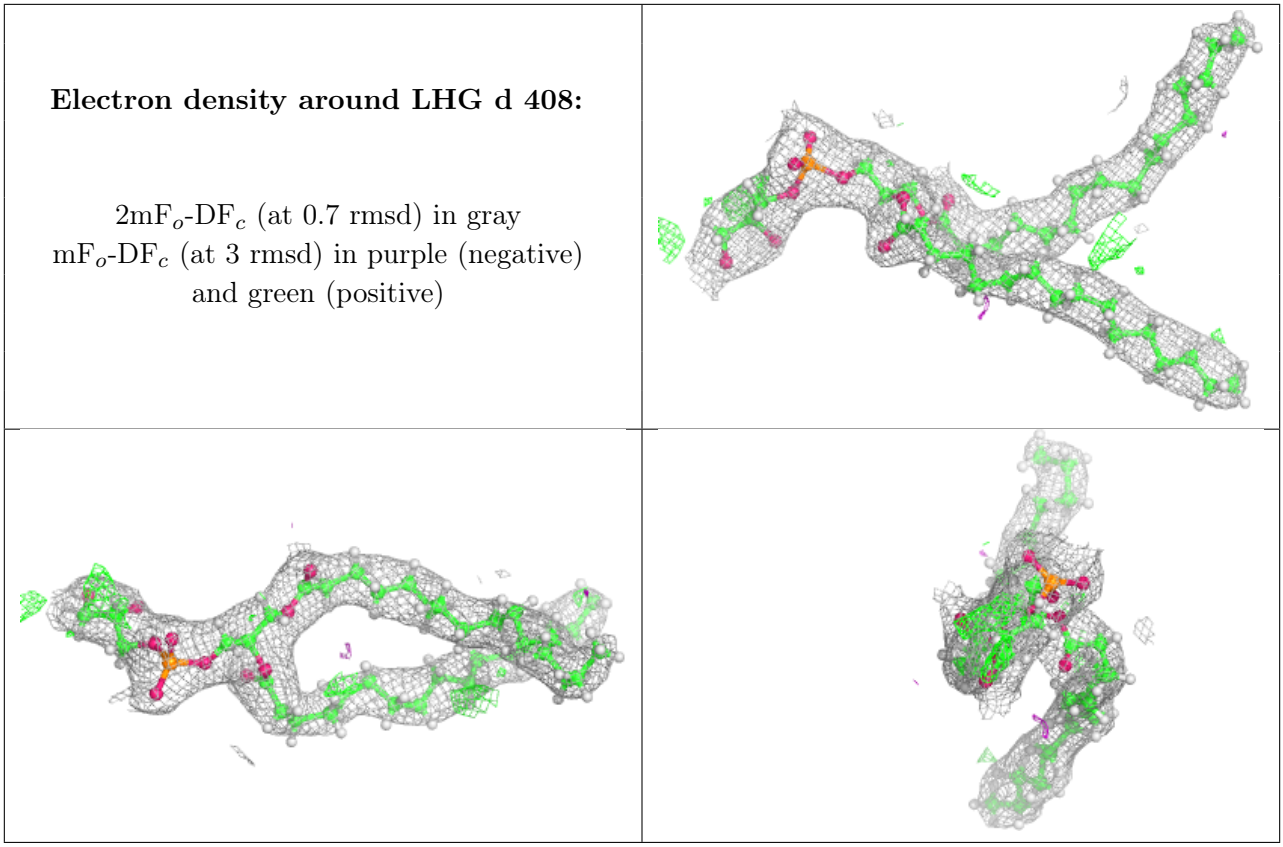
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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)



6.5 Other polymers

There are no such residues in this entry.