Full wwPDB X-ray Structure Validation Report (i)

Apr 22, 2025 – 02:47 AM EDT

PDB ID	:	6W1V / pdb_00006w1v
Title	:	RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution
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Deposited on	:	2020-03-04
Resolution	:	2.09 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:

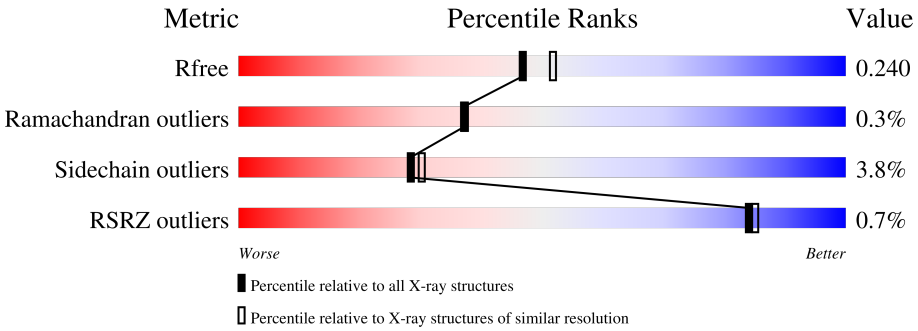
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)

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 2.09 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}	164625	6234 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	344	97%
1	a	344	% 94%
2	B	510	97%

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CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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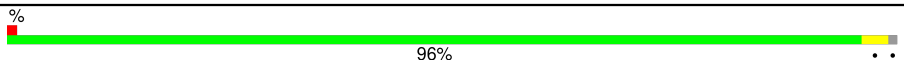
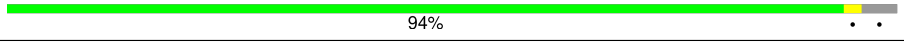
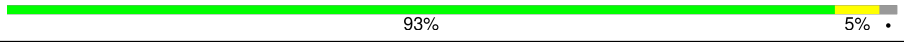
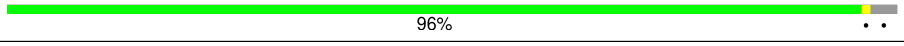
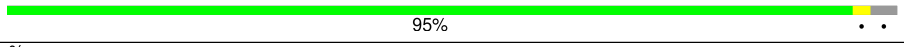
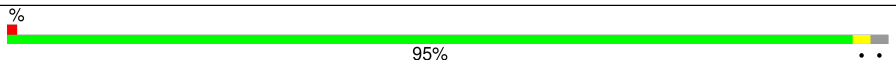
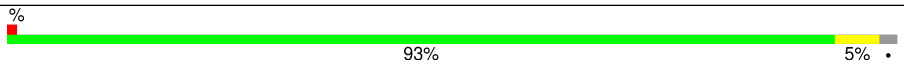
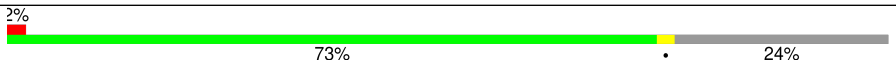
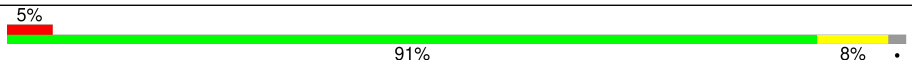
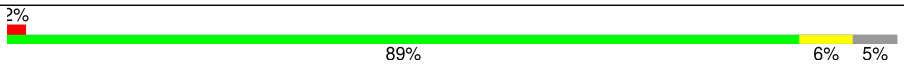
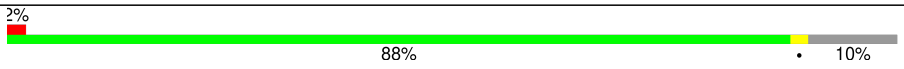
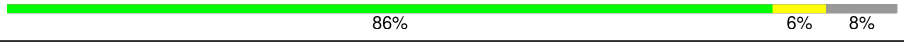
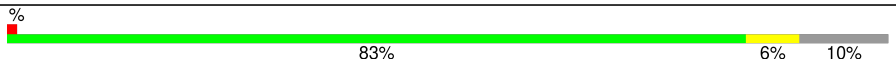
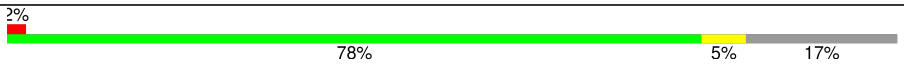
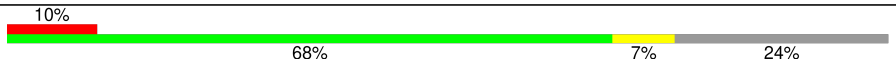
Mol	Chain	Length	Quality of chain
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	
14	r	41	

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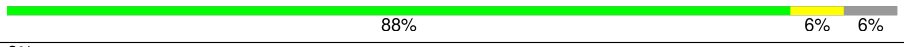
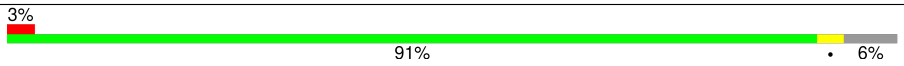
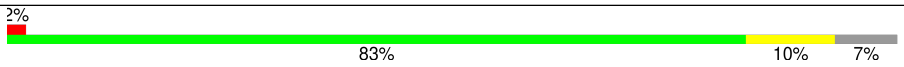
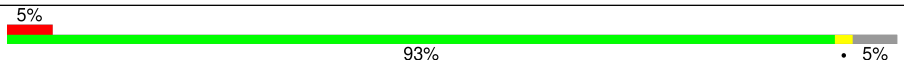
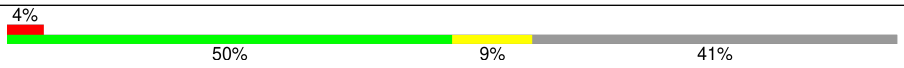
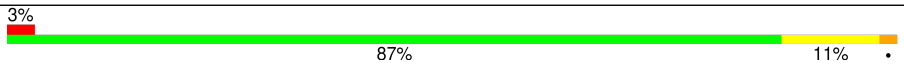
Mol	Chain	Length	Quality of chain
15	T	32	
15	t	32	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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	404	X	-	-	-
22	CLA	B	702	X	-	-	-
22	CLA	B	703	X	-	-	-
22	CLA	B	704	X	-	-	-
22	CLA	B	705	X	-	-	-
22	CLA	B	706	X	-	-	-
22	CLA	B	707	X	-	-	-
22	CLA	B	708	X	-	-	-
22	CLA	B	710	X	-	-	-
22	CLA	B	712	X	-	-	-
22	CLA	B	713	X	-	-	-
22	CLA	B	714	X	-	-	-
22	CLA	B	715	X	-	-	-
22	CLA	B	716	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	H	102	X	-	-	-
22	CLA	a	401	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	b	701	X	-	-	-
22	CLA	b	703	X	-	-	-
22	CLA	b	704	X	-	-	-
22	CLA	b	705	X	-	-	-
22	CLA	b	706	X	-	-	-
22	CLA	b	707	X	-	-	-
22	CLA	b	708	X	-	-	-
22	CLA	b	709	X	-	-	-
22	CLA	b	710	X	-	-	-
22	CLA	b	711	X	-	-	-
22	CLA	b	712	X	-	-	-
22	CLA	b	713	X	-	-	-
22	CLA	b	714	X	-	-	-
22	CLA	b	715	X	-	-	-
22	CLA	b	716	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 106211 atoms, of which 52744 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	66	0
			6084	2030	2971	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6072	2027	2962	513	551	19			

- 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	14	0
			6928	2302	3419	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7073	2343	3490	602	624	14			

- 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	2	0
			5360	1809	2629	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5372	1813	2635	446	466	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
			490	162	250	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			

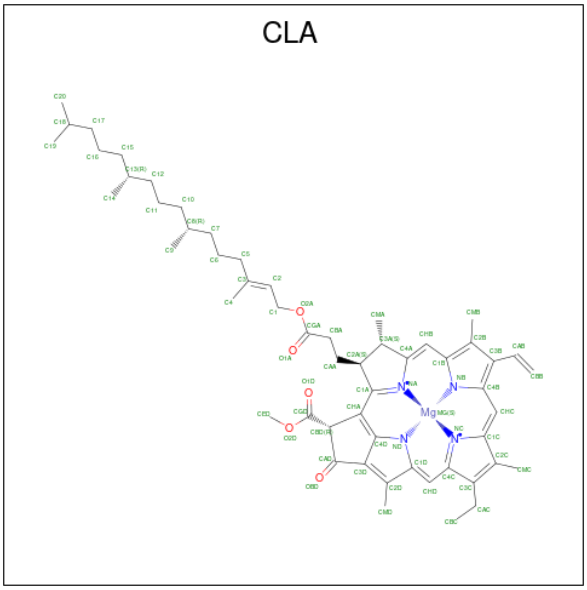
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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 (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: 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 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	A	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0	0

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

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

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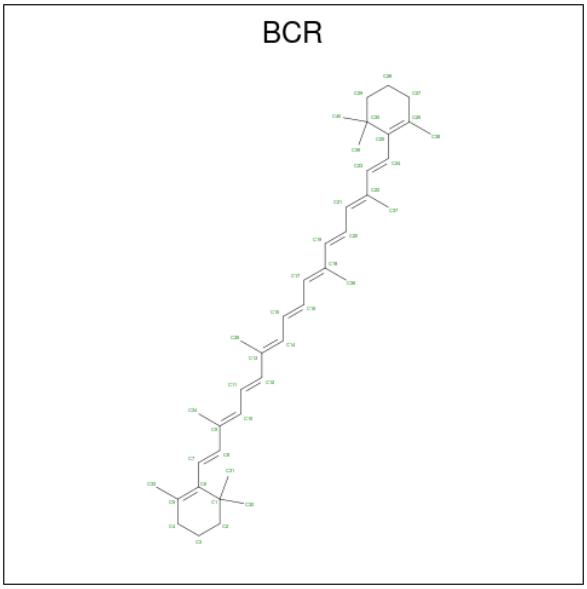
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	H	0	0
			96	40	56		
23	B	1	Total	C	H	0	0
			96	40	56		
23	B	1	Total	C	H	0	0
			96	40	56		
23	B	1	Total	C	H	0	0
			96	40	56		
23	C	1	Total	C	H	0	0
			96	40	56		

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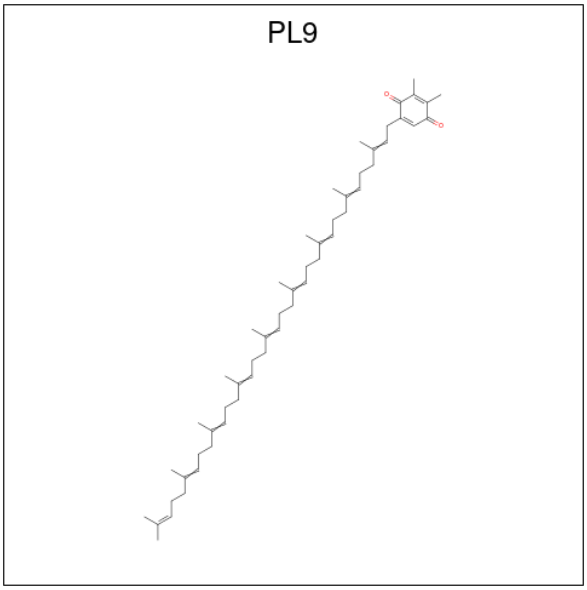
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C H 96 40 56	0	0
23	D	1	Total C H 96 40 56	0	0
23	H	1	Total C H 96 40 56	0	0
23	K	1	Total C H 96 40 56	0	0
23	T	1	Total C H 96 40 56	0	0
23	Y	1	Total C H 96 40 56	0	0
23	a	1	Total C H 96 40 56	0	0
23	b	1	Total C H 96 40 56	0	0
23	b	1	Total C H 96 40 56	0	0
23	b	1	Total C H 96 40 56	0	0
23	c	1	Total C H 96 40 56	0	0
23	c	1	Total C H 96 40 56	0	0
23	d	1	Total C H 96 40 56	0	0
23	h	1	Total C H 96 40 56	0	0
23	k	1	Total C H 96 40 56	0	0
23	k	1	Total C H 96 40 56	0	0
23	t	1	Total C H 96 40 56	0	0

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

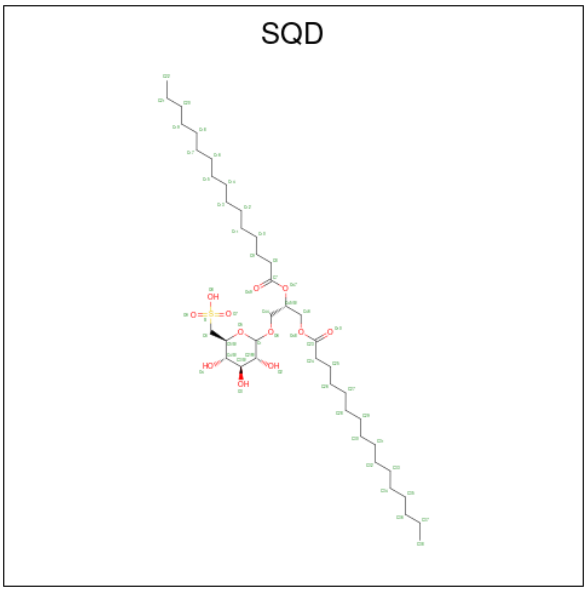
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



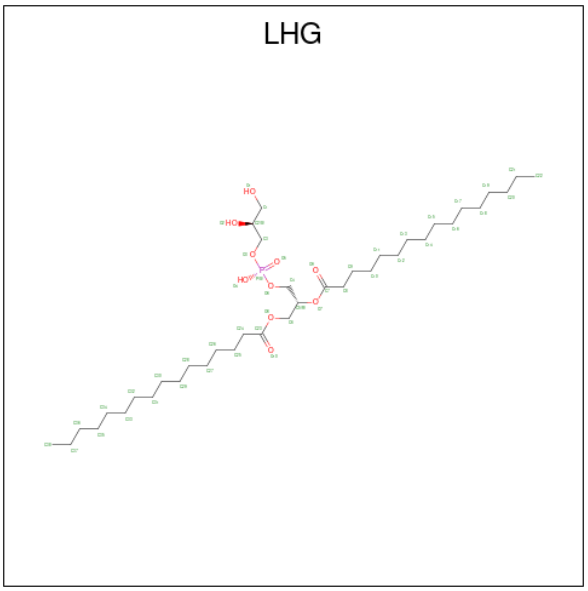
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	H	O	0	0
			135	53	80	2		
25	D	1	Total	C	H	O	0	0
			135	53	80	2		
25	a	1	Total	C	H	O	0	0
			135	53	80	2		
25	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



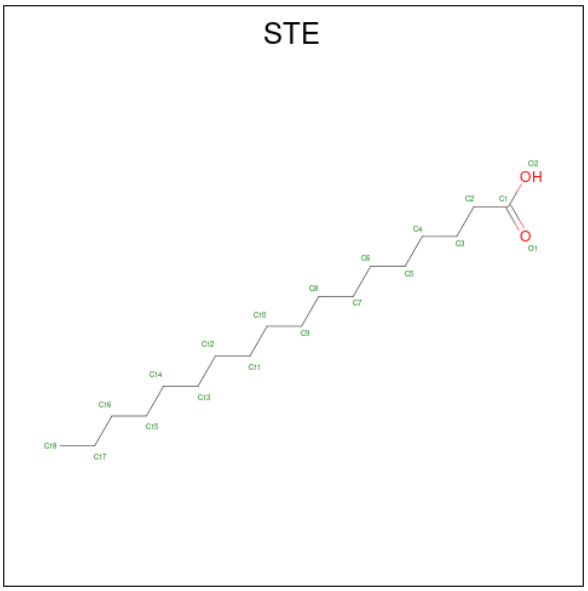
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C H O S 123 39 71 12 1	0	0
26	A	1	Total C H O 104 35 65 4	0	0
26	B	1	Total C H O S 132 41 78 12 1	0	0
26	D	1	Total C H O S 82 25 46 10 1	0	0
26	a	1	Total C H O S 131 41 77 12 1	0	0
26	a	1	Total C H O 92 31 56 5	0	0
26	b	1	Total C H O S 114 36 65 12 1	0	0
26	f	1	Total C H O S 89 28 48 12 1	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
27	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
27	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
27	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
27	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
27	a	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
27	a	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
27	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
27	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
27	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 28 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H 47 16 31	0	0
28	A	1	Total C H 11 5 6	0	0
28	B	1	Total C H O 28 10 16 2	0	0
28	B	1	Total C H O 43 15 26 2	0	0
28	B	1	Total C H O 28 10 16 2	0	0
28	B	1	Total C H O 46 16 28 2	0	0
28	B	1	Total C H 47 16 31	0	0
28	C	1	Total C H O 28 10 16 2	0	0
28	C	1	Total C H 47 16 31	0	0
28	C	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H O 28 10 16 2	0	0
28	E	1	Total C H 17 7 10	0	0
28	H	1	Total C H 53 18 35	0	0
28	H	1	Total C H 20 8 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	I	1	Total C H 41 15 26	0	0
28	J	1	Total C H O 28 10 16 2	0	0
28	M	1	Total C H O 37 13 22 2	0	0
28	M	1	Total C H 26 10 16	0	0
28	T	1	Total C H 44 15 29	0	0
28	X	1	Total C H O 55 18 35 2	0	0
28	Z	1	Total C H 20 8 12	0	0
28	a	1	Total C H 26 10 16	0	0
28	a	1	Total C H O 28 10 16 2	0	0
28	a	1	Total C H 41 15 26	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	b	1	Total C H O 40 14 24 2	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	b	1	Total C H 26 10 16	0	0
28	b	1	Total C H O 55 18 35 2	0	0
28	c	1	Total C H O 28 10 16 2	0	0
28	c	1	Total C H O 55 18 35 2	0	0
28	d	1	Total C H O 43 15 26 2	0	0
28	h	1	Total C H 41 14 27	0	0
28	j	1	Total C H O 28 10 16 2	0	0
28	l	1	Total C H 53 18 35	0	0

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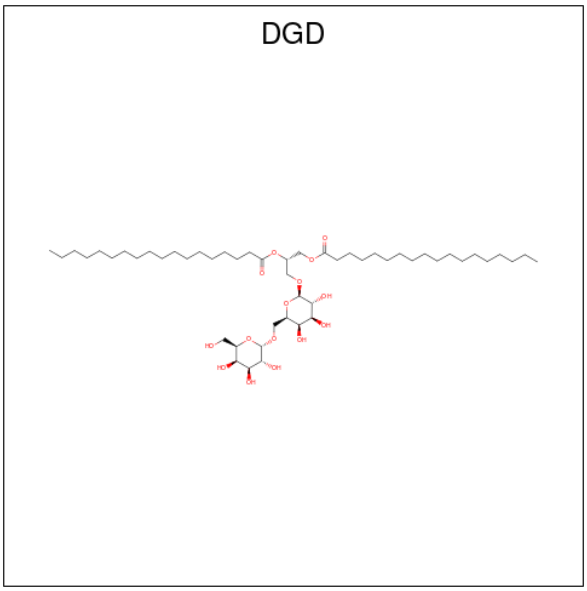
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	m	1	Total	C	H	O	0	0
			28	10	16	2		
28	t	1	Total	C	H	O	0	0
			34	12	20	2		
28	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			143	47	81	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			142	47	80	15		

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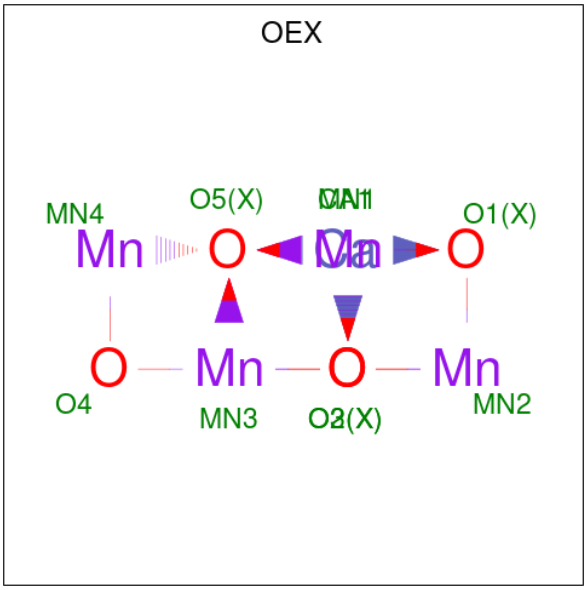
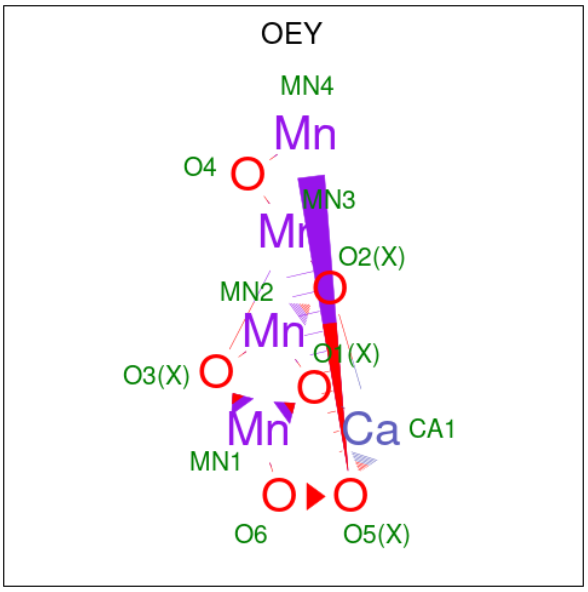
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	h	1	Total C H O 142 47 80 15	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



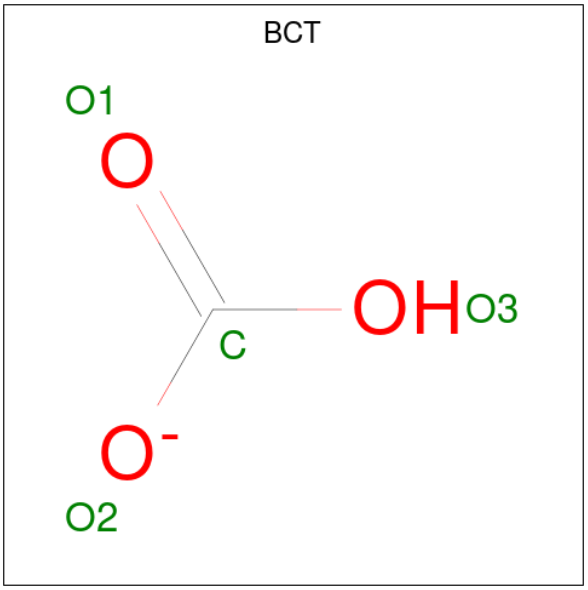
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total Ca Mn O 10 1 4 5	0	1
30	a	1	Total Ca Mn O 10 1 4 5	0	1

- Molecule 31 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: $CaMn_4O_6$).



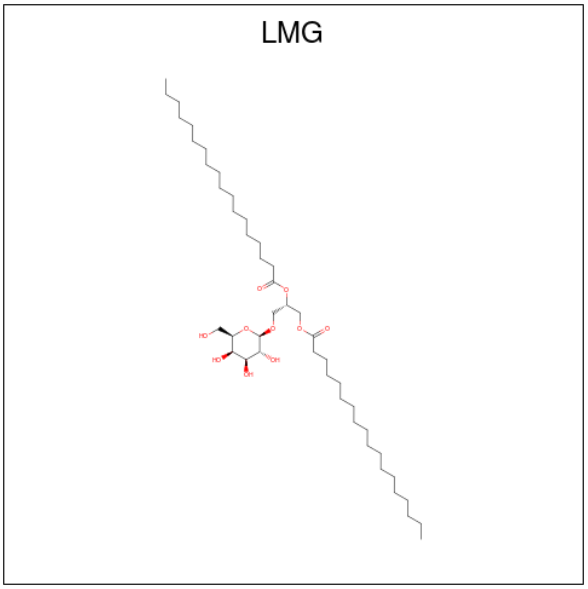
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
31	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			68	24	40	4		
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			123	41	72	10		
33	D	1	Total	C	H	O	0	0
			77	27	45	5		
33	M	1	Total	C	H	O	0	0
			123	41	72	10		
33	a	1	Total	C	H	O	0	0
			141	45	86	10		
33	b	1	Total	C	H	O	0	0
			123	41	72	10		
33	b	1	Total	C	H	O	0	0
			141	45	86	10		
33	c	1	Total	C	H	O	0	0
			81	27	44	10		
33	c	1	Total	C	H	O	0	0
			117	38	69	10		
33	c	1	Total	C	H	O	0	0
			117	39	68	10		

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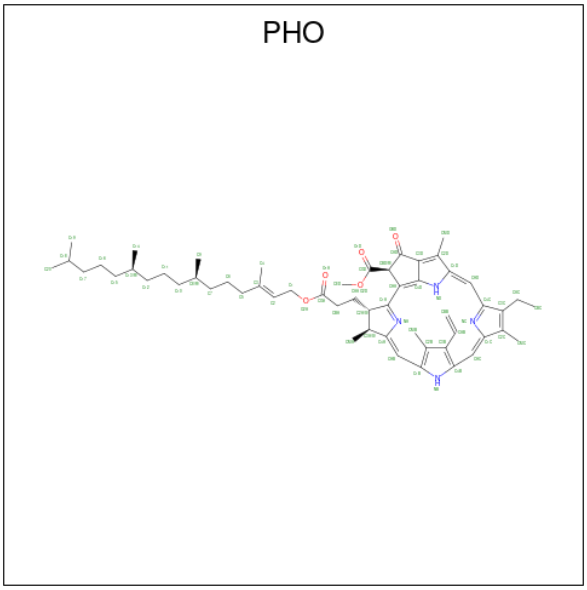
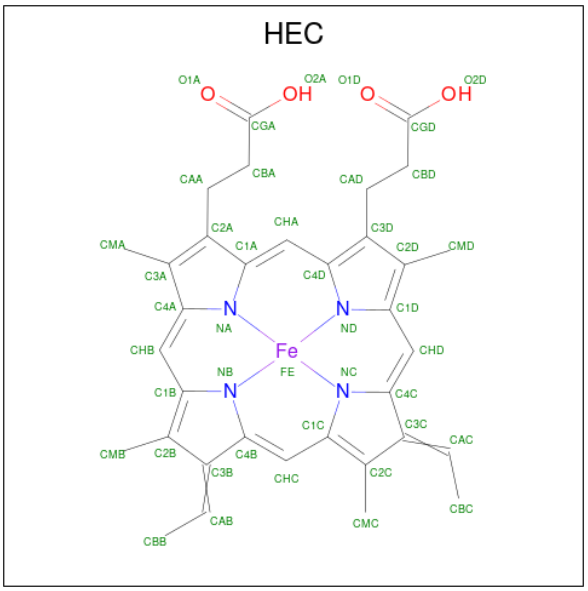
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	145	Total	O	0	8
			145	145		
36	B	233	Total	O	0	0
			233	233		
36	C	168	Total	O	0	0
			168	168		
36	D	115	Total	O	0	0
			115	115		
36	E	37	Total	O	0	0
			37	37		
36	F	6	Total	O	0	0
			6	6		
36	H	35	Total	O	0	0
			35	35		
36	I	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	J	15	Total O 15 15	0	0
36	K	3	Total O 3 3	0	0
36	L	9	Total O 9 9	0	0
36	M	8	Total O 8 8	0	0
36	O	106	Total O 106 106	0	0
36	R	3	Total O 3 3	0	0
36	T	9	Total O 9 9	0	0
36	U	53	Total O 53 53	0	0
36	V	63	Total O 63 63	0	0
36	X	17	Total O 17 17	0	0
36	Y	3	Total O 3 3	0	0
36	a	130	Total O 130 130	0	8
36	b	193	Total O 193 193	0	0
36	c	169	Total O 169 169	0	0
36	d	106	Total O 106 106	0	0
36	e	23	Total O 23 23	0	0
36	f	4	Total O 4 4	0	0
36	h	22	Total O 22 22	0	0
36	i	17	Total O 17 17	0	0
36	j	7	Total O 7 7	0	0
36	k	4	Total O 4 4	0	0

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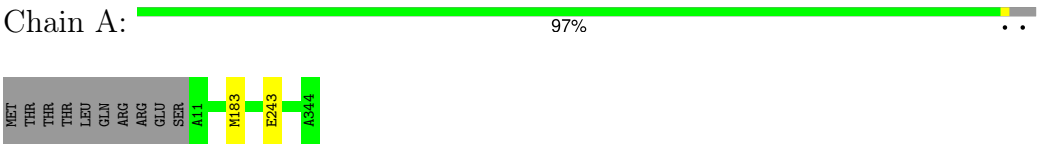
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	l	12	Total O 12 12	0	0
36	m	5	Total O 5 5	0	0
36	o	97	Total O 97 97	0	0
36	r	8	Total O 8 8	0	0
36	t	7	Total O 7 7	0	0
36	u	63	Total O 63 63	0	0
36	v	64	Total O 64 64	0	0
36	x	7	Total O 7 7	0	0
36	y	8	Total O 8 8	0	0
36	z	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

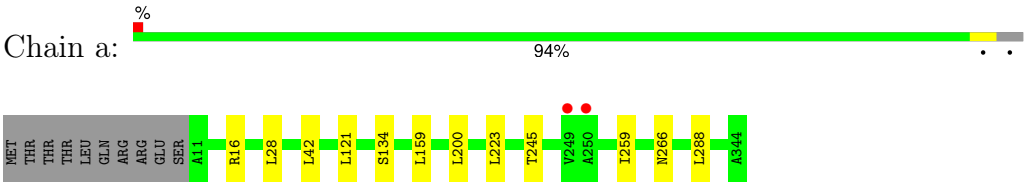
• Molecule 1: Photosystem II protein D1 1

Chain A:



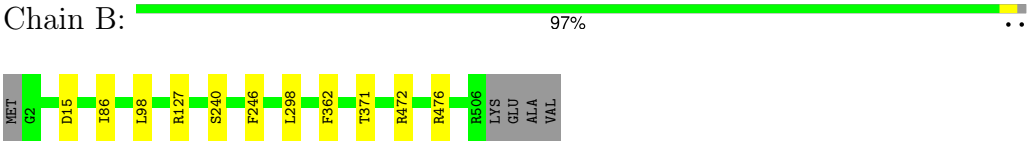
• Molecule 1: Photosystem II protein D1 1

Chain a:



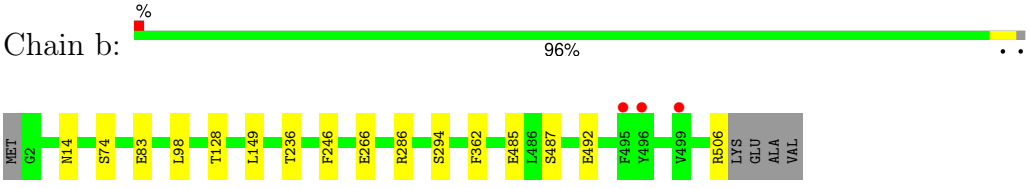
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



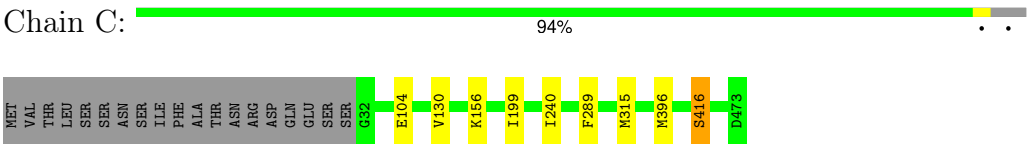
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



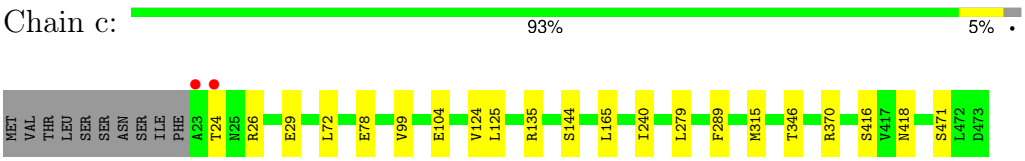
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



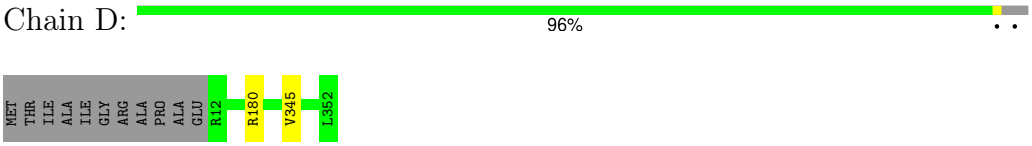
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



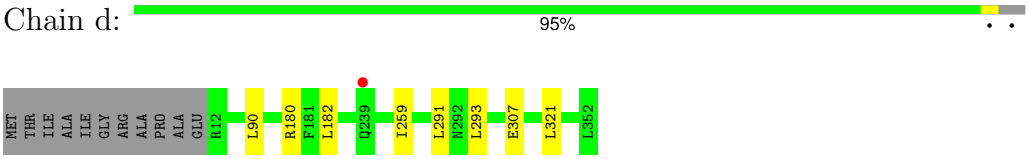
• Molecule 4: Photosystem II D2 protein

Chain D:



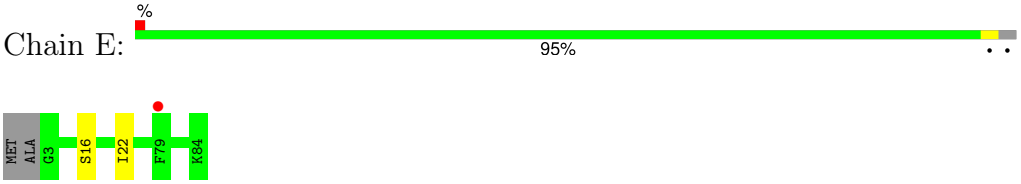
• Molecule 4: Photosystem II D2 protein

Chain d:



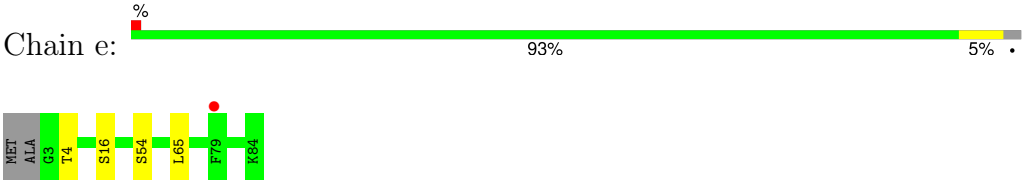
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



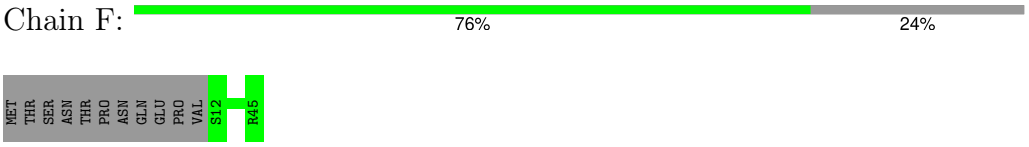
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



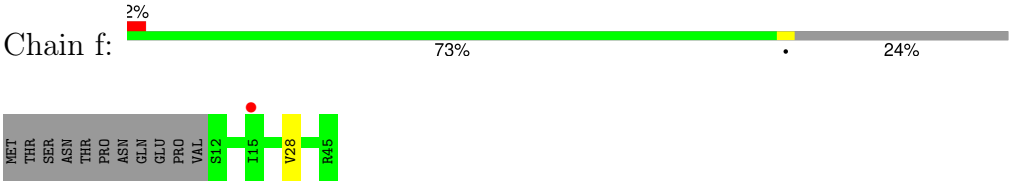
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



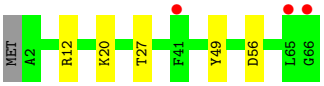
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



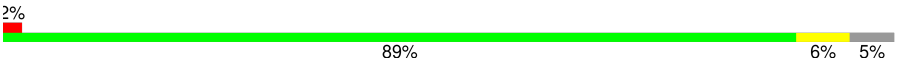
• Molecule 7: Photosystem II reaction center protein H

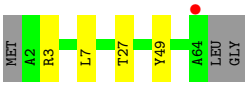
Chain H:



• Molecule 7: Photosystem II reaction center protein H

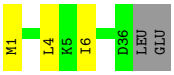
Chain h:





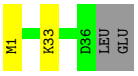
• Molecule 8: Photosystem II reaction center protein I

Chain I:



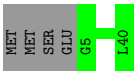
• Molecule 8: Photosystem II reaction center protein I

Chain i:



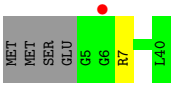
• Molecule 9: Photosystem II reaction center protein J

Chain J:



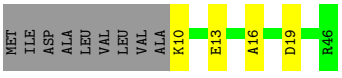
• Molecule 9: Photosystem II reaction center protein J

Chain j:



• Molecule 10: Photosystem II reaction center protein K

Chain K:

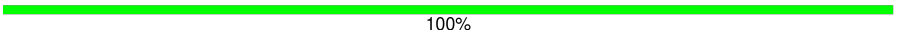


• Molecule 10: Photosystem II reaction center protein K

Chain k:

• Molecule 11: Photosystem II reaction center protein L

Chain L:



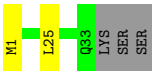
There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem II reaction center protein L

Chain l:

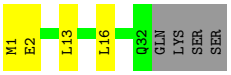
• Molecule 12: Photosystem II reaction center protein M

Chain M:



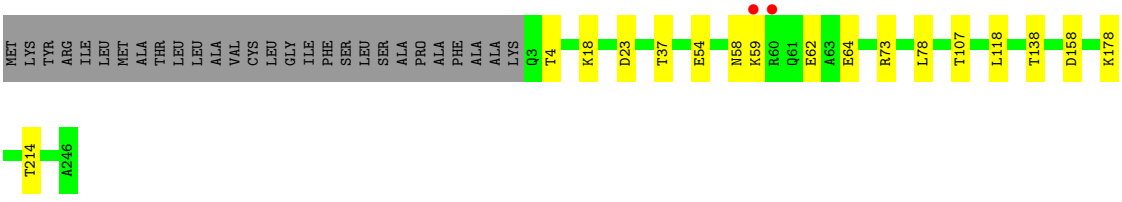
• Molecule 12: Photosystem II reaction center protein M

Chain m:



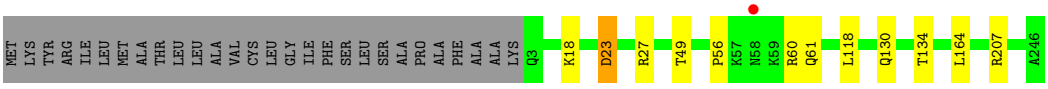
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



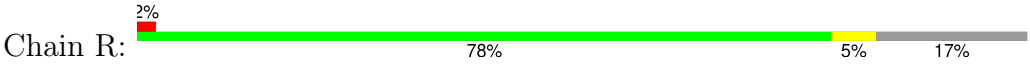
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

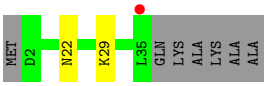
Chain o:



• Molecule 14: Photosystem II protein Y

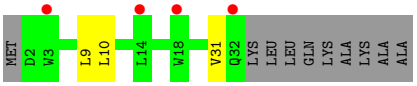
Chain R:





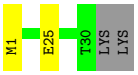
• Molecule 14: Photosystem II protein Y

Chain r:



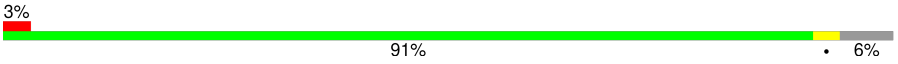
• Molecule 15: Photosystem II reaction center protein T

Chain T:



• Molecule 15: Photosystem II reaction center protein T

Chain t:



• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:

• Molecule 16: Photosystem II 12 kDa extrinsic protein

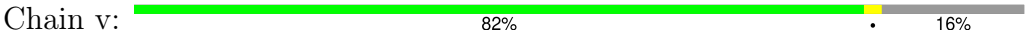
Chain u:

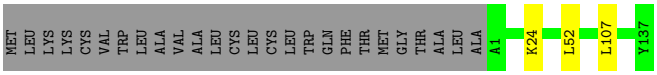
• Molecule 17: Cytochrome c-550

Chain V:

• Molecule 17: Cytochrome c-550

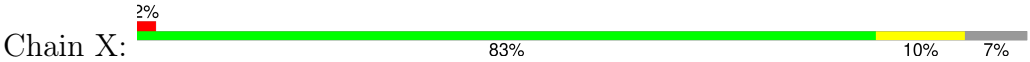
Chain v:

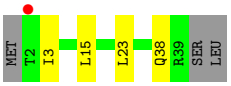




• Molecule 18: Photosystem II reaction center X protein

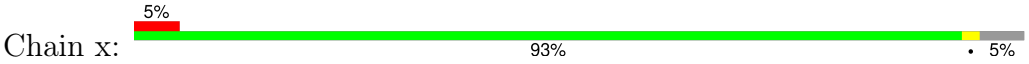
Chain X:





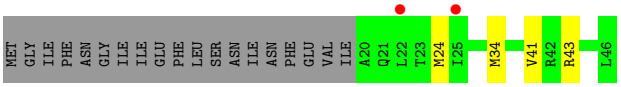
• Molecule 18: Photosystem II reaction center X protein

Chain x:



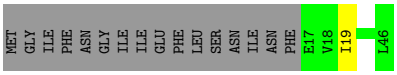
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



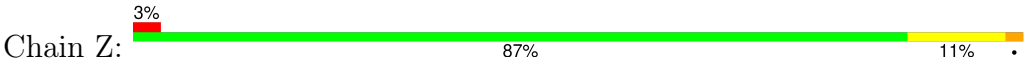
• Molecule 19: Photosystem II reaction center protein Ycf12

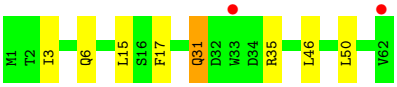
Chain y:



• Molecule 20: Photosystem II reaction center protein Z

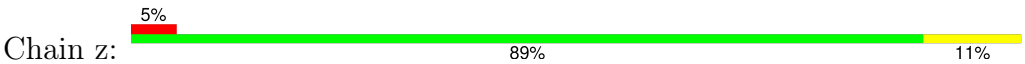
Chain Z:

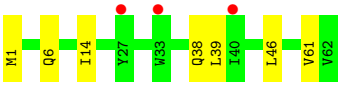




• Molecule 20: Photosystem II reaction center protein Z

Chain z:




M1
Q6
I14
Y27
W33
Q38
L39
I40
L46
V61
V62

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.65-2.09) 84.9 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.182 , 0.241 0.182 , 0.240	Depositor DCC
R_{free} test set	4165 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.3	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	106211	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, LMG, BCR, HEC, DGD, FME, CL, PL9, OEY, BCT, STE, OEX, CLA, PHO, FE2, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.62	0/3227	0.68	2/4397 (0.0%)
1	a	0.62	0/3224	0.68	0/4393
2	B	0.64	0/4161	0.71	1/5669 (0.0%)
2	b	0.64	0/4118	0.68	0/5611
3	C	0.64	0/3647	0.67	1/4965 (0.0%)
3	c	0.60	0/3719	0.68	1/5061 (0.0%)
4	D	0.67	0/2825	0.70	0/3847
4	d	0.65	0/2834	0.71	0/3859
5	E	0.53	0/688	0.58	0/940
5	e	0.49	0/683	0.55	0/932
6	F	0.51	0/284	0.51	0/387
6	f	0.48	0/284	0.62	0/387
7	H	0.65	0/523	0.68	0/713
7	h	0.58	0/511	0.67	0/697
8	I	0.60	0/293	0.61	0/396
8	i	0.68	0/293	0.61	0/396
9	J	0.54	0/263	0.61	0/356
9	j	0.56	0/263	0.59	0/356
10	K	0.55	0/303	0.60	0/416
10	k	0.53	0/303	0.65	0/416
11	L	0.64	0/311	0.72	0/422
11	l	0.68	0/303	0.74	0/412
12	M	0.65	0/249	0.67	0/341
12	m	0.70	0/244	0.67	0/334
13	O	0.61	0/1904	0.73	1/2585 (0.0%)
13	o	0.61	0/1905	0.73	1/2583 (0.0%)
14	R	0.44	0/277	0.60	0/380
14	r	0.41	0/246	0.60	0/339
15	T	0.75	0/257	0.72	0/349
15	t	0.71	0/255	0.64	0/346
16	U	0.58	0/785	0.68	0/1064
16	u	0.62	0/785	0.74	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	V	0.60	0/1085	0.73	1/1473 (0.1%)
17	v	0.58	0/1085	0.67	0/1473
18	X	0.50	0/284	0.60	0/384
18	x	0.41	0/289	0.55	0/391
19	Y	0.43	0/197	0.56	0/264
19	y	0.38	0/219	0.55	0/294
20	Z	0.49	0/490	0.62	0/669
20	z	0.40	0/488	0.51	0/666
All	All	0.61	0/44104	0.68	8/60027 (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
17	V	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	V	63	THR	C-N-CD	-7.20	104.76	120.60
2	B	15	ASP	CB-CG-OD2	-6.76	112.21	118.30
3	C	396	MET	CG-SD-CE	-5.43	91.51	100.20
1	A	183[A]	MET	CA-CB-CG	5.29	122.29	113.30
1	A	183[B]	MET	CA-CB-CG	5.29	122.29	113.30
13	O	158	ASP	CB-CG-OD1	5.28	123.05	118.30
3	c	370	ARG	NE-CZ-NH2	5.10	122.85	120.30
13	o	27	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	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	397/344 (115%)	387 (98%)	10 (2%)	0	100	100
1	a	397/344 (115%)	387 (98%)	9 (2%)	1 (0%)	37	37
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	11 (2%)	1 (0%)	44	45
3	C	454/461 (98%)	440 (97%)	13 (3%)	1 (0%)	44	45
3	c	463/461 (100%)	447 (96%)	15 (3%)	1 (0%)	44	45
4	D	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	8	4
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	33 (94%)	1 (3%)	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	228 (94%)	11 (4%)	4 (2%)	8	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	242/272 (89%)	228 (94%)	12 (5%)	2 (1%)	16 13
14	R	32/41 (78%)	27 (84%)	5 (16%)	0	100 100
14	r	29/41 (71%)	27 (93%)	1 (3%)	1 (3%)	3 1
15	T	28/32 (88%)	28 (100%)	0	0	100 100
15	t	28/32 (88%)	28 (100%)	0	0	100 100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100 100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	12 8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	19 16
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100 100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100 100
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100 100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2 0
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100 100
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7 4
20	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7 4
All	All	5396/5700 (95%)	5212 (97%)	166 (3%)	18 (0%)	37 37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	59	LYS
17	V	64	PRO
14	r	31	VAL
13	O	62	GLU
3	c	416	SER
16	u	53	ALA
19	Y	43	ARG
2	b	294	SER
20	Z	31	GLN
13	O	138	THR
13	o	23	ASP
7	H	12	ARG
13	O	73	ARG
1	a	259	ILE
13	o	56	PRO

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Mol	Chain	Res	Type
20	z	61	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	324/280 (116%)	323 (100%)	1 (0%)	91 94
1	a	323/280 (115%)	311 (96%)	12 (4%)	29 31
2	B	408/407 (100%)	398 (98%)	10 (2%)	42 47
2	b	402/407 (99%)	387 (96%)	15 (4%)	29 31
3	C	356/362 (98%)	348 (98%)	8 (2%)	47 53
3	c	364/362 (101%)	345 (95%)	19 (5%)	19 18
4	D	277/283 (98%)	275 (99%)	2 (1%)	81 87
4	d	278/283 (98%)	270 (97%)	8 (3%)	37 41
5	E	72/73 (99%)	69 (96%)	3 (4%)	25 26
5	e	71/73 (97%)	67 (94%)	4 (6%)	17 16
6	F	28/39 (72%)	28 (100%)	0	100 100
6	f	28/39 (72%)	27 (96%)	1 (4%)	30 32
7	H	54/55 (98%)	50 (93%)	4 (7%)	11 9
7	h	53/55 (96%)	49 (92%)	4 (8%)	11 9
8	I	32/34 (94%)	30 (94%)	2 (6%)	15 13
8	i	32/34 (94%)	31 (97%)	1 (3%)	35 39
9	J	24/28 (86%)	24 (100%)	0	100 100
9	j	24/28 (86%)	23 (96%)	1 (4%)	25 26
10	K	30/37 (81%)	27 (90%)	3 (10%)	6 4
10	k	30/37 (81%)	28 (93%)	2 (7%)	13 11
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	34/35 (97%)	30 (88%)	4 (12%)	4 2
12	M	28/32 (88%)	27 (96%)	1 (4%)	30 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	m	28/32 (88%)	25 (89%)	3 (11%)	5 3
13	O	206/228 (90%)	194 (94%)	12 (6%)	17 15
13	o	207/228 (91%)	197 (95%)	10 (5%)	21 21
14	R	28/33 (85%)	26 (93%)	2 (7%)	12 10
14	r	23/33 (70%)	21 (91%)	2 (9%)	8 6
15	T	26/28 (93%)	25 (96%)	1 (4%)	28 30
15	t	25/28 (89%)	25 (100%)	0	100 100
16	U	84/112 (75%)	82 (98%)	2 (2%)	44 49
16	u	84/112 (75%)	84 (100%)	0	100 100
17	V	117/138 (85%)	115 (98%)	2 (2%)	56 63
17	v	117/138 (85%)	114 (97%)	3 (3%)	41 46
18	X	31/34 (91%)	27 (87%)	4 (13%)	3 2
18	x	31/34 (91%)	30 (97%)	1 (3%)	34 37
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2 1
19	y	22/37 (60%)	21 (96%)	1 (4%)	23 24
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2 1
20	z	51/52 (98%)	45 (88%)	6 (12%)	4 2
All	All	4458/4654 (96%)	4293 (96%)	165 (4%)	28 31

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

Mol	Chain	Res	Type
1	A	243	GLU
2	B	86	ILE
2	B	98	LEU
2	B	127	ARG
2	B	240	SER
2	B	246	PHE
2	B	298	LEU
2	B	362	PHE
2	B	371	THR
2	B	472	ARG
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	156	LYS

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Mol	Chain	Res	Type
3	C	199	ILE
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	180	ARG
4	D	345	VAL
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
7	H	20	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
8	I	4	LEU
8	I	6	ILE
10	K	10	LYS
10	K	13	GLU
10	K	19	ASP
12	M	25	LEU
13	O	4	THR
13	O	18	LYS
13	O	23	ASP
13	O	37	THR
13	O	54	GLU
13	O	58	ASN
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	178	LYS
13	O	214	THR
14	R	22	ASN
14	R	29	LYS
15	T	25	GLU
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
18	X	3	ILE
18	X	15	LEU
18	X	23	LEU

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Mol	Chain	Res	Type
18	X	38	GLN
19	Y	24	MET
19	Y	34	MET
19	Y	41	VAL
20	Z	3	ILE
20	Z	6	GLN
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	134	SER
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	245	THR
1	a	266	ASN
1	a	288	LEU
2	b	14	ASN
2	b	74	SER
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	246	PHE
2	b	266	GLU
2	b	286	ARG
2	b	362	PHE
2	b	485	GLU
2	b	487	SER
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	29	GLU

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Mol	Chain	Res	Type
3	c	72	LEU
3	c	78	GLU
3	c	99	VAL
3	c	104	GLU
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	144	SER
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	346	THR
3	c	418	ASN
3	c	471	SER
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	16	SER
5	e	54	SER
5	e	65	LEU
6	f	28	VAL
7	h	3	ARG
7	h	7	LEU
7	h	27	THR
7	h	49	TYR
8	i	33	LYS
9	j	7	ARG
10	k	10	LYS
10	k	19	ASP
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	2	GLU

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Mol	Chain	Res	Type
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS
13	o	23	ASP
13	o	49	THR
13	o	60	ARG
13	o	61	GLN
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	164	LEU
13	o	207	ARG
14	r	9	LEU
14	r	10	LEU
17	v	24	LYS
17	v	52	LEU
17	v	107	LEU
18	x	2	THR
19	y	19	ILE
20	z	1	MET
20	z	6	GLN
20	z	14	ILE
20	z	38	GLN
20	z	39	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
13	O	3	GLN
13	O	36	GLN
13	O	82	GLN
13	O	88	ASN
18	X	38	GLN
20	Z	6	GLN
20	Z	31	GLN
1	a	19	ASN
1	a	234	ASN
1	a	266	ASN
12	m	5	GLN
13	o	61	GLN

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Mol	Chain	Res	Type
13	o	200	ASN
16	u	78	ASN
18	x	33	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	1.20	1 (12%)	8,9,11	1.45	1 (12%)
8	FME	I	1	8	8,9,10	1.04	1 (12%)	8,9,11	0.95	0
8	FME	i	1	8	8,9,10	1.12	1 (12%)	8,9,11	1.90	3 (37%)
15	FME	T	1	15	8,9,10	1.12	1 (12%)	8,9,11	1.19	1 (12%)
12	FME	M	1	12	8,9,10	1.14	1 (12%)	8,9,11	0.96	0
15	FME	t	1	15	8,9,10	1.45	1 (12%)	8,9,11	0.98	1 (12%)

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
12	FME	m	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	t	1	15	-	2/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.01	1.42	1.46
12	m	1	FME	CA-N	-2.77	1.42	1.46
8	i	1	FME	CA-N	-2.47	1.43	1.46
12	M	1	FME	CA-N	-2.39	1.43	1.46
8	I	1	FME	CA-N	-2.37	1.43	1.46
15	T	1	FME	CB-CA	2.02	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	CA-N-CN	-3.44	117.53	122.82
8	i	1	FME	C-CA-N	2.47	114.27	109.50
8	i	1	FME	O1-CN-N	-2.31	119.35	125.32
15	t	1	FME	CB-CA-N	2.29	114.69	110.52
12	m	1	FME	CA-N-CN	-2.22	119.40	122.82
15	T	1	FME	O1-CN-N	-2.12	119.83	125.32

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 194 ligands modelled in this entry, 6 are monoatomic - leaving 188 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	$\#\|Z\| > 2$
26	SQD	B	723	-	52,54,54	0.96	2 (3%)	62,65,65	1.67	11 (17%)
23	BCR	h	701	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
22	CLA	C	503	-	63,73,73	1.57	9 (14%)	74,113,113	1.35	9 (12%)
26	SQD	b	720	-	47,49,54	0.99	2 (4%)	57,60,65	2.11	14 (24%)
22	CLA	C	512	3	63,73,73	1.46	9 (14%)	74,113,113	1.33	8 (10%)
33	LMG	d	408	-	44,44,55	1.14	6 (13%)	52,52,63	1.45	8 (15%)
22	CLA	C	514	-	63,73,73	1.51	7 (11%)	74,113,113	1.65	11 (14%)
23	BCR	B	718	-	41,41,41	1.15	4 (9%)	56,56,56	1.43	7 (12%)
28	STE	C	521	-	11,11,19	0.89	0	11,11,19	1.38	3 (27%)
26	SQD	A	412	-	38,38,54	1.06	3 (7%)	40,40,65	1.12	3 (7%)
28	STE	H	104	-	17,17,19	0.53	0	16,16,19	0.58	0
22	CLA	b	709	-	63,73,73	1.37	7 (11%)	74,113,113	1.51	8 (10%)
22	CLA	A	404	-	52,62,73	1.66	8 (15%)	60,99,113	1.76	14 (23%)
26	SQD	f	101	-	39,41,54	1.14	5 (12%)	49,52,65	1.71	12 (24%)
23	BCR	k	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.22	5 (8%)
33	LMG	B	721	-	26,26,55	0.77	0	26,26,63	1.33	2 (7%)
29	DGD	c	517	-	63,63,67	1.18	6 (9%)	77,77,81	1.35	10 (12%)
28	STE	T	702	-	14,14,19	0.51	0	13,13,19	0.58	0
33	LMG	b	721	-	51,51,55	0.97	4 (7%)	59,59,63	1.45	7 (11%)
28	STE	t	702	-	13,13,19	0.63	0	13,13,19	1.24	2 (15%)
28	STE	Z	101	-	7,7,19	0.43	0	6,6,19	0.52	0
22	CLA	b	704	-	63,73,73	1.25	6 (9%)	74,113,113	1.79	14 (18%)
27	LHG	A	410	-	48,48,48	0.81	2 (4%)	51,54,54	1.23	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
22	CLA	c	510	-	63,73,73	1.51	7 (11%)	74,113,113	1.77	12 (16%)
35	HEC	v	201	17	32,50,50	2.13	4 (12%)	30,82,82	2.28	7 (23%)
22	CLA	A	403	36	63,73,73	1.37	7 (11%)	74,113,113	1.38	10 (13%)
34	PHO	D	406	-	50,69,69	1.08	6 (12%)	48,99,99	1.36	10 (20%)
27	LHG	d	406	-	48,48,48	0.79	0	51,54,54	1.12	4 (7%)
33	LMG	M	101	-	51,51,55	1.01	3 (5%)	59,59,63	1.42	8 (13%)
34	PHO	D	407	-	50,69,69	1.16	7 (14%)	48,99,99	1.48	8 (16%)
22	CLA	b	706	-	63,73,73	1.61	8 (12%)	74,113,113	1.66	11 (14%)
31	OEY	A	416[B]	36,3,1	0,16,16	-	-	-		
28	STE	A	414	-	4,4,19	0.52	0	3,3,19	0.34	0
33	LMG	D	412	-	31,31,55	1.20	3 (9%)	33,33,63	1.09	2 (6%)
22	CLA	b	716	-	58,68,73	1.54	9 (15%)	68,107,113	1.60	9 (13%)
28	STE	x	101	-	19,19,19	0.80	0	19,19,19	0.75	1 (5%)
23	BCR	D	404	-	41,41,41	1.13	3 (7%)	56,56,56	1.26	7 (12%)
28	STE	C	522	-	15,15,19	0.47	0	14,14,19	0.81	0
23	BCR	b	717	-	41,41,41	1.20	4 (9%)	56,56,56	1.51	11 (19%)
22	CLA	b	703	-	63,73,73	1.47	9 (14%)	74,113,113	1.59	12 (16%)
28	STE	j	101	-	11,11,19	0.81	0	11,11,19	1.52	2 (18%)
22	CLA	c	513	-	63,73,73	1.30	8 (12%)	74,113,113	1.43	9 (12%)
28	STE	b	724	-	15,15,19	0.79	0	15,15,19	0.97	1 (6%)
22	CLA	D	402	36	63,73,73	1.68	8 (12%)	74,113,113	1.26	7 (9%)
22	CLA	b	707	36	63,73,73	1.71	10 (15%)	74,113,113	1.38	11 (14%)
22	CLA	a	404	36	63,73,73	1.55	6 (9%)	74,113,113	1.55	11 (14%)
22	CLA	a	403	-	63,73,73	1.59	7 (11%)	74,113,113	1.62	13 (17%)
22	CLA	c	514	-	63,73,73	1.25	6 (9%)	74,113,113	1.41	9 (12%)
22	CLA	d	401	-	63,73,73	1.29	7 (11%)	74,113,113	1.42	8 (10%)
23	BCR	t	701	-	41,41,41	1.11	3 (7%)	56,56,56	1.41	5 (8%)
28	STE	b	726	-	9,9,19	0.56	0	8,8,19	0.44	0
34	PHO	a	405	-	50,69,69	1.05	3 (6%)	48,99,99	1.28	6 (12%)
35	HEC	e	101	5,6	32,50,50	2.19	4 (12%)	30,82,82	2.61	8 (26%)
22	CLA	D	403	-	63,73,73	1.31	11 (17%)	74,113,113	1.65	12 (16%)
22	CLA	c	507	-	63,73,73	1.38	11 (17%)	74,113,113	1.51	10 (13%)
26	SQD	a	413	-	52,54,54	0.99	6 (11%)	62,65,65	1.84	12 (19%)
28	STE	d	409	-	16,16,19	0.74	0	16,16,19	1.34	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	701	36	63,73,73	1.54	8 (12%)	74,113,113	1.62	7 (9%)
26	SQD	D	409	-	34,36,54	0.96	2 (5%)	42,45,65	1.95	12 (28%)
25	PL9	d	404	-	55,55,55	1.49	8 (14%)	68,69,69	1.74	14 (20%)
28	STE	m	101	-	11,11,19	0.82	0	11,11,19	1.40	2 (18%)
22	CLA	c	511	-	63,73,73	1.44	7 (11%)	74,113,113	1.59	12 (16%)
28	STE	E	102	-	6,6,19	0.42	0	5,5,19	0.57	0
28	STE	B	725	-	17,17,19	0.75	0	17,17,19	0.85	0
22	CLA	B	706	-	63,73,73	1.61	7 (11%)	74,113,113	1.60	12 (16%)
22	CLA	B	713	-	63,73,73	1.43	9 (14%)	74,113,113	1.52	12 (16%)
22	CLA	C	507	-	63,73,73	1.27	6 (9%)	74,113,113	1.39	10 (13%)
27	LHG	a	414	-	41,41,48	0.80	1 (2%)	44,47,54	1.26	3 (6%)
22	CLA	C	506	-	63,73,73	1.41	5 (7%)	74,113,113	1.33	9 (12%)
27	LHG	l	101	-	48,48,48	0.74	1 (2%)	51,54,54	1.14	5 (9%)
22	CLA	c	509	-	62,72,73	1.46	7 (11%)	72,111,113	1.67	14 (19%)
33	LMG	a	419	-	55,55,55	1.31	7 (12%)	63,63,63	1.33	5 (7%)
22	CLA	H	102	36	63,73,73	1.84	10 (15%)	74,113,113	1.64	13 (17%)
28	STE	H	105	-	7,7,19	0.44	0	6,6,19	0.60	0
33	LMG	C	520	-	48,48,55	1.01	3 (6%)	56,56,63	1.35	8 (14%)
32	BCT	A	417	21	3,3,3	1.06	0	2,3,3	3.87	2 (100%)
23	BCR	B	717	-	41,41,41	1.16	3 (7%)	56,56,56	1.30	5 (8%)
22	CLA	B	714	-	63,73,73	1.36	7 (11%)	74,113,113	1.20	7 (9%)
22	CLA	b	714	-	63,73,73	1.41	7 (11%)	74,113,113	1.42	10 (13%)
28	STE	B	720	-	16,16,19	0.64	0	16,16,19	1.35	2 (12%)
35	HEC	E	103	5,6	32,50,50	2.10	3 (9%)	30,82,82	2.65	9 (30%)
22	CLA	C	505	36	57,67,73	1.33	6 (10%)	66,105,113	1.31	8 (12%)
27	LHG	d	407	-	38,38,48	0.89	3 (7%)	41,44,54	1.11	2 (4%)
22	CLA	C	502	-	63,73,73	1.30	11 (17%)	74,113,113	1.43	10 (13%)
22	CLA	C	504	-	63,73,73	1.80	6 (9%)	74,113,113	1.74	16 (21%)
23	BCR	B	719	-	41,41,41	1.13	3 (7%)	56,56,56	1.50	8 (14%)
30	OEX	a	420[A]	36,3,1	0,15,15	-	-	-		
28	STE	a	416	-	9,9,19	0.61	0	8,8,19	0.32	0
22	CLA	B	707	36	63,73,73	1.68	11 (17%)	74,113,113	1.54	5 (6%)
22	CLA	B	704	-	63,73,73	1.62	7 (11%)	74,113,113	1.84	13 (17%)
22	CLA	b	710	36	63,73,73	1.31	10 (15%)	74,113,113	1.38	11 (14%)
28	STE	A	411	-	15,15,19	0.52	0	14,14,19	0.70	0
29	DGD	h	702	-	63,63,67	1.22	7 (11%)	77,77,81	1.57	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	DGD	C	517	-	63,63,67	1.09	5 (7%)	77,77,81	1.30	9 (11%)
28	STE	h	703	-	13,13,19	0.43	0	12,12,19	0.72	0
33	LMG	c	522	-	48,48,55	1.22	4 (8%)	56,56,63	1.25	8 (14%)
28	STE	b	727	-	19,19,19	0.51	0	19,19,19	1.21	2 (10%)
28	STE	I	101	-	14,14,19	0.66	0	13,13,19	0.36	0
33	LMG	C	516	-	48,48,55	0.97	4 (8%)	56,56,63	1.36	6 (10%)
22	CLA	C	510	-	63,73,73	1.42	11 (17%)	74,113,113	1.52	11 (14%)
22	CLA	a	401	36	63,73,73	1.71	6 (9%)	74,113,113	1.68	12 (16%)
25	PL9	a	411	-	55,55,55	0.88	1 (1%)	68,69,69	1.62	10 (14%)
23	BCR	Y	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.17	4 (7%)
23	BCR	A	405	-	41,41,41	1.14	3 (7%)	56,56,56	1.40	8 (14%)
28	STE	E	101	-	11,11,19	0.95	0	11,11,19	0.84	0
32	BCT	a	410	21	3,3,3	1.16	0	2,3,3	3.26	2 (100%)
33	LMG	c	520	-	37,37,55	1.22	5 (13%)	45,45,63	1.30	4 (8%)
23	BCR	k	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.12	3 (5%)
22	CLA	c	506	-	63,73,73	1.26	6 (9%)	74,113,113	1.36	10 (13%)
29	DGD	C	519	-	63,63,67	0.96	5 (7%)	77,77,81	1.42	12 (15%)
23	BCR	b	718	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	6 (10%)
27	LHG	D	411	-	46,46,48	1.24	5 (10%)	49,52,54	1.26	5 (10%)
23	BCR	C	501	-	41,41,41	1.08	3 (7%)	56,56,56	1.17	3 (5%)
28	STE	b	722	-	19,19,19	0.64	0	19,19,19	0.89	0
22	CLA	C	509	-	63,73,73	1.65	6 (9%)	74,113,113	1.56	7 (9%)
23	BCR	a	407	-	41,41,41	1.10	4 (9%)	56,56,56	1.44	13 (23%)
22	CLA	c	502	-	63,73,73	1.26	8 (12%)	74,113,113	1.53	8 (10%)
23	BCR	b	719	-	41,41,41	1.10	2 (4%)	56,56,56	1.41	8 (14%)
28	STE	X	101	-	19,19,19	0.55	0	19,19,19	1.28	1 (5%)
22	CLA	c	504	-	63,73,73	1.54	9 (14%)	74,113,113	1.63	8 (10%)
22	CLA	C	508	36	63,73,73	1.47	7 (11%)	74,113,113	1.64	10 (13%)
28	STE	l	102	-	17,17,19	0.49	0	16,16,19	0.69	0
23	BCR	T	701	-	41,41,41	1.09	4 (9%)	56,56,56	1.36	7 (12%)
27	LHG	L	101	-	48,48,48	0.85	2 (4%)	51,54,54	1.26	4 (7%)
22	CLA	a	406	-	63,73,73	1.58	9 (14%)	74,113,113	1.37	9 (12%)
29	DGD	A	413	-	67,67,67	1.22	9 (13%)	81,81,81	1.54	15 (18%)
23	BCR	C	515	-	41,41,41	1.29	4 (9%)	56,56,56	1.33	7 (12%)
28	STE	c	521	-	19,19,19	0.70	0	19,19,19	1.00	2 (10%)
29	DGD	c	518	-	63,63,67	1.24	9 (14%)	77,77,81	1.43	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	SQD	A	409	-	50,52,54	1.02	4 (8%)	60,63,65	2.02	16 (26%)
23	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.30	6 (10%)
33	LMG	c	523	-	49,49,55	1.00	2 (4%)	57,57,63	1.31	6 (10%)
34	PHO	d	405	-	50,69,69	1.13	5 (10%)	48,99,99	1.34	6 (12%)
22	CLA	B	702	-	63,73,73	1.31	6 (9%)	74,113,113	1.55	12 (16%)
35	HEC	V	201	17	32,50,50	1.96	3 (9%)	30,82,82	2.94	8 (26%)
22	CLA	B	710	36	63,73,73	1.43	7 (11%)	74,113,113	1.51	8 (10%)
22	CLA	c	503	-	63,73,73	1.30	9 (14%)	74,113,113	1.52	10 (13%)
22	CLA	b	711	-	63,73,73	1.47	6 (9%)	74,113,113	1.62	11 (14%)
22	CLA	b	715	-	63,73,73	1.56	9 (14%)	74,113,113	1.50	11 (14%)
28	STE	a	417	-	11,11,19	0.89	1 (9%)	11,11,19	1.01	0
22	CLA	C	513	-	63,73,73	1.75	10 (15%)	74,113,113	1.51	13 (17%)
23	BCR	c	516	-	41,41,41	1.25	3 (7%)	56,56,56	1.43	9 (16%)
25	PL9	D	405	-	55,55,55	1.41	6 (10%)	68,69,69	1.77	15 (22%)
33	LMG	D	408	-	51,51,55	1.00	4 (7%)	59,59,63	1.27	6 (10%)
33	LMG	b	723	-	55,55,55	1.11	5 (9%)	63,63,63	1.46	11 (17%)
27	LHG	D	410	-	48,48,48	0.95	3 (6%)	51,54,54	1.23	4 (7%)
23	BCR	K	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.45	10 (17%)
22	CLA	b	713	-	63,73,73	1.51	9 (14%)	74,113,113	1.71	14 (18%)
25	PL9	A	408	-	55,55,55	1.11	4 (7%)	68,69,69	1.56	14 (20%)
27	LHG	B	722	-	48,48,48	1.10	3 (6%)	51,54,54	1.37	5 (9%)
22	CLA	c	508	36	63,73,73	1.30	6 (9%)	74,113,113	1.41	13 (17%)
31	OEY	a	421[B]	36,3,1	0,16,16	-	-	-		
28	STE	C	523	-	11,11,19	0.86	0	11,11,19	1.02	1 (9%)
28	STE	M	102	-	14,14,19	0.70	0	14,14,19	1.08	0
22	CLA	B	712	-	63,73,73	1.22	3 (4%)	74,113,113	1.60	12 (16%)
22	CLA	D	401	-	63,73,73	1.60	11 (17%)	74,113,113	1.28	7 (9%)
22	CLA	B	716	-	58,68,73	1.49	8 (13%)	68,107,113	1.72	11 (16%)
22	CLA	B	715	-	63,73,73	1.76	8 (12%)	74,113,113	1.55	11 (14%)
29	DGD	H	103	-	63,63,67	1.35	10 (15%)	77,77,81	1.47	11 (14%)
22	CLA	B	708	-	63,73,73	1.46	11 (17%)	74,113,113	1.76	13 (17%)
22	CLA	B	705	-	63,73,73	1.26	7 (11%)	74,113,113	1.44	13 (17%)
22	CLA	b	705	-	63,73,73	1.55	6 (9%)	74,113,113	1.56	10 (13%)
28	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.65	0
28	STE	B	701	-	11,11,19	0.99	0	11,11,19	1.03	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	STE	b	725	-	19,19,19	0.79	0	19,19,19	0.97	1 (5%)
22	CLA	B	709	-	63,73,73	1.34	10 (15%)	74,113,113	1.25	8 (10%)
22	CLA	b	712	-	63,73,73	1.36	9 (14%)	74,113,113	1.50	9 (12%)
22	CLA	B	711	-	63,73,73	1.39	7 (11%)	74,113,113	1.45	10 (13%)
22	CLA	A	402	-	63,73,73	1.64	7 (11%)	74,113,113	1.41	9 (12%)
30	OEX	A	415[A]	36,3,1	0,15,15	-	-	-		
27	LHG	a	412	-	48,48,48	0.88	1 (2%)	51,54,54	1.39	6 (11%)
22	CLA	C	511	-	63,73,73	1.44	7 (11%)	74,113,113	1.38	7 (9%)
22	CLA	b	708	-	63,73,73	1.50	8 (12%)	74,113,113	1.51	12 (16%)
28	STE	c	501	-	11,11,19	0.78	0	11,11,19	1.10	1 (9%)
26	SQD	a	415	-	35,35,54	1.13	2 (5%)	37,37,65	1.35	4 (10%)
29	DGD	c	519	-	63,63,67	1.29	9 (14%)	77,77,81	1.40	13 (16%)
28	STE	a	418	-	14,14,19	0.47	0	13,13,19	0.71	0
23	BCR	d	403	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	8 (14%)
22	CLA	d	402	-	63,73,73	1.33	8 (12%)	74,113,113	1.31	8 (10%)
22	CLA	b	702	-	63,73,73	1.32	8 (12%)	74,113,113	1.62	13 (17%)
29	DGD	C	518	-	63,63,67	1.36	6 (9%)	77,77,81	1.47	12 (15%)
28	STE	J	101	-	11,11,19	0.61	0	11,11,19	1.52	2 (18%)
22	CLA	B	703	-	63,73,73	1.53	9 (14%)	74,113,113	1.32	8 (10%)
22	CLA	c	512	3	63,73,73	1.75	7 (11%)	74,113,113	1.61	7 (9%)
28	STE	B	724	-	11,11,19	0.73	0	11,11,19	1.20	1 (9%)
22	CLA	c	505	36	58,68,73	1.40	8 (13%)	68,107,113	1.56	7 (10%)
28	STE	B	726	-	15,15,19	0.50	0	14,14,19	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	B	723	-	-	28/49/69/69	0/1/1/1
23	BCR	h	701	-	-	7/29/63/63	0/2/2/2
22	CLA	C	503	-	-	8/37/115/115	-
26	SQD	b	720	-	-	21/44/64/69	0/1/1/1
22	CLA	C	512	3	1/1/20/20	6/37/115/115	-
33	LMG	d	408	-	-	12/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	514	-	1/1/20/20	15/37/115/115	-
23	BCR	B	718	-	-	7/29/63/63	0/2/2/2
28	STE	C	521	-	-	2/9/9/17	-
26	SQD	A	412	-	-	15/39/39/69	-
28	STE	H	104	-	-	6/15/15/17	-
22	CLA	b	709	-	1/1/20/20	9/37/115/115	-
22	CLA	A	404	-	1/1/17/20	4/24/102/115	-
26	SQD	f	101	-	-	14/36/56/69	0/1/1/1
23	BCR	k	102	-	-	3/29/63/63	0/2/2/2
33	LMG	B	721	-	-	12/22/22/70	-
29	DGD	c	517	-	-	22/51/91/95	0/2/2/2
28	STE	T	702	-	-	8/12/12/17	-
33	LMG	b	721	-	-	15/46/66/70	0/1/1/1
28	STE	t	702	-	-	4/11/11/17	-
28	STE	Z	101	-	-	3/5/5/17	-
22	CLA	b	704	-	1/1/20/20	7/37/115/115	-
27	LHG	A	410	-	-	28/53/53/53	-
23	BCR	c	515	-	-	11/29/63/63	0/2/2/2
22	CLA	c	510	-	1/1/20/20	10/37/115/115	-
35	HEC	v	201	17	-	2/10/54/54	-
22	CLA	A	403	36	-	10/37/115/115	-
34	PHO	D	406	-	-	4/37/103/103	0/5/6/6
27	LHG	d	406	-	-	14/53/53/53	-
33	LMG	M	101	-	-	24/46/66/70	0/1/1/1
34	PHO	D	407	-	-	2/37/103/103	0/5/6/6
22	CLA	b	706	-	1/1/20/20	8/37/115/115	-
28	STE	A	414	-	-	1/2/2/17	-
33	LMG	D	412	-	-	14/33/33/70	-
22	CLA	b	716	-	1/1/19/20	11/31/109/115	-
28	STE	x	101	-	-	11/17/17/17	-
23	BCR	D	404	-	-	10/29/63/63	0/2/2/2
28	STE	C	522	-	-	3/13/13/17	-
23	BCR	b	717	-	-	8/29/63/63	0/2/2/2
22	CLA	b	703	-	1/1/20/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	j	101	-	-	2/9/9/17	-
22	CLA	c	513	-	1/1/20/20	19/37/115/115	-
28	STE	b	724	-	-	12/13/13/17	-
22	CLA	D	402	36	1/1/20/20	5/37/115/115	-
22	CLA	b	707	36	1/1/20/20	15/37/115/115	-
22	CLA	a	404	36	-	1/37/115/115	-
22	CLA	a	403	-	-	7/37/115/115	-
22	CLA	c	514	-	1/1/20/20	7/37/115/115	-
22	CLA	d	401	-	-	8/37/115/115	-
23	BCR	t	701	-	-	9/29/63/63	0/2/2/2
28	STE	b	726	-	-	4/7/7/17	-
34	PHO	a	405	-	-	5/37/103/103	0/5/6/6
35	HEC	e	101	5,6	-	2/10/54/54	-
22	CLA	c	507	-	1/1/20/20	15/37/115/115	-
22	CLA	D	403	-	-	7/37/115/115	-
26	SQD	a	413	-	-	22/49/69/69	0/1/1/1
28	STE	d	409	-	-	6/14/14/17	-
22	CLA	b	701	36	1/1/20/20	9/37/115/115	-
26	SQD	D	409	-	-	6/28/48/69	0/1/1/1
25	PL9	d	404	-	-	18/53/73/73	0/1/1/1
28	STE	m	101	-	-	2/9/9/17	-
22	CLA	c	511	-	1/1/20/20	9/37/115/115	-
28	STE	E	102	-	-	1/4/4/17	-
28	STE	B	725	-	-	6/15/15/17	-
22	CLA	B	706	-	1/1/20/20	4/37/115/115	-
22	CLA	B	713	-	1/1/20/20	14/37/115/115	-
22	CLA	C	507	-	1/1/20/20	8/37/115/115	-
27	LHG	a	414	-	-	20/46/46/53	-
22	CLA	C	506	-	1/1/20/20	13/37/115/115	-
27	LHG	l	101	-	-	23/53/53/53	-
22	CLA	c	509	-	-	5/36/114/115	-
33	LMG	a	419	-	-	23/50/70/70	0/1/1/1
22	CLA	H	102	36	1/1/20/20	13/37/115/115	-
28	STE	H	105	-	-	3/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	520	-	-	20/43/63/70	0/1/1/1
23	BCR	B	717	-	-	8/29/63/63	0/2/2/2
22	CLA	B	714	-	1/1/20/20	10/37/115/115	-
22	CLA	b	714	-	1/1/20/20	13/37/115/115	-
28	STE	B	720	-	-	9/14/14/17	-
35	HEC	E	103	5,6	-	2/10/54/54	-
22	CLA	C	505	36	1/1/18/20	4/30/108/115	-
27	LHG	d	407	-	-	11/43/43/53	-
22	CLA	C	502	-	1/1/20/20	4/37/115/115	-
22	CLA	C	504	-	1/1/20/20	5/37/115/115	-
23	BCR	B	719	-	-	1/29/63/63	0/2/2/2
28	STE	a	416	-	-	4/7/7/17	-
22	CLA	B	707	36	1/1/20/20	5/37/115/115	-
22	CLA	B	704	-	1/1/20/20	10/37/115/115	-
22	CLA	b	710	36	1/1/20/20	4/37/115/115	-
28	STE	A	411	-	-	7/13/13/17	-
29	DGD	h	702	-	-	14/51/91/95	0/2/2/2
29	DGD	C	517	-	-	21/51/91/95	0/2/2/2
28	STE	h	703	-	-	6/11/11/17	-
33	LMG	c	522	-	-	25/43/63/70	0/1/1/1
28	STE	b	727	-	-	9/17/17/17	-
28	STE	I	101	-	-	4/12/12/17	-
33	LMG	C	516	-	-	18/43/63/70	0/1/1/1
22	CLA	C	510	-	1/1/20/20	13/37/115/115	-
22	CLA	a	401	36	1/1/20/20	5/37/115/115	-
25	PL9	a	411	-	-	20/53/73/73	0/1/1/1
23	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
23	BCR	A	405	-	-	5/29/63/63	0/2/2/2
28	STE	E	101	-	-	5/9/9/17	-
33	LMG	c	520	-	-	12/31/51/70	0/1/1/1
23	BCR	k	101	-	-	13/29/63/63	0/2/2/2
22	CLA	c	506	-	1/1/20/20	11/37/115/115	-
29	DGD	C	519	-	-	15/51/91/95	0/2/2/2
23	BCR	b	718	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	D	411	-	-	21/51/51/53	-
23	BCR	C	501	-	-	12/29/63/63	0/2/2/2
28	STE	b	722	-	-	10/17/17/17	-
22	CLA	C	509	-	-	5/37/115/115	-
23	BCR	a	407	-	-	3/29/63/63	0/2/2/2
22	CLA	c	502	-	1/1/20/20	3/37/115/115	-
23	BCR	b	719	-	-	5/29/63/63	0/2/2/2
28	STE	X	101	-	-	9/17/17/17	-
22	CLA	c	504	-	1/1/20/20	8/37/115/115	-
22	CLA	C	508	36	1/1/20/20	9/37/115/115	-
28	STE	l	102	-	-	5/15/15/17	-
23	BCR	T	701	-	-	4/29/63/63	0/2/2/2
27	LHG	L	101	-	-	20/53/53/53	-
22	CLA	a	406	-	1/1/20/20	10/37/115/115	-
29	DGD	A	413	-	-	27/55/95/95	0/2/2/2
23	BCR	C	515	-	-	6/29/63/63	0/2/2/2
28	STE	c	521	-	-	7/17/17/17	-
29	DGD	c	518	-	-	26/51/91/95	0/2/2/2
26	SQD	A	409	-	-	21/47/67/69	0/1/1/1
23	BCR	H	101	-	-	5/29/63/63	0/2/2/2
33	LMG	c	523	-	-	21/44/64/70	0/1/1/1
34	PHO	d	405	-	-	6/37/103/103	0/5/6/6
22	CLA	B	702	-	1/1/20/20	8/37/115/115	-
35	HEC	V	201	17	-	2/10/54/54	-
22	CLA	B	710	36	1/1/20/20	6/37/115/115	-
22	CLA	c	503	-	1/1/20/20	5/37/115/115	-
22	CLA	b	711	-	1/1/20/20	7/37/115/115	-
22	CLA	b	715	-	1/1/20/20	10/37/115/115	-
28	STE	a	417	-	-	4/9/9/17	-
22	CLA	C	513	-	1/1/20/20	14/37/115/115	-
23	BCR	c	516	-	-	3/29/63/63	0/2/2/2
25	PL9	D	405	-	-	13/53/73/73	0/1/1/1
33	LMG	D	408	-	-	13/46/66/70	0/1/1/1
33	LMG	b	723	-	-	21/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	D	410	-	-	17/53/53/53	-
23	BCR	K	101	-	-	7/29/63/63	0/2/2/2
22	CLA	b	713	-	1/1/20/20	5/37/115/115	-
25	PL9	A	408	-	-	22/53/73/73	0/1/1/1
27	LHG	B	722	-	-	17/53/53/53	-
22	CLA	c	508	36	1/1/20/20	3/37/115/115	-
28	STE	C	523	-	-	6/9/9/17	-
28	STE	M	102	-	-	5/12/12/17	-
22	CLA	B	712	-	1/1/20/20	8/37/115/115	-
22	CLA	D	401	-	1/1/20/20	5/37/115/115	-
22	CLA	B	716	-	1/1/19/20	10/31/109/115	-
22	CLA	B	715	-	1/1/20/20	5/37/115/115	-
29	DGD	H	103	-	-	18/51/91/95	0/2/2/2
22	CLA	B	708	-	1/1/20/20	3/37/115/115	-
22	CLA	B	705	-	1/1/20/20	7/37/115/115	-
22	CLA	b	705	-	1/1/20/20	11/37/115/115	-
28	STE	M	103	-	-	4/7/7/17	-
28	STE	B	701	-	-	4/9/9/17	-
28	STE	b	725	-	-	8/17/17/17	-
22	CLA	B	709	-	-	3/37/115/115	-
22	CLA	b	712	-	1/1/20/20	5/37/115/115	-
22	CLA	B	711	-	-	7/37/115/115	-
22	CLA	A	402	-	1/1/20/20	6/37/115/115	-
27	LHG	a	412	-	-	25/53/53/53	-
22	CLA	C	511	-	1/1/20/20	9/37/115/115	-
22	CLA	b	708	-	1/1/20/20	9/37/115/115	-
28	STE	c	501	-	-	4/9/9/17	-
26	SQD	a	415	-	-	18/37/37/69	-
29	DGD	c	519	-	-	18/51/91/95	0/2/2/2
28	STE	a	418	-	-	4/12/12/17	-
23	BCR	d	403	-	-	10/29/63/63	0/2/2/2
22	CLA	d	402	-	-	7/37/115/115	-
22	CLA	b	702	-	-	8/37/115/115	-
29	DGD	C	518	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	STE	J	101	-	-	4/9/9/17	-
22	CLA	B	703	-	1/1/20/20	11/37/115/115	-
22	CLA	c	512	3	1/1/20/20	12/37/115/115	-
28	STE	B	724	-	-	4/9/9/17	-
22	CLA	c	505	36	1/1/19/20	7/31/109/115	-
28	STE	B	726	-	-	5/13/13/17	-

All (830) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CHB-C4A	8.47	1.40	1.33
22	a	401	CLA	CHB-C4A	8.41	1.40	1.33
22	D	402	CLA	CHB-C4A	8.26	1.40	1.33
22	B	706	CLA	CHB-C4A	8.19	1.40	1.33
22	A	402	CLA	CHB-C4A	8.19	1.40	1.33
22	C	504	CLA	MG-NA	8.03	2.25	2.06
22	c	504	CLA	CHB-C4A	7.60	1.40	1.33
22	B	707	CLA	CHB-C4A	7.56	1.40	1.33
22	B	704	CLA	CHB-C4A	7.54	1.40	1.33
22	C	509	CLA	CHB-C4A	7.31	1.39	1.33
22	B	715	CLA	CHB-C4A	7.20	1.39	1.33
22	c	509	CLA	CHB-C4A	7.07	1.39	1.33
35	e	101	HEC	C2B-C3B	-7.02	1.32	1.40
22	C	513	CLA	MG-ND	-6.94	1.92	2.05
22	H	102	CLA	MG-NA	6.91	2.22	2.06
22	c	511	CLA	CHB-C4A	6.86	1.39	1.33
22	b	701	CLA	CHB-C4A	6.82	1.39	1.33
22	b	707	CLA	MG-ND	-6.72	1.92	2.05
22	C	509	CLA	MG-NA	6.69	2.22	2.06
35	v	201	HEC	C2B-C3B	-6.62	1.33	1.40
22	c	510	CLA	CHB-C4A	6.59	1.39	1.33
22	C	506	CLA	CHB-C4A	6.59	1.39	1.33
22	b	708	CLA	CHB-C4A	6.58	1.39	1.33
22	b	705	CLA	CHB-C4A	6.56	1.39	1.33
35	V	201	HEC	C2B-C3B	-6.53	1.33	1.40
22	a	403	CLA	CHB-C4A	6.48	1.39	1.33
22	A	404	CLA	MG-ND	-6.48	1.92	2.05
22	a	404	CLA	CHB-C4A	6.39	1.39	1.33
22	C	514	CLA	CHB-C4A	6.38	1.39	1.33
22	C	503	CLA	CHB-C4A	6.34	1.39	1.33
22	b	714	CLA	CHB-C4A	6.30	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	715	CLA	CHB-C4A	6.27	1.38	1.33
22	b	705	CLA	MG-ND	6.21	2.18	2.05
22	C	504	CLA	CHB-C4A	6.17	1.38	1.33
22	B	715	CLA	MG-NA	6.12	2.20	2.06
22	B	714	CLA	CHB-C4A	6.11	1.38	1.33
22	a	401	CLA	MG-NA	6.10	2.20	2.06
22	C	511	CLA	CHB-C4A	6.09	1.38	1.33
22	H	102	CLA	MG-ND	-6.08	1.93	2.05
35	E	103	HEC	C3C-C2C	-6.07	1.33	1.40
22	b	706	CLA	MG-NA	6.06	2.20	2.06
22	D	401	CLA	CHB-C4A	6.05	1.38	1.33
22	a	406	CLA	MG-ND	-6.02	1.93	2.05
22	b	716	CLA	CHB-C4A	5.97	1.38	1.33
35	E	103	HEC	C2B-C3B	-5.96	1.34	1.40
22	b	713	CLA	MG-NA	5.95	2.20	2.06
22	b	711	CLA	CHB-C4A	5.91	1.38	1.33
22	B	704	CLA	MG-NC	5.90	2.20	2.06
22	c	508	CLA	CHB-C4A	5.90	1.38	1.33
22	B	703	CLA	CHB-C4A	5.81	1.38	1.33
22	C	513	CLA	CHB-C4A	5.78	1.38	1.33
22	b	703	CLA	MG-NA	5.76	2.20	2.06
22	C	503	CLA	MG-NA	5.72	2.19	2.06
22	b	711	CLA	MG-NA	5.71	2.19	2.06
22	a	406	CLA	CHB-C4A	5.68	1.38	1.33
22	b	712	CLA	MG-ND	-5.67	1.94	2.05
35	e	101	HEC	C3C-C2C	-5.66	1.34	1.40
22	C	508	CLA	CHB-C4A	5.60	1.38	1.33
22	B	710	CLA	CHB-C4A	5.59	1.38	1.33
22	b	707	CLA	MG-NA	5.55	2.19	2.06
22	B	716	CLA	MG-NA	5.53	2.19	2.06
22	B	708	CLA	CHB-C4A	5.47	1.38	1.33
22	c	514	CLA	CHB-C4A	5.47	1.38	1.33
22	D	401	CLA	MG-NA	5.44	2.19	2.06
22	b	713	CLA	CHB-C4A	5.25	1.37	1.33
22	A	404	CLA	CHB-C4A	5.22	1.37	1.33
22	H	102	CLA	CHB-C4A	5.19	1.37	1.33
22	C	513	CLA	MG-NA	5.18	2.18	2.06
22	b	706	CLA	CHB-C4A	5.16	1.37	1.33
35	v	201	HEC	C3C-C2C	-5.15	1.35	1.40
22	C	507	CLA	CHB-C4A	5.09	1.37	1.33
22	a	403	CLA	MG-NC	5.06	2.18	2.06
22	B	716	CLA	CHB-C4A	5.05	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	515	BCR	C1-C6	-5.03	1.47	1.53
22	c	506	CLA	CHB-C4A	5.02	1.37	1.33
22	B	703	CLA	MG-ND	5.02	2.15	2.05
22	C	512	CLA	MG-NA	5.01	2.18	2.06
33	a	419	LMG	C4-C5	5.01	1.63	1.53
35	e	101	HEC	C3D-C2D	4.98	1.52	1.37
35	V	201	HEC	C3C-C2C	-4.98	1.35	1.40
22	B	713	CLA	MG-ND	-4.89	1.96	2.05
22	C	508	CLA	MG-NA	4.88	2.17	2.06
22	B	710	CLA	C3B-C2B	-4.86	1.33	1.40
22	c	502	CLA	CHB-C4A	4.86	1.37	1.33
25	d	404	PL9	C6-C1	-4.86	1.40	1.48
35	E	103	HEC	C3D-C2D	4.82	1.52	1.37
22	B	713	CLA	CHB-C4A	4.81	1.37	1.33
22	a	404	CLA	C1D-ND	4.78	1.44	1.37
35	v	201	HEC	C3D-C2D	4.73	1.51	1.37
22	A	403	CLA	CHB-C4A	4.71	1.37	1.33
22	b	706	CLA	C1D-ND	4.69	1.44	1.37
22	c	507	CLA	CHB-C4A	4.69	1.37	1.33
22	c	510	CLA	MG-ND	4.68	2.15	2.05
22	C	512	CLA	CHB-C4A	4.68	1.37	1.33
22	B	709	CLA	CHB-C4A	4.66	1.37	1.33
22	c	512	CLA	MG-NA	4.66	2.17	2.06
22	b	704	CLA	CHB-C4A	4.65	1.37	1.33
22	c	505	CLA	MG-NC	4.62	2.17	2.06
22	B	711	CLA	CHB-C4A	4.62	1.37	1.33
22	b	709	CLA	MG-ND	-4.61	1.96	2.05
25	d	404	PL9	C3-C4	-4.60	1.42	1.49
22	C	505	CLA	CHB-C4A	4.58	1.37	1.33
22	b	715	CLA	MG-NA	4.57	2.17	2.06
22	B	707	CLA	MG-NA	4.55	2.17	2.06
22	A	402	CLA	MG-NA	4.53	2.17	2.06
22	d	402	CLA	MG-ND	-4.51	1.96	2.05
22	a	404	CLA	MG-NC	4.48	2.16	2.06
27	B	722	LHG	O7-C5	-4.46	1.36	1.46
22	C	510	CLA	CHB-C4A	4.45	1.37	1.33
22	b	703	CLA	CHB-C4A	4.45	1.37	1.33
22	B	712	CLA	CHB-C4A	4.39	1.37	1.33
22	b	707	CLA	CHB-C4A	4.37	1.37	1.33
22	b	702	CLA	CHB-C4A	4.36	1.37	1.33
22	c	503	CLA	CHB-C4A	4.35	1.37	1.33
22	b	702	CLA	MG-NC	-4.35	1.95	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	518	DGD	C4D-C3D	4.30	1.63	1.52
33	c	523	LMG	C4-C5	4.30	1.62	1.53
22	b	709	CLA	CHB-C4A	4.30	1.37	1.33
22	D	402	CLA	MG-NA	4.30	2.16	2.06
25	d	404	PL9	C46-C44	-4.29	1.42	1.51
29	C	518	DGD	C4D-C3D	4.29	1.63	1.52
22	C	514	CLA	MG-NA	4.27	2.16	2.06
23	B	718	BCR	C30-C25	-4.25	1.48	1.53
22	b	716	CLA	MG-ND	4.23	2.14	2.05
22	C	508	CLA	MG-NC	-4.23	1.96	2.06
22	c	513	CLA	CHB-C4A	4.23	1.37	1.33
22	c	512	CLA	CHC-C1C	4.21	1.44	1.34
22	b	710	CLA	CHB-C4A	4.20	1.36	1.33
23	c	515	BCR	C1-C6	-4.20	1.48	1.53
22	C	504	CLA	MG-ND	4.19	2.14	2.05
23	A	405	BCR	C1-C6	-4.17	1.48	1.53
22	B	706	CLA	C3B-C2B	-4.17	1.34	1.40
22	B	702	CLA	CHB-C4A	4.15	1.36	1.33
22	B	711	CLA	CHC-C1C	4.13	1.44	1.34
23	c	516	BCR	C30-C25	-4.12	1.48	1.53
25	D	405	PL9	C6-C1	-4.12	1.41	1.48
29	c	517	DGD	O2G-C2G	-4.08	1.37	1.46
35	V	201	HEC	C3D-C2D	4.07	1.49	1.37
22	b	701	CLA	C1D-ND	4.06	1.43	1.37
22	d	401	CLA	CHB-C4A	4.06	1.36	1.33
22	A	403	CLA	C1D-ND	4.05	1.43	1.37
29	H	103	DGD	O5D-C1E	4.04	1.46	1.40
22	c	505	CLA	CHB-C4A	4.04	1.36	1.33
22	c	512	CLA	MG-NC	4.03	2.15	2.06
25	D	405	PL9	C52-C5	-4.03	1.42	1.50
22	C	511	CLA	MG-NC	4.03	2.15	2.06
22	B	708	CLA	MG-NA	4.02	2.15	2.06
23	b	718	BCR	C30-C25	-3.99	1.48	1.53
22	C	506	CLA	CHC-C1C	3.97	1.44	1.34
22	C	514	CLA	C1D-ND	3.96	1.43	1.37
22	c	507	CLA	MG-ND	-3.96	1.97	2.05
23	K	101	BCR	C30-C25	-3.95	1.48	1.53
22	b	708	CLA	CHC-C1C	3.95	1.44	1.34
22	b	710	CLA	C3B-C2B	-3.94	1.35	1.40
34	d	405	PHO	CAC-C3C	-3.94	1.45	1.52
22	d	402	CLA	CHB-C4A	3.91	1.36	1.33
22	D	403	CLA	MG-NA	3.86	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	715	CLA	CMB-C2B	-3.85	1.43	1.51
22	a	403	CLA	C1D-ND	3.85	1.42	1.37
22	B	715	CLA	CHC-C1C	3.84	1.44	1.34
22	C	502	CLA	CHB-C4A	3.83	1.36	1.33
22	C	512	CLA	MG-ND	-3.82	1.98	2.05
22	B	705	CLA	CHB-C4A	3.81	1.36	1.33
22	B	710	CLA	CHC-C1C	3.81	1.43	1.34
22	B	707	CLA	C1D-ND	3.81	1.42	1.37
22	C	511	CLA	CHC-C1C	3.79	1.43	1.34
22	H	102	CLA	C3B-C2B	-3.79	1.35	1.40
22	b	701	CLA	MG-NC	3.78	2.15	2.06
22	b	706	CLA	MG-NC	3.77	2.15	2.06
22	B	709	CLA	C1D-ND	3.75	1.42	1.37
29	A	413	DGD	O5D-C6D	-3.74	1.37	1.43
23	B	719	BCR	C1-C6	-3.74	1.49	1.53
22	C	510	CLA	MG-ND	3.74	2.13	2.05
22	B	715	CLA	CMB-C2B	-3.74	1.44	1.51
22	c	509	CLA	CHC-C1C	3.73	1.43	1.34
29	H	103	DGD	O1G-C1G	-3.72	1.36	1.45
23	H	101	BCR	C30-C25	-3.71	1.49	1.53
23	c	516	BCR	C1-C6	-3.70	1.49	1.53
22	b	708	CLA	MG-NC	3.69	2.15	2.06
22	H	102	CLA	CHC-C1C	3.69	1.43	1.34
22	b	709	CLA	C1D-ND	3.68	1.42	1.37
26	b	720	SQD	O48-C23	3.68	1.44	1.33
29	h	702	DGD	O2D-C2D	-3.67	1.33	1.43
23	b	717	BCR	C30-C25	-3.67	1.49	1.53
22	b	706	CLA	CHC-C1C	3.67	1.43	1.34
22	C	513	CLA	CHC-C1C	3.66	1.43	1.34
29	c	519	DGD	C6D-C5D	3.65	1.62	1.51
23	b	718	BCR	C1-C6	-3.64	1.49	1.53
22	a	403	CLA	CHC-C1C	3.64	1.43	1.34
22	B	703	CLA	C3B-C2B	-3.64	1.35	1.40
22	c	505	CLA	CHC-C1C	3.64	1.43	1.34
22	B	712	CLA	CHC-C1C	3.63	1.43	1.34
25	A	408	PL9	C7-C3	-3.63	1.46	1.51
33	c	522	LMG	O1-C1	3.63	1.46	1.40
22	C	503	CLA	CHC-C1C	3.63	1.43	1.34
33	D	412	LMG	C7-C8	3.63	1.59	1.51
22	B	706	CLA	MG-NA	3.63	2.14	2.06
29	C	518	DGD	O3G-C3G	-3.63	1.37	1.43
22	B	703	CLA	MG-NC	3.63	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	419	LMG	C4-C3	3.62	1.61	1.52
23	b	717	BCR	C1-C6	-3.61	1.49	1.53
22	C	505	CLA	CHC-C1C	3.59	1.43	1.34
22	c	506	CLA	CHC-C1C	3.58	1.43	1.34
22	b	713	CLA	CMB-C2B	-3.58	1.44	1.51
22	b	704	CLA	CHC-C1C	3.58	1.43	1.34
22	C	509	CLA	CHC-C1C	3.58	1.43	1.34
22	B	710	CLA	CMB-C2B	-3.57	1.44	1.51
26	B	723	SQD	O47-C7	3.56	1.44	1.34
22	D	401	CLA	MG-NC	-3.55	1.97	2.06
26	a	415	SQD	O47-C7	3.54	1.44	1.34
22	C	504	CLA	CHC-C1C	3.53	1.43	1.34
23	b	719	BCR	C30-C25	-3.53	1.49	1.53
33	b	723	LMG	C1-C2	3.53	1.62	1.52
29	c	519	DGD	O5D-C1E	3.53	1.46	1.40
23	Y	101	BCR	C30-C25	-3.52	1.49	1.53
22	c	510	CLA	MG-NA	-3.51	1.97	2.06
26	f	101	SQD	O48-C23	3.51	1.43	1.33
22	A	404	CLA	C1D-ND	3.51	1.42	1.37
22	C	504	CLA	C1D-ND	3.51	1.42	1.37
23	D	404	BCR	C1-C6	-3.50	1.49	1.53
22	c	513	CLA	CHC-C1C	3.50	1.43	1.34
27	D	411	LHG	P-O6	3.49	1.73	1.59
26	A	412	SQD	O47-C45	-3.49	1.41	1.47
22	b	716	CLA	C1D-ND	3.47	1.42	1.37
22	B	712	CLA	C1D-ND	3.47	1.42	1.37
29	c	518	DGD	O2E-C2E	-3.45	1.34	1.43
22	B	711	CLA	C1D-ND	3.45	1.42	1.37
22	C	507	CLA	CHC-C1C	3.45	1.43	1.34
22	D	401	CLA	CMD-C2D	-3.44	1.43	1.50
23	h	701	BCR	C1-C6	-3.44	1.49	1.53
22	d	401	CLA	C1D-ND	3.44	1.42	1.37
22	B	702	CLA	C1D-ND	3.44	1.42	1.37
22	c	511	CLA	CMB-C2B	-3.43	1.44	1.51
22	B	706	CLA	CHC-C1C	3.42	1.43	1.34
22	D	403	CLA	C1D-ND	3.42	1.42	1.37
29	c	519	DGD	C4E-C5E	-3.42	1.45	1.53
22	B	702	CLA	CHC-C1C	3.41	1.43	1.34
22	b	701	CLA	CHC-C1C	3.40	1.42	1.34
22	A	402	CLA	CHC-C1C	3.40	1.42	1.34
22	b	708	CLA	CMB-C2B	-3.39	1.44	1.51
22	b	716	CLA	MG-NC	3.39	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	709	CLA	CMB-C2B	-3.38	1.44	1.51
23	t	701	BCR	C30-C25	-3.38	1.49	1.53
22	B	705	CLA	CHC-C1C	3.36	1.42	1.34
22	b	714	CLA	CMC-C2C	-3.36	1.43	1.50
23	B	717	BCR	C1-C6	-3.36	1.49	1.53
22	b	715	CLA	MG-ND	-3.36	1.99	2.05
22	B	714	CLA	C1D-ND	3.35	1.42	1.37
22	B	715	CLA	MG-NC	3.35	2.14	2.06
22	b	714	CLA	CHC-C1C	3.33	1.42	1.34
29	C	518	DGD	O5D-C6D	-3.33	1.38	1.43
22	b	711	CLA	CHC-C1C	3.33	1.42	1.34
29	C	518	DGD	O5D-C1E	3.32	1.45	1.40
22	b	707	CLA	MG-NC	-3.32	1.98	2.06
22	a	406	CLA	CMC-C2C	-3.32	1.44	1.50
22	C	514	CLA	CHC-C1C	3.32	1.42	1.34
22	b	702	CLA	CHC-C1C	3.31	1.42	1.34
23	k	101	BCR	C1-C6	-3.31	1.49	1.53
22	c	503	CLA	CHC-C1C	3.31	1.42	1.34
26	b	720	SQD	O47-C7	3.31	1.43	1.34
29	h	702	DGD	O2G-C2G	-3.30	1.38	1.46
22	B	704	CLA	MG-NA	3.30	2.14	2.06
22	d	402	CLA	C1D-ND	3.30	1.42	1.37
22	b	710	CLA	C1D-ND	3.29	1.42	1.37
22	D	402	CLA	C1D-ND	3.29	1.42	1.37
27	D	410	LHG	P-O3	3.29	1.72	1.59
22	c	507	CLA	CHC-C1C	3.28	1.42	1.34
22	D	402	CLA	CHC-C1C	3.28	1.42	1.34
22	a	404	CLA	CHC-C1C	3.28	1.42	1.34
26	A	412	SQD	O48-C23	3.28	1.42	1.33
22	B	703	CLA	CHC-C1C	3.27	1.42	1.34
22	c	512	CLA	C1D-ND	3.27	1.42	1.37
22	d	401	CLA	CHC-C1C	3.27	1.42	1.34
22	c	508	CLA	C1D-ND	3.27	1.42	1.37
22	c	514	CLA	CHC-C1C	3.27	1.42	1.34
22	H	102	CLA	C1D-ND	3.26	1.42	1.37
22	d	401	CLA	CMB-C2B	-3.25	1.45	1.51
22	H	102	CLA	CMB-C2B	-3.25	1.45	1.51
22	C	508	CLA	CHC-C1C	3.24	1.42	1.34
22	H	102	CLA	CMC-C2C	-3.23	1.44	1.50
22	C	505	CLA	C1D-ND	3.23	1.42	1.37
27	a	412	LHG	O7-C5	-3.23	1.39	1.46
22	B	704	CLA	CHC-C1C	3.23	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	413	DGD	C6E-C5E	3.23	1.62	1.51
23	B	717	BCR	C30-C25	-3.22	1.49	1.53
27	D	411	LHG	O3-C3	-3.22	1.32	1.44
29	A	413	DGD	C3E-C2E	3.20	1.60	1.52
22	B	707	CLA	CHC-C1C	3.19	1.42	1.34
22	C	502	CLA	MG-ND	-3.18	1.99	2.05
27	d	407	LHG	P-O6	3.17	1.71	1.59
33	D	412	LMG	C9-C8	3.17	1.60	1.50
22	B	715	CLA	C1D-ND	3.17	1.42	1.37
22	D	403	CLA	CHB-C4A	3.17	1.36	1.33
22	b	708	CLA	C1D-ND	3.17	1.42	1.37
22	B	713	CLA	MG-NA	3.16	2.13	2.06
29	C	518	DGD	C1E-C2E	3.16	1.61	1.52
22	c	506	CLA	MG-ND	3.16	2.12	2.05
34	D	407	PHO	CAC-C3C	-3.16	1.46	1.52
22	C	512	CLA	CMB-C2B	-3.15	1.45	1.51
25	D	405	PL9	C21-C19	-3.15	1.44	1.51
22	B	711	CLA	CMB-C2B	-3.14	1.45	1.51
22	b	707	CLA	CHC-C1C	3.14	1.42	1.34
33	c	520	LMG	C1-C2	3.13	1.61	1.52
22	a	401	CLA	CHC-C1C	3.11	1.42	1.34
23	T	701	BCR	C30-C25	-3.11	1.49	1.53
33	a	419	LMG	O8-C9	-3.11	1.38	1.45
22	b	715	CLA	CHC-C1C	3.11	1.42	1.34
23	d	403	BCR	C30-C25	-3.10	1.49	1.53
22	B	708	CLA	CMD-C2D	-3.10	1.44	1.50
23	b	719	BCR	C1-C6	-3.10	1.49	1.53
26	D	409	SQD	O48-C23	3.10	1.42	1.33
22	C	512	CLA	CHC-C1C	3.09	1.42	1.34
22	C	511	CLA	C1D-ND	3.09	1.41	1.37
22	c	514	CLA	CMB-C2B	-3.09	1.45	1.51
22	C	502	CLA	CHC-C1C	3.08	1.42	1.34
22	B	702	CLA	CMB-C2B	-3.08	1.45	1.51
27	D	411	LHG	O8-C6	-3.07	1.38	1.45
22	C	506	CLA	MG-NA	3.07	2.13	2.06
22	B	708	CLA	C1D-ND	3.07	1.41	1.37
26	a	415	SQD	O48-C23	3.07	1.42	1.33
22	B	711	CLA	CMD-C2D	-3.07	1.44	1.50
22	b	707	CLA	C3B-C2B	-3.06	1.36	1.40
22	C	510	CLA	C1D-ND	3.06	1.41	1.37
22	B	714	CLA	C3B-C2B	-3.06	1.36	1.40
22	B	709	CLA	CMD-C2D	-3.06	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	713	CLA	C1D-ND	3.06	1.41	1.37
23	h	701	BCR	C30-C25	-3.06	1.49	1.53
22	B	706	CLA	MG-ND	3.05	2.11	2.05
22	c	513	CLA	C3B-C2B	-3.05	1.36	1.40
22	C	514	CLA	MG-ND	-3.05	1.99	2.05
23	C	501	BCR	C30-C25	-3.04	1.49	1.53
22	b	704	CLA	C1D-ND	3.04	1.41	1.37
33	c	522	LMG	C3-C2	3.04	1.60	1.52
34	a	405	PHO	CBD-CGD	-3.04	1.48	1.52
34	D	406	PHO	CAC-C3C	-3.03	1.46	1.52
22	c	510	CLA	CHC-C1C	3.03	1.42	1.34
33	c	520	LMG	O1-C1	3.02	1.45	1.40
22	B	708	CLA	MG-NC	3.02	2.13	2.06
23	c	515	BCR	C30-C25	-3.02	1.49	1.53
29	A	413	DGD	C1E-C2E	3.02	1.61	1.52
22	a	403	CLA	CMB-C2B	-3.01	1.45	1.51
26	f	101	SQD	O47-C7	3.01	1.42	1.34
22	c	504	CLA	CHC-C1C	3.01	1.42	1.34
22	c	506	CLA	C3B-C2B	-3.01	1.36	1.40
29	h	702	DGD	C1E-C2E	3.00	1.61	1.52
33	b	723	LMG	O7-C8	-3.00	1.39	1.46
22	A	403	CLA	C3B-C2B	-2.99	1.36	1.40
22	C	507	CLA	C1D-ND	2.98	1.41	1.37
34	D	407	PHO	CHA-CBD	-2.98	1.49	1.52
22	c	510	CLA	C1D-ND	2.97	1.41	1.37
22	a	406	CLA	C1C-NC	-2.97	1.33	1.37
22	c	502	CLA	C1D-ND	2.97	1.41	1.37
22	b	703	CLA	C1D-ND	2.97	1.41	1.37
22	c	505	CLA	CMD-C2D	-2.96	1.44	1.50
33	c	520	LMG	C3-C2	2.96	1.60	1.52
22	b	715	CLA	C1D-ND	2.96	1.41	1.37
33	b	721	LMG	O7-C8	-2.95	1.39	1.46
23	C	515	BCR	C36-C18	-2.95	1.44	1.50
22	D	403	CLA	CMC-C2C	-2.95	1.44	1.50
29	C	517	DGD	O2E-C2E	-2.95	1.35	1.43
33	D	408	LMG	C4-C5	2.94	1.59	1.53
22	b	705	CLA	MG-NA	2.94	2.13	2.06
22	C	504	CLA	CMB-C2B	-2.92	1.45	1.51
25	a	411	PL9	C53-C6	-2.92	1.44	1.50
26	a	413	SQD	O48-C23	2.92	1.41	1.33
22	b	716	CLA	CHC-C1C	2.92	1.41	1.34
22	c	502	CLA	CHC-C1C	2.92	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	715	CLA	CMD-C2D	-2.91	1.44	1.50
22	A	404	CLA	MG-NA	-2.91	1.99	2.06
22	B	714	CLA	CHC-C1C	2.91	1.41	1.34
22	a	406	CLA	CMD-C2D	-2.91	1.44	1.50
26	A	412	SQD	O47-C7	2.91	1.42	1.34
22	C	510	CLA	CMB-C2B	-2.90	1.45	1.51
23	k	101	BCR	C30-C25	-2.90	1.50	1.53
34	D	406	PHO	CBD-CGD	-2.89	1.48	1.52
22	b	712	CLA	CMB-C2B	-2.89	1.45	1.51
22	D	401	CLA	C1D-ND	2.89	1.41	1.37
22	b	707	CLA	CMB-C2B	-2.89	1.45	1.51
22	B	703	CLA	CMC-C2C	-2.88	1.44	1.50
27	D	411	LHG	C3-C2	2.88	1.60	1.51
22	a	404	CLA	CMB-C2B	-2.88	1.45	1.51
22	C	510	CLA	CHC-C1C	2.88	1.41	1.34
23	D	404	BCR	C30-C25	-2.86	1.50	1.53
22	B	716	CLA	CMB-C2B	-2.86	1.45	1.51
22	a	406	CLA	CMB-C2B	-2.86	1.45	1.51
22	b	707	CLA	C1D-ND	2.85	1.41	1.37
23	Y	101	BCR	C1-C6	-2.85	1.50	1.53
33	c	522	LMG	C1-C2	2.85	1.60	1.52
22	b	712	CLA	CHB-C4A	2.85	1.35	1.33
26	A	409	SQD	O47-C7	2.85	1.42	1.34
22	C	503	CLA	C3B-C2B	-2.84	1.36	1.40
22	c	511	CLA	C1D-ND	2.84	1.41	1.37
22	A	403	CLA	CHC-C1C	2.82	1.41	1.34
22	c	508	CLA	CMB-C2B	-2.82	1.46	1.51
22	B	709	CLA	CHC-C1C	2.82	1.41	1.34
23	a	407	BCR	C1-C6	-2.82	1.50	1.53
22	C	509	CLA	C1D-ND	2.81	1.41	1.37
29	c	517	DGD	O6D-C1D	2.81	1.49	1.41
22	b	705	CLA	CMB-C2B	-2.81	1.46	1.51
22	B	705	CLA	C3B-C2B	-2.81	1.36	1.40
26	A	409	SQD	O48-C23	2.81	1.41	1.33
22	C	505	CLA	MG-NC	2.80	2.12	2.06
23	T	701	BCR	C38-C26	-2.80	1.46	1.50
22	b	705	CLA	CHC-C1C	2.80	1.41	1.34
22	c	502	CLA	MG-NC	2.80	2.12	2.06
34	D	407	PHO	C3A-C2A	-2.79	1.52	1.54
23	C	501	BCR	C1-C6	-2.79	1.50	1.53
22	C	513	CLA	C1D-ND	2.79	1.41	1.37
22	C	514	CLA	CMC-C2C	-2.79	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	402	CLA	CHC-C1C	2.78	1.41	1.34
27	A	410	LHG	P-O6	2.78	1.70	1.59
22	b	703	CLA	CHC-C1C	2.77	1.41	1.34
33	b	723	LMG	O1-C7	-2.77	1.38	1.43
22	B	709	CLA	MG-ND	2.77	2.11	2.05
27	B	722	LHG	C24-C23	2.77	1.58	1.50
33	d	408	LMG	O8-C9	-2.76	1.39	1.45
22	c	504	CLA	MG-NA	2.76	2.12	2.06
22	c	504	CLA	MG-ND	-2.76	2.00	2.05
33	C	520	LMG	O7-C8	-2.76	1.40	1.46
22	C	507	CLA	MG-ND	-2.76	2.00	2.05
22	b	714	CLA	CMB-C2B	-2.76	1.46	1.51
22	B	713	CLA	CMD-C2D	-2.75	1.45	1.50
22	c	504	CLA	CMC-C2C	-2.75	1.45	1.50
22	D	403	CLA	CMB-C2B	-2.75	1.46	1.51
29	c	518	DGD	C6E-C5E	2.75	1.61	1.51
22	c	504	CLA	C1D-ND	2.75	1.41	1.37
22	B	707	CLA	CMC-C2C	-2.74	1.45	1.50
29	c	517	DGD	C4E-C3E	2.73	1.59	1.52
33	a	419	LMG	C3-C2	2.73	1.59	1.52
22	b	712	CLA	CHC-C1C	2.73	1.41	1.34
23	d	403	BCR	C1-C6	-2.72	1.50	1.53
34	a	405	PHO	O2D-CGD	2.72	1.39	1.33
22	c	507	CLA	C4B-CHC	-2.72	1.33	1.41
22	b	710	CLA	CMB-C2B	-2.72	1.46	1.51
22	b	711	CLA	CMD-C2D	-2.71	1.45	1.50
29	H	103	DGD	C1E-C2E	2.71	1.60	1.52
27	D	411	LHG	C8-C7	-2.71	1.42	1.50
22	B	716	CLA	C1D-ND	2.70	1.41	1.37
22	b	705	CLA	CMD-C2D	-2.70	1.45	1.50
22	B	709	CLA	O2D-CGD	2.70	1.39	1.33
22	D	402	CLA	MG-NC	2.69	2.12	2.06
22	C	510	CLA	CMD-C2D	-2.69	1.45	1.50
22	B	710	CLA	C1D-ND	2.69	1.41	1.37
22	C	513	CLA	CMB-C2B	-2.68	1.46	1.51
22	b	704	CLA	CMB-C2B	-2.68	1.46	1.51
34	D	406	PHO	CHA-CBD	-2.68	1.49	1.52
22	D	402	CLA	MG-ND	2.67	2.11	2.05
29	C	519	DGD	O2G-C2G	-2.67	1.40	1.46
23	T	701	BCR	C1-C6	-2.66	1.50	1.53
33	b	723	LMG	C3-C2	2.66	1.59	1.52
35	v	201	HEC	CAA-C2A	2.66	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	510	CLA	CMB-C2B	-2.65	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.65	1.45	1.50
22	C	514	CLA	CMB-C2B	-2.65	1.46	1.51
22	B	707	CLA	CMB-C2B	-2.65	1.46	1.51
22	B	706	CLA	CMB-C2B	-2.64	1.46	1.51
22	b	716	CLA	CMB-C2B	-2.64	1.46	1.51
22	C	502	CLA	C3B-C2B	-2.64	1.36	1.40
22	b	702	CLA	C1D-ND	2.64	1.41	1.37
29	h	702	DGD	C4E-C3E	2.64	1.59	1.52
33	b	723	LMG	O6-C1	2.64	1.48	1.41
22	c	503	CLA	CMD-C2D	-2.64	1.45	1.50
22	c	503	CLA	C3B-C2B	-2.64	1.36	1.40
22	B	713	CLA	CHC-C1C	2.64	1.41	1.34
33	C	520	LMG	C4-C5	2.63	1.58	1.53
22	c	508	CLA	C3B-C2B	-2.63	1.36	1.40
22	C	508	CLA	CMB-C2B	-2.63	1.46	1.51
29	c	519	DGD	O4E-C4E	-2.62	1.36	1.43
22	b	704	CLA	MG-NA	2.62	2.12	2.06
23	t	701	BCR	C27-C26	-2.62	1.46	1.51
22	a	406	CLA	CHC-C1C	2.62	1.41	1.34
22	C	506	CLA	C1D-ND	2.62	1.41	1.37
22	C	502	CLA	C1D-ND	2.61	1.41	1.37
22	a	406	CLA	C4B-CHC	-2.61	1.33	1.41
29	c	518	DGD	C6D-C5D	2.61	1.59	1.51
33	d	408	LMG	C4-C5	2.61	1.58	1.53
33	d	408	LMG	O7-C8	-2.61	1.40	1.46
22	c	503	CLA	CMB-C2B	-2.60	1.46	1.51
22	A	403	CLA	CMB-C2B	-2.60	1.46	1.51
22	b	710	CLA	CMD-C2D	-2.60	1.45	1.50
29	c	519	DGD	O6D-C5D	-2.60	1.38	1.44
22	c	514	CLA	C1D-ND	2.60	1.41	1.37
26	B	723	SQD	O48-C23	2.59	1.40	1.33
22	b	709	CLA	CHC-C1C	2.59	1.40	1.34
22	b	703	CLA	CMB-C2B	-2.59	1.46	1.51
29	H	103	DGD	C4D-C5D	2.59	1.58	1.53
22	c	513	CLA	CMB-C2B	-2.59	1.46	1.51
22	D	403	CLA	CMD-C2D	-2.58	1.45	1.50
22	B	715	CLA	C3B-C2B	-2.58	1.36	1.40
29	c	519	DGD	O2D-C2D	-2.58	1.36	1.43
22	c	503	CLA	C1D-ND	2.58	1.41	1.37
22	c	511	CLA	CHC-C1C	2.58	1.40	1.34
22	a	401	CLA	MG-ND	2.57	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	CMD-C2D	-2.57	1.45	1.50
26	a	413	SQD	O47-C7	2.56	1.41	1.34
22	c	506	CLA	C1D-ND	2.56	1.41	1.37
22	a	401	CLA	C1D-ND	2.56	1.41	1.37
29	c	518	DGD	C3E-C2E	2.55	1.59	1.52
22	D	403	CLA	C3B-C2B	-2.55	1.36	1.40
22	b	706	CLA	CMD-C2D	-2.55	1.45	1.50
25	D	405	PL9	C11-C9	-2.54	1.46	1.51
29	c	517	DGD	C6D-C5D	2.54	1.59	1.51
22	b	710	CLA	CMC-C2C	-2.54	1.45	1.50
29	C	517	DGD	O2G-C2G	-2.54	1.40	1.46
22	C	510	CLA	O2D-CGD	2.54	1.39	1.33
25	A	408	PL9	C21-C19	2.53	1.56	1.51
22	b	704	CLA	CMD-C2D	-2.53	1.45	1.50
33	D	408	LMG	C9-C8	2.53	1.58	1.50
22	c	504	CLA	C3B-C2B	-2.52	1.37	1.40
22	B	716	CLA	CMC-C2C	-2.52	1.45	1.50
22	b	714	CLA	C1D-ND	2.52	1.41	1.37
22	c	513	CLA	C1D-ND	2.52	1.41	1.37
33	D	408	LMG	O1-C1	2.51	1.44	1.40
22	c	513	CLA	CMC-C2C	-2.51	1.45	1.50
34	d	405	PHO	CBD-CGD	-2.51	1.49	1.52
22	c	509	CLA	CMB-C2B	-2.51	1.46	1.51
22	c	503	CLA	MG-NA	2.51	2.12	2.06
22	B	704	CLA	C1D-ND	2.50	1.41	1.37
22	B	708	CLA	CHC-C1C	2.50	1.40	1.34
22	a	401	CLA	CMB-C2B	-2.50	1.46	1.51
22	B	705	CLA	CMC-C2C	-2.50	1.45	1.50
22	c	507	CLA	C3B-C2B	-2.50	1.37	1.40
26	A	409	SQD	O2-C2	-2.49	1.36	1.43
22	B	708	CLA	C3D-C4D	2.49	1.49	1.44
29	c	519	DGD	C2A-C1A	-2.49	1.43	1.50
23	k	102	BCR	C1-C6	-2.49	1.50	1.53
22	B	707	CLA	CMD-C2D	-2.49	1.45	1.50
23	k	102	BCR	C30-C25	-2.49	1.50	1.53
29	H	103	DGD	O2D-C2D	-2.48	1.36	1.43
29	c	517	DGD	O6E-C5E	-2.48	1.38	1.44
22	c	513	CLA	CMD-C2D	-2.48	1.45	1.50
29	c	517	DGD	C1G-C2G	2.48	1.58	1.50
34	d	405	PHO	CMC-C2C	-2.48	1.45	1.51
22	d	401	CLA	MG-NA	2.48	2.12	2.06
22	B	714	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	721	LMG	O6-C1	2.48	1.48	1.41
23	B	717	BCR	C33-C5	-2.47	1.47	1.50
22	C	507	CLA	C3B-C2B	-2.47	1.37	1.40
22	b	702	CLA	CAC-C3C	-2.47	1.44	1.51
22	B	709	CLA	MG-NA	2.47	2.12	2.06
25	A	408	PL9	C21-C22	2.46	1.61	1.53
34	a	405	PHO	C3B-C2B	-2.46	1.37	1.40
22	A	402	CLA	C3B-C2B	-2.46	1.37	1.40
22	a	404	CLA	CMC-C2C	-2.46	1.45	1.50
22	b	712	CLA	MG-NC	-2.46	2.00	2.06
22	C	502	CLA	C1C-NC	-2.46	1.34	1.37
29	C	518	DGD	C4E-C5E	2.45	1.58	1.53
25	d	404	PL9	C41-C39	-2.45	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.45	1.46	1.51
23	K	101	BCR	C1-C6	-2.45	1.50	1.53
22	b	706	CLA	C3B-C2B	-2.45	1.37	1.40
22	B	706	CLA	C1D-ND	2.45	1.41	1.37
22	c	509	CLA	C1D-ND	2.45	1.41	1.37
22	C	513	CLA	C3B-C2B	-2.44	1.37	1.40
33	a	419	LMG	O7-C10	2.44	1.41	1.34
29	A	413	DGD	C4D-C5D	2.44	1.58	1.53
33	C	516	LMG	C4-C3	2.44	1.58	1.52
27	D	410	LHG	O7-C5	-2.43	1.40	1.46
29	h	702	DGD	O4D-C4D	-2.43	1.36	1.43
22	C	503	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	512	CLA	C4B-CHC	-2.43	1.34	1.41
22	C	510	CLA	MG-NC	-2.42	2.00	2.06
34	d	405	PHO	CMD-C2D	-2.42	1.45	1.51
22	C	502	CLA	MG-NC	2.41	2.12	2.06
22	b	708	CLA	C1D-C2D	2.41	1.50	1.45
23	t	701	BCR	C38-C26	-2.41	1.47	1.50
22	B	714	CLA	C1A-CHA	-2.41	1.33	1.43
22	B	716	CLA	C3B-C2B	-2.41	1.37	1.40
22	B	709	CLA	C4B-CHC	-2.40	1.34	1.41
23	B	718	BCR	C33-C5	-2.40	1.47	1.50
22	B	713	CLA	C3B-C2B	-2.40	1.37	1.40
22	C	505	CLA	C3B-C2B	-2.40	1.37	1.40
22	B	708	CLA	C1D-C2D	2.40	1.50	1.45
22	b	714	CLA	MG-ND	-2.40	2.01	2.05
22	c	502	CLA	CMB-C2B	-2.40	1.46	1.51
22	a	403	CLA	CMC-C2C	-2.39	1.45	1.50
22	C	503	CLA	MG-NC	-2.39	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	707	CLA	CMD-C2D	-2.39	1.45	1.50
22	B	711	CLA	MG-NC	2.39	2.11	2.06
22	C	513	CLA	C1D-C2D	2.39	1.50	1.45
25	d	404	PL9	C53-C6	-2.39	1.45	1.50
22	B	705	CLA	CMB-C2B	-2.38	1.46	1.51
22	d	402	CLA	CMB-C2B	-2.38	1.46	1.51
29	c	519	DGD	O2G-C2G	-2.38	1.41	1.46
34	D	407	PHO	CMB-C2B	-2.38	1.45	1.51
22	c	505	CLA	CMC-C2C	-2.37	1.45	1.50
22	B	713	CLA	C4-C3	-2.37	1.44	1.50
22	B	716	CLA	CMD-C2D	-2.37	1.45	1.50
22	b	713	CLA	CMC-C2C	-2.37	1.45	1.50
22	D	403	CLA	CHC-C1C	2.37	1.40	1.34
22	A	402	CLA	C5-C3	-2.37	1.46	1.51
27	l	101	LHG	C24-C23	-2.37	1.43	1.50
22	b	702	CLA	C4B-CHC	-2.37	1.34	1.41
22	b	712	CLA	C1D-ND	2.37	1.41	1.37
22	B	702	CLA	C3D-C4D	2.37	1.49	1.44
22	D	401	CLA	C4B-CHC	-2.36	1.34	1.41
25	D	405	PL9	C37-C38	-2.36	1.43	1.50
22	B	707	CLA	CMA-C3A	-2.36	1.48	1.53
22	C	502	CLA	CMD-C2D	-2.36	1.45	1.50
27	A	410	LHG	O7-C5	-2.36	1.41	1.46
22	c	505	CLA	MG-ND	-2.36	2.01	2.05
22	c	507	CLA	CMD-C2D	-2.35	1.45	1.50
22	c	508	CLA	C4B-CHC	-2.35	1.34	1.41
22	B	708	CLA	CAC-C3C	-2.35	1.45	1.51
29	H	103	DGD	O6E-C1E	2.34	1.47	1.41
22	c	507	CLA	C1D-ND	2.34	1.40	1.37
22	b	712	CLA	CMC-C2C	-2.33	1.46	1.50
33	M	101	LMG	O4-C4	-2.33	1.37	1.43
22	C	502	CLA	CMC-C2C	-2.33	1.46	1.50
22	a	406	CLA	C1D-ND	2.33	1.40	1.37
22	B	705	CLA	C1C-NC	-2.33	1.34	1.37
29	C	519	DGD	O6D-C5D	-2.33	1.38	1.44
22	c	511	CLA	CMD-C2D	-2.33	1.46	1.50
22	c	507	CLA	CMA-C3A	-2.33	1.48	1.53
22	D	401	CLA	CHC-C1C	2.32	1.40	1.34
22	b	703	CLA	CMD-C2D	-2.32	1.46	1.50
23	B	718	BCR	C36-C18	-2.32	1.46	1.50
25	d	404	PL9	C26-C24	-2.32	1.46	1.51
22	b	711	CLA	C4B-CHC	-2.31	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	401	CLA	MG-ND	-2.31	2.01	2.05
23	b	717	BCR	C33-C5	-2.31	1.47	1.50
22	B	703	CLA	CMD-C2D	-2.31	1.46	1.50
22	A	404	CLA	CMD-C2D	-2.31	1.46	1.50
26	a	413	SQD	O4-C4	-2.31	1.37	1.43
22	B	714	CLA	MG-NA	2.31	2.11	2.06
22	c	504	CLA	CMB-C2B	-2.31	1.47	1.51
22	B	708	CLA	CMB-C2B	-2.30	1.47	1.51
22	A	402	CLA	C1D-ND	2.30	1.40	1.37
23	k	101	BCR	C38-C26	-2.29	1.47	1.50
23	b	717	BCR	C36-C18	-2.29	1.46	1.50
22	D	402	CLA	C1D-C2D	2.29	1.49	1.45
23	b	718	BCR	C36-C18	-2.29	1.46	1.50
22	B	715	CLA	CAC-C3C	-2.28	1.45	1.51
23	C	515	BCR	C30-C25	-2.28	1.50	1.53
22	c	507	CLA	CAC-C3C	-2.28	1.45	1.51
22	c	507	CLA	CMB-C2B	-2.27	1.47	1.51
22	D	401	CLA	CMB-C2B	-2.27	1.47	1.51
22	b	716	CLA	CMD-C2D	-2.27	1.46	1.50
22	C	511	CLA	CMC-C2C	-2.27	1.46	1.50
22	a	403	CLA	MG-ND	-2.26	2.01	2.05
22	A	404	CLA	CHC-C1C	2.26	1.40	1.34
22	b	701	CLA	CMB-C2B	-2.26	1.47	1.51
23	c	516	BCR	C33-C5	-2.26	1.47	1.50
22	H	102	CLA	CMD-C2D	-2.26	1.46	1.50
23	a	407	BCR	C38-C26	-2.26	1.47	1.50
34	D	407	PHO	CMC-C2C	-2.26	1.46	1.51
22	c	512	CLA	CMC-C2C	-2.25	1.46	1.50
22	b	703	CLA	C4B-CHC	-2.25	1.34	1.41
22	B	716	CLA	CHC-C1C	2.25	1.40	1.34
22	c	505	CLA	C1D-ND	2.25	1.40	1.37
27	a	414	LHG	P-O6	2.25	1.68	1.59
22	b	713	CLA	C4B-CHC	-2.25	1.34	1.41
33	d	408	LMG	O1-C7	-2.25	1.39	1.43
22	c	505	CLA	CMB-C2B	-2.24	1.47	1.51
22	d	402	CLA	O2D-CGD	2.24	1.38	1.33
33	D	408	LMG	O2-C2	-2.24	1.37	1.43
22	B	708	CLA	CMA-C3A	-2.24	1.48	1.53
29	c	518	DGD	O5D-C1E	2.24	1.43	1.40
25	d	404	PL9	C37-C38	-2.24	1.43	1.50
22	D	403	CLA	C4B-CHC	-2.23	1.34	1.41
27	D	410	LHG	O8-C6	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	721	LMG	C4-C3	2.23	1.58	1.52
22	c	509	CLA	CMC-C2C	-2.23	1.46	1.50
22	B	710	CLA	C1A-CHA	-2.23	1.33	1.43
33	a	419	LMG	C12-C11	2.23	1.60	1.52
29	h	702	DGD	O2E-C2E	-2.22	1.37	1.43
22	b	702	CLA	CMD-C2D	-2.22	1.46	1.50
22	B	707	CLA	C3B-C2B	-2.21	1.37	1.40
22	c	506	CLA	CMC-C2C	-2.21	1.46	1.50
22	A	403	CLA	CMD-C2D	-2.21	1.46	1.50
22	C	511	CLA	MG-NA	2.21	2.11	2.06
22	C	502	CLA	CMB-C2B	-2.21	1.47	1.51
25	D	405	PL9	C3-C4	-2.21	1.46	1.49
22	c	514	CLA	C3B-C2B	-2.21	1.37	1.40
22	C	505	CLA	CMB-C2B	-2.21	1.47	1.51
33	M	101	LMG	C4-C3	2.20	1.58	1.52
22	c	503	CLA	CMC-C2C	-2.20	1.46	1.50
33	c	522	LMG	C9-C8	2.20	1.57	1.50
22	b	710	CLA	C3D-C4D	2.20	1.49	1.44
22	C	511	CLA	CMD-C2D	-2.19	1.46	1.50
22	B	710	CLA	CMA-C3A	-2.19	1.48	1.53
22	b	703	CLA	MG-ND	2.19	2.10	2.05
29	H	103	DGD	O3E-C3E	-2.19	1.37	1.43
22	c	503	CLA	C4B-CHC	-2.19	1.34	1.41
22	C	510	CLA	CMC-C2C	-2.19	1.46	1.50
22	C	512	CLA	C1D-ND	2.18	1.40	1.37
22	b	709	CLA	MG-NA	2.18	2.11	2.06
33	C	516	LMG	O6-C5	-2.18	1.39	1.44
22	D	403	CLA	C3D-C4D	2.18	1.49	1.44
22	C	502	CLA	C1D-C2D	2.18	1.49	1.45
22	c	513	CLA	MG-NC	-2.18	2.01	2.06
27	L	101	LHG	O2-C2	2.18	1.49	1.43
22	b	710	CLA	C4C-C3C	2.18	1.48	1.45
22	D	401	CLA	C1A-CHA	-2.17	1.34	1.43
22	c	510	CLA	C3B-C2B	-2.17	1.37	1.40
22	c	511	CLA	MG-NA	2.17	2.11	2.06
22	b	716	CLA	CMC-C2C	-2.17	1.46	1.50
23	A	405	BCR	C38-C26	-2.17	1.47	1.50
27	L	101	LHG	O8-C23	2.17	1.39	1.33
22	B	713	CLA	C5-C3	-2.17	1.46	1.51
27	d	407	LHG	O8-C23	2.17	1.39	1.33
22	b	713	CLA	CMD-C2D	-2.17	1.46	1.50
22	d	401	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	CMB-C2B	-2.17	1.47	1.51
22	c	508	CLA	CHC-C1C	2.16	1.39	1.34
29	c	518	DGD	O3E-C3E	-2.16	1.37	1.43
22	C	506	CLA	CMC-C2C	-2.16	1.46	1.50
22	C	509	CLA	C3D-C4D	2.16	1.49	1.44
22	c	502	CLA	CMC-C2C	-2.16	1.46	1.50
22	C	510	CLA	O2A-CGA	2.16	1.39	1.33
22	b	712	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	709	CLA	C3B-C2B	-2.16	1.37	1.40
22	d	401	CLA	CMD-C2D	-2.16	1.46	1.50
29	A	413	DGD	C4D-C3D	2.16	1.57	1.52
22	b	714	CLA	CAC-C3C	-2.15	1.45	1.51
22	B	713	CLA	CMB-C2B	-2.15	1.47	1.51
22	d	402	CLA	CMC-C2C	-2.15	1.46	1.50
26	a	413	SQD	O47-C45	-2.15	1.41	1.46
23	A	405	BCR	C33-C5	-2.14	1.47	1.50
22	C	512	CLA	CMC-C2C	-2.14	1.46	1.50
22	B	707	CLA	CAC-C3C	-2.14	1.45	1.51
23	a	407	BCR	C30-C25	-2.14	1.51	1.53
27	d	407	LHG	C6-C5	2.13	1.57	1.50
22	c	502	CLA	C3B-C2B	-2.13	1.37	1.40
22	b	701	CLA	O2A-CGA	2.13	1.39	1.33
33	c	520	LMG	O7-C10	2.13	1.39	1.35
29	C	519	DGD	C2A-C1A	-2.12	1.44	1.50
33	d	408	LMG	O6-C5	-2.12	1.39	1.44
29	A	413	DGD	O3G-C1D	2.12	1.43	1.40
34	D	406	PHO	CMD-C2D	-2.12	1.46	1.51
22	b	710	CLA	CHC-C1C	2.12	1.39	1.34
29	h	702	DGD	O3G-C1D	2.12	1.43	1.40
22	B	702	CLA	C1D-C2D	2.12	1.49	1.45
34	d	405	PHO	CAA-C2A	-2.12	1.49	1.54
22	c	509	CLA	CMA-C3A	-2.12	1.48	1.53
29	C	519	DGD	O3G-C3G	-2.11	1.40	1.43
22	b	701	CLA	CMD-C2D	-2.11	1.46	1.50
22	H	102	CLA	C1C-NC	-2.11	1.34	1.37
26	f	101	SQD	O3-C3	-2.11	1.37	1.43
22	C	508	CLA	C1D-ND	2.11	1.40	1.37
22	C	513	CLA	C5-C3	-2.11	1.46	1.51
22	b	715	CLA	C3B-C2B	-2.11	1.37	1.40
33	c	520	LMG	C7-C8	2.11	1.57	1.50
22	b	702	CLA	CMB-C2B	-2.10	1.47	1.51
26	D	409	SQD	O3-C3	-2.10	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	103	DGD	C3E-C2E	2.10	1.57	1.52
23	a	407	BCR	C35-C13	-2.10	1.46	1.50
22	d	402	CLA	C1A-CHA	-2.10	1.34	1.43
34	D	407	PHO	C3B-C2B	-2.10	1.37	1.40
33	D	412	LMG	O8-C28	2.10	1.39	1.33
35	e	101	HEC	C4B-C3B	2.10	1.46	1.43
29	C	517	DGD	C4D-C3D	2.09	1.57	1.52
22	c	504	CLA	O2D-CGD	2.09	1.38	1.33
33	a	419	LMG	C6-C5	2.09	1.58	1.51
23	B	719	BCR	C30-C25	-2.09	1.51	1.53
22	B	711	CLA	MG-ND	2.09	2.09	2.05
29	A	413	DGD	C4E-C5E	2.09	1.57	1.53
22	C	509	CLA	C1D-C2D	2.08	1.49	1.45
29	H	103	DGD	O2G-C2G	-2.08	1.41	1.46
22	C	503	CLA	CMC-C2C	-2.08	1.46	1.50
22	B	707	CLA	MG-NC	2.08	2.11	2.06
22	C	510	CLA	MG-NA	2.08	2.11	2.06
22	b	708	CLA	C3D-C4D	2.08	1.48	1.44
34	D	406	PHO	CMC-C2C	-2.08	1.46	1.51
27	B	722	LHG	P-O6	2.08	1.67	1.59
26	a	413	SQD	O2-C2	-2.08	1.37	1.43
22	B	703	CLA	CMB-C2B	-2.08	1.47	1.51
22	c	509	CLA	CMD-C2D	-2.07	1.46	1.50
22	C	503	CLA	CAC-C3C	-2.07	1.45	1.51
22	b	713	CLA	CAC-C3C	-2.07	1.45	1.51
33	c	523	LMG	C1-C2	2.06	1.58	1.52
22	b	713	CLA	CAA-C2A	-2.06	1.50	1.54
22	b	706	CLA	CMB-C2B	-2.06	1.47	1.51
22	c	514	CLA	CMC-C2C	-2.06	1.46	1.50
22	b	701	CLA	CMC-C2C	-2.06	1.46	1.50
23	C	501	BCR	C27-C26	-2.06	1.47	1.51
22	A	404	CLA	C4B-CHC	-2.06	1.35	1.41
22	C	503	CLA	MG-ND	-2.05	2.01	2.05
22	C	512	CLA	CMD-C2D	-2.05	1.46	1.50
23	B	718	BCR	C1-C6	-2.05	1.51	1.53
22	c	502	CLA	C4B-CHC	-2.05	1.35	1.41
33	M	101	LMG	C4-C5	2.05	1.57	1.53
22	b	703	CLA	CMC-C2C	-2.05	1.46	1.50
23	T	701	BCR	C27-C26	-2.05	1.47	1.51
22	A	404	CLA	CMB-C2B	-2.05	1.47	1.51
25	A	408	PL9	C37-C38	2.05	1.56	1.50
22	b	707	CLA	C1A-CHA	-2.04	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	b	721	LMG	C1-C2	2.04	1.58	1.52
26	f	101	SQD	O2-C2	-2.04	1.37	1.43
29	C	517	DGD	C4E-C3E	2.04	1.57	1.52
26	A	409	SQD	O4-C4	-2.04	1.37	1.43
22	b	709	CLA	C3D-C4D	2.04	1.48	1.44
23	B	719	BCR	C31-C1	-2.04	1.49	1.53
22	B	704	CLA	CMD-C2D	-2.04	1.46	1.50
29	c	518	DGD	O3D-C3D	-2.04	1.37	1.43
22	b	712	CLA	C3B-C2B	-2.03	1.37	1.40
22	b	708	CLA	C3C-C2C	2.03	1.41	1.36
22	b	715	CLA	C4B-CHC	-2.03	1.35	1.41
23	D	404	BCR	C38-C26	-2.03	1.47	1.50
22	B	704	CLA	CMB-C2B	-2.03	1.47	1.51
26	a	413	SQD	O5-C5	-2.03	1.39	1.44
26	f	101	SQD	O4-C4	-2.03	1.37	1.43
34	D	406	PHO	CMB-C2B	-2.03	1.46	1.51
33	C	520	LMG	C6-C5	2.03	1.58	1.51
22	B	703	CLA	C1A-CHA	-2.02	1.34	1.43
33	C	516	LMG	O1-C7	-2.02	1.40	1.43
22	B	709	CLA	CMC-C2C	-2.02	1.46	1.50
33	d	408	LMG	O3-C3	-2.02	1.37	1.43
22	A	403	CLA	CAA-C2A	-2.02	1.50	1.54
33	C	516	LMG	C4-C5	2.02	1.57	1.53
22	b	710	CLA	C4B-CHC	-2.02	1.35	1.41
23	C	515	BCR	C31-C1	-2.02	1.49	1.53
22	b	711	CLA	CMB-C2B	-2.02	1.47	1.51
34	D	407	PHO	CMD-C2D	-2.02	1.46	1.51
29	c	519	DGD	C1D-C2D	2.02	1.58	1.52
22	c	507	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	705	CLA	CMD-C2D	-2.02	1.46	1.50
29	C	517	DGD	O1G-C1G	-2.02	1.40	1.45
29	H	103	DGD	C4E-C5E	2.01	1.57	1.53
22	b	716	CLA	CAC-C3C	-2.01	1.45	1.51
29	C	519	DGD	O1G-C1G	-2.01	1.40	1.45
29	A	413	DGD	C3G-C2G	2.01	1.57	1.50
22	D	401	CLA	CAC-C3C	-2.01	1.46	1.51
22	c	511	CLA	CAC-C3C	-2.01	1.46	1.51
29	c	518	DGD	C1E-C2E	2.01	1.58	1.52
25	d	404	PL9	C10-C9	-2.01	1.45	1.50
22	D	402	CLA	CAC-C3C	-2.01	1.46	1.51
22	A	402	CLA	C1C-NC	-2.01	1.34	1.37
28	a	417	STE	O1-C1	2.01	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	CAA-C2A	-2.00	1.50	1.54

All (1332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	704	CLA	C4A-NA-C1A	9.71	111.11	106.68
35	V	201	HEC	CBB-CAB-C3B	-9.69	104.82	127.49
22	c	510	CLA	C4A-NA-C1A	9.37	110.95	106.68
22	b	701	CLA	C4A-NA-C1A	9.34	110.94	106.68
22	c	512	CLA	C4A-NA-C1A	9.27	110.91	106.68
35	E	103	HEC	CBC-CAC-C3C	-9.03	106.36	127.49
22	B	707	CLA	C4A-NA-C1A	8.99	110.78	106.68
22	c	504	CLA	C4A-NA-C1A	8.94	110.76	106.68
26	b	720	SQD	O6-C1-C2	8.84	121.70	108.27
26	a	413	SQD	O6-C1-C2	8.24	120.79	108.27
22	a	401	CLA	C4A-NA-C1A	8.15	110.40	106.68
22	b	704	CLA	C4A-NA-C1A	8.02	110.34	106.68
22	B	715	CLA	C4A-NA-C1A	7.76	110.22	106.68
22	B	706	CLA	C4A-NA-C1A	7.71	110.20	106.68
22	B	716	CLA	C4A-NA-C1A	7.53	110.11	106.68
22	H	102	CLA	C4A-NA-C1A	7.38	110.05	106.68
35	e	101	HEC	CBC-CAC-C3C	-7.37	110.24	127.49
22	C	514	CLA	C4A-NA-C1A	7.28	110.00	106.68
22	C	504	CLA	C4A-NA-C1A	7.26	109.99	106.68
26	A	409	SQD	O6-C1-C2	7.25	119.29	108.27
22	c	509	CLA	C4A-NA-C1A	7.13	109.93	106.68
22	C	509	CLA	C4A-NA-C1A	7.02	109.88	106.68
35	v	201	HEC	CBB-CAB-C3B	-6.91	111.32	127.49
22	C	508	CLA	C4A-NA-C1A	6.87	109.81	106.68
22	a	403	CLA	CMB-C2B-C1B	-6.79	118.51	128.46
22	D	403	CLA	C4A-NA-C1A	6.74	109.75	106.68
22	b	713	CLA	C4A-NA-C1A	6.53	109.66	106.68
35	V	201	HEC	CBC-CAC-C3C	-6.46	112.36	127.49
25	D	405	PL9	C7-C3-C4	6.40	122.18	116.91
22	c	502	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	c	514	CLA	C4A-NA-C1A	6.35	109.58	106.68
35	e	101	HEC	CBD-CAD-C3D	-6.35	101.86	112.54
22	B	708	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	b	709	CLA	CMB-C2B-C1B	-6.28	119.26	128.46
22	b	706	CLA	C4A-NA-C1A	6.25	109.53	106.68
35	v	201	HEC	CBC-CAC-C3C	-6.23	112.90	127.49
22	b	715	CLA	CMB-C2B-C1B	-6.10	119.52	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	708	CLA	O2D-CGD-O1D	-5.97	112.23	123.85
22	c	505	CLA	C4A-NA-C1A	5.79	109.32	106.68
35	V	201	HEC	CBD-CAD-C3D	-5.77	102.84	112.54
35	E	103	HEC	CBD-CAD-C3D	-5.73	102.90	112.54
22	A	404	CLA	CMB-C2B-C1B	-5.73	120.06	128.46
26	D	409	SQD	O6-C1-C2	5.71	116.95	108.27
22	C	502	CLA	C4A-NA-C1A	5.70	109.28	106.68
22	c	505	CLA	CMB-C2B-C1B	-5.69	120.12	128.46
25	a	411	PL9	C7-C3-C4	5.65	121.57	116.91
22	b	711	CLA	C4A-NA-C1A	5.65	109.26	106.68
22	b	705	CLA	CMB-C2B-C1B	-5.63	120.21	128.46
22	A	402	CLA	CMB-C2B-C1B	-5.62	120.22	128.46
22	B	708	CLA	O2D-CGD-CBD	5.58	120.98	111.23
22	d	401	CLA	CMB-C2B-C1B	-5.55	120.33	128.46
22	c	503	CLA	C4A-NA-C1A	5.53	109.20	106.68
22	b	716	CLA	CMB-C2B-C1B	-5.49	120.42	128.46
25	d	404	PL9	C40-C39-C41	5.46	124.70	115.23
22	C	512	CLA	C4A-NA-C1A	5.39	109.14	106.68
22	B	716	CLA	CMB-C2B-C1B	-5.38	120.58	128.46
22	C	511	CLA	C4A-NA-C1A	5.37	109.13	106.68
26	B	723	SQD	O6-C1-C2	5.36	116.41	108.27
22	C	503	CLA	C4A-NA-C1A	5.32	109.11	106.68
22	b	703	CLA	CMB-C2B-C1B	-5.32	120.66	128.46
26	b	720	SQD	O7-S-C6	5.27	114.63	106.76
22	C	509	CLA	CMB-C2B-C1B	-5.20	120.83	128.46
22	c	511	CLA	C4A-NA-C1A	5.18	109.04	106.68
22	D	402	CLA	C4A-NA-C1A	5.18	109.04	106.68
22	D	403	CLA	O2D-CGD-O1D	-5.17	113.78	123.85
22	B	702	CLA	CMB-C2B-C1B	-5.15	120.91	128.46
22	c	502	CLA	O2D-CGD-O1D	-5.13	113.87	123.85
22	b	714	CLA	C4A-NA-C1A	5.11	109.01	106.68
22	c	507	CLA	C4A-NA-C1A	5.09	109.00	106.68
29	A	413	DGD	C4E-C3E-C2E	-5.09	101.89	110.83
22	B	712	CLA	CMB-C2B-C1B	-5.04	121.08	128.46
22	b	715	CLA	C4A-NA-C1A	5.00	108.96	106.68
35	e	101	HEC	CBA-CAA-C2A	-4.97	104.36	112.55
22	a	403	CLA	CMB-C2B-C3B	4.96	134.59	124.68
22	B	710	CLA	O2D-CGD-O1D	-4.95	114.22	123.85
25	D	405	PL9	C30-C29-C31	-4.93	106.67	115.23
33	b	723	LMG	C1-O6-C5	-4.91	104.14	113.72
35	V	201	HEC	C1D-C2D-C3D	-4.89	103.60	107.00
22	b	702	CLA	CMB-C2B-C1B	-4.88	121.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	402	CLA	CMB-C2B-C3B	4.87	134.42	124.68
22	C	504	CLA	CMB-C2B-C1B	-4.84	121.36	128.46
22	d	402	CLA	CMB-C2B-C1B	-4.82	121.39	128.46
22	C	507	CLA	C4A-NA-C1A	4.79	108.86	106.68
22	b	708	CLA	C4A-NA-C1A	4.78	108.86	106.68
22	a	404	CLA	CMB-C2B-C1B	-4.78	121.45	128.46
22	B	711	CLA	C4A-NA-C1A	4.76	108.85	106.68
22	c	511	CLA	O2D-CGD-O1D	-4.75	114.60	123.85
27	L	101	LHG	O4-P-O5	4.75	134.54	112.44
22	C	507	CLA	CMB-C2B-C1B	-4.74	121.52	128.46
22	C	510	CLA	C4A-NA-C1A	4.73	108.84	106.68
22	b	708	CLA	CMB-C2B-C1B	-4.72	121.55	128.46
22	C	506	CLA	C4A-NA-C1A	4.72	108.83	106.68
22	a	404	CLA	C4A-NA-C1A	4.70	108.82	106.68
25	d	404	PL9	C7-C3-C4	4.70	120.78	116.91
22	c	504	CLA	C11-C12-C13	-4.69	100.36	115.97
22	b	704	CLA	C1-C2-C3	-4.69	118.52	126.20
22	B	711	CLA	CMB-C2B-C1B	-4.68	121.60	128.46
22	b	712	CLA	CMB-C2B-C1B	-4.67	121.61	128.46
22	B	705	CLA	O2D-CGD-O1D	-4.65	114.80	123.85
22	B	704	CLA	CMB-C2B-C1B	-4.65	121.65	128.46
35	e	101	HEC	CBB-CAB-C3B	-4.64	116.63	127.49
22	C	508	CLA	CMB-C2B-C1B	-4.62	121.69	128.46
22	B	712	CLA	C4A-NA-C1A	4.59	108.77	106.68
22	b	716	CLA	O2D-CGD-O1D	-4.57	114.96	123.85
27	a	414	LHG	O4-P-O5	4.52	133.46	112.44
22	b	706	CLA	CMB-C2B-C1B	-4.50	121.86	128.46
26	D	409	SQD	O8-S-C6	4.50	114.66	105.97
27	A	410	LHG	O4-P-O5	4.50	133.37	112.44
22	b	713	CLA	CMB-C2B-C1B	-4.49	121.87	128.46
22	b	716	CLA	CMB-C2B-C3B	4.49	133.66	124.68
35	v	201	HEC	CMC-C2C-C1C	-4.49	121.88	128.46
22	C	514	CLA	C4-C3-C5	4.48	123.01	115.23
22	B	712	CLA	CMB-C2B-C3B	4.48	133.63	124.68
22	D	403	CLA	CMB-C2B-C1B	-4.48	121.90	128.46
22	C	511	CLA	CMB-C2B-C1B	-4.47	121.90	128.46
29	H	103	DGD	O3G-C3G-C2G	-4.45	99.99	110.82
22	b	705	CLA	C4A-NA-C1A	4.45	108.71	106.68
26	A	409	SQD	O7-S-C6	4.44	113.39	106.76
22	d	401	CLA	CMB-C2B-C3B	4.44	133.55	124.68
26	f	101	SQD	O9-S-O7	-4.44	99.39	113.82
22	b	706	CLA	O2D-CGD-O1D	-4.41	115.26	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	711	CLA	O2D-CGD-O1D	-4.40	115.29	123.85
22	b	702	CLA	CHB-C4A-NA	4.38	130.72	124.40
22	b	713	CLA	C1-C2-C3	-4.38	119.02	126.20
25	A	408	PL9	C7-C3-C4	4.37	120.51	116.91
23	b	717	BCR	C2-C1-C6	4.37	116.79	110.44
32	A	417	BCT	O2-C-O1	4.35	130.81	119.68
22	b	711	CLA	CMB-C2B-C1B	-4.35	122.09	128.46
27	D	411	LHG	O4-P-O5	4.33	132.61	112.44
22	c	511	CLA	CMB-C2B-C1B	-4.33	122.11	128.46
27	a	412	LHG	O4-P-O5	4.32	132.53	112.44
22	b	712	CLA	C1B-CHB-C4A	-4.32	121.81	130.04
22	B	713	CLA	C4A-NA-C1A	4.30	108.64	106.68
22	B	702	CLA	O2D-CGD-CBD	4.30	118.75	111.23
22	c	513	CLA	C4A-NA-C1A	4.30	108.64	106.68
22	A	404	CLA	CMB-C2B-C3B	4.30	133.27	124.68
35	V	201	HEC	CMC-C2C-C1C	-4.28	122.18	128.46
22	b	712	CLA	CHB-C4A-NA	4.28	130.57	124.40
26	A	409	SQD	C1-C2-C3	-4.24	101.08	110.01
26	A	409	SQD	O8-S-C6	4.24	114.16	105.97
22	a	401	CLA	CMB-C2B-C1B	-4.23	122.26	128.46
33	d	408	LMG	O1-C1-C2	-4.22	101.86	108.27
22	a	406	CLA	C4A-NA-C1A	4.22	108.61	106.68
26	D	409	SQD	O9-S-C6	4.22	113.06	106.76
35	E	103	HEC	CMB-C2B-C1B	-4.21	122.29	128.46
29	c	518	DGD	O3G-C3G-C2G	-4.21	100.59	110.82
26	A	409	SQD	O9-S-O7	-4.20	100.17	113.82
22	c	507	CLA	CMB-C2B-C1B	-4.17	122.34	128.46
23	B	717	BCR	C2-C1-C6	4.16	116.48	110.44
22	B	713	CLA	CMB-C2B-C1B	-4.16	122.36	128.46
22	c	509	CLA	O2D-CGD-O1D	-4.15	115.76	123.85
23	B	719	BCR	C2-C1-C6	4.14	116.46	110.44
22	b	702	CLA	CMB-C2B-C3B	4.12	132.92	124.68
34	D	407	PHO	O1D-CGD-CBD	4.12	130.97	124.72
27	d	407	LHG	O4-P-O5	4.12	131.60	112.44
25	a	411	PL9	C22-C23-C24	-4.12	118.20	127.62
22	B	705	CLA	O1D-CGD-CBD	4.12	132.64	124.52
22	B	716	CLA	CMB-C2B-C3B	4.12	132.91	124.68
22	b	709	CLA	CMB-C2B-C3B	4.11	132.89	124.68
22	c	505	CLA	CMB-C2B-C3B	4.10	132.88	124.68
22	A	403	CLA	CMB-C2B-C1B	-4.10	122.45	128.46
26	f	101	SQD	O6-C1-C2	4.10	114.50	108.27
25	a	411	PL9	C7-C3-C2	-4.10	118.56	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	413	SQD	C1-O5-C5	-4.08	105.75	113.72
22	C	504	CLA	C4D-CHA-C1A	4.04	126.07	121.24
22	B	702	CLA	CMB-C2B-C3B	4.04	132.76	124.68
22	b	702	CLA	C4A-NA-C1A	4.03	108.52	106.68
27	D	410	LHG	O4-P-O5	4.03	131.18	112.44
22	c	506	CLA	C4A-NA-C1A	4.03	108.52	106.68
22	c	513	CLA	C1-C2-C3	-4.02	119.61	126.20
22	C	514	CLA	CMB-C2B-C1B	-4.02	122.57	128.46
22	B	707	CLA	CMB-C2B-C1B	-4.01	122.58	128.46
26	B	723	SQD	O47-C7-C8	3.99	120.11	111.48
22	d	402	CLA	CMB-C2B-C3B	3.99	132.65	124.68
22	b	707	CLA	CMB-C2B-C1B	-3.99	122.61	128.46
22	C	510	CLA	CMB-C2B-C1B	-3.99	122.61	128.46
33	a	419	LMG	C1-C2-C3	-3.99	101.62	110.01
22	b	703	CLA	O2D-CGD-O1D	-3.97	116.11	123.85
22	C	511	CLA	CMB-C2B-C3B	3.97	132.62	124.68
22	b	703	CLA	CMB-C2B-C3B	3.97	132.61	124.68
27	d	406	LHG	O4-P-O5	3.97	130.89	112.44
22	b	713	CLA	O2D-CGD-CBD	3.95	118.14	111.23
22	C	508	CLA	O2D-CGD-O1D	-3.95	116.15	123.85
22	b	712	CLA	C4A-NA-C1A	3.95	108.48	106.68
22	C	512	CLA	CMB-C2B-C1B	-3.94	122.69	128.46
22	C	513	CLA	C4A-NA-C1A	3.93	108.47	106.68
25	D	405	PL9	C7-C3-C2	-3.93	118.76	123.39
22	b	710	CLA	CAC-C3C-C4C	3.92	129.89	124.79
29	h	702	DGD	O3G-C3G-C2G	-3.91	101.30	110.82
22	B	703	CLA	C4A-NA-C1A	3.91	108.46	106.68
22	b	714	CLA	CMB-C2B-C1B	-3.88	122.77	128.46
22	c	513	CLA	CHB-C4A-NA	3.87	129.99	124.40
22	B	713	CLA	C1-C2-C3	-3.87	119.86	126.20
22	c	508	CLA	O2D-CGD-O1D	-3.86	116.34	123.85
26	B	723	SQD	O5-C5-C4	3.86	116.65	109.70
27	B	722	LHG	O4-P-O5	3.85	130.34	112.44
34	d	405	PHO	O1D-CGD-CBD	3.84	130.54	124.72
22	H	102	CLA	CAA-CBA-CGA	-3.84	102.31	113.21
22	b	705	CLA	C4-C3-C5	3.82	121.86	115.23
27	l	101	LHG	O4-P-O5	3.82	130.19	112.44
22	c	502	CLA	CMB-C2B-C1B	-3.81	122.87	128.46
29	C	519	DGD	O3G-C3G-C2G	-3.81	101.55	110.82
26	A	409	SQD	C1-O5-C5	-3.81	106.28	113.72
22	B	710	CLA	C4A-NA-C1A	3.81	108.42	106.68
22	b	706	CLA	O2D-CGD-CBD	3.80	117.87	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	716	CLA	C4A-NA-C1A	3.79	108.41	106.68
22	C	513	CLA	CHB-C4A-NA	3.79	129.88	124.40
25	D	405	PL9	C22-C23-C24	-3.79	118.94	127.62
29	C	518	DGD	O3G-C3G-C2G	-3.79	101.60	110.82
22	C	508	CLA	CMB-C2B-C3B	3.78	132.23	124.68
26	f	101	SQD	O7-S-C6	3.78	112.39	106.76
22	B	708	CLA	CMB-C2B-C1B	-3.78	122.92	128.46
35	E	103	HEC	CMC-C2C-C1C	-3.77	122.93	128.46
29	C	517	DGD	O3G-C3G-C2G	-3.77	101.66	110.82
22	B	710	CLA	O2D-CGD-CBD	3.76	117.81	111.23
34	D	406	PHO	CMB-C2B-C3B	3.76	132.20	124.68
32	a	410	BCT	O2-C-O1	3.76	129.29	119.68
22	c	514	CLA	CMB-C2B-C1B	-3.76	122.95	128.46
22	c	509	CLA	CHB-C4A-NA	3.76	129.82	124.40
27	a	412	LHG	O8-C23-C24	3.75	123.28	111.83
26	f	101	SQD	O5-C5-C4	3.75	116.45	109.70
22	B	709	CLA	C4A-NA-C1A	3.75	108.39	106.68
26	b	720	SQD	O48-C23-C24	3.74	123.23	111.83
22	A	404	CLA	C1B-CHB-C4A	-3.74	122.91	130.04
26	B	723	SQD	O7-S-C6	3.73	112.33	106.76
22	C	513	CLA	C1-C2-C3	-3.73	120.08	126.20
22	c	513	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
29	C	518	DGD	O5D-C6D-C5D	-3.73	101.01	109.42
23	B	718	BCR	C29-C30-C25	3.72	115.84	110.44
22	C	509	CLA	CMB-C2B-C3B	3.71	132.10	124.68
22	c	510	CLA	O2A-CGA-O1A	-3.71	114.34	123.63
26	D	409	SQD	C1-C2-C3	-3.71	102.20	110.01
29	H	103	DGD	C3E-C4E-C5E	-3.71	103.51	110.23
26	A	409	SQD	O47-C7-C8	3.71	119.50	111.48
26	a	415	SQD	O48-C23-O10	-3.69	114.39	123.63
22	b	716	CLA	O2D-CGD-CBD	3.69	117.68	111.23
22	D	401	CLA	CMB-C2B-C1B	-3.68	123.07	128.46
22	B	704	CLA	CMB-C2B-C3B	3.68	132.03	124.68
22	a	404	CLA	O2D-CGD-CBD	3.67	117.65	111.23
26	a	413	SQD	O9-S-O7	-3.67	101.89	113.82
22	b	711	CLA	O2D-CGD-CBD	3.67	117.64	111.23
22	b	701	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
27	B	722	LHG	O8-C23-C24	3.65	122.97	111.83
22	d	401	CLA	C4A-NA-C1A	3.65	108.34	106.68
22	C	504	CLA	C7-C6-C5	-3.64	103.55	113.26
22	B	712	CLA	C16-C15-C13	-3.64	103.86	115.97
22	b	701	CLA	CHB-C4A-NA	3.64	129.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	710	CLA	CHB-C4A-NA	3.64	129.65	124.40
22	b	705	CLA	CMB-C2B-C3B	3.63	131.94	124.68
28	d	409	STE	O2-C1-C2	3.63	125.47	114.00
22	A	404	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
29	C	518	DGD	O2D-C2D-C1D	-3.61	101.47	110.08
22	c	503	CLA	CMB-C2B-C1B	-3.61	123.16	128.46
26	b	720	SQD	O47-C7-C8	3.61	119.29	111.48
22	c	503	CLA	C1B-CHB-C4A	-3.59	123.20	130.04
23	B	718	BCR	C15-C14-C13	-3.57	122.27	127.28
33	a	419	LMG	C1-O6-C5	-3.56	106.76	113.72
28	j	101	STE	O2-C1-C2	3.56	125.26	114.00
22	a	403	CLA	C1B-CHB-C4A	-3.56	123.25	130.04
35	E	103	HEC	CMB-C2B-C3B	3.56	130.00	125.82
22	B	713	CLA	CMB-C2B-C3B	3.56	131.79	124.68
22	b	709	CLA	C4A-NA-C1A	3.56	108.30	106.68
22	b	704	CLA	CMB-C2B-C1B	-3.54	123.27	128.46
25	d	404	PL9	C42-C43-C44	-3.54	119.52	127.62
33	b	721	LMG	O1-C1-C2	-3.54	102.89	108.27
22	b	706	CLA	CMB-C2B-C3B	3.54	131.75	124.68
22	D	403	CLA	CMB-C2B-C3B	3.53	131.74	124.68
22	C	502	CLA	O2D-CGD-O1D	-3.53	116.97	123.85
22	B	705	CLA	C7-C6-C5	-3.53	103.85	113.26
35	E	103	HEC	CBA-CAA-C2A	-3.53	106.74	112.55
22	b	703	CLA	C4A-NA-C1A	3.52	108.29	106.68
26	B	723	SQD	O9-S-O7	-3.50	102.43	113.82
22	c	502	CLA	O2D-CGD-CBD	3.50	117.34	111.23
35	V	201	HEC	CMC-C2C-C3C	3.49	129.93	125.82
22	c	510	CLA	CMB-C2B-C1B	-3.49	123.35	128.46
22	b	714	CLA	CHD-C1D-ND	-3.49	119.90	124.80
22	D	401	CLA	C1B-CHB-C4A	-3.48	123.39	130.04
23	T	701	BCR	C27-C26-C25	3.48	127.41	122.70
22	a	404	CLA	CHB-C4A-NA	3.48	129.43	124.40
29	h	702	DGD	C4E-C3E-C2E	-3.48	104.72	110.83
22	c	510	CLA	CHB-C4A-NA	3.48	129.42	124.40
33	C	520	LMG	O1-C1-C2	-3.48	102.99	108.27
29	A	413	DGD	O3G-C3G-C2G	-3.48	102.36	110.82
22	C	502	CLA	CMB-C2B-C1B	-3.47	123.37	128.46
22	b	715	CLA	CMB-C2B-C3B	3.47	131.61	124.68
22	b	704	CLA	CHB-C4A-NA	3.46	129.40	124.40
26	a	415	SQD	O47-C7-C8	3.46	118.97	111.48
26	b	720	SQD	O5-C5-C4	3.46	115.94	109.70
33	d	408	LMG	O2-C2-C1	-3.46	101.83	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	406	CLA	CMB-C2B-C1B	-3.46	123.39	128.46
22	c	512	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
27	a	412	LHG	O8-C23-O10	-3.46	114.98	123.63
22	B	702	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
35	E	103	HEC	CBB-CAB-C3B	-3.45	119.42	127.49
22	c	505	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
22	b	709	CLA	C1B-CHB-C4A	-3.43	123.49	130.04
22	H	102	CLA	CAA-C2A-C3A	-3.42	103.75	113.00
22	B	710	CLA	C1B-CHB-C4A	-3.42	123.51	130.04
22	B	712	CLA	C11-C12-C13	-3.42	104.59	115.97
22	b	704	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
22	b	710	CLA	C1B-CHB-C4A	-3.42	123.52	130.04
22	c	510	CLA	CHD-C1D-ND	-3.42	119.99	124.80
22	a	404	CLA	CMB-C2B-C3B	3.41	131.50	124.68
34	D	407	PHO	CMB-C2B-C3B	3.41	131.50	124.68
35	e	101	HEC	CMC-C2C-C1C	-3.39	123.48	128.46
23	b	718	BCR	C36-C18-C17	-3.39	117.32	122.82
25	A	408	PL9	C7-C3-C2	-3.39	119.39	123.39
23	b	717	BCR	C36-C18-C17	-3.39	117.33	122.82
22	c	508	CLA	C4A-NA-C1A	3.39	108.22	106.68
22	B	704	CLA	CHB-C4A-NA	3.38	129.28	124.40
22	C	504	CLA	CMB-C2B-C3B	3.37	131.41	124.68
23	T	701	BCR	C7-C8-C9	-3.36	121.26	126.23
22	C	511	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
23	A	405	BCR	C27-C26-C25	3.36	127.24	122.70
22	B	711	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
22	b	716	CLA	C1B-CHB-C4A	-3.35	123.64	130.04
23	c	516	BCR	C27-C26-C25	3.35	127.23	122.70
22	b	702	CLA	C1B-CHB-C4A	-3.34	123.67	130.04
22	C	507	CLA	CMB-C2B-C3B	3.33	131.34	124.68
32	A	417	BCT	O3-C-O1	-3.33	111.16	119.68
26	a	413	SQD	O8-S-C6	3.33	112.40	105.97
23	D	404	BCR	C3-C4-C5	-3.31	108.15	114.06
23	K	101	BCR	C11-C10-C9	-3.31	122.63	127.28
34	d	405	PHO	O2D-CGD-O1D	-3.31	117.41	123.85
22	B	702	CLA	C4A-NA-C1A	3.31	108.19	106.68
25	d	404	PL9	C36-C34-C33	-3.31	113.74	121.17
33	C	516	LMG	O6-C1-O1	-3.31	102.23	110.04
22	D	403	CLA	O2D-CGD-CBD	3.31	117.01	111.23
23	k	102	BCR	C2-C1-C6	3.31	115.24	110.44
22	b	705	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
22	a	406	CLA	O2A-CGA-O1A	-3.30	115.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	H	101	BCR	C2-C1-C6	3.30	115.23	110.44
23	B	719	BCR	C29-C30-C25	3.30	115.23	110.44
23	K	101	BCR	C2-C1-C6	3.29	115.22	110.44
22	b	712	CLA	CMB-C2B-C3B	3.29	131.25	124.68
25	d	404	PL9	C37-C38-C39	-3.29	120.10	127.62
22	B	704	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
22	c	507	CLA	CHB-C4A-NA	3.29	129.14	124.40
26	a	415	SQD	O48-C23-C24	3.28	121.84	111.83
22	a	404	CLA	C1B-CHB-C4A	-3.28	123.78	130.04
23	a	407	BCR	C2-C1-C6	3.25	115.17	110.44
22	c	509	CLA	CHD-C1D-ND	-3.25	120.23	124.80
34	D	407	PHO	O2D-CGD-O1D	-3.25	117.52	123.85
22	c	508	CLA	CMB-C2B-C1B	-3.25	123.69	128.46
22	B	714	CLA	C4-C3-C5	3.25	120.86	115.23
26	A	409	SQD	O47-C7-O49	-3.23	116.15	123.70
22	c	503	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
33	b	721	LMG	O3-C3-C2	-3.23	102.77	110.38
22	d	401	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
22	b	713	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
22	a	401	CLA	CMC-C2C-C1C	3.22	130.07	125.03
25	A	408	PL9	C20-C19-C21	3.22	120.81	115.23
26	a	413	SQD	C1-C2-C3	-3.21	103.26	110.01
25	A	408	PL9	C36-C34-C33	-3.21	113.96	121.17
22	b	703	CLA	C4-C3-C5	3.21	120.80	115.23
22	c	503	CLA	O1D-CGD-CBD	3.21	130.84	124.52
22	c	503	CLA	CMB-C2B-C3B	3.21	131.09	124.68
22	b	708	CLA	CMB-C2B-C3B	3.20	131.09	124.68
22	C	508	CLA	CHB-C4A-NA	3.20	129.02	124.40
22	B	711	CLA	CMB-C2B-C3B	3.20	131.07	124.68
22	B	710	CLA	O2A-CGA-O1A	-3.20	115.63	123.63
22	c	504	CLA	CHB-C4A-NA	3.20	129.01	124.40
22	B	702	CLA	CHD-C1D-ND	-3.20	120.31	124.80
22	a	404	CLA	CAC-C3C-C4C	3.19	128.95	124.79
28	m	101	STE	O2-C1-O1	-3.19	115.13	123.33
29	h	702	DGD	C1D-O6D-C5D	-3.19	107.50	113.72
22	D	402	CLA	CMB-C2B-C1B	-3.18	123.79	128.46
23	c	515	BCR	C2-C1-C6	3.18	115.06	110.44
22	b	702	CLA	O2D-CGD-CBD	3.17	116.78	111.23
25	a	411	PL9	C35-C34-C36	3.17	120.73	115.23
33	c	522	LMG	C1-O6-C5	-3.17	107.53	113.72
22	c	512	CLA	O2D-CGD-CBD	3.16	116.76	111.23
22	b	708	CLA	O2D-CGD-O1D	-3.16	117.69	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	520	LMG	O2-C2-C1	-3.16	102.55	110.08
29	h	702	DGD	O2D-C2D-C1D	-3.15	102.56	110.08
22	b	703	CLA	C1B-CHB-C4A	-3.15	124.03	130.04
34	a	405	PHO	C1-C2-C3	-3.15	121.04	126.20
22	A	403	CLA	CMB-C2B-C3B	3.15	130.97	124.68
23	b	719	BCR	C2-C1-C6	3.14	115.01	110.44
22	B	707	CLA	CMB-C2B-C3B	3.14	130.95	124.68
22	c	506	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
22	c	507	CLA	CMB-C2B-C3B	3.13	130.94	124.68
33	b	723	LMG	C3-C4-C5	-3.12	104.58	110.23
22	b	703	CLA	O2D-CGD-CBD	3.11	116.67	111.23
22	B	714	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
22	C	505	CLA	O2A-CGA-O1A	-3.11	115.85	123.63
22	C	514	CLA	C6-C5-C3	3.11	121.03	113.47
23	d	403	BCR	C27-C26-C25	3.11	126.90	122.70
22	A	404	CLA	O2D-CGD-CBD	3.11	116.66	111.23
26	b	720	SQD	O2-C2-C1	3.10	117.47	110.08
22	c	511	CLA	CMB-C2B-C3B	3.10	130.88	124.68
22	H	102	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
22	B	714	CLA	CHB-C4A-NA	3.10	128.87	124.40
29	c	517	DGD	O3G-C3G-C2G	-3.10	103.29	110.82
22	C	510	CLA	CMB-C2B-C3B	3.09	130.86	124.68
26	B	723	SQD	O48-C23-O10	-3.09	115.89	123.63
35	v	201	HEC	CMB-C2B-C1B	-3.09	123.93	128.46
22	B	708	CLA	CMB-C2B-C3B	3.09	130.85	124.68
23	d	403	BCR	C2-C1-C6	3.08	114.91	110.44
22	b	711	CLA	CMB-C2B-C3B	3.08	130.83	124.68
22	b	707	CLA	C4-C3-C5	3.08	120.57	115.23
22	b	710	CLA	C1-C2-C3	-3.07	121.16	126.20
34	d	405	PHO	C1-C2-C3	-3.07	121.16	126.20
22	b	715	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
23	C	515	BCR	C15-C16-C17	-3.07	117.23	123.52
26	B	723	SQD	O48-C23-C24	3.07	121.19	111.83
25	D	405	PL9	C32-C33-C34	-3.06	120.61	127.62
22	B	715	CLA	O2D-CGD-CBD	3.06	116.58	111.23
25	d	404	PL9	C22-C23-C24	-3.06	120.62	127.62
22	C	514	CLA	O2A-CGA-O1A	-3.06	115.98	123.63
22	B	706	CLA	O2A-CGA-O1A	-3.06	115.98	123.63
23	B	719	BCR	C3-C4-C5	-3.05	108.61	114.06
23	t	701	BCR	C31-C1-C6	3.05	115.03	110.24
22	C	514	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
22	a	401	CLA	CMB-C2B-C3B	3.05	130.78	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	V	201	HEC	CMB-C2B-C1B	-3.05	123.99	128.46
28	m	101	STE	O2-C1-C2	3.05	123.63	114.00
34	d	405	PHO	CMC-C2C-C3C	3.05	130.69	124.94
22	B	713	CLA	CAC-C3C-C4C	3.04	128.75	124.79
23	C	515	BCR	C36-C18-C17	-3.04	117.89	122.82
23	b	719	BCR	C37-C22-C21	-3.03	117.90	122.82
22	c	507	CLA	C1-O2A-CGA	3.03	123.98	116.65
35	e	101	HEC	CMB-C2B-C1B	-3.03	124.02	128.46
22	B	716	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
22	c	507	CLA	C1B-CHB-C4A	-3.03	124.27	130.04
25	D	405	PL9	C42-C43-C44	-3.02	120.70	127.62
22	C	513	CLA	CMB-C2B-C1B	-3.02	124.04	128.46
22	a	403	CLA	O1D-CGD-CBD	3.01	130.46	124.52
22	A	403	CLA	C1B-CHB-C4A	-3.01	124.30	130.04
29	H	103	DGD	O2D-C2D-C1D	-3.01	102.91	110.08
22	b	707	CLA	CMB-C2B-C3B	3.00	130.69	124.68
22	B	702	CLA	CHB-C4A-NA	3.00	128.73	124.40
22	b	714	CLA	C1B-CHB-C4A	-3.00	124.31	130.04
22	c	511	CLA	O1D-CGD-CBD	3.00	130.44	124.52
22	D	402	CLA	CMB-C2B-C3B	3.00	130.67	124.68
22	C	513	CLA	O2A-CGA-O1A	-2.99	116.14	123.63
22	C	505	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
26	a	415	SQD	O49-C7-C8	-2.99	112.10	123.78
25	a	411	PL9	C36-C34-C33	-2.98	114.47	121.17
22	B	714	CLA	C1B-CHB-C4A	-2.98	124.35	130.04
22	C	513	CLA	O2D-CGD-CBD	2.98	116.44	111.23
22	b	714	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
22	B	713	CLA	C4-C3-C5	2.98	120.40	115.23
22	A	403	CLA	CED-O2D-CGD	-2.98	109.16	115.92
26	D	409	SQD	O48-C23-C24	2.97	120.91	111.83
29	C	518	DGD	C1D-O6D-C5D	-2.97	107.92	113.72
26	a	413	SQD	O47-C7-O49	-2.97	116.76	123.70
22	d	402	CLA	C1B-CHB-C4A	-2.97	124.37	130.04
22	c	514	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
23	B	717	BCR	C29-C30-C25	2.97	114.75	110.44
22	b	701	CLA	O1D-CGD-CBD	2.97	130.37	124.52
26	b	720	SQD	O9-S-O7	-2.97	104.17	113.82
29	C	519	DGD	O6D-C1D-O3G	-2.96	103.06	110.04
22	c	514	CLA	CHB-C4A-NA	2.95	128.66	124.40
26	f	101	SQD	C1-C2-C3	-2.95	103.81	110.01
22	C	511	CLA	C1B-CHB-C4A	-2.94	124.42	130.04
26	A	409	SQD	O48-C23-O10	-2.94	116.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	706	CLA	C1B-CHB-C4A	-2.94	124.43	130.04
22	C	502	CLA	O2A-CGA-O1A	-2.94	116.27	123.63
22	b	702	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
22	b	707	CLA	C1-O2A-CGA	2.94	123.76	116.65
22	B	708	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
23	a	407	BCR	C40-C30-C25	2.93	114.84	110.24
23	b	717	BCR	C29-C30-C25	2.93	114.70	110.44
29	c	519	DGD	O3G-C3G-C2G	-2.93	103.69	110.82
26	D	409	SQD	O48-C23-O10	-2.93	116.30	123.63
29	h	702	DGD	CDB-CCB-CBB	-2.93	99.55	114.37
23	c	516	BCR	C2-C1-C6	2.93	114.69	110.44
23	h	701	BCR	C27-C26-C25	2.93	126.66	122.70
29	c	517	DGD	C4E-C3E-C2E	-2.93	105.69	110.83
26	b	720	SQD	C1-C2-C3	-2.93	103.85	110.01
25	d	404	PL9	C41-C39-C38	-2.92	114.60	121.17
22	D	401	CLA	C1-C2-C3	-2.92	121.42	126.20
22	B	713	CLA	CHB-C4A-NA	2.91	128.60	124.40
35	v	201	HEC	CBD-CAD-C3D	-2.91	107.65	112.54
23	C	501	BCR	C2-C1-C6	2.91	114.66	110.44
33	D	408	LMG	C3-C4-C5	-2.91	104.96	110.23
25	A	408	PL9	C25-C24-C26	2.89	120.25	115.23
22	c	502	CLA	CMB-C2B-C3B	2.89	130.47	124.68
22	b	713	CLA	CMB-C2B-C3B	2.89	130.46	124.68
23	D	404	BCR	C2-C1-C6	2.89	114.64	110.44
22	c	507	CLA	CBC-CAC-C3C	-2.89	104.60	112.42
23	B	719	BCR	C15-C16-C17	-2.89	117.61	123.52
22	B	704	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
22	b	713	CLA	CHB-C4A-NA	2.88	128.56	124.40
23	d	403	BCR	C38-C26-C25	-2.88	121.35	124.48
22	C	505	CLA	CMB-C2B-C1B	-2.87	124.25	128.46
23	B	718	BCR	C35-C13-C14	-2.87	118.16	122.82
26	b	720	SQD	O5-C1-C2	-2.87	104.47	110.37
23	c	516	BCR	C15-C16-C17	-2.87	117.65	123.52
22	B	709	CLA	CMB-C2B-C3B	2.86	130.41	124.68
33	D	408	LMG	O3-C3-C2	-2.86	103.63	110.38
26	a	413	SQD	C3-C4-C5	2.86	115.42	110.23
22	b	710	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
22	B	715	CLA	CHB-C4A-NA	2.86	128.53	124.40
29	c	518	DGD	O6D-C1D-O3G	-2.86	103.30	110.04
22	b	710	CLA	CHB-C4A-NA	2.85	128.52	124.40
22	B	709	CLA	CMB-C2B-C1B	-2.85	124.28	128.46
27	B	722	LHG	O8-C23-O10	-2.85	116.50	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	521	STE	C3-C2-C1	-2.85	107.07	114.51
22	B	706	CLA	CHB-C4A-NA	2.85	128.51	124.40
22	C	513	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
22	B	715	CLA	CMB-C2B-C1B	-2.84	124.29	128.46
33	D	408	LMG	O1-C1-C2	-2.84	103.96	108.27
22	D	403	CLA	C1B-CHB-C4A	-2.84	124.62	130.04
22	c	509	CLA	CMB-C2B-C1B	-2.84	124.30	128.46
22	C	514	CLA	CMB-C2B-C3B	2.84	130.35	124.68
23	b	717	BCR	C27-C26-C25	2.84	126.54	122.70
22	d	401	CLA	C1B-CHB-C4A	-2.84	124.63	130.04
22	C	509	CLA	CHD-C1D-ND	-2.84	120.81	124.80
22	b	714	CLA	CHB-C4A-NA	2.83	128.49	124.40
29	H	103	DGD	C1E-O6E-C5E	2.83	119.25	113.72
22	B	706	CLA	C6-C5-C3	-2.83	106.57	113.47
22	B	703	CLA	C3B-C4B-NB	-2.83	105.55	109.21
22	c	512	CLA	CMB-C2B-C1B	-2.83	124.31	128.46
29	A	413	DGD	O3G-C1D-C2D	-2.83	103.98	108.27
22	b	708	CLA	C3B-C4B-NB	-2.83	105.56	109.21
22	B	705	CLA	CHD-C1D-ND	-2.82	120.83	124.80
23	C	515	BCR	C2-C1-C6	2.82	114.54	110.44
34	D	406	PHO	OBD-CAD-CBD	-2.82	121.68	125.82
23	b	719	BCR	C36-C18-C17	-2.82	118.25	122.82
26	B	723	SQD	C3-C4-C5	2.82	115.34	110.23
25	D	405	PL9	C20-C19-C21	2.82	120.12	115.23
22	c	507	CLA	C4-C3-C2	-2.82	116.39	123.63
22	B	712	CLA	CHB-C4A-NA	2.82	128.47	124.40
35	e	101	HEC	CMC-C2C-C3C	-2.82	122.51	125.82
23	h	701	BCR	C15-C16-C17	-2.81	117.77	123.52
22	A	402	CLA	C4A-NA-C1A	2.81	107.96	106.68
29	h	702	DGD	O3E-C3E-C2E	-2.81	103.75	110.38
22	b	709	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	c	510	CLA	CMB-C2B-C3B	2.81	130.29	124.68
29	c	517	DGD	CDB-CCB-CBB	-2.81	100.18	114.37
34	a	405	PHO	OBD-CAD-CBD	-2.81	121.71	125.82
23	c	516	BCR	C8-C9-C10	2.80	123.41	119.01
33	b	723	LMG	O1-C7-C8	-2.80	104.01	110.82
22	C	507	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
34	a	405	PHO	CMB-C2B-C3B	2.80	130.27	124.68
26	b	720	SQD	C3-C4-C5	2.79	115.30	110.23
28	J	101	STE	C3-C2-C1	-2.79	107.23	114.51
29	A	413	DGD	O5D-C6D-C5D	-2.79	103.14	109.42
22	A	402	CLA	CHB-C4A-NA	2.78	128.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	720	SQD	O9-S-C6	2.78	110.91	106.76
23	B	718	BCR	C38-C26-C25	-2.78	121.45	124.48
22	C	507	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
22	C	506	CLA	CMB-C2B-C1B	-2.78	124.39	128.46
33	b	723	LMG	O7-C10-O9	-2.77	117.22	123.70
22	B	716	CLA	CAA-CBA-CGA	-2.77	105.34	113.21
22	D	401	CLA	CMB-C2B-C3B	2.76	130.21	124.68
22	A	404	CLA	CHB-C4A-NA	2.76	128.39	124.40
33	M	101	LMG	C1-C2-C3	-2.76	104.20	110.01
33	b	721	LMG	O7-C10-O9	-2.76	117.25	123.70
33	M	101	LMG	O7-C10-O9	-2.76	117.26	123.70
33	c	520	LMG	O6-C1-O1	-2.76	103.53	110.04
26	A	412	SQD	O47-C7-C8	2.76	117.44	111.48
23	Y	101	BCR	C27-C26-C25	2.75	126.43	122.70
28	x	101	STE	C3-C2-C1	-2.75	107.32	114.51
22	C	510	CLA	CHD-C1D-ND	-2.75	120.93	124.80
22	B	702	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
22	B	713	CLA	C7-C6-C5	-2.74	105.95	113.26
22	a	401	CLA	C2A-C1A-CHA	2.74	128.62	123.87
22	b	716	CLA	CHB-C4A-NA	2.73	128.35	124.40
23	c	516	BCR	C35-C13-C14	-2.73	118.39	122.82
22	c	508	CLA	C2C-C1C-NC	2.73	112.85	109.98
29	c	518	DGD	C3E-C4E-C5E	-2.73	105.29	110.23
22	C	507	CLA	O1D-CGD-CBD	2.73	129.90	124.52
25	d	404	PL9	C47-C48-C49	-2.72	118.56	127.64
34	D	407	PHO	C1B-NB-C4B	2.72	112.69	107.09
22	H	102	CLA	C1B-CHB-C4A	-2.72	124.85	130.04
25	A	408	PL9	C32-C33-C34	-2.72	121.39	127.62
22	C	510	CLA	CED-O2D-CGD	2.72	122.09	115.92
22	b	702	CLA	C1-C2-C3	-2.72	121.74	126.20
26	f	101	SQD	O47-C7-O49	-2.72	117.35	123.70
22	a	401	CLA	CHB-C4A-NA	2.72	128.32	124.40
22	c	510	CLA	C1B-CHB-C4A	-2.72	124.86	130.04
22	A	404	CLA	C2C-C1C-NC	2.72	112.83	109.98
22	c	510	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
22	c	503	CLA	CED-O2D-CGD	2.71	122.07	115.92
23	T	701	BCR	C31-C1-C6	2.71	114.49	110.24
23	k	102	BCR	C27-C26-C25	2.71	126.36	122.70
33	M	101	LMG	C1-O6-C5	-2.71	108.43	113.72
22	b	710	CLA	CAA-CBA-CGA	-2.71	105.52	113.21
29	A	413	DGD	O2D-C2D-C1D	-2.70	103.63	110.08
22	a	403	CLA	CHA-C4D-ND	2.70	138.12	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	k	101	BCR	C38-C26-C25	-2.70	121.54	124.48
26	B	723	SQD	O8-S-C6	2.70	111.18	105.97
23	B	717	BCR	C38-C26-C25	-2.69	121.55	124.48
22	C	509	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
25	a	411	PL9	C37-C38-C39	-2.69	121.47	127.62
22	b	707	CLA	C6-C7-C8	-2.69	107.03	115.97
23	b	718	BCR	C30-C25-C26	-2.69	118.97	122.64
33	b	721	LMG	O1-C7-C8	-2.68	104.29	110.82
23	D	404	BCR	C27-C26-C25	2.68	126.33	122.70
22	B	714	CLA	CMB-C2B-C1B	-2.68	124.53	128.46
32	a	410	BCT	O3-C-O1	-2.68	112.82	119.68
22	D	401	CLA	C4A-NA-C1A	2.68	107.90	106.68
22	c	507	CLA	O1D-CGD-CBD	2.68	129.80	124.52
23	k	102	BCR	C24-C23-C22	-2.68	122.27	126.23
22	b	705	CLA	O1D-CGD-CBD	2.68	129.80	124.52
27	D	410	LHG	C18-C17-C16	-2.68	100.84	114.37
23	B	718	BCR	C3-C4-C5	-2.68	109.28	114.06
22	A	404	CLA	CHD-C1D-ND	-2.68	121.04	124.80
22	B	707	CLA	C1B-CHB-C4A	-2.67	124.94	130.04
22	C	503	CLA	CMD-C2D-C3D	2.67	133.82	127.69
29	c	519	DGD	O6D-C1D-O3G	-2.67	103.73	110.04
22	b	707	CLA	C4A-NA-C1A	2.67	107.90	106.68
23	B	718	BCR	C2-C1-C6	2.67	114.32	110.44
23	t	701	BCR	C1-C6-C5	-2.67	118.99	122.64
23	t	701	BCR	C27-C26-C25	2.67	126.31	122.70
22	B	713	CLA	O2A-CGA-O1A	-2.67	116.96	123.63
26	a	413	SQD	O7-S-C6	2.67	110.74	106.76
22	b	704	CLA	C11-C12-C13	-2.67	107.11	115.97
22	b	712	CLA	O1D-CGD-CBD	2.66	129.77	124.52
26	A	409	SQD	O48-C23-C24	2.66	119.95	111.83
33	c	523	LMG	C1-O6-C5	-2.66	108.53	113.72
23	d	403	BCR	C24-C23-C22	-2.66	122.30	126.23
26	f	101	SQD	C45-O47-C7	2.66	124.16	117.80
23	b	718	BCR	C27-C26-C25	2.66	126.30	122.70
23	D	404	BCR	C24-C23-C22	-2.66	122.31	126.23
22	C	512	CLA	CMB-C2B-C3B	2.65	129.99	124.68
33	b	723	LMG	O8-C28-O10	-2.65	116.99	123.63
28	d	409	STE	O2-C1-O1	-2.65	116.51	123.33
23	K	101	BCR	C15-C16-C17	-2.65	118.09	123.52
34	D	407	PHO	C1-C2-C3	-2.65	121.86	126.20
23	b	718	BCR	C8-C7-C6	-2.65	119.93	127.00
22	C	510	CLA	CHB-C4A-NA	2.65	128.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	513	CLA	CHD-C1D-ND	-2.64	121.08	124.80
22	B	713	CLA	CHA-C1A-NA	-2.64	120.40	126.39
23	T	701	BCR	C2-C1-C6	2.64	114.28	110.44
23	b	717	BCR	C15-C14-C13	-2.64	123.57	127.28
22	B	709	CLA	C1B-CHB-C4A	-2.64	125.00	130.04
22	c	503	CLA	CHB-C4A-NA	2.64	128.21	124.40
22	B	712	CLA	O2D-CGD-CBD	2.64	115.84	111.23
22	H	102	CLA	C1-C2-C3	-2.64	121.88	126.20
33	M	101	LMG	C38-C37-C36	-2.64	101.05	114.37
28	b	725	STE	C3-C2-C1	-2.64	107.63	114.51
22	B	710	CLA	CMD-C2D-C3D	2.63	133.73	127.69
22	B	710	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
29	C	519	DGD	O2D-C2D-C1D	-2.63	103.81	110.08
22	C	513	CLA	C6-C5-C3	-2.63	107.06	113.47
23	H	101	BCR	C16-C15-C14	-2.63	118.14	123.52
22	b	708	CLA	CHB-C4A-NA	2.63	128.19	124.40
29	C	517	DGD	C4E-C3E-C2E	-2.63	106.22	110.83
29	H	103	DGD	C1D-C2D-C3D	-2.62	104.50	110.01
29	C	518	DGD	O4D-C4D-C3D	2.62	116.55	110.38
22	b	701	CLA	CMB-C2B-C1B	-2.62	124.62	128.46
22	C	513	CLA	C1B-CHB-C4A	-2.62	125.05	130.04
29	C	518	DGD	C3D-C4D-C5D	-2.62	105.49	110.23
22	c	505	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
22	b	702	CLA	CHC-C1C-NC	2.61	128.25	124.31
23	d	403	BCR	C16-C15-C14	-2.61	118.17	123.52
23	H	101	BCR	C27-C26-C25	2.61	126.23	122.70
22	c	508	CLA	O1D-CGD-CBD	2.61	129.66	124.52
23	b	719	BCR	C12-C13-C14	-2.61	114.91	119.01
29	C	517	DGD	C6D-O5D-C1E	2.61	119.39	113.80
22	c	506	CLA	CMB-C2B-C1B	-2.61	124.64	128.46
22	c	509	CLA	CHD-C1D-C2D	2.60	130.90	125.49
27	B	722	LHG	C20-C19-C18	-2.60	101.21	114.37
22	b	711	CLA	CHD-C1D-ND	-2.60	121.14	124.80
33	a	419	LMG	C9-C8-C7	-2.60	105.73	111.78
22	b	703	CLA	CHD-C1D-ND	-2.59	121.16	124.80
23	a	407	BCR	C29-C30-C25	2.59	114.20	110.44
22	c	511	CLA	C1B-CHB-C4A	-2.59	125.11	130.04
29	h	702	DGD	C3D-C4D-C5D	-2.58	105.55	110.23
22	C	505	CLA	C4-C3-C5	2.58	119.71	115.23
29	A	413	DGD	C3G-C2G-C1G	-2.58	105.77	111.78
25	a	411	PL9	C40-C39-C41	2.58	119.70	115.23
29	C	519	DGD	CBB-CAB-C9B	-2.58	101.35	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	409	SQD	O9-S-O7	-2.57	105.46	113.82
25	A	408	PL9	C35-C34-C33	-2.57	117.02	123.63
22	c	509	CLA	O2D-CGD-CBD	2.57	115.72	111.23
23	k	101	BCR	C27-C26-C25	2.57	126.18	122.70
22	C	504	CLA	C1B-CHB-C4A	-2.57	125.14	130.04
25	A	408	PL9	C27-C28-C29	-2.57	121.75	127.62
22	B	703	CLA	C4-C3-C5	2.57	119.68	115.23
22	b	711	CLA	CMC-C2C-C1C	-2.57	121.03	125.03
22	c	513	CLA	CHC-C1C-NC	2.56	128.17	124.31
23	A	405	BCR	C16-C15-C14	-2.56	118.28	123.52
22	c	508	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
26	a	413	SQD	O9-S-C6	2.56	110.58	106.76
22	c	514	CLA	CMB-C2B-C3B	2.56	129.80	124.68
22	c	506	CLA	C4D-C3D-CAD	-2.56	105.33	108.11
22	C	512	CLA	CHB-C4A-NA	2.56	128.09	124.40
33	d	408	LMG	O6-C1-O1	-2.56	104.01	110.04
26	b	720	SQD	C45-O47-C7	2.55	123.91	117.80
23	t	701	BCR	C36-C18-C19	2.55	121.99	118.09
26	A	409	SQD	C3-C4-C5	2.55	114.86	110.23
22	B	703	CLA	C1B-CHB-C4A	-2.55	125.17	130.04
29	c	519	DGD	O5D-C1E-C2E	2.55	112.15	108.27
22	C	505	CLA	C6-C5-C3	2.55	119.68	113.47
22	B	706	CLA	CHD-C1D-ND	-2.55	121.22	124.80
22	B	702	CLA	C1B-CHB-C4A	-2.54	125.19	130.04
22	a	403	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
26	D	409	SQD	C3-C4-C5	2.54	114.84	110.23
22	H	102	CLA	C4-C3-C5	2.54	119.64	115.23
22	c	508	CLA	C1B-CHB-C4A	-2.54	125.19	130.04
29	A	413	DGD	C3E-C4E-C5E	-2.54	105.62	110.23
22	B	712	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
22	B	705	CLA	C4A-NA-C1A	2.54	107.84	106.68
29	C	518	DGD	O6D-C1D-O3G	-2.54	104.05	110.04
29	H	103	DGD	O3G-C1D-C2D	-2.54	104.42	108.27
26	f	101	SQD	C44-O6-C1	2.53	119.22	113.80
22	B	709	CLA	CAC-C3C-C4C	2.53	128.08	124.79
22	b	708	CLA	CHD-C1D-ND	-2.53	121.24	124.80
22	C	512	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
29	A	413	DGD	CDB-CCB-CBB	-2.52	101.61	114.37
22	b	710	CLA	CHA-C1A-NA	-2.52	120.68	126.39
34	a	405	PHO	CMA-C3A-C4A	-2.52	109.18	114.61
22	C	506	CLA	C1B-CHB-C4A	-2.52	125.23	130.04
28	C	523	STE	C3-C2-C1	-2.52	107.93	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	405	PL9	C37-C38-C39	-2.52	121.86	127.62
22	H	102	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
22	C	514	CLA	CHB-C4A-NA	2.52	128.03	124.40
34	D	406	PHO	C5-C3-C2	2.51	126.81	121.17
29	c	517	DGD	O3G-C1D-C2D	-2.51	104.45	108.27
22	d	402	CLA	C1D-ND-C4D	-2.51	104.55	106.31
22	c	504	CLA	C7-C6-C5	-2.51	106.57	113.26
22	C	511	CLA	O2D-CGD-CBD	2.51	115.62	111.23
22	b	712	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
27	l	101	LHG	O8-C23-O10	-2.51	117.36	123.63
22	D	402	CLA	CHB-C4A-NA	2.51	128.02	124.40
25	A	408	PL9	O1-C4-C3	-2.51	118.09	120.73
28	B	720	STE	C3-C2-C1	-2.50	107.97	114.51
22	B	712	CLA	CHD-C4C-C3C	-2.50	121.13	124.77
22	C	504	CLA	CHD-C1D-ND	-2.50	121.28	124.80
23	Y	101	BCR	C15-C16-C17	-2.50	118.41	123.52
22	C	503	CLA	C16-C17-C18	-2.50	104.79	115.94
22	C	502	CLA	O2D-CGD-CBD	2.50	115.59	111.23
23	H	101	BCR	C38-C26-C25	-2.49	121.76	124.48
28	J	101	STE	O2-C1-C2	2.49	121.87	114.00
22	b	712	CLA	C11-C12-C13	-2.49	107.68	115.97
33	c	523	LMG	O6-C1-O1	-2.49	104.16	110.04
22	A	404	CLA	C1D-ND-C4D	-2.49	104.57	106.31
25	d	404	PL9	C7-C3-C2	-2.49	120.45	123.39
23	K	101	BCR	C15-C14-C13	-2.48	123.79	127.28
33	D	412	LMG	O7-C10-O9	-2.48	117.90	123.70
22	b	707	CLA	CED-O2D-CGD	2.48	121.55	115.92
29	c	517	DGD	CAB-C9B-C8B	-2.48	101.82	114.37
22	B	706	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
22	a	403	CLA	C4A-NA-C1A	2.48	107.81	106.68
29	C	517	DGD	C6B-C5B-C4B	-2.48	101.83	114.37
22	C	507	CLA	C4-C3-C5	2.48	119.53	115.23
25	a	411	PL9	C26-C24-C23	-2.48	115.60	121.17
22	H	102	CLA	CHB-C4A-NA	2.48	127.98	124.40
29	H	103	DGD	C3G-C2G-C1G	-2.48	106.01	111.78
23	h	701	BCR	C36-C18-C17	-2.48	118.80	122.82
29	C	517	DGD	O1G-C1A-C2A	-2.48	104.28	111.83
22	A	403	CLA	C4A-NA-C1A	2.48	107.81	106.68
23	K	101	BCR	C24-C23-C22	-2.47	122.58	126.23
22	B	704	CLA	C2D-C1D-ND	-2.47	107.68	110.13
23	C	515	BCR	C38-C26-C25	-2.47	121.79	124.48
22	C	506	CLA	CHB-C4A-NA	2.47	127.96	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	514	CLA	C1-C2-C3	-2.46	122.16	126.20
22	a	401	CLA	C4D-CHA-C1A	2.46	124.18	121.24
22	A	403	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
23	a	407	BCR	C39-C30-C25	-2.46	106.38	110.24
23	K	101	BCR	C38-C26-C25	-2.46	121.80	124.48
33	c	522	LMG	O2-C2-C1	-2.46	104.22	110.08
33	C	516	LMG	C40-C39-C38	-2.46	101.95	114.37
23	h	701	BCR	C7-C8-C9	-2.46	122.60	126.23
22	C	510	CLA	C1B-CHB-C4A	-2.45	125.36	130.04
33	M	101	LMG	C9-C8-C7	-2.45	106.06	111.78
28	B	724	STE	C3-C2-C1	-2.45	108.10	114.51
22	H	102	CLA	CHA-C4D-ND	2.45	137.61	132.55
22	C	512	CLA	CHA-C1A-NA	-2.45	120.84	126.39
22	B	716	CLA	C4D-CHA-C1A	2.45	124.17	121.24
22	A	402	CLA	C11-C12-C13	-2.45	107.83	115.97
22	a	406	CLA	CAC-C3C-C4C	2.45	127.97	124.79
22	c	510	CLA	C11-C10-C8	-2.45	107.84	115.97
22	a	406	CLA	C1B-CHB-C4A	-2.44	125.38	130.04
22	B	702	CLA	C16-C15-C13	-2.44	107.84	115.97
29	c	517	DGD	O6D-C1D-O3G	-2.44	104.27	110.04
25	a	411	PL9	O2-C1-C2	-2.44	116.27	121.83
22	B	712	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
26	a	413	SQD	O48-C23-C24	2.44	119.28	111.83
22	C	511	CLA	CHB-C4A-NA	2.44	127.92	124.40
26	D	409	SQD	C46-C45-C44	-2.44	105.79	113.67
22	C	510	CLA	CMC-C2C-C1C	-2.44	121.22	125.03
27	d	406	LHG	C11-C10-C9	-2.44	102.04	114.37
23	b	717	BCR	C3-C4-C5	-2.44	109.71	114.06
33	c	522	LMG	O7-C10-O9	-2.44	118.01	123.70
22	A	404	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
23	C	515	BCR	C27-C26-C25	2.43	125.99	122.70
22	b	714	CLA	CMB-C2B-C3B	2.43	129.55	124.68
22	C	510	CLA	C9-C8-C10	-2.43	102.60	111.27
33	b	723	LMG	O6-C5-C6	2.43	112.47	106.44
29	h	702	DGD	C4B-C3B-C2B	-2.43	104.19	113.13
26	A	412	SQD	O47-C45-C44	2.43	113.41	107.96
22	B	706	CLA	C3B-C4B-NB	-2.43	106.07	109.21
23	B	718	BCR	C27-C26-C25	2.43	125.99	122.70
33	b	723	LMG	O1-C1-C2	-2.43	104.58	108.27
22	C	504	CLA	C4D-C3D-CAD	-2.43	105.47	108.11
34	D	406	PHO	C1A-C2A-C3A	-2.43	100.53	102.84
33	C	516	LMG	C36-C35-C34	-2.43	102.09	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	708	CLA	CHD-C1D-ND	-2.43	121.39	124.80
22	d	401	CLA	C4-C3-C5	2.42	119.44	115.23
25	D	405	PL9	C12-C13-C14	-2.42	122.08	127.62
25	D	405	PL9	C41-C39-C38	-2.42	115.73	121.17
22	b	708	CLA	O2D-CGD-CBD	2.42	115.47	111.23
22	b	709	CLA	O2A-CGA-O1A	-2.42	117.57	123.63
23	d	403	BCR	C33-C5-C6	-2.42	121.84	124.48
29	A	413	DGD	C1D-C2D-C3D	-2.42	104.91	110.01
23	A	405	BCR	C2-C1-C6	2.42	113.96	110.44
22	B	716	CLA	C1B-CHB-C4A	-2.42	125.42	130.04
22	C	509	CLA	O2D-CGD-CBD	2.42	115.46	111.23
22	b	707	CLA	CHA-C1A-NA	-2.42	120.91	126.39
26	A	409	SQD	O4-C4-C3	-2.42	104.67	110.38
22	C	513	CLA	CHD-C1D-ND	-2.42	121.40	124.80
33	D	408	LMG	O2-C2-C1	-2.42	104.31	110.08
22	C	503	CLA	CMD-C2D-C1D	-2.42	120.47	124.73
22	c	508	CLA	CMB-C2B-C3B	2.42	129.51	124.68
34	D	406	PHO	CMA-C3A-C2A	-2.42	104.80	114.13
22	c	502	CLA	CHD-C1D-ND	-2.42	121.40	124.80
22	C	504	CLA	C3A-C2A-C1A	2.42	104.96	101.34
22	a	401	CLA	CMD-C2D-C3D	2.41	133.23	127.69
22	c	509	CLA	CHD-C4C-NC	2.41	127.97	124.23
22	B	703	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
22	B	706	CLA	O2D-CGD-CBD	2.41	115.44	111.23
22	B	703	CLA	CMB-C2B-C3B	2.41	129.50	124.68
23	c	515	BCR	C16-C17-C18	-2.41	123.90	127.28
22	C	505	CLA	C4A-NA-C1A	2.41	107.78	106.68
26	b	720	SQD	O10-C23-C24	-2.40	114.38	123.78
35	E	103	HEC	C1D-C2D-C3D	-2.40	105.32	107.00
22	c	514	CLA	C1B-CHB-C4A	-2.40	125.46	130.04
29	c	519	DGD	O1G-C1A-C2A	-2.40	104.51	111.83
22	B	702	CLA	CHC-C1C-NC	2.40	127.93	124.31
22	c	511	CLA	C7-C6-C5	-2.40	106.86	113.26
22	B	713	CLA	C1B-CHB-C4A	-2.40	125.47	130.04
27	A	410	LHG	O8-C23-O10	-2.40	117.63	123.63
22	b	714	CLA	CAC-C3C-C4C	2.40	127.91	124.79
22	B	711	CLA	O2D-CGD-CBD	2.40	115.42	111.23
23	C	501	BCR	C27-C26-C25	2.40	125.94	122.70
33	C	516	LMG	C9-C8-C7	-2.40	106.20	111.78
23	B	717	BCR	C3-C4-C5	-2.39	109.79	114.06
25	A	408	PL9	O2-C1-C2	-2.39	116.38	121.83
23	B	719	BCR	C8-C7-C6	-2.39	120.60	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	715	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
23	c	516	BCR	C1-C6-C5	-2.39	119.37	122.64
33	c	522	LMG	C3-C4-C5	-2.39	105.89	110.23
27	a	412	LHG	C11-C10-C9	-2.39	102.28	114.37
25	d	404	PL9	C35-C34-C36	2.39	119.38	115.23
22	B	715	CLA	C5-C3-C2	-2.39	115.80	121.17
22	c	511	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	b	704	CLA	CMB-C2B-C3B	2.39	129.46	124.68
23	c	515	BCR	C24-C23-C22	-2.39	122.70	126.23
23	A	405	BCR	C37-C22-C21	-2.39	118.94	122.82
22	a	406	CLA	CMB-C2B-C3B	2.39	129.46	124.68
29	h	702	DGD	C4D-C3D-C2D	-2.39	106.64	110.83
22	a	403	CLA	CHB-C4A-NA	2.39	127.84	124.40
29	C	518	DGD	CDB-CCB-CBB	-2.39	102.31	114.37
22	c	512	CLA	O1A-CGA-CBA	2.39	133.11	123.78
23	c	515	BCR	C27-C26-C25	2.39	125.93	122.70
22	b	713	CLA	CHA-C1A-NA	-2.38	121.00	126.39
23	b	717	BCR	C8-C7-C6	-2.38	120.64	127.00
22	B	708	CLA	C6-C7-C8	-2.38	108.05	115.97
34	D	407	PHO	CMC-C2C-C3C	2.38	129.43	124.94
22	D	403	CLA	O1D-CGD-CBD	2.38	129.21	124.52
22	d	402	CLA	CGD-CBD-CAD	-2.38	103.14	110.85
22	B	709	CLA	CAA-CBA-CGA	-2.38	106.46	113.21
29	h	702	DGD	O5E-C6E-C5E	-2.38	103.25	111.33
33	c	522	LMG	C9-C8-C7	-2.37	106.25	111.78
22	D	401	CLA	CHB-C4A-NA	2.37	127.83	124.40
22	b	711	CLA	CMC-C2C-C3C	2.37	132.57	126.15
28	C	521	STE	O2-C1-C2	2.37	121.50	114.00
25	D	405	PL9	C7-C8-C9	-2.37	122.74	126.83
22	c	509	CLA	CHC-C1C-NC	2.37	127.88	124.31
22	b	706	CLA	CHB-C4A-NA	2.37	127.82	124.40
33	c	520	LMG	C9-C8-C7	-2.37	106.26	111.78
22	B	711	CLA	C7-C6-C5	-2.37	106.95	113.26
26	B	723	SQD	C1-C2-C3	-2.36	105.04	110.01
29	c	518	DGD	O3G-C1D-C2D	-2.36	104.68	108.27
22	b	702	CLA	CHD-C1D-ND	-2.36	121.48	124.80
23	b	717	BCR	C15-C16-C17	-2.36	118.69	123.52
22	C	506	CLA	CMB-C2B-C3B	2.36	129.40	124.68
23	B	719	BCR	C30-C25-C26	-2.36	119.41	122.64
22	C	508	CLA	O1D-CGD-CBD	2.36	129.17	124.52
28	t	702	STE	O2-C1-C2	2.36	121.45	114.00
22	A	404	CLA	C4A-NA-C1A	2.36	107.75	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	510	CLA	CHD-C4C-NC	2.36	127.88	124.23
22	a	401	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
23	b	719	BCR	C16-C15-C14	-2.35	118.71	123.52
23	D	404	BCR	C7-C8-C9	-2.35	122.76	126.23
23	C	515	BCR	C37-C22-C21	-2.35	119.01	122.82
22	B	715	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
22	b	705	CLA	CHD-C1D-ND	-2.35	121.50	124.80
23	b	717	BCR	C11-C10-C9	-2.35	123.98	127.28
22	B	704	CLA	C1D-ND-C4D	2.35	107.96	106.31
29	c	519	DGD	O2G-C1B-C2B	-2.35	106.41	111.48
29	c	517	DGD	C5B-C4B-C3B	-2.34	102.52	114.37
22	C	506	CLA	CHD-C1D-ND	-2.34	121.50	124.80
22	a	406	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
22	c	508	CLA	CHA-C1A-NA	-2.34	121.10	126.39
29	c	519	DGD	C8B-C7B-C6B	-2.34	102.56	114.37
33	b	723	LMG	O5-C6-C5	-2.33	103.38	111.33
22	b	714	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
27	a	414	LHG	O8-C23-C24	2.33	118.95	111.83
26	D	409	SQD	O8-S-O9	-2.33	105.56	111.40
22	B	711	CLA	CHD-C4C-NC	2.33	127.85	124.23
22	B	714	CLA	O1D-CGD-CBD	2.33	129.12	124.52
22	a	403	CLA	C4-C3-C5	2.33	119.28	115.23
22	A	404	CLA	C4-C3-C5	2.33	119.27	115.23
29	c	518	DGD	C3G-C2G-C1G	-2.33	106.35	111.78
22	c	508	CLA	C7-C6-C5	-2.33	107.06	113.26
22	C	504	CLA	C6-C7-C8	-2.33	108.23	115.97
23	b	719	BCR	C15-C16-C17	-2.33	118.76	123.52
22	b	709	CLA	O1D-CGD-CBD	2.33	129.11	124.52
22	C	504	CLA	C6-C5-C3	2.33	119.13	113.47
22	D	402	CLA	CAA-C2A-C1A	-2.32	104.36	111.97
33	b	721	LMG	O6-C1-O1	-2.32	104.55	110.04
22	b	713	CLA	CHA-C4D-ND	2.32	137.34	132.55
23	b	717	BCR	C38-C26-C25	-2.32	121.95	124.48
23	d	403	BCR	C3-C4-C5	-2.32	109.92	114.06
22	D	403	CLA	CHB-C4A-NA	2.32	127.75	124.40
33	d	408	LMG	C7-O1-C1	-2.32	108.82	113.80
29	c	518	DGD	O2E-C2E-C1E	-2.32	104.55	110.08
22	D	402	CLA	C1B-CHB-C4A	-2.32	125.62	130.04
22	b	707	CLA	CHB-C4A-NA	2.32	127.75	124.40
22	b	705	CLA	CHD-C1D-C2D	2.32	130.31	125.49
26	a	413	SQD	O48-C23-O10	-2.32	117.83	123.63
29	C	519	DGD	C7B-C6B-C5B	-2.32	102.65	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	413	DGD	CBB-CAB-C9B	-2.32	102.66	114.37
22	b	707	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
22	c	504	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
22	C	508	CLA	C1B-CHB-C4A	-2.31	125.63	130.04
25	A	408	PL9	O2-C1-C6	2.31	124.16	120.48
23	t	701	BCR	C15-C16-C17	-2.31	118.79	123.52
33	d	408	LMG	C3-C4-C5	-2.31	106.04	110.23
23	C	501	BCR	C15-C16-C17	-2.31	118.80	123.52
22	a	401	CLA	C1B-CHB-C4A	-2.31	125.64	130.04
22	a	404	CLA	CMA-C3A-C4A	-2.31	105.57	111.77
22	c	503	CLA	CHD-C1D-ND	-2.31	121.56	124.80
22	b	711	CLA	CHB-C4A-NA	2.31	127.73	124.40
22	B	705	CLA	C4D-CHA-C1A	2.30	123.99	121.24
22	B	705	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
22	b	707	CLA	C6-C5-C3	2.30	119.08	113.47
29	h	702	DGD	O6E-C5E-C4E	2.30	113.84	109.70
27	d	407	LHG	C26-C25-C24	2.30	121.58	113.13
28	B	701	STE	O2-C1-O1	-2.30	117.42	123.33
29	c	519	DGD	CDB-CCB-CBB	-2.30	102.74	114.37
22	b	702	CLA	CHC-C1C-C2C	-2.30	120.43	126.94
22	b	715	CLA	CHC-C1C-NC	2.30	127.77	124.31
23	Y	101	BCR	C37-C22-C21	-2.30	119.09	122.82
23	A	405	BCR	C38-C26-C25	-2.30	121.98	124.48
27	A	410	LHG	C11-C10-C9	-2.30	102.76	114.37
33	d	408	LMG	C31-C30-C29	-2.29	104.70	113.13
26	A	409	SQD	O5-C1-O6	2.29	115.46	110.04
22	b	713	CLA	C7-C6-C5	-2.29	107.15	113.26
29	A	413	DGD	O6E-C1E-O5D	-2.29	104.63	110.04
35	v	201	HEC	CMC-C2C-C3C	2.29	128.51	125.82
27	D	411	LHG	O8-C6-C5	-2.29	101.79	108.40
22	A	402	CLA	C1B-CHB-C4A	-2.29	125.67	130.04
23	k	102	BCR	C15-C16-C17	-2.29	118.84	123.52
33	C	520	LMG	O1-C7-C8	-2.29	105.25	110.82
29	C	517	DGD	CDB-CCB-CBB	-2.29	102.81	114.37
25	A	408	PL9	C20-C19-C18	-2.29	117.76	123.63
28	b	724	STE	O2-C1-C2	2.29	121.22	114.00
33	D	408	LMG	C38-C37-C36	-2.28	102.82	114.37
25	d	404	PL9	C50-C49-C48	-2.28	115.80	122.66
22	D	403	CLA	C1-C2-C3	-2.28	122.46	126.20
33	d	408	LMG	O7-C10-O9	-2.28	118.37	123.70
22	A	403	CLA	CHD-C1D-ND	-2.28	121.59	124.80
22	d	401	CLA	CHA-C4D-ND	2.28	137.25	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	715	CLA	C1B-CHB-C4A	-2.28	125.69	130.04
22	b	703	CLA	C11-C12-C13	-2.28	108.39	115.97
22	B	704	CLA	O2D-CGD-CBD	2.28	115.21	111.23
22	C	514	CLA	O1D-CGD-CBD	2.28	129.01	124.52
29	A	413	DGD	C3G-O3G-C1D	2.28	118.68	113.80
22	c	505	CLA	O1D-CGD-CBD	2.27	129.00	124.52
23	A	405	BCR	C36-C18-C17	-2.27	119.13	122.82
22	b	704	CLA	CHD-C1D-ND	-2.27	121.61	124.80
23	K	101	BCR	C31-C1-C6	2.27	113.80	110.24
22	a	406	CLA	CHA-C1A-NA	-2.27	121.25	126.39
29	c	519	DGD	O1G-C1G-C2G	-2.27	101.85	108.40
22	H	102	CLA	C2A-C1A-CHA	2.27	127.81	123.87
22	c	510	CLA	CHC-C1C-NC	2.27	127.73	124.31
29	h	702	DGD	C1E-O6E-C5E	2.27	118.15	113.72
29	C	519	DGD	C1D-C2D-C3D	-2.27	105.24	110.01
34	d	405	PHO	O2A-CGA-O1A	-2.27	117.95	123.63
23	a	407	BCR	C27-C26-C25	2.27	125.77	122.70
22	B	703	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
23	T	701	BCR	C3-C4-C5	-2.27	110.01	114.06
22	D	403	CLA	CMD-C2D-C1D	-2.27	120.73	124.73
22	B	716	CLA	CHA-C4D-ND	2.26	137.22	132.55
22	b	713	CLA	C2C-C1C-NC	2.26	112.36	109.98
22	B	715	CLA	CHA-C1A-NA	-2.26	121.27	126.39
22	b	713	CLA	C16-C15-C13	-2.26	108.45	115.97
26	f	101	SQD	O5-C1-C2	-2.26	105.73	110.37
33	c	523	LMG	C9-C8-C7	-2.26	106.52	111.78
25	d	404	PL9	C12-C13-C14	-2.26	122.45	127.62
22	B	705	CLA	OBD-CAD-C3D	2.26	133.70	128.42
22	C	505	CLA	CHC-C1C-NC	2.26	127.71	124.31
22	C	507	CLA	C1B-CHB-C4A	-2.26	125.74	130.04
22	b	711	CLA	C6-C5-C3	2.25	118.96	113.47
27	d	406	LHG	C18-C17-C16	-2.25	102.98	114.37
22	D	401	CLA	O2D-CGD-CBD	2.25	115.17	111.23
35	V	201	HEC	O1D-CGD-CBD	-2.25	115.96	123.09
23	a	407	BCR	C21-C20-C19	-2.25	116.69	123.20
33	c	523	LMG	O8-C28-O10	-2.25	118.01	123.63
22	C	502	CLA	CAA-CBA-CGA	-2.25	106.83	113.21
22	B	709	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
29	C	519	DGD	CDB-CCB-CBB	-2.25	103.02	114.37
34	d	405	PHO	C1B-NB-C4B	2.24	111.70	107.09
23	b	719	BCR	C28-C27-C26	-2.24	110.06	114.06
22	B	705	CLA	CHB-C4A-NA	2.24	127.64	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	CHB-C4A-NA	2.24	127.64	124.40
22	C	506	CLA	CED-O2D-CGD	2.24	121.00	115.92
27	a	412	LHG	O8-C6-C5	-2.24	101.94	108.40
34	a	405	PHO	O2A-CGA-O1A	-2.24	118.03	123.63
22	b	716	CLA	C4-C3-C5	2.24	119.11	115.23
29	C	517	DGD	O6D-C1D-O3G	-2.24	104.75	110.04
22	B	705	CLA	C4D-C3D-CAD	-2.24	105.67	108.11
22	b	704	CLA	CHD-C1D-C2D	2.24	130.14	125.49
22	d	402	CLA	CHA-C1A-NA	-2.24	121.33	126.39
22	B	702	CLA	CHD-C1D-C2D	2.24	130.14	125.49
25	A	408	PL9	C12-C13-C14	-2.23	122.51	127.62
22	b	708	CLA	CHA-C1A-NA	-2.23	121.33	126.39
28	b	727	STE	O2-C1-C2	2.23	121.05	114.00
22	b	708	CLA	C1B-CHB-C4A	-2.23	125.79	130.04
22	B	713	CLA	C2A-C1A-CHA	2.23	127.74	123.87
33	C	516	LMG	O3-C3-C2	-2.23	105.12	110.38
22	C	514	CLA	C3A-C2A-C1A	2.23	104.67	101.34
22	c	513	CLA	O1D-CGD-CBD	2.23	128.91	124.52
22	C	508	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
23	H	101	BCR	C16-C17-C18	-2.22	124.16	127.28
22	c	506	CLA	CMB-C2B-C3B	2.22	129.12	124.68
23	T	701	BCR	C38-C26-C27	-2.22	108.86	113.60
22	c	505	CLA	CHD-C4C-NC	2.22	127.68	124.23
26	D	409	SQD	C1-O5-C5	-2.22	109.38	113.72
22	C	513	CLA	CMB-C2B-C3B	2.22	129.12	124.68
22	d	402	CLA	C3D-C4D-ND	2.22	113.60	109.99
22	A	403	CLA	CMD-C2D-C1D	2.22	128.64	124.73
23	c	516	BCR	C38-C26-C25	-2.22	122.06	124.48
22	d	402	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
22	a	406	CLA	CHB-C4A-NA	2.22	127.60	124.40
23	b	717	BCR	C36-C18-C19	2.22	121.47	118.09
22	B	712	CLA	C1B-CHB-C4A	-2.21	125.82	130.04
33	M	101	LMG	O3-C3-C2	-2.21	105.16	110.38
29	A	413	DGD	C8B-C7B-C6B	-2.21	103.20	114.37
23	H	101	BCR	C29-C30-C25	2.21	113.65	110.44
29	H	103	DGD	CDB-CCB-CBB	-2.21	103.20	114.37
34	D	407	PHO	C1A-C2A-C3A	-2.21	100.74	102.84
23	b	718	BCR	C2-C1-C6	2.21	113.65	110.44
22	c	509	CLA	C1-C2-C3	-2.21	122.58	126.20
29	H	103	DGD	C3D-C4D-C5D	-2.20	106.24	110.23
22	c	514	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
22	b	715	CLA	O2D-CGD-CBD	2.20	115.08	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	405	PL9	C40-C39-C41	2.20	119.05	115.23
22	C	508	CLA	CAA-CBA-CGA	-2.20	106.96	113.21
22	B	708	CLA	CHD-C4C-NC	2.20	127.64	124.23
22	c	509	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
22	C	503	CLA	CHA-C1A-NA	-2.20	121.41	126.39
22	B	708	CLA	CHB-C4A-NA	2.20	127.57	124.40
29	h	702	DGD	O5D-C6D-C5D	-2.20	104.47	109.42
22	b	709	CLA	CHA-C1A-NA	-2.20	121.42	126.39
33	b	721	LMG	C12-C11-C10	-2.20	105.65	113.69
29	H	103	DGD	CAB-C9B-C8B	-2.19	103.27	114.37
22	a	403	CLA	C11-C10-C8	-2.19	108.67	115.97
22	b	705	CLA	C16-C15-C13	-2.19	108.68	115.97
33	c	522	LMG	C40-C39-C38	-2.19	103.29	114.37
34	D	406	PHO	C1-C2-C3	-2.19	122.61	126.20
22	d	401	CLA	O1D-CGD-CBD	2.19	128.84	124.52
26	B	723	SQD	C25-C24-C23	-2.19	105.67	113.69
22	B	703	CLA	CHD-C4C-NC	2.19	127.62	124.23
22	C	514	CLA	C5-C3-C2	-2.19	116.26	121.17
22	b	710	CLA	C2C-C1C-NC	2.19	112.28	109.98
22	C	503	CLA	C4D-C3D-CAD	-2.19	105.73	108.11
26	D	409	SQD	O4-C4-C3	-2.19	105.22	110.38
22	b	712	CLA	C1-C2-C3	-2.19	122.62	126.20
22	a	403	CLA	O2D-CGD-O1D	-2.18	119.59	123.85
22	b	704	CLA	C6-C7-C8	-2.18	108.71	115.97
22	C	506	CLA	C6-C5-C3	2.18	118.79	113.47
22	B	708	CLA	C3C-C4C-NC	-2.18	107.63	110.43
22	C	502	CLA	CMB-C2B-C3B	2.18	129.04	124.68
33	d	408	LMG	O3-C3-C2	-2.18	105.23	110.38
23	B	719	BCR	C1-C6-C5	-2.18	119.66	122.64
22	c	509	CLA	CMB-C2B-C3B	2.18	129.04	124.68
23	c	516	BCR	C36-C18-C17	-2.18	119.28	122.82
22	b	714	CLA	O2D-CGD-CBD	2.18	115.04	111.23
23	a	407	BCR	C11-C10-C9	-2.18	124.22	127.28
22	C	510	CLA	C2A-C3A-C4A	2.18	105.39	101.87
23	B	717	BCR	C15-C16-C17	-2.18	119.07	123.52
22	C	502	CLA	C1B-CHB-C4A	-2.17	125.89	130.04
33	C	520	LMG	C38-C37-C36	-2.17	103.38	114.37
23	B	719	BCR	C40-C30-C29	-2.17	100.61	108.95
33	C	516	LMG	C1-C2-C3	-2.17	105.44	110.01
22	c	504	CLA	CHD-C1D-ND	-2.17	121.75	124.80
22	b	708	CLA	C11-C10-C8	-2.17	108.75	115.97
35	v	201	HEC	CAD-CBD-CGD	-2.17	107.99	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	h	702	DGD	O6D-C1D-C2D	-2.17	105.92	110.37
22	C	503	CLA	C16-C15-C13	-2.17	108.76	115.97
22	c	506	CLA	CHD-C1D-ND	-2.17	121.75	124.80
22	C	504	CLA	CMA-C3A-C4A	2.17	117.59	111.77
29	c	519	DGD	C5B-C4B-C3B	-2.16	103.43	114.37
22	A	404	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
33	M	101	LMG	O6-C1-O1	-2.16	104.94	110.04
22	c	511	CLA	C6-C5-C3	-2.16	108.21	113.47
22	B	706	CLA	C4-C3-C5	2.16	118.97	115.23
33	c	523	LMG	C38-C37-C36	-2.16	103.47	114.37
22	C	504	CLA	O1D-CGD-CBD	2.16	128.77	124.52
27	l	101	LHG	O8-C23-C24	2.16	118.41	111.83
22	c	504	CLA	C4-C3-C5	2.16	118.97	115.23
22	B	711	CLA	C9-C8-C10	-2.15	103.59	111.27
22	A	402	CLA	C7-C6-C5	-2.15	107.52	113.26
22	b	703	CLA	CHD-C1D-C2D	2.15	129.97	125.49
33	C	520	LMG	O3-C3-C2	-2.15	105.30	110.38
22	b	702	CLA	C4-C3-C5	2.15	118.97	115.23
27	l	101	LHG	C27-C26-C25	-2.15	103.48	114.37
29	c	517	DGD	C8B-C7B-C6B	-2.15	103.48	114.37
29	C	519	DGD	O3E-C3E-C2E	-2.15	105.30	110.38
29	C	517	DGD	CBB-CAB-C9B	-2.15	103.49	114.37
22	c	502	CLA	O1D-CGD-CBD	2.15	128.76	124.52
22	C	504	CLA	C5-C3-C2	-2.15	116.34	121.17
33	b	721	LMG	C40-C39-C38	-2.15	103.49	114.37
23	T	701	BCR	C1-C6-C5	-2.15	119.69	122.64
25	d	404	PL9	C20-C19-C21	2.15	118.96	115.23
22	C	509	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
33	C	520	LMG	C1-O6-C5	-2.15	109.53	113.72
22	a	403	CLA	C17-C16-C15	-2.15	103.65	113.28
23	b	718	BCR	C15-C14-C13	-2.15	124.27	127.28
27	L	101	LHG	C36-C35-C34	-2.15	103.51	114.37
28	C	521	STE	O2-C1-O1	-2.15	117.81	123.33
25	D	405	PL9	C36-C34-C33	-2.15	116.35	121.17
25	A	408	PL9	C22-C23-C24	-2.15	122.71	127.62
22	c	506	CLA	CMD-C2D-C3D	2.15	132.61	127.69
22	b	706	CLA	CAC-C3C-C4C	-2.15	122.00	124.79
25	d	404	PL9	O1-C4-C3	-2.15	118.47	120.73
22	c	512	CLA	CHB-C4A-NA	2.14	127.50	124.40
23	a	407	BCR	C37-C22-C23	2.14	121.36	118.09
23	a	407	BCR	C34-C9-C10	-2.14	119.34	122.82
27	D	411	LHG	C11-C10-C9	-2.14	103.53	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	515	BCR	C11-C10-C9	-2.14	124.27	127.28
22	c	506	CLA	C11-C10-C8	-2.14	108.85	115.97
22	b	713	CLA	C2A-C1A-CHA	2.14	127.58	123.87
22	c	509	CLA	CED-O2D-CGD	-2.14	111.06	115.92
22	b	704	CLA	O1D-CGD-CBD	2.14	128.74	124.52
28	j	101	STE	O2-C1-O1	-2.14	117.83	123.33
33	M	101	LMG	C6-C5-C4	-2.14	107.77	113.02
29	c	518	DGD	O4D-C4D-C3D	2.14	115.42	110.38
22	A	402	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
29	A	413	DGD	C2G-O2G-C1B	2.14	122.91	117.80
33	c	520	LMG	C40-C39-C38	-2.14	103.56	114.37
22	b	711	CLA	CHD-C1D-C2D	2.14	129.93	125.49
22	b	701	CLA	CMB-C2B-C3B	2.13	128.95	124.68
27	L	101	LHG	O10-C23-C24	-2.13	115.44	123.78
26	A	409	SQD	O49-C7-C8	-2.13	115.44	123.78
22	c	511	CLA	O2D-CGD-CBD	2.13	114.96	111.23
27	d	406	LHG	C20-C19-C18	-2.13	103.59	114.37
33	c	522	LMG	O8-C28-O10	-2.13	118.30	123.63
26	a	413	SQD	O47-C7-C8	2.13	116.09	111.48
33	D	408	LMG	O8-C28-O10	-2.13	118.30	123.63
22	B	708	CLA	C1B-CHB-C4A	-2.13	125.98	130.04
22	c	512	CLA	C11-C12-C13	-2.13	108.89	115.97
22	C	504	CLA	O2A-C1-C2	-2.13	99.92	108.11
22	a	403	CLA	C9-C8-C10	-2.13	103.69	111.27
23	Y	101	BCR	C2-C1-C6	2.13	113.53	110.44
22	C	507	CLA	CAA-C2A-C1A	-2.13	105.00	111.97
29	C	519	DGD	O3G-C1D-C2D	-2.13	105.04	108.27
22	b	706	CLA	C1-C2-C3	-2.12	122.72	126.20
22	c	503	CLA	CHD-C1D-C2D	2.12	129.91	125.49
22	B	708	CLA	C1-O2A-CGA	2.12	121.79	116.65
22	b	706	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
22	b	715	CLA	CHA-C1A-NA	-2.12	121.58	126.39
27	a	414	LHG	C11-C10-C9	-2.12	103.64	114.37
26	f	101	SQD	O8-S-C6	2.12	110.06	105.97
22	c	502	CLA	CED-O2D-CGD	-2.12	111.11	115.92
29	A	413	DGD	C5B-C4B-C3B	-2.12	103.67	114.37
22	c	513	CLA	CHD-C1D-C2D	2.12	129.89	125.49
23	d	403	BCR	C30-C25-C26	-2.12	119.75	122.64
28	X	101	STE	C15-C14-C13	-2.11	103.68	114.37
33	b	723	LMG	C40-C39-C38	-2.11	103.68	114.37
22	A	403	CLA	CHA-C1A-NA	-2.11	121.61	126.39
26	f	101	SQD	O9-S-C6	2.11	109.91	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
22	B	705	CLA	C1-O2A-CGA	-2.11	111.54	116.65
26	b	720	SQD	O47-C45-C46	2.11	115.91	108.34
22	b	703	CLA	OBD-CAD-C3D	2.11	133.35	128.42
29	h	702	DGD	CAB-C9B-C8B	-2.11	103.71	114.37
22	c	509	CLA	C1B-CHB-C4A	-2.11	126.02	130.04
33	B	721	LMG	O8-C28-O10	-2.10	117.92	123.33
34	a	405	PHO	C1B-NB-C4B	2.10	111.41	107.09
22	B	716	CLA	CHA-C1A-NA	-2.10	121.64	126.39
23	A	405	BCR	C7-C8-C9	-2.10	123.13	126.23
33	C	520	LMG	C6-C5-C4	-2.10	107.87	113.02
23	a	407	BCR	C15-C16-C17	-2.10	119.23	123.52
28	b	727	STE	C3-C2-C1	-2.10	109.04	114.51
27	D	411	LHG	C27-C26-C25	-2.10	103.77	114.37
22	c	504	CLA	C6-C5-C3	2.09	118.57	113.47
22	c	511	CLA	C1-C2-C3	-2.09	122.77	126.20
22	A	403	CLA	C2A-C1A-CHA	2.09	127.50	123.87
22	B	716	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
22	B	715	CLA	CAC-C3C-C4C	2.09	127.51	124.79
22	D	403	CLA	CMD-C2D-C3D	2.09	132.49	127.69
22	b	704	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	C	513	CLA	OBD-CAD-C3D	2.09	133.30	128.42
23	k	102	BCR	C7-C8-C9	-2.09	123.14	126.23
22	c	508	CLA	CMC-C2C-C3C	2.09	131.80	126.15
22	C	508	CLA	C1-O2A-CGA	2.09	121.71	116.65
23	A	405	BCR	C8-C7-C6	-2.09	121.42	127.00
29	c	519	DGD	C1D-C2D-C3D	-2.09	105.61	110.01
23	K	101	BCR	C7-C8-C9	-2.09	123.14	126.23
22	A	404	CLA	CHC-C1C-C2C	-2.09	121.02	126.94
22	b	715	CLA	CHC-C1C-C2C	-2.09	121.02	126.94
26	f	101	SQD	O48-C23-C24	2.09	118.20	111.83
34	D	406	PHO	O2A-CGA-O1A	-2.09	118.41	123.63
29	c	519	DGD	O3E-C3E-C2E	-2.09	105.45	110.38
27	D	410	LHG	C15-C14-C13	-2.09	103.81	114.37
22	C	504	CLA	C2A-C1A-CHA	2.09	127.49	123.87
22	B	704	CLA	C2A-C3A-C4A	2.09	105.24	101.87
22	b	706	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
23	a	407	BCR	C30-C25-C26	-2.08	119.79	122.64
29	c	519	DGD	O2D-C2D-C3D	-2.08	105.47	110.38
29	c	518	DGD	C7A-C6A-C5A	-2.08	103.85	114.37
22	b	710	CLA	CMB-C2B-C1B	-2.08	125.41	128.46
22	H	102	CLA	C4D-CHA-C1A	2.08	123.73	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	704	CLA	C1B-CHB-C4A	-2.08	126.07	130.04
25	D	405	PL9	C50-C49-C48	-2.08	116.42	122.66
22	B	704	CLA	C6-C7-C8	-2.08	109.06	115.97
22	C	503	CLA	C4D-CHA-C1A	2.08	123.72	121.24
22	B	706	CLA	O1A-CGA-CBA	2.08	131.90	123.78
22	a	404	CLA	O2D-CGD-O1D	-2.08	119.81	123.85
22	B	715	CLA	CHC-C1C-NC	2.08	127.44	124.31
22	c	511	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
22	c	506	CLA	CHB-C4A-NA	2.07	127.39	124.40
22	B	715	CLA	C2A-C1A-CHA	2.07	127.46	123.87
29	C	519	DGD	C3G-C2G-C1G	-2.07	106.96	111.78
33	a	419	LMG	C7-O1-C1	2.07	118.23	113.80
22	C	503	CLA	CMB-C2B-C1B	-2.07	125.42	128.46
22	B	716	CLA	O2D-CGD-CBD	2.07	114.85	111.23
29	c	517	DGD	C4A-C3A-C2A	-2.07	105.52	113.13
33	D	412	LMG	C38-C37-C36	-2.07	103.91	114.37
28	t	702	STE	C3-C2-C1	-2.07	109.11	114.51
23	c	516	BCR	C7-C8-C9	-2.07	123.18	126.23
22	B	712	CLA	CBC-CAC-C3C	2.07	118.02	112.42
29	H	103	DGD	O2G-C1B-O1B	-2.07	118.88	123.70
33	c	520	LMG	C1-O6-C5	-2.06	109.69	113.72
28	c	521	STE	C15-C14-C13	-2.06	103.93	114.37
23	K	101	BCR	C27-C26-C25	2.06	125.49	122.70
27	D	410	LHG	C20-C19-C18	-2.06	103.94	114.37
22	b	704	CLA	C4-C3-C5	2.06	118.81	115.23
22	c	508	CLA	CHD-C1D-ND	-2.06	121.90	124.80
35	E	103	HEC	O2D-CGD-CBD	2.06	120.51	114.00
22	b	716	CLA	CHD-C1D-ND	-2.06	121.90	124.80
26	A	409	SQD	C9-C8-C7	-2.06	106.15	113.69
22	B	705	CLA	C1B-CHB-C4A	-2.06	126.11	130.04
33	b	723	LMG	O6-C1-O1	-2.06	105.18	110.04
22	B	706	CLA	CHD-C4C-C3C	-2.06	121.77	124.77
23	a	407	BCR	C7-C8-C9	-2.06	123.19	126.23
29	C	519	DGD	CDA-CCA-CBA	-2.06	103.97	114.37
22	c	508	CLA	C1C-C2C-C3C	-2.05	104.82	106.98
22	B	705	CLA	CHD-C1D-C2D	2.05	129.76	125.49
23	k	101	BCR	C33-C5-C6	-2.05	122.24	124.48
22	b	701	CLA	C1B-CHB-C4A	-2.05	126.13	130.04
22	H	102	CLA	CHA-C1A-NA	-2.05	121.75	126.39
26	A	409	SQD	O5-C5-C4	2.05	113.39	109.70
27	A	410	LHG	C18-C17-C16	-2.05	104.01	114.37
22	c	510	CLA	O1D-CGD-CBD	2.05	128.56	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	517	DGD	C7B-C6B-C5B	-2.05	104.01	114.37
22	B	704	CLA	C1B-CHB-C4A	-2.05	126.13	130.04
22	a	401	CLA	C11-C10-C8	-2.05	109.16	115.97
22	b	710	CLA	CHC-C1C-C2C	-2.05	121.14	126.94
27	B	722	LHG	C18-C17-C16	-2.05	104.02	114.37
29	c	517	DGD	O3E-C3E-C2E	-2.05	105.55	110.38
22	B	706	CLA	CHD-C4C-NC	2.05	127.40	124.23
33	C	520	LMG	C31-C30-C29	-2.04	105.62	113.13
22	B	715	CLA	CHA-C4D-ND	2.04	136.77	132.55
33	c	522	LMG	O3-C3-C2	-2.04	105.56	110.38
35	e	101	HEC	CMD-C2D-C1D	-2.04	125.46	128.46
22	C	512	CLA	C4-C3-C5	2.04	118.77	115.23
22	C	513	CLA	CBA-CAA-C2A	-2.04	107.72	113.79
22	c	507	CLA	CGD-CBD-CAD	-2.04	104.24	110.85
29	h	702	DGD	O3E-C3E-C4E	2.04	115.18	110.38
27	L	101	LHG	C17-C16-C15	-2.04	104.06	114.37
23	c	515	BCR	C11-C10-C9	-2.04	124.42	127.28
22	a	404	CLA	C4D-C3D-CAD	-2.04	105.89	108.11
27	a	412	LHG	C5-O7-C7	-2.04	112.92	117.80
23	K	101	BCR	C34-C9-C10	-2.04	119.52	122.82
22	B	709	CLA	CMD-C2D-C3D	2.04	132.36	127.69
22	b	702	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
33	a	419	LMG	O7-C10-O9	-2.04	118.94	123.70
22	b	703	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
26	A	412	SQD	O48-C23-O10	-2.03	118.54	123.63
22	b	710	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
22	A	402	CLA	C6-C5-C3	2.03	118.42	113.47
27	l	101	LHG	C11-C10-C9	-2.03	104.09	114.37
22	c	513	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
22	B	711	CLA	C11-C12-C13	-2.03	109.21	115.97
22	b	715	CLA	CHB-C4A-NA	2.03	127.33	124.40
29	c	518	DGD	O2D-C2D-C1D	-2.03	105.24	110.08
22	b	708	CLA	C2A-C1A-CHA	2.03	127.39	123.87
23	a	407	BCR	C8-C7-C6	-2.03	121.58	127.00
28	B	720	STE	C4-C3-C2	-2.03	105.68	113.13
22	a	404	CLA	CHC-C1C-NC	2.03	127.36	124.31
29	c	518	DGD	C7B-C6B-C5B	-2.03	104.12	114.37
29	c	519	DGD	C3D-C4D-C5D	-2.03	106.56	110.23
23	h	701	BCR	C38-C26-C25	-2.03	122.27	124.48
34	D	406	PHO	C6-C5-C3	2.02	118.40	113.47
22	C	502	CLA	CHD-C1D-ND	-2.02	121.95	124.80
28	c	521	STE	O2-C1-C2	2.02	120.39	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	O2D-CGD-CBD	2.02	114.77	111.23
22	B	704	CLA	CMC-C2C-C3C	2.02	131.62	126.15
22	B	711	CLA	C1-C2-C3	-2.02	122.88	126.20
22	D	403	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
29	C	518	DGD	C7B-C6B-C5B	-2.02	104.15	114.37
22	D	402	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
25	a	411	PL9	C12-C13-C14	-2.02	123.00	127.62
25	D	405	PL9	O2-C1-C2	-2.02	117.24	121.83
34	D	406	PHO	C1B-NB-C4B	2.02	111.24	107.09
29	h	702	DGD	O2E-C2E-C3E	-2.02	105.62	110.38
22	b	713	CLA	C1B-CHB-C4A	-2.02	126.19	130.04
22	b	705	CLA	C1-O2A-CGA	-2.02	111.77	116.65
29	c	518	DGD	CDB-CCB-CBB	-2.01	104.18	114.37
33	B	721	LMG	O7-C10-O9	-2.01	118.15	123.33
22	C	512	CLA	C2A-C1A-CHA	2.01	127.36	123.87
27	D	411	LHG	O3-P-O5	-2.01	100.95	108.94
22	C	506	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
29	C	518	DGD	C5B-C4B-C3B	-2.01	104.19	114.37
29	C	518	DGD	C1D-C2D-C3D	-2.01	105.78	110.01
22	B	707	CLA	C4D-CHA-C1A	2.01	123.64	121.24
22	C	507	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	D	404	BCR	C38-C26-C25	-2.01	122.29	124.48
22	C	502	CLA	CHD-C1D-C2D	2.01	129.67	125.49
22	c	514	CLA	C11-C12-C13	-2.01	109.29	115.97
23	D	404	BCR	C10-C11-C12	-2.01	117.38	123.20
29	C	518	DGD	C3E-C4E-C5E	-2.01	106.59	110.23
23	b	719	BCR	C23-C24-C25	-2.01	121.64	127.00
22	a	401	CLA	O2D-CGD-CBD	2.01	114.74	111.23
29	C	519	DGD	C4D-C3D-C2D	-2.01	107.31	110.83
33	c	523	LMG	C20-C19-C18	-2.00	104.23	114.37
34	D	406	PHO	O2D-CGD-CBD	2.00	113.15	110.95
34	D	407	PHO	CMD-C2D-C3D	2.00	128.69	124.68
33	b	723	LMG	O2-C2-C1	-2.00	105.30	110.08
22	B	714	CLA	C3B-C4B-NB	-2.00	106.62	109.21
28	c	501	STE	O2-C1-C2	2.00	120.33	114.00

All (58) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	404	CLA	ND
22	B	702	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	703	CLA	ND
22	B	704	CLA	ND
22	B	705	CLA	ND
22	B	706	CLA	ND
22	B	707	CLA	ND
22	B	708	CLA	ND
22	B	710	CLA	ND
22	B	712	CLA	ND
22	B	713	CLA	ND
22	B	714	CLA	ND
22	B	715	CLA	ND
22	B	716	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	508	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	C	514	CLA	ND
22	D	401	CLA	ND
22	D	402	CLA	ND
22	H	102	CLA	ND
22	a	401	CLA	ND
22	a	406	CLA	ND
22	b	701	CLA	ND
22	b	703	CLA	ND
22	b	704	CLA	ND
22	b	705	CLA	ND
22	b	706	CLA	ND
22	b	707	CLA	ND
22	b	708	CLA	ND
22	b	709	CLA	ND
22	b	710	CLA	ND
22	b	711	CLA	ND
22	b	712	CLA	ND
22	b	713	CLA	ND
22	b	714	CLA	ND
22	b	715	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	716	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	c	514	CLA	ND

All (1755) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	705	CLA	C11-C12-C13-C14
22	B	714	CLA	CAD-CBD-CGD-O1D
22	B	714	CLA	CAD-CBD-CGD-O2D
22	B	714	CLA	C4-C3-C5-C6
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	C6-C7-C8-C9
22	D	403	CLA	CBD-CGD-O2D-CED
22	H	102	CLA	CAD-CBD-CGD-O1D
22	H	102	CLA	CAD-CBD-CGD-O2D
22	b	714	CLA	CAD-CBD-CGD-O1D
22	b	714	CLA	CAD-CBD-CGD-O2D
22	b	716	CLA	CHA-CBD-CGD-O1D
22	b	716	CLA	CHA-CBD-CGD-O2D
22	b	716	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
22	c	514	CLA	CBD-CGD-O2D-CED
23	A	405	BCR	C20-C21-C22-C37
23	B	718	BCR	C16-C17-C18-C36
23	C	501	BCR	C11-C12-C13-C35
23	C	501	BCR	C17-C18-C19-C20
23	C	515	BCR	C11-C10-C9-C34
23	C	515	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	D	404	BCR	C20-C21-C22-C23
23	D	404	BCR	C20-C21-C22-C37
23	D	404	BCR	C21-C22-C23-C24
23	D	404	BCR	C23-C24-C25-C26
23	D	404	BCR	C23-C24-C25-C30
23	H	101	BCR	C7-C8-C9-C10
23	K	101	BCR	C14-C15-C16-C17
23	T	701	BCR	C7-C8-C9-C34
23	Y	101	BCR	C1-C6-C7-C8
23	Y	101	BCR	C5-C6-C7-C8
23	Y	101	BCR	C20-C21-C22-C37
23	Y	101	BCR	C37-C22-C23-C24
23	b	717	BCR	C7-C8-C9-C34
23	b	717	BCR	C35-C13-C14-C15
23	b	717	BCR	C20-C21-C22-C37
23	c	515	BCR	C16-C17-C18-C19
23	c	515	BCR	C18-C19-C20-C21
23	d	403	BCR	C10-C11-C12-C13
23	k	101	BCR	C7-C8-C9-C10
23	k	101	BCR	C7-C8-C9-C34
23	k	101	BCR	C17-C18-C19-C20
23	t	701	BCR	C11-C10-C9-C34
23	t	701	BCR	C11-C12-C13-C14
23	t	701	BCR	C11-C12-C13-C35
25	A	408	PL9	C12-C13-C14-C15
25	A	408	PL9	C12-C13-C14-C16
25	A	408	PL9	C22-C23-C24-C25
25	A	408	PL9	C22-C23-C24-C26
25	A	408	PL9	C32-C33-C34-C36
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C37-C38-C39-C41
25	D	405	PL9	C32-C33-C34-C36
25	D	405	PL9	C37-C38-C39-C40
25	a	411	PL9	C12-C13-C14-C16
25	a	411	PL9	C22-C23-C24-C25
25	a	411	PL9	C22-C23-C24-C26
25	a	411	PL9	C32-C33-C34-C36
25	a	411	PL9	C42-C43-C44-C45
25	d	404	PL9	C32-C33-C34-C36
26	A	409	SQD	O6-C44-C45-O47
26	B	723	SQD	O5-C1-O6-C44
26	B	723	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
26	B	723	SQD	C8-C7-O47-C45
26	a	413	SQD	O47-C45-C46-O48
26	a	415	SQD	C8-C7-O47-C45
26	b	720	SQD	C8-C7-O47-C45
26	b	720	SQD	O10-C23-O48-C46
26	b	720	SQD	C24-C23-O48-C46
26	f	101	SQD	O5-C1-O6-C44
26	f	101	SQD	O49-C7-O47-C45
26	f	101	SQD	C8-C7-O47-C45
27	A	410	LHG	O1-C1-C2-C3
27	A	410	LHG	C3-O3-P-O5
27	B	722	LHG	O1-C1-C2-O2
27	B	722	LHG	O1-C1-C2-C3
27	B	722	LHG	C1-C2-C3-O3
27	B	722	LHG	C3-O3-P-O4
27	B	722	LHG	C3-O3-P-O5
27	B	722	LHG	C3-O3-P-O6
27	D	410	LHG	O1-C1-C2-C3
27	D	410	LHG	C3-O3-P-O4
27	D	410	LHG	C3-O3-P-O5
27	D	410	LHG	C3-O3-P-O6
27	D	410	LHG	C4-O6-P-O3
27	D	410	LHG	C4-O6-P-O4
27	D	411	LHG	C3-O3-P-O5
27	D	411	LHG	C3-O3-P-O6
27	L	101	LHG	C3-O3-P-O4
27	L	101	LHG	C4-O6-P-O3
27	L	101	LHG	C4-O6-P-O4
27	a	412	LHG	O1-C1-C2-C3
27	a	412	LHG	C3-O3-P-O6
27	a	412	LHG	C4-O6-P-O5
27	a	414	LHG	C3-O3-P-O5
27	a	414	LHG	C3-O3-P-O6
27	d	406	LHG	C3-O3-P-O4
27	d	406	LHG	C3-O3-P-O6
27	d	406	LHG	C4-O6-P-O3
27	d	406	LHG	C4-O6-P-O4
27	l	101	LHG	C3-O3-P-O4
27	l	101	LHG	C4-O6-P-O3
27	l	101	LHG	C4-O6-P-O4
27	l	101	LHG	C4-O6-P-O5
33	C	516	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
33	c	522	LMG	C11-C10-O7-C8
33	c	523	LMG	O6-C1-O1-C7
33	c	523	LMG	C29-C28-O8-C9
22	C	506	CLA	C4C-C3C-CAC-CBC
22	C	506	CLA	C2C-C3C-CAC-CBC
22	b	714	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	CBD-CGD-O2D-CED
22	b	714	CLA	CBD-CGD-O2D-CED
33	c	523	LMG	O10-C28-O8-C9
25	d	404	PL9	C47-C48-C49-C50
25	d	404	PL9	C47-C48-C49-C51
26	f	101	SQD	O10-C23-O48-C46
27	a	414	LHG	O10-C23-O8-C6
22	D	403	CLA	O1D-CGD-O2D-CED
22	b	716	CLA	O1D-CGD-O2D-CED
22	c	509	CLA	O1D-CGD-O2D-CED
22	c	514	CLA	O1D-CGD-O2D-CED
34	d	405	PHO	CBD-CGD-O2D-CED
33	c	522	LMG	O10-C28-O8-C9
26	B	723	SQD	O49-C7-O47-C45
26	a	415	SQD	O49-C7-O47-C45
26	b	720	SQD	O49-C7-O47-C45
29	A	413	DGD	O1B-C1B-O2G-C2G
33	D	412	LMG	O9-C10-O7-C8
33	b	723	LMG	O9-C10-O7-C8
22	C	510	CLA	C3-C5-C6-C7
22	b	714	CLA	C3-C5-C6-C7
26	f	101	SQD	C24-C23-O48-C46
22	c	513	CLA	CBD-CGD-O2D-CED
34	D	407	PHO	CBD-CGD-O2D-CED
29	A	413	DGD	C2B-C1B-O2G-C2G
33	C	516	LMG	C11-C10-O7-C8
22	C	514	CLA	C4-C3-C5-C6
22	b	705	CLA	C4-C3-C5-C6
22	b	716	CLA	C4-C3-C5-C6
25	A	408	PL9	C25-C24-C26-C27
25	A	408	PL9	C40-C39-C41-C42
22	B	714	CLA	C2-C3-C5-C6
22	b	705	CLA	C2-C3-C5-C6
25	a	411	PL9	C33-C34-C36-C37
26	a	415	SQD	O10-C23-O48-C46
33	M	101	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	C	514	CLA	C3-C5-C6-C7
22	b	701	CLA	C3-C5-C6-C7
26	B	723	SQD	C24-C23-O48-C46
26	D	409	SQD	C24-C23-O48-C46
27	A	410	LHG	C24-C23-O8-C6
27	a	414	LHG	C24-C23-O8-C6
25	A	408	PL9	C32-C33-C34-C35
25	a	411	PL9	C12-C13-C14-C15
25	d	404	PL9	C42-C43-C44-C45
33	C	516	LMG	O6-C5-C6-O5
33	c	522	LMG	O9-C10-O7-C8
25	a	411	PL9	C47-C48-C49-C51
22	b	702	CLA	C3-C5-C6-C7
22	c	511	CLA	CBD-CGD-O2D-CED
27	B	722	LHG	O2-C2-C3-O3
27	D	410	LHG	O2-C2-C3-O3
27	D	411	LHG	O2-C2-C3-O3
22	C	510	CLA	O1D-CGD-O2D-CED
33	c	522	LMG	C29-C28-O8-C9
29	h	702	DGD	O6E-C5E-C6E-O5E
33	c	522	LMG	C4-C5-C6-O5
33	C	520	LMG	C11-C10-O7-C8
33	D	412	LMG	C11-C10-O7-C8
27	l	101	LHG	C7-C8-C9-C10
33	C	516	LMG	C4-C5-C6-O5
22	a	406	CLA	CBA-CGA-O2A-C1
33	a	419	LMG	C29-C28-O8-C9
22	b	703	CLA	C4-C3-C5-C6
22	b	704	CLA	C4-C3-C5-C6
22	A	404	CLA	C2-C3-C5-C6
22	b	703	CLA	C2-C3-C5-C6
25	A	408	PL9	C18-C19-C21-C22
25	A	408	PL9	C23-C24-C26-C27
25	A	408	PL9	C34-C36-C37-C38
25	A	408	PL9	C44-C46-C47-C48
25	D	405	PL9	C34-C36-C37-C38
25	a	411	PL9	C19-C21-C22-C23
25	a	411	PL9	C24-C26-C27-C28
25	d	404	PL9	C34-C36-C37-C38
33	c	520	LMG	O6-C5-C6-O5
22	a	406	CLA	O1A-CGA-O2A-C1
27	A	410	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	CBD-CGD-O2D-CED
27	B	722	LHG	C28-C29-C30-C31
25	D	405	PL9	C12-C13-C14-C15
25	a	411	PL9	C32-C33-C34-C35
33	c	520	LMG	O9-C10-O7-C8
25	A	408	PL9	C47-C48-C49-C50
33	b	723	LMG	O10-C28-O8-C9
26	a	415	SQD	C24-C23-O48-C46
33	M	101	LMG	C29-C28-O8-C9
34	d	405	PHO	O1D-CGD-O2D-CED
26	a	413	SQD	C12-C13-C14-C15
22	A	404	CLA	C4-C3-C5-C6
22	b	707	CLA	C4-C3-C5-C6
25	d	404	PL9	C40-C39-C41-C42
22	C	514	CLA	C2-C3-C5-C6
22	b	707	CLA	C2-C3-C5-C6
22	b	716	CLA	C2-C3-C5-C6
25	D	405	PL9	C38-C39-C41-C42
25	d	404	PL9	C33-C34-C36-C37
25	d	404	PL9	C38-C39-C41-C42
22	A	403	CLA	C14-C13-C15-C16
22	B	703	CLA	C11-C12-C13-C14
22	B	707	CLA	C14-C13-C15-C16
22	B	713	CLA	C11-C12-C13-C14
22	B	714	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	C	514	CLA	C6-C7-C8-C9
22	D	401	CLA	C11-C10-C8-C9
22	b	705	CLA	C11-C10-C8-C9
22	b	707	CLA	C11-C10-C8-C9
22	b	711	CLA	C14-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C12-C13-C14
22	c	512	CLA	C14-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C9
33	c	520	LMG	C4-C5-C6-O5
33	c	523	LMG	C4-C5-C6-O5
22	c	513	CLA	O1D-CGD-O2D-CED
26	B	723	SQD	C2-C1-O6-C44
22	b	709	CLA	CBD-CGD-O2D-CED
23	B	718	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	C	501	BCR	C36-C18-C19-C20
23	C	501	BCR	C37-C22-C23-C24
23	H	101	BCR	C11-C12-C13-C35
23	K	101	BCR	C37-C22-C23-C24
23	b	719	BCR	C37-C22-C23-C24
23	c	515	BCR	C36-C18-C19-C20
23	c	516	BCR	C37-C22-C23-C24
23	d	403	BCR	C37-C22-C23-C24
23	h	701	BCR	C11-C12-C13-C35
23	k	101	BCR	C37-C22-C23-C24
33	c	522	LMG	O6-C5-C6-O5
23	d	403	BCR	C21-C22-C23-C24
33	c	520	LMG	C11-C10-O7-C8
22	b	715	CLA	C15-C16-C17-C18
27	l	101	LHG	C23-C24-C25-C26
22	C	510	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
27	d	407	LHG	C33-C34-C35-C36
23	d	403	BCR	C14-C15-C16-C17
22	C	509	CLA	C15-C16-C17-C18
22	a	406	CLA	C5-C6-C7-C8
22	C	503	CLA	C3-C5-C6-C7
29	H	103	DGD	C1A-C2A-C3A-C4A
22	C	506	CLA	C10-C11-C12-C13
22	C	514	CLA	C15-C16-C17-C18
22	B	711	CLA	C12-C13-C15-C16
22	b	706	CLA	C11-C10-C8-C7
22	b	701	CLA	C13-C15-C16-C17
28	c	521	STE	C1-C2-C3-C4
22	C	510	CLA	C8-C10-C11-C12
22	D	401	CLA	C15-C16-C17-C18
26	A	412	SQD	C23-C24-C25-C26
33	D	412	LMG	C10-C11-C12-C13
33	c	522	LMG	C10-C11-C12-C13
22	B	713	CLA	C8-C10-C11-C12
22	C	507	CLA	C15-C16-C17-C18
22	H	102	CLA	C15-C16-C17-C18
22	b	711	CLA	C13-C15-C16-C17
22	b	711	CLA	C15-C16-C17-C18
22	b	715	CLA	C8-C10-C11-C12
22	c	510	CLA	C10-C11-C12-C13
22	B	706	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	712	CLA	C13-C15-C16-C17
22	C	510	CLA	C5-C6-C7-C8
22	C	513	CLA	C13-C15-C16-C17
22	D	402	CLA	C15-C16-C17-C18
22	d	402	CLA	C5-C6-C7-C8
27	a	412	LHG	C23-C24-C25-C26
27	a	414	LHG	C23-C24-C25-C26
28	b	725	STE	C1-C2-C3-C4
33	b	723	LMG	C28-C29-C30-C31
22	H	102	CLA	C3-C5-C6-C7
29	C	518	DGD	O6E-C1E-O5D-C6D
22	B	714	CLA	C13-C15-C16-C17
22	D	403	CLA	C10-C11-C12-C13
22	b	703	CLA	C13-C15-C16-C17
22	b	713	CLA	C13-C15-C16-C17
27	A	410	LHG	O2-C2-C3-O3
27	a	412	LHG	O2-C2-C3-O3
33	a	419	LMG	O10-C28-O8-C9
28	b	724	STE	C1-C2-C3-C4
33	M	101	LMG	C28-C29-C30-C31
22	C	504	CLA	C5-C6-C7-C8
22	d	402	CLA	C10-C11-C12-C13
22	c	511	CLA	O1D-CGD-O2D-CED
26	A	412	SQD	C17-C18-C19-C20
29	h	702	DGD	C4E-C5E-C6E-O5E
34	D	407	PHO	O1D-CGD-O2D-CED
22	B	714	CLA	CBD-CGD-O2D-CED
22	C	502	CLA	CBD-CGD-O2D-CED
33	c	523	LMG	O6-C5-C6-O5
26	D	409	SQD	O10-C23-O48-C46
29	c	518	DGD	C1A-C2A-C3A-C4A
29	c	518	DGD	C1B-C2B-C3B-C4B
22	B	716	CLA	C5-C6-C7-C8
22	b	701	CLA	C8-C10-C11-C12
22	c	506	CLA	C5-C6-C7-C8
22	H	102	CLA	CBA-CGA-O2A-C1
33	C	520	LMG	C29-C28-O8-C9
33	d	408	LMG	C28-C29-C30-C31
27	A	410	LHG	C1-C2-C3-O3
27	D	410	LHG	C1-C2-C3-O3
27	a	412	LHG	C1-C2-C3-O3
22	b	706	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	CBA-CGA-O2A-C1
26	a	413	SQD	C24-C23-O48-C46
22	B	707	CLA	C13-C15-C16-C17
22	D	402	CLA	C13-C15-C16-C17
22	b	714	CLA	C8-C10-C11-C12
22	c	512	CLA	C13-C15-C16-C17
25	a	411	PL9	C47-C48-C49-C50
22	B	705	CLA	C8-C10-C11-C12
22	C	507	CLA	C8-C10-C11-C12
22	B	715	CLA	C5-C6-C7-C8
22	c	509	CLA	C10-C11-C12-C13
22	B	716	CLA	C3-C5-C6-C7
33	b	723	LMG	C11-C10-O7-C8
22	C	514	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C10-C8-C9
25	D	405	PL9	C27-C28-C29-C30
25	d	404	PL9	C7-C8-C9-C10
26	f	101	SQD	C2-C1-O6-C44
29	C	518	DGD	C2E-C1E-O5D-C6D
29	c	518	DGD	C2E-C1E-O5D-C6D
33	D	412	LMG	C29-C28-O8-C9
22	C	503	CLA	C16-C17-C18-C20
23	A	405	BCR	C35-C13-C14-C15
23	B	717	BCR	C11-C10-C9-C34
23	B	717	BCR	C35-C13-C14-C15
23	B	717	BCR	C16-C17-C18-C36
23	B	717	BCR	C20-C21-C22-C37
23	B	718	BCR	C35-C13-C14-C15
23	B	718	BCR	C20-C21-C22-C37
23	B	719	BCR	C16-C17-C18-C36
23	C	501	BCR	C11-C10-C9-C34
23	C	501	BCR	C16-C17-C18-C36
23	D	404	BCR	C11-C10-C9-C34
23	Y	101	BCR	C11-C10-C9-C34
23	a	407	BCR	C11-C10-C9-C34
23	b	717	BCR	C11-C10-C9-C34
23	b	719	BCR	C35-C13-C14-C15
23	b	719	BCR	C16-C17-C18-C36
23	b	719	BCR	C20-C21-C22-C37
23	c	515	BCR	C11-C10-C9-C34
23	c	515	BCR	C16-C17-C18-C36
23	d	403	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	h	701	BCR	C35-C13-C14-C15
23	h	701	BCR	C16-C17-C18-C36
23	k	101	BCR	C35-C13-C14-C15
23	k	101	BCR	C16-C17-C18-C36
23	k	101	BCR	C20-C21-C22-C37
23	D	404	BCR	C36-C18-C19-C20
23	T	701	BCR	C11-C12-C13-C35
33	D	412	LMG	O10-C28-O8-C9
27	d	407	LHG	O1-C1-C2-C3
26	b	720	SQD	C46-C45-O47-C7
22	b	702	CLA	C16-C17-C18-C20
22	b	707	CLA	C16-C17-C18-C20
22	b	716	CLA	C11-C12-C13-C14
22	c	507	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C20
22	c	507	CLA	O1A-CGA-O2A-C1
29	C	519	DGD	O1A-C1A-O1G-C1G
22	b	707	CLA	C10-C11-C12-C13
23	B	717	BCR	C12-C13-C14-C15
23	B	717	BCR	C20-C21-C22-C23
23	C	515	BCR	C20-C21-C22-C23
23	K	101	BCR	C11-C10-C9-C8
23	K	101	BCR	C20-C21-C22-C23
23	T	701	BCR	C12-C13-C14-C15
23	b	717	BCR	C12-C13-C14-C15
23	b	718	BCR	C16-C17-C18-C19
23	c	515	BCR	C20-C21-C22-C23
23	d	403	BCR	C16-C17-C18-C19
23	d	403	BCR	C20-C21-C22-C23
23	h	701	BCR	C11-C10-C9-C8
23	h	701	BCR	C16-C17-C18-C19
23	t	701	BCR	C11-C10-C9-C8
23	t	701	BCR	C12-C13-C14-C15
28	B	701	STE	C5-C6-C7-C8
29	c	518	DGD	O6E-C1E-O5D-C6D
26	B	723	SQD	O10-C23-O48-C46
33	b	721	LMG	C29-C28-O8-C9
22	a	404	CLA	C13-C15-C16-C17
22	c	507	CLA	C15-C16-C17-C18
22	H	102	CLA	C2-C1-O2A-CGA
22	a	401	CLA	C16-C17-C18-C19
22	b	716	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C19
22	C	509	CLA	O1D-CGD-O2D-CED
26	B	723	SQD	C11-C10-C9-C8
28	B	724	STE	C2-C3-C4-C5
28	C	521	STE	C5-C6-C7-C8
29	C	518	DGD	C5A-C6A-C7A-C8A
29	C	519	DGD	CBA-CCA-CDA-CEA
29	c	519	DGD	CBA-CCA-CDA-CEA
33	C	520	LMG	C31-C32-C33-C34
33	b	723	LMG	C13-C14-C15-C16
23	D	404	BCR	C14-C15-C16-C17
26	A	409	SQD	C26-C27-C28-C29
26	b	720	SQD	C24-C25-C26-C27
27	A	410	LHG	C17-C18-C19-C20
28	H	104	STE	C9-C10-C11-C12
28	T	702	STE	C9-C10-C11-C12
28	X	101	STE	C4-C5-C6-C7
28	Z	101	STE	C11-C12-C13-C14
29	c	519	DGD	C3A-C4A-C5A-C6A
33	a	419	LMG	C21-C22-C23-C24
33	c	522	LMG	C13-C14-C15-C16
26	a	415	SQD	C11-C10-C9-C8
26	a	415	SQD	C16-C17-C18-C19
26	b	720	SQD	C26-C27-C28-C29
27	A	410	LHG	C11-C10-C9-C8
27	L	101	LHG	C17-C18-C19-C20
27	d	406	LHG	C29-C30-C31-C32
28	b	725	STE	C12-C13-C14-C15
28	b	727	STE	C14-C15-C16-C17
29	A	413	DGD	C2B-C3B-C4B-C5B
26	B	723	SQD	C13-C14-C15-C16
26	a	413	SQD	C29-C30-C31-C32
27	A	410	LHG	C34-C35-C36-C37
27	l	101	LHG	C12-C13-C14-C15
27	l	101	LHG	C14-C15-C16-C17
28	c	521	STE	C11-C12-C13-C14
29	c	517	DGD	C4A-C5A-C6A-C7A
33	M	101	LMG	C12-C13-C14-C15
27	D	410	LHG	O1-C1-C2-O2
27	a	412	LHG	O1-C1-C2-O2
27	d	407	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C18-C19-C20-C21
33	c	523	LMG	C12-C13-C14-C15
22	C	506	CLA	C5-C6-C7-C8
27	A	410	LHG	C23-C24-C25-C26
27	D	411	LHG	C7-C8-C9-C10
33	c	523	LMG	C28-C29-C30-C31
26	B	723	SQD	C11-C12-C13-C14
33	c	520	LMG	C36-C37-C38-C39
22	B	706	CLA	C16-C17-C18-C20
22	a	401	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
22	c	513	CLA	C2A-CAA-CBA-CGA
22	b	707	CLA	C8-C10-C11-C12
26	A	412	SQD	C32-C33-C34-C35
28	x	101	STE	C7-C8-C9-C10
22	c	504	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
27	D	411	LHG	C33-C34-C35-C36
28	I	101	STE	C10-C11-C12-C13
28	b	724	STE	C6-C7-C8-C9
33	b	723	LMG	C23-C24-C25-C26
26	b	720	SQD	C23-C24-C25-C26
22	c	513	CLA	CBA-CGA-O2A-C1
28	B	725	STE	C9-C10-C11-C12
28	c	521	STE	C10-C11-C12-C13
29	C	518	DGD	C6A-C7A-C8A-C9A
33	B	721	LMG	C32-C33-C34-C35
33	B	721	LMG	C33-C34-C35-C36
33	M	101	LMG	C35-C36-C37-C38
33	c	522	LMG	C30-C31-C32-C33
28	C	523	STE	C7-C8-C9-C10
25	a	411	PL9	C35-C34-C36-C37
26	A	409	SQD	C12-C13-C14-C15
28	B	725	STE	C11-C12-C13-C14
33	c	522	LMG	C11-C12-C13-C14
22	C	505	CLA	C2-C3-C5-C6
33	C	520	LMG	C38-C39-C40-C41
22	B	706	CLA	C5-C6-C7-C8
22	b	708	CLA	C5-C6-C7-C8
22	b	715	CLA	C5-C6-C7-C8
22	c	513	CLA	C5-C6-C7-C8
26	f	101	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	a	412	LHG	C7-C8-C9-C10
23	k	101	BCR	C19-C20-C21-C22
22	B	706	CLA	C16-C17-C18-C19
22	B	710	CLA	C16-C17-C18-C20
22	D	402	CLA	C16-C17-C18-C20
22	b	707	CLA	C16-C17-C18-C19
22	b	715	CLA	C16-C17-C18-C19
26	A	409	SQD	C16-C17-C18-C19
27	A	410	LHG	C30-C31-C32-C33
27	D	411	LHG	C10-C11-C12-C13
28	E	101	STE	C3-C4-C5-C6
29	c	519	DGD	C8B-C9B-CAB-CBB
33	D	408	LMG	C31-C32-C33-C34
26	B	723	SQD	C18-C19-C20-C21
27	d	406	LHG	C32-C33-C34-C35
29	A	413	DGD	C9A-CAA-CBA-CCA
29	h	702	DGD	C2B-C3B-C4B-C5B
33	c	522	LMG	C15-C16-C17-C18
26	f	101	SQD	C27-C28-C29-C30
27	L	101	LHG	C14-C15-C16-C17
28	a	416	STE	C6-C7-C8-C9
28	h	703	STE	C10-C11-C12-C13
29	H	103	DGD	C8B-C9B-CAB-CBB
33	a	419	LMG	C41-C42-C43-C44
33	b	721	LMG	C17-C18-C19-C20
26	A	412	SQD	C12-C13-C14-C15
26	A	412	SQD	C14-C15-C16-C17
27	L	101	LHG	C31-C32-C33-C34
27	a	412	LHG	C16-C17-C18-C19
27	l	101	LHG	C9-C10-C11-C12
28	B	701	STE	C2-C3-C4-C5
28	I	101	STE	C2-C3-C4-C5
28	X	101	STE	C7-C8-C9-C10
28	b	724	STE	C3-C4-C5-C6
28	l	102	STE	C4-C5-C6-C7
28	t	702	STE	C11-C10-C9-C8
29	A	413	DGD	CBB-CCB-CDB-CEB
33	D	412	LMG	C14-C15-C16-C17
33	a	419	LMG	C33-C34-C35-C36
22	H	102	CLA	O1A-CGA-O2A-C1
29	c	519	DGD	O1A-C1A-O1G-C1G
27	a	414	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
28	M	103	STE	C4-C5-C6-C7
29	C	517	DGD	C5B-C6B-C7B-C8B
33	D	408	LMG	C36-C37-C38-C39
33	b	723	LMG	C18-C19-C20-C21
27	A	410	LHG	C29-C30-C31-C32
27	L	101	LHG	C18-C19-C20-C21
28	b	725	STE	C14-C15-C16-C17
22	A	402	CLA	C15-C16-C17-C18
27	A	410	LHG	C33-C34-C35-C36
28	T	702	STE	C13-C14-C15-C16
29	c	517	DGD	C4B-C5B-C6B-C7B
33	c	523	LMG	C34-C35-C36-C37
22	B	712	CLA	C16-C17-C18-C20
22	C	514	CLA	C16-C17-C18-C19
22	c	513	CLA	O1A-CGA-O2A-C1
23	C	501	BCR	C1-C6-C7-C8
23	C	501	BCR	C5-C6-C7-C8
23	H	101	BCR	C23-C24-C25-C26
23	b	717	BCR	C1-C6-C7-C8
23	b	717	BCR	C5-C6-C7-C8
23	c	515	BCR	C23-C24-C25-C30
23	k	101	BCR	C1-C6-C7-C8
23	k	101	BCR	C5-C6-C7-C8
27	L	101	LHG	C12-C13-C14-C15
29	h	702	DGD	C6B-C7B-C8B-C9B
33	C	516	LMG	C35-C36-C37-C38
22	C	511	CLA	C8-C10-C11-C12
27	D	411	LHG	C15-C16-C17-C18
29	H	103	DGD	C6A-C7A-C8A-C9A
33	b	723	LMG	C30-C31-C32-C33
22	b	709	CLA	O1D-CGD-O2D-CED
26	a	415	SQD	C10-C11-C12-C13
26	f	101	SQD	C25-C26-C27-C28
28	X	101	STE	C3-C4-C5-C6
28	x	101	STE	C2-C3-C4-C5
33	a	419	LMG	C13-C14-C15-C16
28	B	720	STE	C1-C2-C3-C4
26	B	723	SQD	C33-C34-C35-C36
26	b	720	SQD	C27-C28-C29-C30
29	c	519	DGD	C7A-C8A-C9A-CAA
33	B	721	LMG	C14-C15-C16-C17
33	b	721	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
34	a	405	PHO	CBD-CGD-O2D-CED
29	A	413	DGD	C8B-C9B-CAB-CBB
29	c	519	DGD	CCA-CDA-CEA-CFA
27	D	411	LHG	C25-C26-C27-C28
27	d	407	LHG	C31-C32-C33-C34
28	B	726	STE	C11-C12-C13-C14
28	c	521	STE	C9-C10-C11-C12
29	C	518	DGD	C8B-C9B-CAB-CBB
29	H	103	DGD	C6B-C7B-C8B-C9B
33	D	408	LMG	C38-C39-C40-C41
23	C	501	BCR	C18-C19-C20-C21
23	T	701	BCR	C18-C19-C20-C21
23	t	701	BCR	C10-C11-C12-C13
22	B	703	CLA	C2-C3-C5-C6
22	b	704	CLA	C2-C3-C5-C6
22	c	507	CLA	C16-C17-C18-C19
26	A	409	SQD	C10-C11-C12-C13
27	L	101	LHG	C29-C30-C31-C32
27	a	412	LHG	C11-C10-C9-C8
27	a	414	LHG	C17-C18-C19-C20
29	c	517	DGD	C7A-C8A-C9A-CAA
28	E	101	STE	C1-C2-C3-C4
22	C	506	CLA	CBA-CGA-O2A-C1
22	C	514	CLA	CBA-CGA-O2A-C1
33	b	723	LMG	C29-C28-O8-C9
22	b	701	CLA	C14-C13-C15-C16
26	a	413	SQD	C15-C16-C17-C18
28	M	102	STE	C9-C10-C11-C12
22	C	511	CLA	C13-C15-C16-C17
26	A	409	SQD	C14-C15-C16-C17
33	M	101	LMG	C37-C38-C39-C40
29	A	413	DGD	O6D-C1D-O3G-C3G
29	c	517	DGD	O6E-C1E-O5D-C6D
23	k	101	BCR	C14-C15-C16-C17
26	B	723	SQD	C27-C28-C29-C30
27	A	410	LHG	C24-C25-C26-C27
28	T	702	STE	C12-C13-C14-C15
28	d	409	STE	C5-C6-C7-C8
28	x	101	STE	C3-C4-C5-C6
29	c	518	DGD	C2A-C3A-C4A-C5A
29	c	518	DGD	C7A-C8A-C9A-CAA
33	a	419	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
33	c	523	LMG	C2-C1-O1-C7
22	D	403	CLA	C13-C15-C16-C17
22	H	102	CLA	C10-C11-C12-C13
22	b	704	CLA	C15-C16-C17-C18
27	D	411	LHG	C29-C30-C31-C32
27	D	411	LHG	C30-C31-C32-C33
28	T	702	STE	C5-C6-C7-C8
33	b	721	LMG	C39-C40-C41-C42
26	A	409	SQD	C32-C33-C34-C35
26	a	413	SQD	C10-C11-C12-C13
28	A	411	STE	C4-C5-C6-C7
33	C	520	LMG	C37-C38-C39-C40
28	B	726	STE	C11-C10-C9-C8
28	M	103	STE	C3-C4-C5-C6
28	b	722	STE	C7-C8-C9-C10
28	b	727	STE	C6-C7-C8-C9
33	B	721	LMG	C31-C32-C33-C34
33	C	520	LMG	C30-C31-C32-C33
22	c	513	CLA	C15-C16-C17-C18
23	h	701	BCR	C15-C16-C17-C18
22	b	715	CLA	C16-C17-C18-C20
26	A	409	SQD	C8-C7-O47-C45
28	a	417	STE	C4-C5-C6-C7
27	D	411	LHG	O9-C7-O7-C5
29	C	517	DGD	O1B-C1B-O2G-C2G
27	A	410	LHG	C10-C11-C12-C13
29	h	702	DGD	C9B-CAB-CBB-CCB
27	d	406	LHG	C12-C13-C14-C15
22	b	713	CLA	C10-C11-C12-C13
26	a	415	SQD	C14-C15-C16-C17
28	b	727	STE	C9-C10-C11-C12
28	b	722	STE	C1-C2-C3-C4
29	C	517	DGD	C7B-C8B-C9B-CAB
29	c	517	DGD	C9B-CAB-CBB-CCB
23	B	717	BCR	C17-C18-C19-C20
33	a	419	LMG	C8-C7-O1-C1
27	l	101	LHG	C26-C27-C28-C29
29	C	519	DGD	C4B-C5B-C6B-C7B
22	C	503	CLA	C16-C17-C18-C19
29	c	518	DGD	CAB-CBB-CCB-CDB
22	C	506	CLA	C4-C3-C5-C6
27	L	101	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	d	407	LHG	C27-C28-C29-C30
28	H	105	STE	C7-C8-C9-C10
33	D	408	LMG	C17-C18-C19-C20
22	a	406	CLA	C2C-C3C-CAC-CBC
22	B	705	CLA	C10-C11-C12-C13
22	B	711	CLA	C13-C15-C16-C17
29	c	519	DGD	C9B-CAB-CBB-CCB
28	B	701	STE	C3-C4-C5-C6
28	h	703	STE	C7-C8-C9-C10
33	b	723	LMG	C12-C13-C14-C15
33	c	522	LMG	C39-C40-C41-C42
27	B	722	LHG	C26-C27-C28-C29
29	C	518	DGD	CCB-CDB-CEB-CFB
26	D	409	SQD	C44-C45-C46-O48
26	a	413	SQD	C24-C25-C26-C27
29	c	517	DGD	O6D-C5D-C6D-O5D
29	C	517	DGD	O6E-C5E-C6E-O5E
33	d	408	LMG	O6-C5-C6-O5
27	a	412	LHG	C17-C18-C19-C20
28	d	409	STE	C10-C11-C12-C13
33	C	520	LMG	C17-C18-C19-C20
33	M	101	LMG	C14-C15-C16-C17
22	B	710	CLA	C8-C10-C11-C12
22	b	705	CLA	C5-C6-C7-C8
22	B	703	CLA	C16-C17-C18-C19
27	D	411	LHG	C11-C10-C9-C8
28	T	702	STE	C11-C12-C13-C14
33	b	721	LMG	C37-C38-C39-C40
33	b	723	LMG	C11-C12-C13-C14
22	C	506	CLA	O1A-CGA-O2A-C1
28	J	101	STE	C3-C4-C5-C6
28	j	101	STE	C4-C5-C6-C7
33	c	522	LMG	C33-C34-C35-C36
33	C	516	LMG	C10-C11-C12-C13
22	B	704	CLA	C2C-C3C-CAC-CBC
22	b	714	CLA	C15-C16-C17-C18
22	c	508	CLA	C8-C10-C11-C12
26	A	409	SQD	C30-C31-C32-C33
26	b	720	SQD	C29-C30-C31-C32
28	X	101	STE	C13-C14-C15-C16
28	t	702	STE	C6-C7-C8-C9
33	c	522	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
33	D	408	LMG	O6-C5-C6-O5
26	a	415	SQD	C11-C12-C13-C14
27	D	411	LHG	C12-C13-C14-C15
29	A	413	DGD	C2A-C3A-C4A-C5A
27	l	101	LHG	C17-C18-C19-C20
33	c	523	LMG	C15-C16-C17-C18
33	C	516	LMG	C16-C17-C18-C19
22	B	703	CLA	C8-C10-C11-C12
26	B	723	SQD	C9-C10-C11-C12
27	a	412	LHG	C30-C31-C32-C33
27	l	101	LHG	C24-C25-C26-C27
33	a	419	LMG	C18-C19-C20-C21
33	b	723	LMG	C32-C33-C34-C35
26	D	409	SQD	C26-C27-C28-C29
22	B	703	CLA	C4-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
25	d	404	PL9	C13-C14-C16-C17
27	D	411	LHG	C1-C2-C3-O3
26	a	413	SQD	C16-C17-C18-C19
27	a	414	LHG	C16-C17-C18-C19
28	X	101	STE	C6-C7-C8-C9
33	c	523	LMG	C18-C19-C20-C21
28	H	104	STE	C5-C6-C7-C8
29	c	519	DGD	C6B-C7B-C8B-C9B
26	B	723	SQD	C45-C46-O48-C23
28	B	725	STE	C5-C6-C7-C8
26	A	412	SQD	C10-C11-C12-C13
26	a	413	SQD	C26-C27-C28-C29
28	A	411	STE	C6-C7-C8-C9
29	C	519	DGD	C3A-C4A-C5A-C6A
33	D	408	LMG	C16-C17-C18-C19
33	c	522	LMG	C34-C35-C36-C37
22	C	514	CLA	C16-C17-C18-C20
27	A	410	LHG	O1-C1-C2-O2
27	B	722	LHG	C9-C10-C11-C12
29	C	519	DGD	C6A-C7A-C8A-C9A
29	H	103	DGD	C5A-C6A-C7A-C8A
29	c	519	DGD	C9A-CAA-CBA-CCA
22	B	704	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	a	413	SQD	C30-C31-C32-C33
26	a	413	SQD	C34-C35-C36-C37
28	B	720	STE	C11-C12-C13-C14
33	b	723	LMG	C16-C17-C18-C19
22	C	514	CLA	O1A-CGA-O2A-C1
28	b	724	STE	C5-C6-C7-C8
33	c	522	LMG	C38-C39-C40-C41
33	c	523	LMG	C29-C30-C31-C32
33	d	408	LMG	C30-C31-C32-C33
22	b	716	CLA	C5-C6-C7-C8
22	c	513	CLA	C13-C15-C16-C17
28	c	521	STE	C7-C8-C9-C10
33	C	516	LMG	C38-C39-C40-C41
22	B	704	CLA	C12-C13-C15-C16
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	C	513	CLA	C11-C12-C13-C15
22	b	703	CLA	C6-C7-C8-C10
22	b	711	CLA	C11-C12-C13-C15
22	b	711	CLA	C12-C13-C15-C16
22	b	715	CLA	C12-C13-C15-C16
22	c	512	CLA	C12-C13-C15-C16
22	d	402	CLA	C11-C12-C13-C15
28	b	724	STE	C11-C10-C9-C8
33	c	522	LMG	C40-C41-C42-C43
22	B	716	CLA	C11-C12-C13-C14
22	a	403	CLA	C16-C17-C18-C20
22	c	504	CLA	C15-C16-C17-C18
27	a	412	LHG	C32-C33-C34-C35
22	B	704	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	a	406	CLA	C14-C13-C15-C16
22	b	708	CLA	C11-C12-C13-C14
22	b	709	CLA	C14-C13-C15-C16
22	c	505	CLA	C11-C10-C8-C9
22	d	402	CLA	C11-C12-C13-C14
29	c	519	DGD	C4B-C5B-C6B-C7B
26	a	415	SQD	C24-C25-C26-C27
33	D	408	LMG	C14-C15-C16-C17
29	A	413	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
22	B	711	CLA	C8-C10-C11-C12
29	C	519	DGD	C2B-C3B-C4B-C5B
26	B	723	SQD	C16-C17-C18-C19
22	c	512	CLA	C15-C16-C17-C18
26	B	723	SQD	O6-C44-C45-C46
26	a	413	SQD	C44-C45-C46-O48
26	a	415	SQD	C44-C45-C46-O48
26	A	409	SQD	C11-C10-C9-C8
27	A	410	LHG	C32-C33-C34-C35
28	l	102	STE	C10-C11-C12-C13
29	A	413	DGD	CCB-CDB-CEB-CFB
26	A	412	SQD	C18-C19-C20-C21
27	a	412	LHG	C15-C16-C17-C18
28	E	101	STE	C4-C5-C6-C7
28	a	416	STE	C3-C4-C5-C6
33	M	101	LMG	C38-C39-C40-C41
22	A	402	CLA	C2C-C3C-CAC-CBC
28	I	101	STE	C11-C10-C9-C8
29	h	702	DGD	C3B-C4B-C5B-C6B
29	c	517	DGD	O6E-C5E-C6E-O5E
22	B	716	CLA	C11-C12-C13-C15
22	a	403	CLA	C16-C17-C18-C19
22	b	702	CLA	C16-C17-C18-C19
28	B	726	STE	C4-C5-C6-C7
28	Z	101	STE	C13-C14-C15-C16
33	c	523	LMG	C32-C33-C34-C35
29	C	519	DGD	C7B-C8B-C9B-CAB
33	C	520	LMG	C39-C40-C41-C42
22	B	714	CLA	O1D-CGD-O2D-CED
23	C	515	BCR	C16-C17-C18-C36
23	t	701	BCR	C20-C21-C22-C37
22	B	715	CLA	C13-C15-C16-C17
27	a	412	LHG	C18-C19-C20-C21
29	c	517	DGD	CBA-CCA-CDA-CEA
27	d	407	LHG	C23-C24-C25-C26
27	D	410	LHG	C11-C10-C9-C8
25	A	408	PL9	C43-C44-C46-C47
22	c	504	CLA	C5-C6-C7-C8
27	a	412	LHG	C28-C29-C30-C31
22	B	702	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C20
28	l	102	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	M	101	LMG	C13-C14-C15-C16
28	x	101	STE	C5-C6-C7-C8
33	c	523	LMG	C38-C39-C40-C41
33	b	723	LMG	O6-C5-C6-O5
27	a	414	LHG	C11-C12-C13-C14
29	c	517	DGD	C4D-C5D-C6D-O5D
27	B	722	LHG	C12-C13-C14-C15
28	b	724	STE	C7-C8-C9-C10
28	b	727	STE	C11-C12-C13-C14
29	c	518	DGD	CAA-CBA-CCA-CDA
22	C	513	CLA	O2A-C1-C2-C3
26	B	723	SQD	C46-C45-O47-C7
27	L	101	LHG	C11-C12-C13-C14
27	L	101	LHG	C13-C14-C15-C16
28	d	409	STE	C11-C12-C13-C14
29	A	413	DGD	C4B-C5B-C6B-C7B
33	c	520	LMG	C35-C36-C37-C38
23	B	717	BCR	C18-C19-C20-C21
23	C	515	BCR	C18-C19-C20-C21
28	H	104	STE	C6-C7-C8-C9
28	c	521	STE	C4-C5-C6-C7
29	C	517	DGD	C8B-C9B-CAB-CBB
29	c	519	DGD	C7B-C8B-C9B-CAB
28	a	416	STE	C2-C3-C4-C5
28	b	726	STE	C3-C4-C5-C6
28	b	722	STE	C14-C15-C16-C17
33	D	412	LMG	C33-C34-C35-C36
33	b	721	LMG	C11-C10-O7-C8
22	B	716	CLA	O1A-CGA-O2A-C1
27	D	411	LHG	C27-C28-C29-C30
27	l	101	LHG	C10-C11-C12-C13
28	c	521	STE	C11-C10-C9-C8
29	A	413	DGD	C5B-C6B-C7B-C8B
22	A	404	CLA	C6-C7-C8-C9
33	C	516	LMG	C32-C33-C34-C35
25	d	404	PL9	C30-C29-C31-C32
34	D	406	PHO	C4-C3-C5-C6
34	D	406	PHO	C2-C3-C5-C6
28	A	414	STE	C11-C10-C9-C8
28	x	101	STE	C9-C10-C11-C12
22	b	704	CLA	C16-C17-C18-C19
27	l	101	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
28	b	722	STE	C12-C13-C14-C15
29	H	103	DGD	C9A-CAA-CBA-CCA
33	a	419	LMG	C23-C24-C25-C26
28	B	720	STE	C12-C13-C14-C15
29	C	519	DGD	CDB-CEB-CFB-CGB
29	c	519	DGD	CDA-CEA-CFA-CGA
33	c	520	LMG	C40-C41-C42-C43
26	A	409	SQD	O47-C45-C46-O48
26	a	413	SQD	O6-C44-C45-O47
26	b	720	SQD	O47-C45-C46-O48
33	C	520	LMG	O1-C7-C8-O7
27	D	410	LHG	C17-C18-C19-C20
28	H	105	STE	C6-C7-C8-C9
22	B	716	CLA	CBA-CGA-O2A-C1
27	D	410	LHG	C10-C11-C12-C13
29	c	517	DGD	C7B-C8B-C9B-CAB
33	M	101	LMG	C15-C16-C17-C18
33	a	419	LMG	O8-C28-C29-C30
28	h	703	STE	C12-C13-C14-C15
29	C	518	DGD	C6B-C7B-C8B-C9B
22	C	513	CLA	C3-C5-C6-C7
29	c	518	DGD	C7B-C8B-C9B-CAB
29	C	517	DGD	CDA-CEA-CFA-CGA
22	B	710	CLA	C15-C16-C17-C18
25	d	404	PL9	C44-C46-C47-C48
26	A	409	SQD	C17-C18-C19-C20
28	M	103	STE	C7-C8-C9-C10
28	M	102	STE	C11-C10-C9-C8
29	H	103	DGD	C4A-C5A-C6A-C7A
33	D	412	LMG	C35-C36-C37-C38
25	d	404	PL9	C37-C38-C39-C40
28	B	725	STE	C12-C13-C14-C15
28	b	727	STE	C5-C6-C7-C8
29	h	702	DGD	CAA-CBA-CCA-CDA
22	d	402	CLA	C15-C16-C17-C18
33	M	101	LMG	C33-C34-C35-C36
28	a	417	STE	C7-C8-C9-C10
22	C	508	CLA	C16-C17-C18-C19
34	D	406	PHO	C16-C17-C18-C20
22	C	511	CLA	C4-C3-C5-C6
22	c	513	CLA	C4-C3-C5-C6
27	d	406	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	b	725	STE	C3-C4-C5-C6
26	b	720	SQD	C19-C20-C21-C22
26	A	412	SQD	C27-C28-C29-C30
29	C	518	DGD	C3A-C4A-C5A-C6A
33	c	522	LMG	C31-C32-C33-C34
33	C	520	LMG	O9-C10-O7-C8
22	B	704	CLA	C11-C12-C13-C14
22	C	507	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C12-C13-C14
22	H	102	CLA	C14-C13-C15-C16
22	b	702	CLA	C6-C7-C8-C9
22	b	715	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C10-C8-C9
28	T	702	STE	C10-C11-C12-C13
28	a	418	STE	C10-C11-C12-C13
22	A	403	CLA	C13-C15-C16-C17
22	B	712	CLA	C10-C11-C12-C13
22	b	706	CLA	C8-C10-C11-C12
22	b	707	CLA	C13-C15-C16-C17
27	a	412	LHG	C29-C30-C31-C32
28	B	720	STE	C3-C4-C5-C6
28	b	726	STE	C4-C5-C6-C7
28	x	101	STE	C11-C10-C9-C8
22	C	507	CLA	C13-C15-C16-C17
22	c	514	CLA	C13-C15-C16-C17
27	d	407	LHG	C35-C36-C37-C38
29	C	519	DGD	C9B-CAB-CBB-CCB
27	L	101	LHG	C30-C31-C32-C33
29	A	413	DGD	CBA-CCA-CDA-CEA
29	C	517	DGD	C6B-C7B-C8B-C9B
33	M	101	LMG	C17-C18-C19-C20
33	a	419	LMG	C32-C33-C34-C35
33	M	101	LMG	C40-C41-C42-C43
33	c	523	LMG	C20-C21-C22-C23
27	A	410	LHG	O6-C4-C5-C6
27	A	410	LHG	C26-C27-C28-C29
29	A	413	DGD	CDA-CEA-CFA-CGA
22	A	403	CLA	C11-C10-C8-C7
22	B	704	CLA	C11-C12-C13-C15
22	B	705	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	714	CLA	C6-C7-C8-C10
22	C	507	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C7
22	C	514	CLA	C6-C7-C8-C10
22	b	702	CLA	C6-C7-C8-C10
22	b	708	CLA	C11-C12-C13-C15
22	b	709	CLA	C12-C13-C15-C16
22	c	505	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C12-C13-C15
22	D	401	CLA	C10-C11-C12-C13
27	L	101	LHG	C19-C20-C21-C22
28	h	703	STE	C15-C16-C17-C18
28	H	104	STE	C11-C10-C9-C8
29	H	103	DGD	C7A-C8A-C9A-CAA
22	b	704	CLA	C16-C17-C18-C20
28	X	101	STE	C11-C10-C9-C8
29	c	517	DGD	CAB-CBB-CCB-CDB
22	c	506	CLA	C4-C3-C5-C6
26	A	409	SQD	C28-C29-C30-C31
29	C	518	DGD	C4A-C5A-C6A-C7A
27	D	410	LHG	C25-C26-C27-C28
33	c	520	LMG	C34-C35-C36-C37
33	C	516	LMG	C36-C37-C38-C39
22	B	703	CLA	C15-C16-C17-C18
22	b	708	CLA	C13-C15-C16-C17
28	H	105	STE	C5-C6-C7-C8
29	c	517	DGD	C1B-C2B-C3B-C4B
23	k	101	BCR	C36-C18-C19-C20
22	A	404	CLA	C5-C6-C7-C8
28	l	102	STE	C1-C2-C3-C4
29	c	517	DGD	C3B-C4B-C5B-C6B
29	c	519	DGD	C6A-C7A-C8A-C9A
26	A	412	SQD	C7-C8-C9-C10
28	B	725	STE	C2-C3-C4-C5
28	b	726	STE	C7-C8-C9-C10
28	m	101	STE	C5-C6-C7-C8
22	a	403	CLA	C2C-C3C-CAC-CBC
26	A	409	SQD	C44-C45-C46-O48
27	A	410	LHG	C4-C5-C6-O8
29	A	413	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	O1-C7-C8-C9
33	M	101	LMG	C7-C8-C9-O8
33	a	419	LMG	O1-C7-C8-C9
33	c	522	LMG	O1-C7-C8-C9
33	c	522	LMG	C7-C8-C9-O8
28	C	523	STE	C6-C7-C8-C9
26	a	413	SQD	C17-C18-C19-C20
26	a	413	SQD	C28-C29-C30-C31
28	C	522	STE	C6-C7-C8-C9
22	b	702	CLA	CBD-CGD-O2D-CED
33	D	412	LMG	O1-C7-C8-C9
22	C	513	CLA	C10-C11-C12-C13
29	C	518	DGD	C4B-C5B-C6B-C7B
29	c	519	DGD	O6D-C5D-C6D-O5D
25	d	404	PL9	C15-C14-C16-C17
26	a	413	SQD	C11-C10-C9-C8
28	E	101	STE	C5-C6-C7-C8
22	C	511	CLA	C2-C3-C5-C6
22	c	513	CLA	C2-C3-C5-C6
27	A	410	LHG	C35-C36-C37-C38
27	A	410	LHG	C27-C28-C29-C30
27	d	407	LHG	C30-C31-C32-C33
22	B	712	CLA	C16-C17-C18-C19
22	c	504	CLA	C16-C17-C18-C19
28	C	521	STE	C3-C4-C5-C6
33	c	523	LMG	C30-C31-C32-C33
23	B	718	BCR	C23-C24-C25-C30
23	C	501	BCR	C23-C24-C25-C30
23	H	101	BCR	C23-C24-C25-C30
23	d	403	BCR	C23-C24-C25-C30
29	c	518	DGD	CDA-CEA-CFA-CGA
33	C	520	LMG	C40-C41-C42-C43
27	l	101	LHG	C16-C17-C18-C19
28	x	101	STE	C4-C5-C6-C7
22	c	512	CLA	C8-C10-C11-C12
26	A	409	SQD	C31-C32-C33-C34
26	a	413	SQD	C18-C19-C20-C21
33	b	723	LMG	C19-C20-C21-C22
26	B	723	SQD	C19-C20-C21-C22
28	A	411	STE	C15-C16-C17-C18
28	T	702	STE	C6-C7-C8-C9
22	B	703	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	A	413	DGD	O2G-C2G-C3G-O3G
33	c	522	LMG	O1-C7-C8-O7
27	d	406	LHG	C17-C18-C19-C20
22	c	506	CLA	C2-C3-C5-C6
25	a	411	PL9	C13-C14-C16-C17
26	D	409	SQD	C30-C31-C32-C33
27	B	722	LHG	C27-C28-C29-C30
29	c	518	DGD	C8B-C9B-CAB-CBB
22	B	702	CLA	C16-C17-C18-C19
27	A	410	LHG	C12-C13-C14-C15
28	B	724	STE	C3-C4-C5-C6
28	B	725	STE	C1-C2-C3-C4
27	L	101	LHG	O10-C23-O8-C6
22	C	511	CLA	C6-C7-C8-C9
22	C	514	CLA	C11-C10-C8-C9
22	H	102	CLA	C6-C7-C8-C9
22	b	711	CLA	C11-C12-C13-C14
22	b	714	CLA	C6-C7-C8-C9
22	b	715	CLA	C11-C10-C8-C9
22	c	513	CLA	C11-C12-C13-C14
28	A	411	STE	C12-C13-C14-C15
29	H	103	DGD	CDA-CEA-CFA-CGA
28	b	725	STE	C7-C8-C9-C10
33	b	721	LMG	C33-C34-C35-C36
27	l	101	LHG	C32-C33-C34-C35
23	A	405	BCR	C14-C15-C16-C17
29	H	103	DGD	C8A-C9A-CAA-CBA
22	B	710	CLA	C16-C17-C18-C19
22	d	401	CLA	C16-C17-C18-C20
26	B	723	SQD	C28-C29-C30-C31
28	b	722	STE	C5-C6-C7-C8
33	D	408	LMG	C39-C40-C41-C42
33	a	419	LMG	C30-C31-C32-C33
28	A	411	STE	C3-C4-C5-C6
33	D	408	LMG	O10-C28-O8-C9
29	h	702	DGD	CBA-CCA-CDA-CEA
29	H	103	DGD	CDB-CEB-CFB-CGB
25	d	404	PL9	C28-C29-C31-C32
26	b	720	SQD	C30-C31-C32-C33
26	f	101	SQD	C24-C25-C26-C27
28	E	102	STE	C4-C5-C6-C7
28	b	724	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	c	519	DGD	CCB-CDB-CEB-CFB
33	D	408	LMG	C30-C31-C32-C33
33	M	101	LMG	C32-C33-C34-C35
23	H	101	BCR	C20-C21-C22-C37
23	K	101	BCR	C35-C13-C14-C15
23	Y	101	BCR	C16-C17-C18-C36
23	c	515	BCR	C35-C13-C14-C15
23	t	701	BCR	C35-C13-C14-C15
22	B	705	CLA	C3-C5-C6-C7
22	B	703	CLA	C13-C15-C16-C17
22	b	714	CLA	C5-C6-C7-C8
27	a	414	LHG	C15-C16-C17-C18
34	a	405	PHO	O1D-CGD-O2D-CED
22	D	402	CLA	C16-C17-C18-C19
29	C	518	DGD	C2B-C3B-C4B-C5B
33	d	408	LMG	C40-C41-C42-C43
27	B	722	LHG	C18-C19-C20-C21
22	A	403	CLA	C11-C12-C13-C15
22	B	702	CLA	C12-C13-C15-C16
22	B	707	CLA	C12-C13-C15-C16
22	B	713	CLA	C11-C12-C13-C15
22	C	508	CLA	C11-C12-C13-C15
22	C	509	CLA	C11-C10-C8-C7
22	b	705	CLA	C12-C13-C15-C16
22	b	707	CLA	C6-C7-C8-C10
22	b	715	CLA	C11-C10-C8-C7
22	c	509	CLA	C11-C10-C8-C7
22	d	401	CLA	C11-C12-C13-C15
22	d	402	CLA	C12-C13-C15-C16
26	A	412	SQD	C11-C12-C13-C14
33	c	523	LMG	C37-C38-C39-C40
28	B	720	STE	C9-C10-C11-C12
33	D	412	LMG	C16-C17-C18-C19
22	c	510	CLA	C8-C10-C11-C12
23	c	516	BCR	C21-C22-C23-C24
26	f	101	SQD	C28-C29-C30-C31
29	C	518	DGD	C2G-C3G-O3G-C1D
29	c	518	DGD	C2G-C3G-O3G-C1D
22	b	712	CLA	C13-C15-C16-C17
28	b	727	STE	C4-C5-C6-C7
33	c	520	LMG	C38-C39-C40-C41
22	d	401	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	c	517	DGD	O1B-C1B-O2G-C2G
33	d	408	LMG	C37-C38-C39-C40
29	H	103	DGD	O2G-C1B-C2B-C3B
28	b	727	STE	C3-C4-C5-C6
22	c	512	CLA	CBD-CGD-O2D-CED
22	B	703	CLA	C10-C11-C12-C13
22	C	511	CLA	C15-C16-C17-C18
33	D	412	LMG	C9-C8-O7-C10
33	c	523	LMG	C9-C8-O7-C10
26	b	720	SQD	C11-C12-C13-C14
29	C	517	DGD	C2B-C3B-C4B-C5B
26	A	409	SQD	C27-C28-C29-C30
28	b	722	STE	C4-C5-C6-C7
23	c	515	BCR	C12-C13-C14-C15
27	a	414	LHG	O6-C4-C5-O7
29	c	518	DGD	O6D-C1D-O3G-C3G
33	C	520	LMG	O6-C1-O1-C7
29	c	518	DGD	CBB-CCB-CDB-CEB
26	A	409	SQD	O6-C44-C45-C46
26	a	413	SQD	O6-C44-C45-C46
27	d	407	LHG	C26-C27-C28-C29
29	C	518	DGD	CAA-CBA-CCA-CDA
25	a	411	PL9	C15-C14-C16-C17
28	a	417	STE	C2-C3-C4-C5
29	C	519	DGD	C6B-C7B-C8B-C9B
33	M	101	LMG	C19-C20-C21-C22
27	d	406	LHG	C31-C32-C33-C34
28	J	101	STE	C5-C6-C7-C8
27	A	410	LHG	O7-C5-C6-O8
27	a	414	LHG	O7-C5-C6-O8
29	C	517	DGD	O1G-C1G-C2G-O2G
29	c	517	DGD	O1G-C1G-C2G-O2G
33	b	723	LMG	O7-C8-C9-O8
22	C	510	CLA	C14-C13-C15-C16
22	c	509	CLA	C11-C10-C8-C9
22	A	403	CLA	C16-C17-C18-C19
27	B	722	LHG	C29-C30-C31-C32
27	a	412	LHG	C14-C15-C16-C17
28	b	727	STE	C2-C3-C4-C5
29	C	519	DGD	C8A-C9A-CAA-CBA
33	D	412	LMG	C15-C16-C17-C18
33	c	520	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
22	B	711	CLA	C15-C16-C17-C18
26	a	415	SQD	C30-C31-C32-C33
33	b	723	LMG	C14-C15-C16-C17
33	b	723	LMG	C34-C35-C36-C37
28	C	523	STE	C2-C3-C4-C5
22	A	402	CLA	C4C-C3C-CAC-CBC
29	c	517	DGD	C5B-C6B-C7B-C8B
29	c	517	DGD	C2E-C1E-O5D-C6D
22	B	705	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C20
22	c	504	CLA	C16-C17-C18-C20
33	b	723	LMG	C40-C41-C42-C43
28	E	101	STE	C7-C8-C9-C10
29	A	413	DGD	O6D-C5D-C6D-O5D
22	c	506	CLA	C15-C16-C17-C18
28	B	726	STE	C14-C15-C16-C17
27	D	411	LHG	C9-C10-C11-C12
22	b	706	CLA	C16-C17-C18-C20
28	B	720	STE	C10-C11-C12-C13
26	a	413	SQD	C31-C32-C33-C34
29	H	103	DGD	CCB-CDB-CEB-CFB
26	B	723	SQD	C10-C11-C12-C13
27	D	411	LHG	C17-C18-C19-C20
23	b	719	BCR	C11-C12-C13-C35
28	T	702	STE	C15-C16-C17-C18
33	b	721	LMG	C15-C16-C17-C18
22	C	514	CLA	C1A-C2A-CAA-CBA
22	a	401	CLA	C1A-C2A-CAA-CBA
33	c	520	LMG	C29-C28-O8-C9
28	a	418	STE	C11-C10-C9-C8
25	A	408	PL9	C28-C29-C31-C32
25	a	411	PL9	C38-C39-C41-C42
23	D	404	BCR	C17-C18-C19-C20
25	a	411	PL9	C42-C43-C44-C46
27	a	412	LHG	C33-C34-C35-C36
25	d	404	PL9	C32-C33-C34-C35
26	A	412	SQD	C34-C35-C36-C37
28	b	724	STE	C2-C3-C4-C5
33	D	412	LMG	C34-C35-C36-C37
33	d	408	LMG	C32-C33-C34-C35
33	c	520	LMG	C31-C32-C33-C34
22	B	713	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	713	CLA	C12-C13-C15-C16
22	B	716	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10
22	C	511	CLA	C11-C10-C8-C7
22	C	513	CLA	C12-C13-C15-C16
22	b	703	CLA	C11-C12-C13-C15
22	b	707	CLA	C11-C12-C13-C15
22	c	502	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C12-C13-C15
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C10-C8-C7
22	c	513	CLA	C12-C13-C15-C16
22	c	514	CLA	C12-C13-C15-C16
22	A	402	CLA	C16-C17-C18-C19
22	b	706	CLA	C16-C17-C18-C19
34	D	406	PHO	C16-C17-C18-C19
33	C	520	LMG	O10-C28-O8-C9
22	b	714	CLA	C13-C15-C16-C17
28	X	101	STE	C12-C13-C14-C15
28	h	703	STE	C5-C6-C7-C8
28	H	104	STE	C7-C8-C9-C10
28	m	101	STE	C2-C3-C4-C5
27	A	410	LHG	O6-C4-C5-O7
29	h	702	DGD	C7B-C8B-C9B-CAB
29	C	517	DGD	C4D-C5D-C6D-O5D
26	a	413	SQD	C8-C7-O47-C45
22	A	403	CLA	C11-C10-C8-C9
22	A	403	CLA	C11-C12-C13-C14
22	B	702	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C12-C13-C14
22	C	509	CLA	C11-C10-C8-C9
22	C	511	CLA	C11-C10-C8-C9
22	a	406	CLA	C11-C12-C13-C14
22	b	701	CLA	C11-C12-C13-C14
22	b	705	CLA	C14-C13-C15-C16
22	b	706	CLA	C14-C13-C15-C16
22	d	402	CLA	C14-C13-C15-C16
27	a	412	LHG	C25-C26-C27-C28
25	D	405	PL9	C47-C48-C49-C51
22	B	713	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	C8-C10-C11-C12
28	B	726	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C8A-C9A-CAA-CBA
22	B	711	CLA	O1D-CGD-O2D-CED
26	A	409	SQD	C11-C12-C13-C14
33	C	520	LMG	C19-C20-C21-C22
33	D	408	LMG	C12-C13-C14-C15
29	c	518	DGD	C5A-C6A-C7A-C8A
29	C	517	DGD	O6D-C5D-C6D-O5D
26	a	415	SQD	O47-C45-C46-O48
33	M	101	LMG	O7-C8-C9-O8
33	a	419	LMG	O1-C7-C8-O7
33	c	522	LMG	O7-C8-C9-O8
22	c	507	CLA	C8-C10-C11-C12
22	c	505	CLA	C11-C12-C13-C15
27	a	414	LHG	C4-C5-C6-O8
29	C	517	DGD	O1G-C1G-C2G-C3G
33	C	520	LMG	C32-C33-C34-C35
22	b	703	CLA	C8-C10-C11-C12
22	b	704	CLA	C3-C5-C6-C7
29	A	413	DGD	CFA-CGA-CHA-CIA
29	C	519	DGD	CBB-CCB-CDB-CEB
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	707	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	CAD-CBD-CGD-O2D
33	d	408	LMG	C36-C37-C38-C39
29	H	103	DGD	CAB-CBB-CCB-CDB
29	C	519	DGD	C2A-C1A-O1G-C1G
26	b	720	SQD	O5-C1-O6-C44
33	C	516	LMG	O6-C1-O1-C7
22	A	402	CLA	C16-C17-C18-C20
28	d	409	STE	C2-C3-C4-C5
27	B	722	LHG	C17-C18-C19-C20
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	b	707	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
23	B	718	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	C46-C45-O47-C7
27	L	101	LHG	C3-O3-P-O6
27	L	101	LHG	C4-O6-P-O5
27	a	412	LHG	C3-O3-P-O5
27	a	414	LHG	C3-O3-P-O4
27	d	406	LHG	C4-O6-P-O5
29	A	413	DGD	CEB-CFB-CGB-CHB
23	D	404	BCR	C37-C22-C23-C24
33	C	516	LMG	C15-C16-C17-C18
28	a	417	STE	C1-C2-C3-C4
26	a	415	SQD	C29-C30-C31-C32
28	b	727	STE	C11-C10-C9-C8
33	d	408	LMG	C35-C36-C37-C38
25	A	408	PL9	C4-C3-C7-C8
33	B	721	LMG	C29-C30-C31-C32
22	b	701	CLA	C10-C11-C12-C13
33	a	419	LMG	C9-C8-O7-C10
26	a	415	SQD	C31-C32-C33-C34
22	B	716	CLA	C10-C11-C12-C13
22	b	714	CLA	C2-C3-C5-C6
29	C	517	DGD	C3A-C4A-C5A-C6A
33	d	408	LMG	C15-C16-C17-C18
22	B	705	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C19
22	c	505	CLA	C11-C12-C13-C14
27	a	414	LHG	O6-C4-C5-C6
22	A	403	CLA	C6-C7-C8-C9
22	B	702	CLA	C11-C12-C13-C14
22	b	702	CLA	C11-C10-C8-C9
22	b	703	CLA	C6-C7-C8-C9
22	b	707	CLA	C6-C7-C8-C9
22	b	707	CLA	C11-C12-C13-C14
22	b	716	CLA	C11-C10-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	507	CLA	C14-C13-C15-C16
33	a	419	LMG	C17-C18-C19-C20
22	c	507	CLA	C6-C7-C8-C10
22	c	510	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C12-C13-C15
22	c	506	CLA	C13-C15-C16-C17
23	c	516	BCR	C12-C13-C14-C15
22	B	715	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C16-C17-C18-C19
28	b	722	STE	C13-C14-C15-C16
29	c	518	DGD	C5B-C6B-C7B-C8B
29	C	518	DGD	O1A-C1A-O1G-C1G
29	H	103	DGD	C4B-C5B-C6B-C7B
29	A	413	DGD	C6B-C7B-C8B-C9B
29	A	413	DGD	C4D-C5D-C6D-O5D
33	b	721	LMG	C19-C20-C21-C22
26	B	723	SQD	C32-C33-C34-C35
28	c	501	STE	C7-C8-C9-C10
33	a	419	LMG	O7-C8-C9-O8
29	h	702	DGD	O2G-C1B-C2B-C3B
22	c	512	CLA	CBA-CGA-O2A-C1
22	b	709	CLA	C16-C17-C18-C20
22	c	506	CLA	C16-C17-C18-C20
33	b	721	LMG	C22-C23-C24-C25
29	C	519	DGD	C1A-C2A-C3A-C4A
28	H	104	STE	C11-C12-C13-C14
29	H	103	DGD	C3B-C4B-C5B-C6B
29	c	518	DGD	C9B-CAB-CBB-CCB
22	b	714	CLA	C4-C3-C5-C6
26	a	415	SQD	C17-C18-C19-C20
29	c	519	DGD	C5A-C6A-C7A-C8A
28	b	722	STE	C2-C3-C4-C5
29	h	702	DGD	CBB-CCB-CDB-CEB
22	C	502	CLA	O1D-CGD-O2D-CED
27	A	410	LHG	C8-C7-O7-C5
25	D	405	PL9	C42-C43-C44-C46
26	B	723	SQD	C14-C15-C16-C17
28	t	702	STE	C3-C4-C5-C6
29	C	517	DGD	CBB-CCB-CDB-CEB
27	a	414	LHG	C14-C15-C16-C17
29	c	518	DGD	C5D-C6D-O5D-C1E
27	D	410	LHG	C11-C12-C13-C14
23	k	102	BCR	C13-C14-C15-C16
27	d	406	LHG	C7-C8-C9-C10
33	B	721	LMG	C28-C29-C30-C31
28	j	101	STE	C7-C8-C9-C10
33	a	419	LMG	C31-C32-C33-C34
33	d	408	LMG	C10-C11-C12-C13
28	M	103	STE	C2-C3-C4-C5
26	f	101	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	C4C-C3C-CAC-CBC
22	B	713	CLA	C6-C7-C8-C9
22	B	713	CLA	C14-C13-C15-C16
22	C	503	CLA	C6-C7-C8-C9
22	b	703	CLA	C11-C12-C13-C14
22	c	506	CLA	C6-C7-C8-C9
22	c	513	CLA	C14-C13-C15-C16
29	h	702	DGD	C5B-C6B-C7B-C8B
22	b	706	CLA	C10-C11-C12-C13
29	A	413	DGD	CCA-CDA-CEA-CFA
22	B	713	CLA	C16-C17-C18-C19
33	C	516	LMG	C29-C28-O8-C9
22	B	707	CLA	C15-C16-C17-C18
25	A	408	PL9	C12-C11-C9-C10
33	C	516	LMG	C12-C13-C14-C15
23	k	101	BCR	C15-C16-C17-C18
22	C	512	CLA	C13-C15-C16-C17
22	A	403	CLA	C16-C17-C18-C20
22	B	713	CLA	C16-C17-C18-C20
22	C	503	CLA	C6-C7-C8-C10
22	a	406	CLA	C12-C13-C15-C16
22	B	708	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
33	D	408	LMG	C32-C33-C34-C35
27	a	414	LHG	C28-C29-C30-C31
22	D	403	CLA	C16-C17-C18-C20
28	C	523	STE	C4-C5-C6-C7
33	C	516	LMG	O1-C7-C8-O7
22	H	102	CLA	C3A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
27	l	101	LHG	C18-C19-C20-C21
33	M	101	LMG	C36-C37-C38-C39
33	a	419	LMG	C22-C23-C24-C25
29	H	103	DGD	C5B-C6B-C7B-C8B
28	a	418	STE	C1-C2-C3-C4
22	c	510	CLA	C13-C15-C16-C17
22	a	406	CLA	C15-C16-C17-C18
23	K	101	BCR	C13-C14-C15-C16
22	B	704	CLA	C10-C11-C12-C13
23	a	407	BCR	C11-C12-C13-C35
23	t	701	BCR	C7-C8-C9-C34
27	D	411	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
22	C	504	CLA	C10-C11-C12-C13
27	D	411	LHG	C13-C14-C15-C16
28	b	724	STE	O1-C1-C2-C3
23	C	501	BCR	C11-C12-C13-C14
22	C	507	CLA	C4-C3-C5-C6
28	a	418	STE	C5-C6-C7-C8
28	c	501	STE	C2-C3-C4-C5
33	B	721	LMG	O7-C10-C11-C12
35	v	201	HEC	CAD-CBD-CGD-O2D
22	B	712	CLA	O1A-CGA-O2A-C1
33	b	723	LMG	C7-C8-C9-O8
28	A	411	STE	C7-C8-C9-C10
29	A	413	DGD	C4E-C5E-C6E-O5E
27	a	412	LHG	C27-C28-C29-C30
33	M	101	LMG	C30-C31-C32-C33
33	d	408	LMG	O10-C28-O8-C9
22	B	710	CLA	C14-C13-C15-C16
22	C	508	CLA	C14-C13-C15-C16
22	a	403	CLA	C14-C13-C15-C16
22	b	706	CLA	C11-C10-C8-C9
22	c	502	CLA	C11-C12-C13-C14
22	c	507	CLA	C6-C7-C8-C9
22	d	401	CLA	C6-C7-C8-C9
26	b	720	SQD	C10-C11-C12-C13
29	c	517	DGD	C2A-C3A-C4A-C5A
26	A	409	SQD	C13-C14-C15-C16
26	a	415	SQD	C15-C16-C17-C18
29	c	518	DGD	C4A-C5A-C6A-C7A
27	D	410	LHG	C34-C35-C36-C37
28	B	724	STE	O2-C1-C2-C3
33	C	516	LMG	C9-C8-O7-C10
33	M	101	LMG	C9-C8-O7-C10
35	V	201	HEC	CAD-CBD-CGD-O2D
28	h	703	STE	C11-C10-C9-C8
22	C	507	CLA	C2-C3-C5-C6
26	A	409	SQD	C33-C34-C35-C36
29	c	519	DGD	C3B-C4B-C5B-C6B
22	c	510	CLA	CAA-CBA-CGA-O2A
22	B	702	CLA	C1A-C2A-CAA-CBA
27	B	722	LHG	C24-C25-C26-C27
22	b	708	CLA	C4C-C3C-CAC-CBC
27	l	101	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C13-C14-C15-C16
23	A	405	BCR	C1-C6-C7-C8
23	B	718	BCR	C23-C24-C25-C26
23	C	501	BCR	C23-C24-C25-C26
23	c	515	BCR	C23-C24-C25-C26
23	d	403	BCR	C23-C24-C25-C26
29	c	518	DGD	CCB-CDB-CEB-CFB
28	b	722	STE	O1-C1-C2-C3
33	c	522	LMG	C36-C37-C38-C39
27	d	407	LHG	C2-C3-O3-P
28	M	102	STE	C4-C5-C6-C7
28	l	102	STE	C9-C10-C11-C12
22	C	506	CLA	CBD-CGD-O2D-CED
22	B	704	CLA	C4C-C3C-CAC-CBC
22	H	102	CLA	C4-C3-C5-C6
22	b	701	CLA	C4-C3-C5-C6
25	A	408	PL9	C15-C14-C16-C17
28	I	101	STE	C12-C13-C14-C15
27	l	101	LHG	C29-C30-C31-C32
28	b	725	STE	C4-C5-C6-C7
28	M	102	STE	O1-C1-C2-C3
22	A	403	CLA	C6-C7-C8-C10
22	B	702	CLA	C11-C12-C13-C15
22	B	703	CLA	C11-C12-C13-C15
22	B	715	CLA	C11-C12-C13-C15
22	C	514	CLA	C11-C10-C8-C7
22	D	401	CLA	C11-C10-C8-C7
22	a	403	CLA	C12-C13-C15-C16
22	b	701	CLA	C11-C12-C13-C15
22	b	705	CLA	C11-C10-C8-C7
22	c	512	CLA	C6-C7-C8-C10
22	c	513	CLA	C6-C7-C8-C10
22	d	401	CLA	C6-C7-C8-C10
22	b	710	CLA	C2A-CAA-CBA-CGA
33	c	522	LMG	C42-C43-C44-C45
33	B	721	LMG	O9-C10-C11-C12
28	X	101	STE	C5-C6-C7-C8
33	C	516	LMG	C14-C15-C16-C17
25	a	411	PL9	C4-C3-C7-C8
28	b	724	STE	O2-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O1D
33	b	721	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	b	718	BCR	C36-C18-C19-C20
22	a	406	CLA	C4-C3-C5-C6
22	H	102	CLA	C2-C3-C5-C6
29	c	518	DGD	C3B-C4B-C5B-C6B
33	a	419	LMG	C12-C13-C14-C15
22	d	401	CLA	C2-C1-O2A-CGA
22	b	705	CLA	C10-C11-C12-C13
22	c	506	CLA	C16-C17-C18-C19
33	B	721	LMG	C34-C35-C36-C37
28	B	724	STE	O1-C1-C2-C3
22	B	704	CLA	C11-C10-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	b	705	CLA	C11-C12-C13-C14
22	c	514	CLA	C14-C13-C15-C16
27	l	101	LHG	C28-C29-C30-C31
28	b	724	STE	C10-C11-C12-C13
22	A	402	CLA	C13-C15-C16-C17
28	b	725	STE	O1-C1-C2-C3
22	c	511	CLA	C15-C16-C17-C18
33	b	723	LMG	C29-C30-C31-C32
25	d	404	PL9	C45-C44-C46-C47
22	B	712	CLA	C8-C10-C11-C12
28	C	523	STE	O2-C1-C2-C3
26	D	409	SQD	C27-C28-C29-C30
27	D	410	LHG	C13-C14-C15-C16
27	B	722	LHG	C16-C17-C18-C19
25	A	408	PL9	C29-C31-C32-C33
26	b	720	SQD	C44-C45-C46-O48
29	c	517	DGD	O1G-C1G-C2G-C3G
33	M	101	LMG	O1-C7-C8-C9
28	M	102	STE	O2-C1-C2-C3
35	V	201	HEC	CAD-CBD-CGD-O1D
33	D	412	LMG	O1-C7-C8-O7
22	c	502	CLA	C2A-CAA-CBA-CGA
28	x	101	STE	C1-C2-C3-C4
22	C	510	CLA	C10-C11-C12-C13
22	B	709	CLA	C4-C3-C5-C6
34	a	405	PHO	C4-C3-C5-C6
29	C	517	DGD	C5A-C6A-C7A-C8A
29	h	702	DGD	O1B-C1B-C2B-C3B
29	C	517	DGD	O1G-C1A-C2A-C3A
22	b	715	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	c	519	DGD	C8A-C9A-CAA-CBA
28	b	722	STE	O2-C1-C2-C3
26	b	720	SQD	C13-C14-C15-C16
29	C	517	DGD	O1A-C1A-O1G-C1G
22	b	705	CLA	C15-C16-C17-C18
22	B	710	CLA	CBD-CGD-O2D-CED
23	a	407	BCR	C20-C21-C22-C37
28	c	501	STE	O2-C1-C2-C3
29	c	518	DGD	C9A-CAA-CBA-CCA
22	C	512	CLA	CBD-CGD-O2D-CED
22	a	403	CLA	CBD-CGD-O2D-CED
27	a	412	LHG	C10-C11-C12-C13
28	x	101	STE	C10-C11-C12-C13
33	b	721	LMG	C14-C15-C16-C17
28	b	726	STE	C1-C2-C3-C4
26	A	412	SQD	C8-C7-O47-C45
29	C	517	DGD	O6E-C1E-O5D-C6D
27	D	411	LHG	C14-C15-C16-C17
22	B	704	CLA	C11-C10-C8-C7
22	b	705	CLA	C11-C12-C13-C15
33	B	721	LMG	C30-C31-C32-C33
22	B	711	CLA	C14-C13-C15-C16
22	B	715	CLA	C11-C12-C13-C14
22	B	716	CLA	C6-C7-C8-C9
22	C	512	CLA	C6-C7-C8-C9
22	b	713	CLA	C11-C12-C13-C14
27	a	412	LHG	C34-C35-C36-C37
33	B	721	LMG	O10-C28-C29-C30
22	B	713	CLA	C13-C15-C16-C17
22	B	703	CLA	C2A-CAA-CBA-CGA
25	A	408	PL9	C7-C8-C9-C11
27	L	101	LHG	C27-C28-C29-C30
22	b	712	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C4-C3-C5-C6
34	d	405	PHO	C3A-C2A-CAA-CBA
28	J	101	STE	C2-C3-C4-C5
33	C	516	LMG	C30-C31-C32-C33
28	t	702	STE	C2-C3-C4-C5
26	A	412	SQD	C33-C34-C35-C36
33	C	520	LMG	C2-C1-O1-C7
28	B	720	STE	O2-C1-C2-C3
28	C	523	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	b	720	SQD	C14-C15-C16-C17
28	C	522	STE	C11-C12-C13-C14
28	x	101	STE	C11-C12-C13-C14
29	c	518	DGD	CBA-CCA-CDA-CEA
33	B	721	LMG	C16-C17-C18-C19
22	B	712	CLA	CBA-CGA-O2A-C1
28	X	101	STE	C15-C16-C17-C18
34	a	405	PHO	C5-C6-C7-C8
28	Z	101	STE	C10-C11-C12-C13
34	d	405	PHO	C4C-C3C-CAC-CBC
27	A	410	LHG	C31-C32-C33-C34
22	C	513	CLA	O1A-CGA-O2A-C1
22	b	716	CLA	C8-C10-C11-C12
22	c	503	CLA	C16-C17-C18-C19
29	C	517	DGD	CCA-CDA-CEA-CFA
27	d	406	LHG	O1-C1-C2-O2
33	c	522	LMG	C16-C17-C18-C19
27	L	101	LHG	O9-C7-O7-C5
25	D	405	PL9	C33-C34-C36-C37
23	h	701	BCR	C13-C14-C15-C16
22	b	709	CLA	C15-C16-C17-C18
27	D	411	LHG	C16-C17-C18-C19
29	c	518	DGD	C8A-C9A-CAA-CBA
28	B	720	STE	O1-C1-C2-C3
22	C	506	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C12-C13-C14
26	a	415	SQD	O48-C23-C24-C25
27	d	406	LHG	C33-C34-C35-C36
23	b	717	BCR	C21-C22-C23-C24
29	c	518	DGD	C6A-C7A-C8A-C9A
26	b	720	SQD	C16-C17-C18-C19
22	C	503	CLA	C4-C3-C5-C6
34	d	405	PHO	C2C-C3C-CAC-CBC
22	c	511	CLA	CAA-CBA-CGA-O2A
29	c	517	DGD	O1G-C1A-C2A-C3A
22	B	713	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	C11-C10-C8-C7
22	C	514	CLA	C11-C12-C13-C15
22	D	402	CLA	C6-C7-C8-C10
22	a	401	CLA	C12-C13-C15-C16
22	b	701	CLA	C12-C13-C15-C16
22	b	707	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	b	708	CLA	C11-C10-C8-C7
28	b	725	STE	O2-C1-C2-C3
23	A	405	BCR	C5-C6-C7-C8
23	k	102	BCR	C23-C24-C25-C26
23	k	102	BCR	C23-C24-C25-C30
28	B	701	STE	C7-C8-C9-C10
22	D	401	CLA	C2-C1-O2A-CGA
22	c	511	CLA	C2-C1-O2A-CGA
33	b	721	LMG	C35-C36-C37-C38
22	B	709	CLA	C2-C3-C5-C6
25	D	405	PL9	C28-C29-C31-C32
34	a	405	PHO	C2-C3-C5-C6
27	a	414	LHG	C11-C10-C9-C8
29	A	413	DGD	C7A-C8A-C9A-CAA
29	H	103	DGD	CCA-CDA-CEA-CFA
22	b	714	CLA	C2A-CAA-CBA-CGA
28	c	501	STE	O1-C1-C2-C3
22	b	712	CLA	CAA-CBA-CGA-O2A
27	L	101	LHG	O7-C7-C8-C9
33	a	419	LMG	O7-C10-C11-C12
25	a	411	PL9	C16-C17-C18-C19
22	b	712	CLA	C10-C11-C12-C13
22	c	510	CLA	C15-C16-C17-C18
26	a	413	SQD	O47-C7-C8-C9
33	b	721	LMG	O8-C28-C29-C30
33	d	408	LMG	O7-C10-C11-C12
29	h	702	DGD	CAB-CBB-CCB-CDB
22	b	708	CLA	C2C-C3C-CAC-CBC
27	l	101	LHG	O7-C7-C8-C9
22	d	401	CLA	C2C-C3C-CAC-CBC
26	B	723	SQD	O47-C7-C8-C9
33	c	523	LMG	O8-C28-C29-C30
27	a	412	LHG	C26-C27-C28-C29
33	D	408	LMG	C21-C22-C23-C24
28	J	101	STE	C6-C7-C8-C9
35	e	101	HEC	CAD-CBD-CGD-O2D
22	C	513	CLA	C14-C13-C15-C16
22	D	403	CLA	C11-C12-C13-C14
22	b	710	CLA	C14-C13-C15-C16
27	a	414	LHG	O7-C7-C8-C9
27	A	410	LHG	C18-C19-C20-C21
22	b	711	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	C	504	CLA	C1A-C2A-CAA-CBA
35	E	103	HEC	CAD-CBD-CGD-O1D
33	M	101	LMG	O6-C1-O1-C7
25	D	405	PL9	C41-C42-C43-C44
35	e	101	HEC	CAD-CBD-CGD-O1D
23	d	403	BCR	C17-C18-C19-C20
23	K	101	BCR	C15-C16-C17-C18
23	c	515	BCR	C15-C16-C17-C18
27	l	101	LHG	C5-C6-O8-C23
22	B	708	CLA	CBA-CGA-O2A-C1
22	B	714	CLA	C2A-CAA-CBA-CGA
26	B	723	SQD	C23-C24-C25-C26
22	B	713	CLA	CAA-CBA-CGA-O2A
22	b	713	CLA	CAA-CBA-CGA-O2A
26	f	101	SQD	C30-C31-C32-C33
35	E	103	HEC	CAD-CBD-CGD-O2D
26	f	101	SQD	C5-C6-S-O7
25	D	405	PL9	C30-C29-C31-C32
22	C	507	CLA	C2-C1-O2A-CGA
27	d	407	LHG	C24-C25-C26-C27
22	C	512	CLA	C6-C7-C8-C10
22	b	704	CLA	C11-C12-C13-C15
22	b	710	CLA	C10-C11-C12-C13
28	x	101	STE	C12-C13-C14-C15
28	B	720	STE	C7-C8-C9-C10
29	C	519	DGD	C7A-C8A-C9A-CAA
22	B	707	CLA	C8-C10-C11-C12
22	B	713	CLA	C10-C11-C12-C13
22	b	710	CLA	C13-C15-C16-C17
22	B	716	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	C8-C10-C11-C12
22	b	708	CLA	C16-C17-C18-C19
29	c	517	DGD	CAA-CBA-CCA-CDA
25	a	411	PL9	C14-C16-C17-C18
22	B	702	CLA	C3A-C2A-CAA-CBA
23	C	515	BCR	C11-C10-C9-C8
28	d	409	STE	C6-C7-C8-C9
22	c	514	CLA	O1A-CGA-O2A-C1
22	B	709	CLA	C13-C15-C16-C17
27	a	414	LHG	O9-C7-C8-C9
22	b	702	CLA	C2A-CAA-CBA-CGA
22	B	711	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	708	CLA	C11-C10-C8-C9
22	d	401	CLA	C11-C12-C13-C14
28	C	522	STE	C15-C16-C17-C18
26	A	409	SQD	O10-C23-C24-C25
26	A	412	SQD	O10-C23-C24-C25
29	c	518	DGD	O1B-C1B-C2B-C3B
33	C	520	LMG	C33-C34-C35-C36
22	b	709	CLA	O1A-CGA-O2A-C1
22	b	712	CLA	CAA-CBA-CGA-O1A
29	A	413	DGD	O1B-C1B-C2B-C3B
22	b	709	CLA	C13-C15-C16-C17
26	B	723	SQD	C24-C25-C26-C27
22	B	712	CLA	CAA-CBA-CGA-O2A
26	B	723	SQD	O48-C23-C24-C25
22	C	513	CLA	CBA-CGA-O2A-C1
22	c	511	CLA	CAA-CBA-CGA-O1A
27	D	410	LHG	C28-C29-C30-C31
22	C	512	CLA	C8-C10-C11-C12
34	d	405	PHO	C5-C6-C7-C8
33	M	101	LMG	C8-C7-O1-C1
33	b	721	LMG	C8-C7-O1-C1
33	c	523	LMG	C8-C7-O1-C1
33	M	101	LMG	O1-C7-C8-O7
27	l	101	LHG	O9-C7-C8-C9
29	C	517	DGD	O1B-C1B-C2B-C3B
22	C	502	CLA	C2A-CAA-CBA-CGA
29	A	413	DGD	O6E-C5E-C6E-O5E
22	b	713	CLA	CAA-CBA-CGA-O1A
25	D	405	PL9	C21-C22-C23-C24
22	c	503	CLA	C13-C15-C16-C17
28	a	416	STE	C1-C2-C3-C4
22	a	406	CLA	C2-C3-C5-C6
28	b	724	STE	C11-C12-C13-C14
22	c	507	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	a	401	CLA	C2C-C3C-CAC-CBC
29	c	517	DGD	O1B-C1B-C2B-C3B
22	B	708	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	O1D-CGD-O2D-CED
26	a	413	SQD	C14-C15-C16-C17
26	b	720	SQD	C25-C26-C27-C28
25	d	404	PL9	C21-C22-C23-C24

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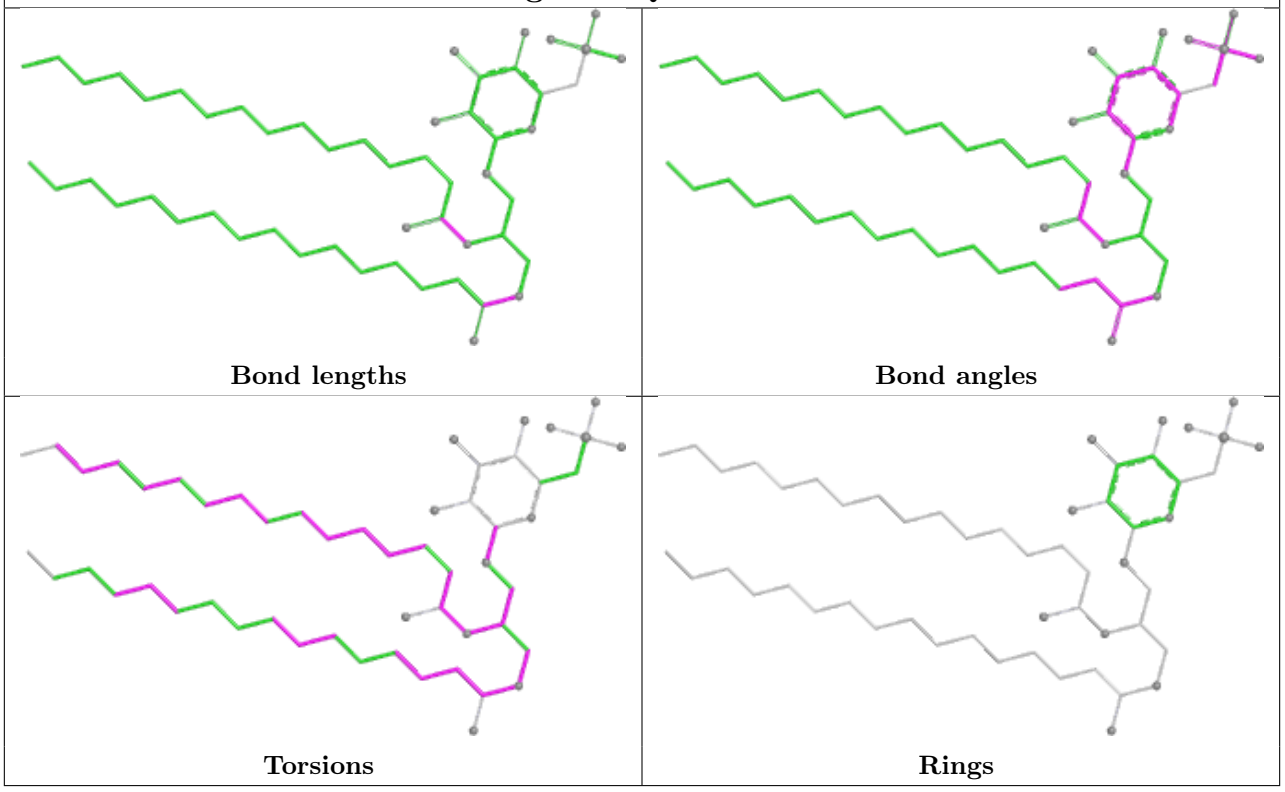
Mol	Chain	Res	Type	Atoms
28	A	411	STE	C10-C11-C12-C13
33	c	523	LMG	O10-C28-C29-C30
29	A	413	DGD	O2G-C1B-C2B-C3B
28	d	409	STE	O2-C1-C2-C3
26	B	723	SQD	O49-C7-C8-C9
33	a	419	LMG	C35-C36-C37-C38
22	b	709	CLA	CBA-CGA-O2A-C1
22	c	503	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

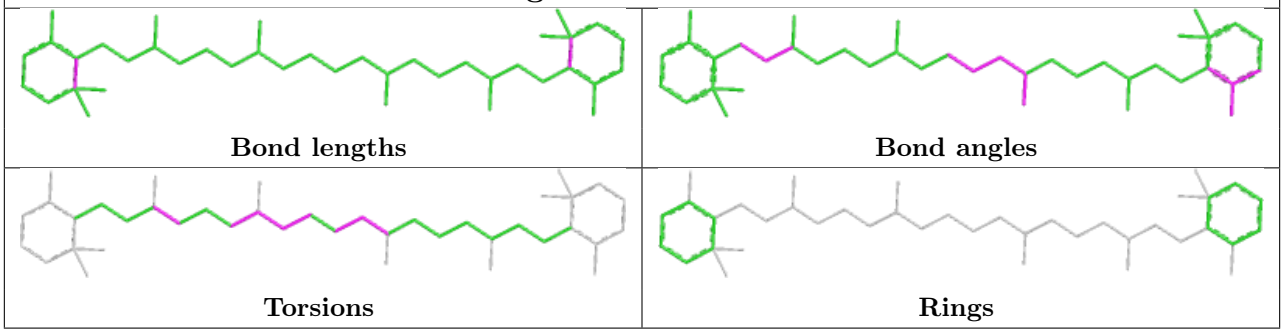
No monomer is involved in short contacts.

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

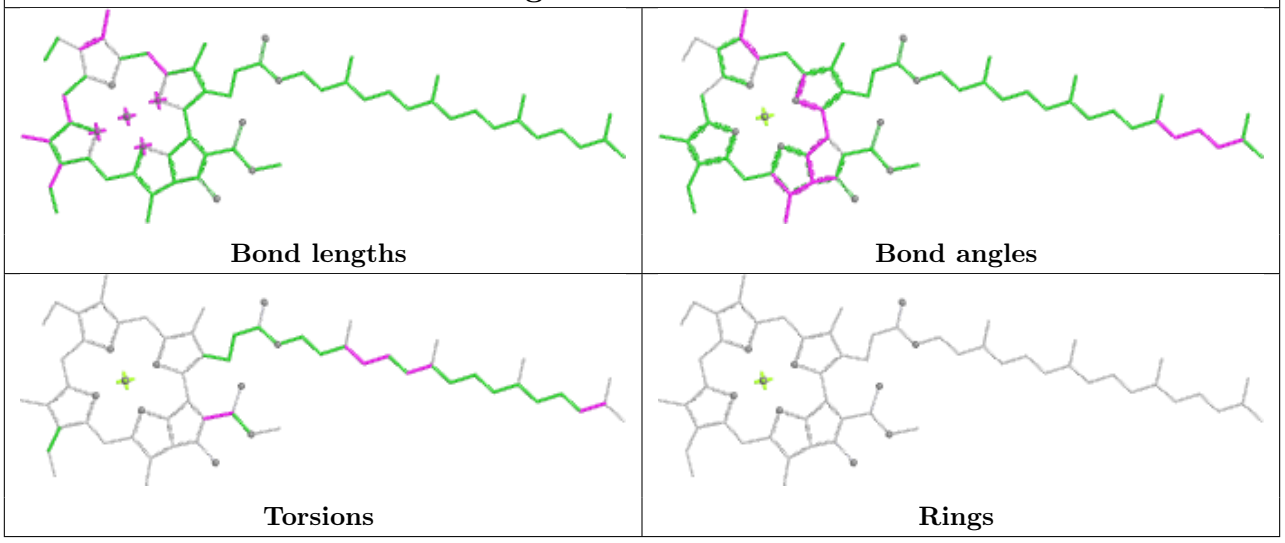
Ligand SQD B 723



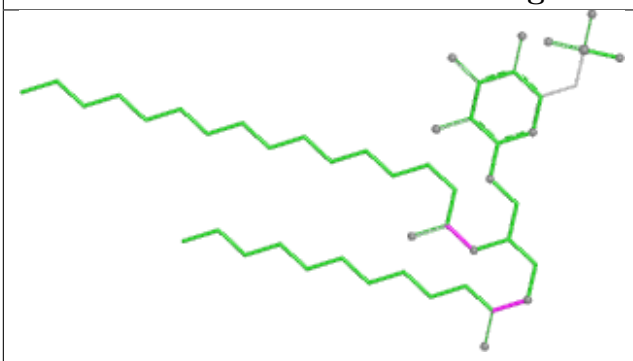
Ligand BCR h 701



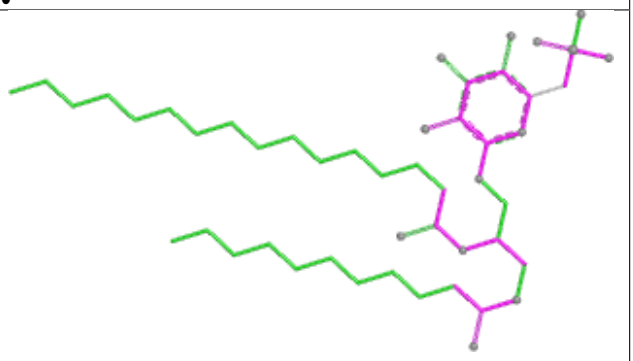
Ligand CLA C 503



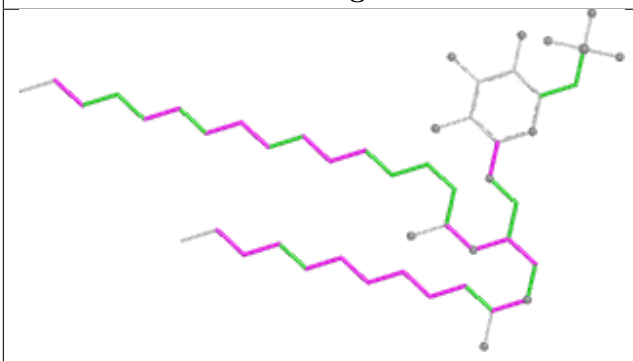
Ligand SQD b 720



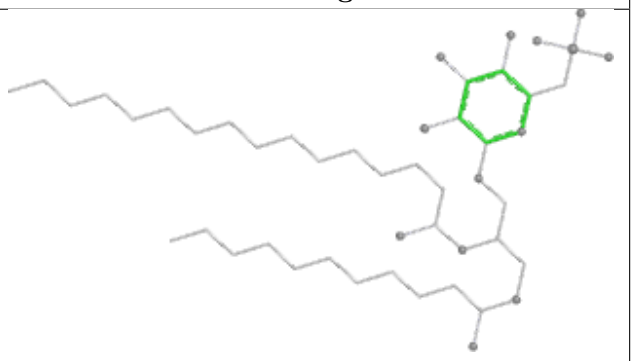
Bond lengths



Bond angles

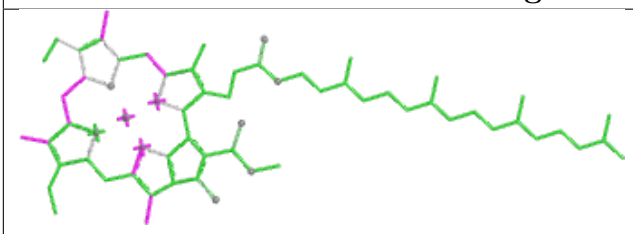


Torsions

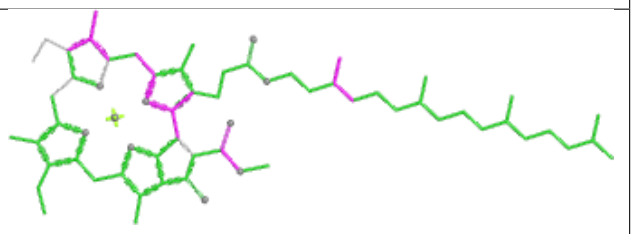


Rings

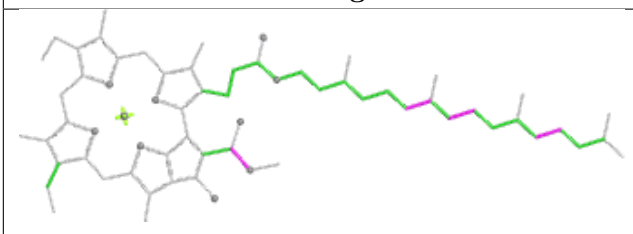
Ligand CLA C 512



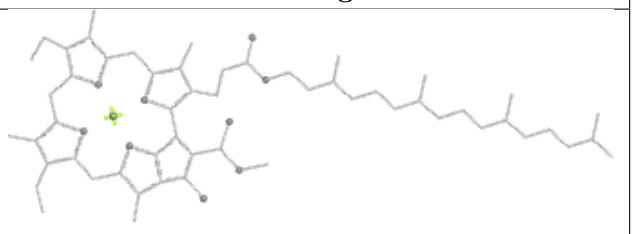
Bond lengths



Bond angles

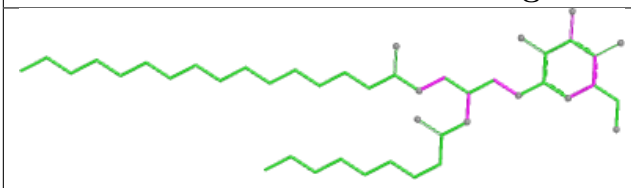


Torsions

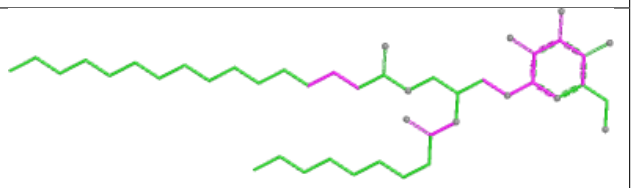


Rings

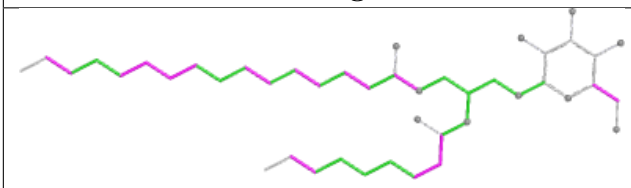
Ligand LMG d 408



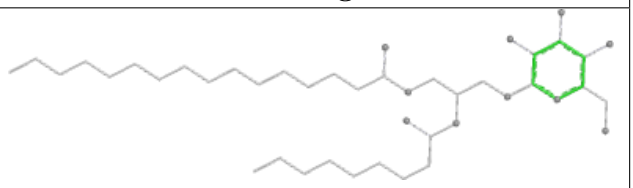
Bond lengths



Bond angles

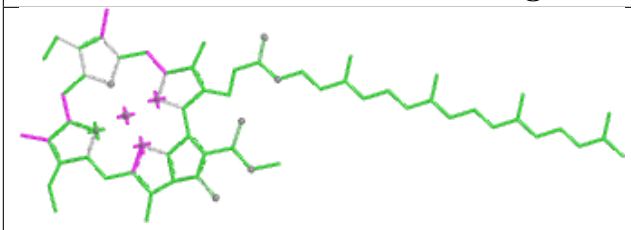


Torsions

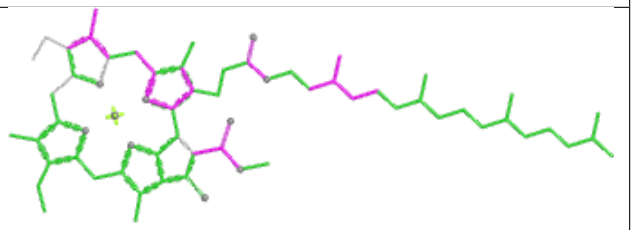


Rings

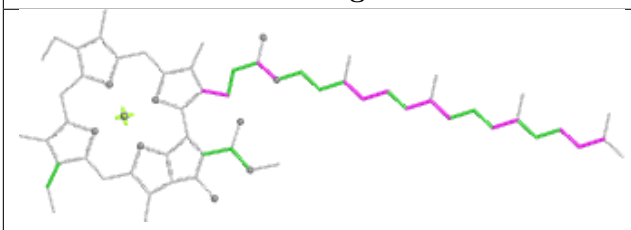
Ligand CLA C 514



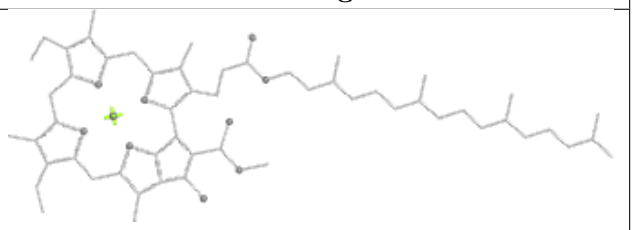
Bond lengths



Bond angles

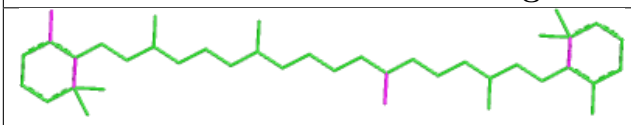


Torsions

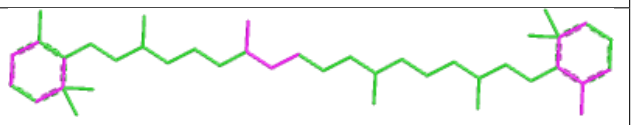


Rings

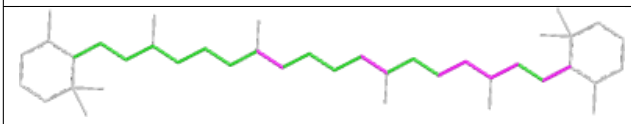
Ligand BCR B 718



Bond lengths



Bond angles



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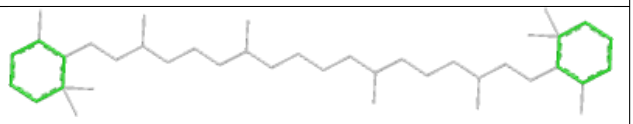
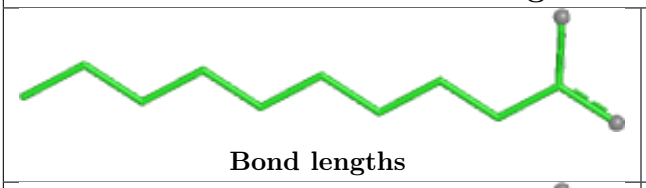
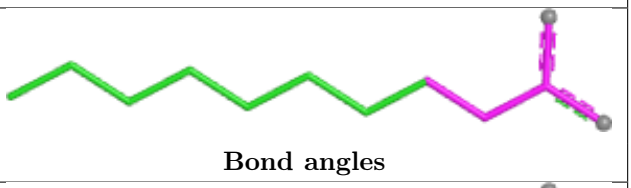
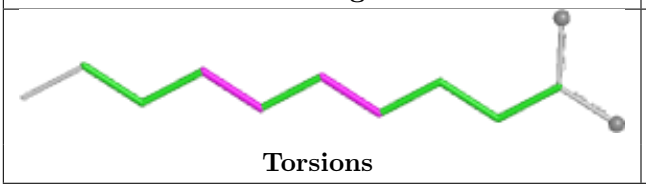


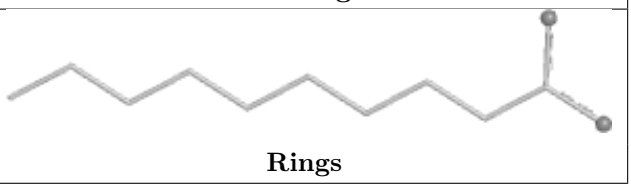
Rings

Ligand STE C 521

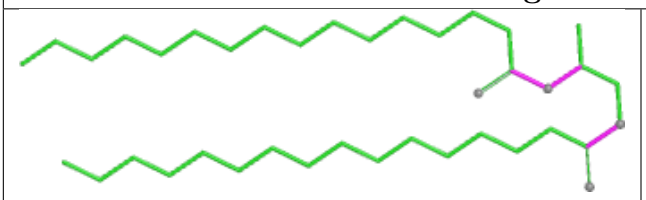

Bond lengths

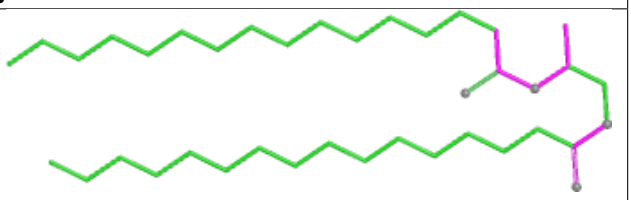

Bond angles

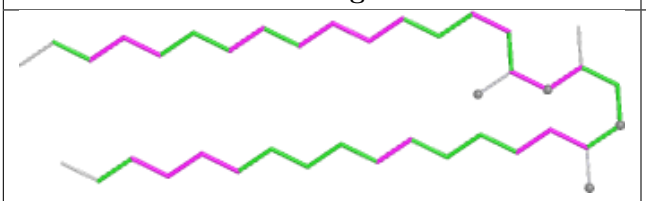

Torsions

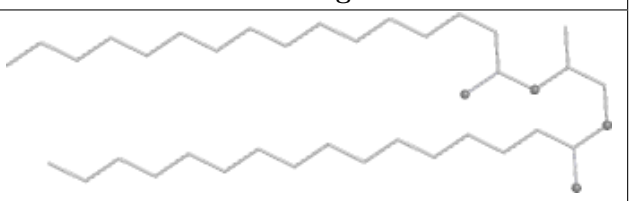

Rings

Ligand SQD A 412


Bond lengths


Bond angles

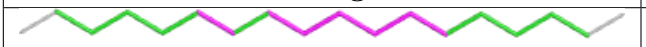

Torsions


Rings

Ligand STE H 104


Bond lengths


Bond angles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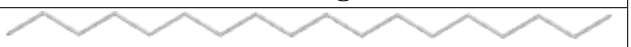
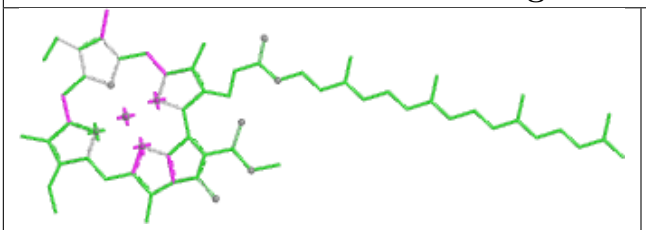
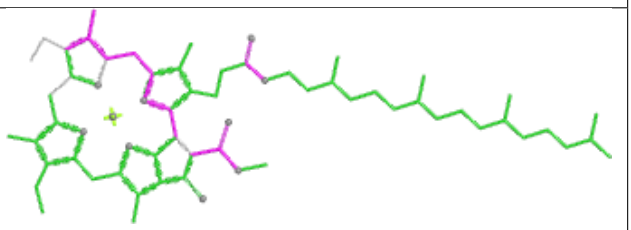
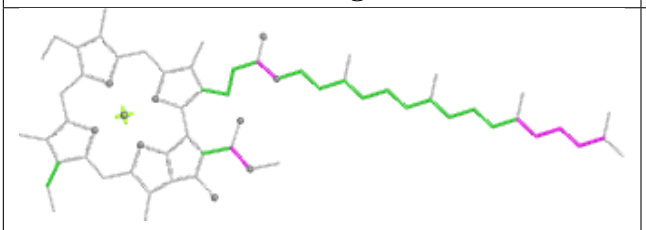
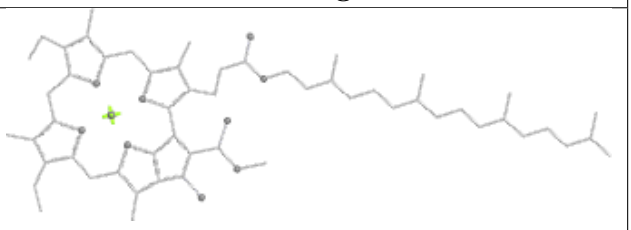

Rings

Ligand CLA b 709

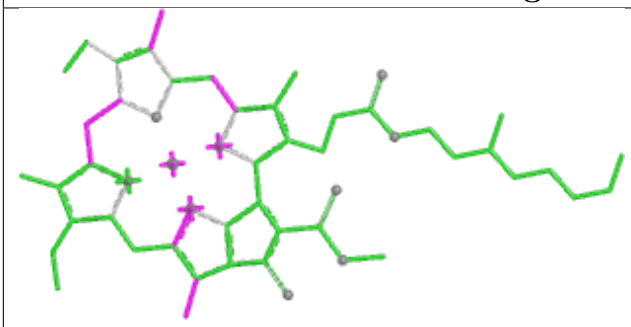

Bond lengths


Bond angles

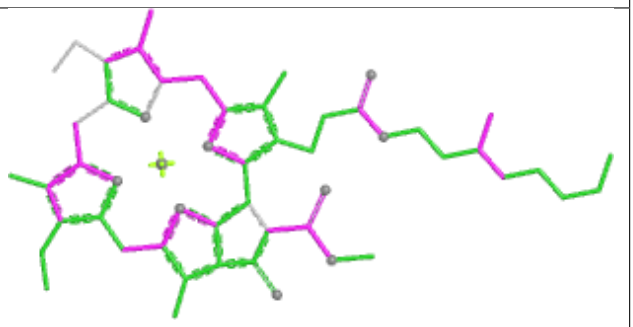

Torsions


Rings

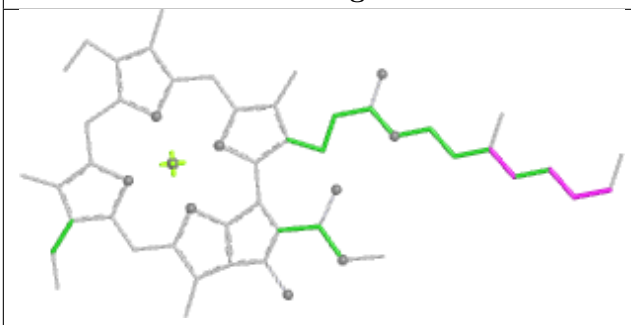
Ligand CLA A 404



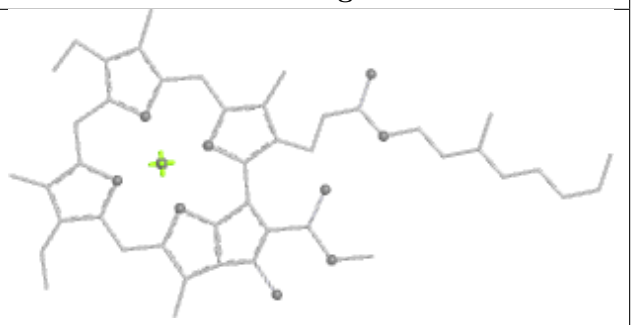
Bond lengths



Bond angles

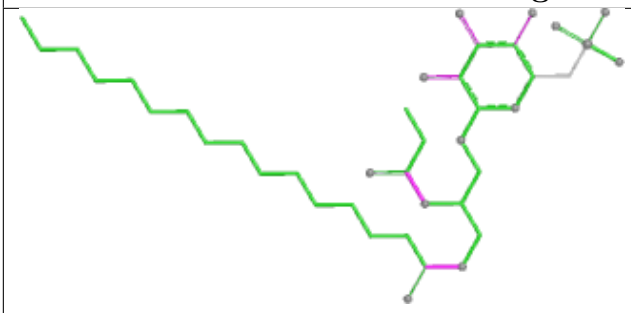


Torsions

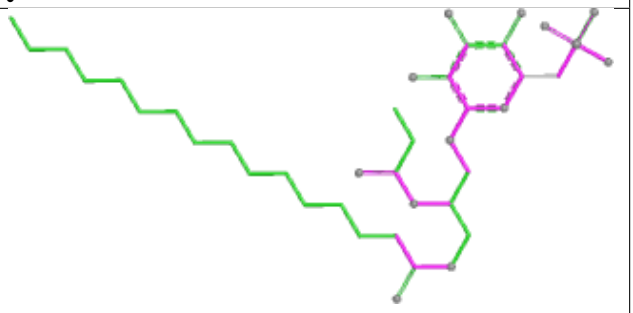


Rings

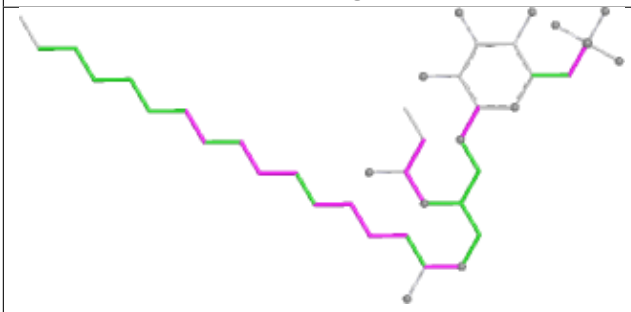
Ligand SQD f 101



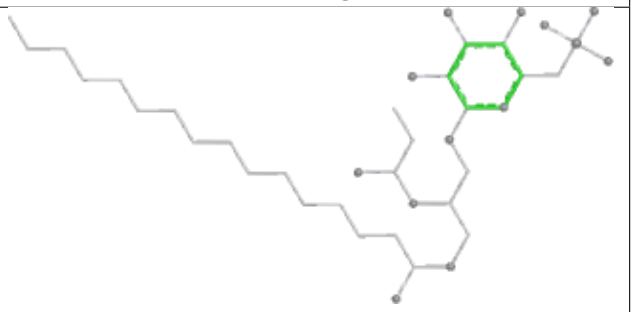
Bond lengths



Bond angles

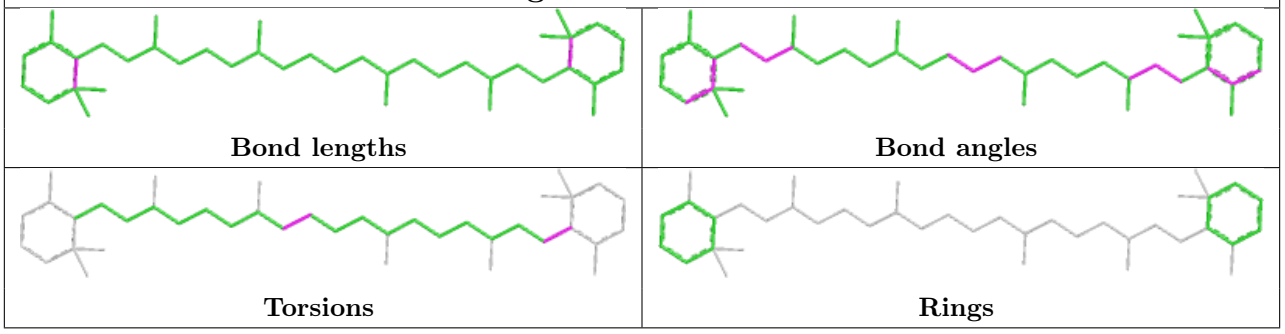


Torsions

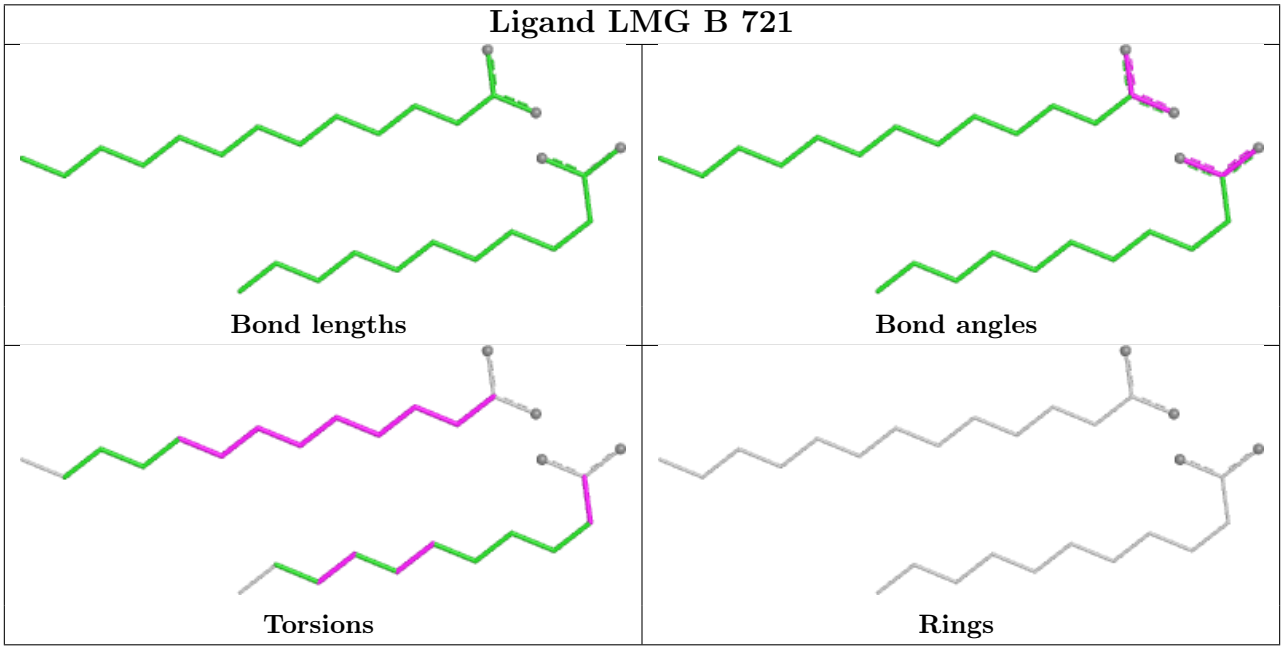


Rings

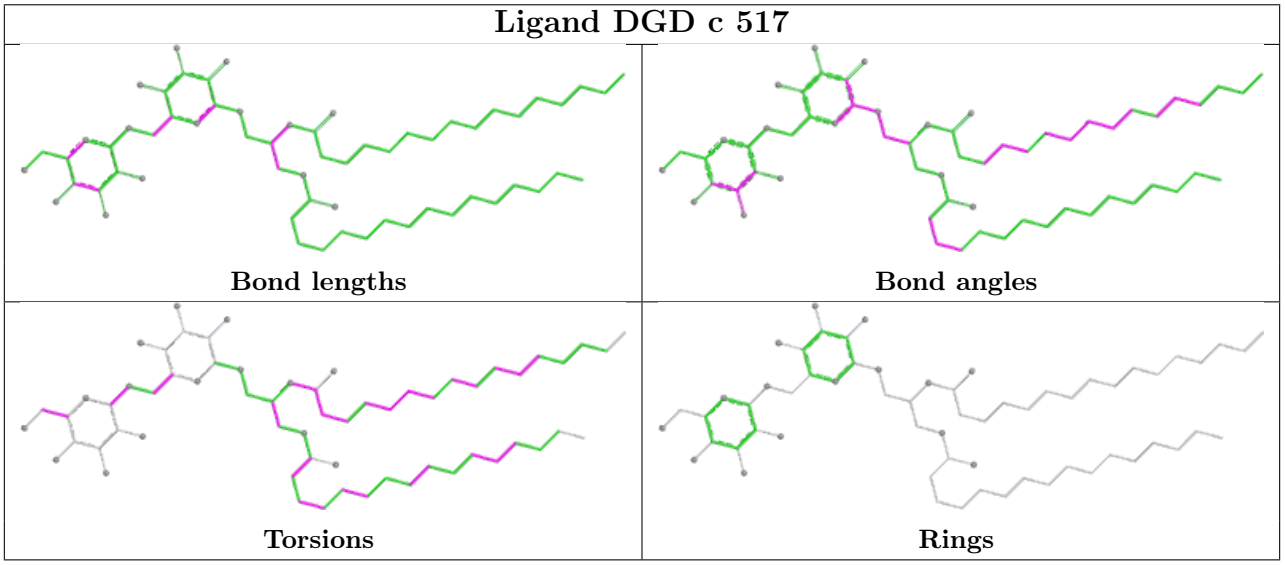
Ligand BCR k 102



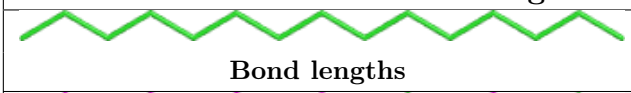
Ligand LMG B 721

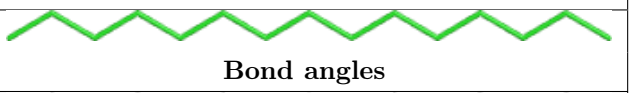


Ligand DGD c 517

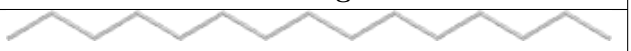


Ligand STE T 702

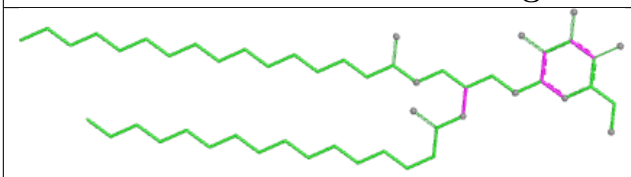

Bond lengths


Bond angles


Torsions


Rings

Ligand LMG b 721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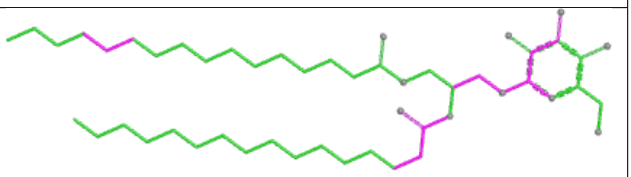
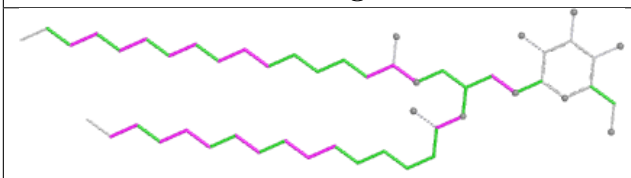
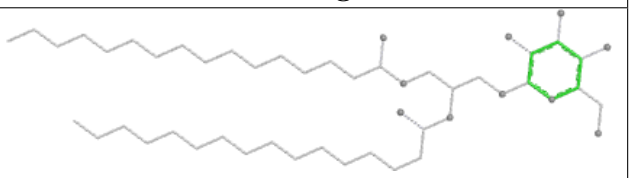
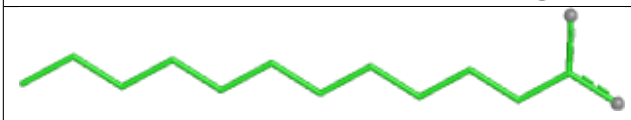
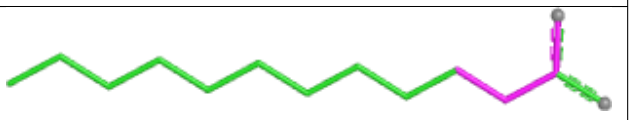

Bond angles

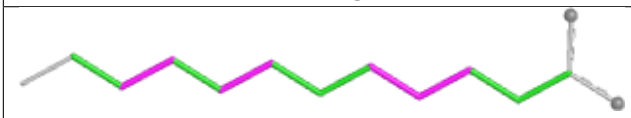

Torsions

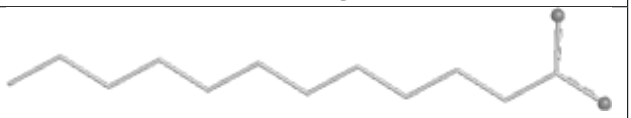

Rings

Ligand STE t 702

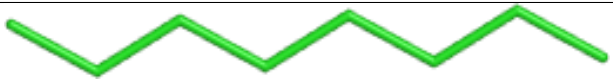

Bond lengths

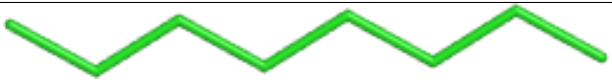

Bond angles

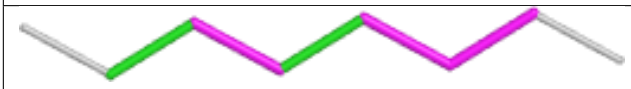

Torsions


Rings

Ligand STE Z 101

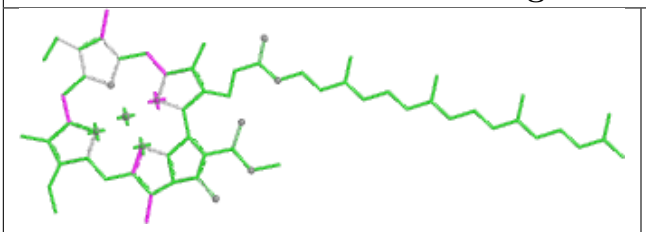

Bond lengths


Bond angles

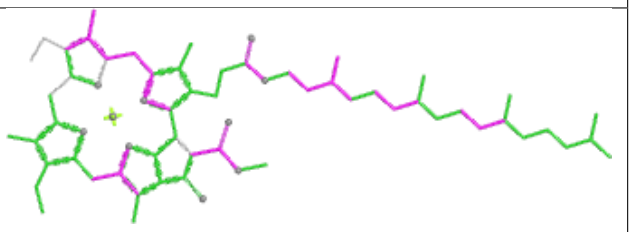

Torsions


Rings

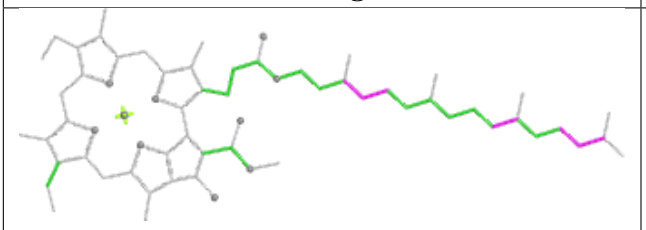
Ligand CLA b 704



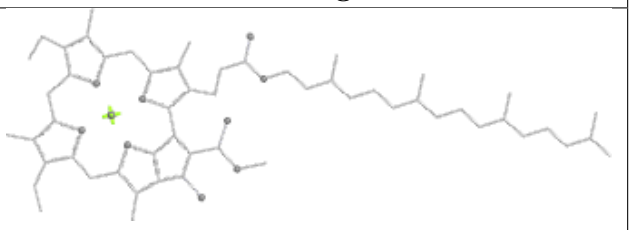
Bond lengths



Bond angles

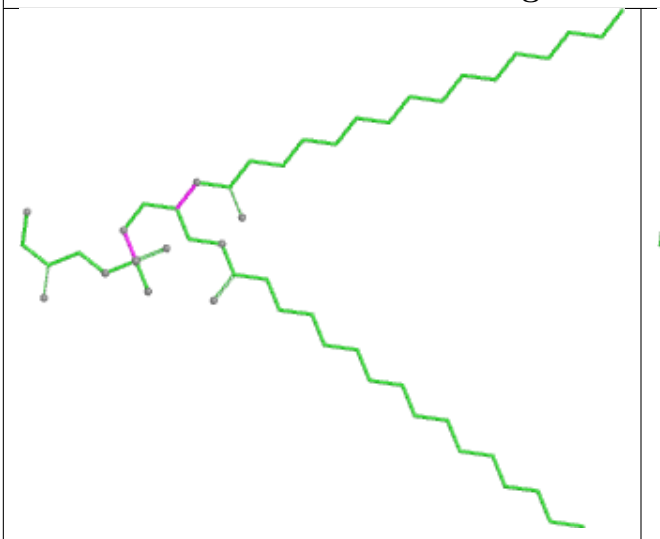


Torsions



Rings

Ligand LHG A 410



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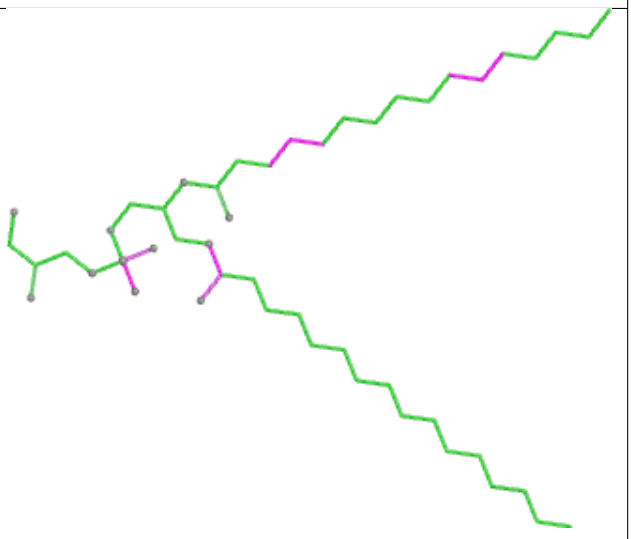
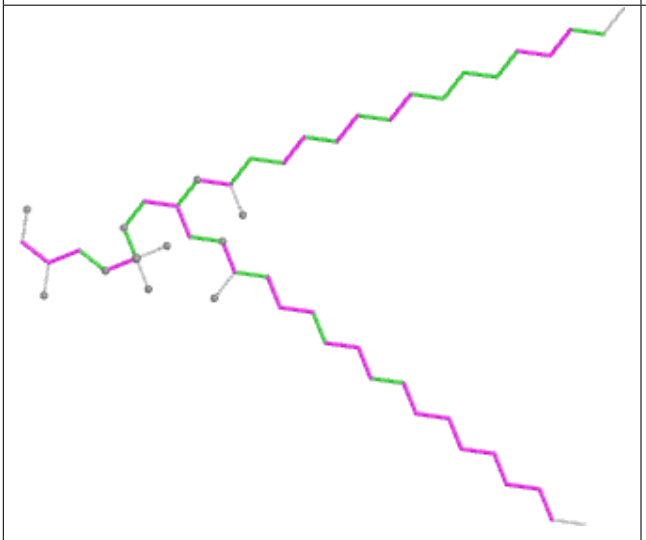


Bond angles



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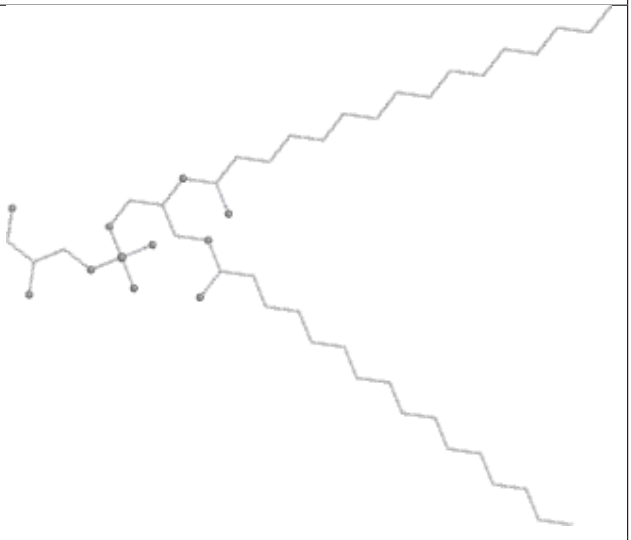
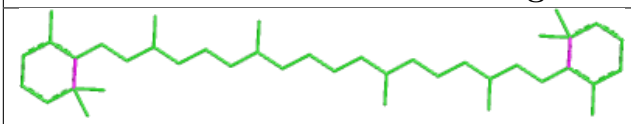


Rings

Ligand BCR c 515



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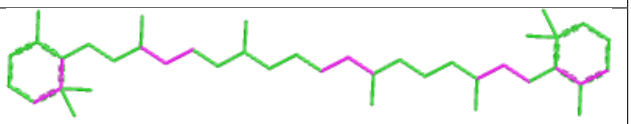
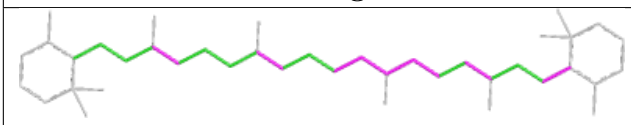


Bond angles



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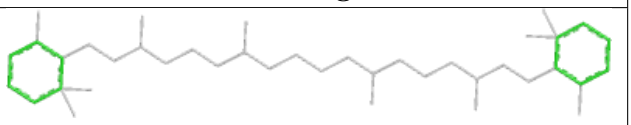
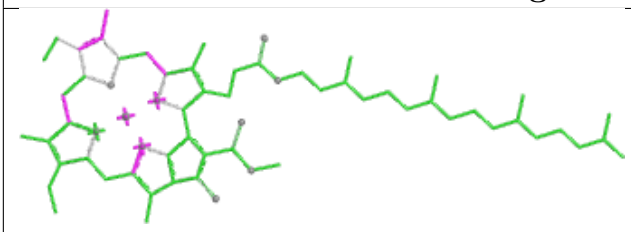


Rings

Ligand CLA c 510



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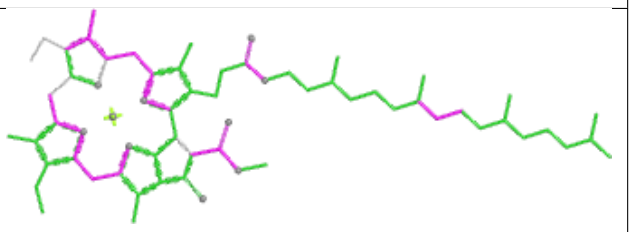
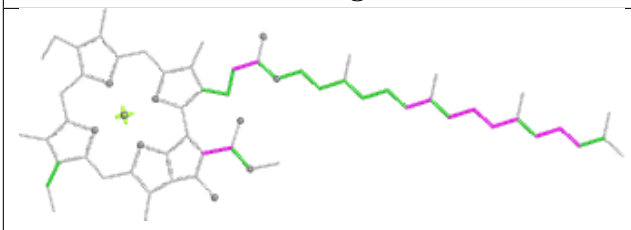


Bond angles



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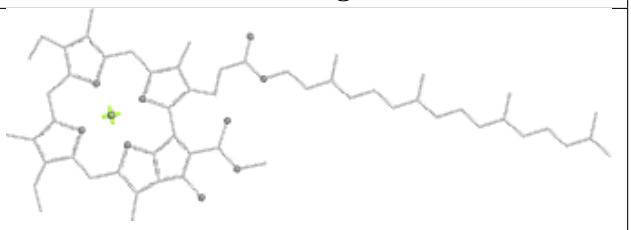
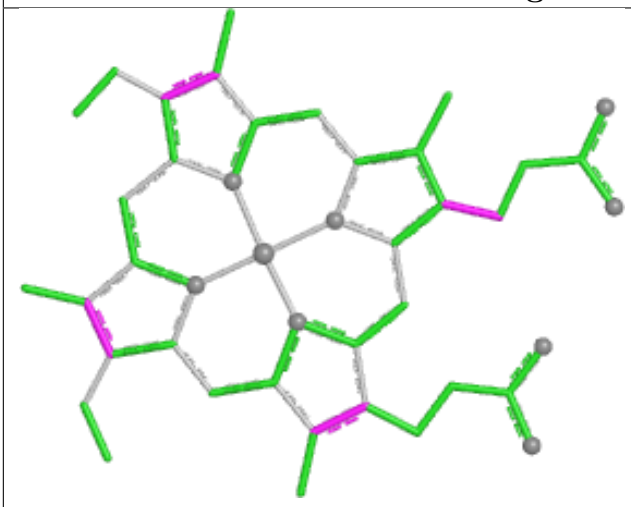


Rings

Ligand HEC v 201



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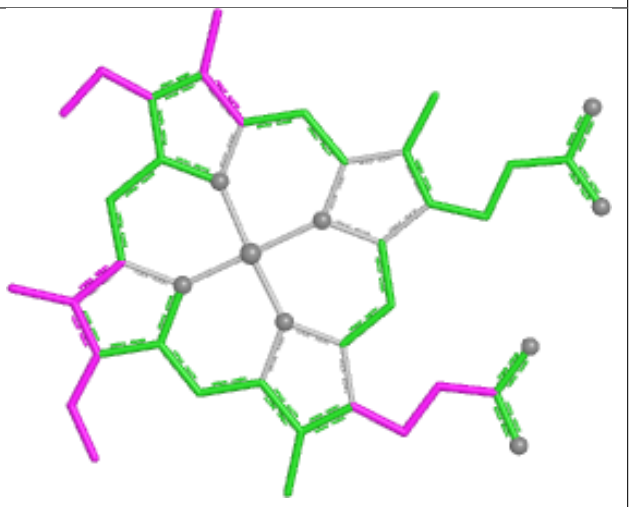
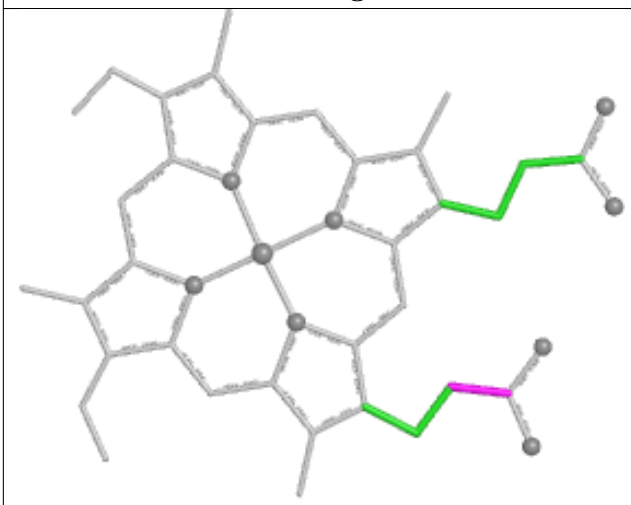


Bond angles



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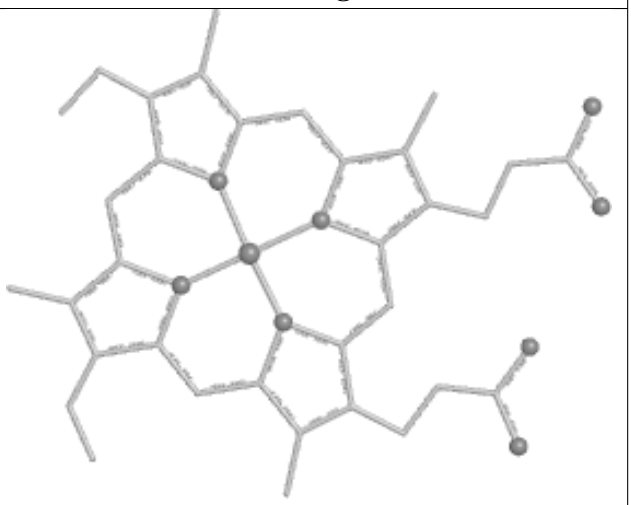
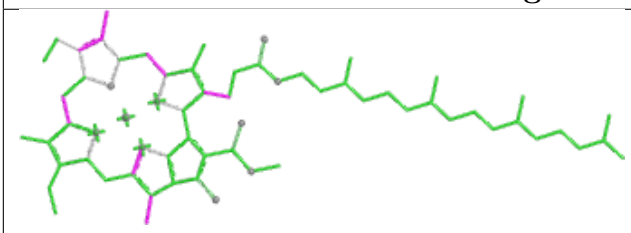


Rings

Ligand CLA A 403



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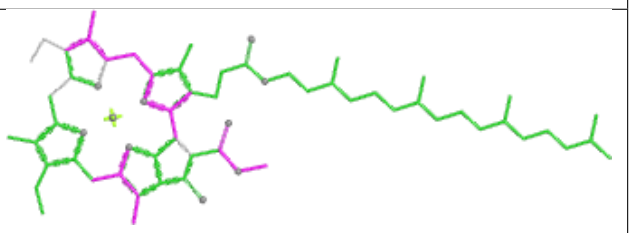
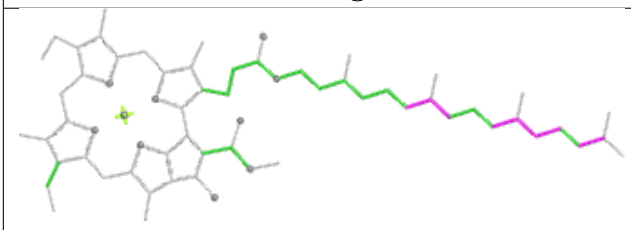


Bond angles



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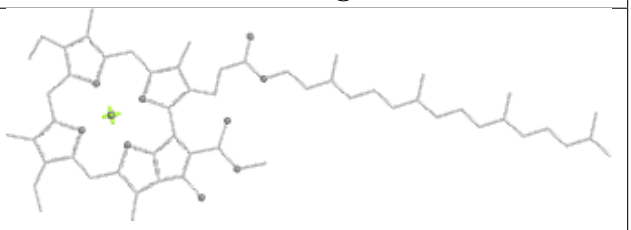
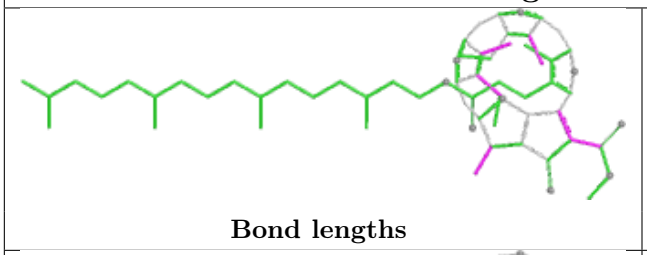


Rings

Ligand PHO D 406



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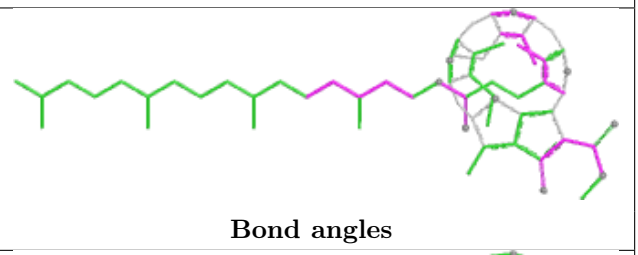

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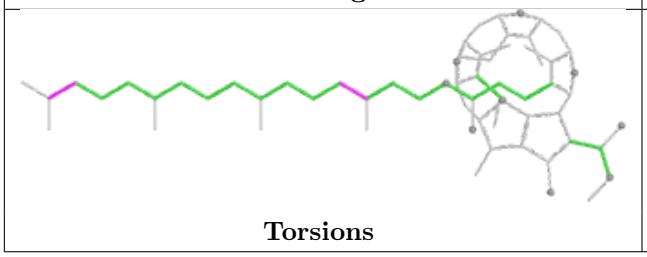
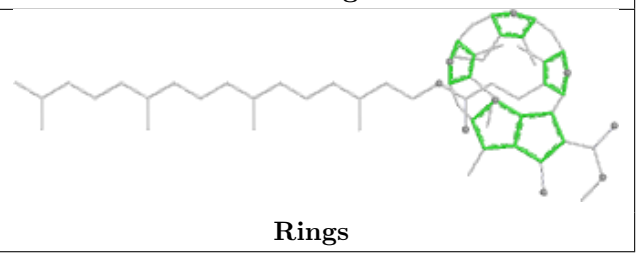
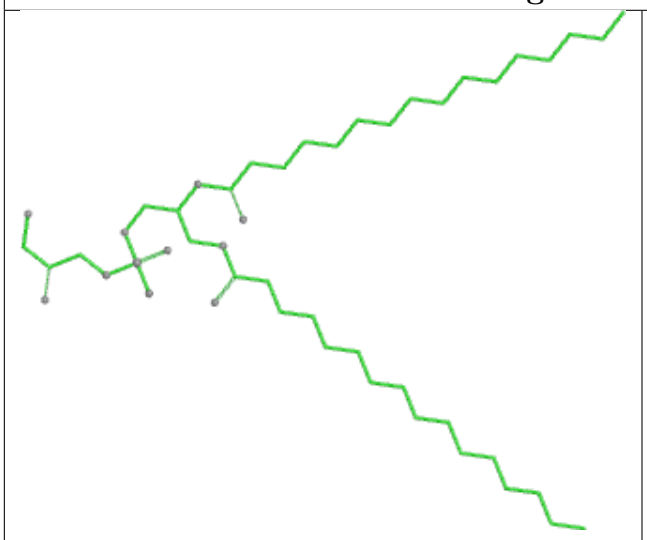


Torsions



Rings

Ligand LHG d 406



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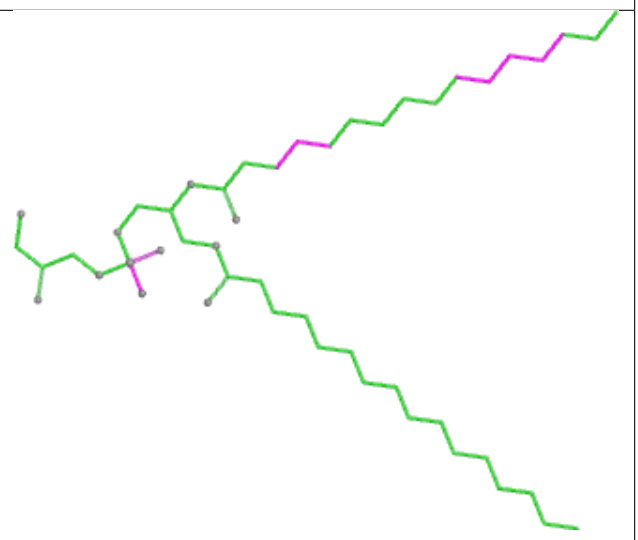
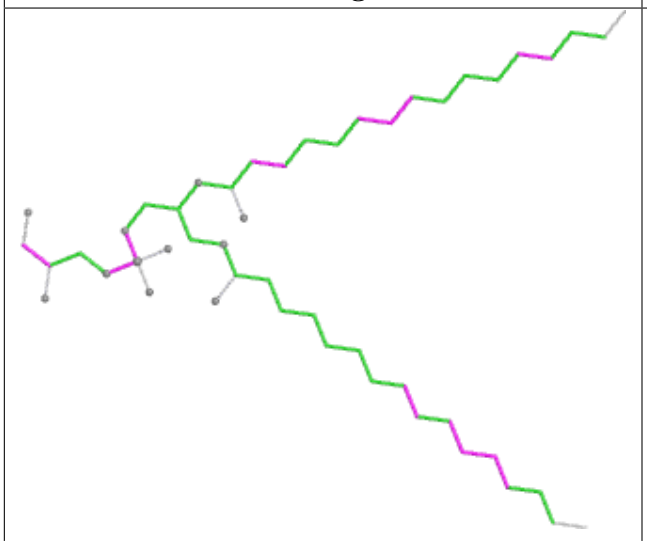


Bond angles



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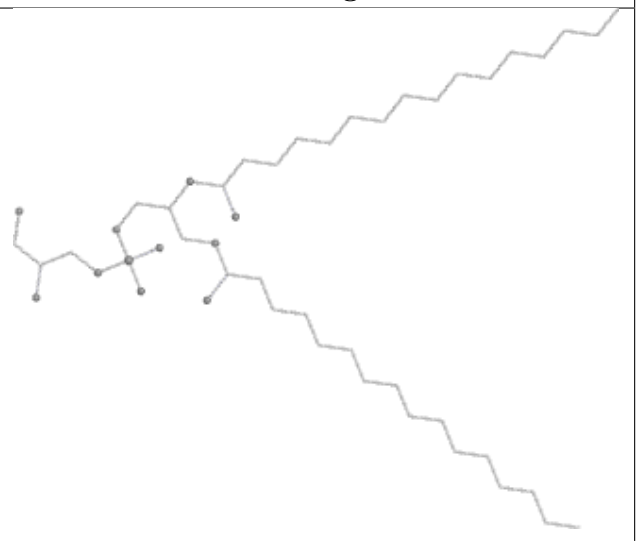
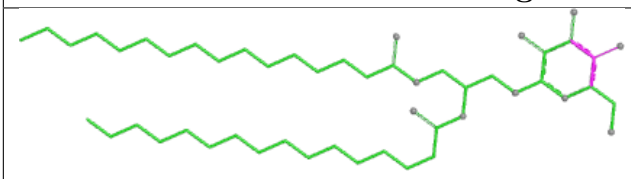


Rings

Ligand LMG M 101



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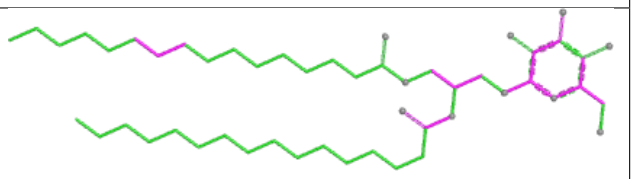
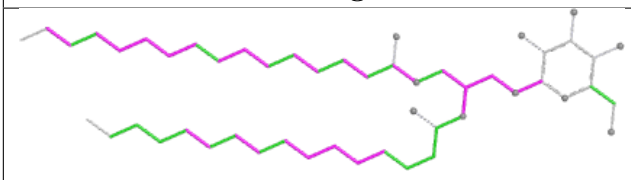


Bond angles



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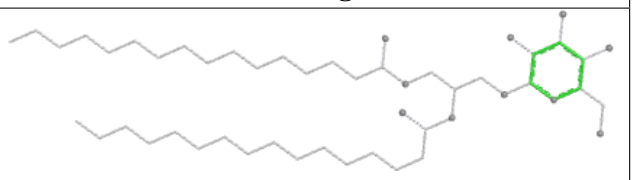
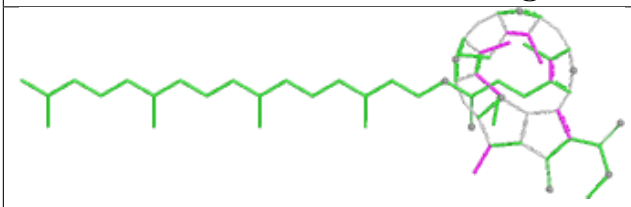


Rings

Ligand PHO D 407



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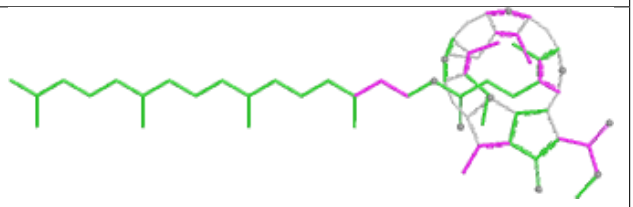
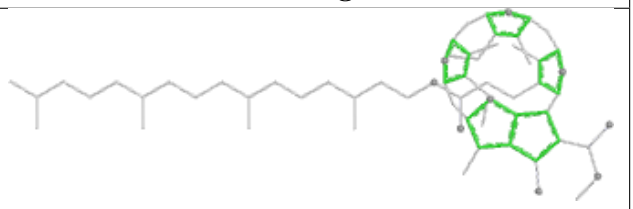


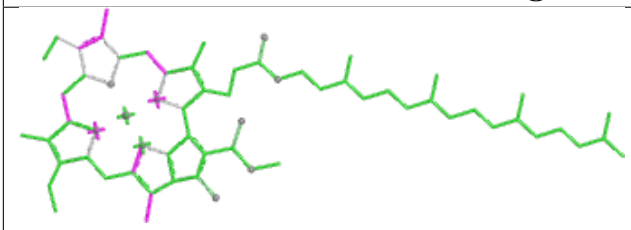
Bond angles

Torsions



Rings

Ligand CLA b 706



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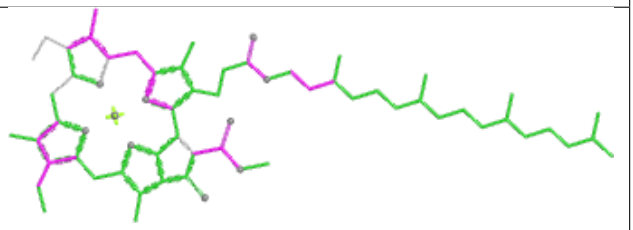
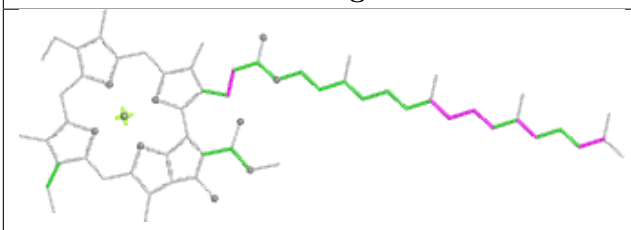


Bond angles



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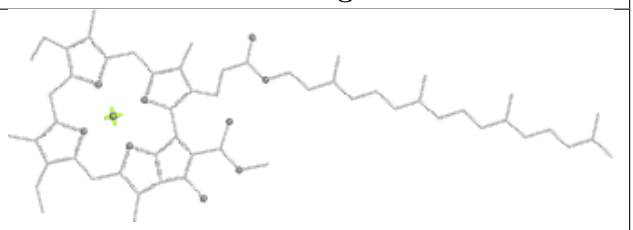
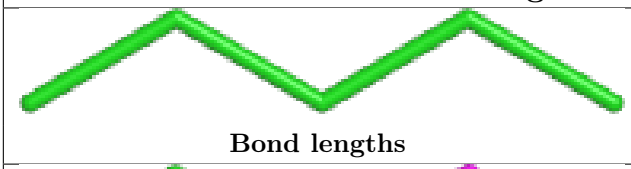


Rings

Ligand STE A 414



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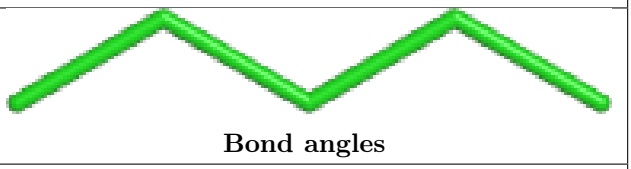
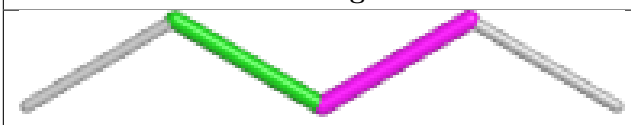


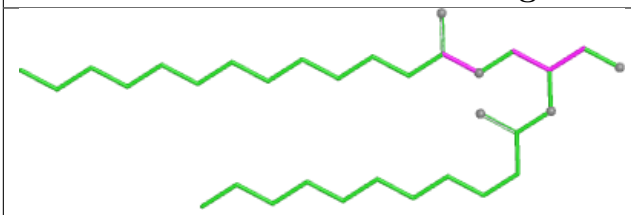
Bond angles



Torsions

Rings

Ligand LMG D 412



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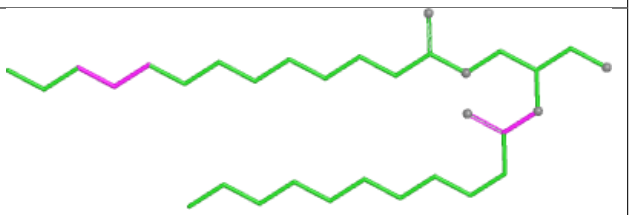
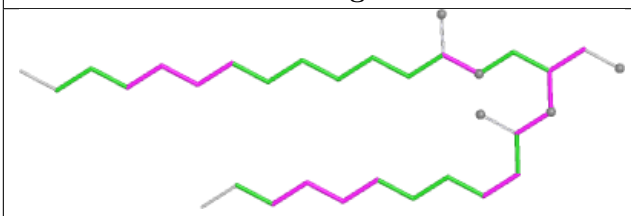
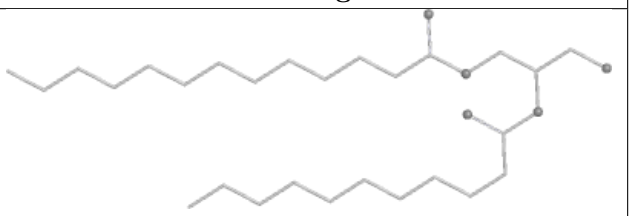


Bond angles

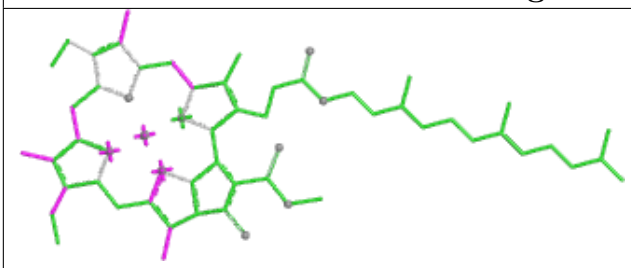


Torsions



Rings

Ligand CLA b 716



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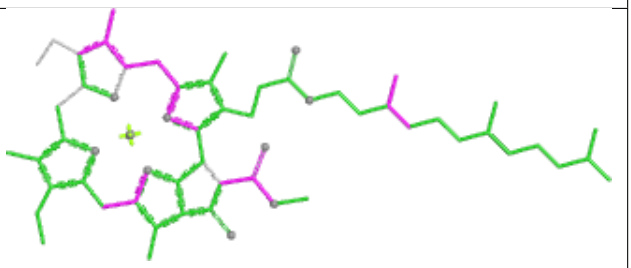
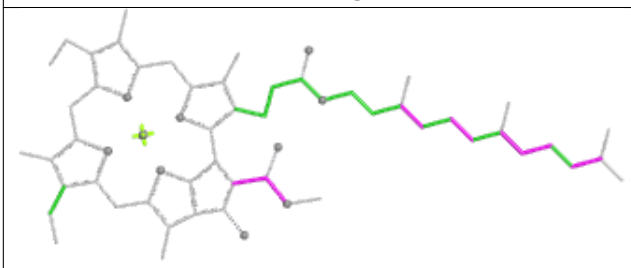
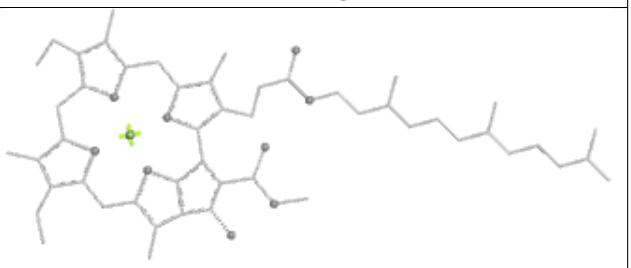


Bond angles

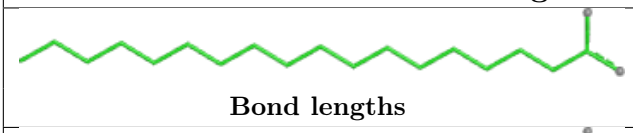


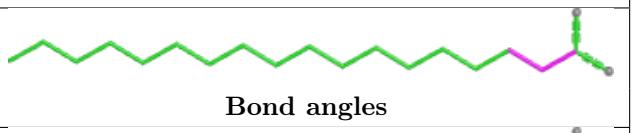
Torsions



Rings

Ligand STE x 101


Bond lengths


Bond angles

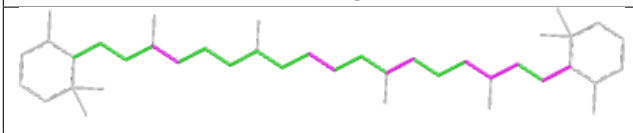

Torsions

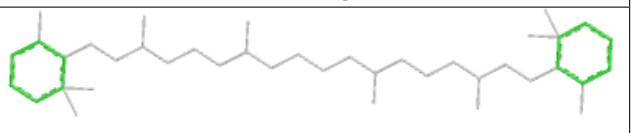

Rings

Ligand BCR D 404

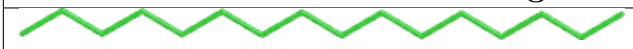

Bond lengths


Bond angles

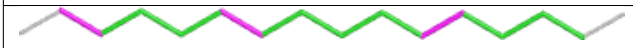

Torsions


Rings

Ligand STE C 522

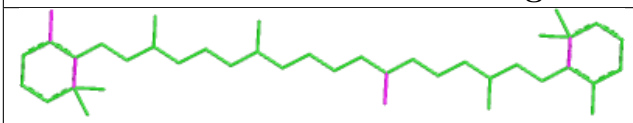

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR b 717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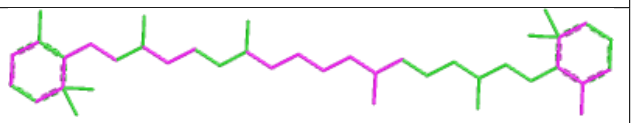
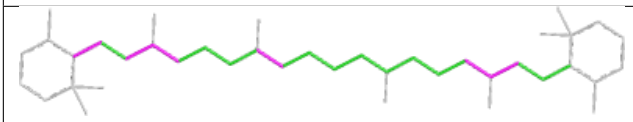

Bond angles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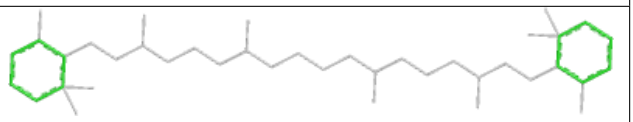
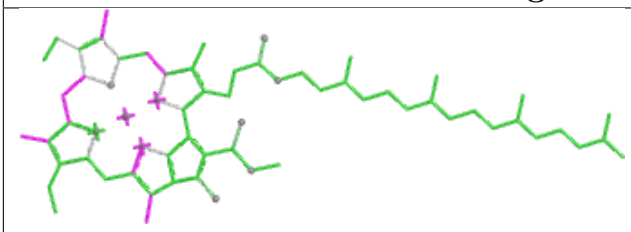
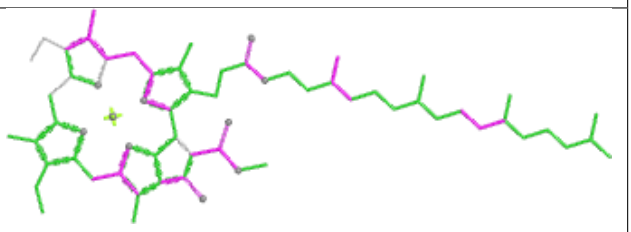

Rings

Ligand CLA b 703



Bond lengths



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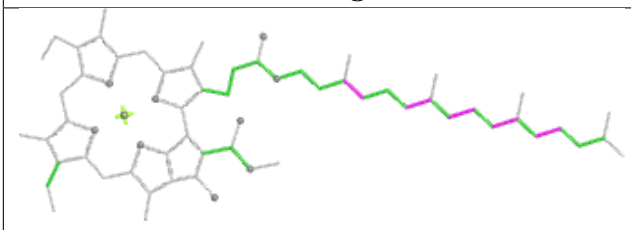

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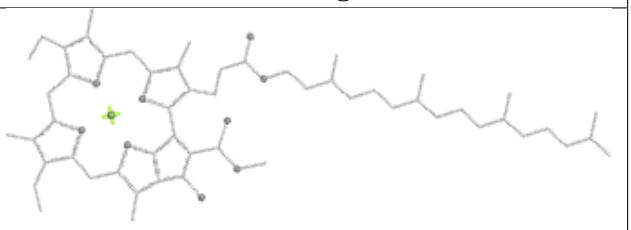
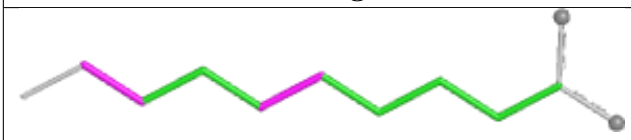


Rings

Ligand STE j 101

Bond lengths

Bond angles



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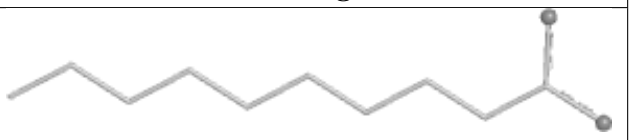
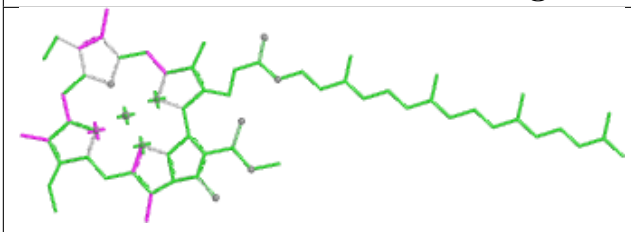


Rings

Ligand CLA c 513



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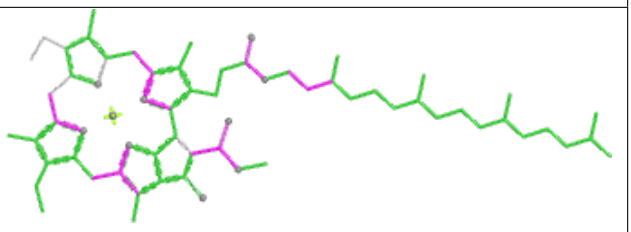

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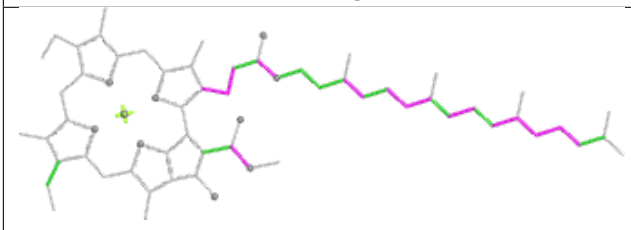

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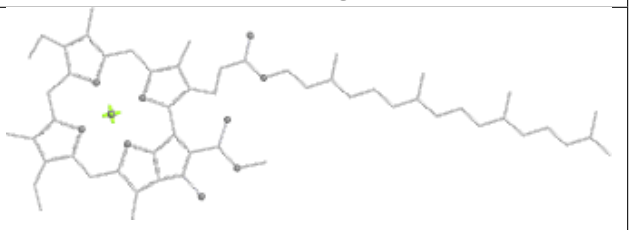
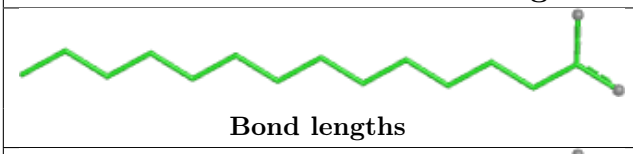


Rings

Ligand STE b 724



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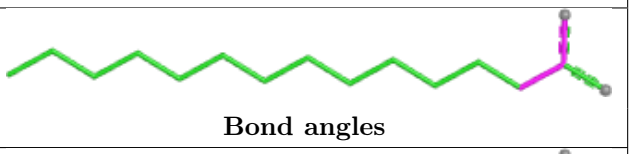

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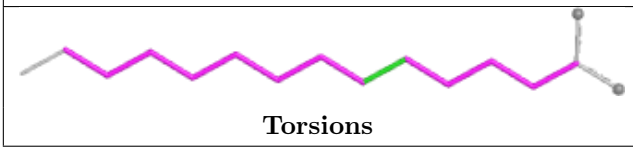

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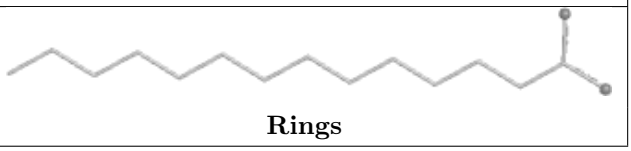
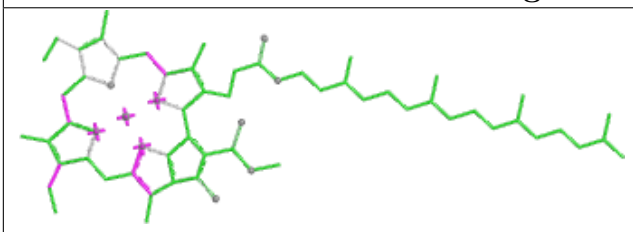


Rings

Ligand CLA D 402



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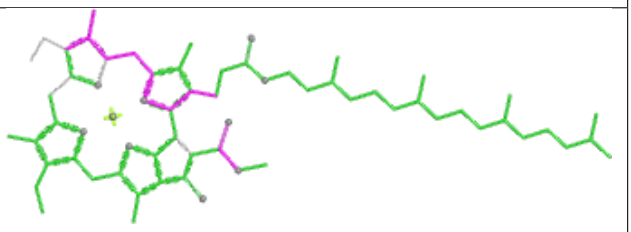

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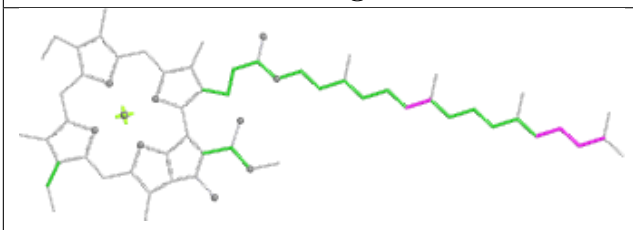

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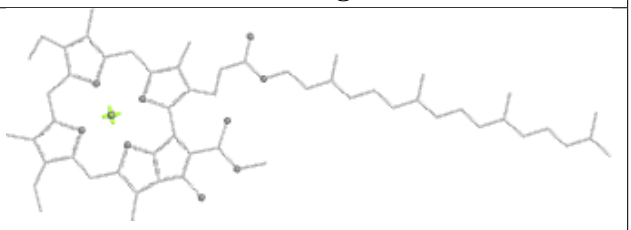
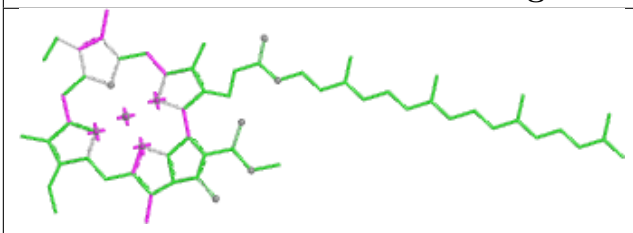


Rings

Ligand CLA b 707



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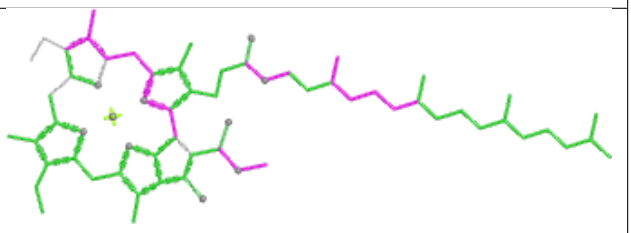
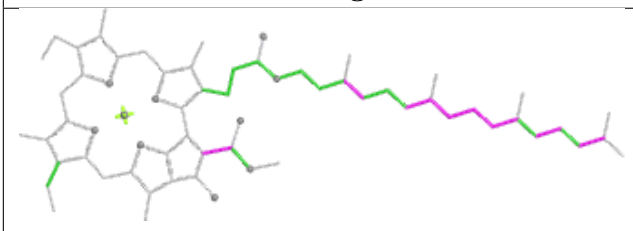


Bond angles



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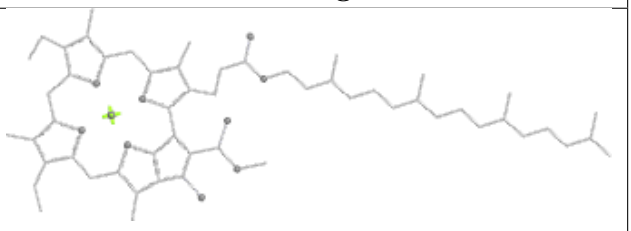
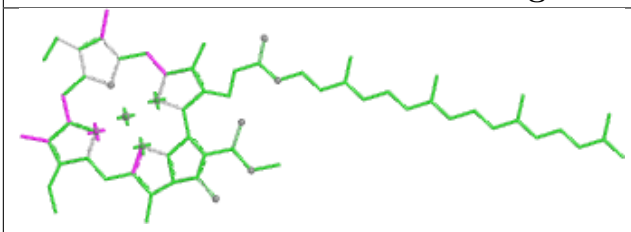


Rings

Ligand CLA a 404



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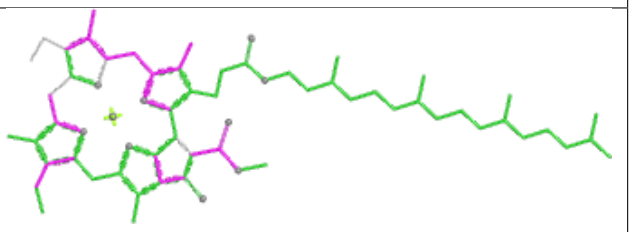

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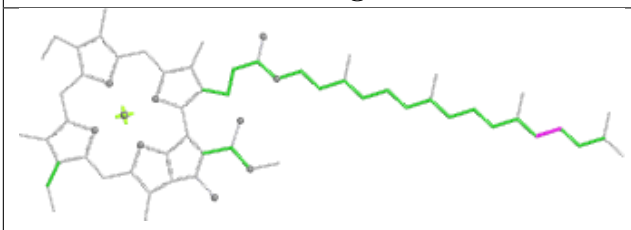

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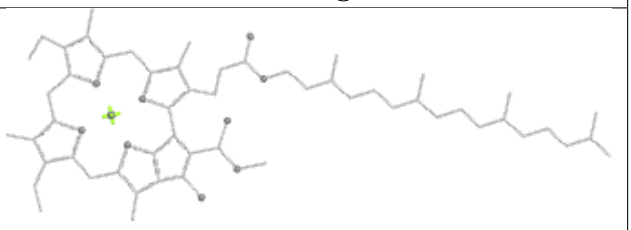
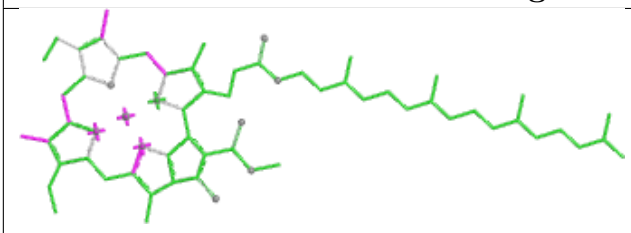


Rings

Ligand CLA a 403



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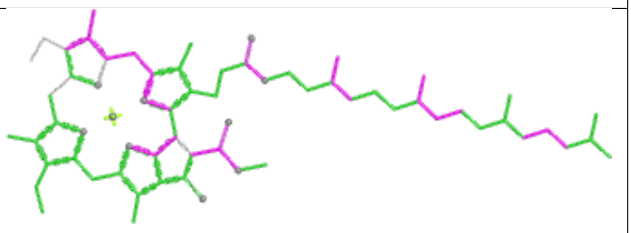
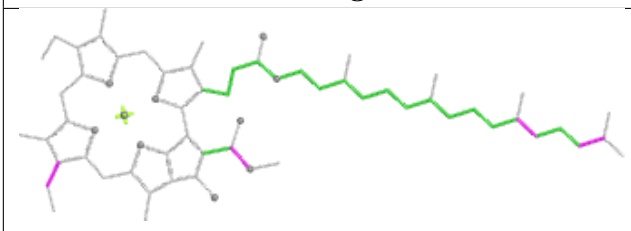


Bond angles



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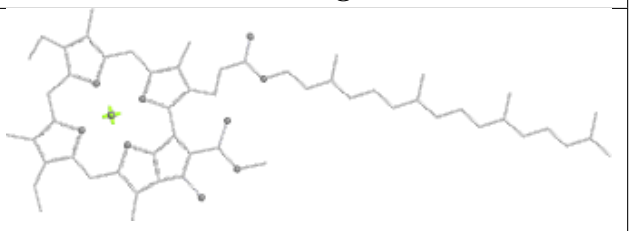
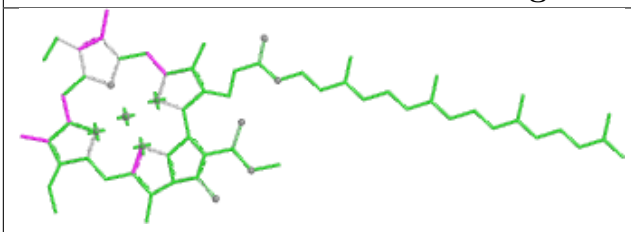


Rings

Ligand CLA c 514



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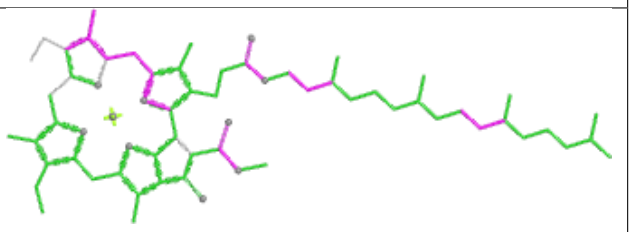

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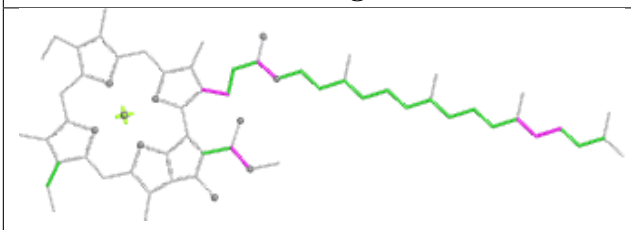

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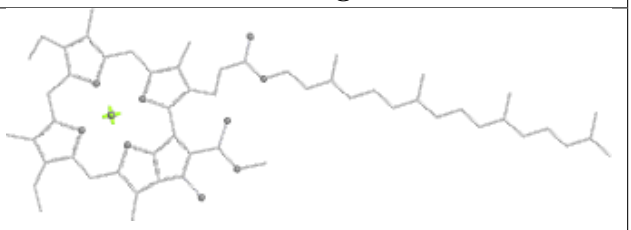
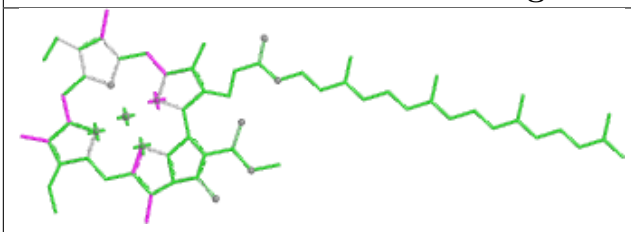


Rings

Ligand CLA d 401



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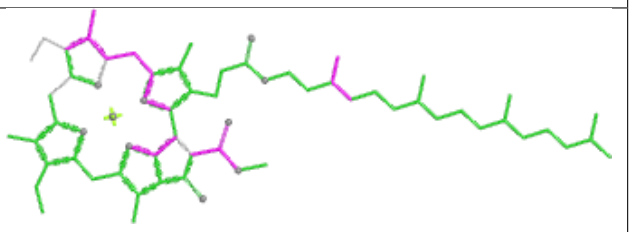
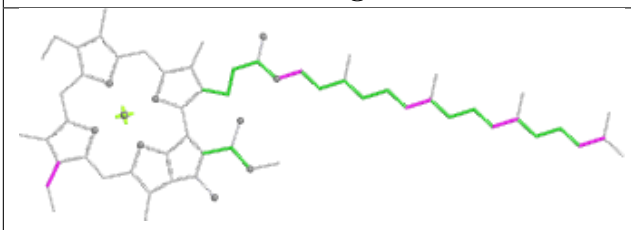


Bond angles



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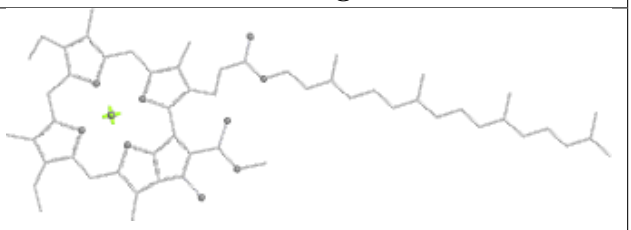
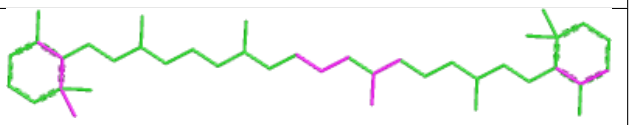


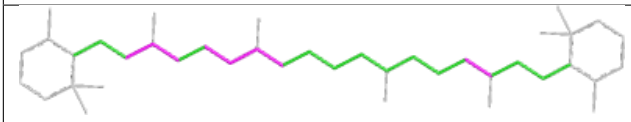
Rings

Ligand BCR t 701

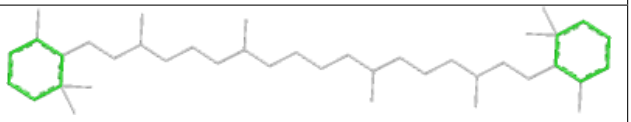
Bond lengths



Bond angles



Torsions



Rings

Ligand STE b 726

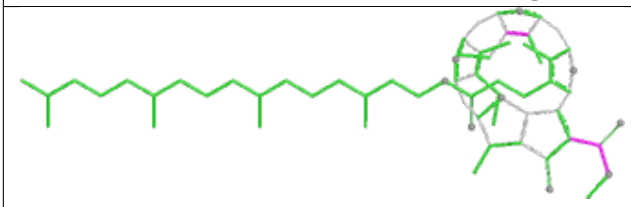
Bond lengths

Bond angles

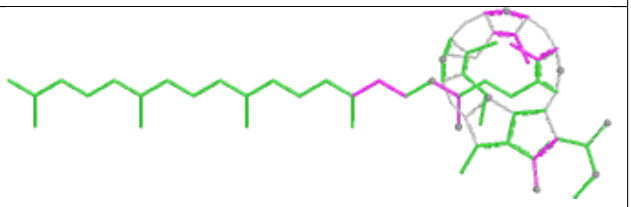
Torsions

Rings

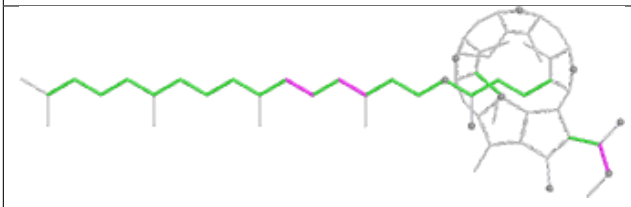
Ligand PHO a 405



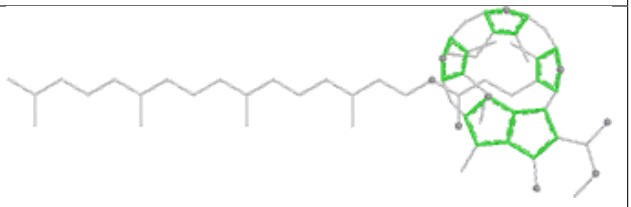
Bond lengths



Bond angles

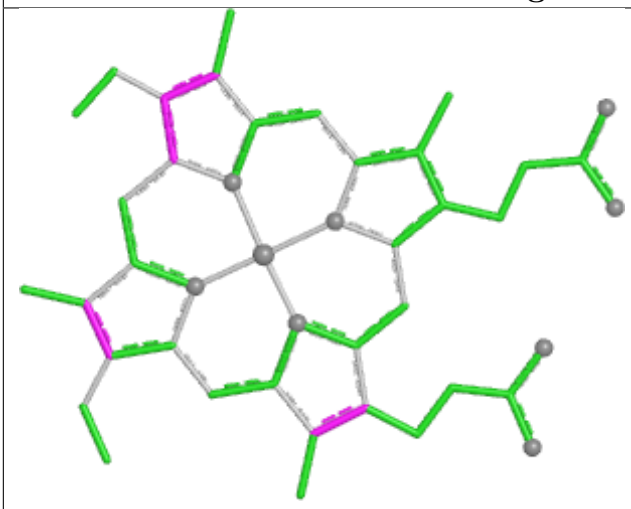


Torsions

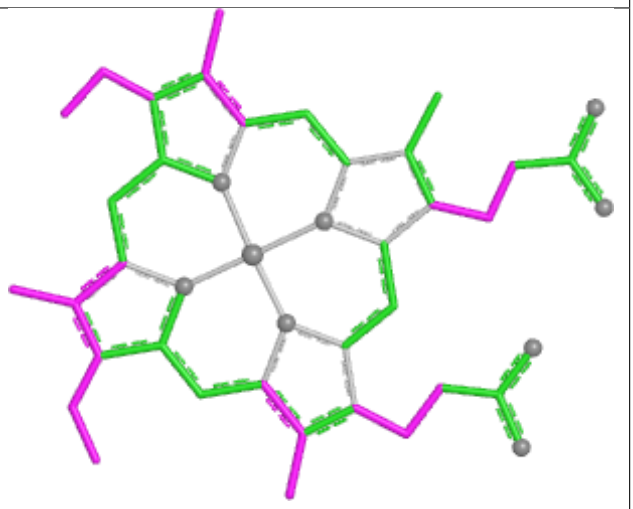


Rings

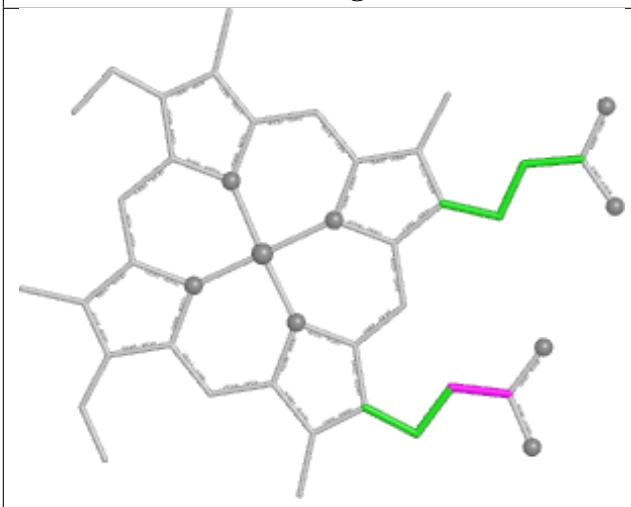
Ligand HEC e 101



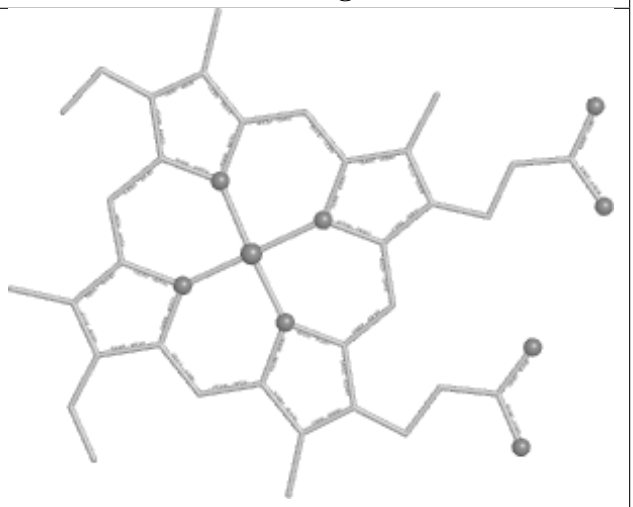
Bond lengths



Bond angles

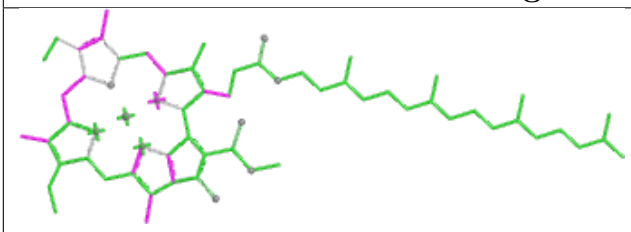


Torsions

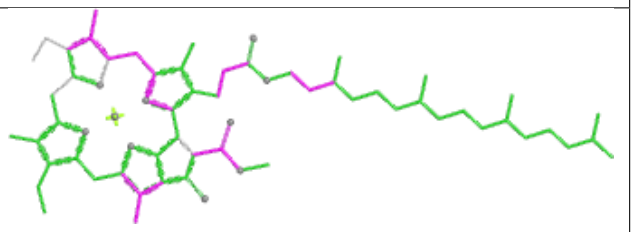


Rings

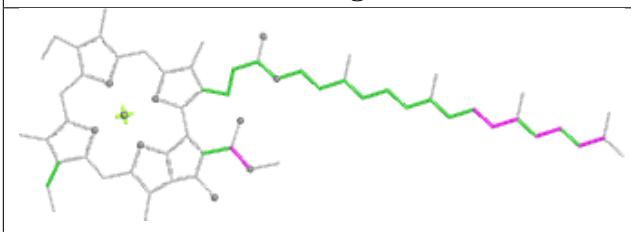
Ligand CLA D 403



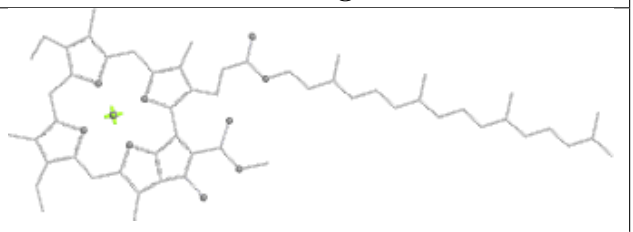
Bond lengths



Bond angles

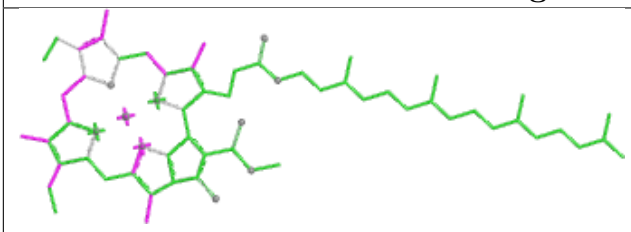


Torsions



Rings

Ligand CLA c 507



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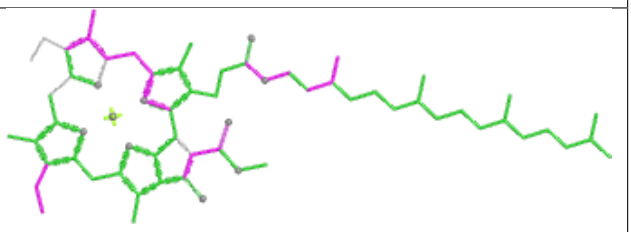
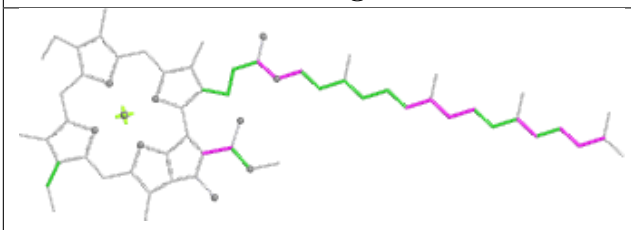
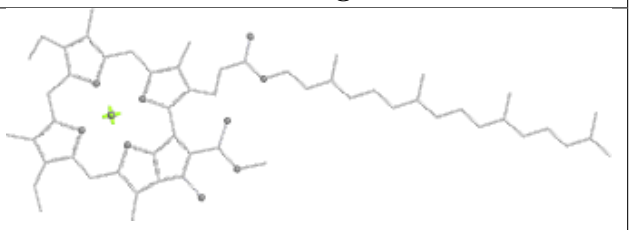


Bond angles

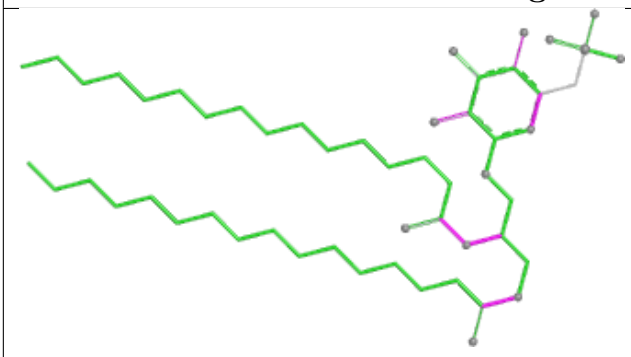


Torsions



Rings

Ligand SQD a 413



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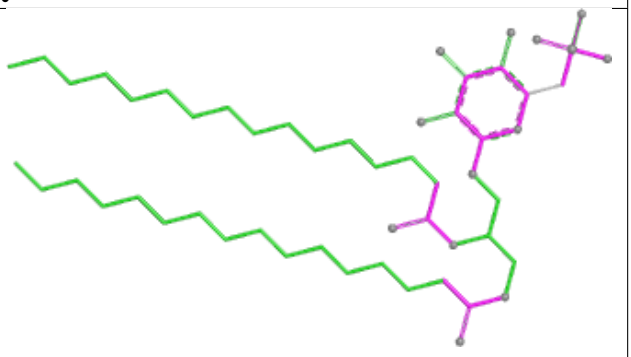
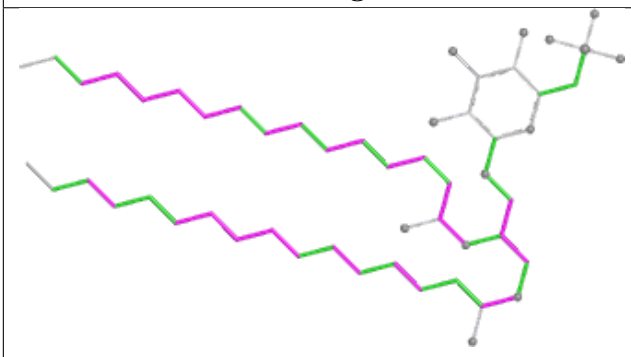
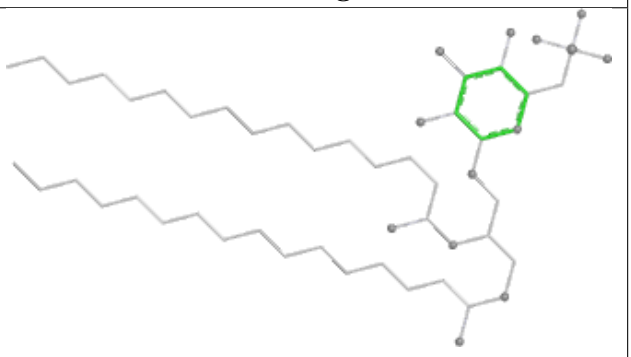


Bond angles

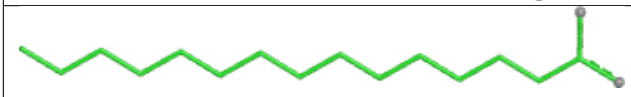


Torsions



Rings

Ligand STE d 409



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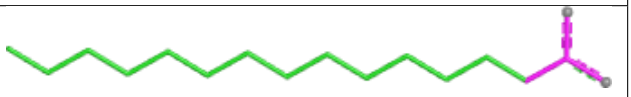
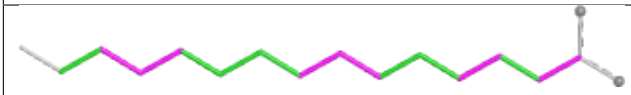


Bond angles



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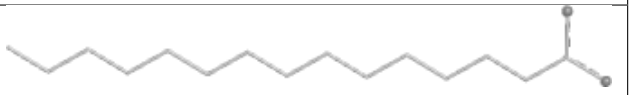
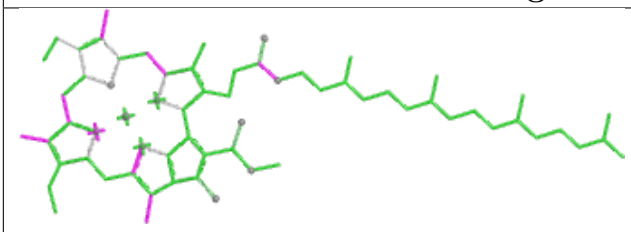


Rings

Ligand CLA b 701



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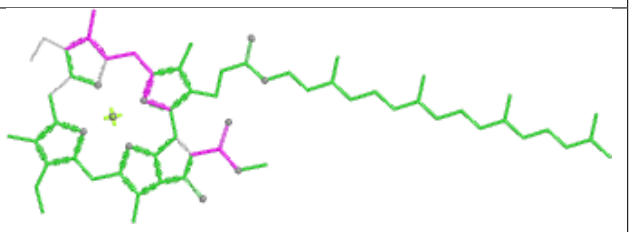
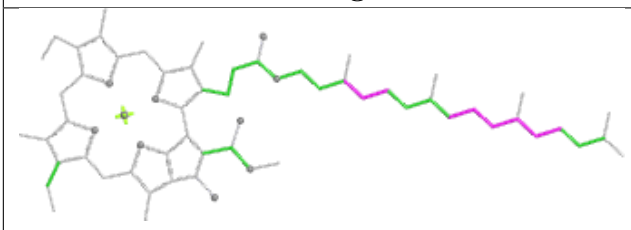


Bond angles



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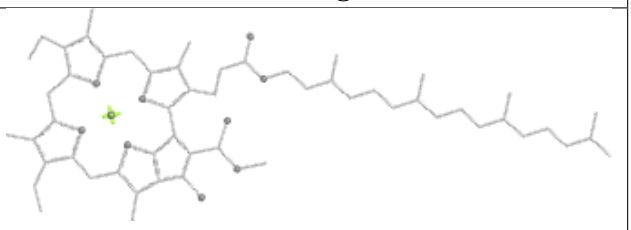
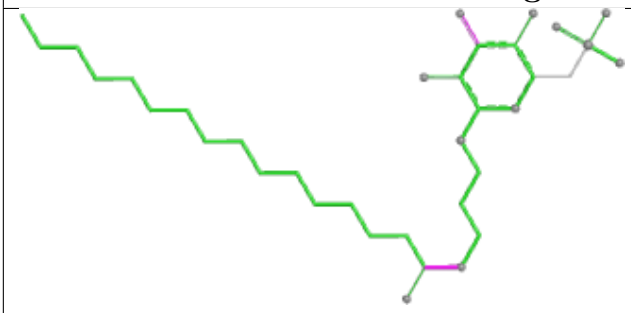


Rings

Ligand SQD D 409



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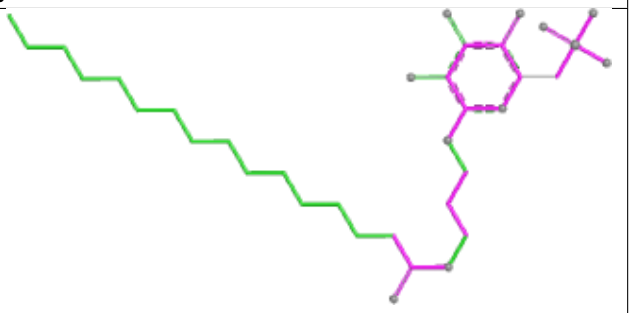
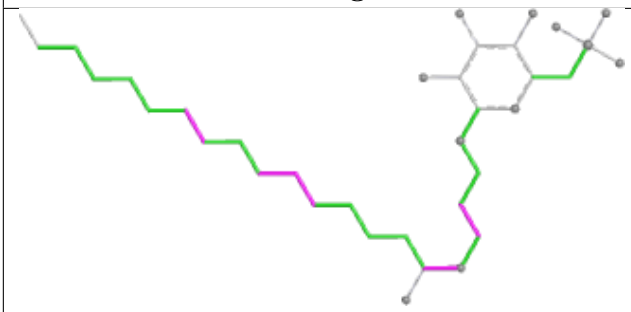


Bond angles



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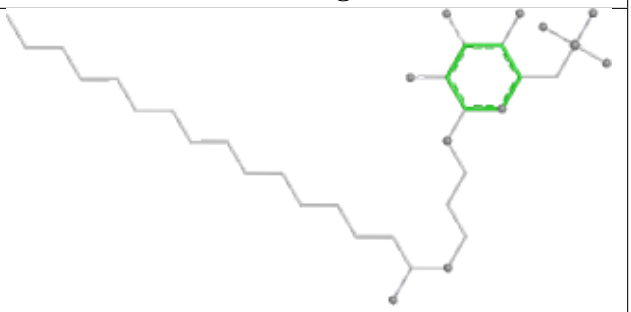
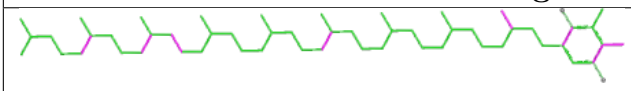


Rings

Ligand PL9 d 404



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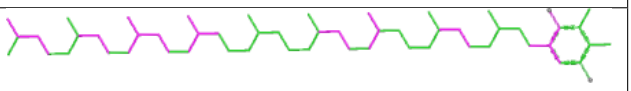
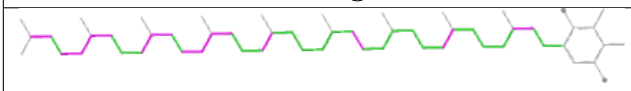


Bond angles



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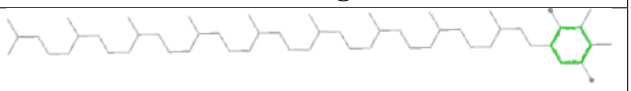
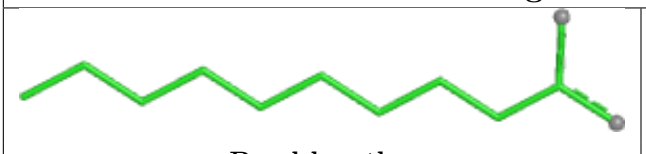


Rings

Ligand STE m 101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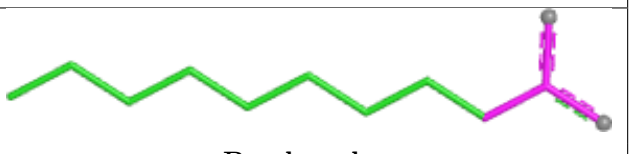
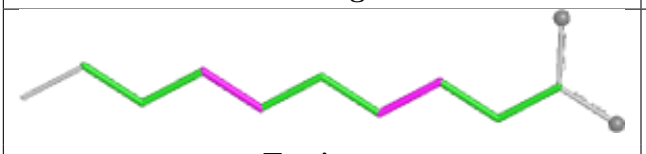

Bond angles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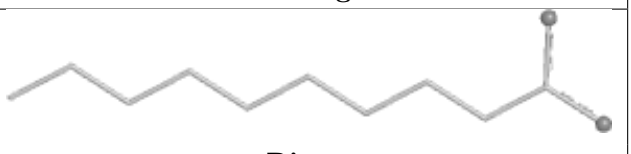
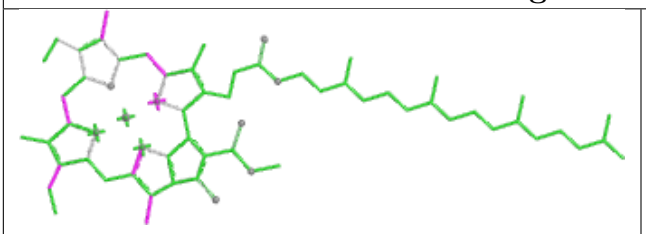

Rings

Ligand CLA c 511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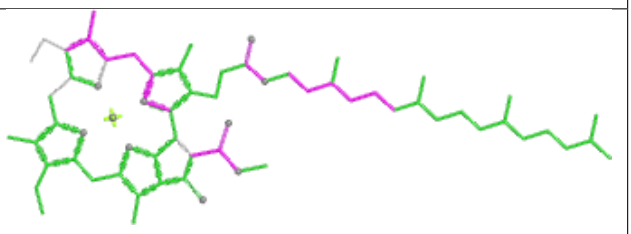
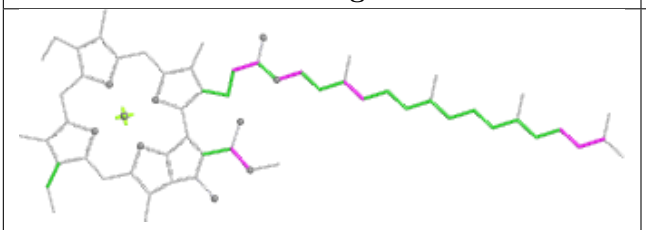

Bond angles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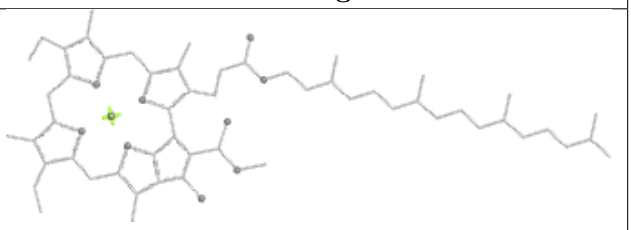
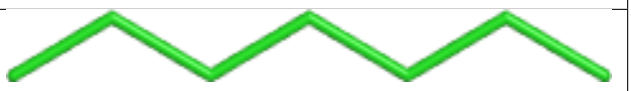
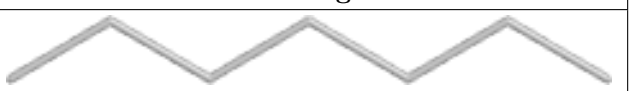

Rings

Ligand STE E 102

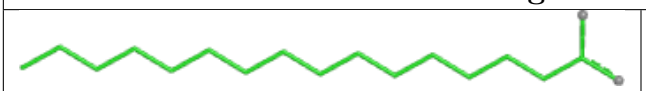

Bond lengths


Bond angles


Torsions


Rings

Ligand STE B 725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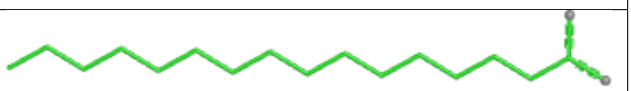
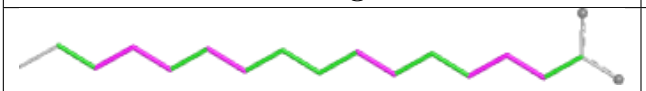

Bond angles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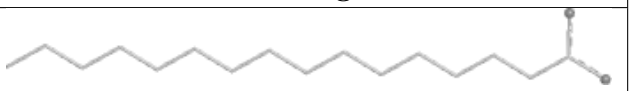
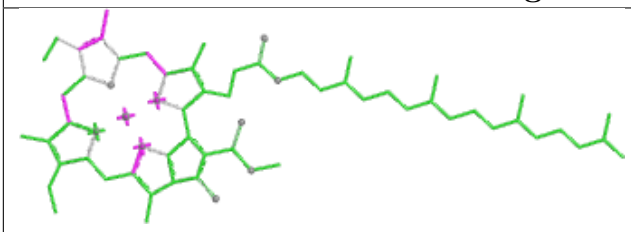
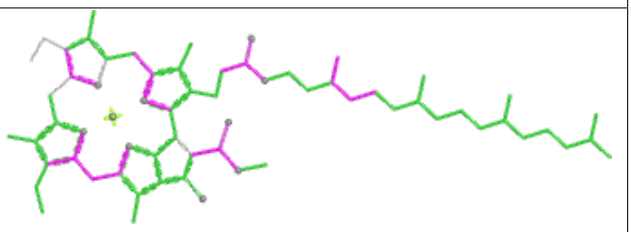

Rings

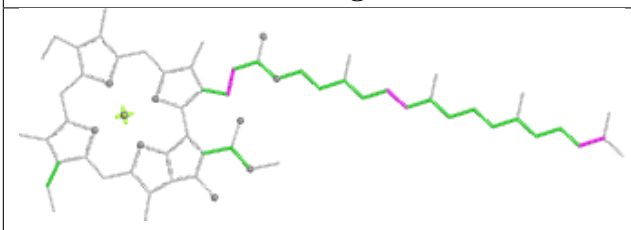
Ligand CLA B 706



Bond lengths



Bond angles



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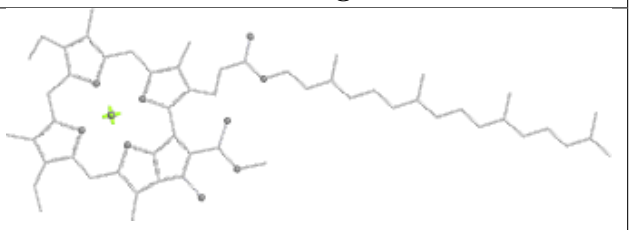
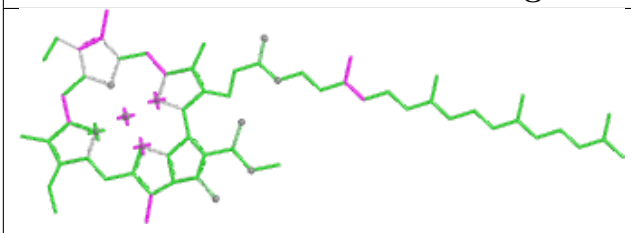
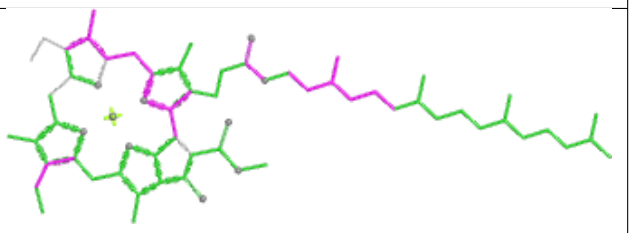


Rings

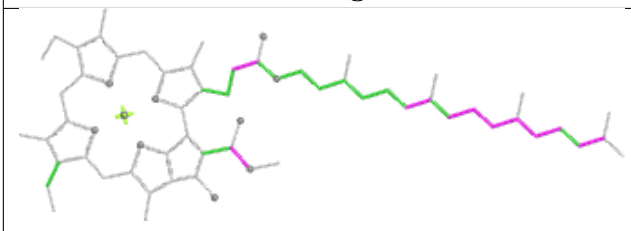
Ligand CLA B 713



Bond lengths



Bond angles



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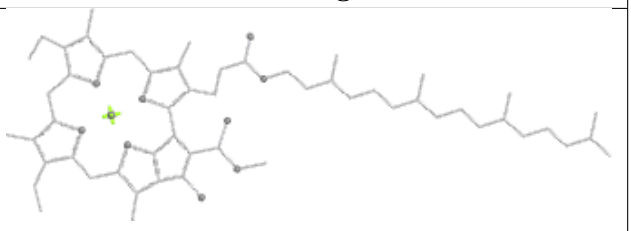
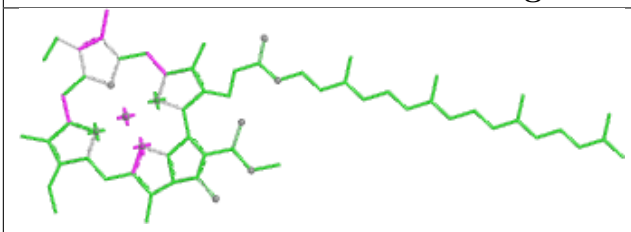
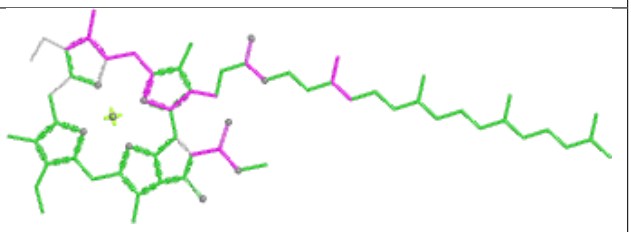


Rings

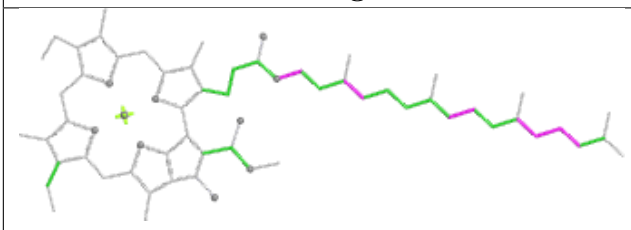
Ligand CLA C 507



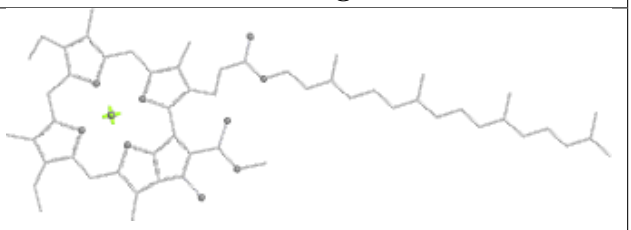
Bond lengths



Bond angles

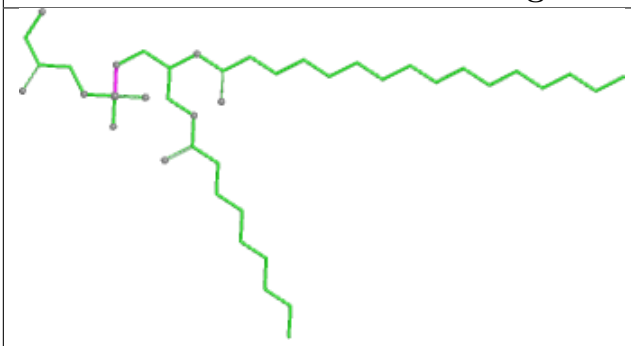


Torsions

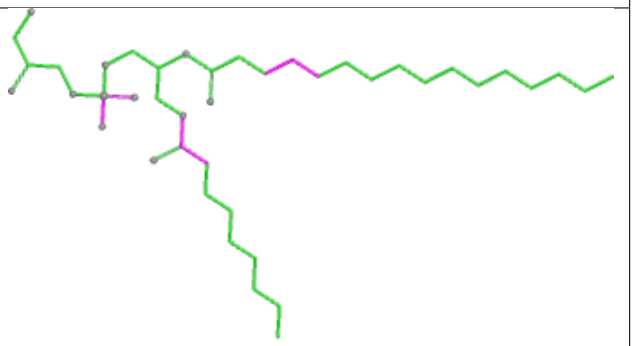


Rings

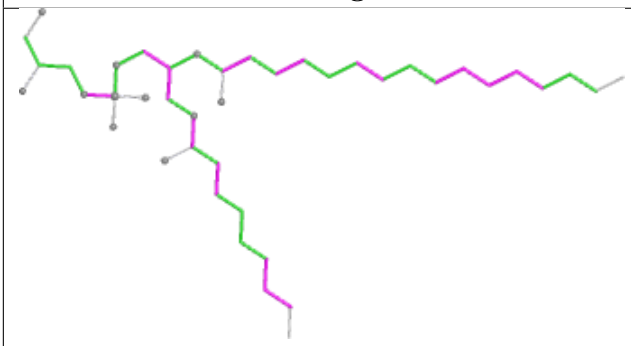
Ligand LHG a 414



Bond lengths



Bond angles



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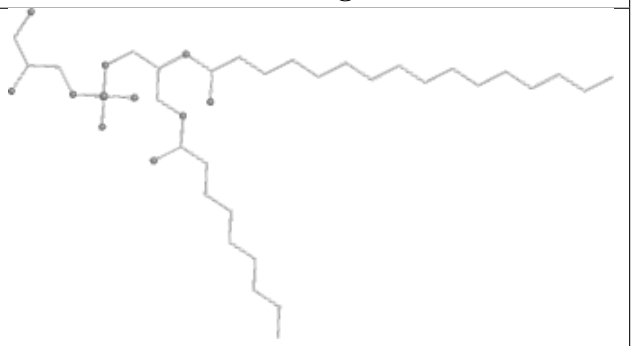
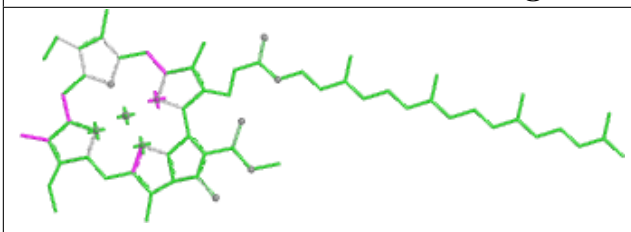
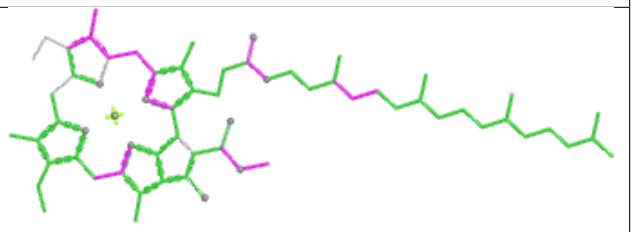


Rings

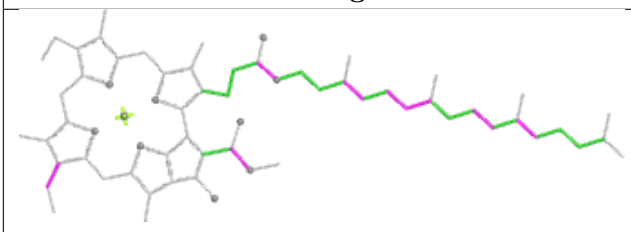
Ligand CLA C 506



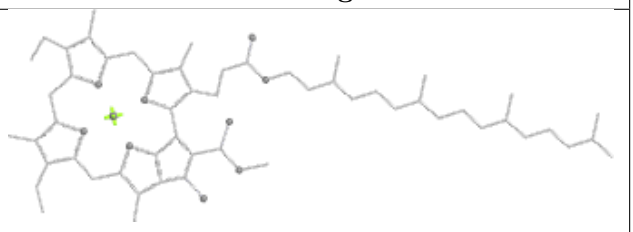
Bond lengths



Bond angles

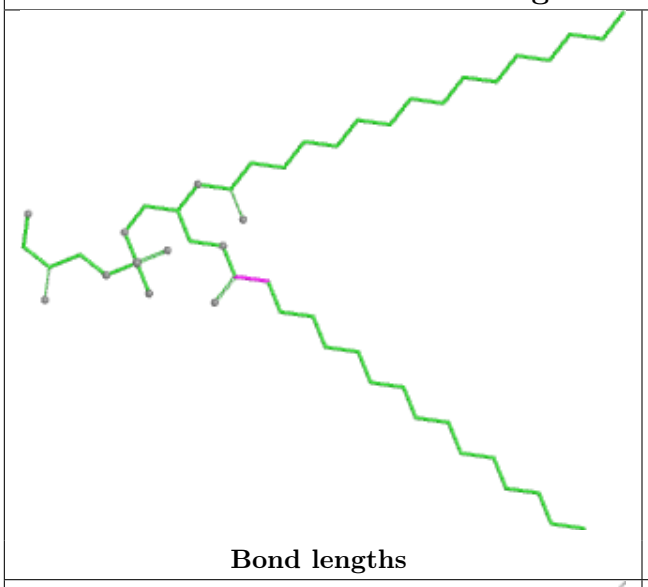


Torsions



Rings

Ligand LHG l 101



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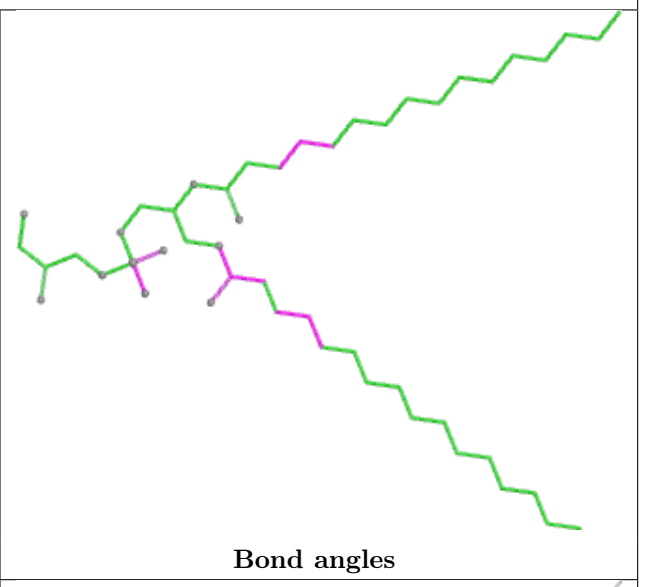
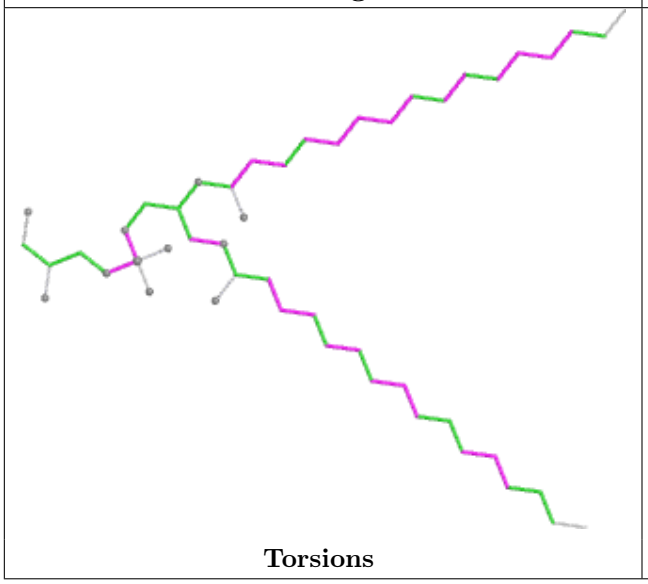


Bond angles



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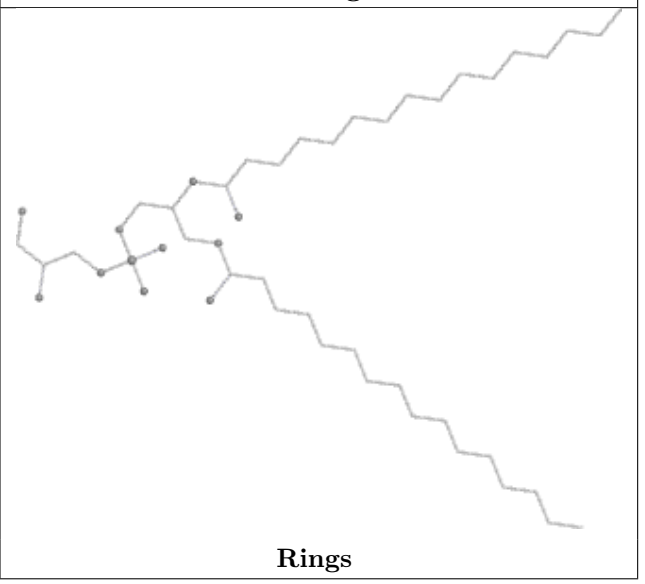
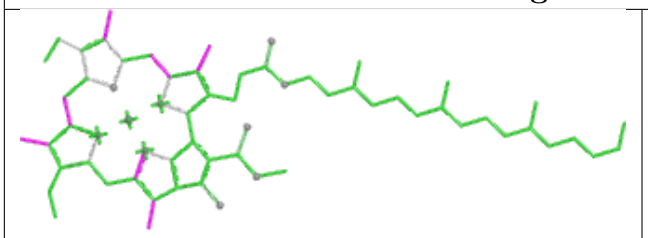
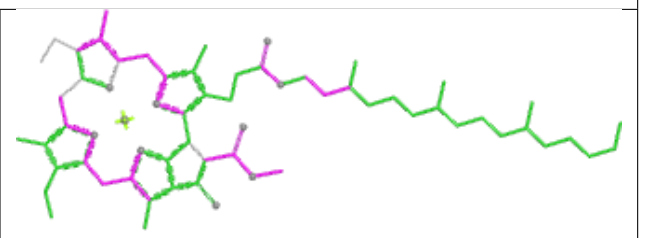


Rings

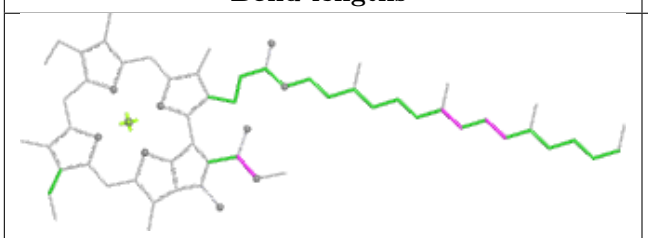
Ligand CLA c 509



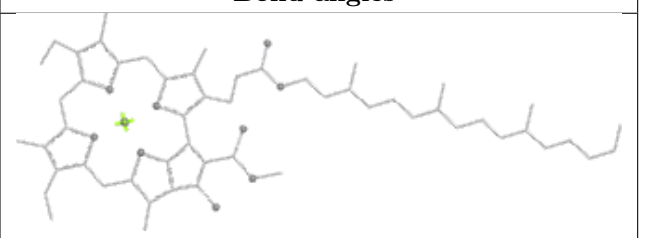
Bond lengths



Bond angles

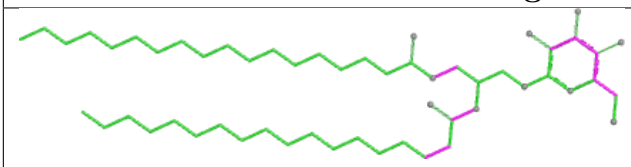


Torsions



Rings

Ligand LMG a 419



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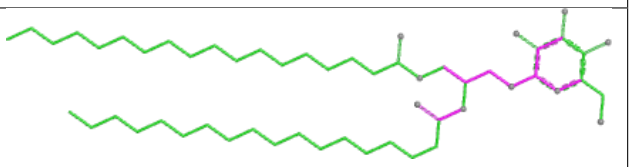
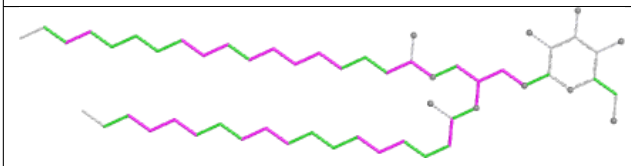
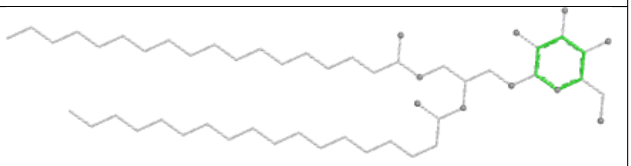


Bond angles

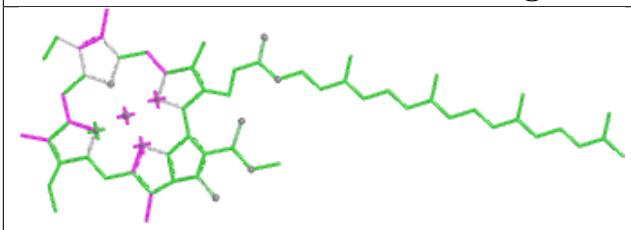


Torsions

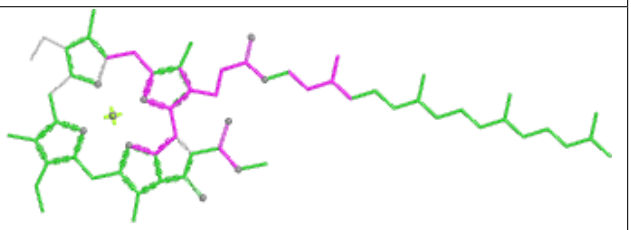


Rings

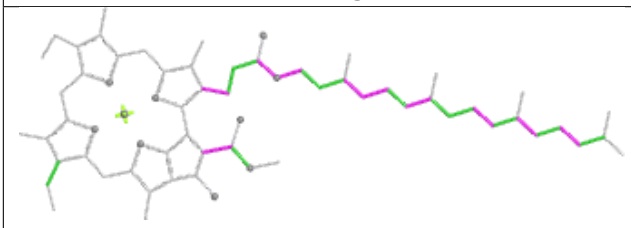
Ligand CLA H 102



Bond lengths



Bond angles



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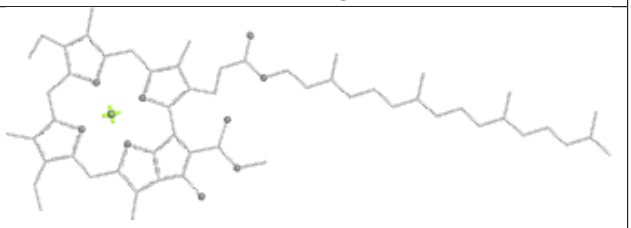
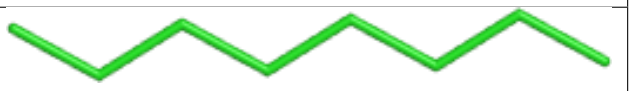


Rings

Ligand STE H 105

Bond lengths

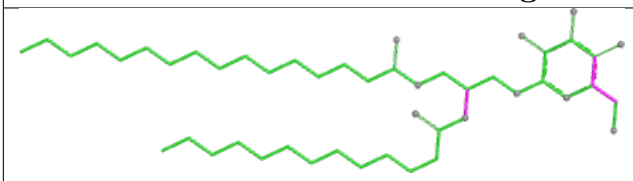


Bond angles

Torsions

Rings

Ligand LMG C 520



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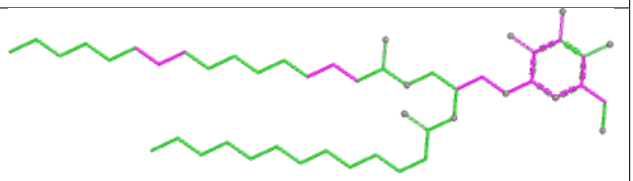
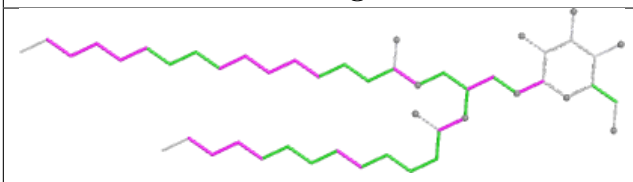


Bond angles



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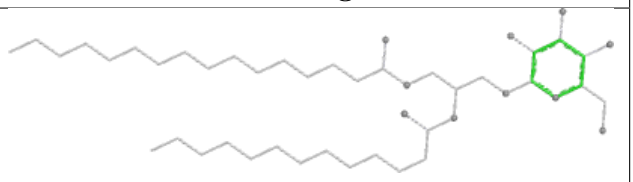
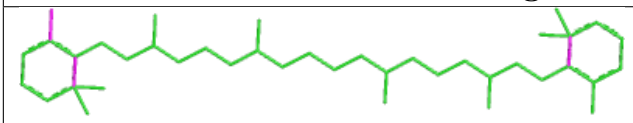
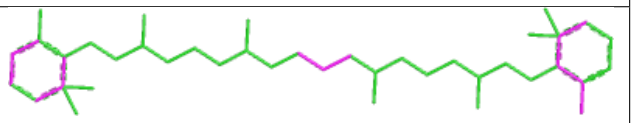


Rings

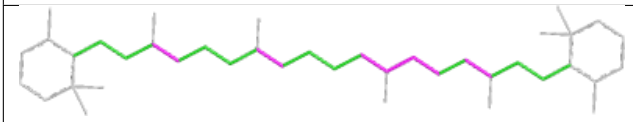
Ligand BCR B 717



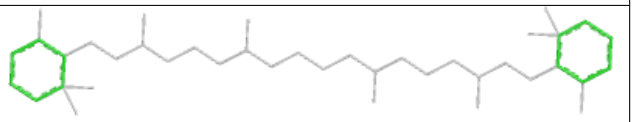
Bond lengths



Bond angles

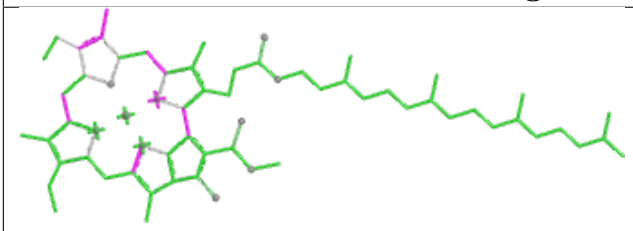


Torsions

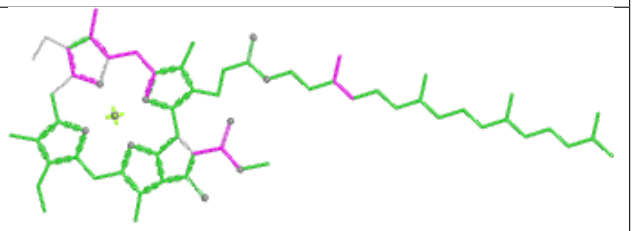


Rings

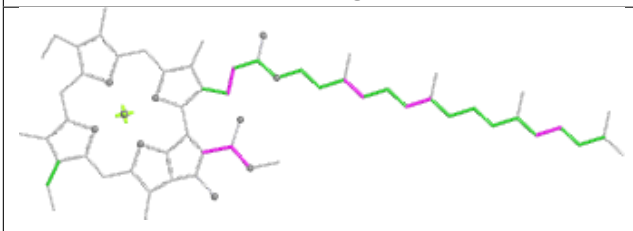
Ligand CLA B 714



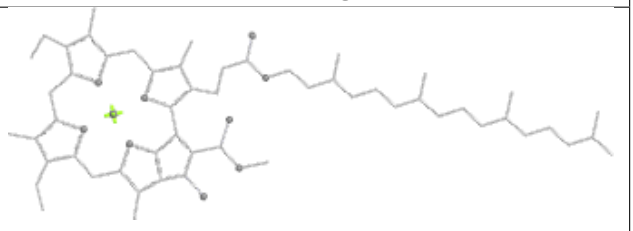
Bond lengths



Bond angles

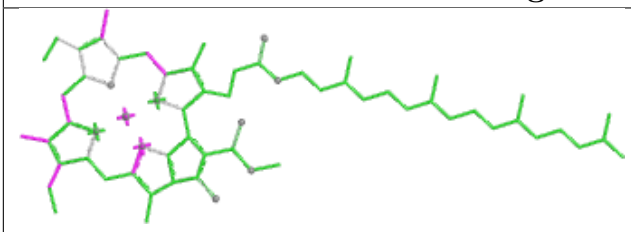


Torsions

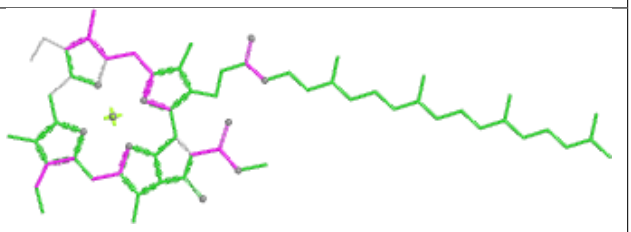


Rings

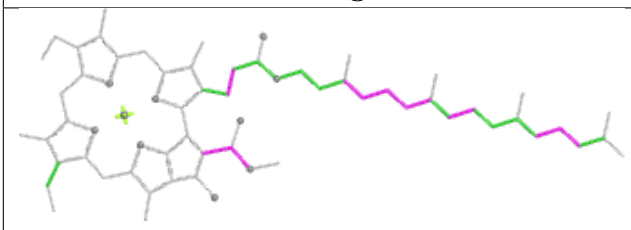
Ligand CLA b 714



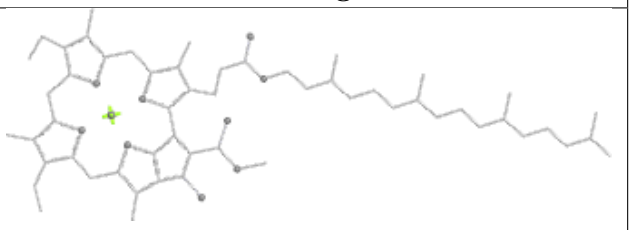
Bond lengths



Bond angles

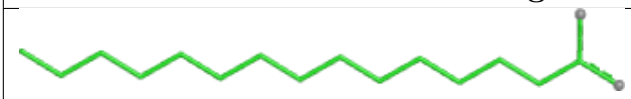


Torsions



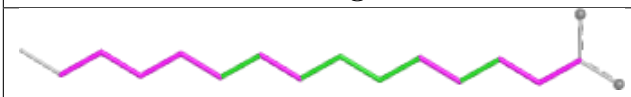
Rings

Ligand STE B 720

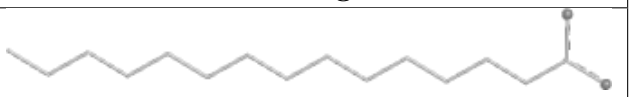


Bond lengths

Bond angles

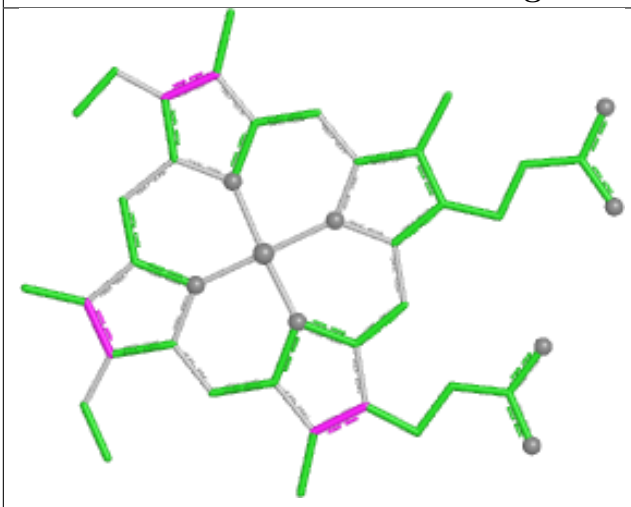


Torsions

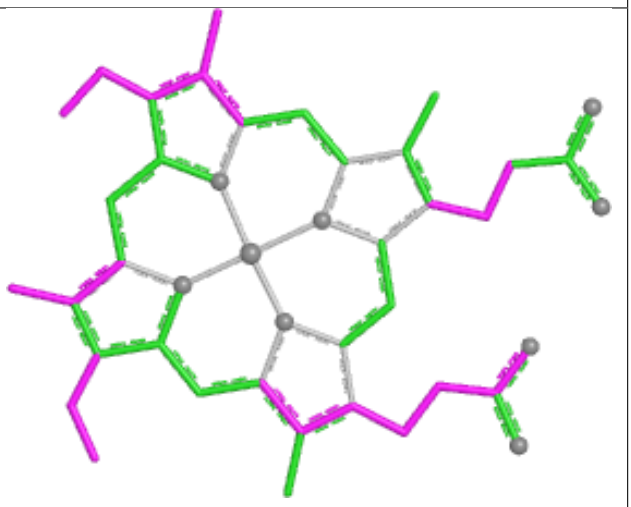


Rings

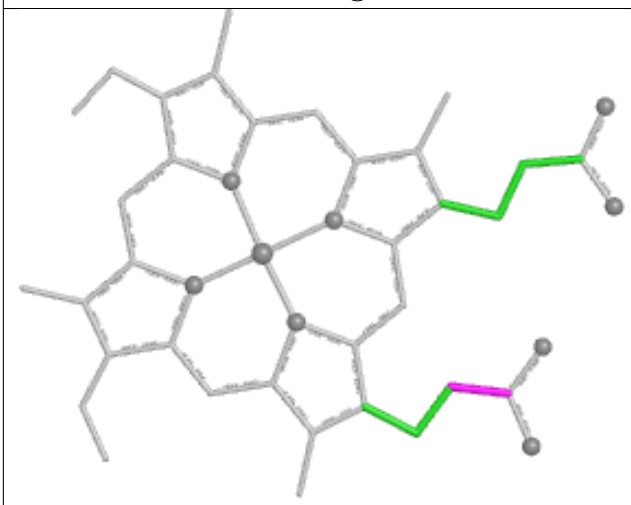
Ligand HEC E 103



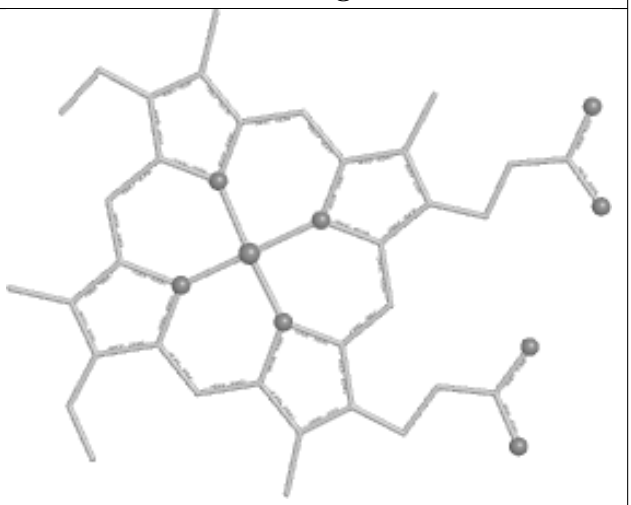
Bond lengths



Bond angles

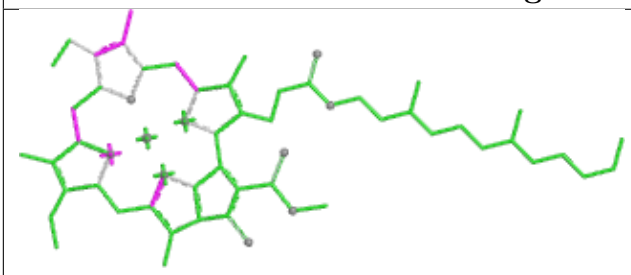


Torsions



Rings

Ligand CLA C 505



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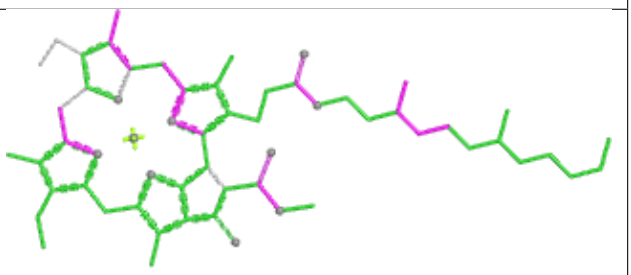
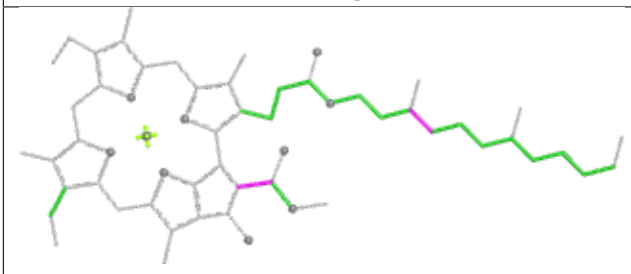


Bond angles



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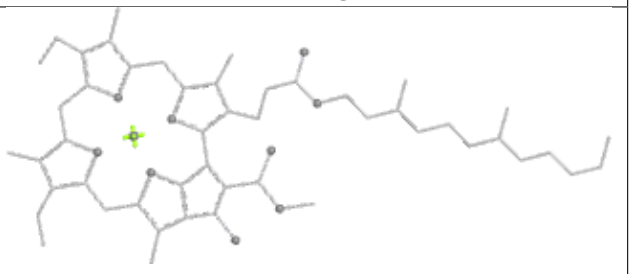
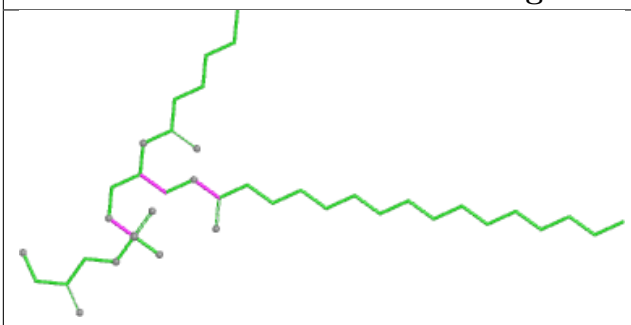


Rings

Ligand LHG d 407



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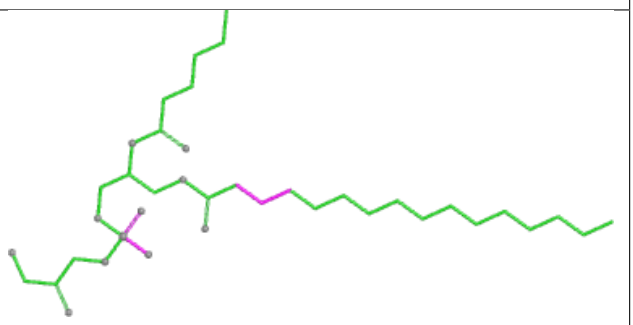
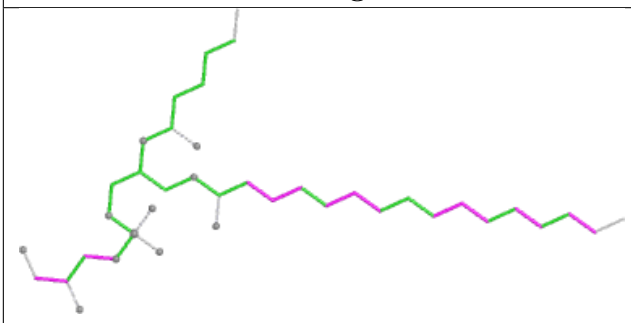
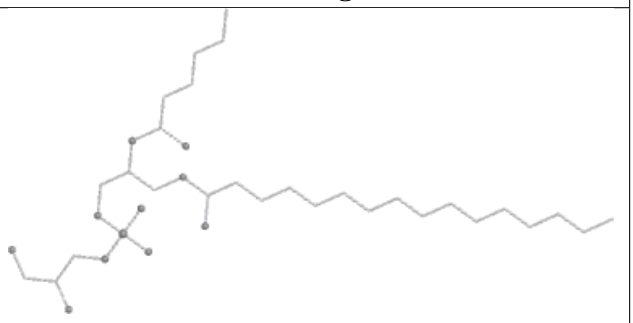


Bond angles

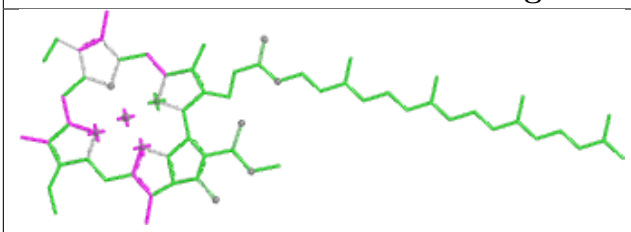


Torsions

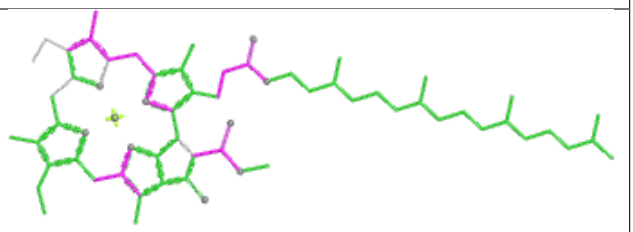


Rings

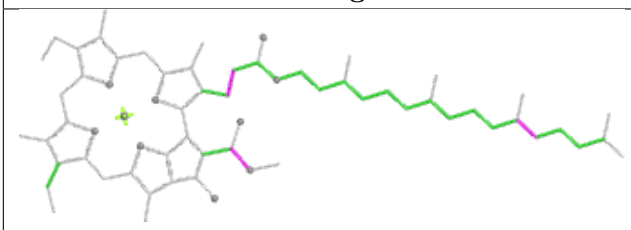
Ligand CLA C 502



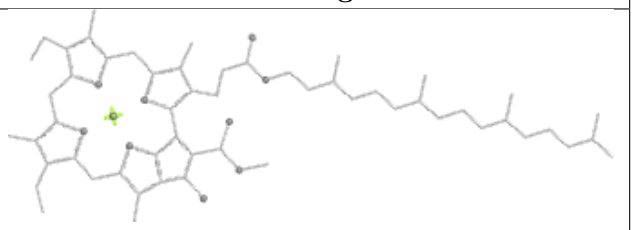
Bond lengths



Bond angles

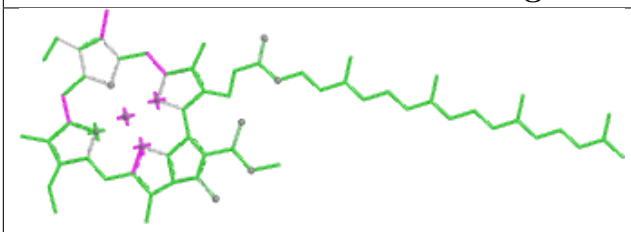


Torsions

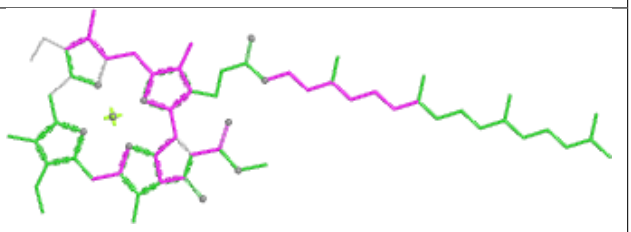


Rings

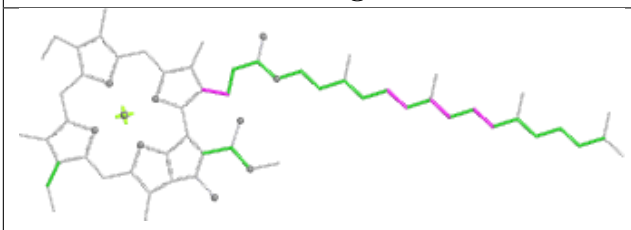
Ligand CLA C 504



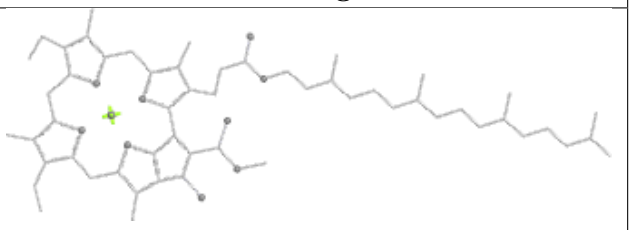
Bond lengths



Bond angles



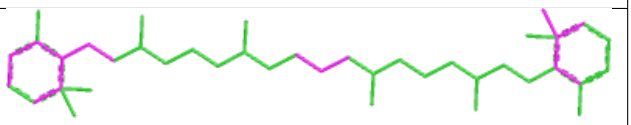
Torsions



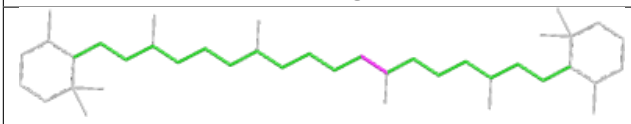
Rings

Ligand BCR B 719

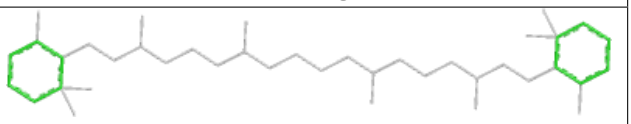
Bond lengths



Bond angles



Torsions



Rings

Ligand STE a 416

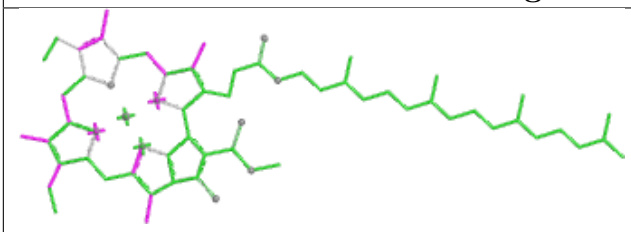
Bond lengths

Bond angles

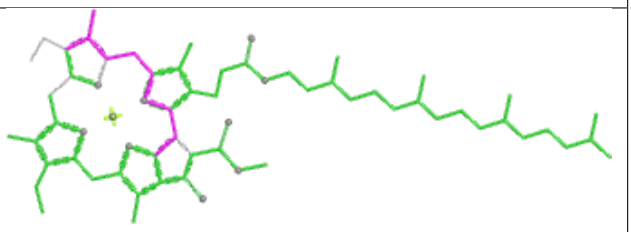
Torsions

Rings

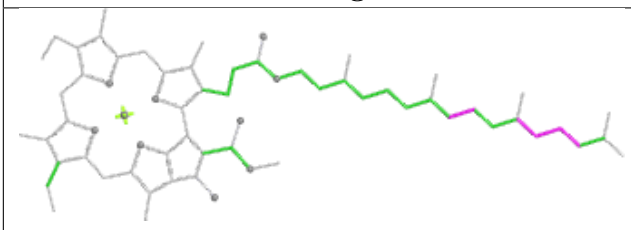
Ligand CLA B 707



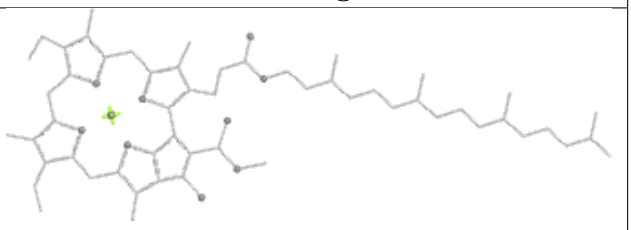
Bond lengths



Bond angles

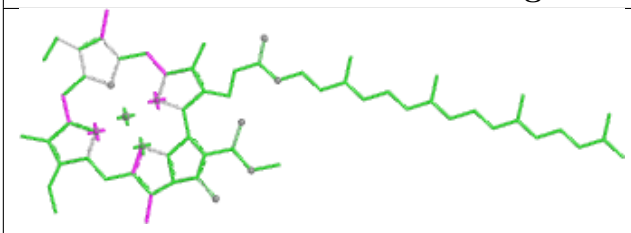


Torsions

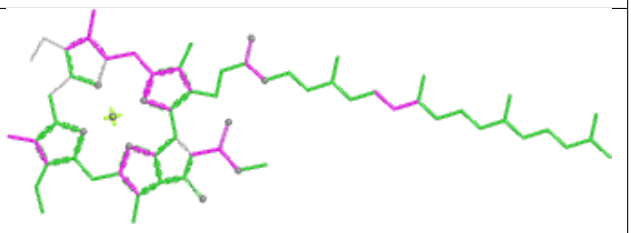


Rings

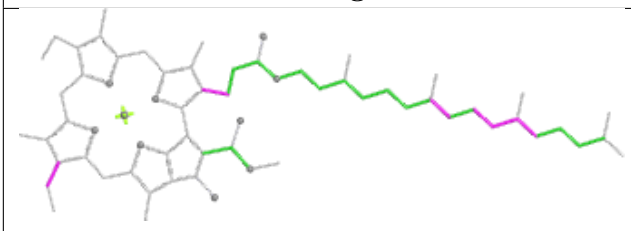
Ligand CLA B 704



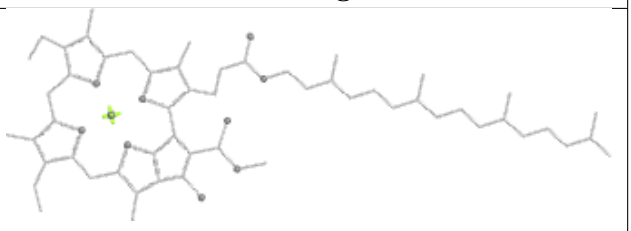
Bond lengths



Bond angles

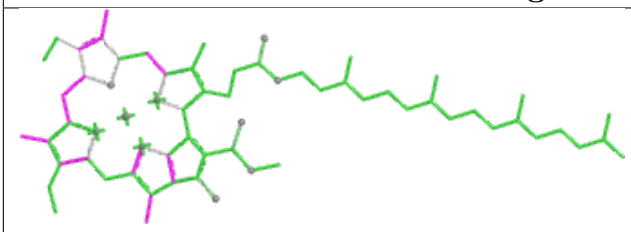


Torsions

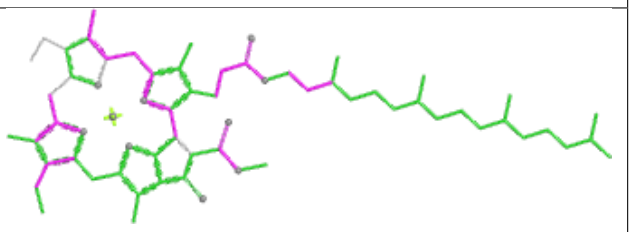


Rings

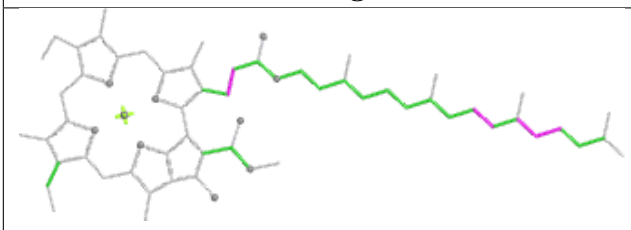
Ligand CLA b 710



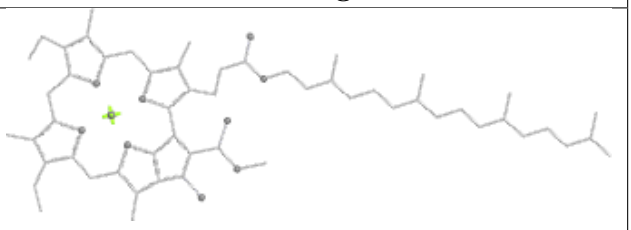
Bond lengths



Bond angles

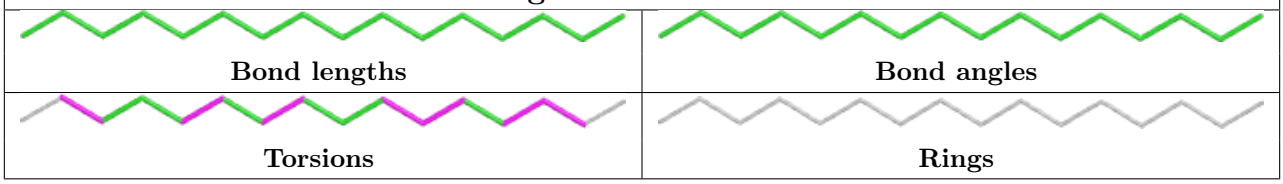


Torsions

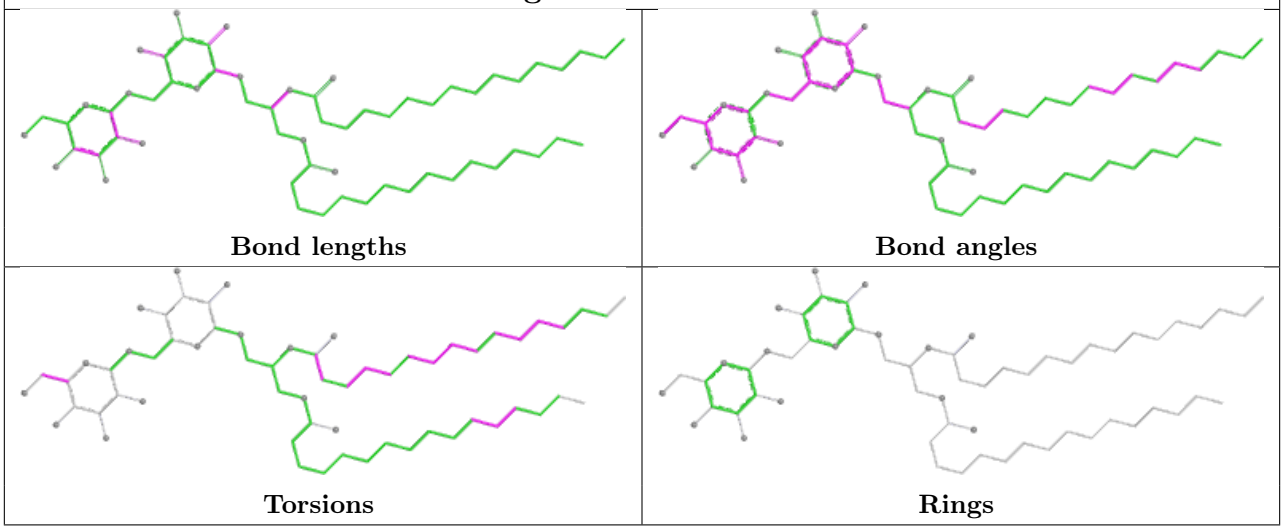


Rings

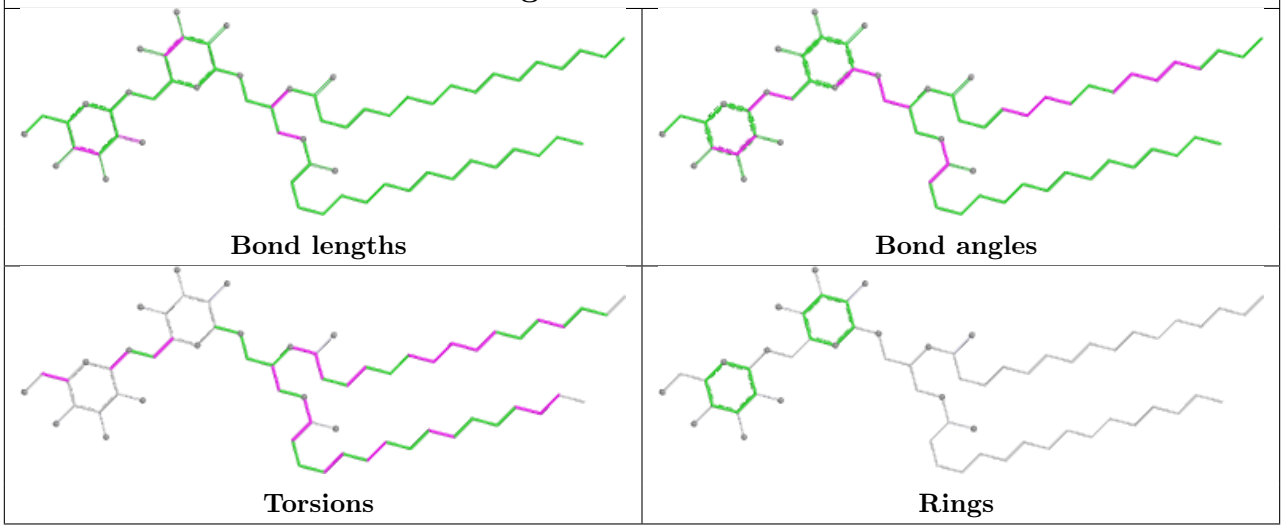
Ligand STE A 411



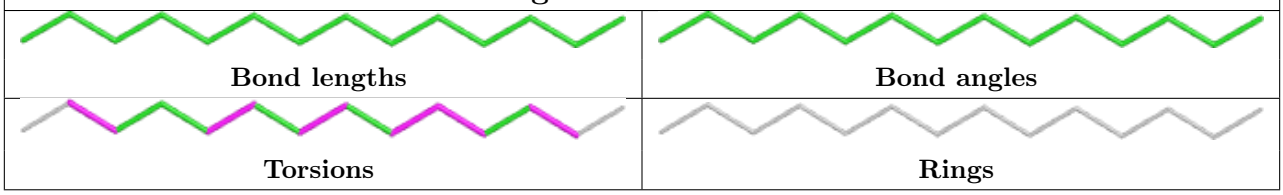
Ligand DGD h 702



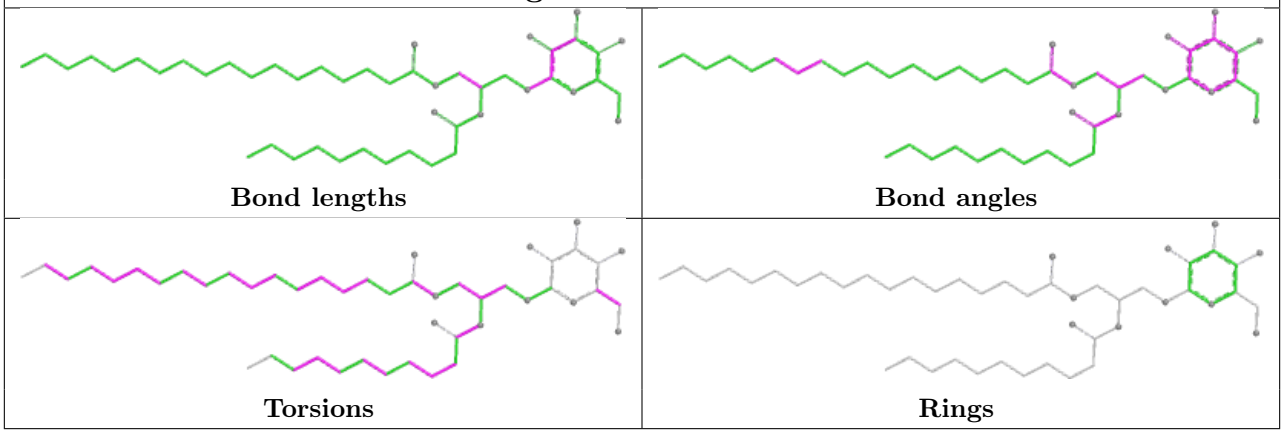
Ligand DGD C 517



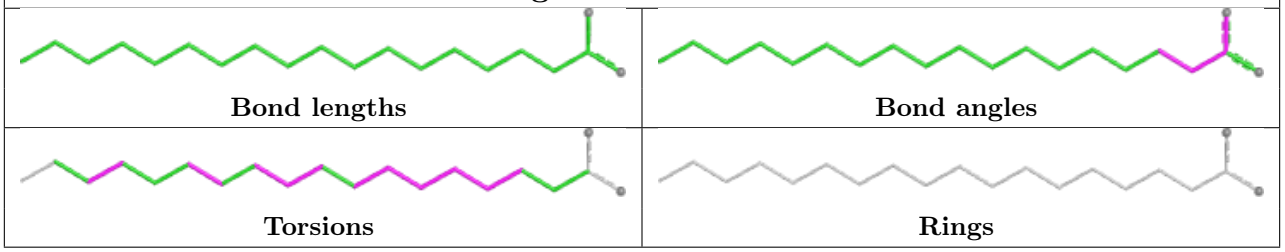
Ligand STE h 703



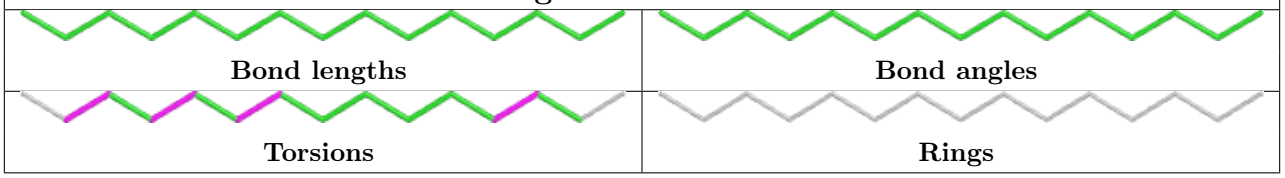
Ligand LMG c 522



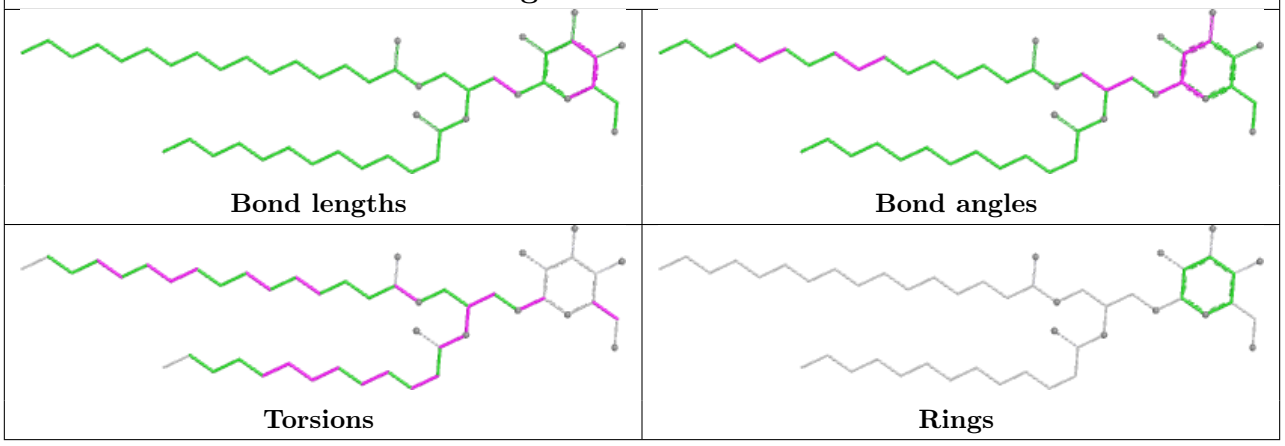
Ligand STE b 727



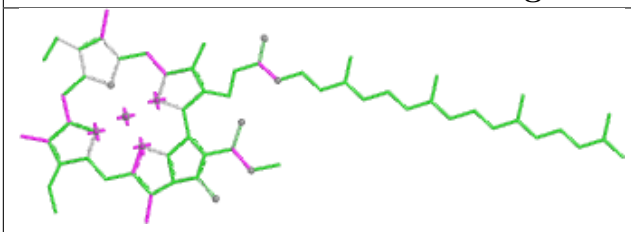
Ligand STE I 101



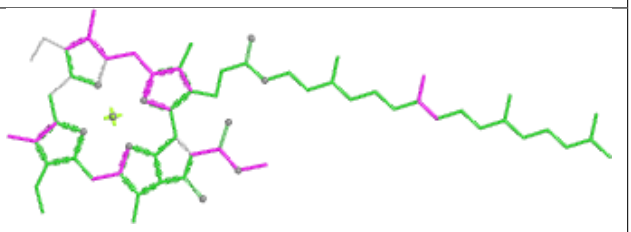
Ligand LMG C 516



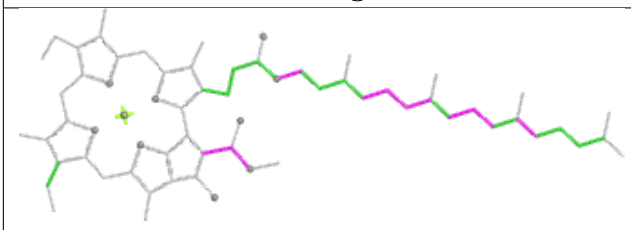
Ligand CLA C 510



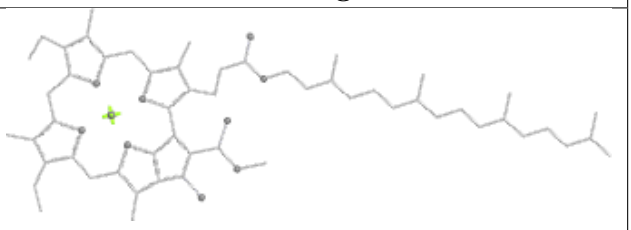
Bond lengths



Bond angles

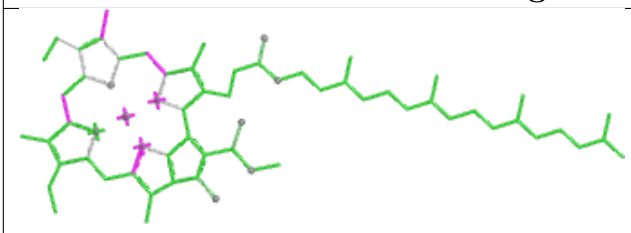


Torsions

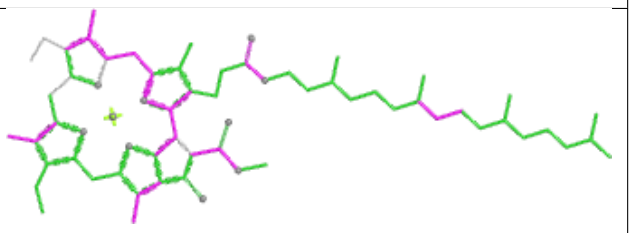


Rings

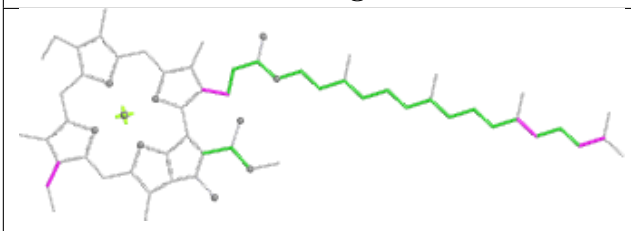
Ligand CLA a 401



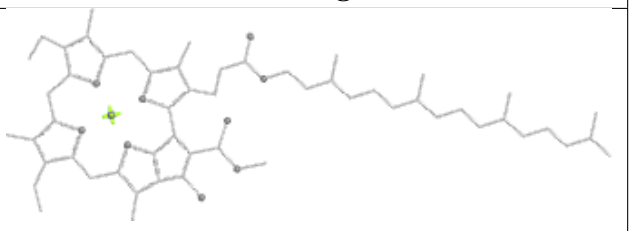
Bond lengths



Bond angles

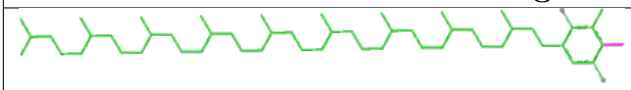


Torsions

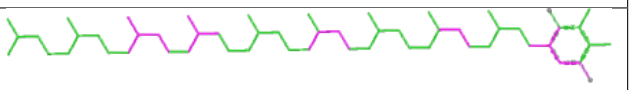


Rings

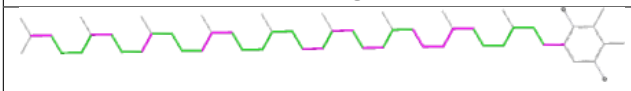
Ligand PL9 a 411



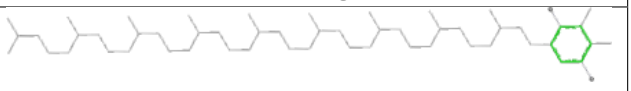
Bond lengths



Bond angles

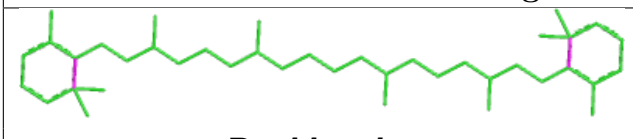


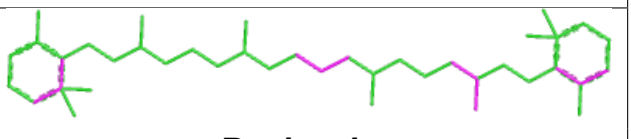
Torsions

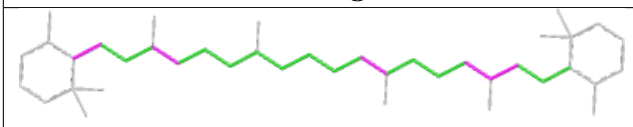


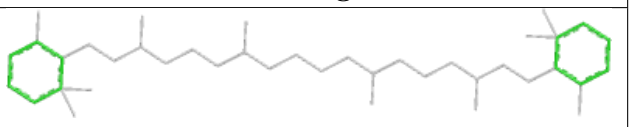
Rings

Ligand BCR Y 101


Bond lengths

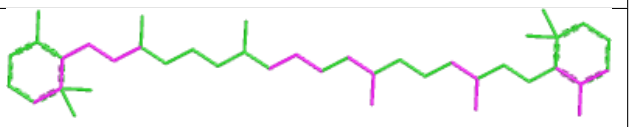

Bond angles

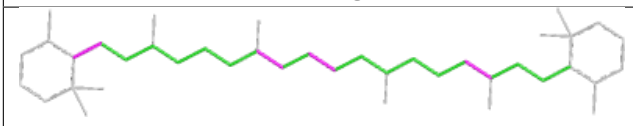

Torsions

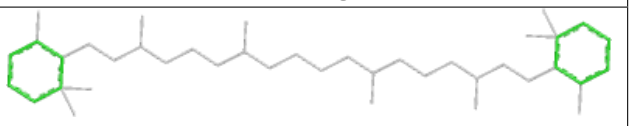

Rings

Ligand BCR A 405

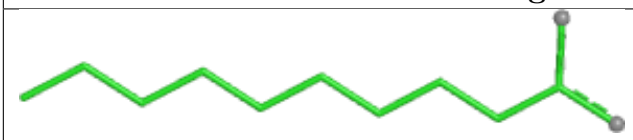

Bond lengths

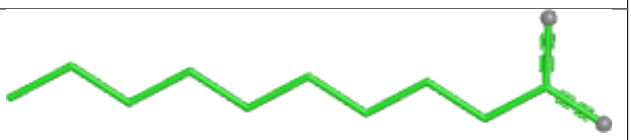

Bond angles

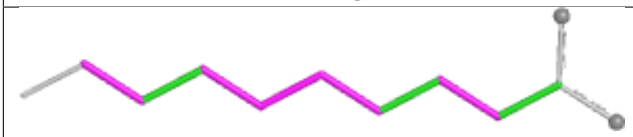

Torsions

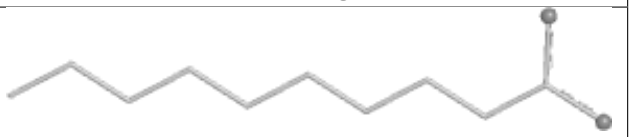

Rings

Ligand STE E 101

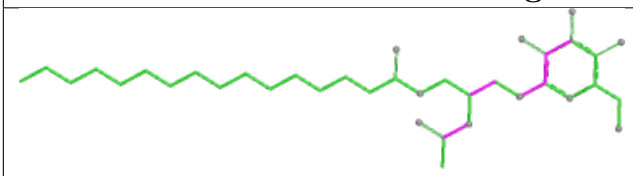

Bond lengths

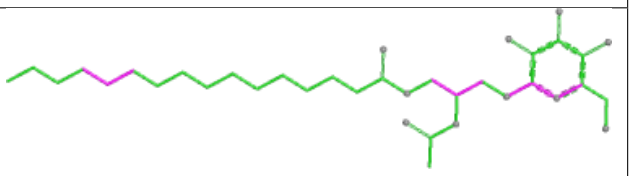

Bond angles

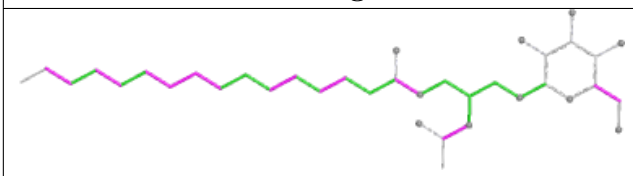

Torsions

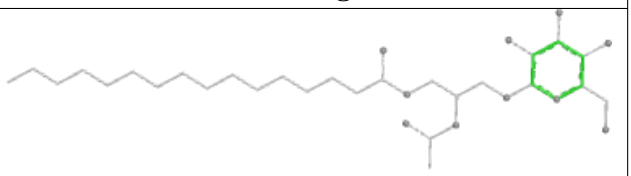

Rings

Ligand LMG c 520

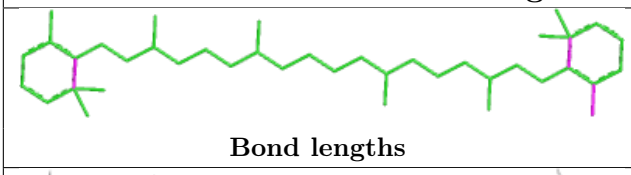

Bond lengths


Bond angles

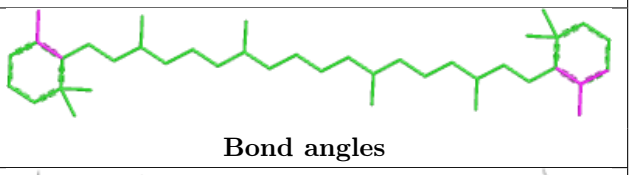

Torsions


Rings

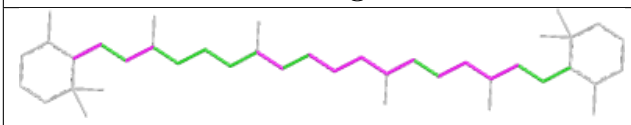
Ligand BCR k 101



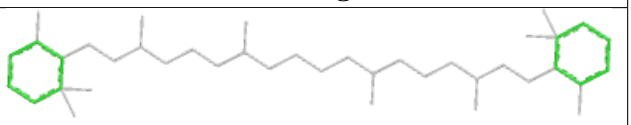
Bond lengths



Bond angles

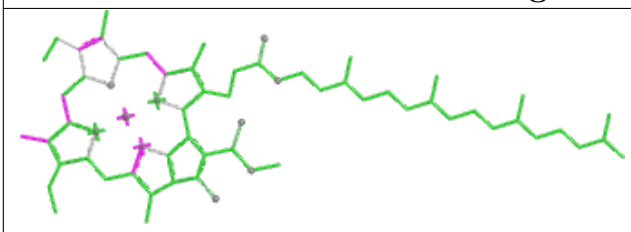


Torsions

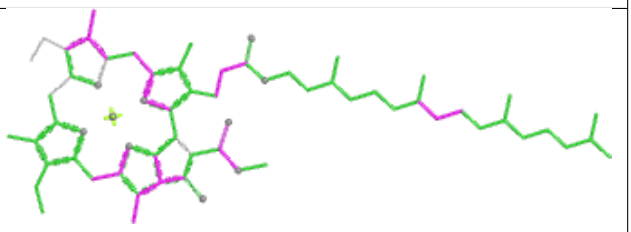


Rings

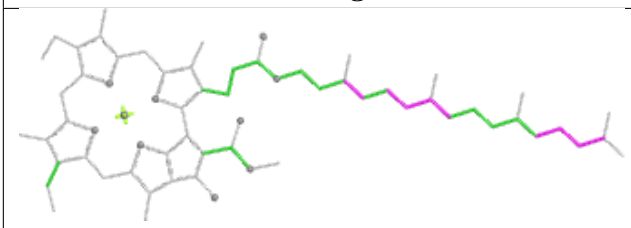
Ligand CLA c 506



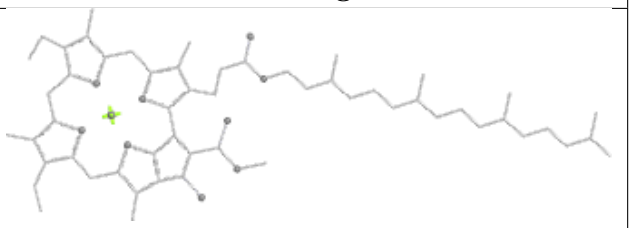
Bond lengths



Bond angles

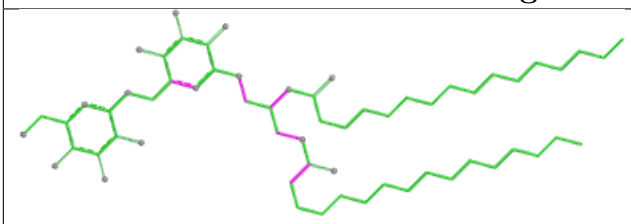


Torsions

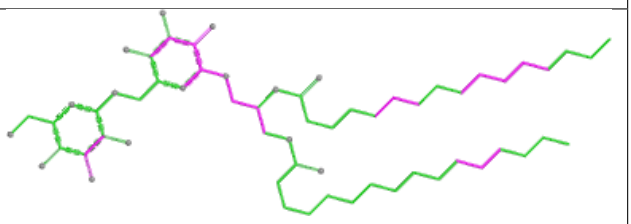


Rings

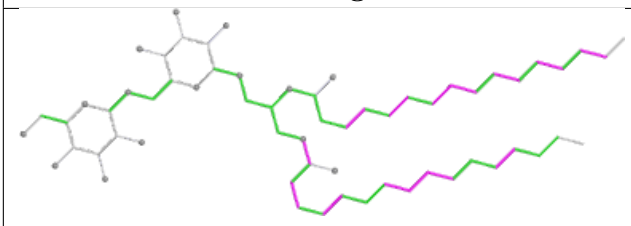
Ligand DGD C 519



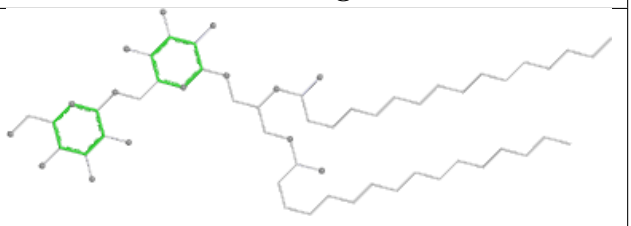
Bond lengths



Bond angles

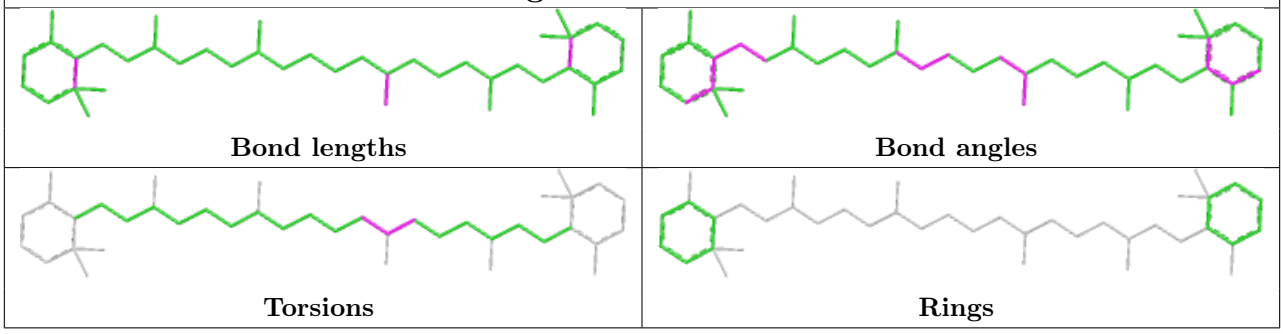


Torsions

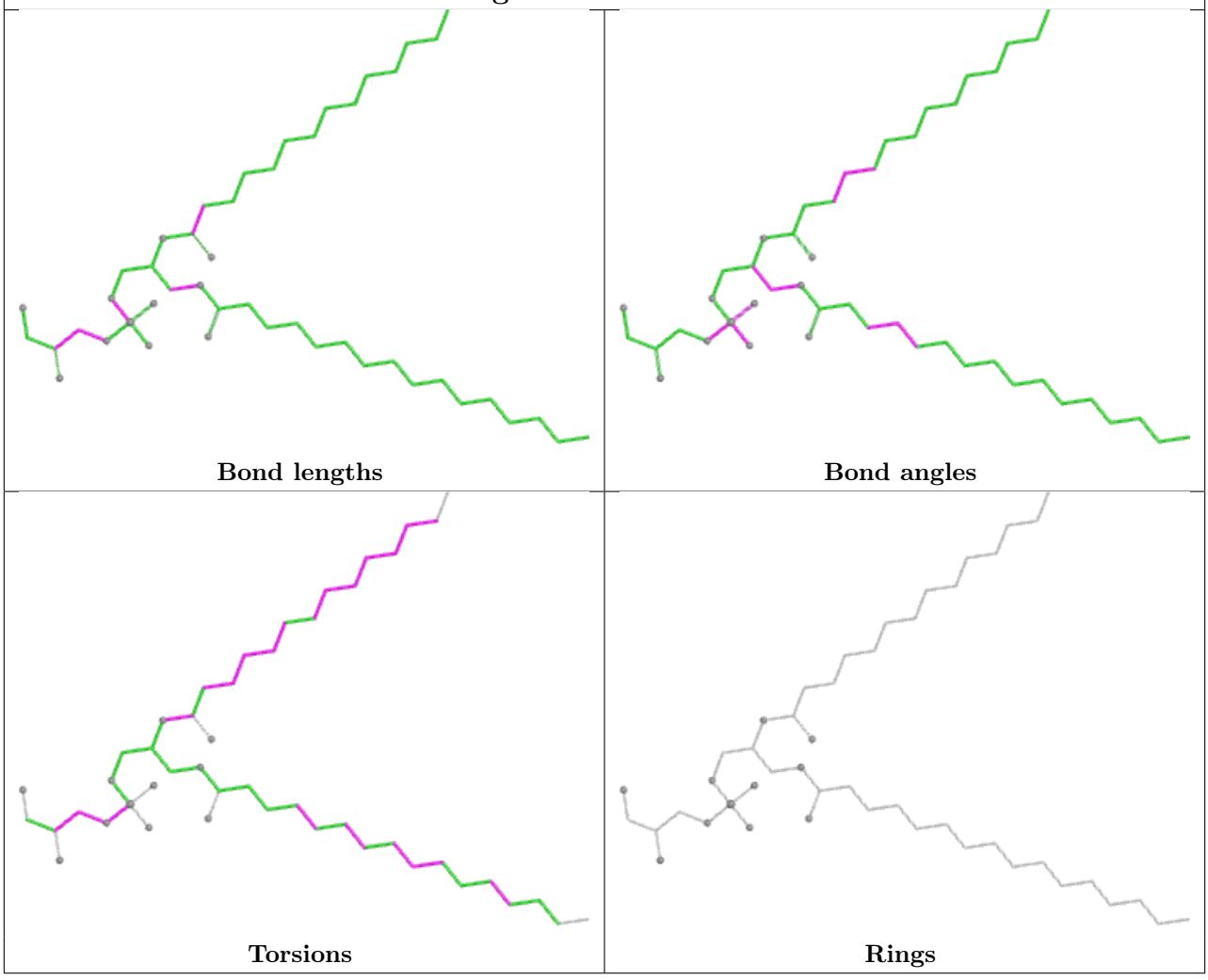


Rings

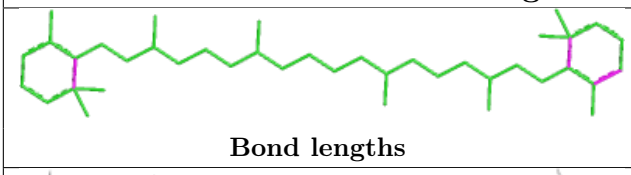
Ligand BCR b 718

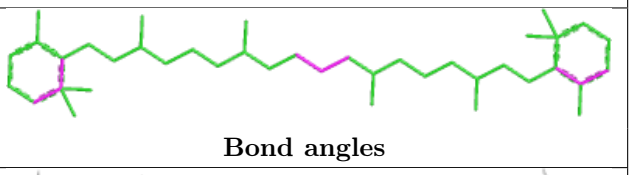


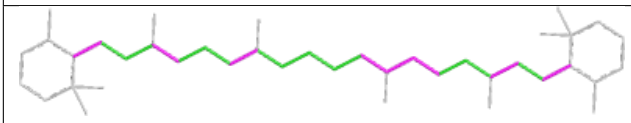
Ligand LHG D 411

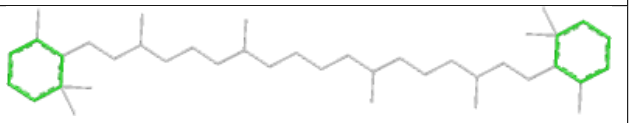


Ligand BCR C 501


Bond lengths


Bond angles

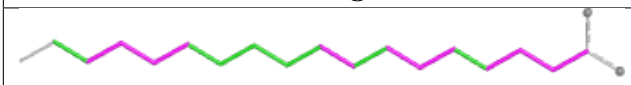

Torsions


Rings

Ligand STE b 722

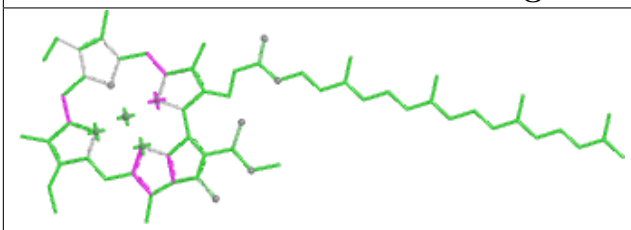

Bond lengths

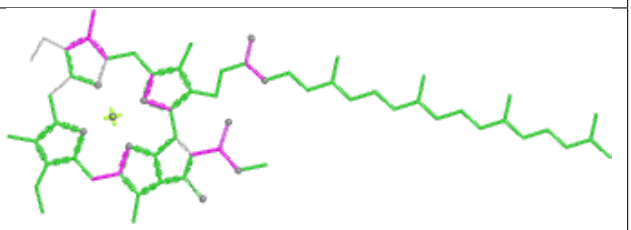

Bond angles

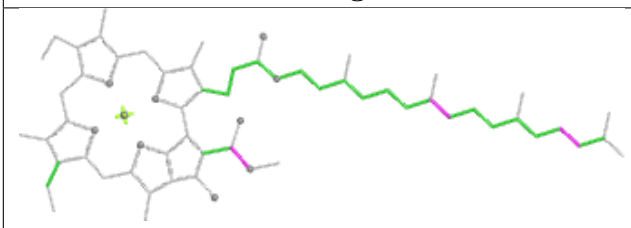

Torsions

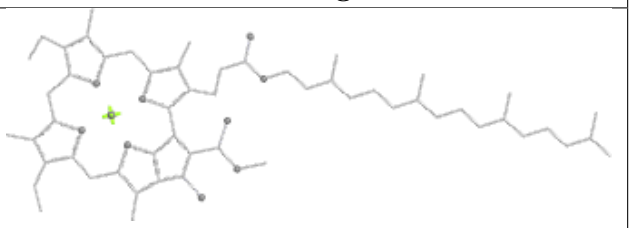

Rings

Ligand CLA C 509


Bond lengths

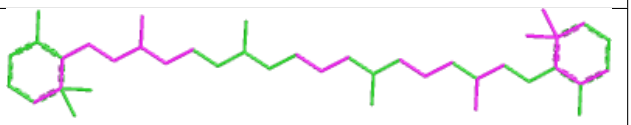

Bond angles

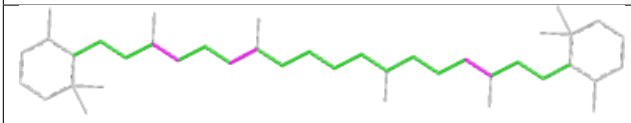

Torsions

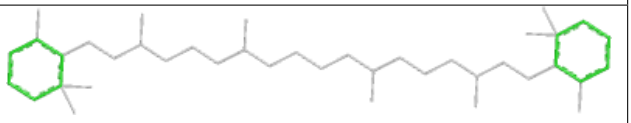

Rings

Ligand BCR a 407

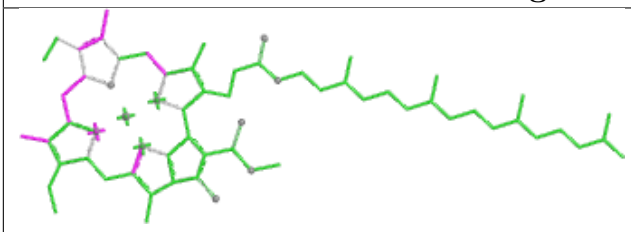

Bond lengths


Bond angles

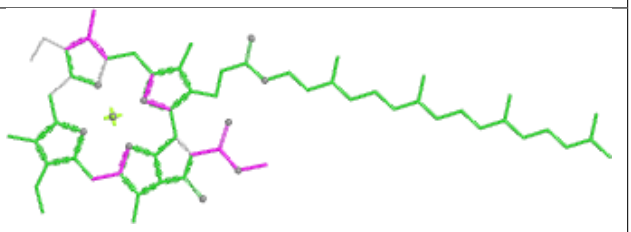

Torsions


Rings

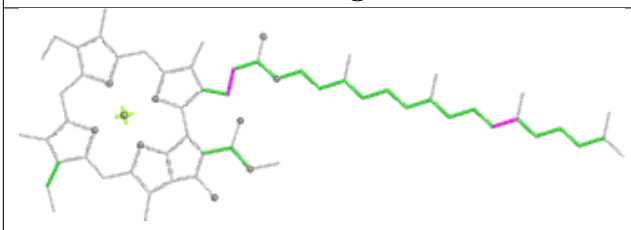
Ligand CLA c 502



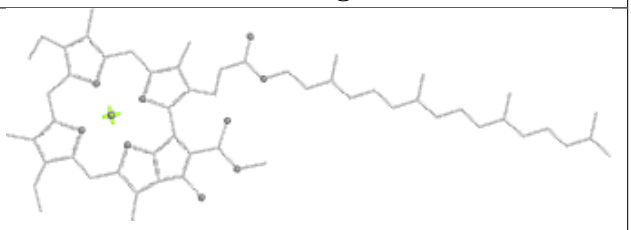
Bond lengths



Bond angles



Torsions

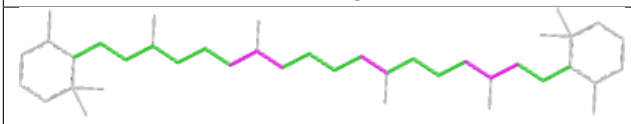


Rings

Ligand BCR b 719

Bond lengths

Bond angles



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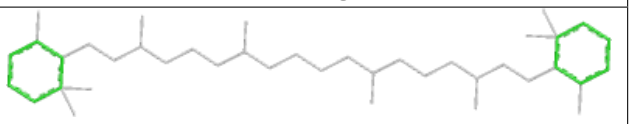
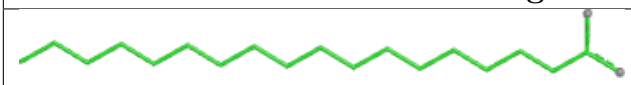
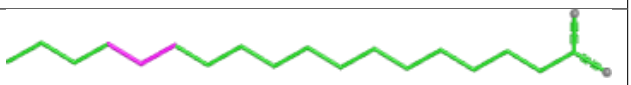


Rings

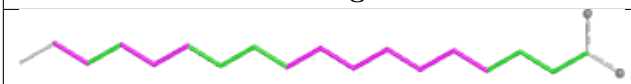
Ligand STE X 101



Bond lengths



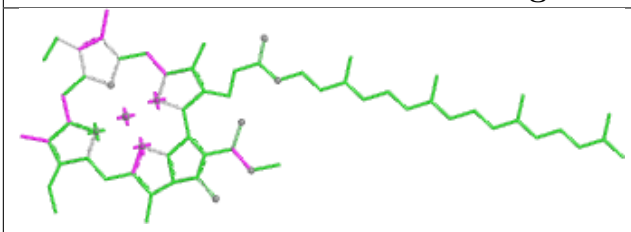
Bond angles

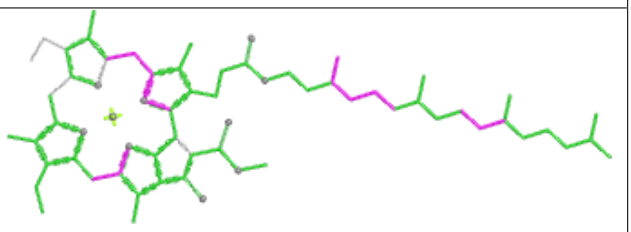


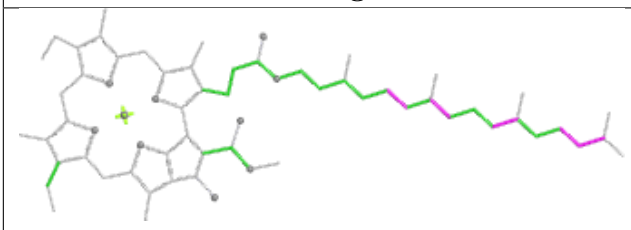
Torsions

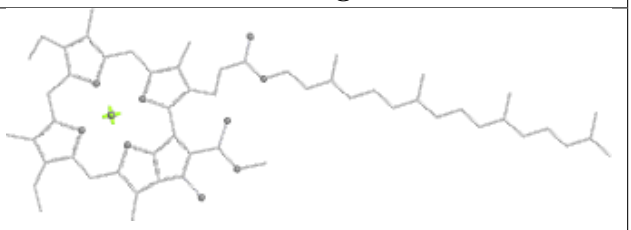
Rings

Ligand CLA c 504

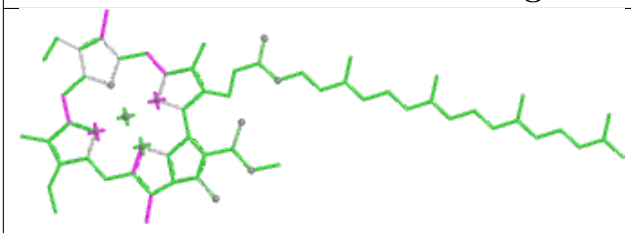

Bond lengths

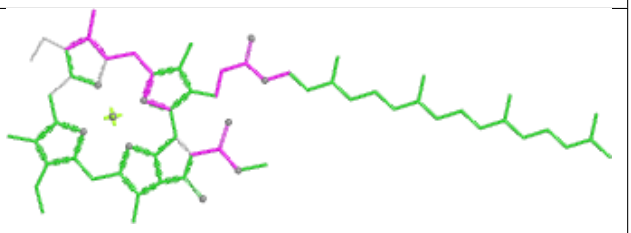

Bond angles

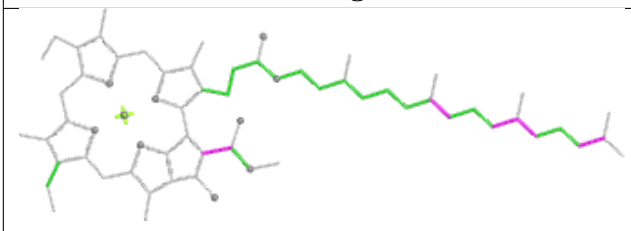

Torsions

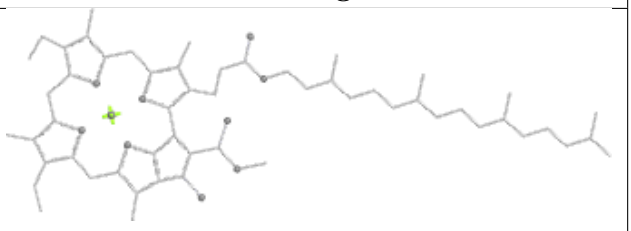

Rings

Ligand CLA C 508


Bond lengths

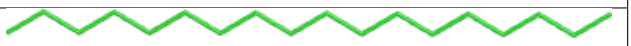

Bond angles


Torsions

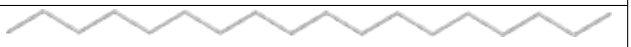

Rings

Ligand STE l 102

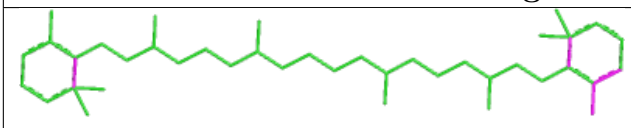

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR T 701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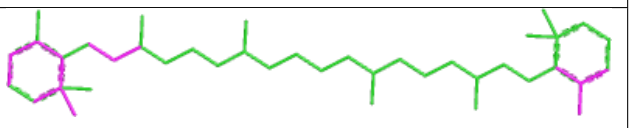
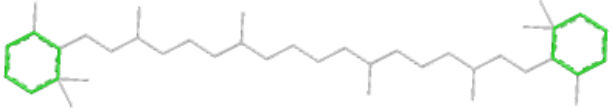
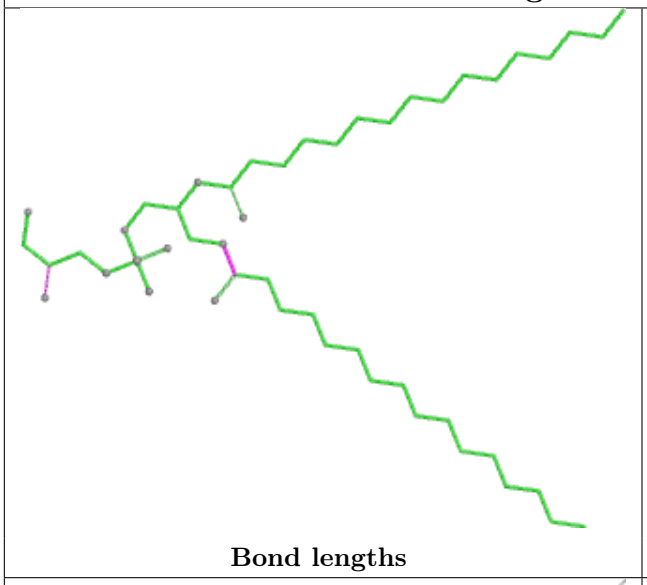

Bond angles

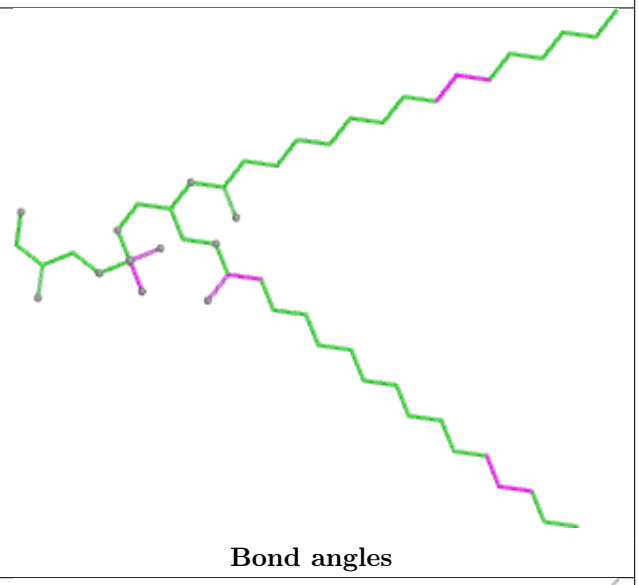

Torsions


Rings

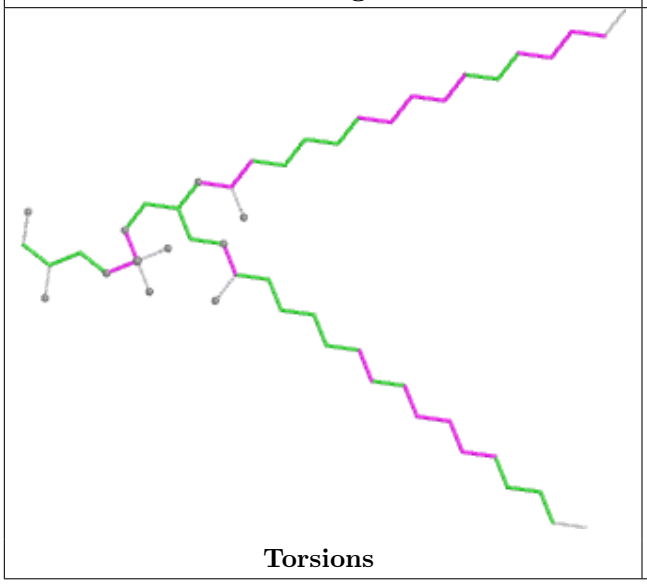
Ligand LHG L 101



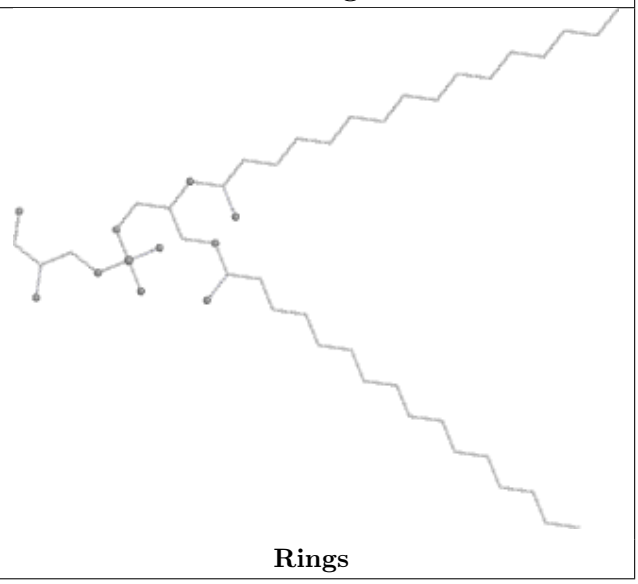
Bond lengths



Bond angles

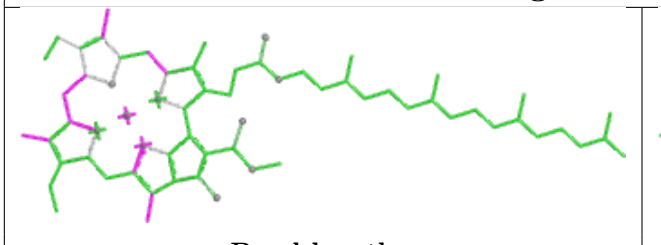


Torsions

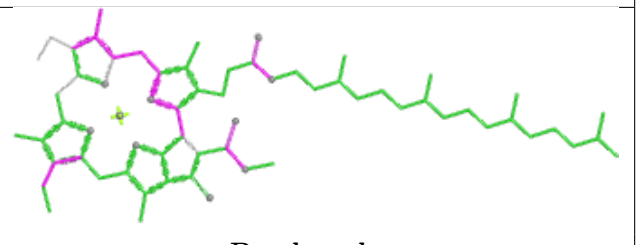


Rings

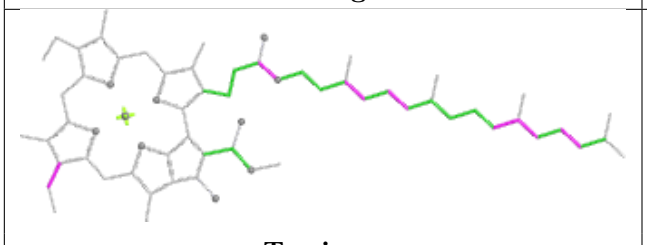
Ligand CLA a 406



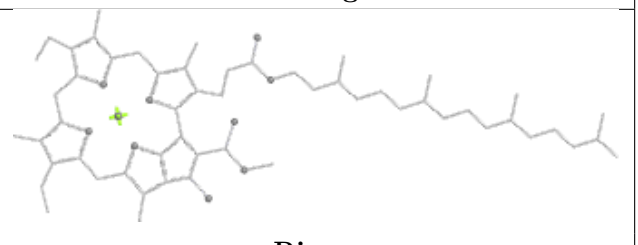
Bond lengths



Bond angles

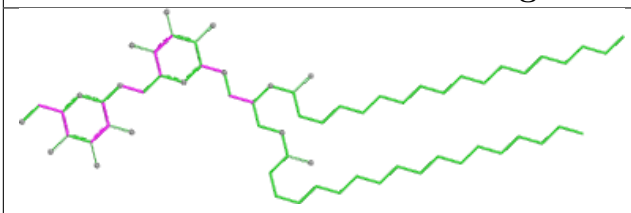


Torsions

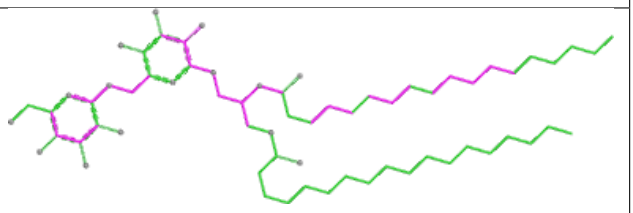


Rings

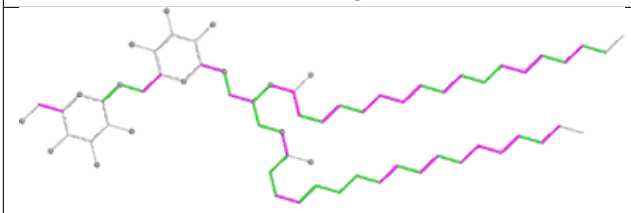
Ligand DGD A 413



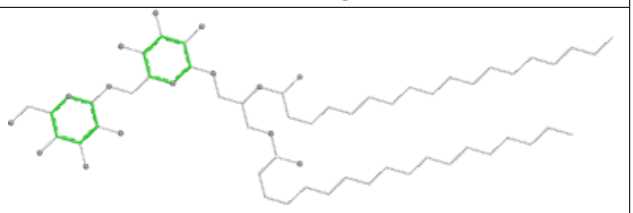
Bond lengths



Bond angles

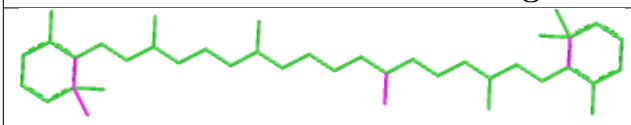


Torsions

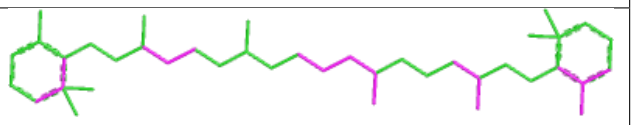


Rings

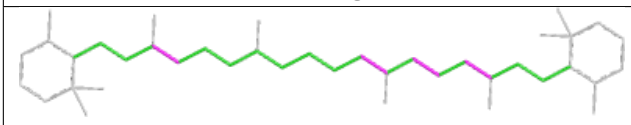
Ligand BCR C 515



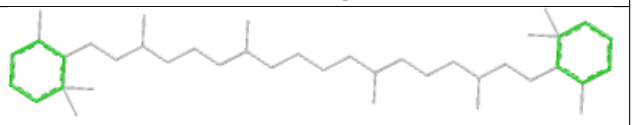
Bond lengths



Bond angles



Torsions

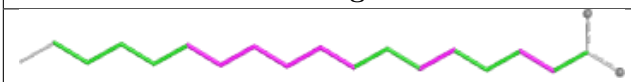


Rings

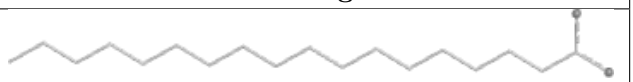
Ligand STE c 521

Bond lengths

Bond angles

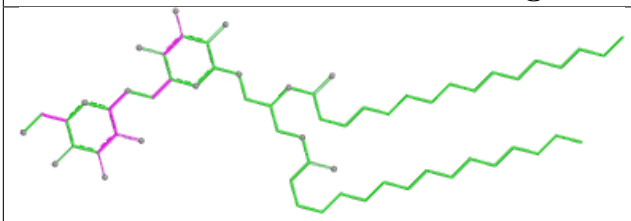


Torsions

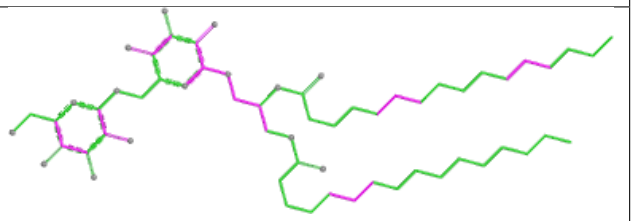


Rings

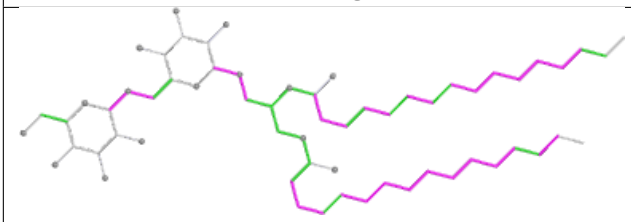
Ligand DGD c 518



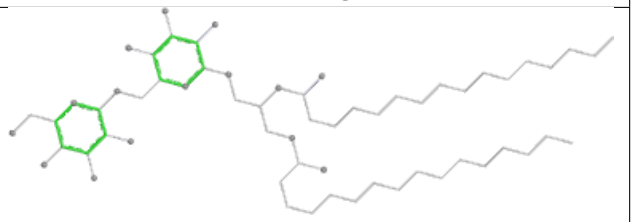
Bond lengths



Bond angles

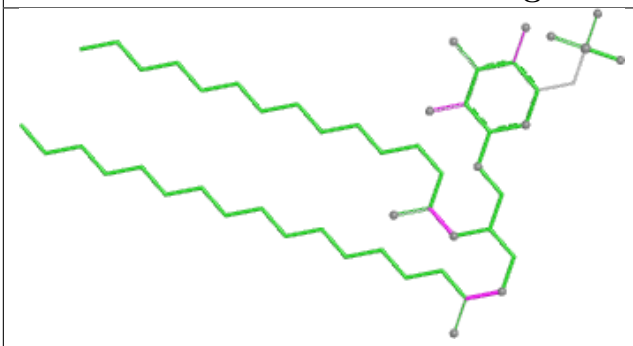


Torsions



Rings

Ligand SQD A 409



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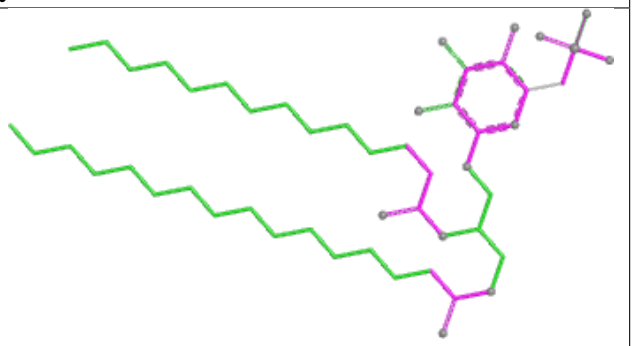
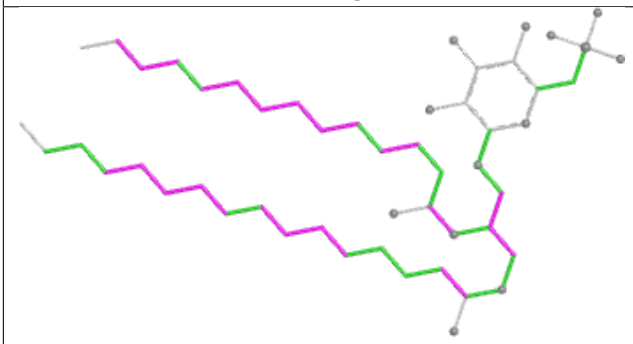


Bond angles



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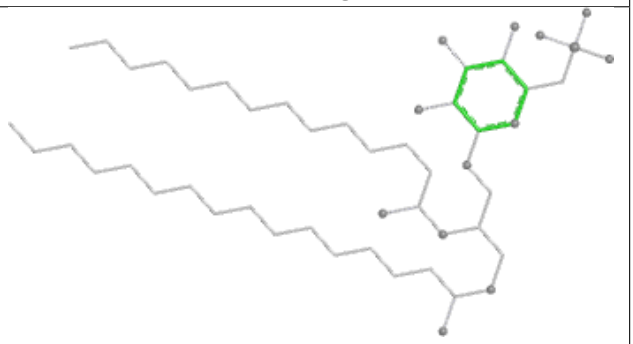
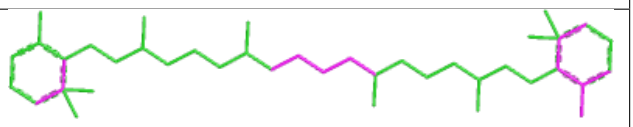


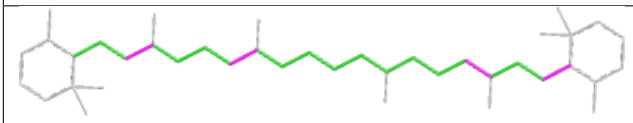
Rings

Ligand BCR H 101

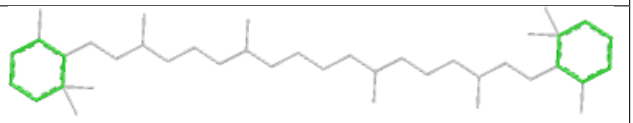
Bond lengths



Bond angles

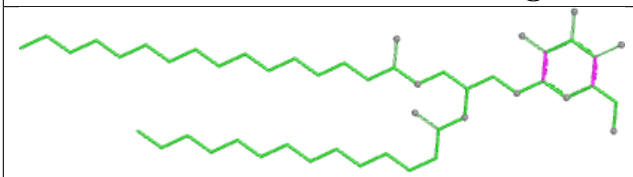


Torsions



Rings

Ligand LMG c 523



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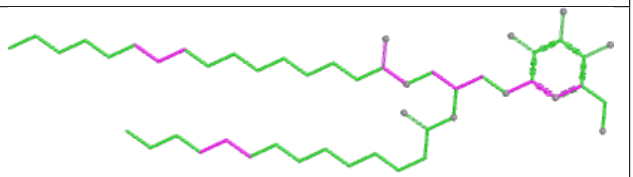
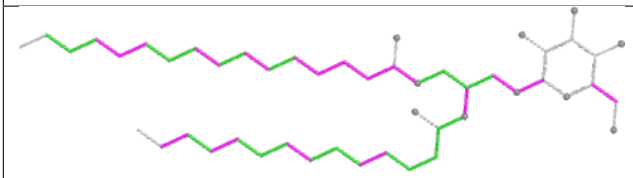


Bond angles



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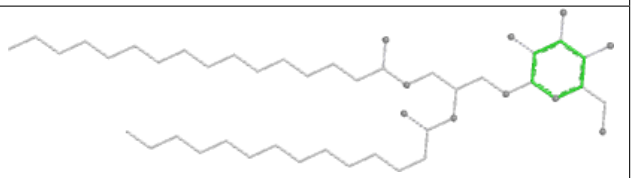
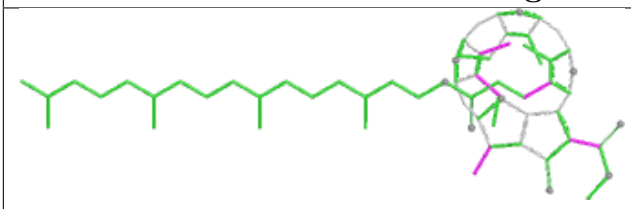


Rings

Ligand PHO d 405



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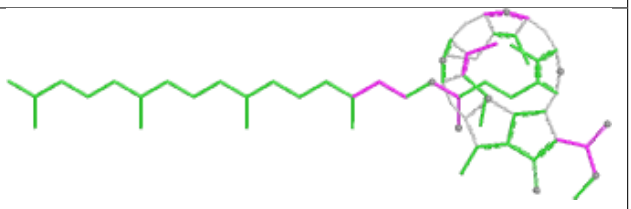
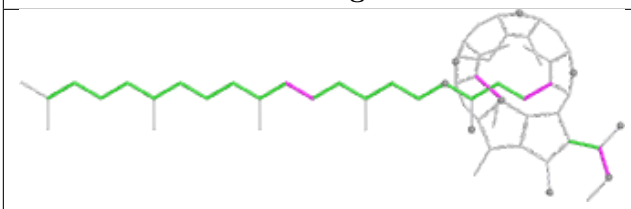


Bond angles



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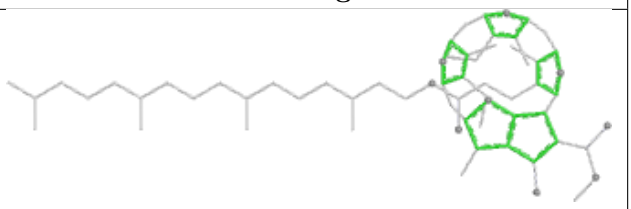
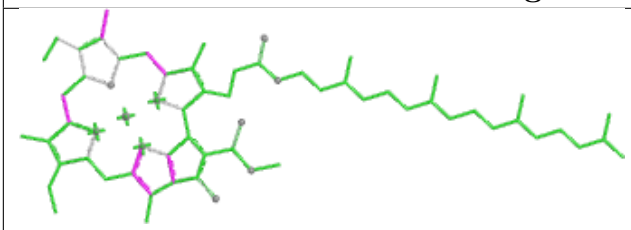


Rings

Ligand CLA B 702



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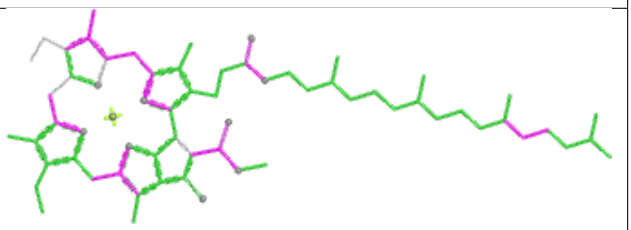
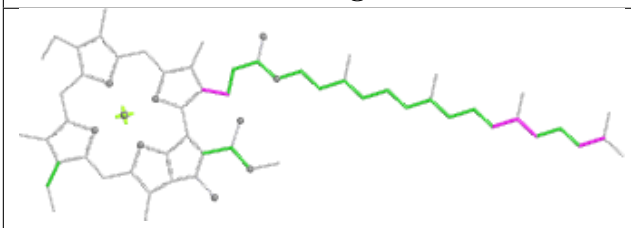


Bond angles



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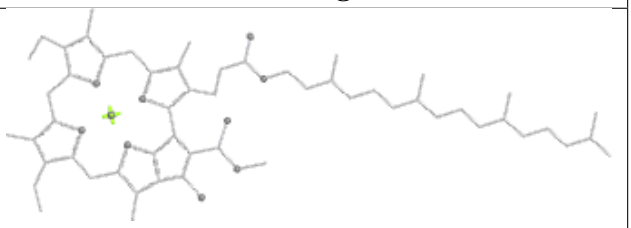
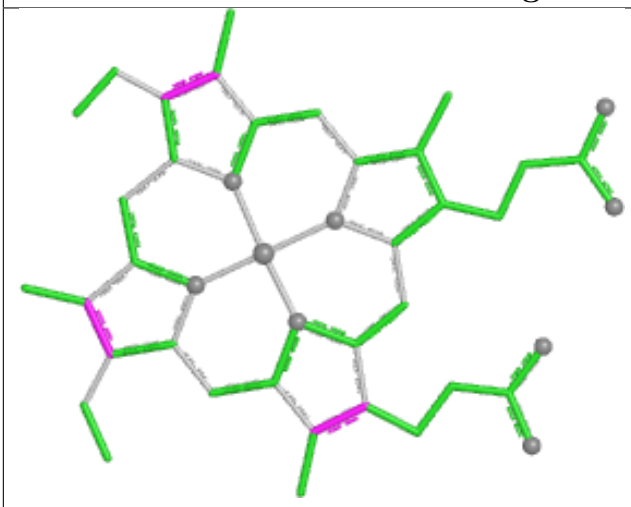


Rings

Ligand HEC V 201



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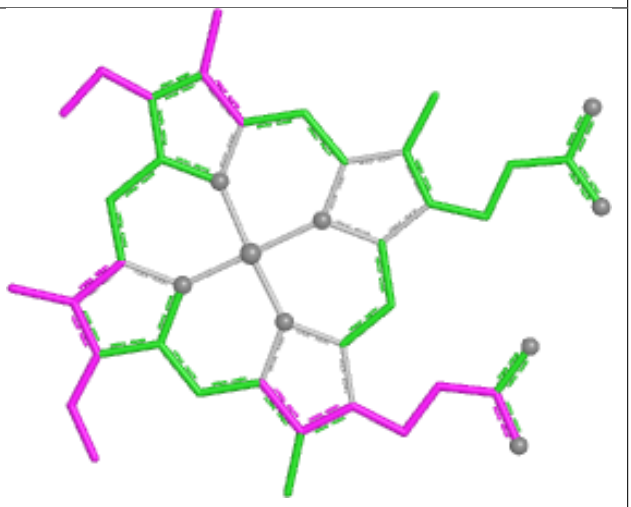
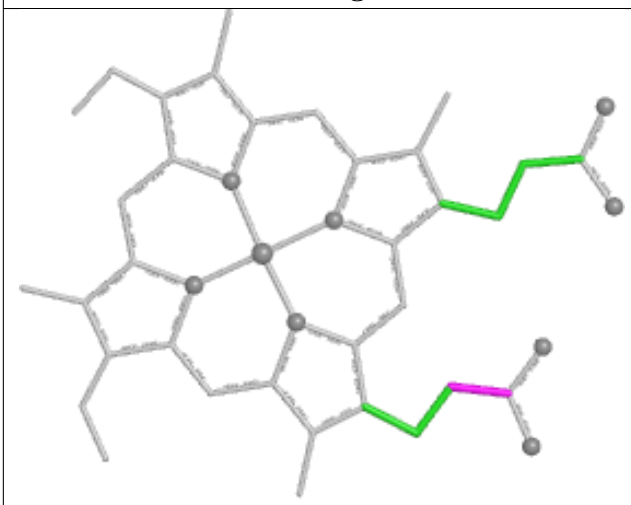


Bond angles



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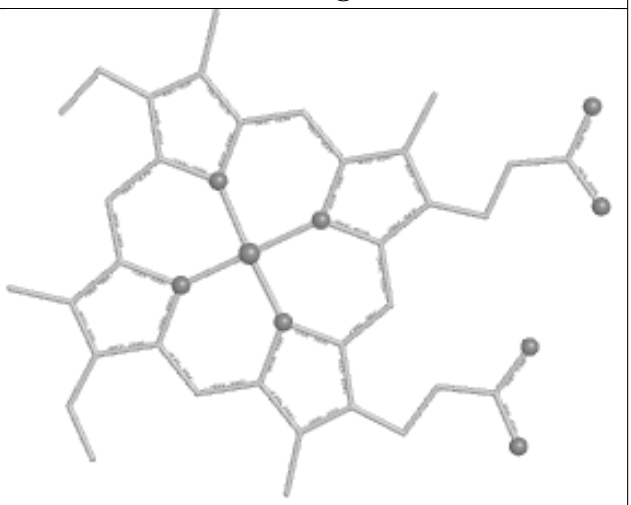
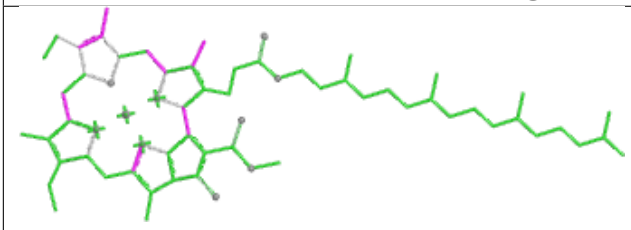


Rings

Ligand CLA B 710



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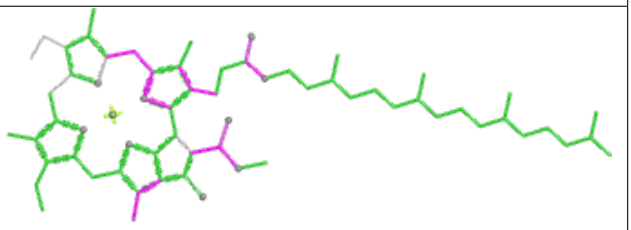
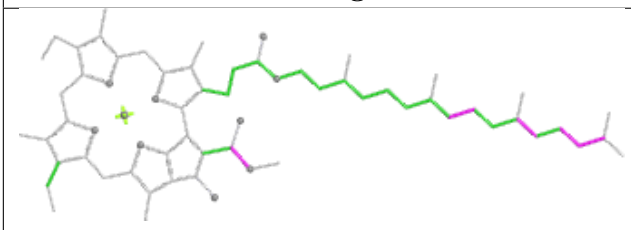


Bond angles



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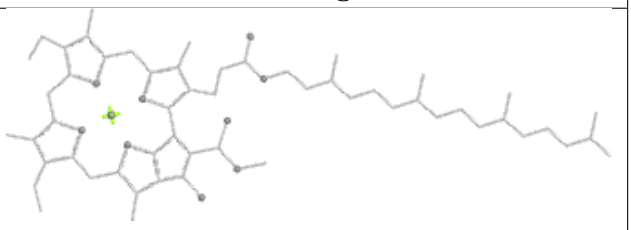
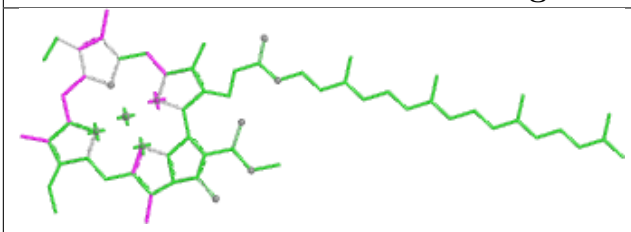


Rings

Ligand CLA c 503



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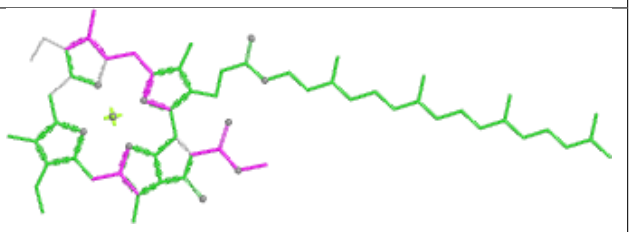
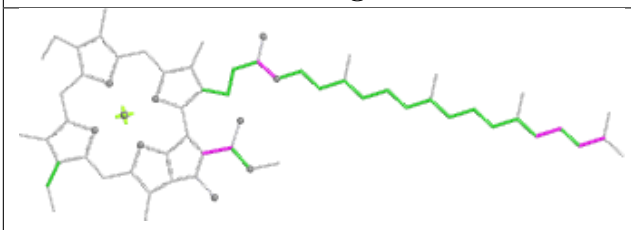


Bond angles



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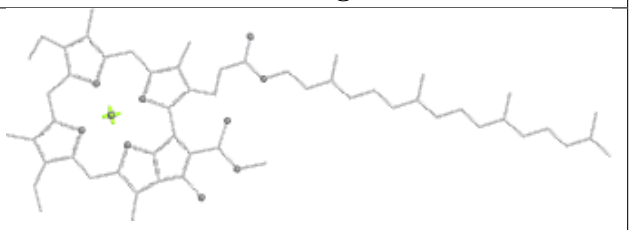
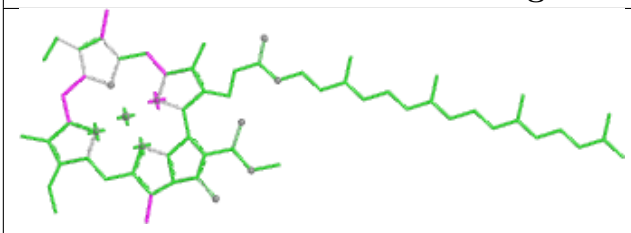


Rings

Ligand CLA b 711



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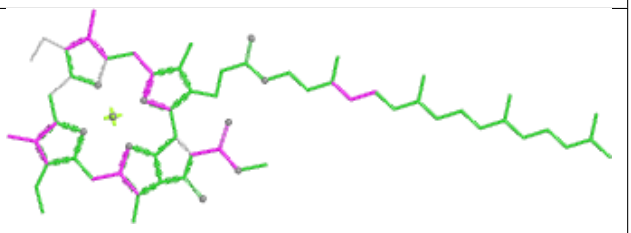
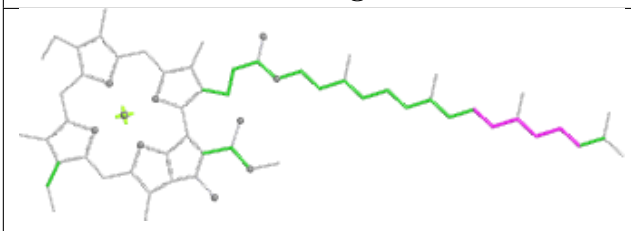


Bond angles



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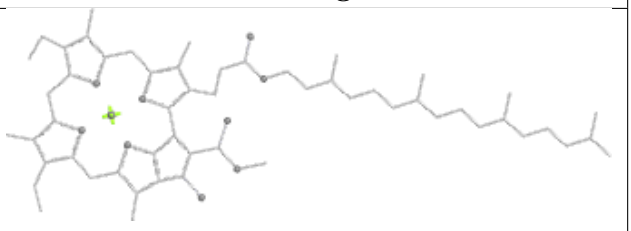
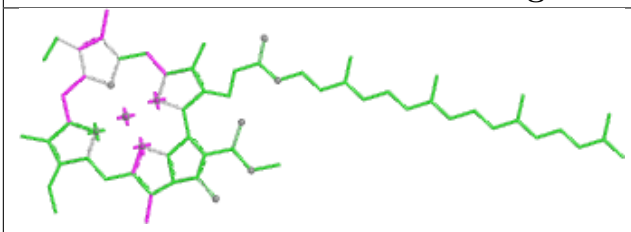


Rings

Ligand CLA b 715



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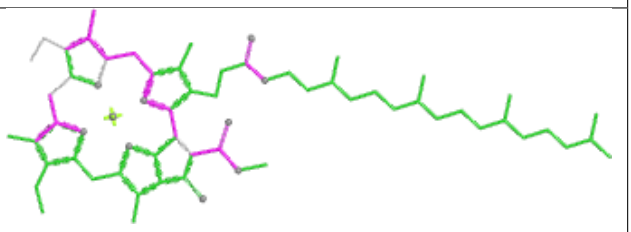
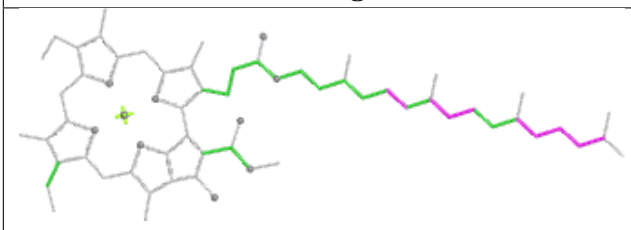


Bond angles



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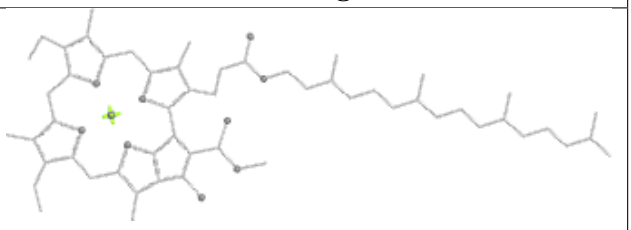
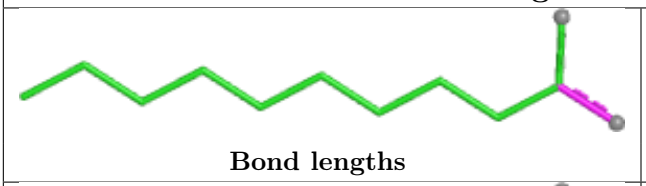
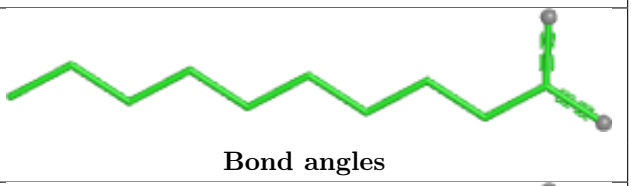
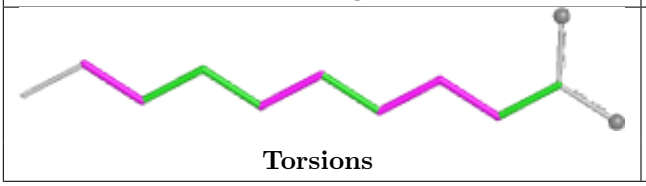


Rings

Ligand STE a 417


Bond lengths


Bond angles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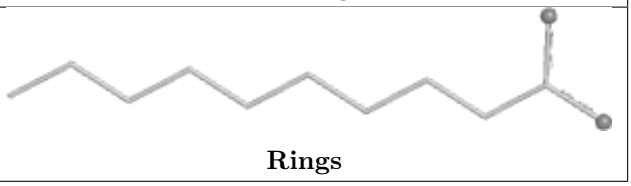
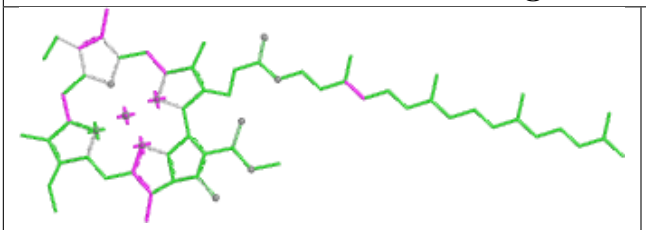
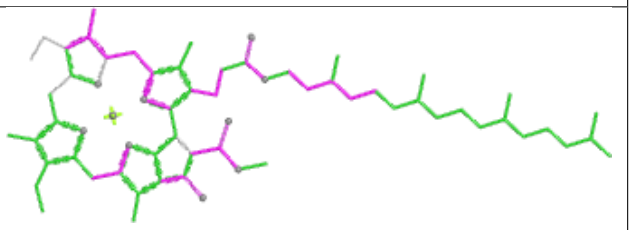
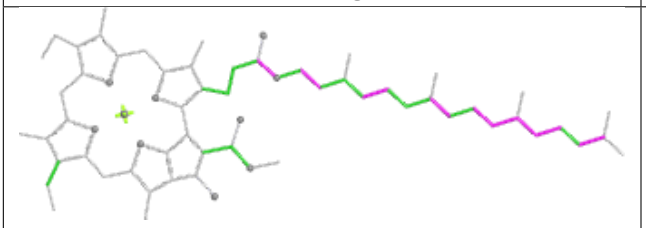

Rings

Ligand CLA C 513


Bond lengths


Bond angles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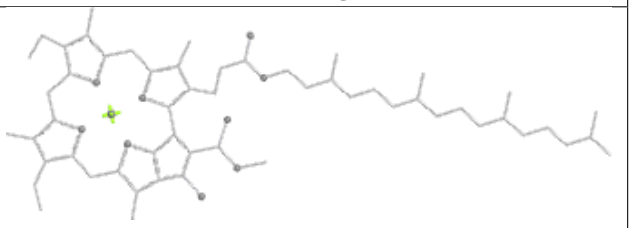
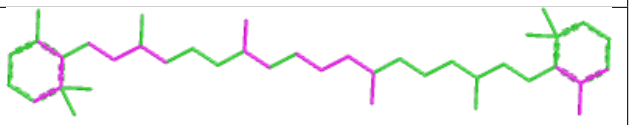
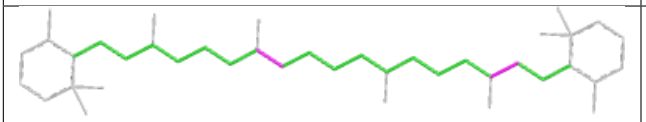

Rings

Ligand BCR c 516


Bond lengths


Bond angles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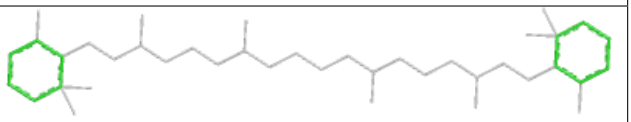
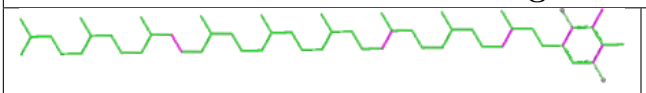

Rings

Ligand PL9 D 405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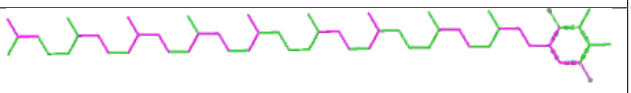
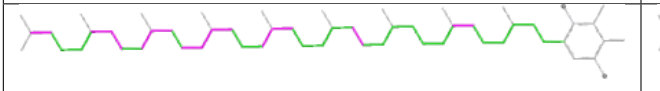
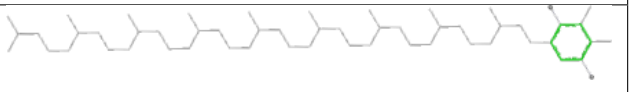
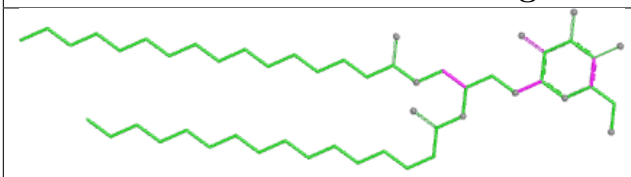

Bond angles

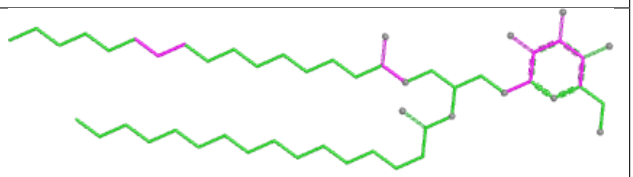

Torsions


Rings

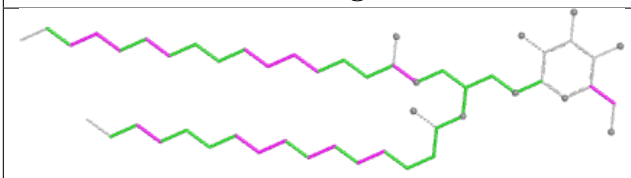
Ligand LMG D 408



Bond lengths



Bond angles



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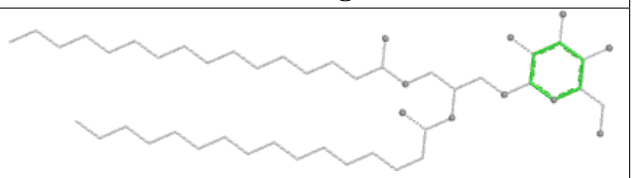
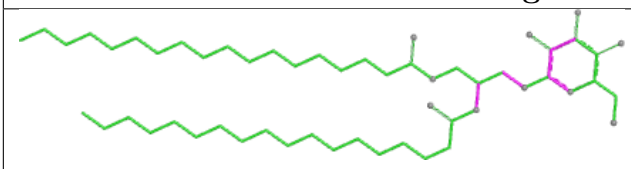


Rings

Ligand LMG b 723



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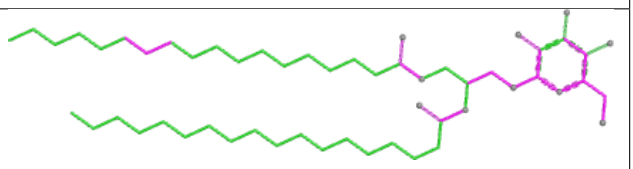
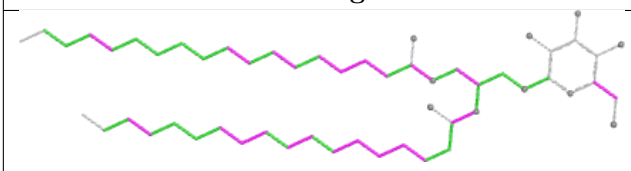


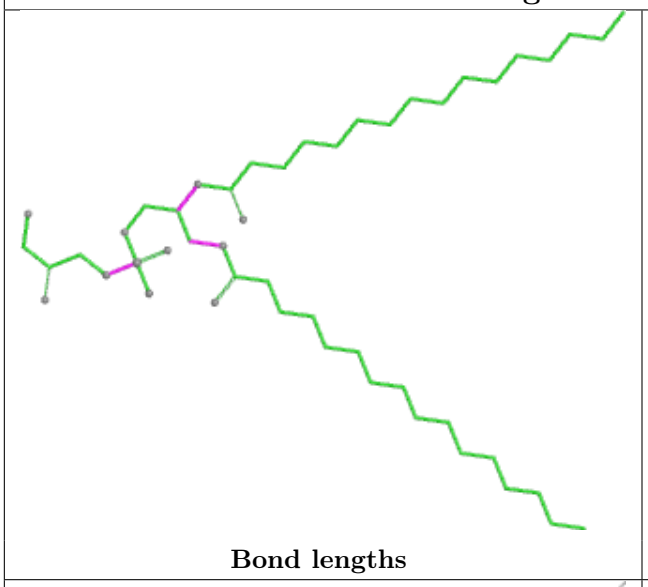
Bond angles



Torsions

Rings

Ligand LHG D 410



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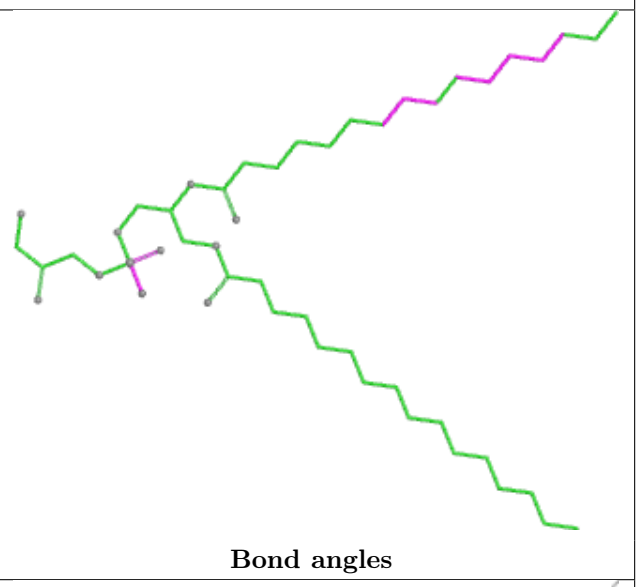

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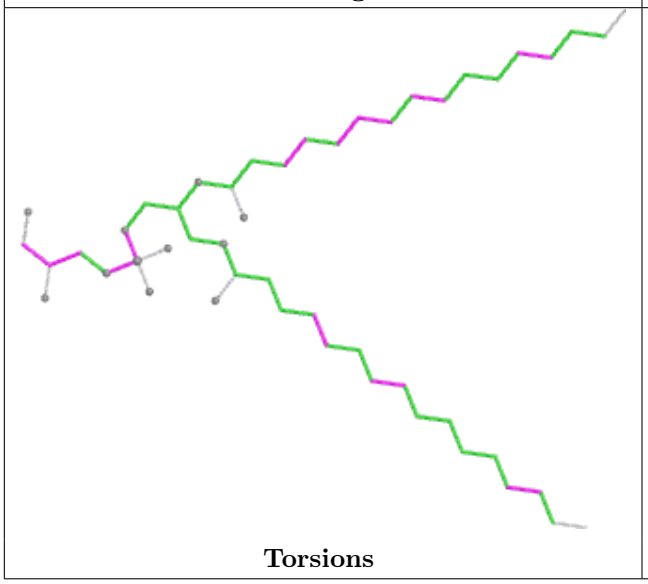

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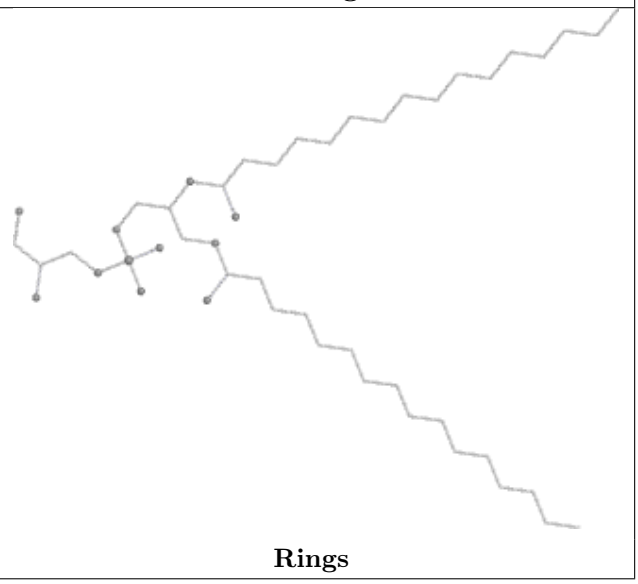
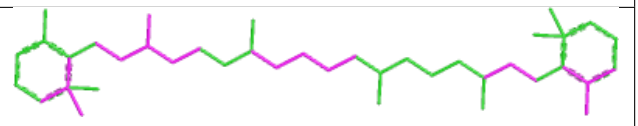


Rings

Ligand BCR K 101

Bond lengths



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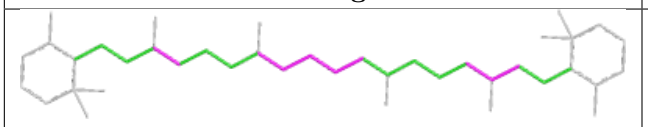

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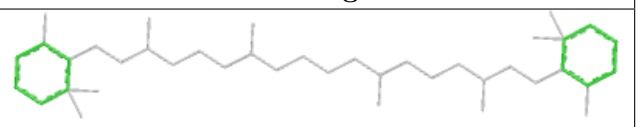
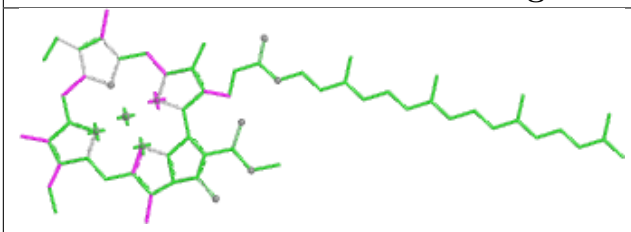
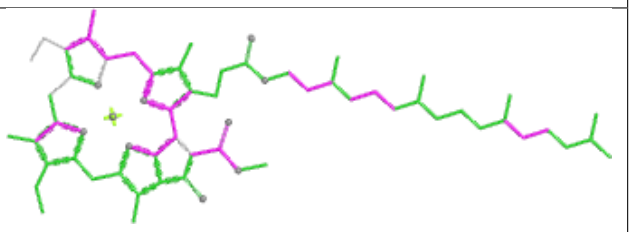


Rings

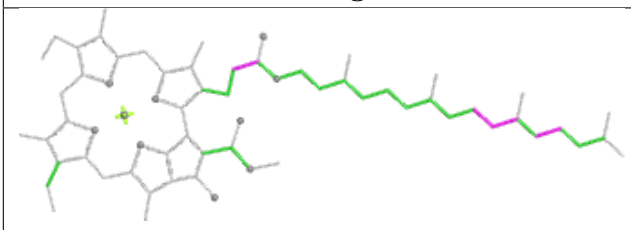
Ligand CLA b 713



Bond lengths



Bond angles



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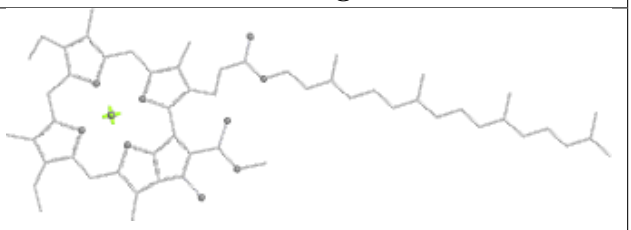
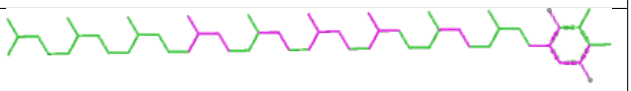


Rings

Ligand PL9 A 408

Bond lengths



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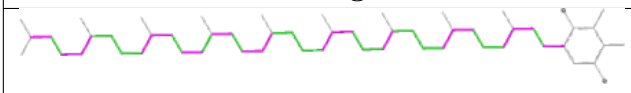

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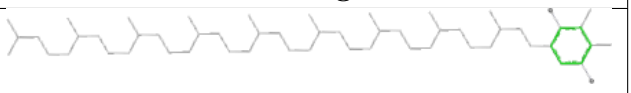
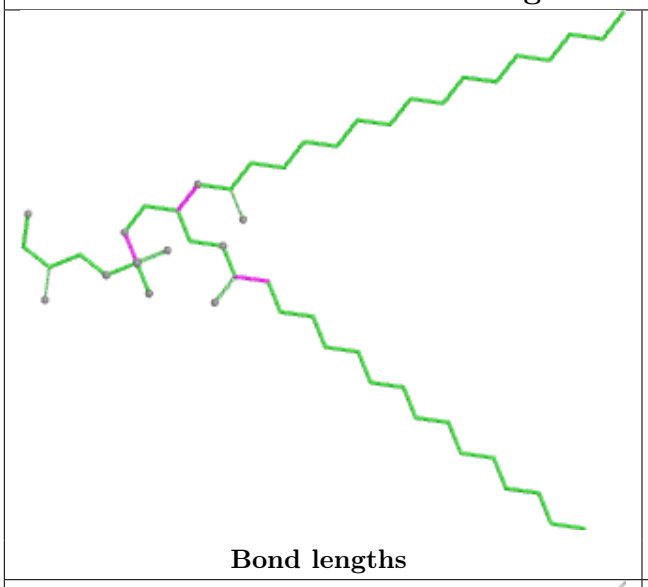


Rings

Ligand LHG B 722



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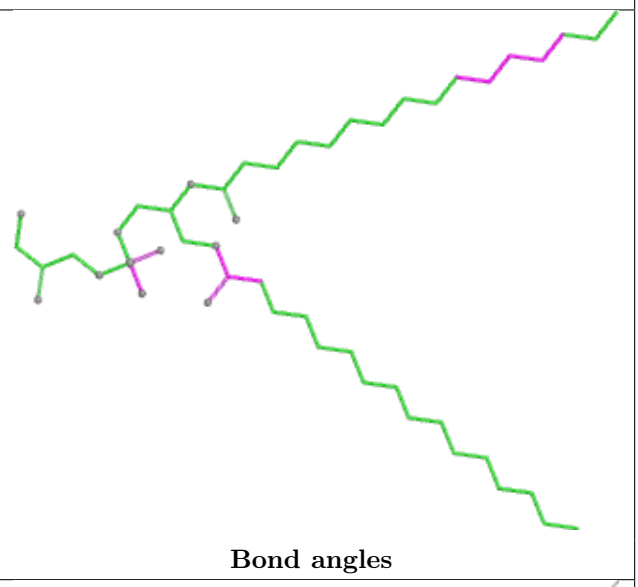
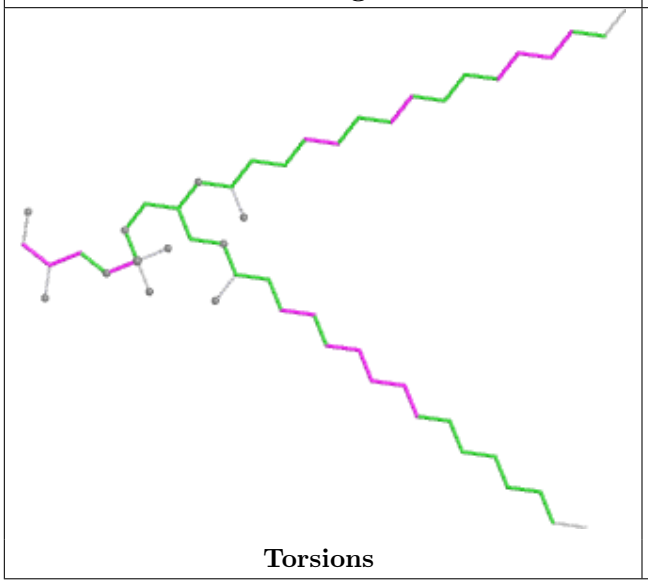


Bond angles



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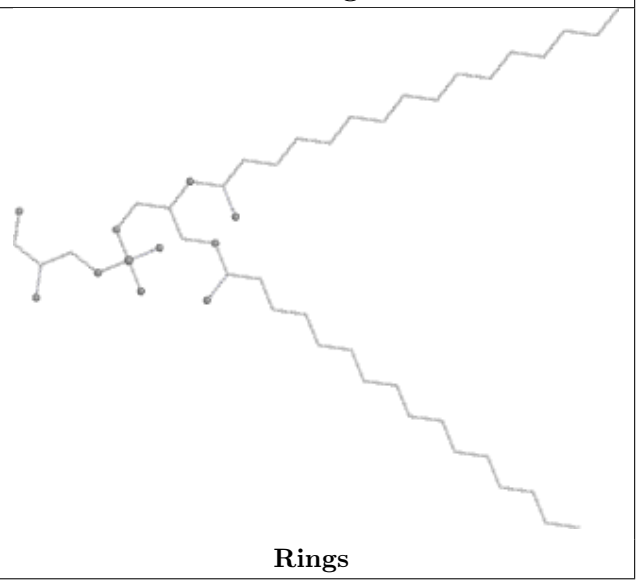
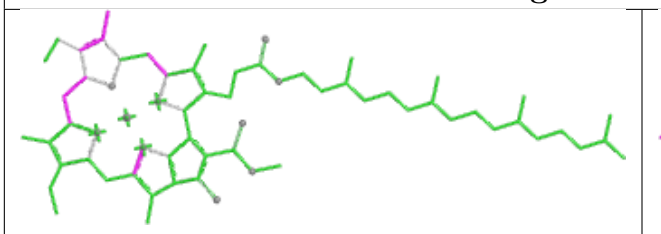
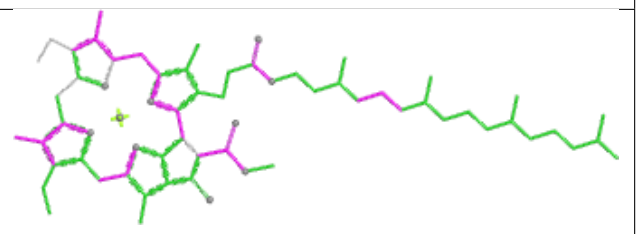


Rings

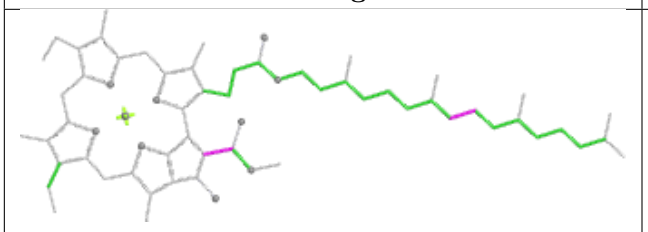
Ligand CLA c 508



Bond lengths



Bond angles



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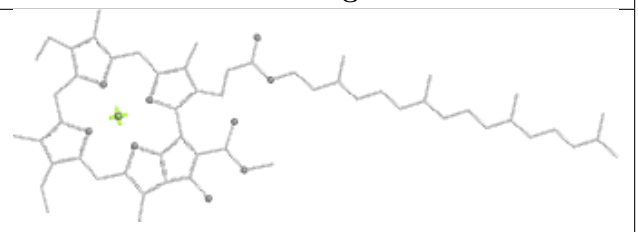
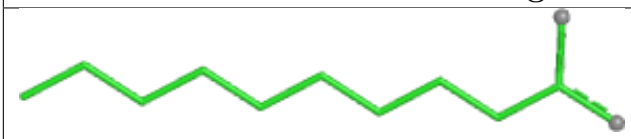
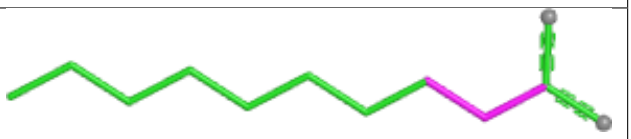
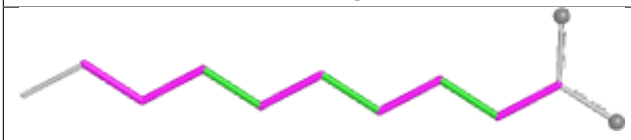
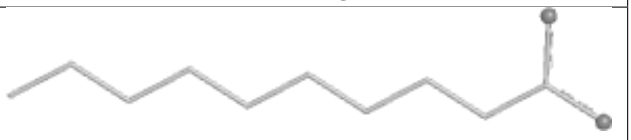
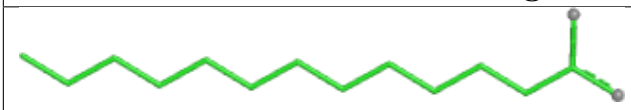
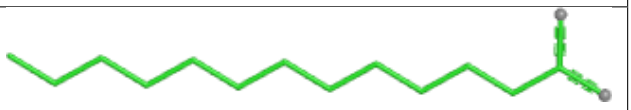
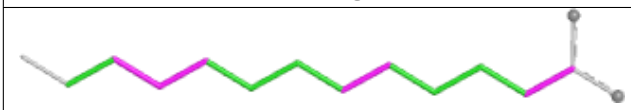
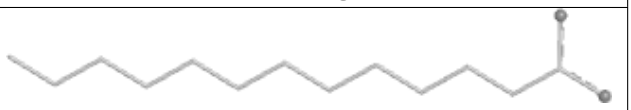
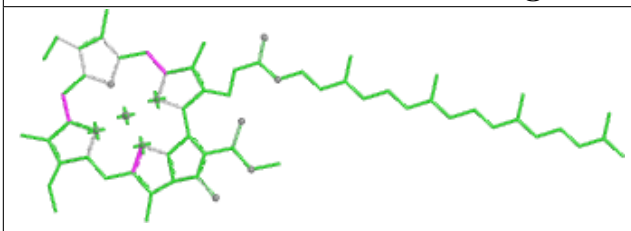
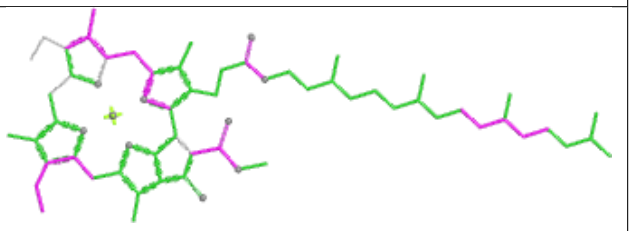
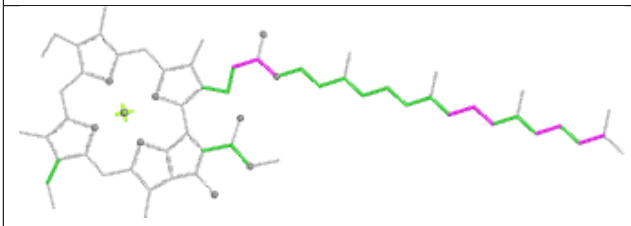
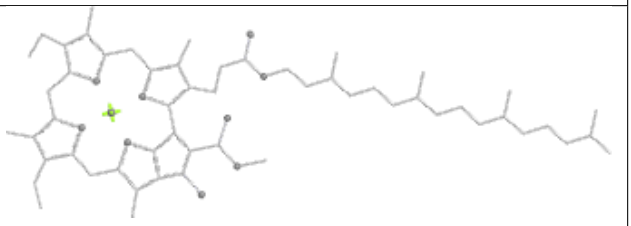
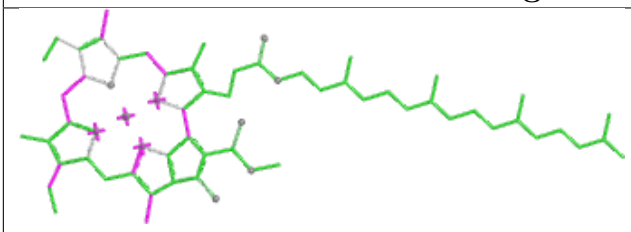
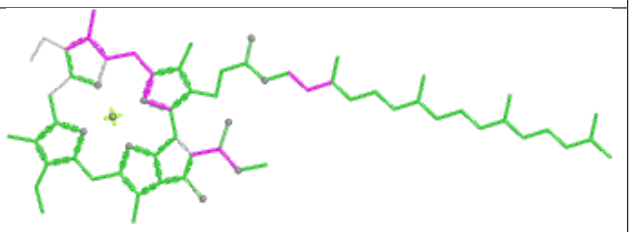
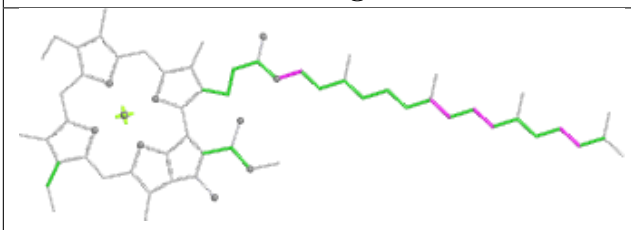
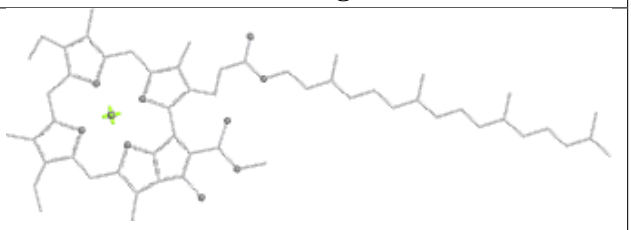


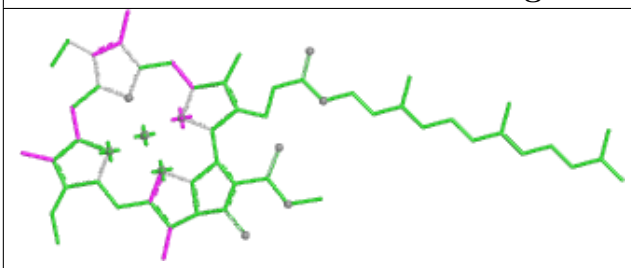
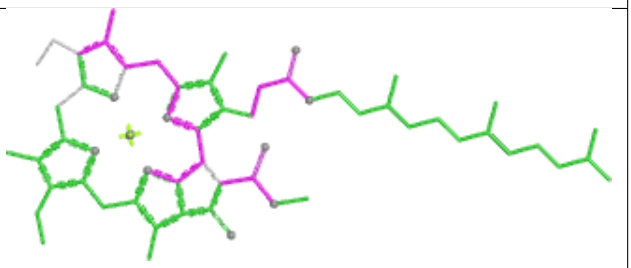
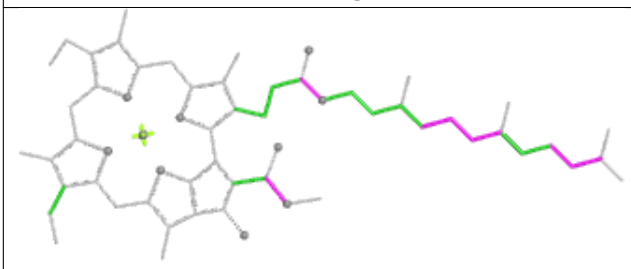
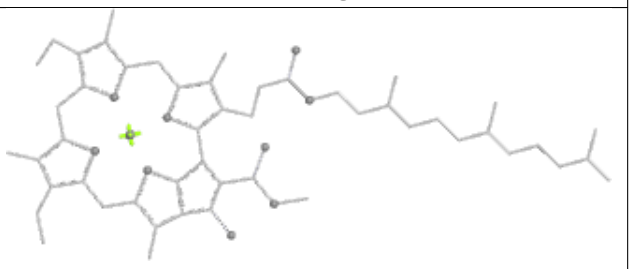
Rings

Ligand STE C 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

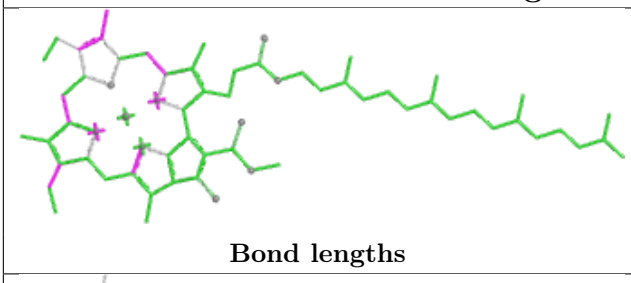
Ligand STE M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 712	
 Bond lengths	 Bond angles
 Torsions	 Rings

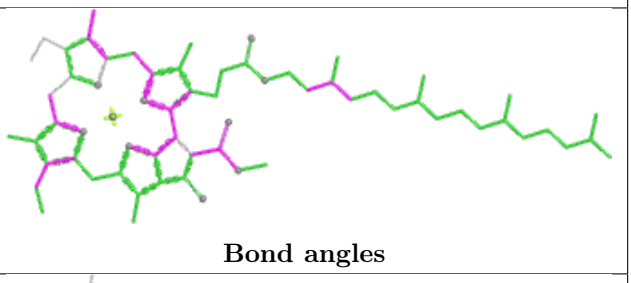
Ligand CLA D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 716	
 Bond lengths	 Bond angles
 Torsions	 Rings

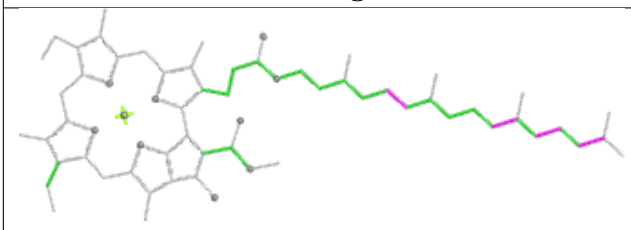
Ligand CLA B 715



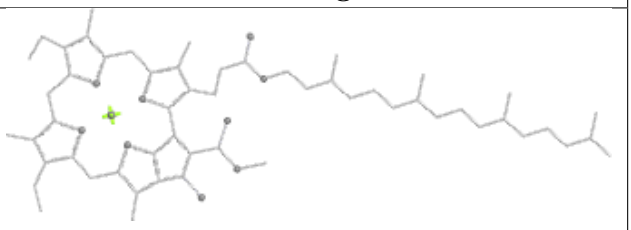
Bond lengths



Bond angles

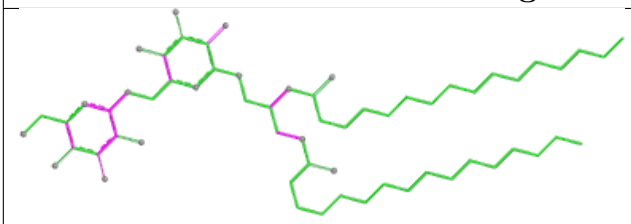


Torsions

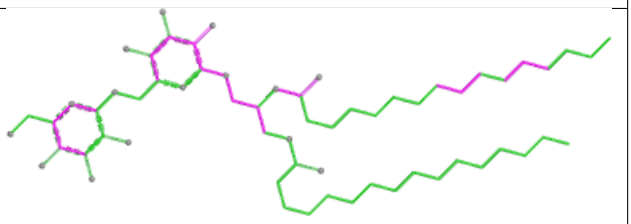


Rings

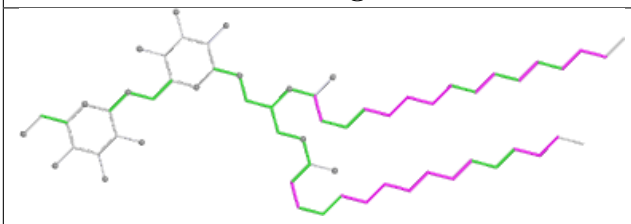
Ligand DGD H 103



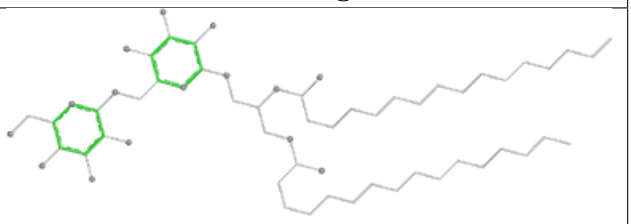
Bond lengths



Bond angles

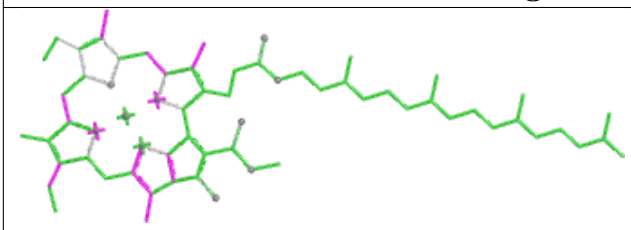


Torsions

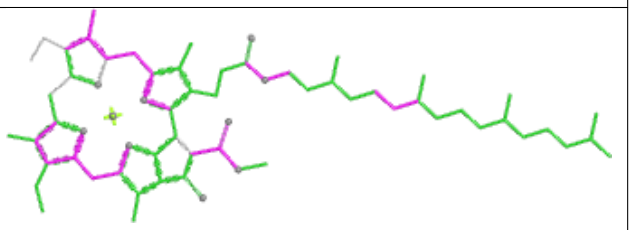


Rings

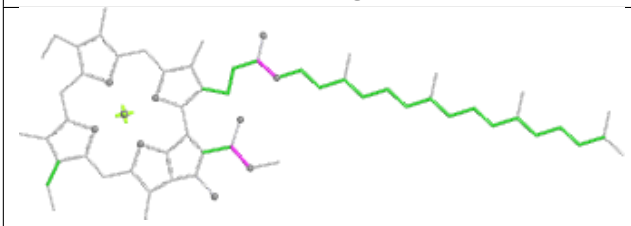
Ligand CLA B 708



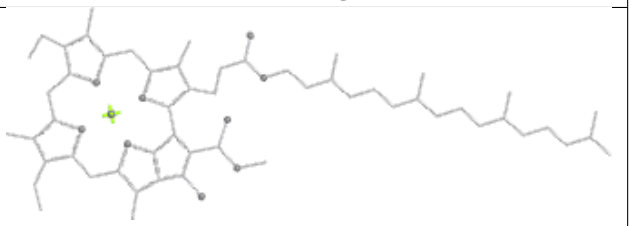
Bond lengths



Bond angles

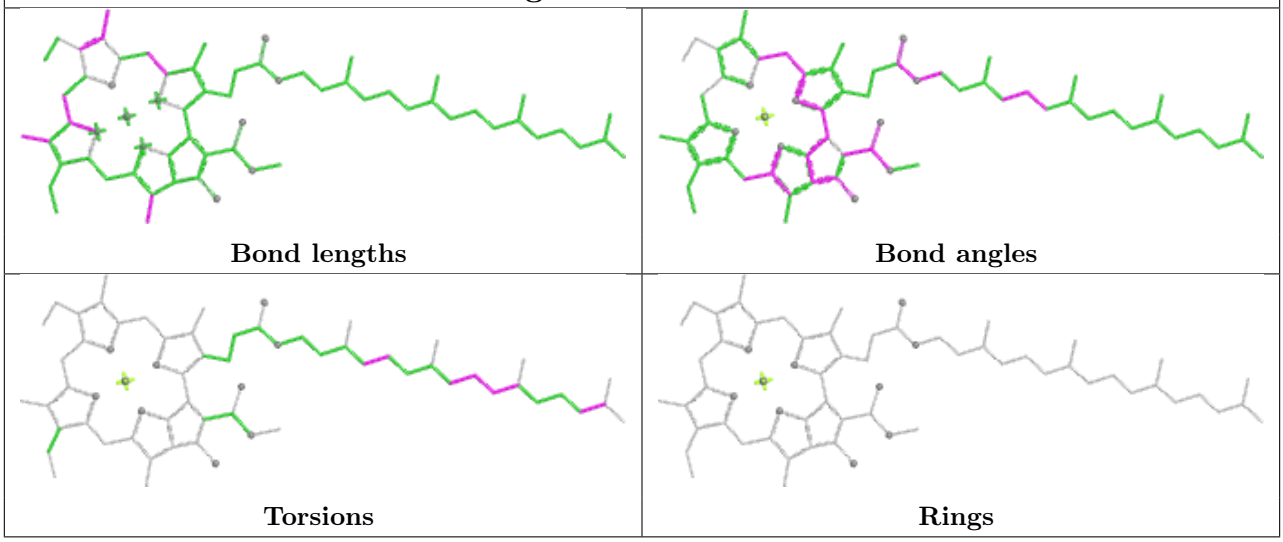


Torsions

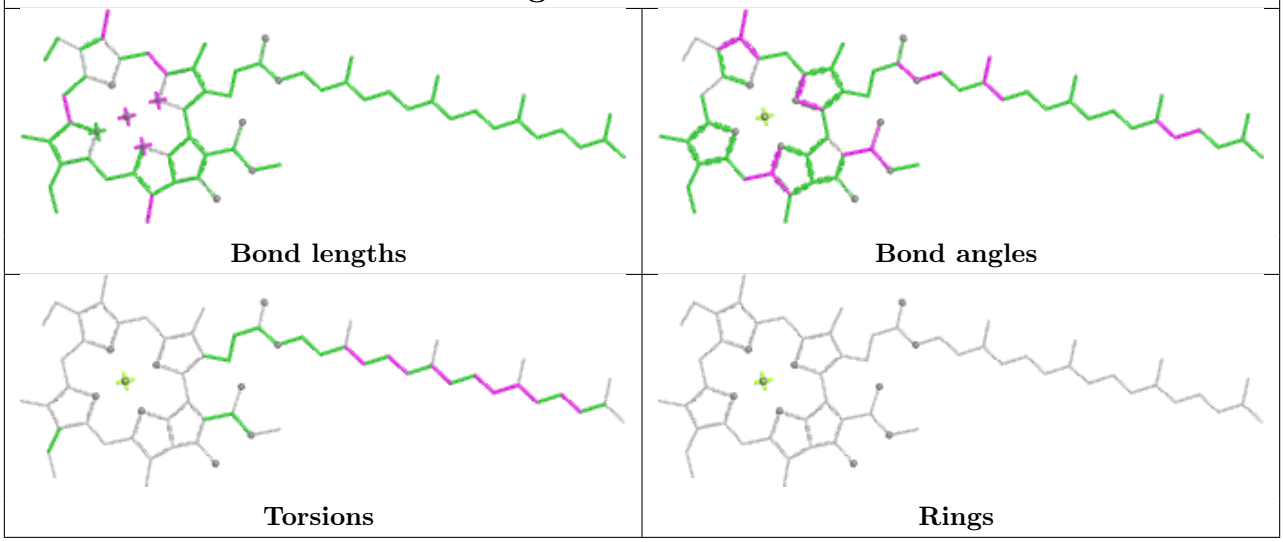


Rings

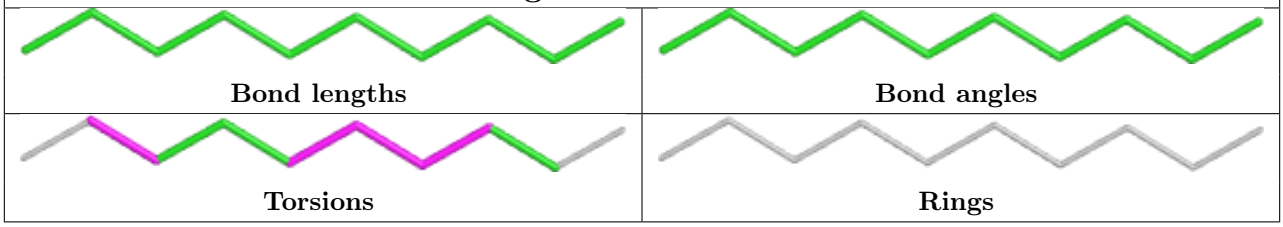
Ligand CLA B 705



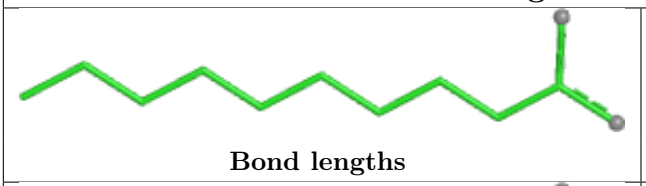
Ligand CLA b 705



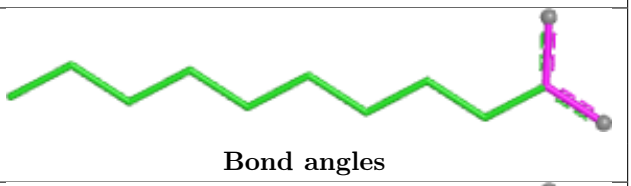
Ligand STE M 103



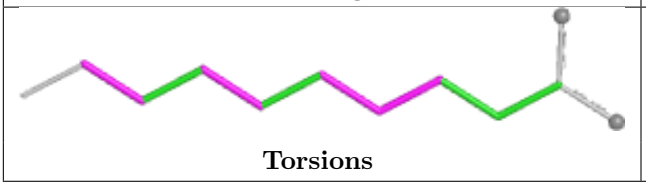
Ligand STE B 701



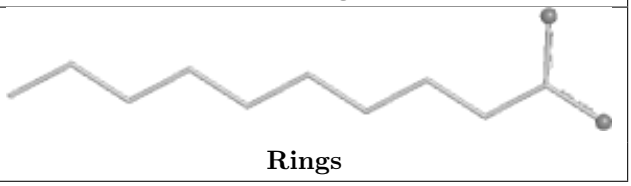
Bond lengths



Bond angles

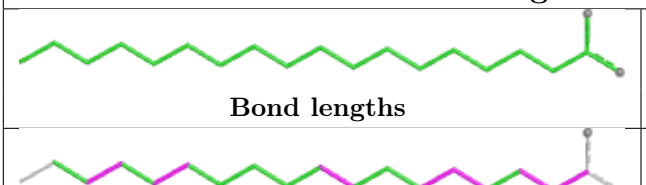


Torsions

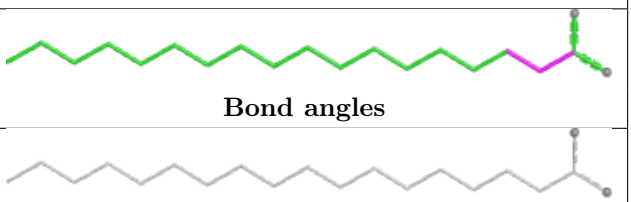


Rings

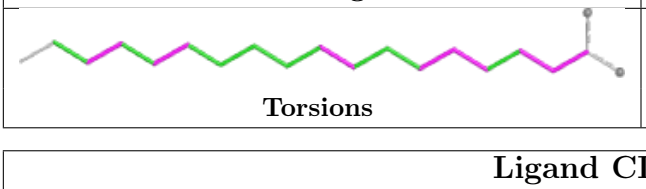
Ligand STE b 725



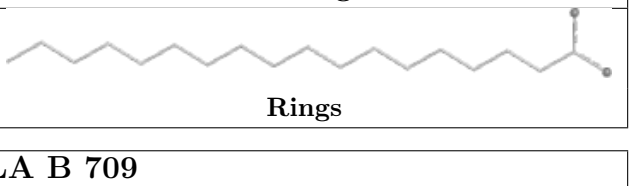
Bond lengths



Bond angles

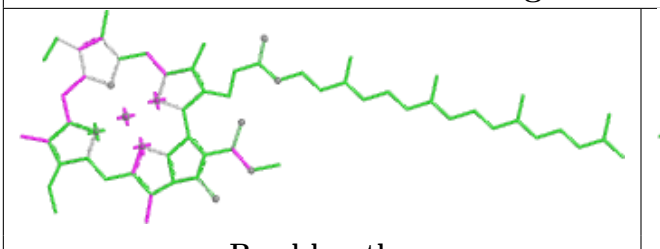


Torsions

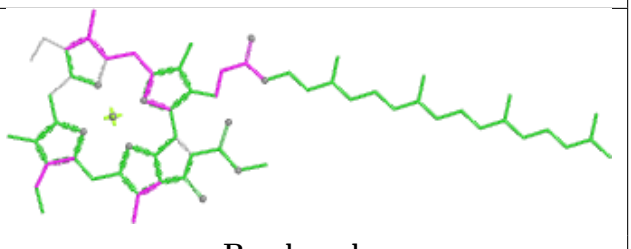


Rings

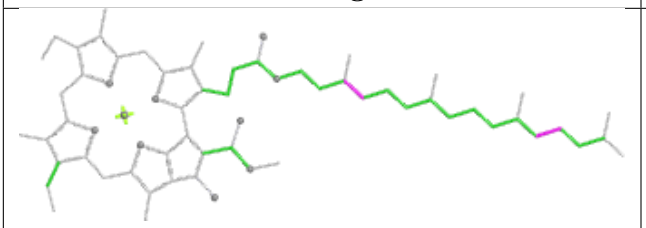
Ligand CLA B 709



Bond lengths



Bond angles



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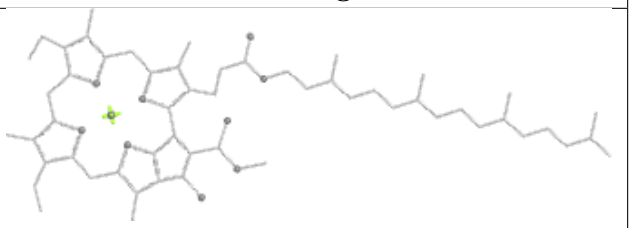
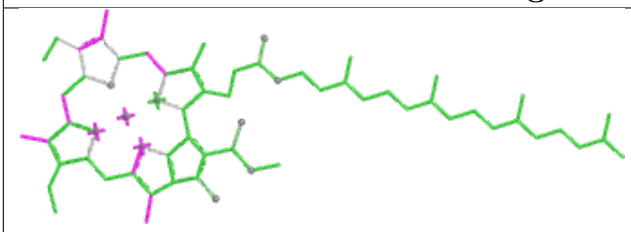


Rings

Ligand CLA b 712



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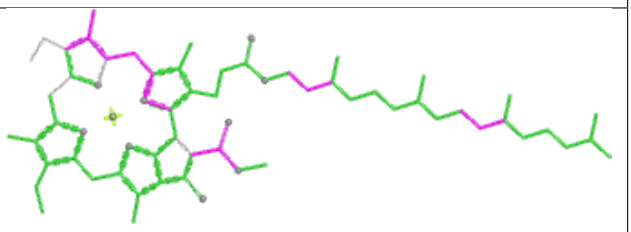
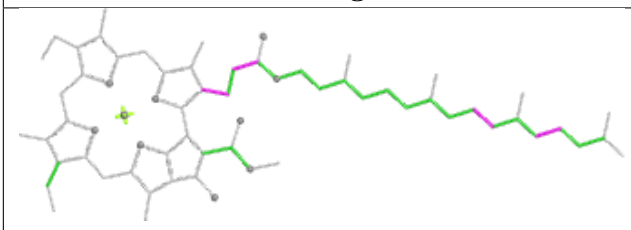
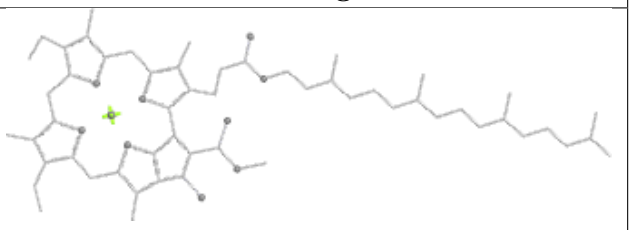


Bond angles

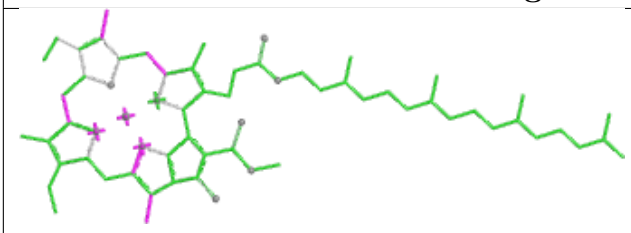


Torsions



Rings

Ligand CLA B 711



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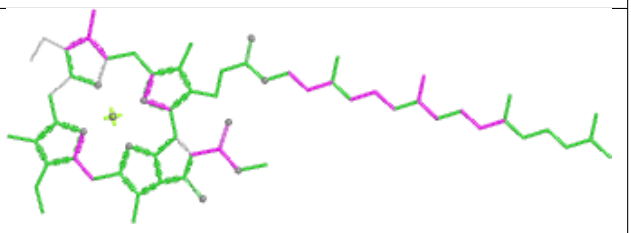
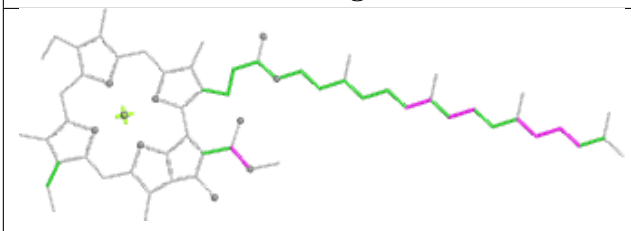
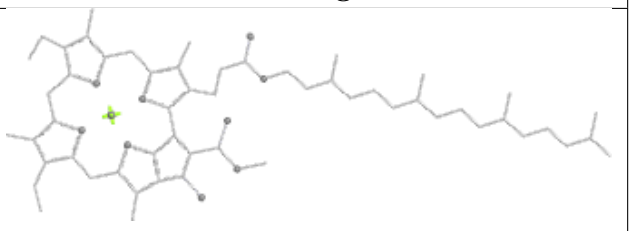


Bond angles

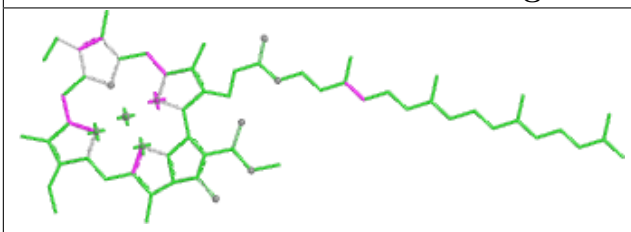


Torsions



Rings

Ligand CLA A 402



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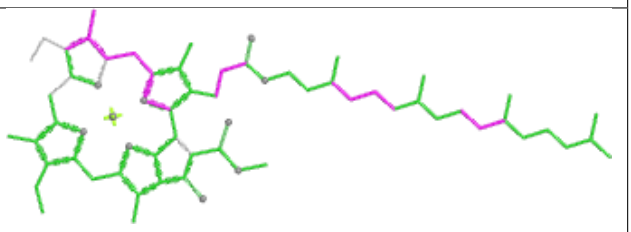
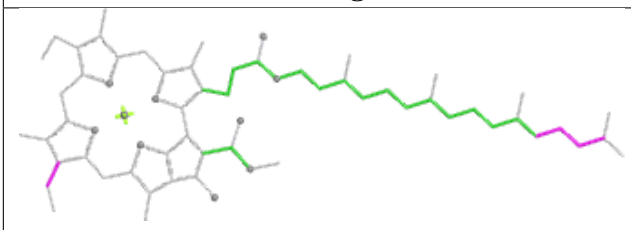
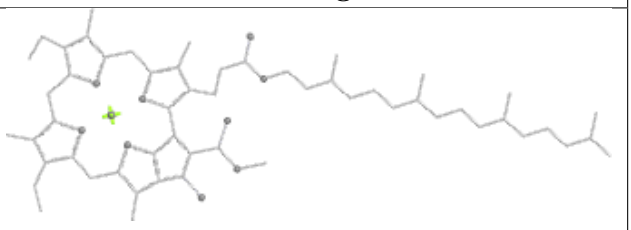


Bond angles

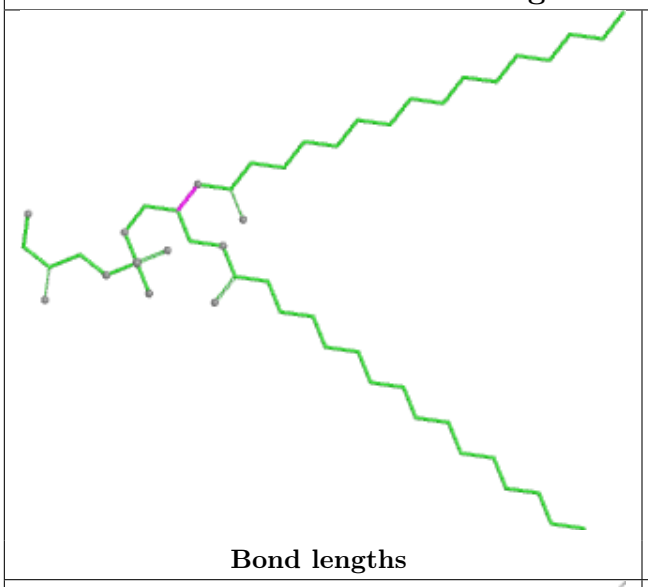


Torsions

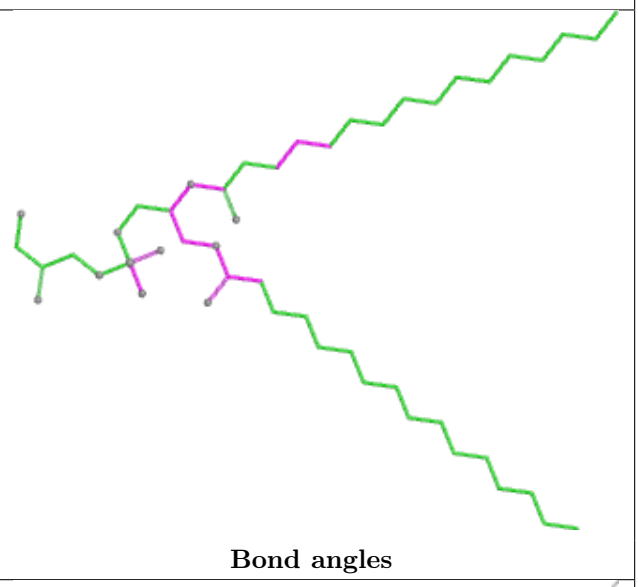


Rings

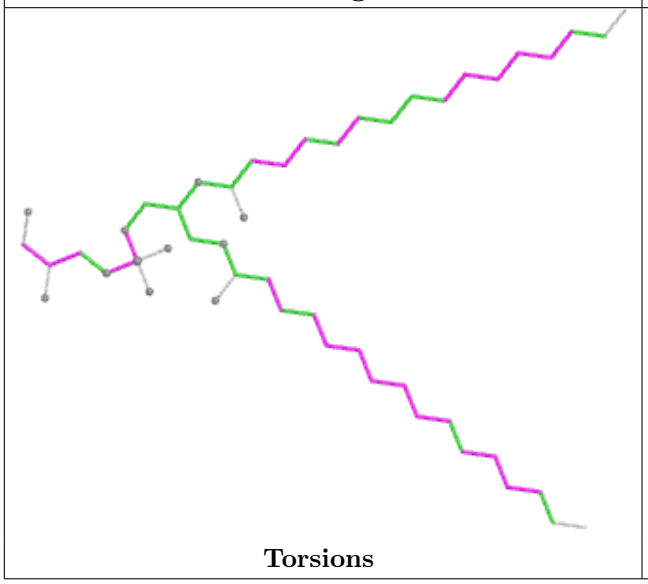
Ligand LHG a 412



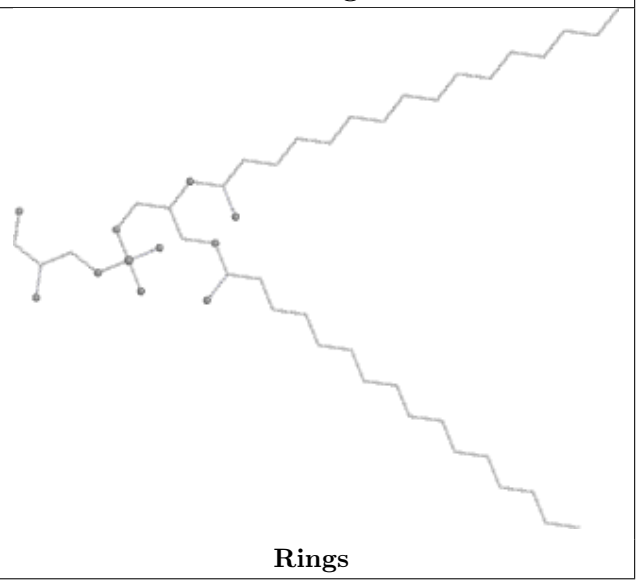
Bond lengths



Bond angles

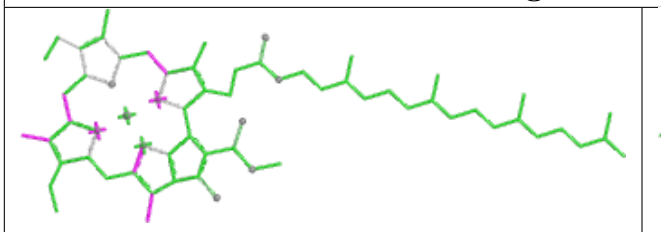


Torsions

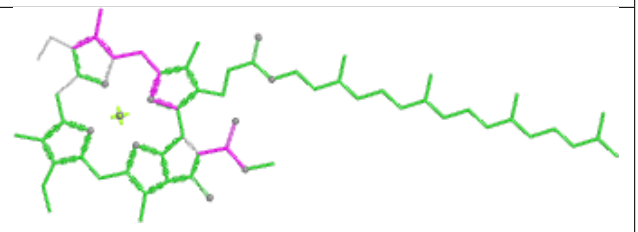


Rings

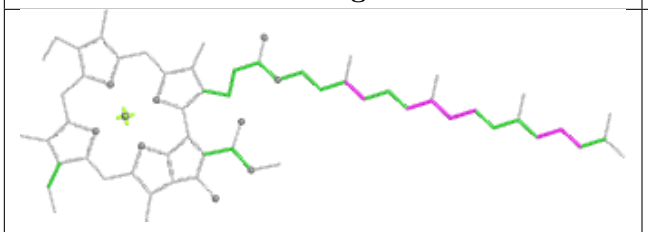
Ligand CLA C 511



Bond lengths



Bond angles



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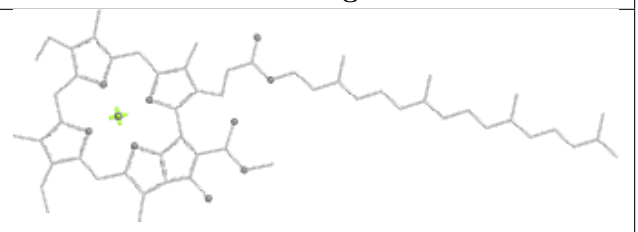
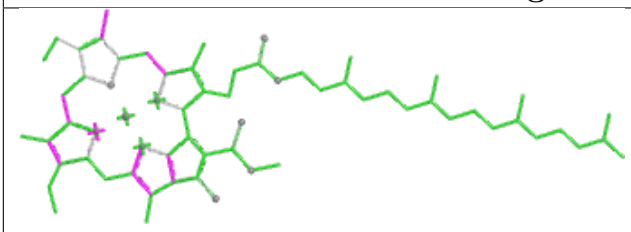


Rings

Ligand CLA b 708



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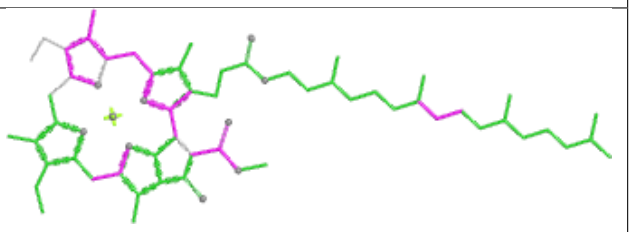
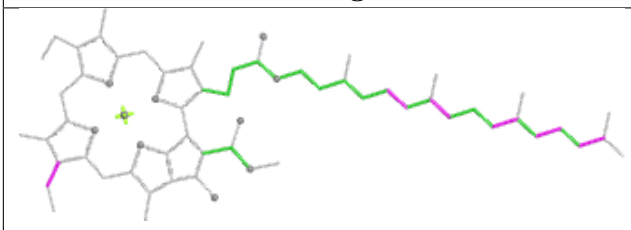


Bond angles



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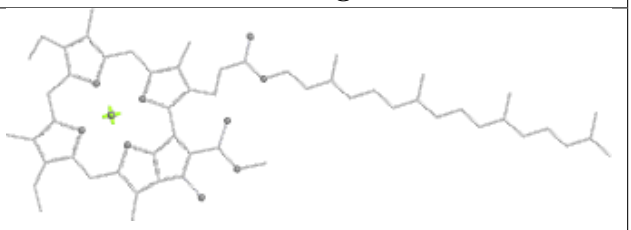
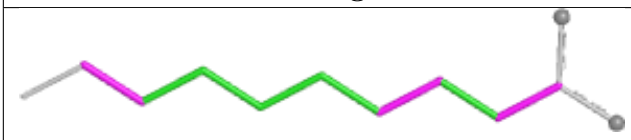


Rings

Ligand STE c 501

Bond lengths

Bond angles



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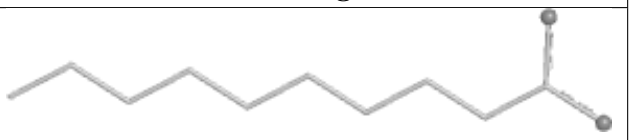
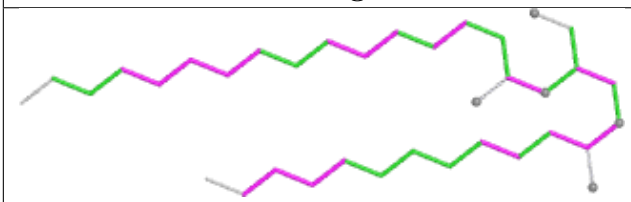


Rings

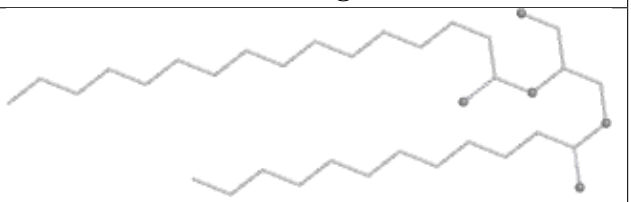
Ligand SQD a 415

Bond lengths

Bond angles

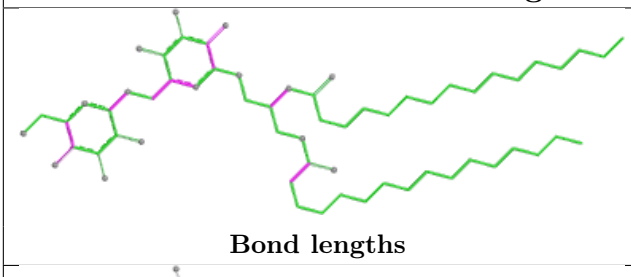


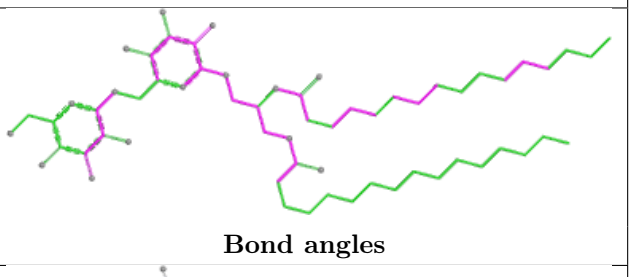
Torsions

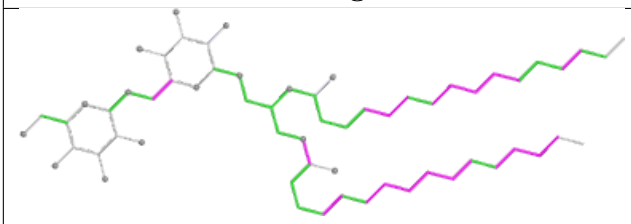


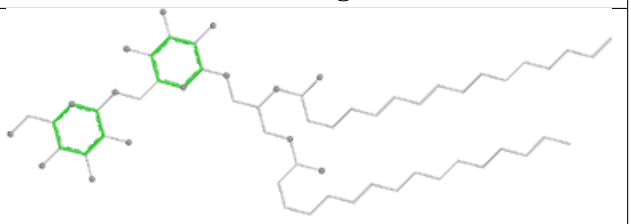
Rings

Ligand DGD c 519


Bond lengths


Bond angles


Torsions


Rings

Ligand STE a 418

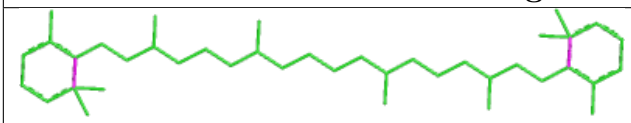

Bond lengths

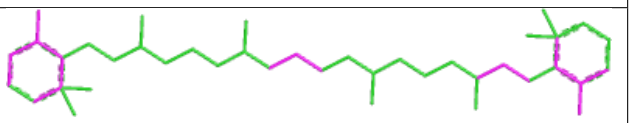

Bond angles

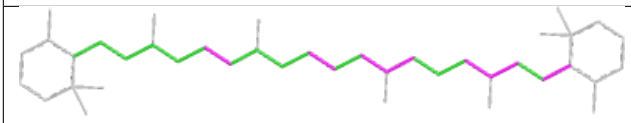

Torsions

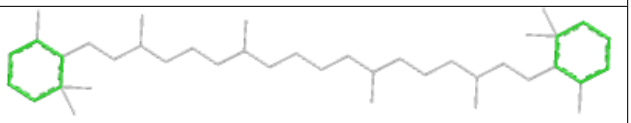

Rings

Ligand BCR d 403

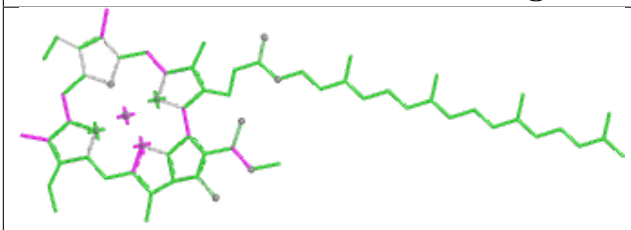

Bond lengths

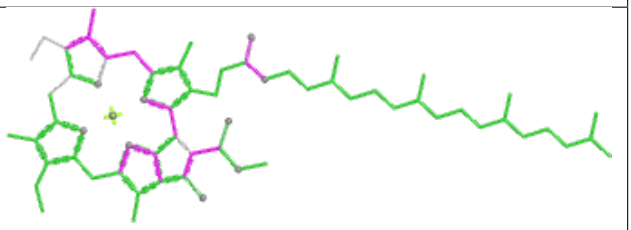

Bond angles

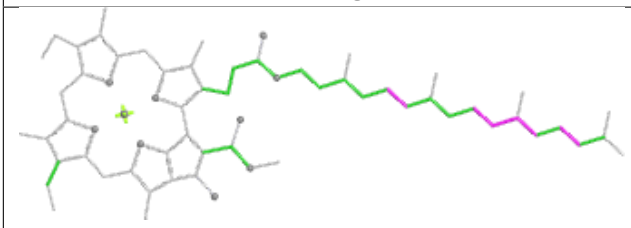

Torsions

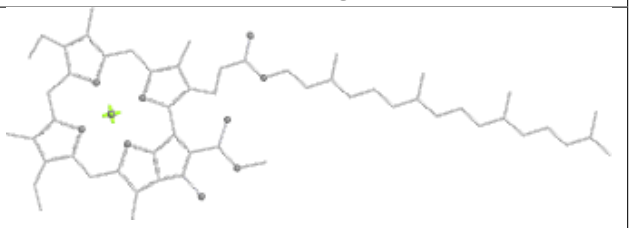

Rings

Ligand CLA d 402

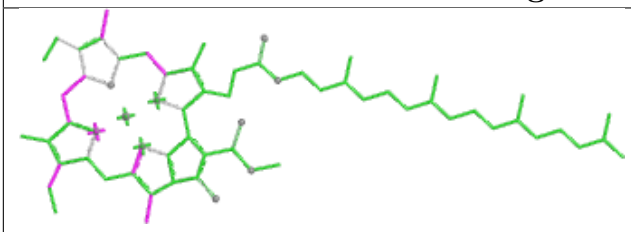

Bond lengths


Bond angles

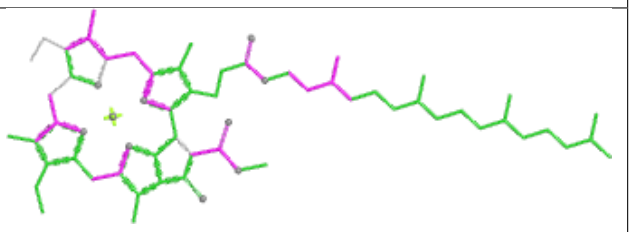

Torsions


Rings

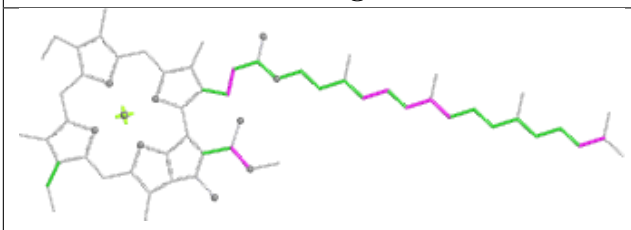
Ligand CLA b 702



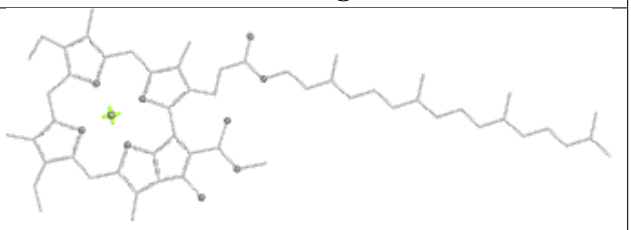
Bond lengths



Bond angles

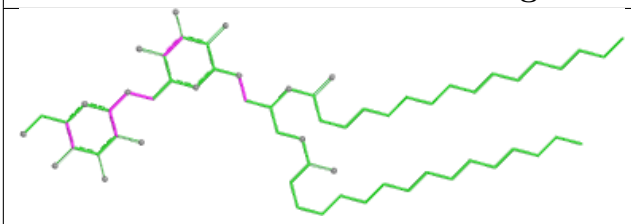


Torsions

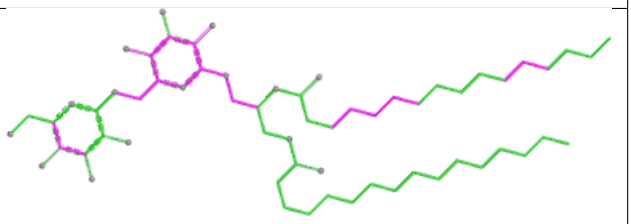


Rings

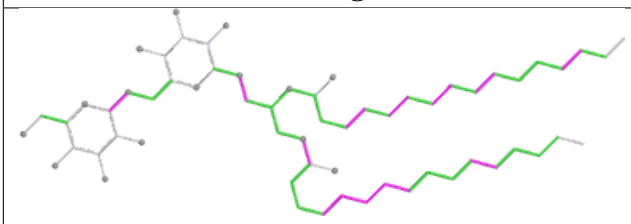
Ligand DGD C 518



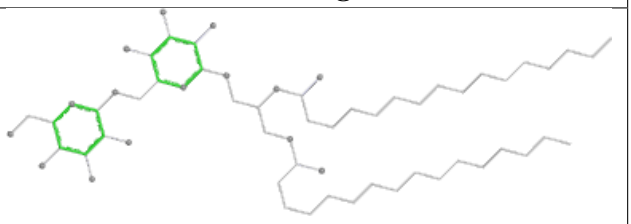
Bond lengths



Bond angles

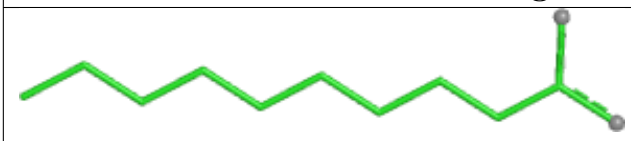


Torsions

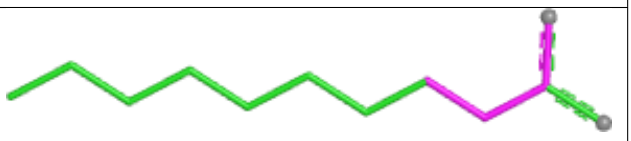


Rings

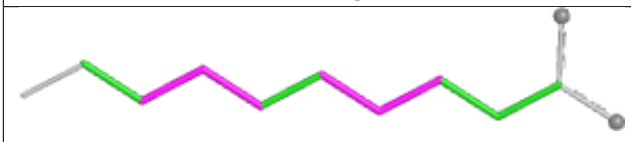
Ligand STE J 101



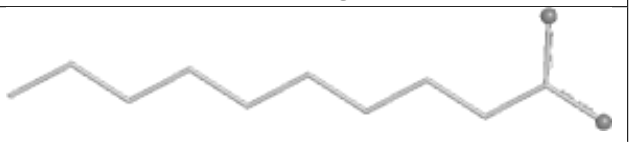
Bond lengths



Bond angles

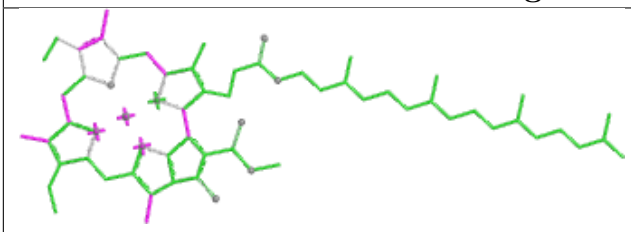


Torsions

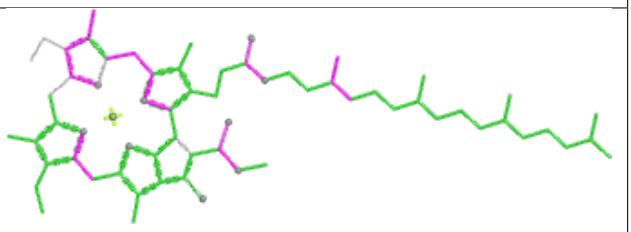


Rings

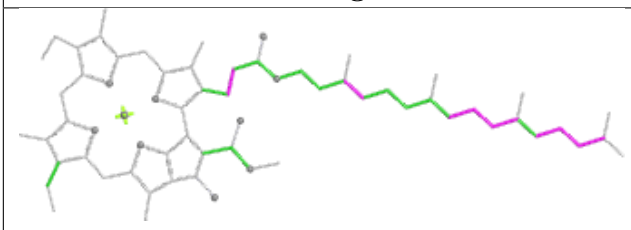
Ligand CLA B 703



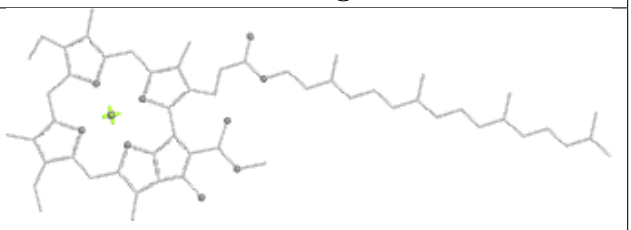
Bond lengths



Bond angles

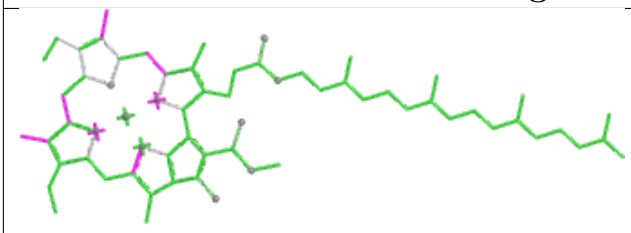


Torsions

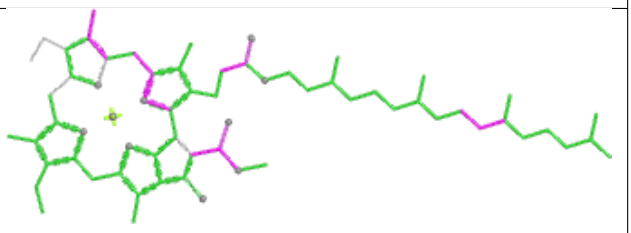


Rings

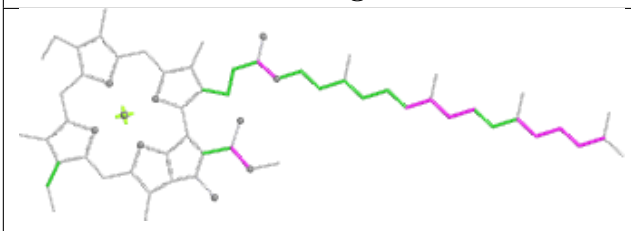
Ligand CLA c 512



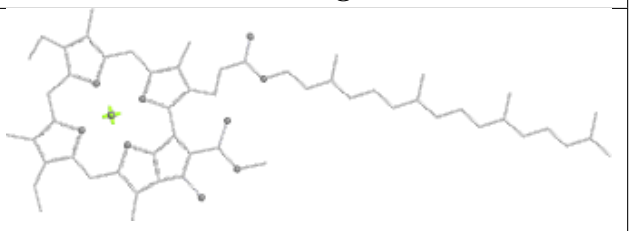
Bond lengths



Bond angles

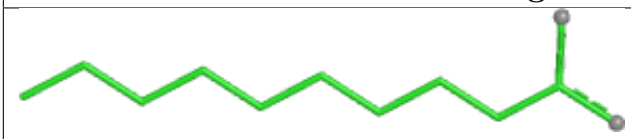


Torsions

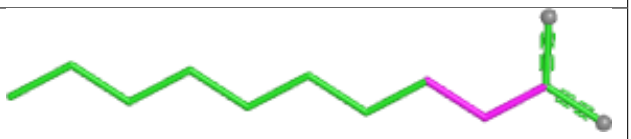


Rings

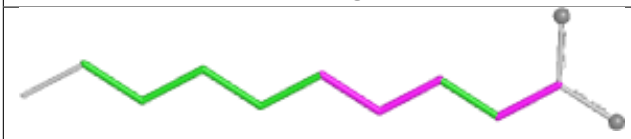
Ligand STE B 724



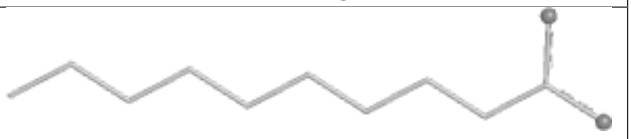
Bond lengths



Bond angles

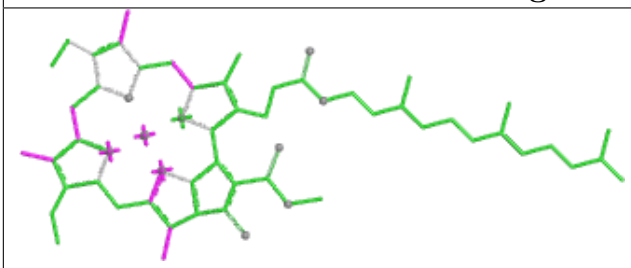


Torsions

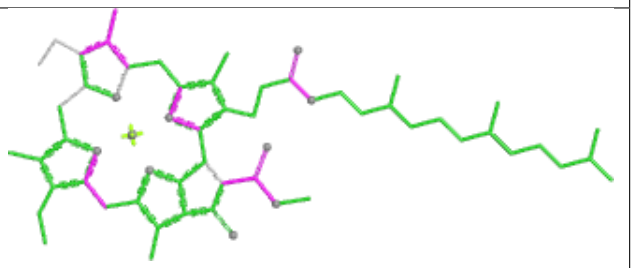


Rings

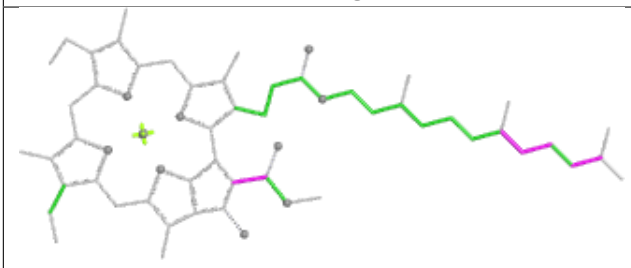
Ligand CLA c 505



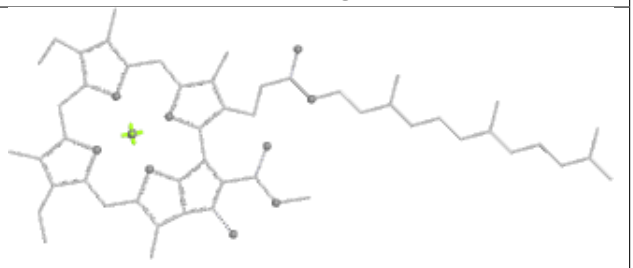
Bond lengths



Bond angles

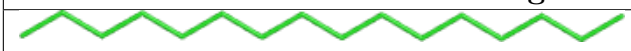


Torsions



Rings

Ligand STE B 726



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.51	0 100 100	12, 31, 56, 88	64 (19%)
1	a	334/344 (97%)	-0.42	2 (0%) 85 86	14, 33, 63, 91	64 (19%)
2	B	505/510 (99%)	-0.51	0 100 100	18, 36, 67, 100	4 (0%)
2	b	505/510 (99%)	-0.39	3 (0%) 85 86	26, 40, 79, 117	0
3	C	442/461 (95%)	-0.44	0 100 100	15, 40, 57, 90	11 (2%)
3	c	451/461 (97%)	-0.35	2 (0%) 89 90	15, 43, 69, 101	12 (2%)
4	D	341/352 (96%)	-0.63	0 100 100	16, 34, 52, 88	2 (0%)
4	d	341/352 (96%)	-0.47	1 (0%) 90 91	16, 37, 65, 83	3 (0%)
5	E	82/84 (97%)	0.16	1 (1%) 76 77	35, 57, 76, 88	1 (1%)
5	e	82/84 (97%)	0.17	1 (1%) 76 77	41, 64, 85, 87	0
6	F	34/45 (75%)	-0.18	0 100 100	42, 49, 73, 90	0
6	f	34/45 (75%)	0.08	1 (2%) 54 55	44, 54, 86, 99	0
7	H	65/66 (98%)	-0.28	3 (4%) 38 40	36, 45, 64, 75	0
7	h	63/66 (95%)	-0.02	1 (1%) 70 71	43, 55, 68, 81	0
8	I	35/38 (92%)	-0.44	0 100 100	35, 42, 77, 88	0
8	i	35/38 (92%)	-0.27	0 100 100	34, 45, 78, 85	0
9	J	36/40 (90%)	-0.22	0 100 100	35, 54, 83, 100	0
9	j	36/40 (90%)	0.09	1 (2%) 55 57	44, 56, 89, 104	0
10	K	37/46 (80%)	-0.01	0 100 100	48, 58, 79, 87	0
10	k	37/46 (80%)	0.10	0 100 100	53, 61, 76, 86	0
11	L	37/37 (100%)	-0.64	0 100 100	28, 35, 70, 75	0
11	l	36/37 (97%)	-0.65	0 100 100	25, 34, 80, 95	0
12	M	32/36 (88%)	-0.57	0 100 100	28, 38, 61, 76	0
12	m	31/36 (86%)	-0.61	0 100 100	27, 38, 54, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.29	2 (0%) 82 83	26, 45, 85, 139	1 (0%)
13	o	244/272 (89%)	-0.33	1 (0%) 89 90	27, 44, 86, 128	0
14	R	34/41 (82%)	0.98	1 (2%) 54 55	68, 86, 101, 114	0
14	r	31/41 (75%)	1.33	4 (12%) 9 9	85, 108, 125, 139	0
15	T	29/32 (90%)	-0.66	0 100 100	29, 34, 69, 80	0
15	t	29/32 (90%)	-0.50	1 (3%) 48 50	29, 36, 85, 92	0
16	U	97/134 (72%)	-0.28	0 100 100	33, 48, 76, 94	0
16	u	97/134 (72%)	-0.34	0 100 100	33, 44, 63, 82	0
17	V	137/163 (84%)	-0.44	0 100 100	32, 43, 59, 85	0
17	v	137/163 (84%)	-0.25	0 100 100	31, 51, 75, 89	0
18	X	38/41 (92%)	-0.12	1 (2%) 57 59	46, 57, 82, 88	0
18	x	39/41 (95%)	0.13	2 (5%) 34 36	54, 66, 96, 113	0
19	Y	27/46 (58%)	0.84	2 (7%) 22 24	58, 82, 96, 105	0
19	y	30/46 (65%)	0.53	0 100 100	66, 79, 94, 105	0
20	Z	62/62 (100%)	0.59	2 (3%) 50 52	58, 73, 117, 131	0
20	z	62/62 (100%)	0.58	3 (4%) 36 38	58, 77, 117, 129	0
All	All	5302/5700 (93%)	-0.33	35 (0%) 84 85	12, 42, 81, 139	162 (3%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	R	35	LEU	4.0
13	o	58	ASN	3.7
14	r	32	GLN	3.7
13	O	60	ARG	3.6
15	t	30	THR	3.1
5	e	79	PHE	3.0
14	r	14	LEU	3.0
2	b	495	PHE	2.9
3	c	23	ALA	2.9
1	a	250	ALA	2.9
9	j	6	GLY	2.8
20	Z	33	TRP	2.8
20	z	33	TRP	2.8
19	Y	22	LEU	2.8
7	H	41	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	2.8
20	z	27	TYR	2.7
18	x	40	SER	2.6
7	h	64	ALA	2.6
20	z	40	ILE	2.6
2	b	499	VAL	2.5
14	r	18	TRP	2.4
20	Z	62	VAL	2.4
4	d	239	GLN	2.4
1	a	249	VAL	2.3
13	O	59	LYS	2.3
19	Y	25	ILE	2.3
5	E	79	PHE	2.3
6	f	15	ILE	2.2
14	r	3	TRP	2.2
18	X	2	THR	2.1
18	x	2	THR	2.1
2	b	496	TYR	2.1
7	H	66	GLY	2.1
3	c	24	THR	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
8	FME	I	1	10/11	0.93	0.09	39,52,68,71	0
15	FME	t	1	10/11	0.94	0.08	29,46,71,71	0
15	FME	T	1	10/11	0.95	0.08	27,47,63,64	0
12	FME	M	1	10/11	0.95	0.08	41,50,66,80	0
8	FME	i	1	10/11	0.96	0.09	38,48,60,62	0
12	FME	m	1	10/11	0.96	0.07	34,48,69,82	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
28	STE	b	726	10/20	0.75	0.16	43,56,67,75	0
28	STE	I	101	15/20	0.77	0.17	40,55,81,86	0
28	STE	H	104	18/20	0.77	0.17	43,76,86,92	0
28	STE	b	725	20/20	0.81	0.14	45,63,80,83	0
33	LMG	c	522	48/55	0.81	0.14	35,77,108,113	0
28	STE	a	416	10/20	0.82	0.14	30,64,69,73	0
28	STE	B	726	16/20	0.82	0.14	43,64,79,86	0
25	PL9	A	408	55/55	0.82	0.16	44,70,86,96	0
28	STE	b	727	20/20	0.82	0.14	43,67,93,95	0
28	STE	c	501	12/20	0.82	0.11	55,68,85,93	0
33	LMG	b	723	55/55	0.82	0.15	45,73,94,109	0
27	LHG	A	410	49/49	0.82	0.13	45,80,104,115	0
28	STE	A	414	5/20	0.83	0.22	41,57,71,71	0
27	LHG	a	414	42/49	0.83	0.14	45,87,109,127	0
28	STE	E	101	12/20	0.83	0.16	56,79,85,90	0
28	STE	h	703	14/20	0.84	0.16	43,66,89,90	0
28	STE	a	417	12/20	0.84	0.12	51,64,76,77	0
28	STE	a	418	15/20	0.84	0.16	36,61,76,79	0
28	STE	C	522	16/20	0.85	0.12	38,53,66,67	0
25	PL9	a	411	55/55	0.85	0.15	42,69,93,98	0
28	STE	E	102	7/20	0.85	0.15	49,62,76,76	0
28	STE	A	411	16/20	0.85	0.14	34,47,74,75	0
28	STE	x	101	20/20	0.85	0.12	45,62,75,81	0
29	DGD	A	413	66/66	0.85	0.11	42,64,79,94	0
33	LMG	a	419	55/55	0.85	0.14	35,62,103,143	0
28	STE	b	724	16/20	0.85	0.14	52,66,82,85	0
28	STE	H	105	8/20	0.85	0.15	47,58,69,69	0
28	STE	C	523	12/20	0.86	0.13	33,46,58,69	0
26	SQD	A	412	39/54	0.86	0.13	38,64,94,99	0
28	STE	c	521	20/20	0.86	0.11	39,57,79,84	0
26	SQD	a	415	36/54	0.86	0.12	25,59,84,92	0
33	LMG	c	520	37/55	0.86	0.12	44,70,84,92	0
28	STE	m	101	12/20	0.86	0.12	42,57,70,79	0
28	STE	J	101	12/20	0.87	0.12	48,67,71,71	0
28	STE	B	720	17/20	0.87	0.11	30,50,62,73	0
33	LMG	D	412	32/55	0.87	0.12	37,57,80,84	0
22	CLA	b	701	65/65	0.87	0.11	48,68,91,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	STE	C	521	12/20	0.87	0.10	34,52,63,66	0
26	SQD	f	101	41/54	0.87	0.13	55,88,106,108	0
26	SQD	B	723	54/54	0.87	0.10	37,60,94,106	0
33	LMG	C	520	48/55	0.88	0.12	43,70,88,94	0
28	STE	l	102	18/20	0.88	0.12	37,50,81,85	0
28	STE	B	724	12/20	0.88	0.10	40,51,66,66	0
28	STE	B	725	18/20	0.88	0.11	37,54,75,81	0
28	STE	j	101	12/20	0.88	0.11	41,57,67,69	0
33	LMG	C	516	48/55	0.88	0.10	38,59,78,100	0
28	STE	t	702	14/20	0.89	0.10	34,53,65,67	0
26	SQD	D	409	36/54	0.89	0.12	48,76,93,99	0
28	STE	B	701	12/20	0.89	0.13	46,61,86,87	0
28	STE	b	722	20/20	0.89	0.10	35,54,74,77	0
28	STE	d	409	17/20	0.89	0.11	42,55,64,68	0
26	SQD	b	720	49/54	0.90	0.09	37,59,91,109	0
22	CLA	C	514	65/65	0.90	0.10	40,65,98,108	0
33	LMG	b	721	51/55	0.90	0.10	34,52,76,93	0
33	LMG	B	721	28/55	0.90	0.11	33,50,62,68	0
23	BCR	c	515	40/40	0.90	0.10	45,61,76,80	0
23	BCR	h	701	40/40	0.90	0.11	37,56,75,86	0
28	STE	Z	101	8/20	0.91	0.14	39,57,68,68	0
23	BCR	d	403	40/40	0.91	0.10	36,54,93,108	0
33	LMG	M	101	51/55	0.91	0.09	30,48,73,79	0
23	BCR	K	101	40/40	0.91	0.11	42,57,71,79	0
26	SQD	a	413	54/54	0.91	0.10	41,64,90,97	0
23	BCR	k	101	40/40	0.91	0.10	36,63,79,87	0
28	STE	T	702	15/20	0.91	0.11	39,54,81,81	0
28	STE	X	101	20/20	0.91	0.10	33,49,69,79	0
33	LMG	c	523	49/55	0.91	0.10	34,57,82,100	0
22	CLA	c	513	65/65	0.92	0.10	40,59,95,110	0
23	BCR	Y	101	40/40	0.92	0.09	40,54,75,77	0
29	DGD	h	702	62/66	0.92	0.09	32,48,61,73	0
23	BCR	H	101	40/40	0.92	0.09	34,48,61,78	0
28	STE	M	102	15/20	0.92	0.10	34,51,65,75	0
28	STE	M	103	10/20	0.92	0.09	34,47,51,58	0
23	BCR	k	102	40/40	0.92	0.10	40,54,68,71	0
22	CLA	c	514	65/65	0.93	0.10	43,71,109,112	0
33	LMG	D	408	51/55	0.93	0.10	34,55,84,90	0
23	BCR	B	718	40/40	0.93	0.07	22,39,53,54	0
23	BCR	B	719	40/40	0.93	0.07	22,42,58,64	0
29	DGD	C	518	62/66	0.93	0.09	35,52,99,119	0
29	DGD	H	103	62/66	0.93	0.08	28,46,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	DGD	c	518	62/66	0.93	0.09	32,53,87,94	0
23	BCR	C	501	40/40	0.93	0.10	38,56,70,74	0
23	BCR	D	404	40/40	0.93	0.09	26,42,91,98	0
22	CLA	H	102	65/65	0.93	0.09	30,60,95,107	0
22	CLA	C	511	65/65	0.94	0.08	32,48,65,80	0
27	LHG	d	407	39/49	0.94	0.08	33,49,68,71	0
22	CLA	C	513	65/65	0.94	0.10	35,56,93,98	0
32	BCT	a	410	4/4	0.94	0.09	30,32,44,53	0
26	SQD	A	409	52/54	0.94	0.09	27,61,89,95	0
23	BCR	b	717	40/40	0.94	0.07	27,41,52,56	0
23	BCR	b	719	40/40	0.94	0.07	33,48,65,76	0
22	CLA	c	509	64/65	0.94	0.09	31,47,87,108	0
23	BCR	c	516	40/40	0.94	0.09	30,43,58,70	0
22	CLA	c	510	65/65	0.94	0.09	33,48,63,69	0
23	BCR	C	515	40/40	0.94	0.07	25,39,51,59	0
22	CLA	c	512	65/65	0.94	0.09	38,55,71,74	0
22	CLA	C	504	65/65	0.94	0.07	30,45,56,58	0
27	LHG	B	722	49/49	0.94	0.09	29,46,70,77	0
27	LHG	a	412	49/49	0.94	0.10	30,48,76,83	0
29	DGD	C	519	62/66	0.94	0.08	32,49,69,84	0
33	LMG	d	408	44/55	0.94	0.09	34,53,82,87	0
22	CLA	C	509	65/65	0.95	0.08	27,44,105,117	0
22	CLA	C	510	65/65	0.95	0.08	27,45,63,74	0
22	CLA	B	709	65/65	0.95	0.07	23,38,52,56	0
23	BCR	t	701	40/40	0.95	0.06	22,38,54,56	0
22	CLA	d	402	65/65	0.95	0.09	28,49,81,95	0
25	PL9	D	405	55/55	0.95	0.06	23,33,48,54	0
23	BCR	A	405	40/40	0.95	0.06	24,36,47,53	0
25	PL9	d	404	55/55	0.95	0.06	21,34,43,47	0
29	DGD	C	517	62/66	0.95	0.09	23,42,75,85	0
23	BCR	B	717	40/40	0.95	0.07	24,41,58,62	0
22	CLA	b	702	65/65	0.95	0.08	28,42,63,66	0
22	CLA	b	706	65/65	0.95	0.08	23,39,75,80	0
22	CLA	b	709	65/65	0.95	0.07	27,47,68,80	0
29	DGD	c	519	62/66	0.95	0.08	28,55,83,95	0
22	CLA	b	714	65/65	0.95	0.07	22,40,73,86	0
22	CLA	b	715	65/65	0.95	0.08	27,42,60,65	0
22	CLA	b	716	60/65	0.95	0.09	29,46,92,95	0
22	CLA	c	503	65/65	0.95	0.07	27,45,68,75	0
23	BCR	T	701	40/40	0.95	0.07	28,41,57,60	0
22	CLA	c	504	65/65	0.95	0.07	23,44,56,64	0
27	LHG	D	411	47/49	0.95	0.09	24,49,85,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	BCR	a	407	40/40	0.95	0.06	23,34,50,54	0
22	CLA	c	507	65/65	0.95	0.09	30,48,97,104	0
23	BCR	b	718	40/40	0.95	0.06	27,39,52,55	0
27	LHG	l	101	49/49	0.95	0.07	31,44,53,61	0
22	CLA	c	508	65/65	0.95	0.07	26,43,60,64	0
22	CLA	C	512	65/65	0.95	0.08	30,52,67,74	0
22	CLA	C	507	65/65	0.95	0.09	26,44,83,94	0
22	CLA	c	511	65/65	0.95	0.07	34,49,63,75	0
34	PHO	a	405	64/64	0.95	0.06	18,32,41,46	0
34	PHO	d	405	64/64	0.95	0.06	28,39,48,63	0
27	LHG	L	101	49/49	0.96	0.07	31,41,55,65	0
22	CLA	b	705	65/65	0.96	0.06	19,35,49,61	0
22	CLA	B	715	65/65	0.96	0.07	24,36,67,75	0
27	LHG	d	406	49/49	0.96	0.07	26,45,56,62	0
22	CLA	b	707	65/65	0.96	0.08	19,36,68,75	0
22	CLA	b	708	65/65	0.96	0.07	28,44,64,66	0
22	CLA	C	503	65/65	0.96	0.06	30,44,57,62	0
22	CLA	b	710	65/65	0.96	0.07	24,38,49,61	0
22	CLA	b	712	65/65	0.96	0.07	23,36,47,52	0
22	CLA	b	713	65/65	0.96	0.07	18,36,67,82	0
22	CLA	A	403	65/65	0.96	0.09	21,35,88,102	0
22	CLA	C	505	59/65	0.96	0.07	28,43,75,85	0
22	CLA	C	506	65/65	0.96	0.08	23,41,69,80	0
22	CLA	c	502	65/65	0.96	0.07	27,41,52,56	0
22	CLA	B	702	65/65	0.96	0.06	25,36,56,64	0
29	DGD	c	517	62/66	0.96	0.08	24,42,78,87	0
22	CLA	C	508	65/65	0.96	0.07	25,42,57,63	0
22	CLA	c	505	60/65	0.96	0.07	34,47,77,84	0
22	CLA	c	506	65/65	0.96	0.08	25,41,69,76	0
32	BCT	A	417	4/4	0.96	0.07	25,31,36,43	0
22	CLA	B	704	65/65	0.96	0.07	20,32,76,78	0
22	CLA	B	705	65/65	0.96	0.06	15,31,45,52	0
22	CLA	B	706	65/65	0.96	0.07	24,37,81,90	0
22	CLA	A	402	65/65	0.96	0.06	15,29,44,57	0
22	CLA	B	710	65/65	0.96	0.07	17,33,45,48	0
22	CLA	B	711	65/65	0.96	0.06	18,30,50,56	0
22	CLA	D	402	65/65	0.96	0.06	15,27,51,56	0
22	CLA	B	712	65/65	0.96	0.07	20,31,45,54	0
22	CLA	a	401	65/65	0.96	0.06	21,32,41,47	0
22	CLA	a	403	65/65	0.96	0.06	19,31,42,58	0
22	CLA	a	404	65/65	0.96	0.09	27,42,102,112	0
22	CLA	a	406	65/65	0.96	0.07	18,38,76,81	0

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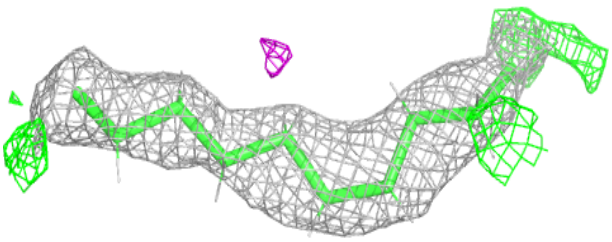
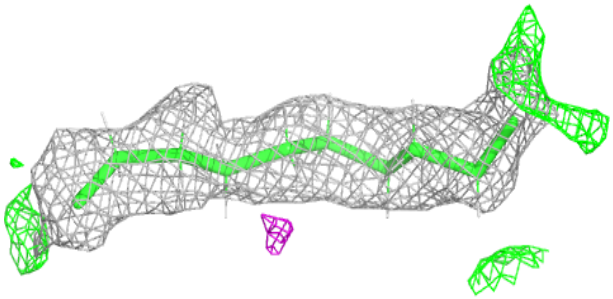
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	B	713	65/65	0.96	0.07	19,32,72,74	0
22	CLA	B	714	65/65	0.96	0.08	19,37,78,96	0
34	PHO	D	406	64/64	0.96	0.06	16,28,37,42	0
34	PHO	D	407	64/64	0.96	0.06	23,32,44,51	0
27	LHG	D	410	49/49	0.96	0.07	21,40,54,65	0
22	CLA	b	704	65/65	0.96	0.08	21,37,84,97	0
35	HEC	e	101	43/43	0.96	0.09	42,59,80,88	0
22	CLA	C	502	65/65	0.97	0.06	22,36,50,61	0
22	CLA	B	707	65/65	0.97	0.07	17,35,65,75	0
22	CLA	B	708	65/65	0.97	0.06	19,36,54,59	0
22	CLA	D	401	65/65	0.97	0.06	14,29,57,68	0
22	CLA	B	703	65/65	0.97	0.06	20,33,57,65	0
22	CLA	D	403	65/65	0.97	0.08	24,42,107,122	0
22	CLA	b	711	65/65	0.97	0.06	22,34,59,64	0
22	CLA	d	401	65/65	0.97	0.06	20,36,54,62	0
22	CLA	b	703	65/65	0.97	0.07	24,37,68,78	0
35	HEC	E	103	43/43	0.97	0.09	34,51,70,74	0
22	CLA	B	716	60/65	0.97	0.09	23,39,87,103	0
24	CL	A	406	1/1	0.98	0.04	29,29,29,29	0
22	CLA	A	404	54/65	0.98	0.05	17,31,61,68	0
35	HEC	V	201	43/43	0.98	0.06	17,33,43,50	0
30	OEX	A	415[A]	10/10	0.98	0.04	32,35,38,40	10
35	HEC	v	201	43/43	0.98	0.06	26,37,51,52	0
30	OEX	a	420[A]	10/10	0.99	0.03	29,35,39,39	10
31	OEY	A	416[B]	11/11	0.99	0.03	14,24,29,31	11
24	CL	a	408	1/1	0.99	0.04	28,28,28,28	0
24	CL	a	409	1/1	0.99	0.07	28,28,28,28	0
24	CL	A	407	1/1	0.99	0.06	27,27,27,27	0
31	OEY	a	421[B]	11/11	1.00	0.02	19,25,29,33	11
21	FE2	A	401	1/1	1.00	0.01	29,29,29,29	0
21	FE2	a	402	1/1	1.00	0.02	33,33,33,33	0

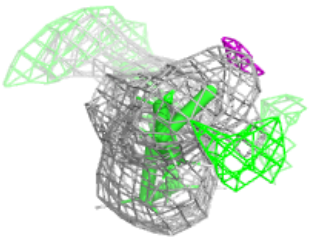
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE b 726:

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

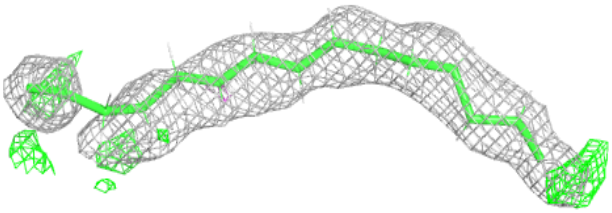


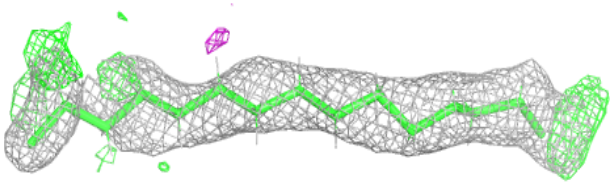


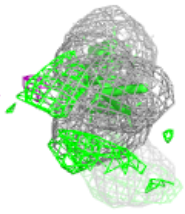


Electron density around STE I 101:

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

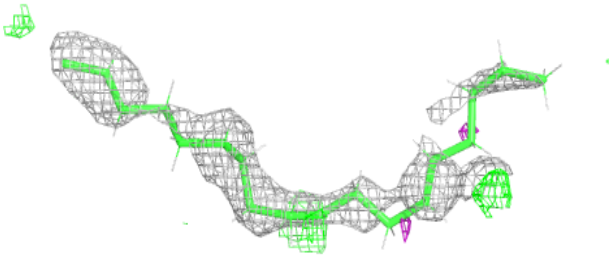


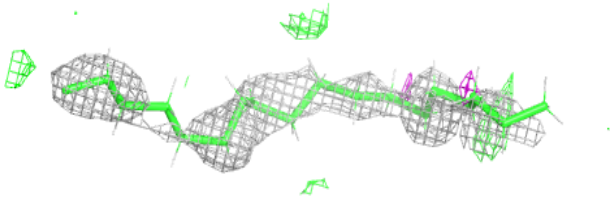


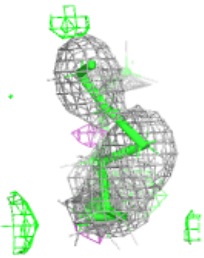


Electron density around STE H 104:

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

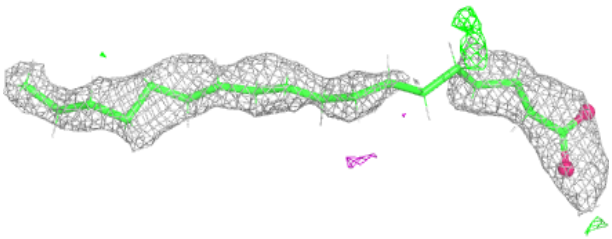


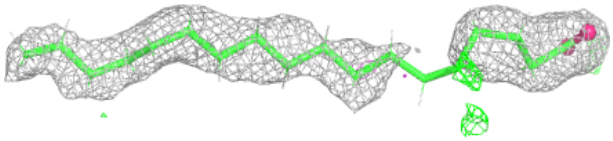


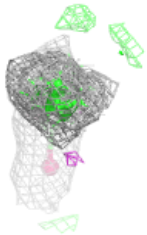


Electron density around STE b 725:

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

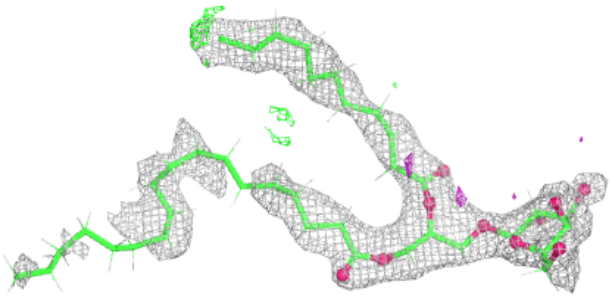


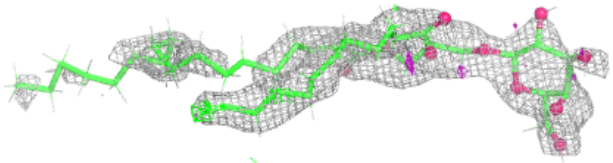




Electron density around LMG c 522:

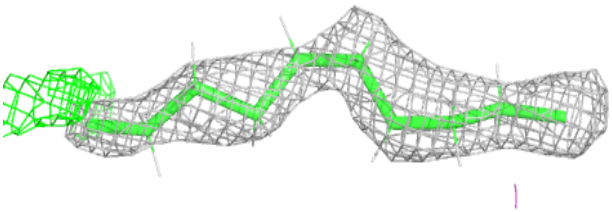
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

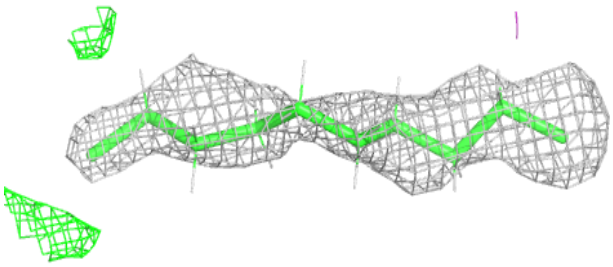


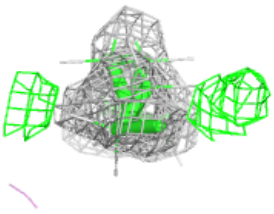


Electron density around STE a 416:

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

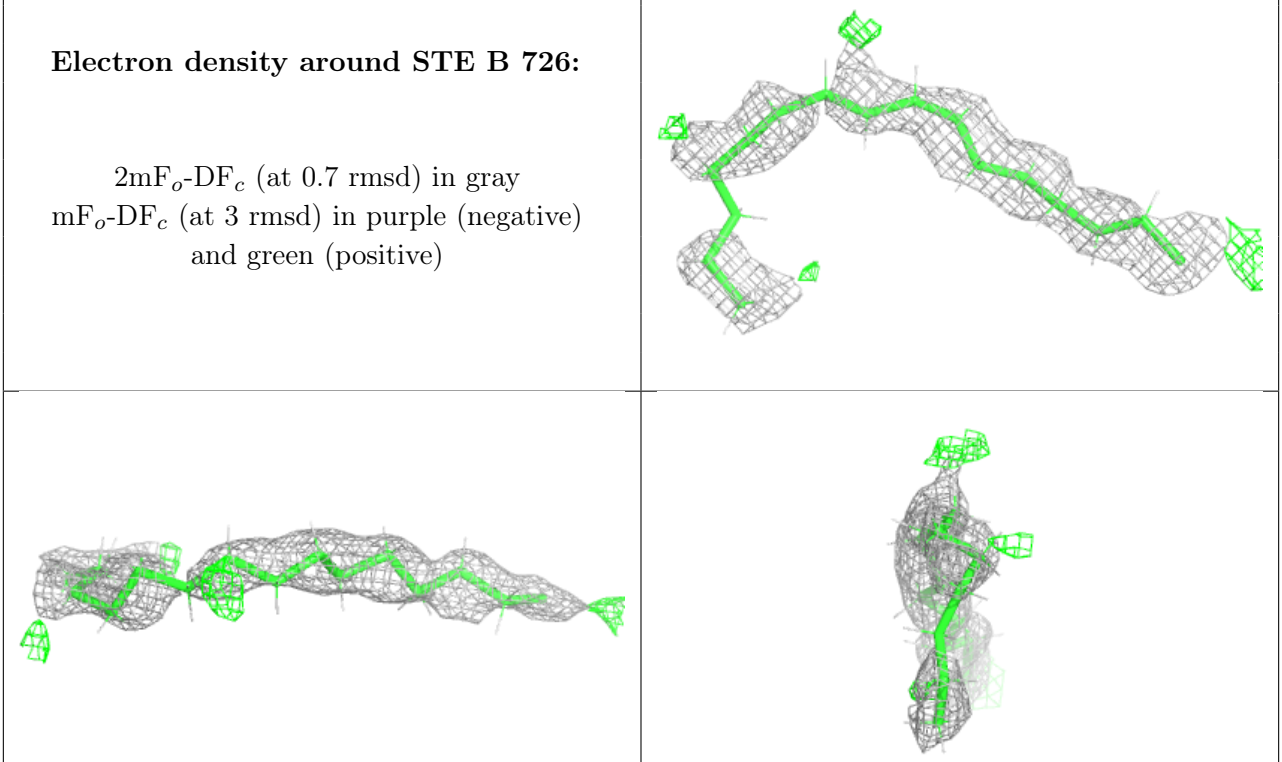






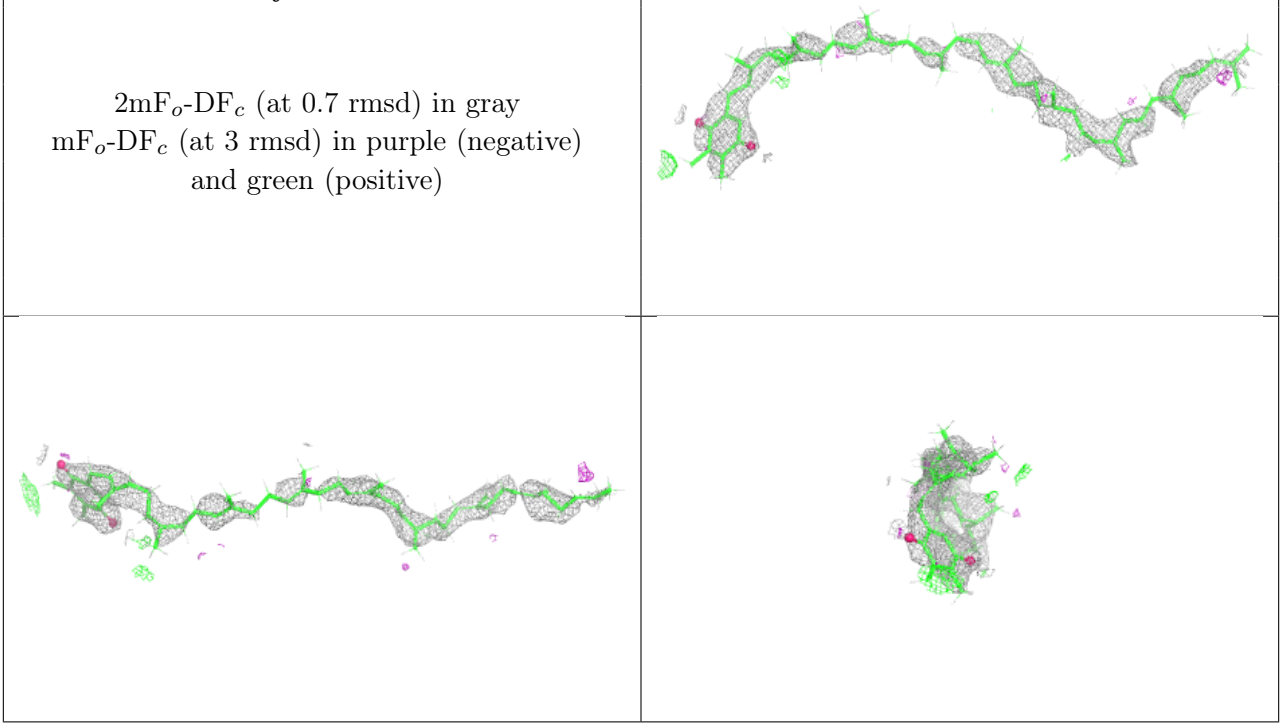
Electron density around STE B 726:

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



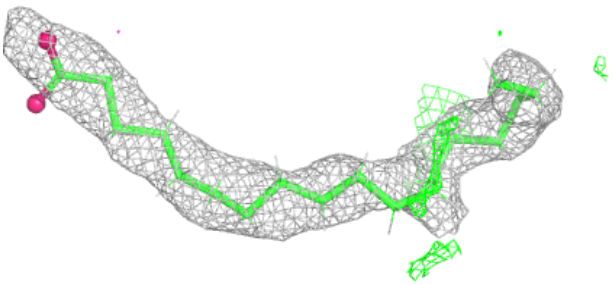
Electron density around PL9 A 408:

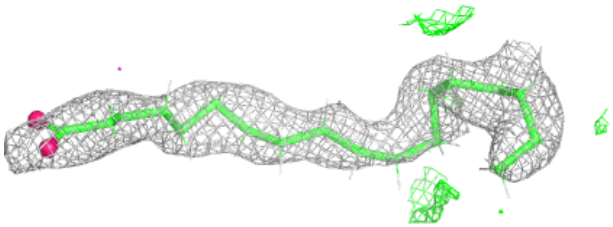
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

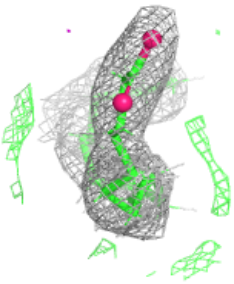


Electron density around STE b 727:

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

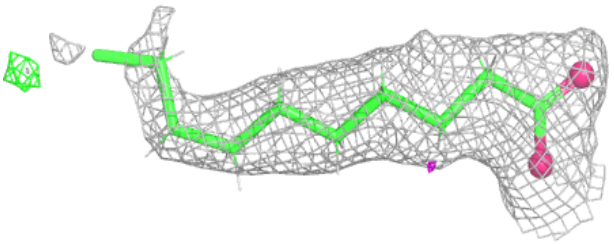


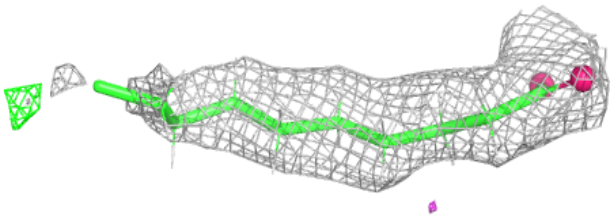


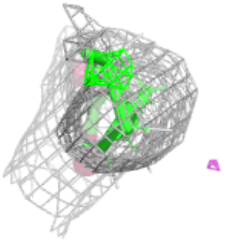


Electron density around STE c 501:

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

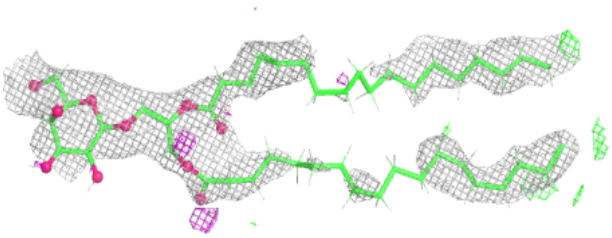


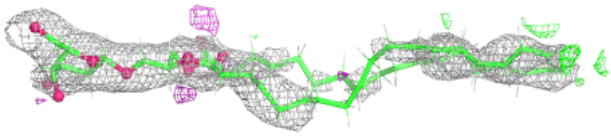




Electron density around LMG b 723:

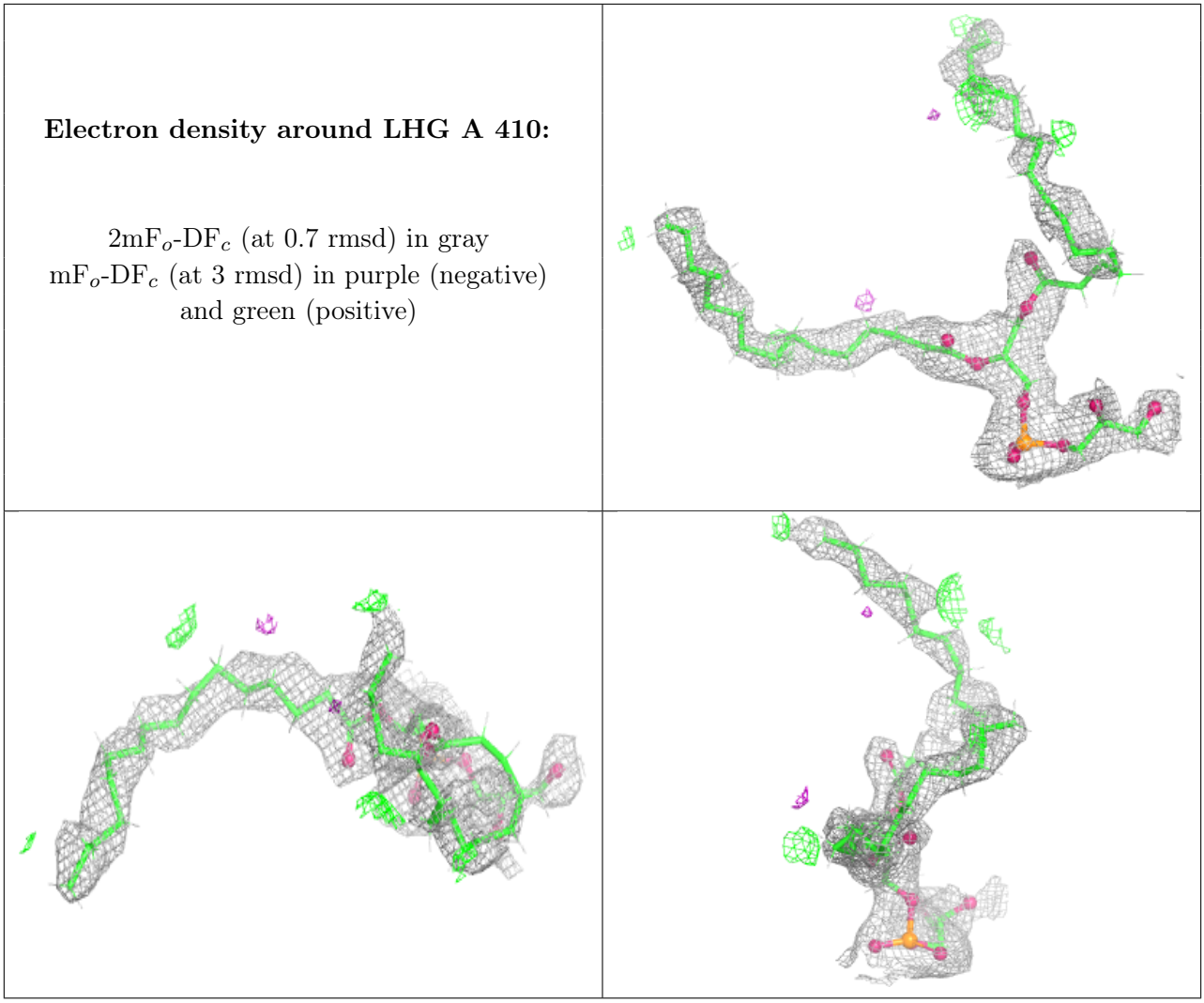
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





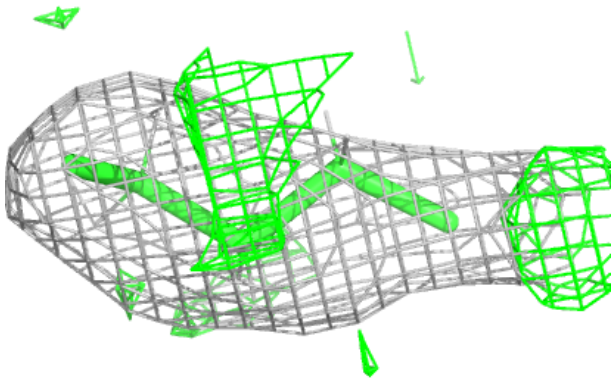
Electron density around LHG A 410:

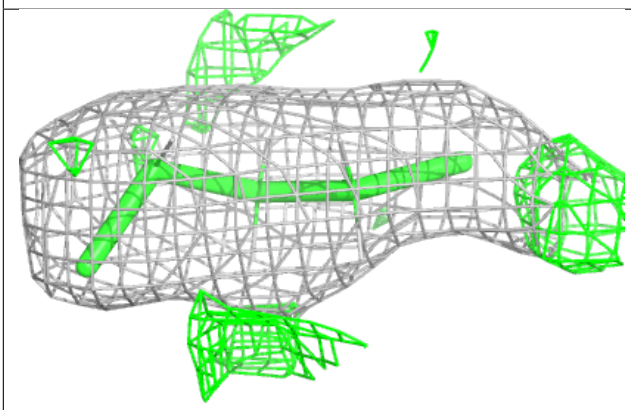
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

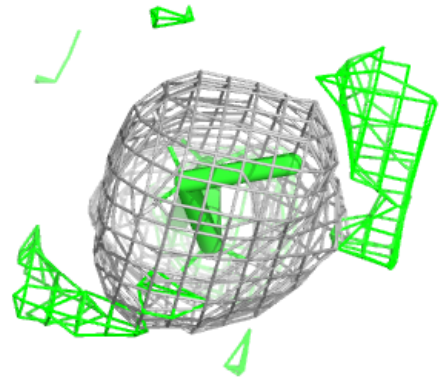


Electron density around STE A 414:

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

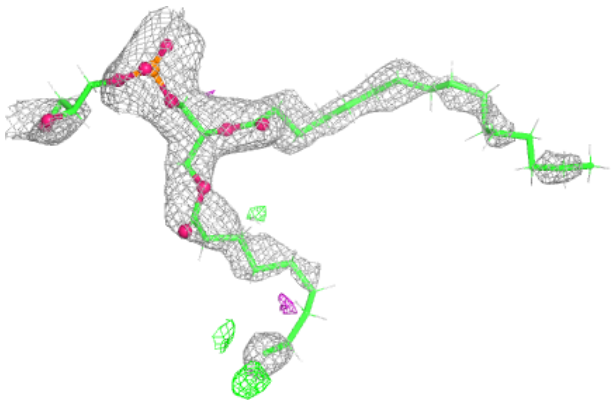


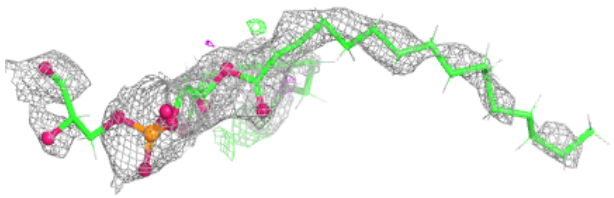


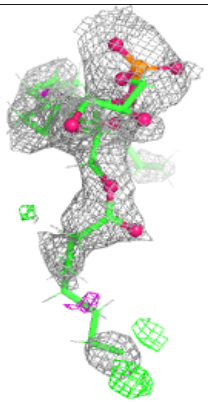


Electron density around LHG a 414:

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

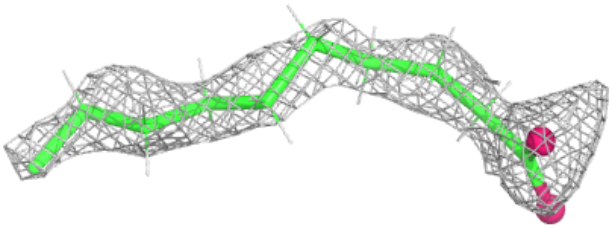


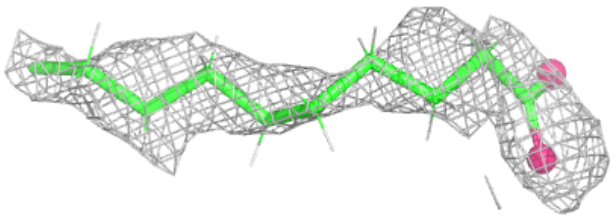


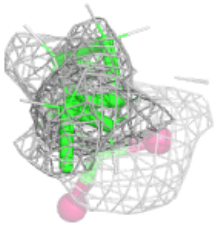


Electron density around STE E 101:

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

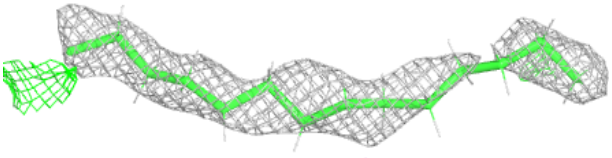


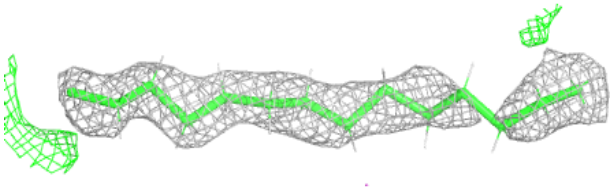


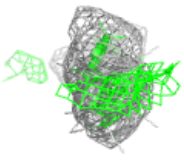


Electron density around STE h 703:

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

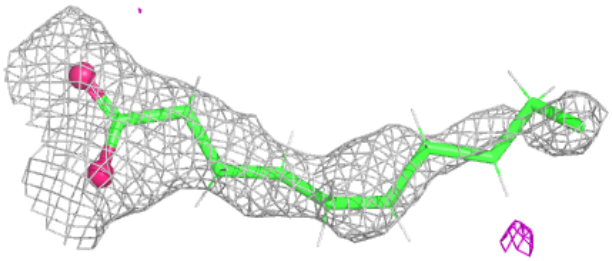


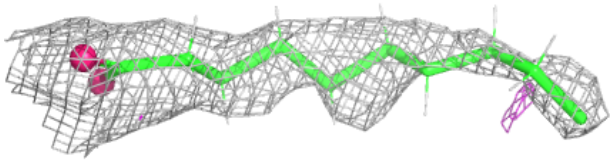


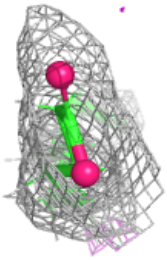


Electron density around STE a 417:

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

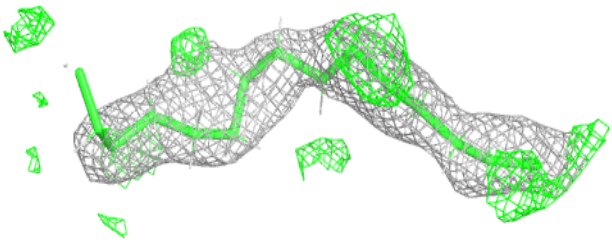


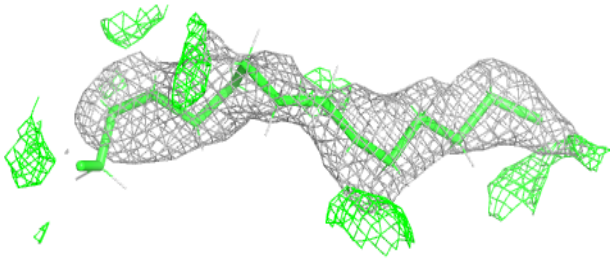


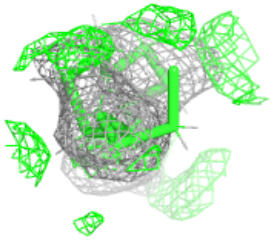


Electron density around STE a 418:

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

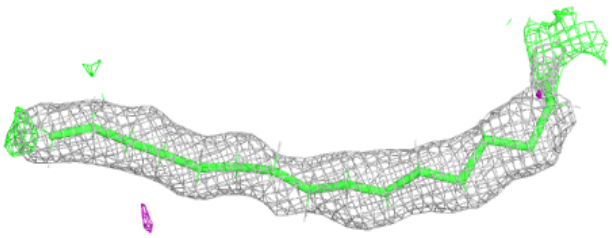


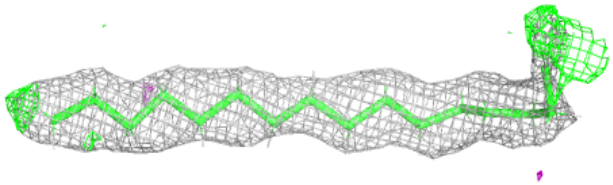


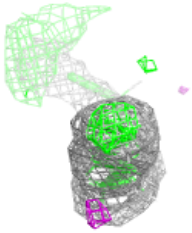


Electron density around STE C 522:

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

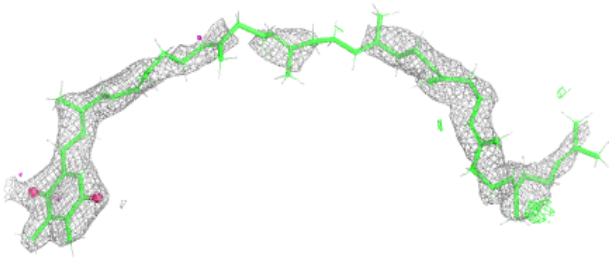


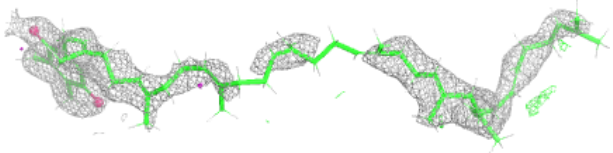


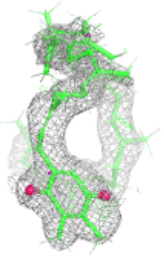


Electron density around PL9 a 411:

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

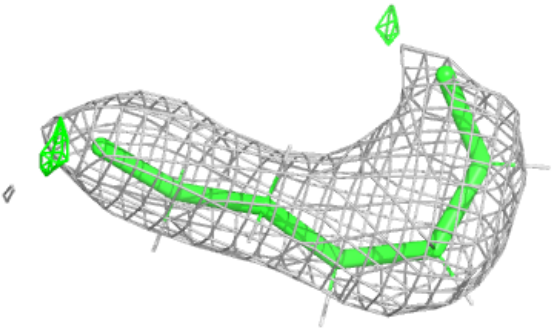


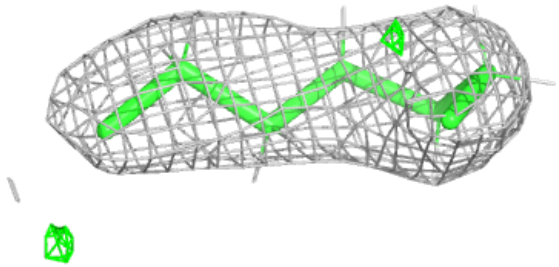


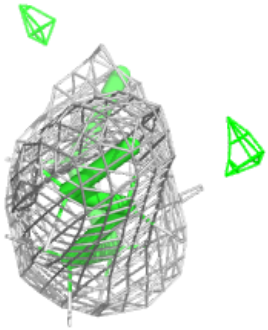


Electron density around STE E 102:

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

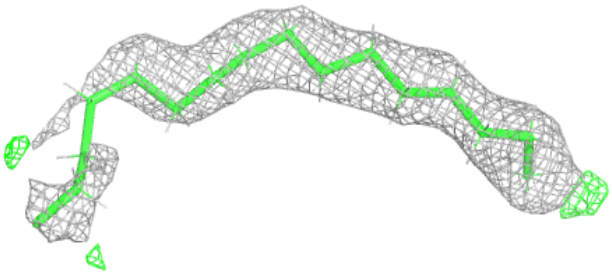


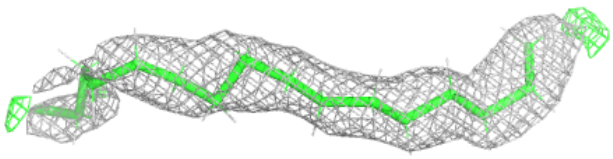


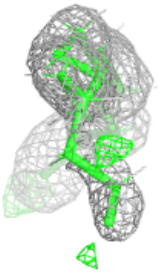


Electron density around STE A 411:

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

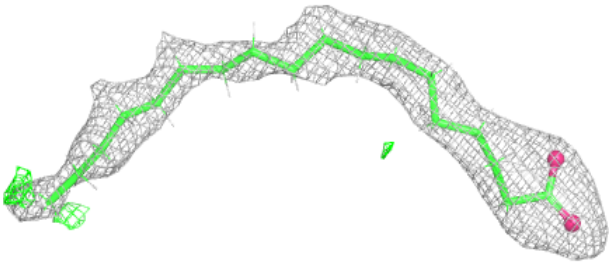


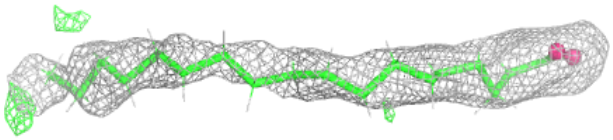


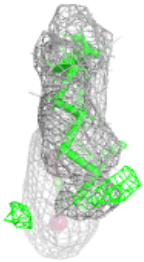


Electron density around STE x 101:

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

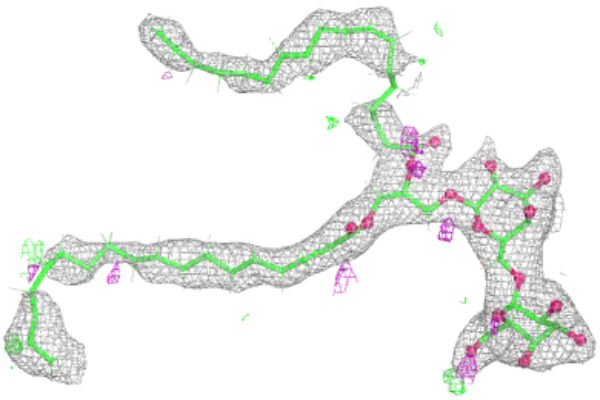


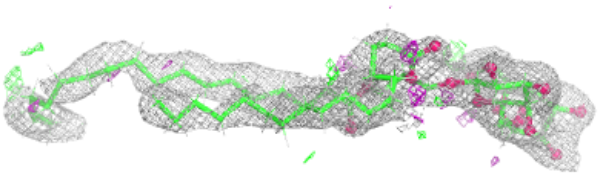


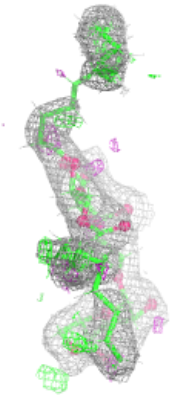


Electron density around DGD A 413:

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

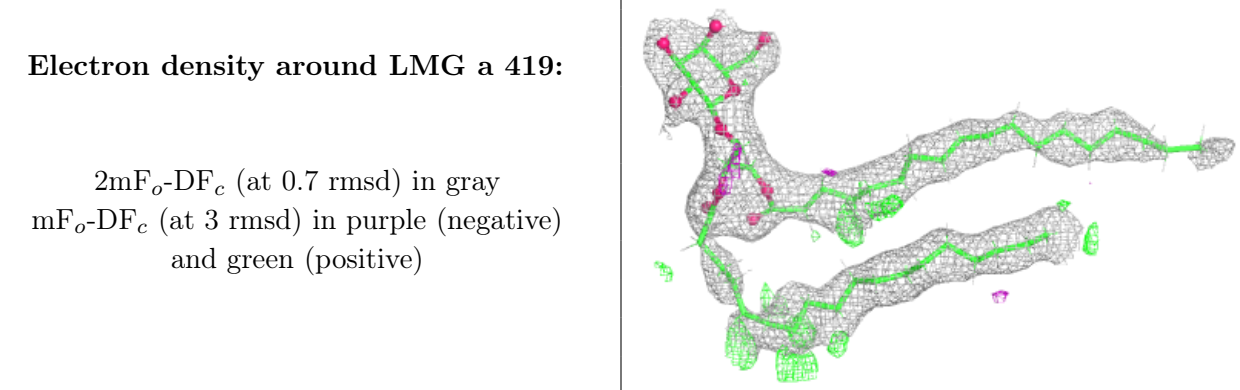






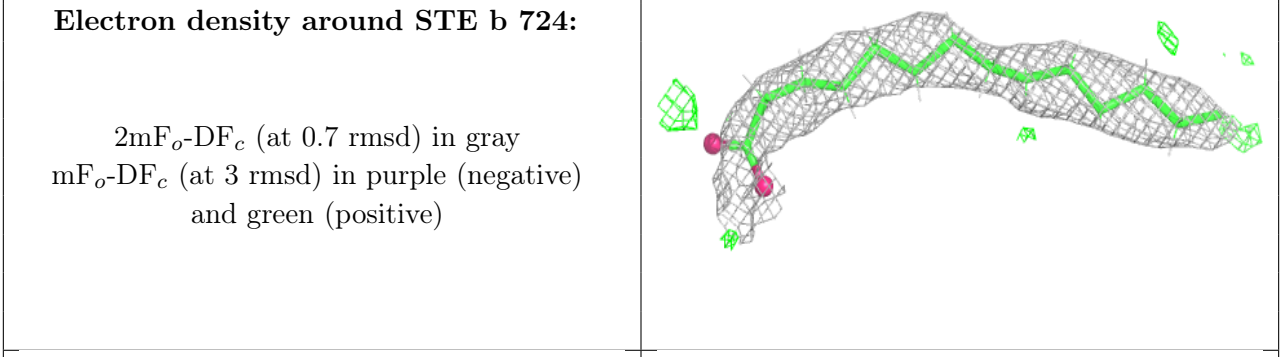
Electron density around LMG a 419:

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



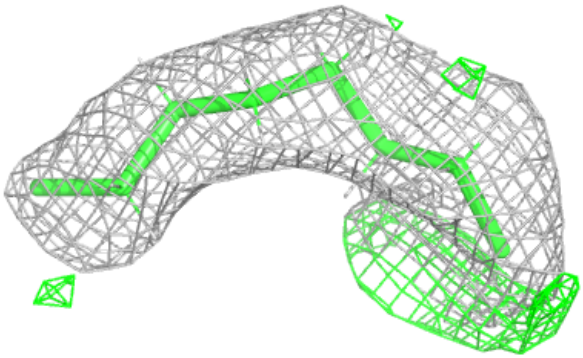
Electron density around STE b 724:

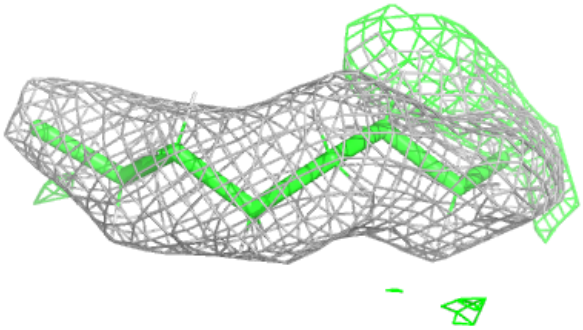
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

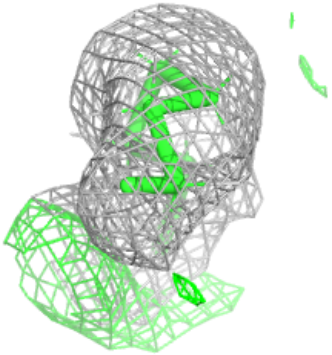


Electron density around STE H 105:

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

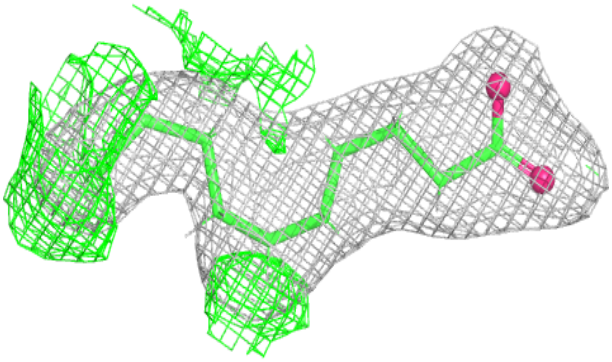


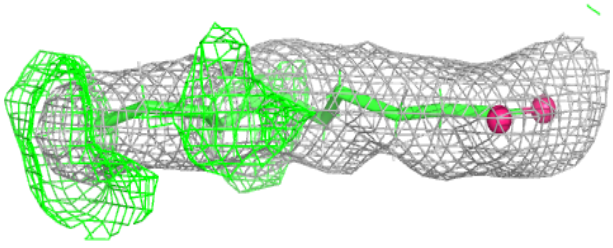


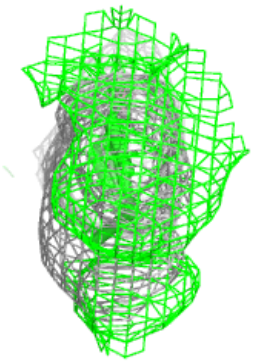


Electron density around STE C 523:

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

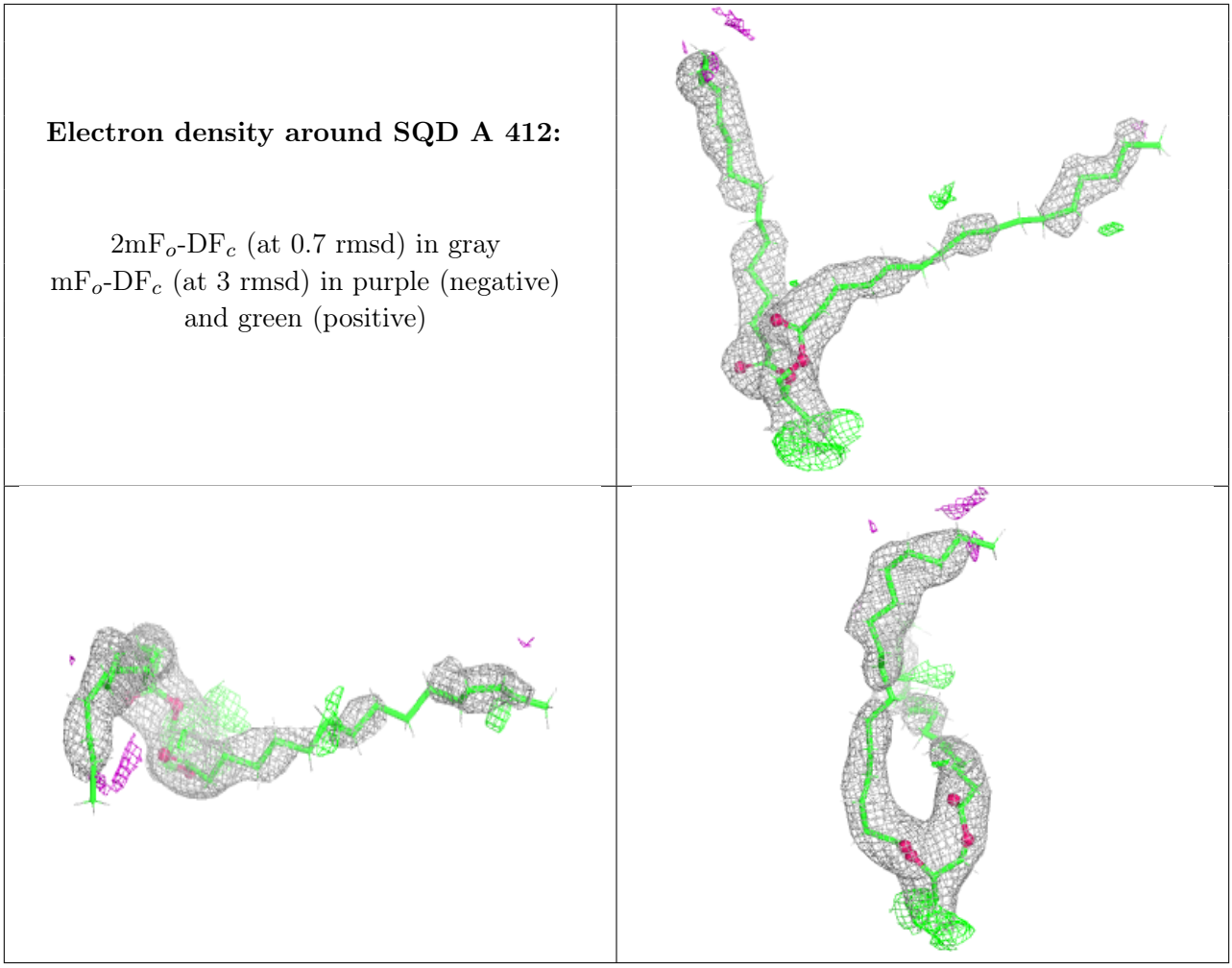






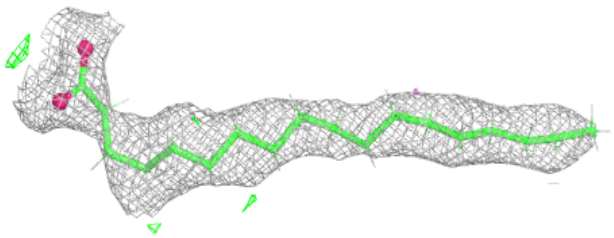
Electron density around SQD A 412:

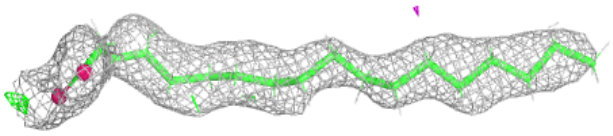
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

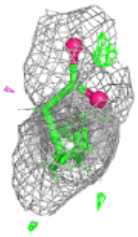


Electron density around STE c 521:

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

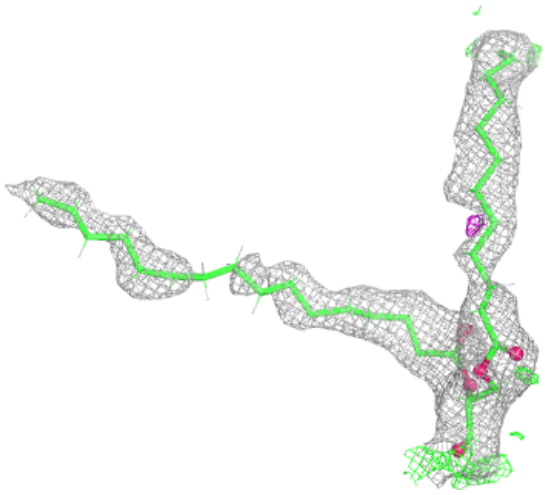


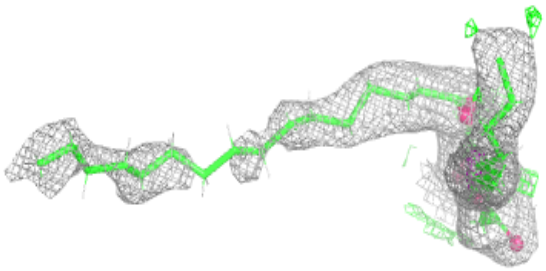


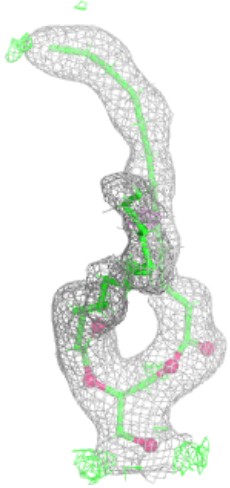


Electron density around SQD a 415:

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

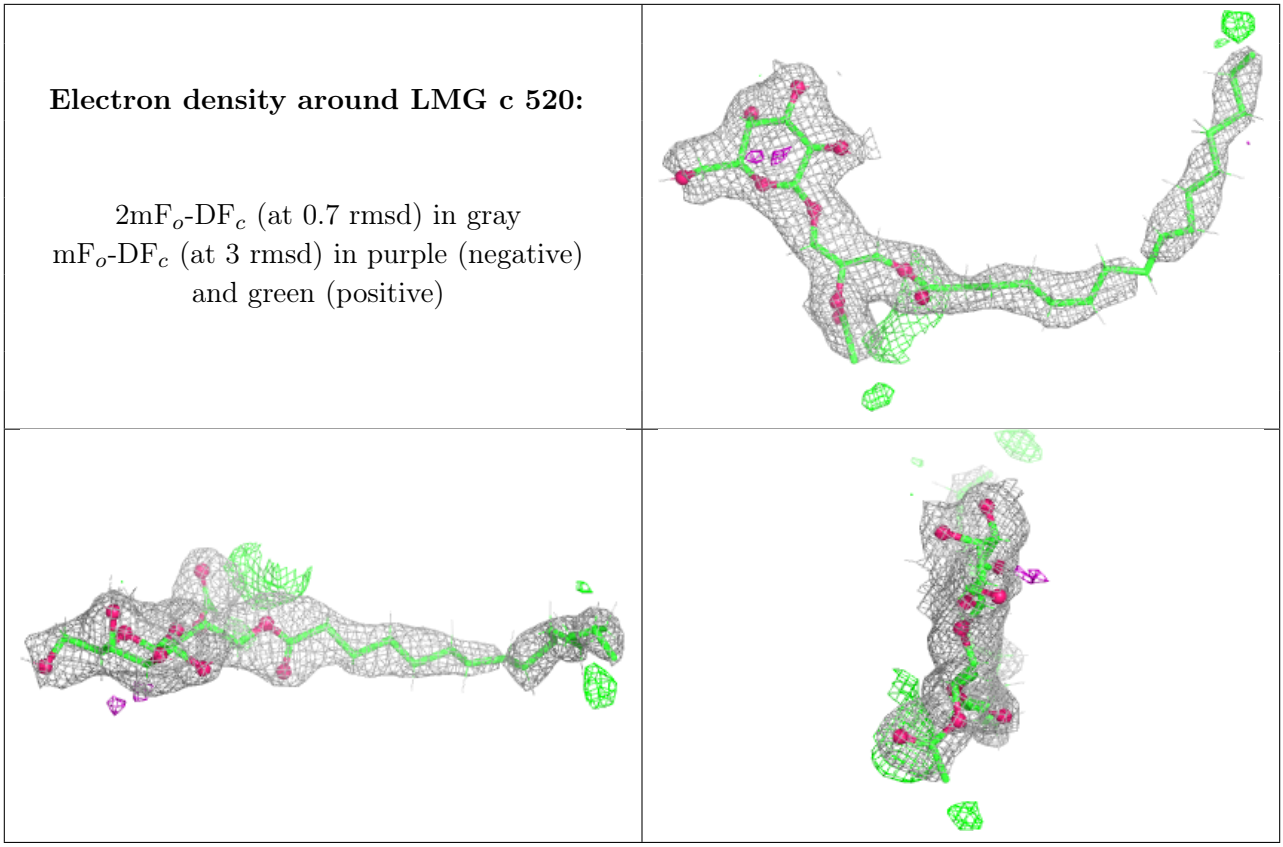






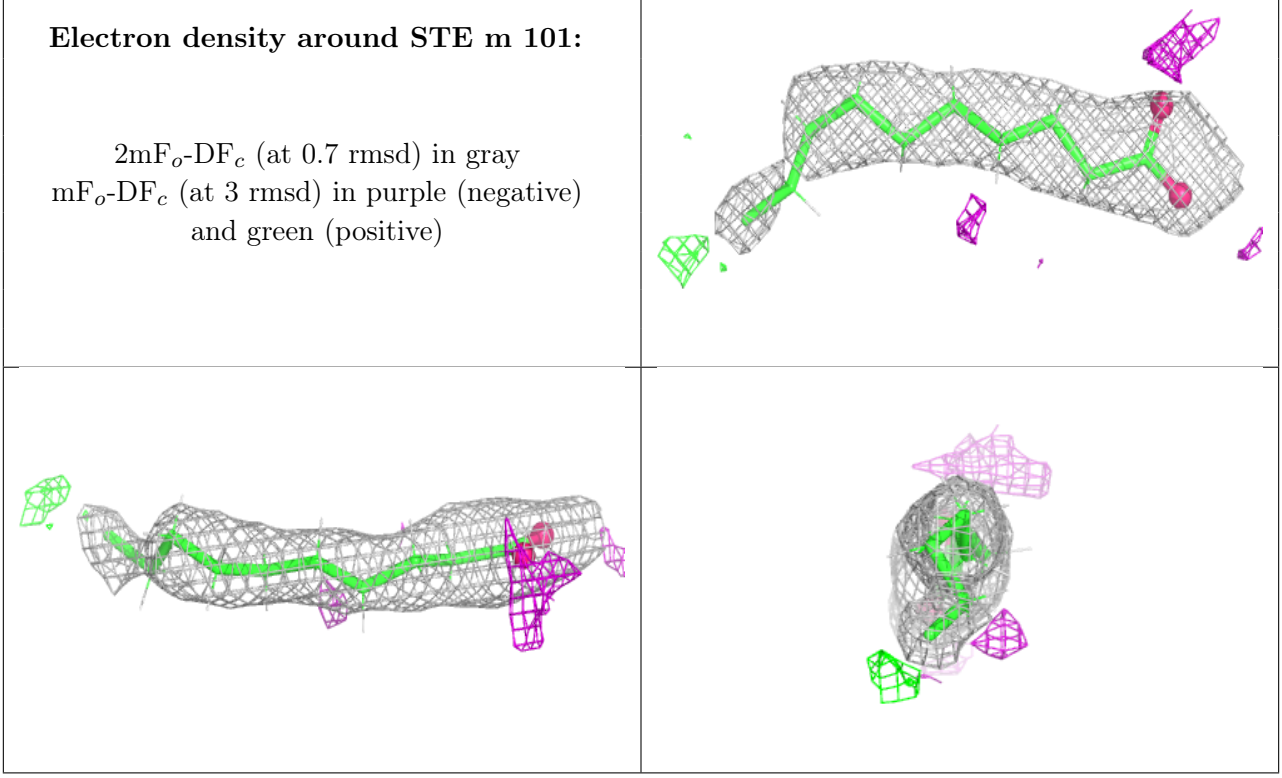
Electron density around LMG c 520:

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



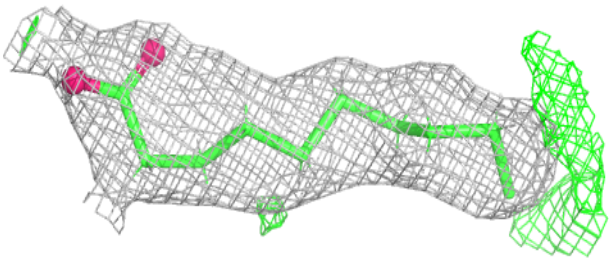
Electron density around STE m 101:

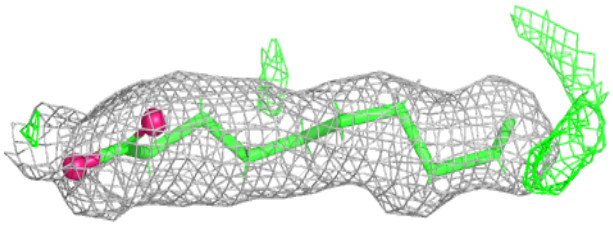
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

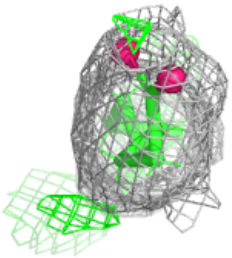


Electron density around STE J 101:

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

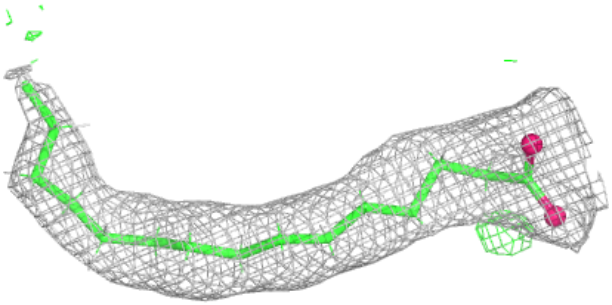


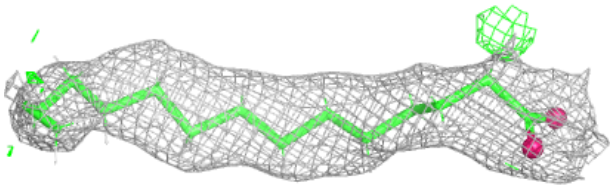


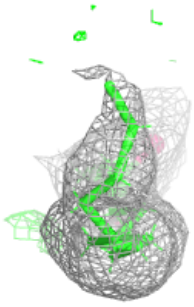


Electron density around STE B 720:

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

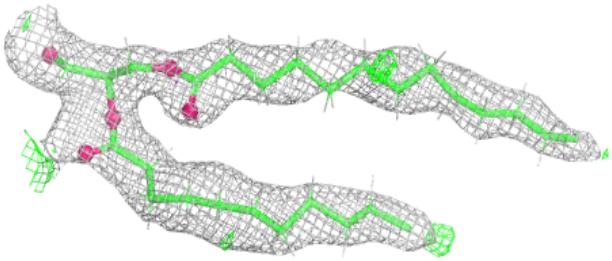


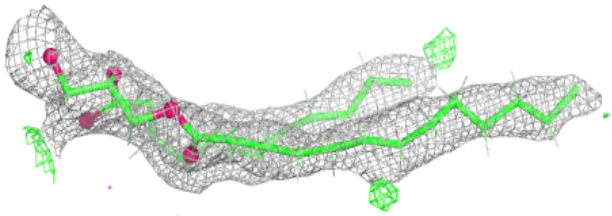


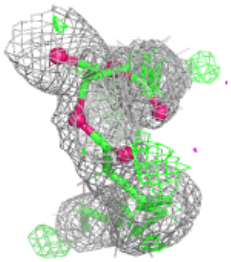


Electron density around LMG D 412:

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

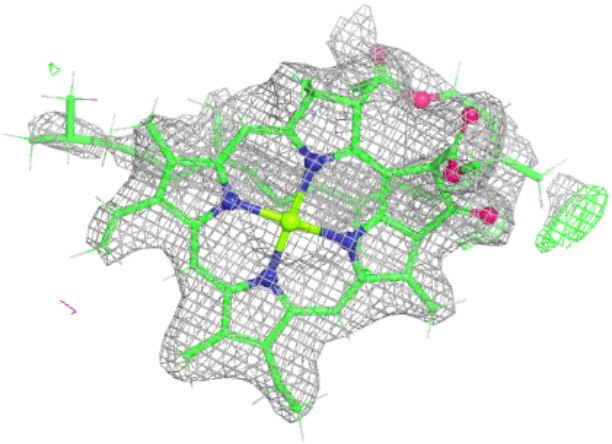


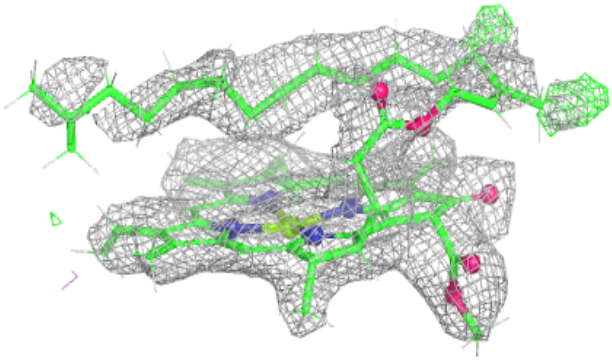




Electron density around CLA b 701:

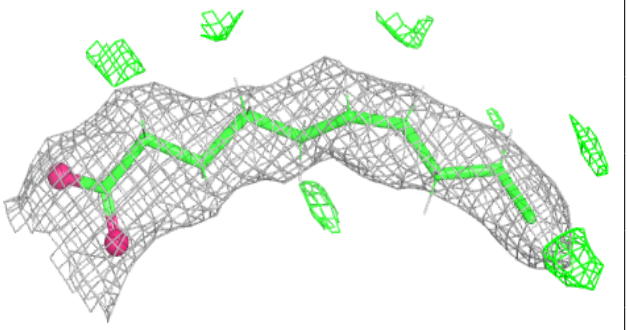
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

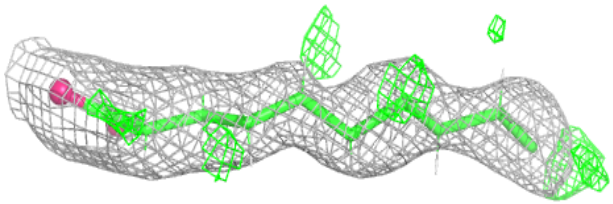


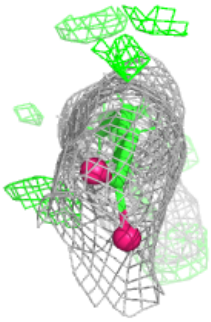


Electron density around STE C 521:

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

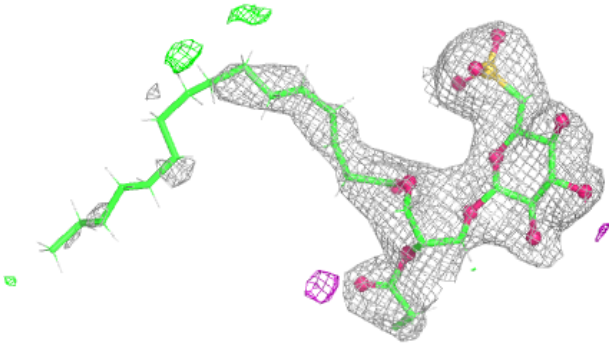


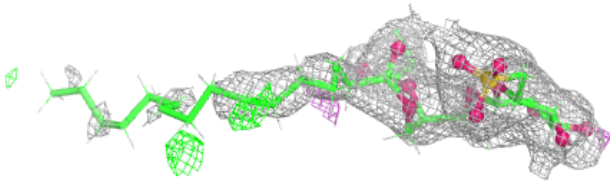


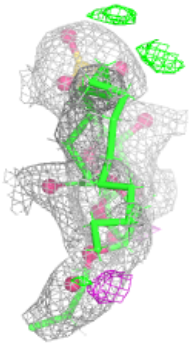


Electron density around SQD f 101:

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

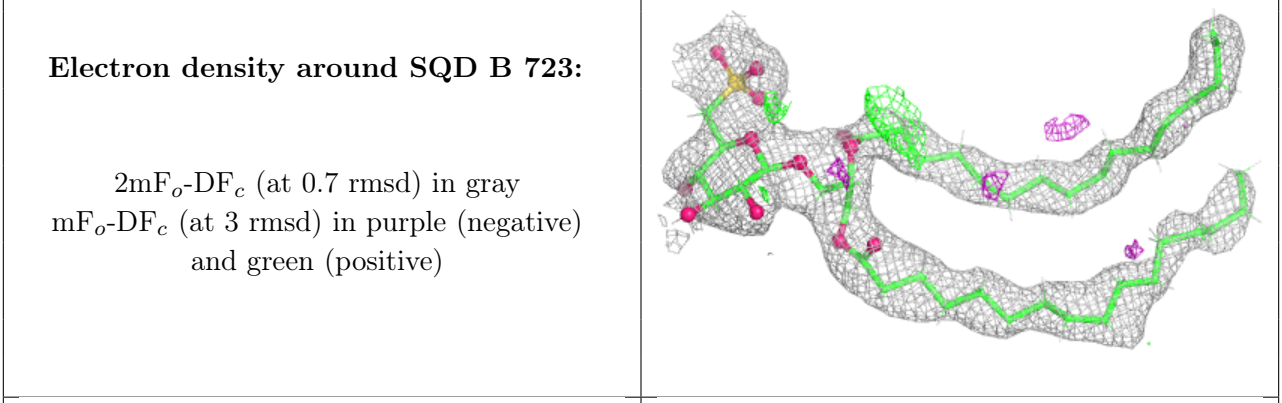


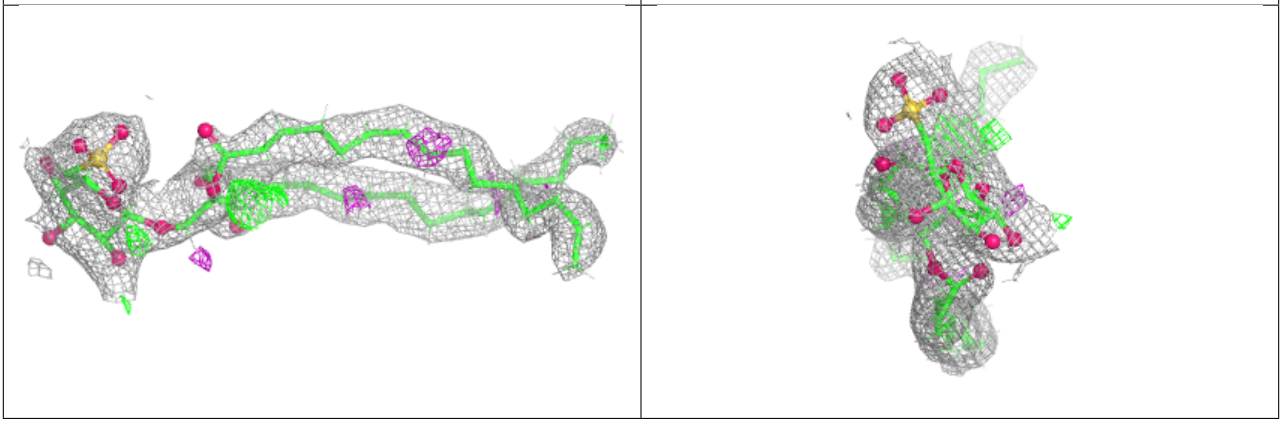




Electron density around SQD B 723:

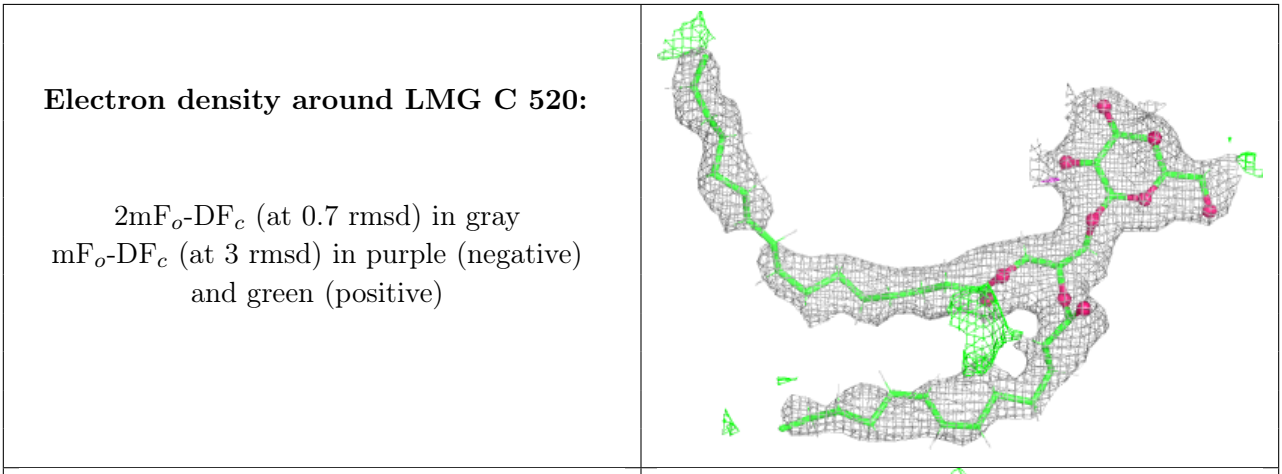
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

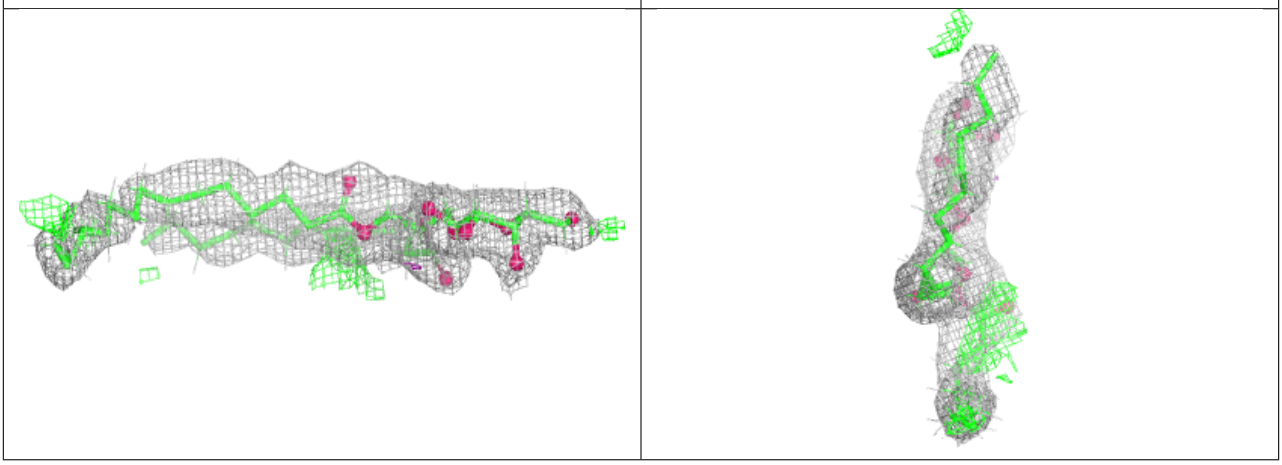




Electron density around LMG C 520:

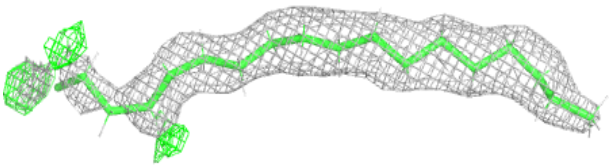
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

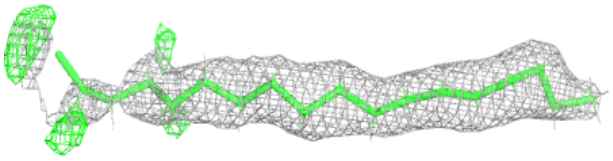


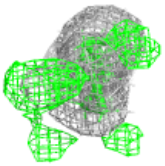


Electron density around STE l 102:

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

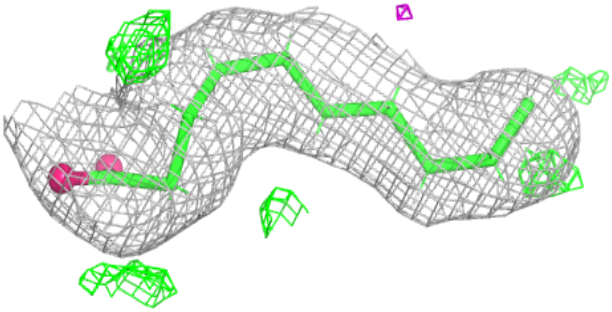


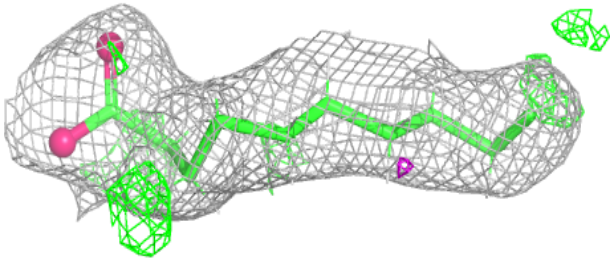


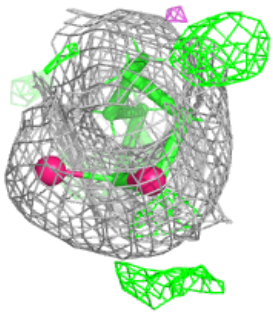


Electron density around STE B 724:

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

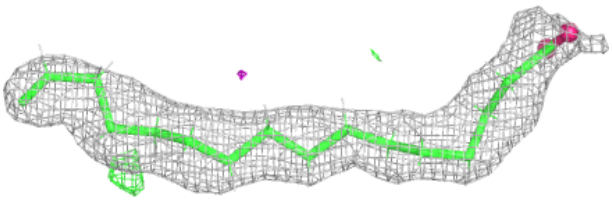


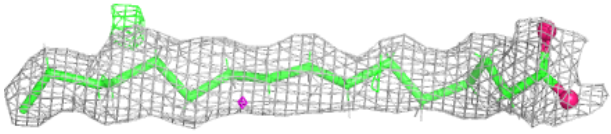


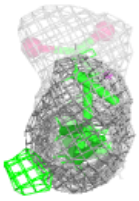


Electron density around STE B 725:

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

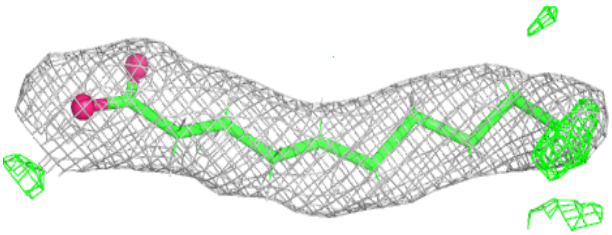


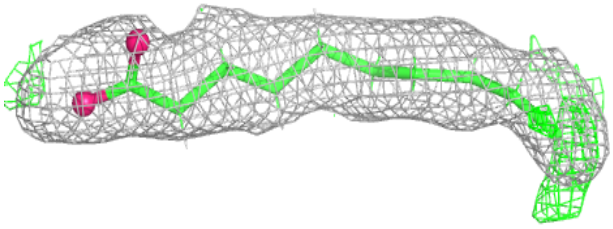


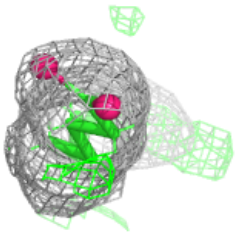


Electron density around STE j 101:

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

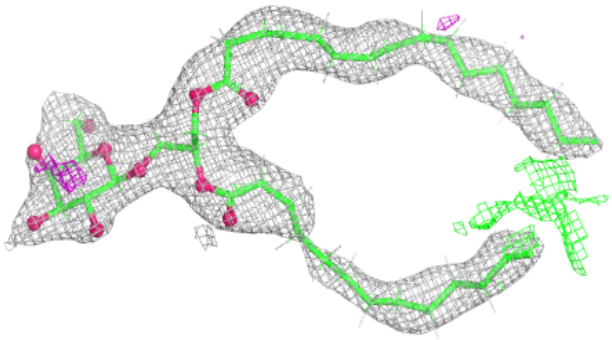


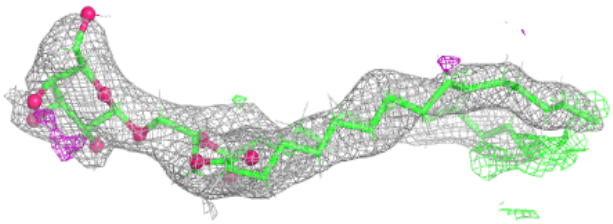




Electron density around LMG C 516:

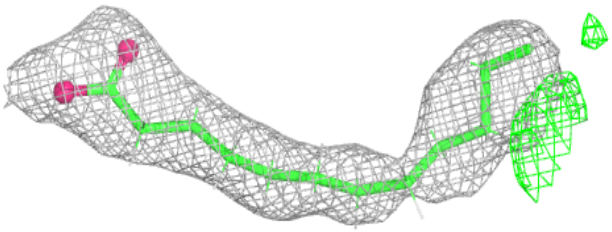
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

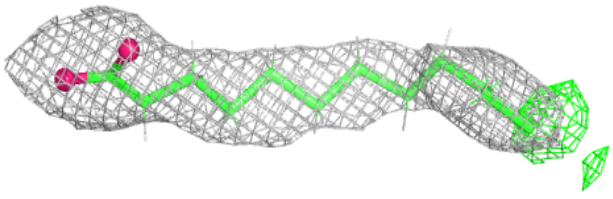


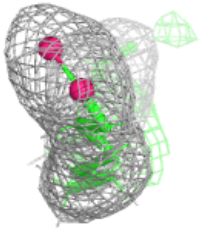


Electron density around STE t 702:

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

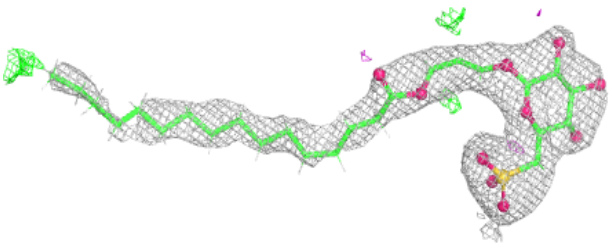


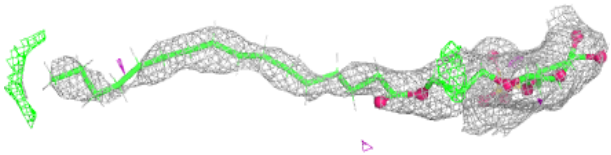


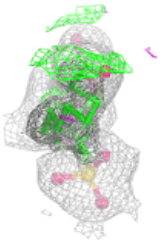


Electron density around SQD D 409:

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

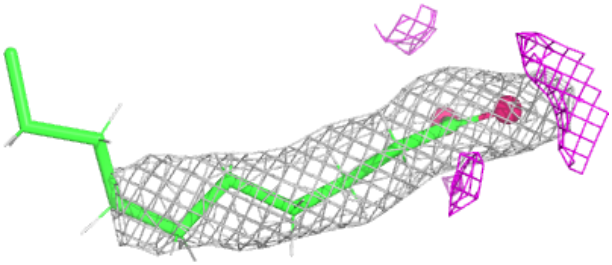


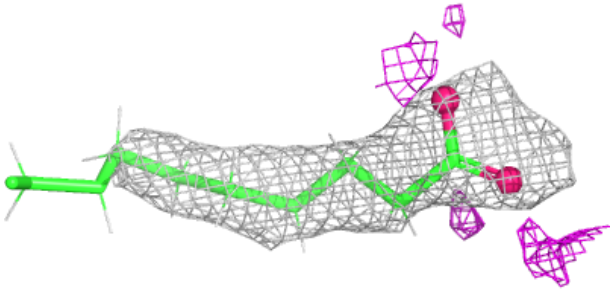


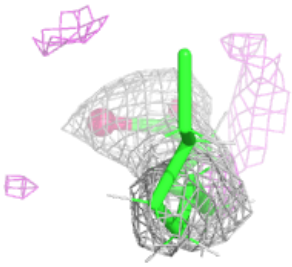


Electron density around STE B 701:

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

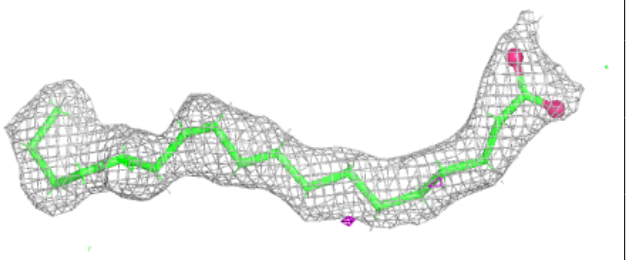


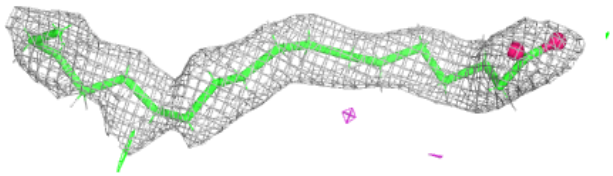


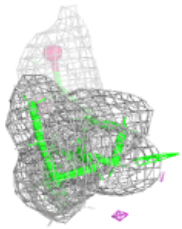


Electron density around STE b 722:

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

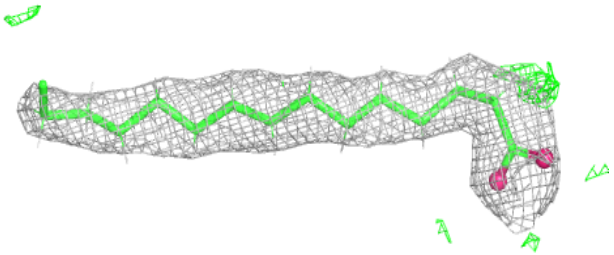


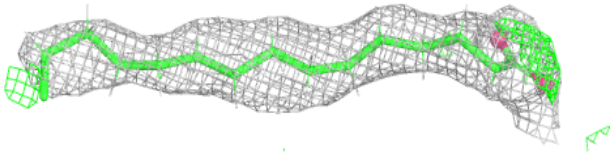


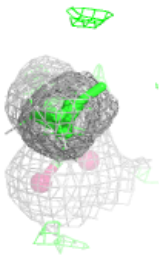


Electron density around STE d 409:

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

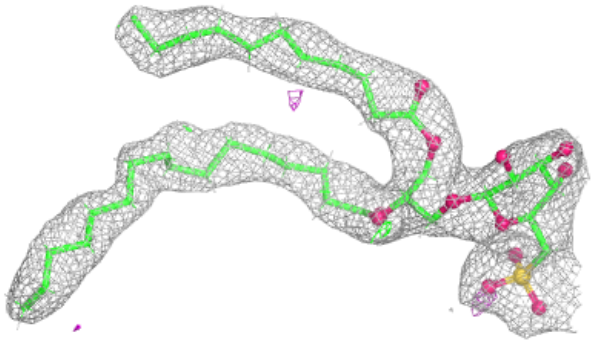


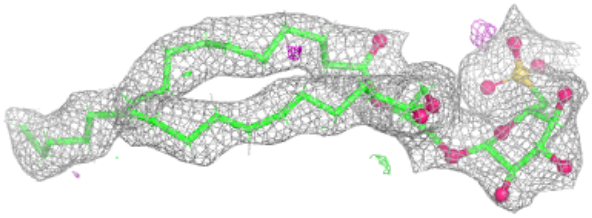


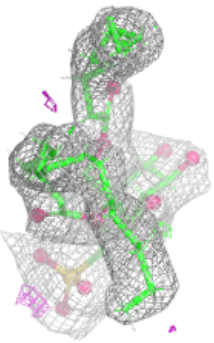


Electron density around SQD b 720:

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

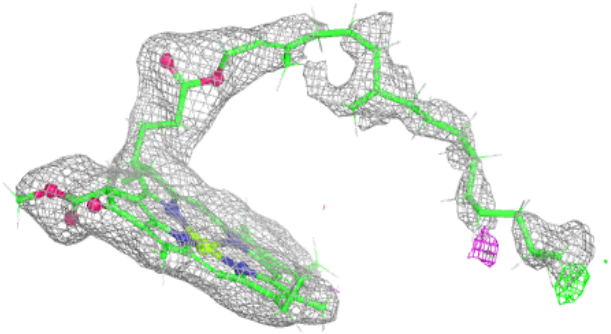


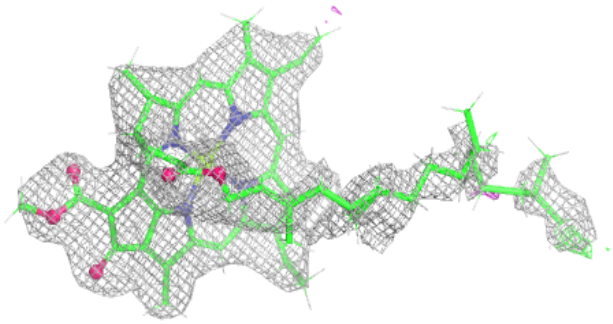


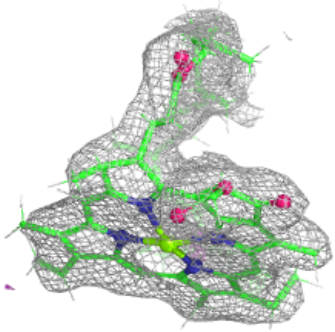


Electron density around CLA C 514:

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

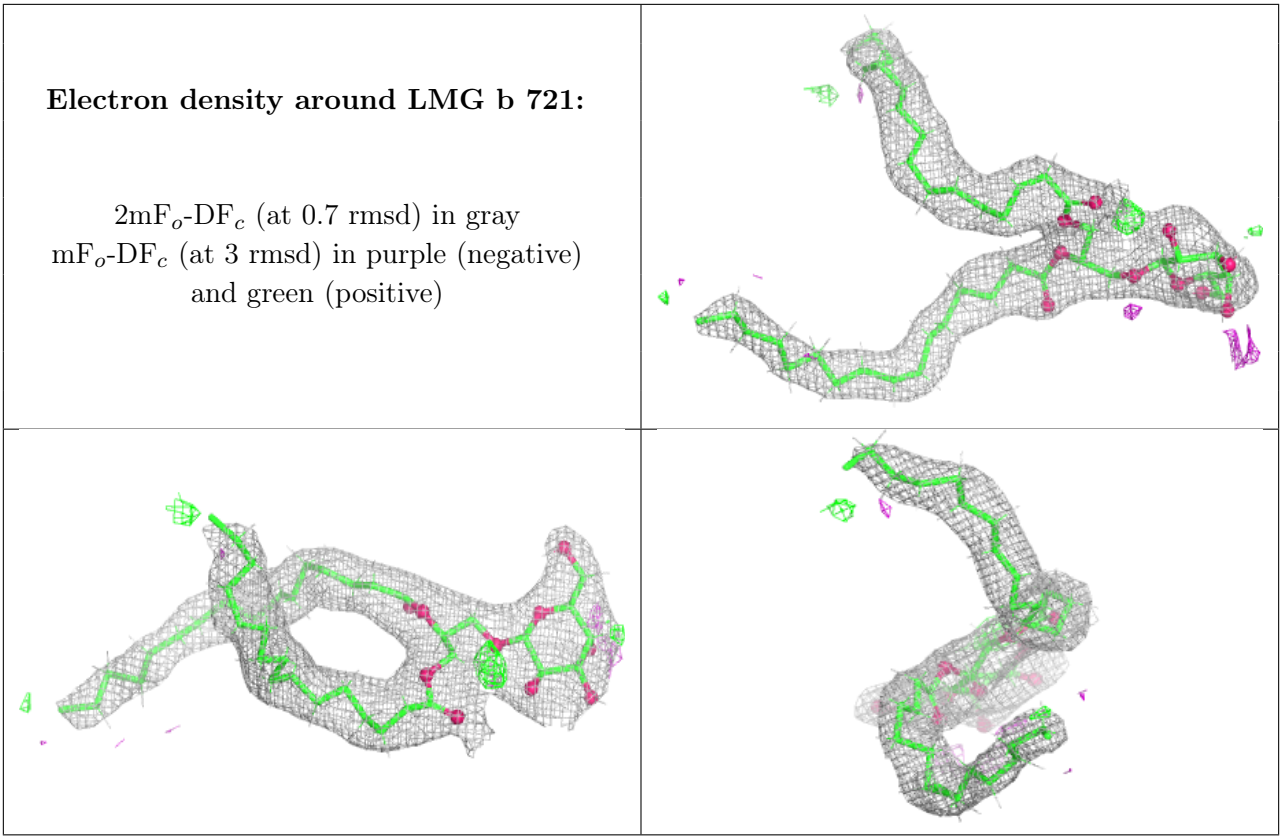






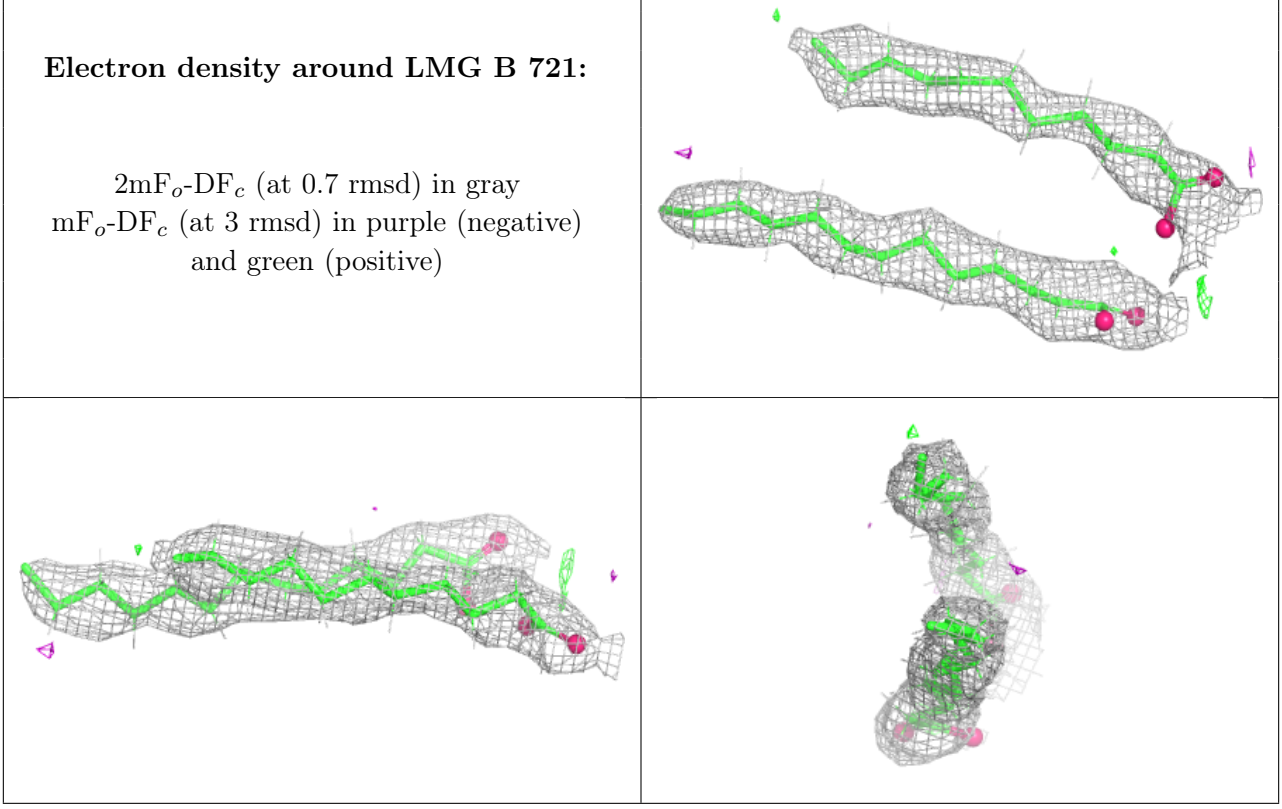
Electron density around LMG b 721:

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



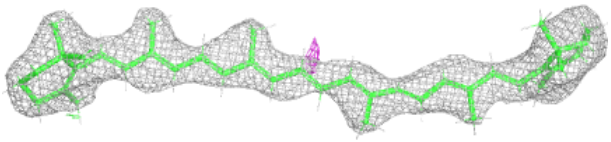
Electron density around LMG B 721:

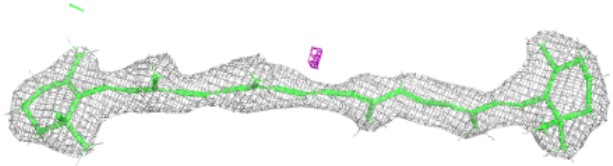
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

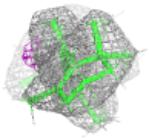


Electron density around BCR c 515:

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

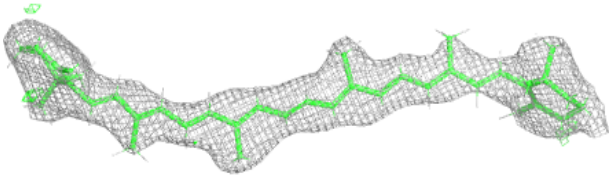


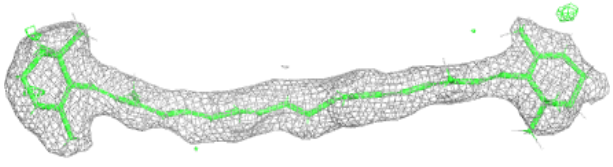


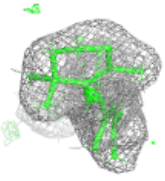


Electron density around BCR h 701:

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

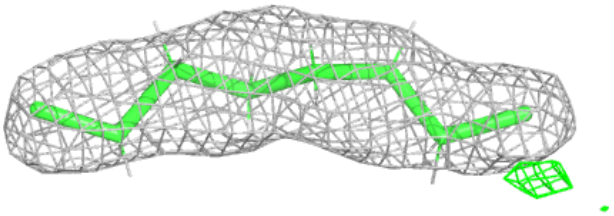


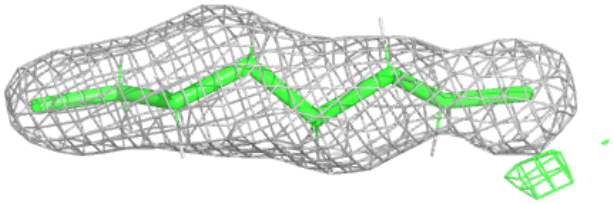


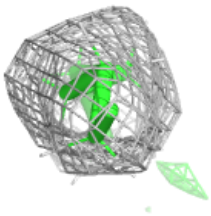


Electron density around STE Z 101:

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

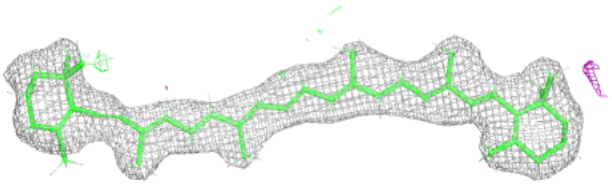


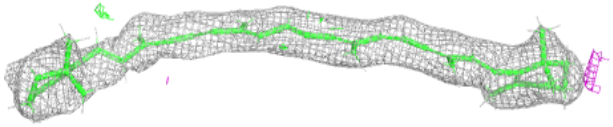


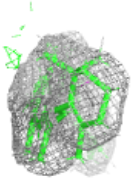


Electron density around BCR d 403:

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

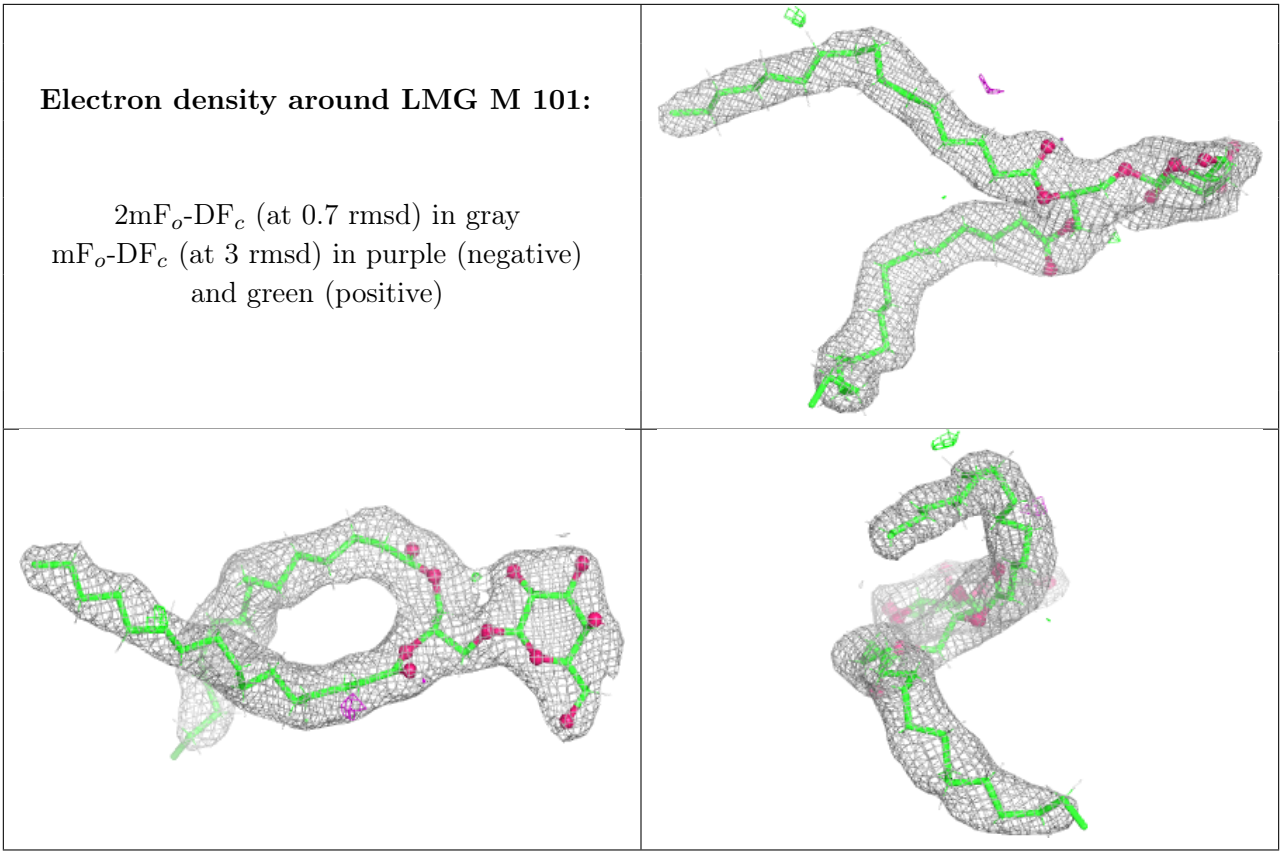






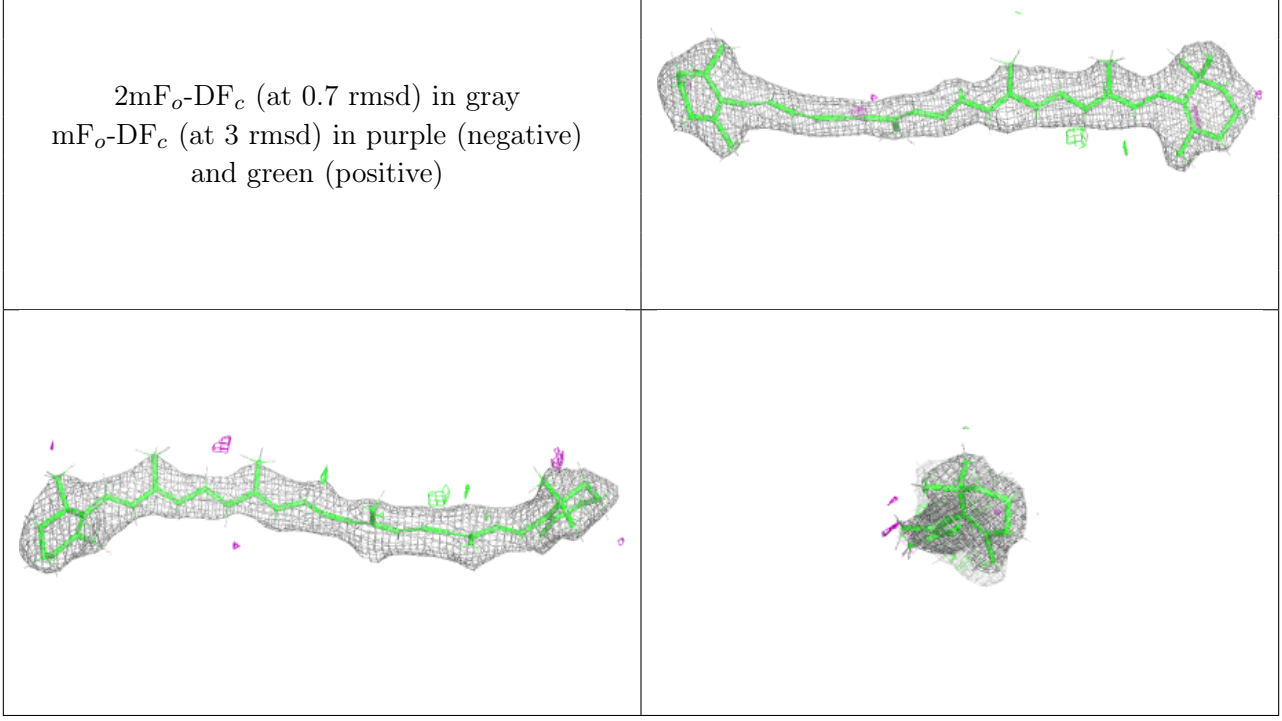
Electron density around LMG M 101:

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



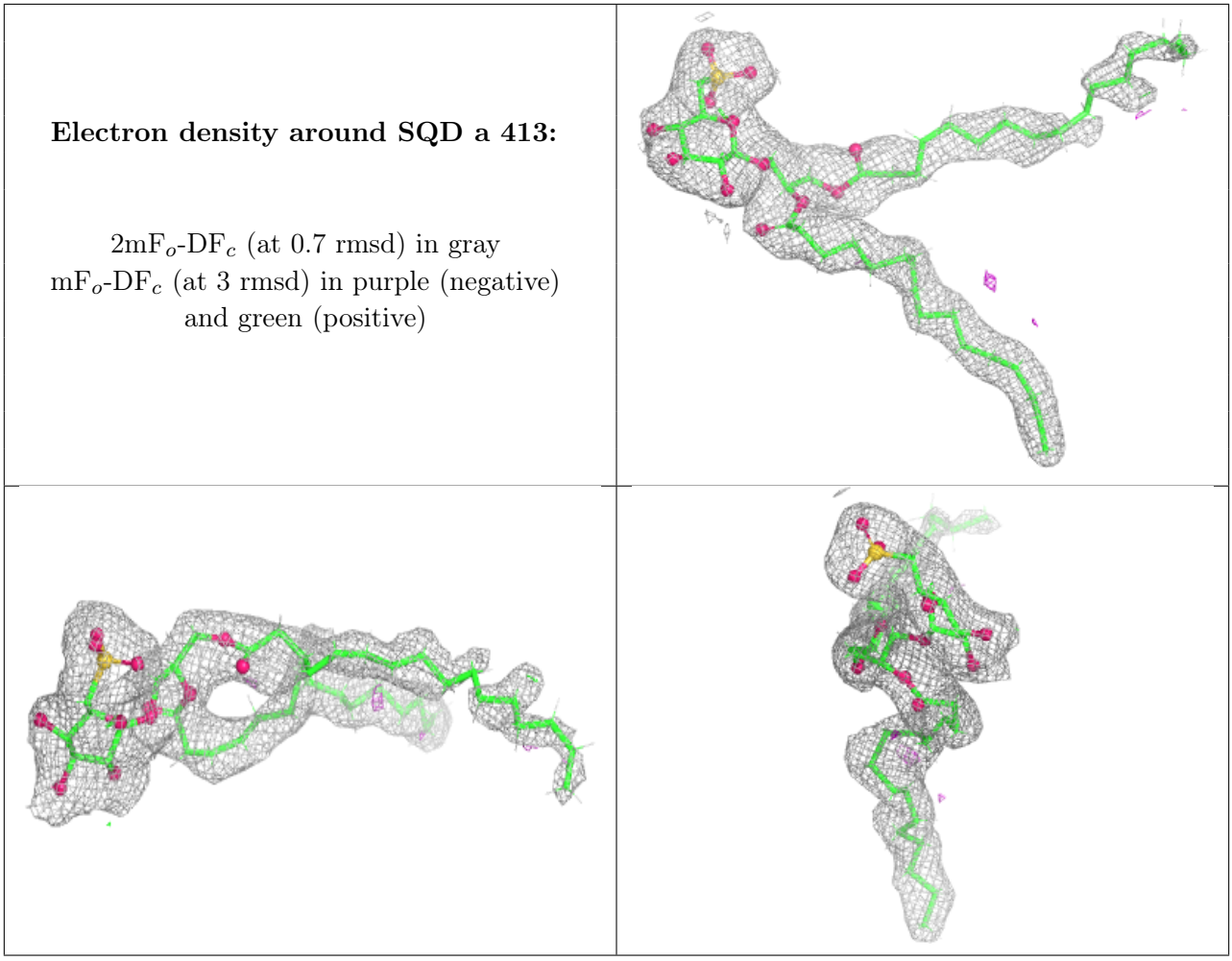
Electron density around BCR K 101:

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



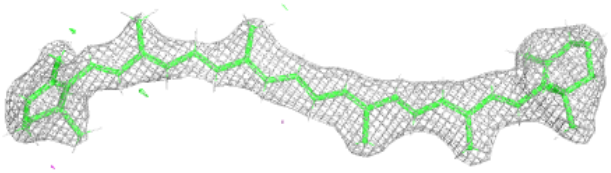
Electron density around SQD a 413:

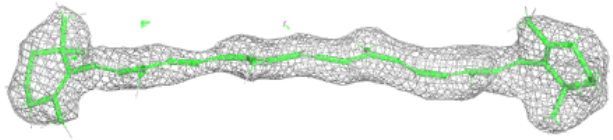
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

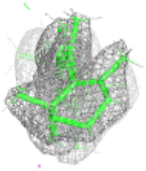


Electron density around BCR k 101:

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

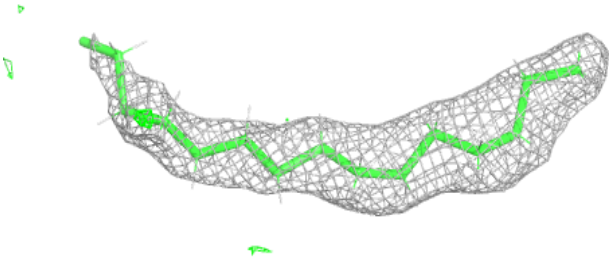


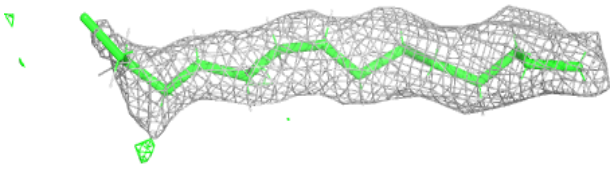


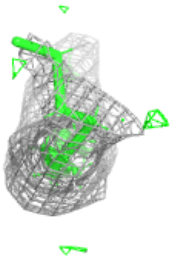


Electron density around STE T 702:

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

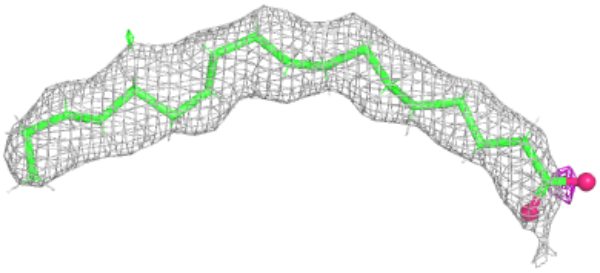


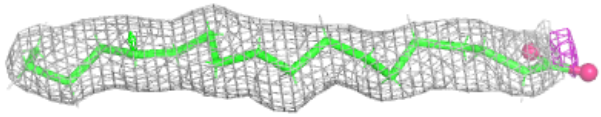


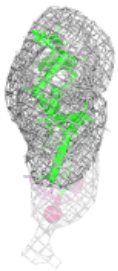


Electron density around STE X 101:

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

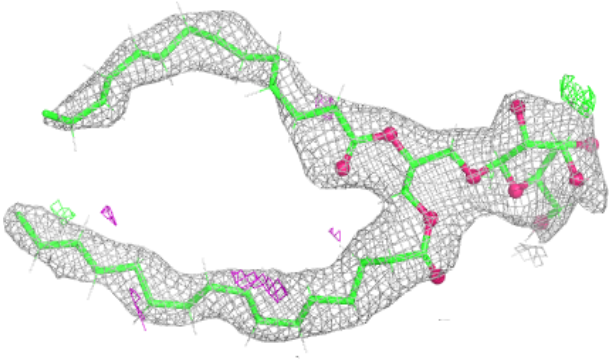


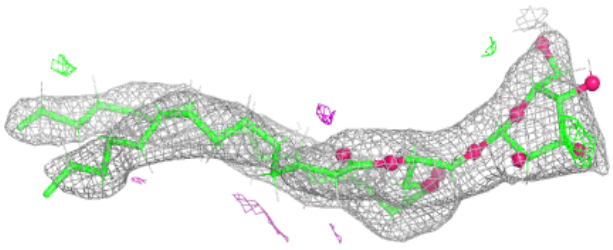


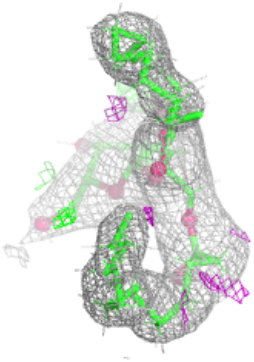


Electron density around LMG c 523:

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

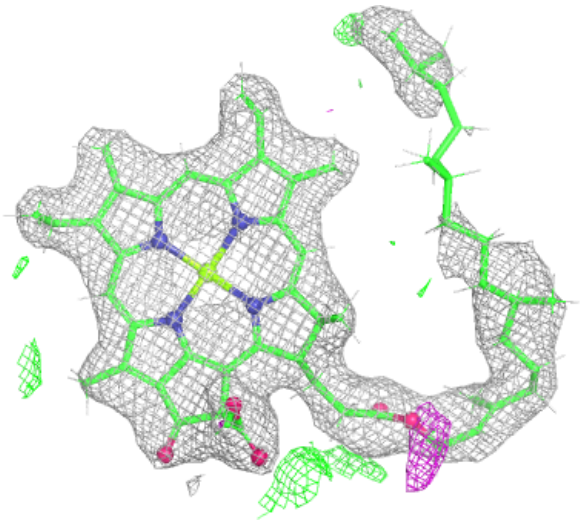


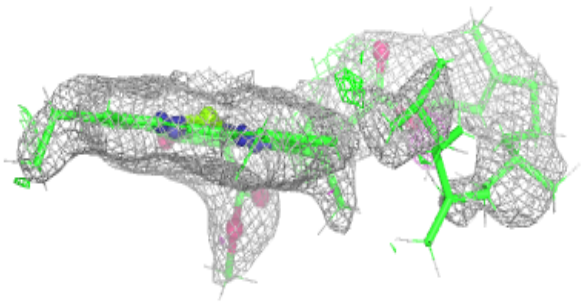


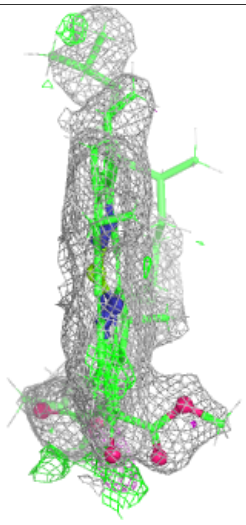


Electron density around CLA c 513:

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

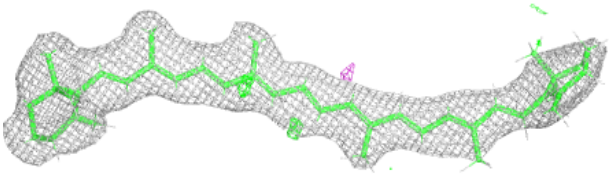


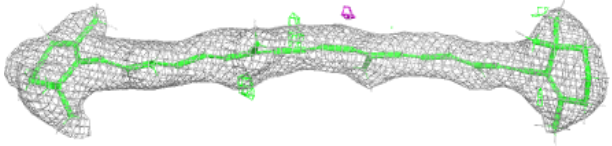


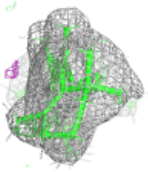


Electron density around BCR Y 101:

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

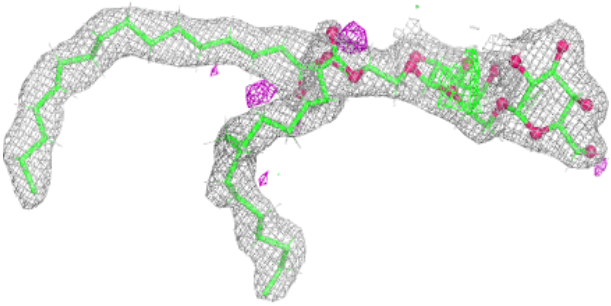


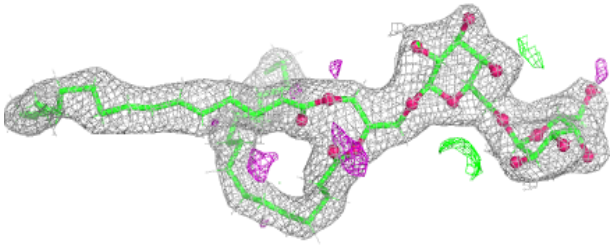




Electron density around DGD h 702:

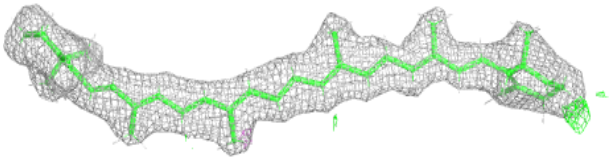
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

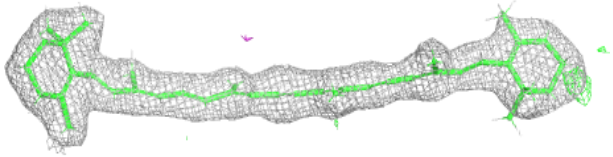


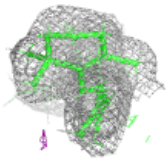


Electron density around BCR H 101:

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

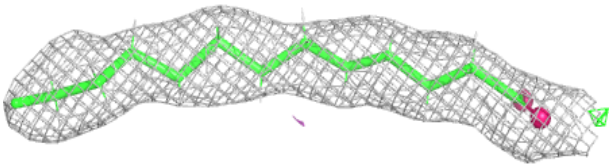


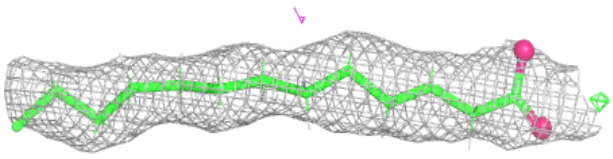


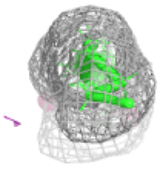


Electron density around STE M 102:

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

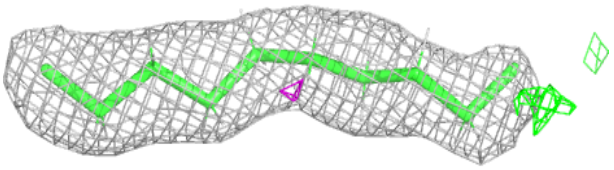


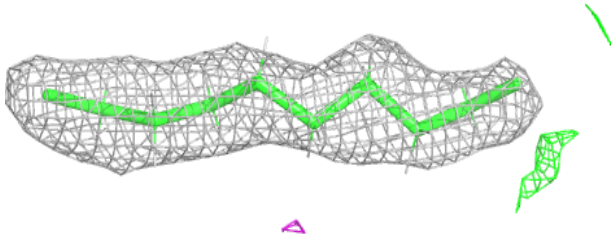


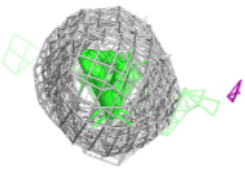


Electron density around STE M 103:

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

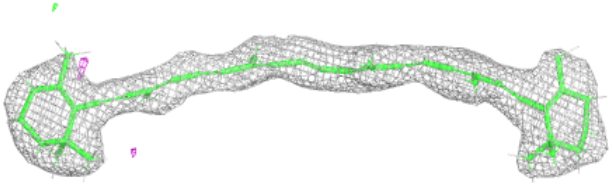


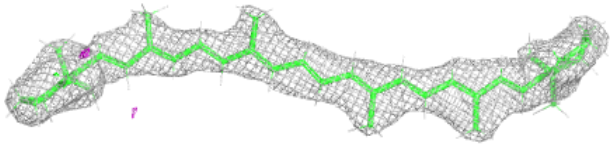


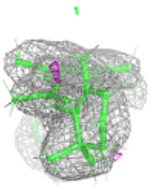


Electron density around BCR k 102:

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

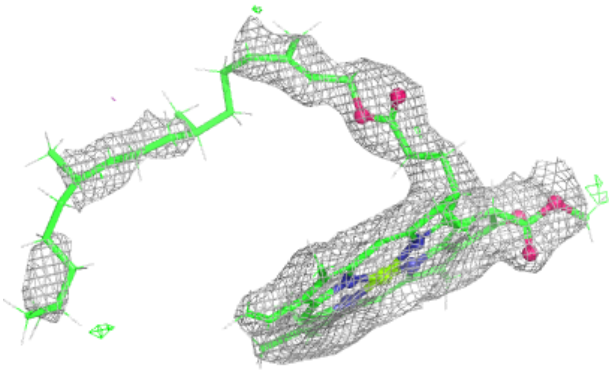


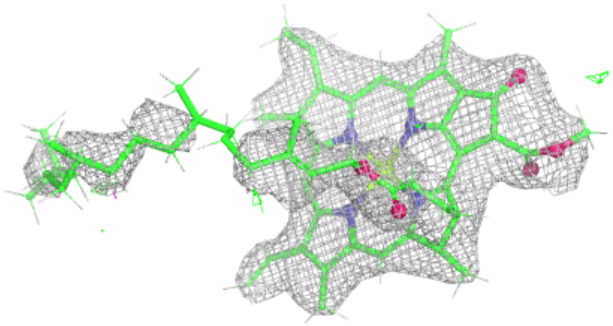


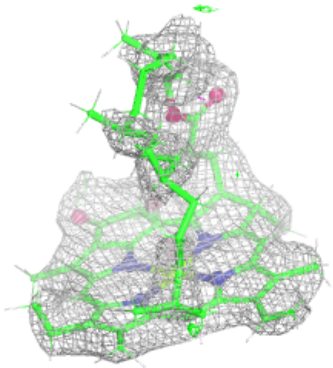


Electron density around CLA c 514:

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

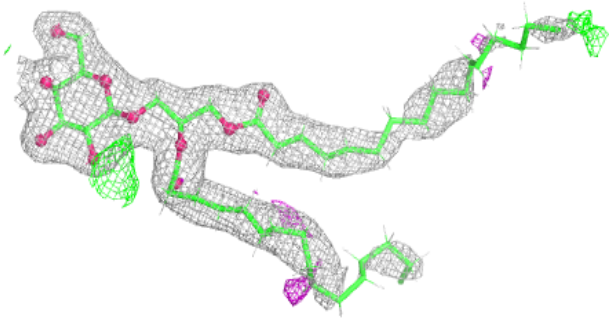


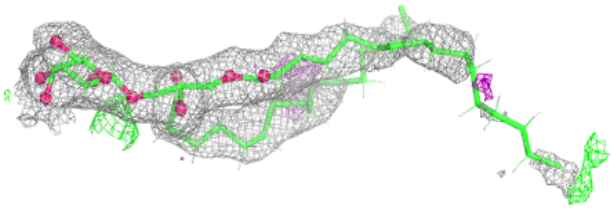




Electron density around LMG D 408:

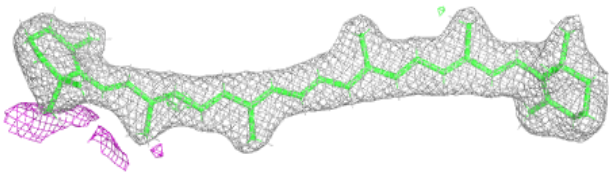
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

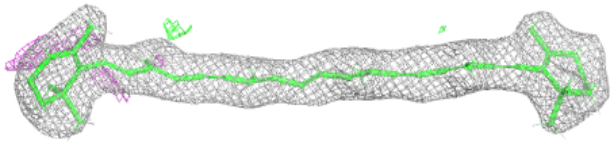


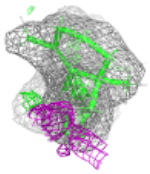


Electron density around BCR B 718:

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

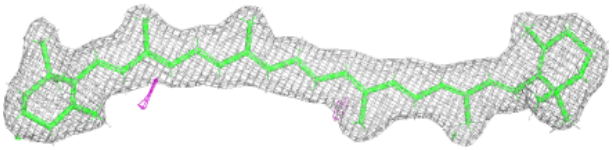


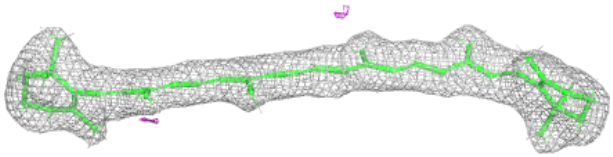


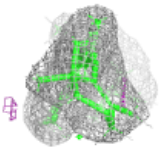


Electron density around BCR B 719:

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

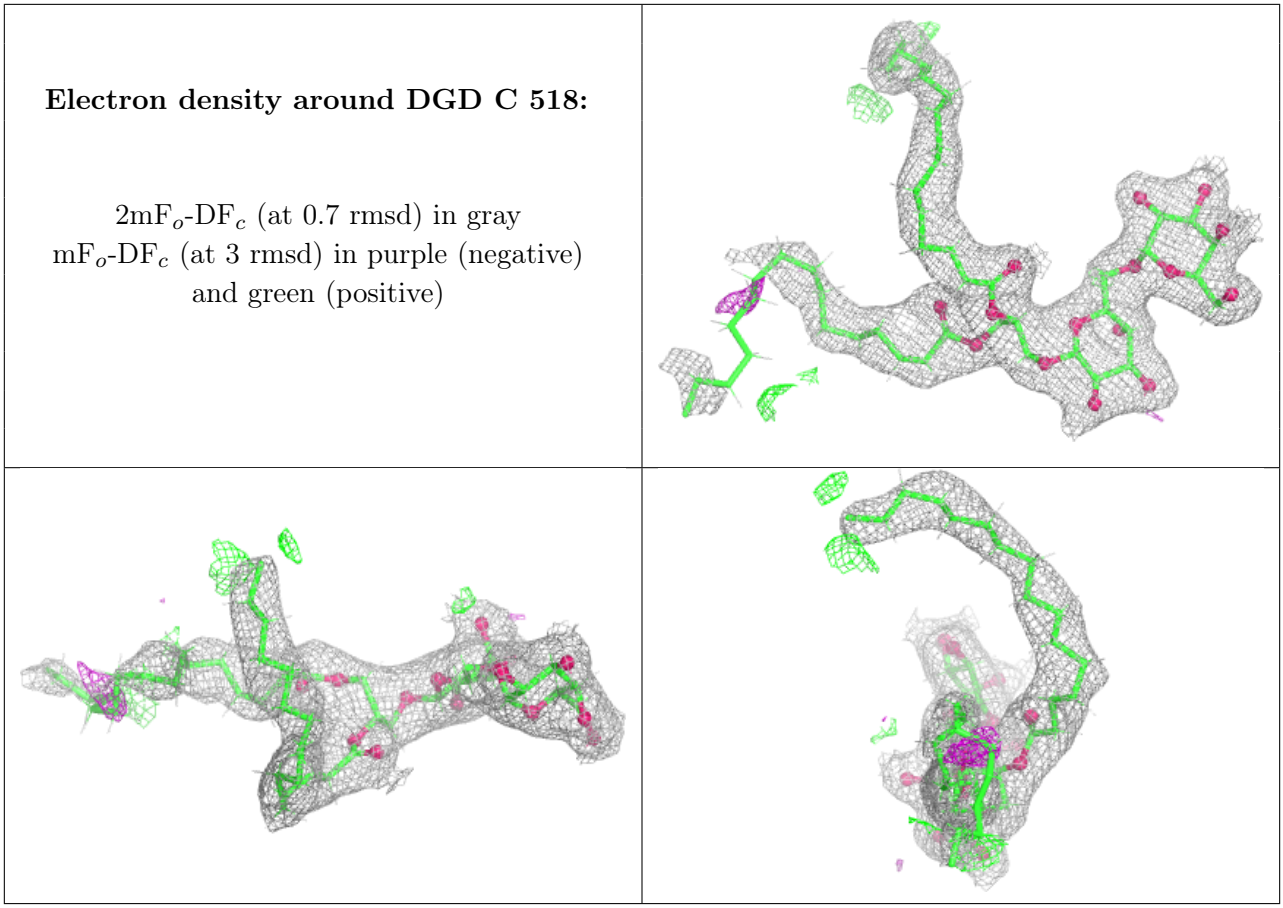






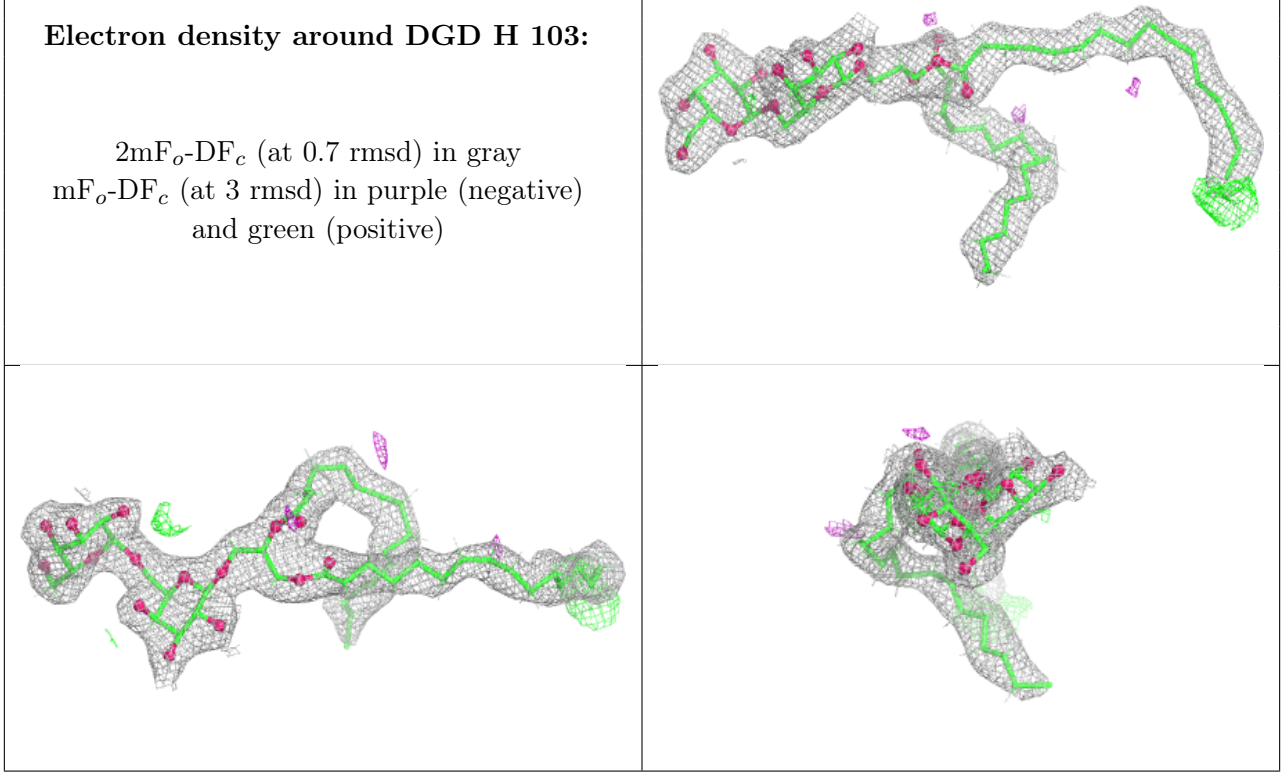
Electron density around DGD C 518:

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



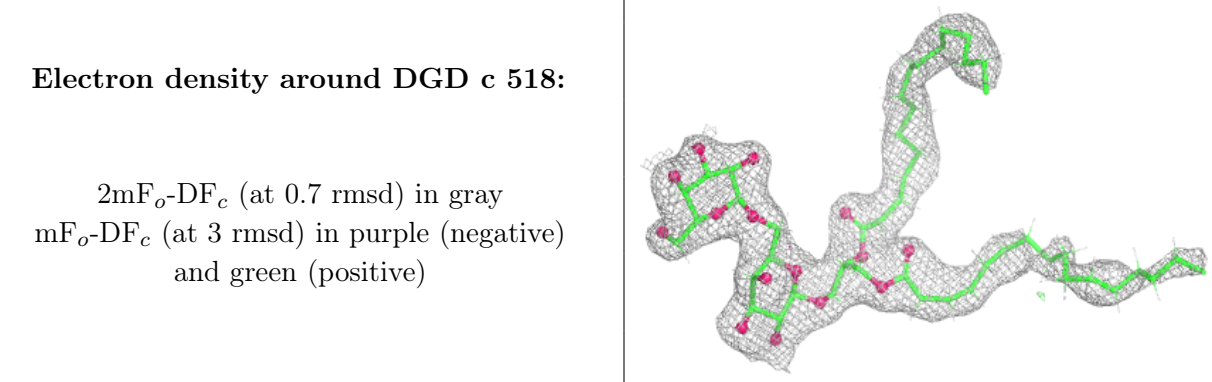
Electron density around DGD H 103:

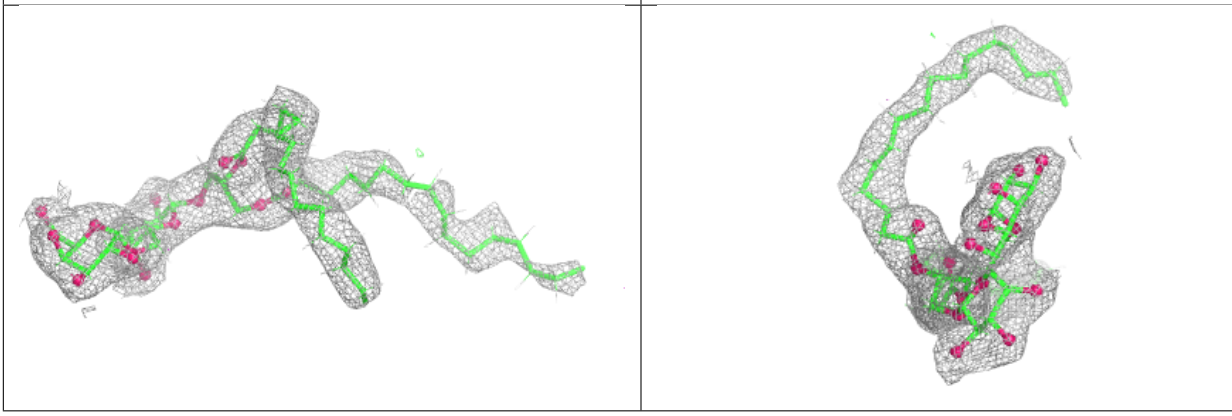
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD c 518:

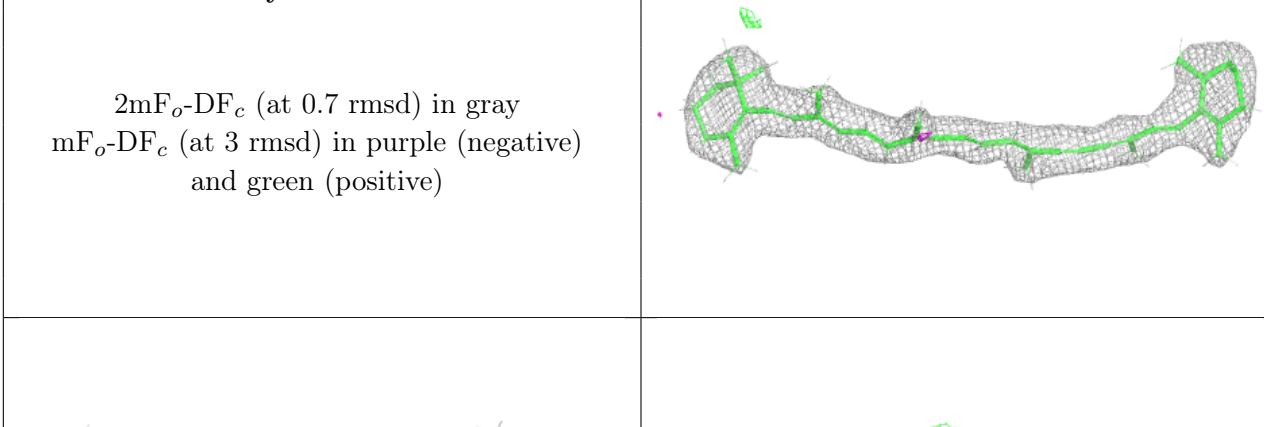
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

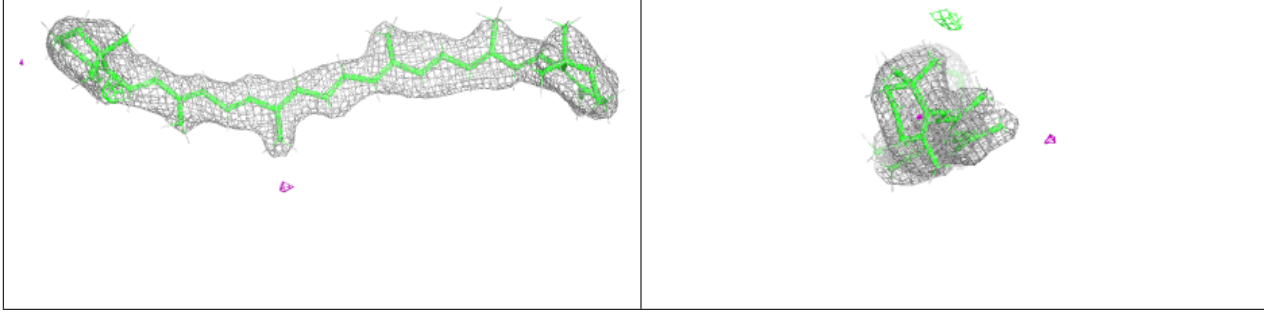




Electron density around BCR C 501:

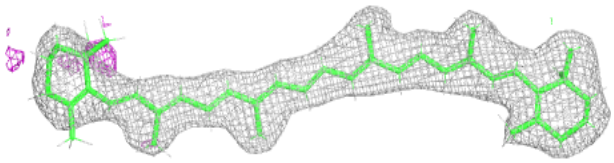
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

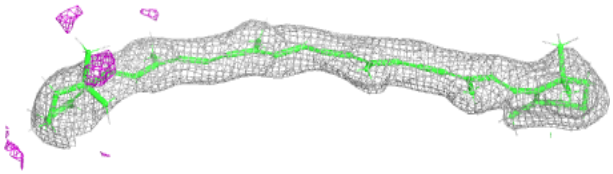


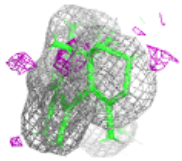


Electron density around BCR D 404:

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

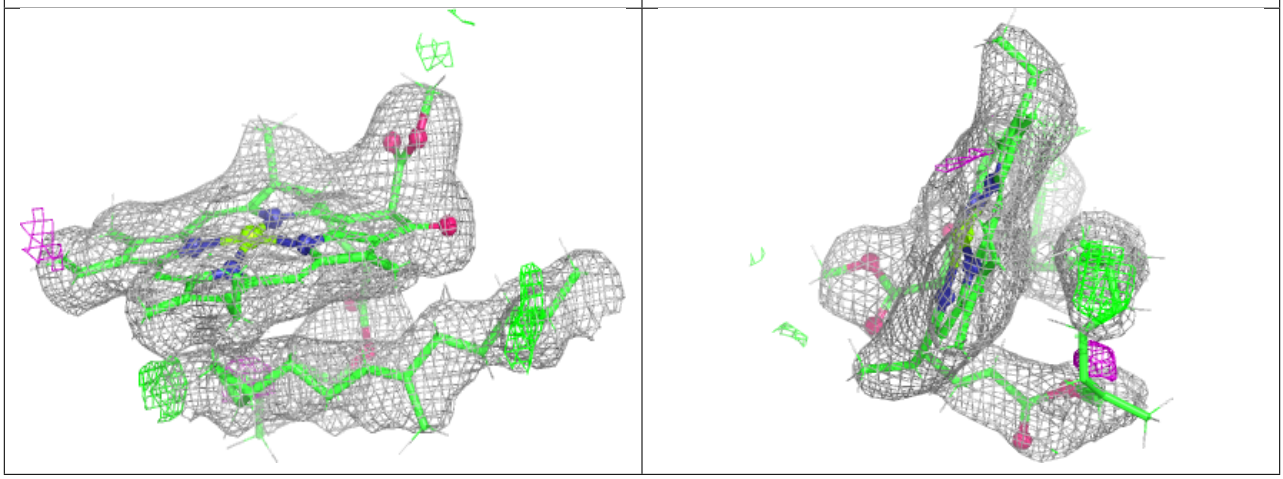






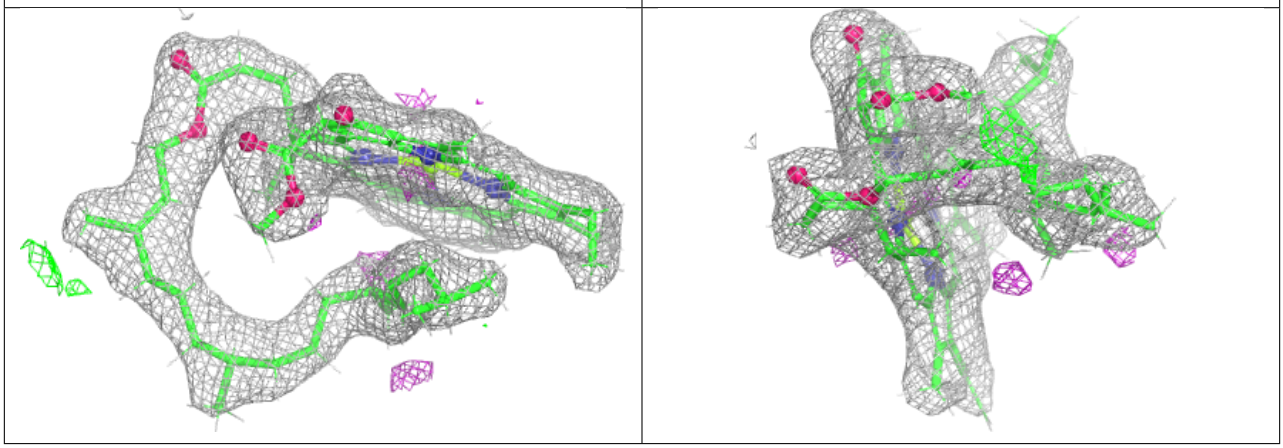
Electron density around CLA H 102:

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



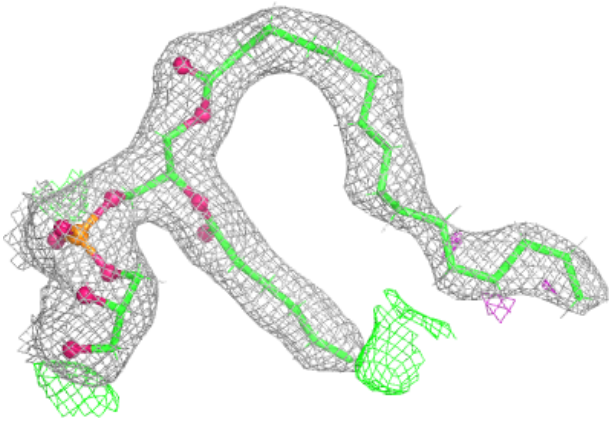
Electron density around CLA C 511:

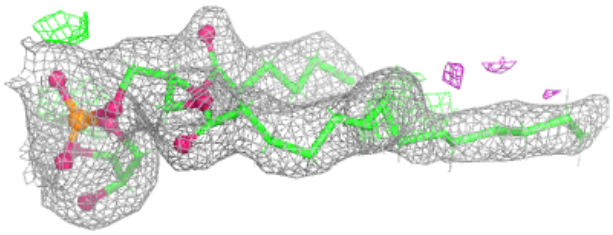
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

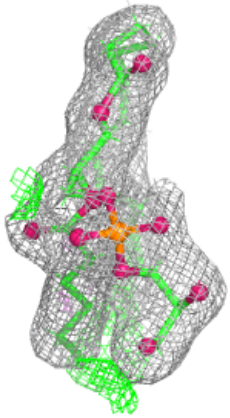


Electron density around LHG d 407:

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

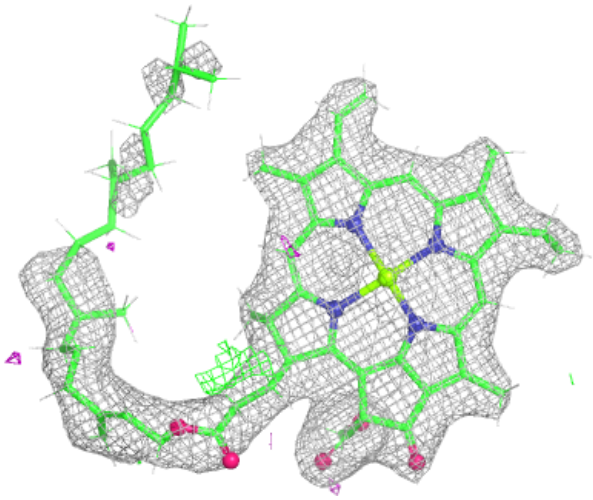


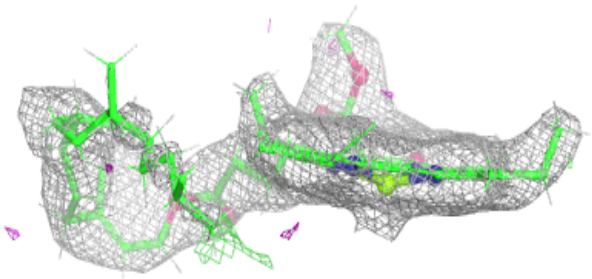


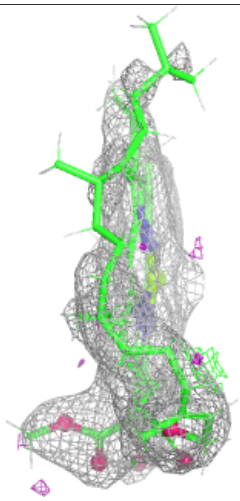


Electron density around CLA C 513:

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

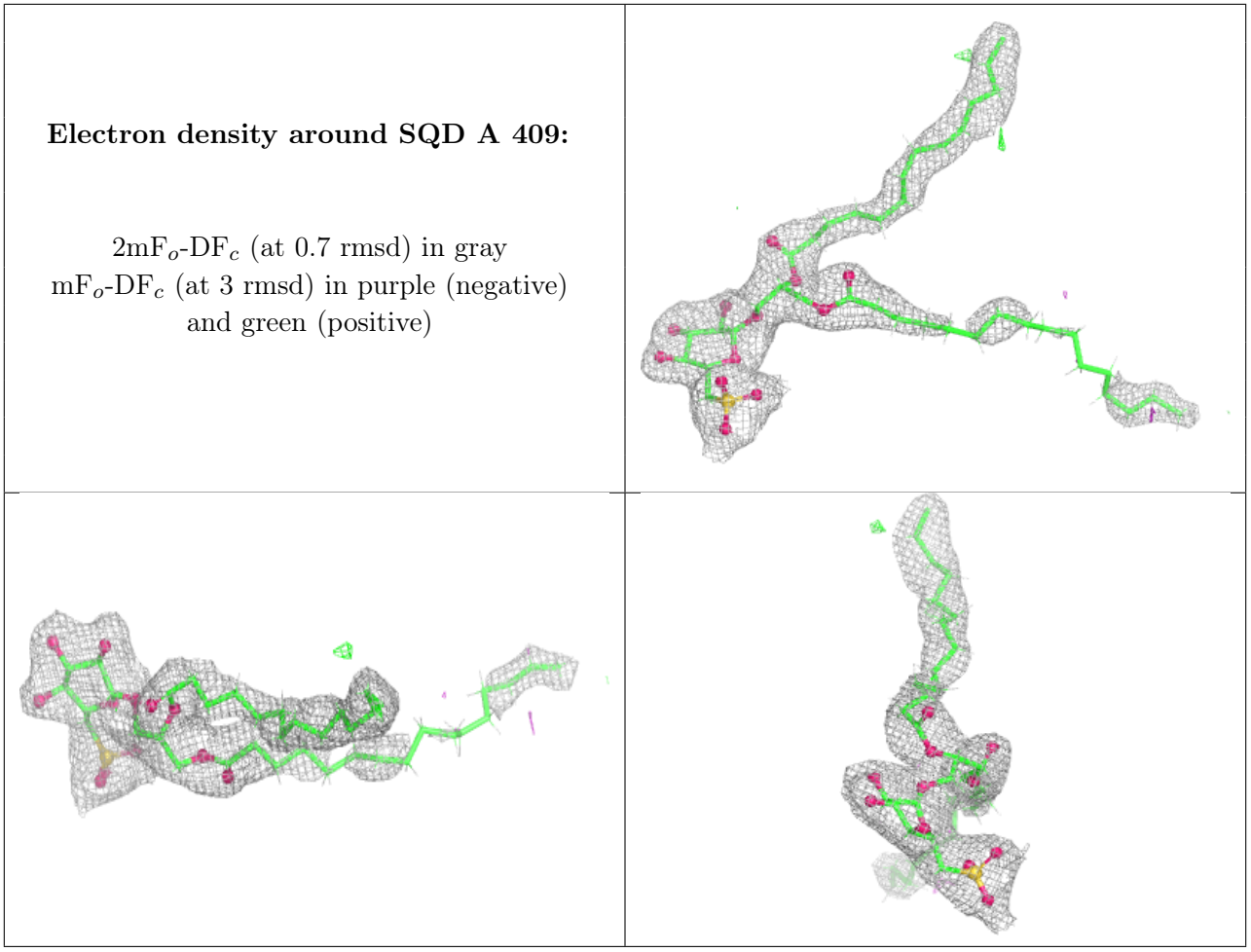






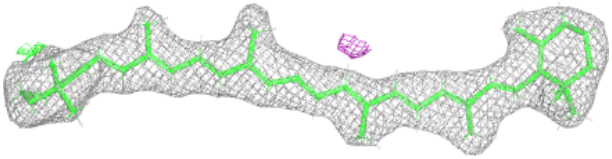
Electron density around SQD A 409:

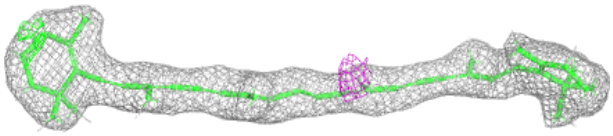
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

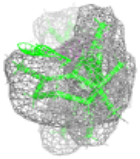


Electron density around BCR b 717:

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

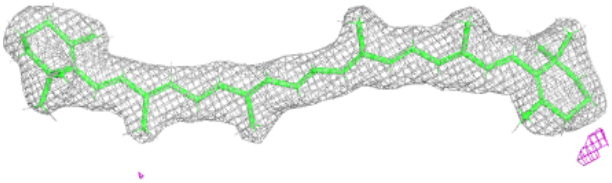


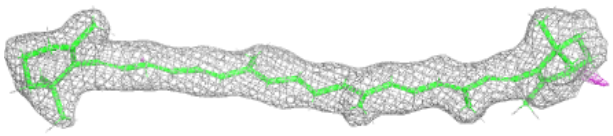


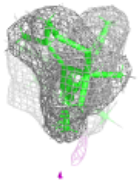


Electron density around BCR b 719:

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

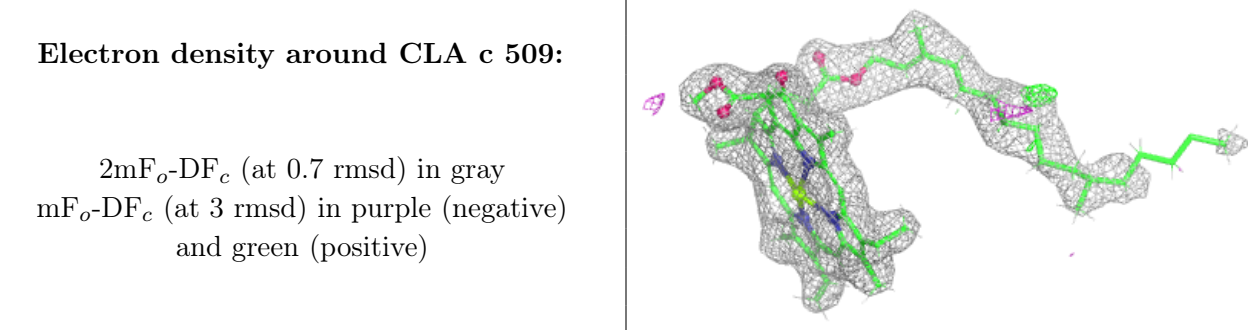






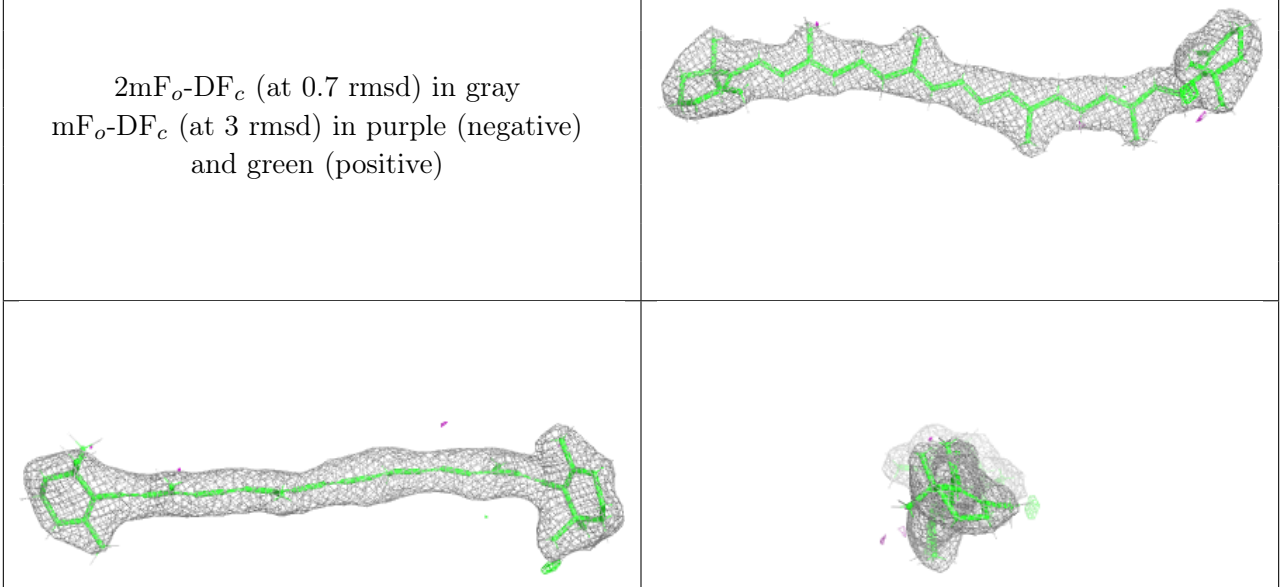
Electron density around CLA c 509:

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



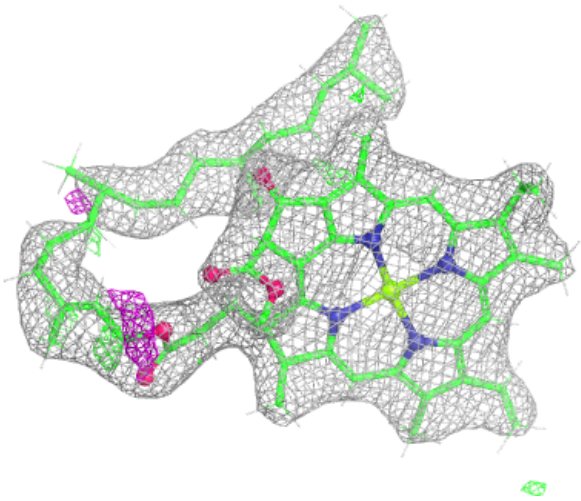
Electron density around BCR c 516:

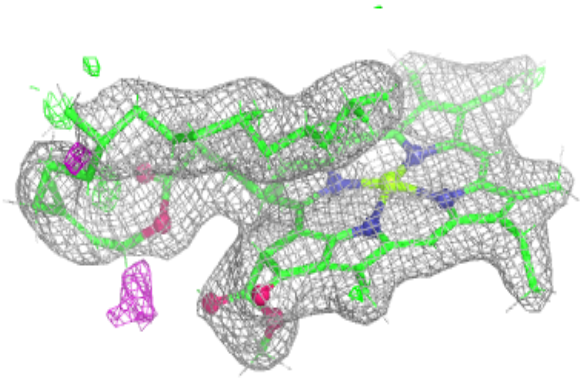
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

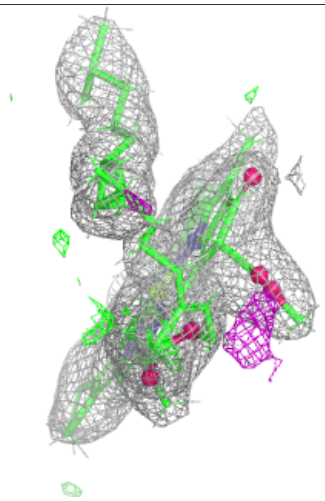


Electron density around CLA c 510:

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

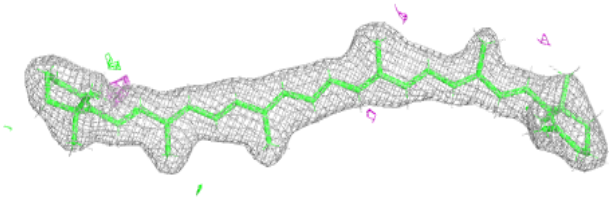


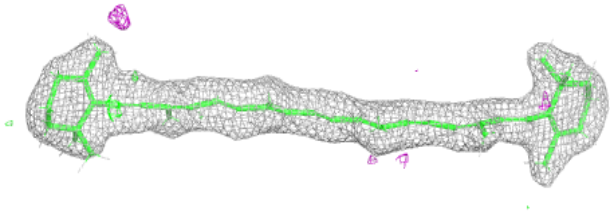


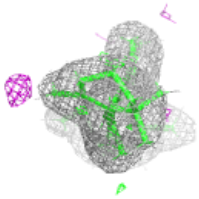


Electron density around BCR C 515:

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

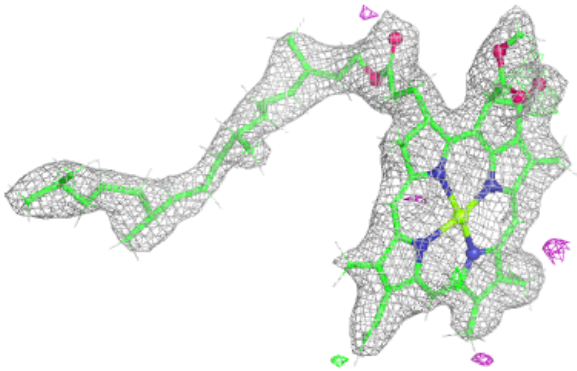


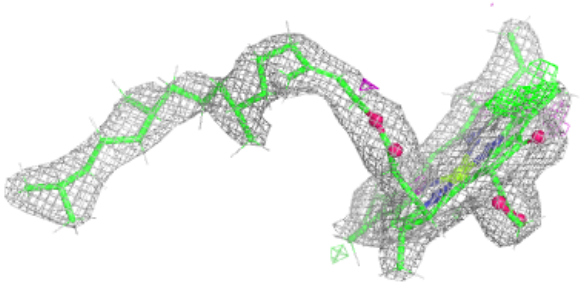


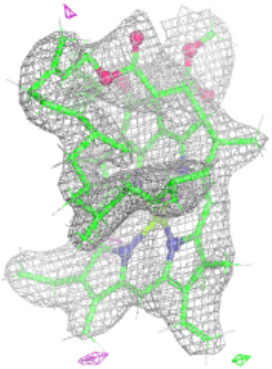


Electron density around CLA c 512:

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

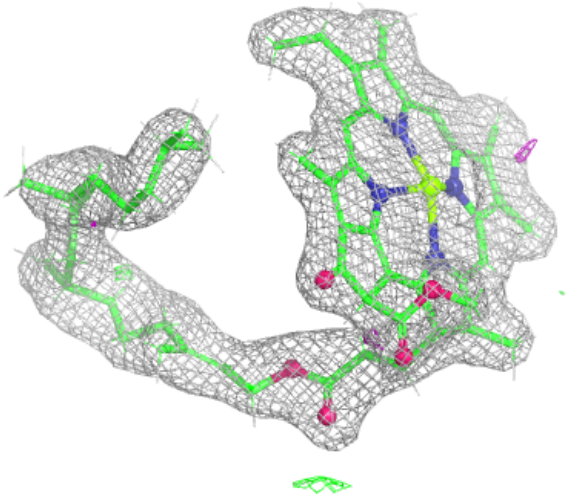


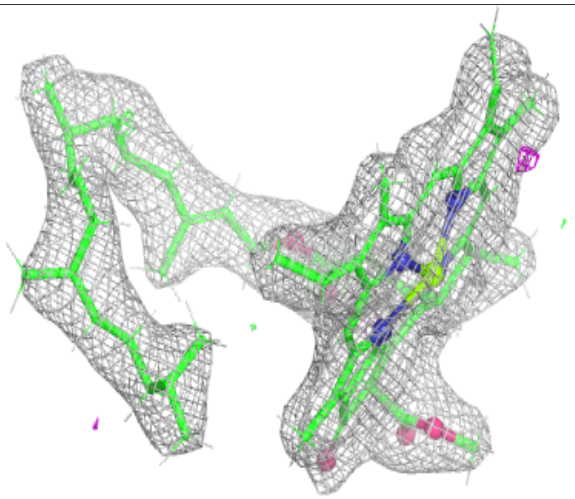


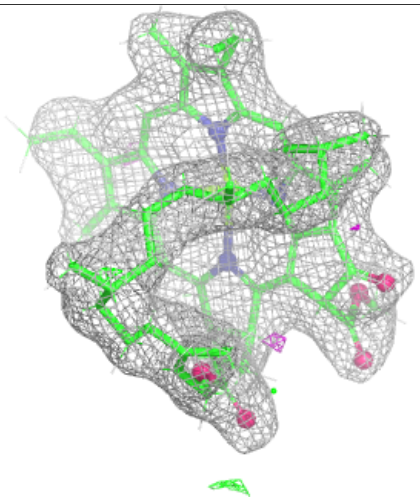


Electron density around CLA C 504:

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

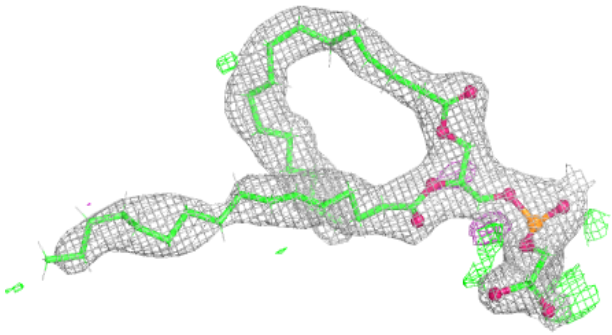


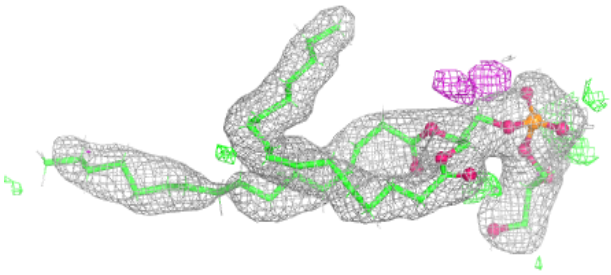


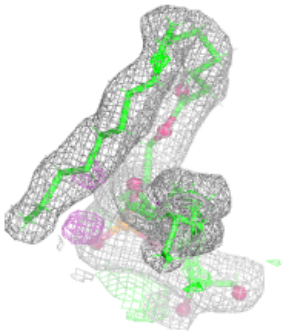


Electron density around LHG B 722:

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

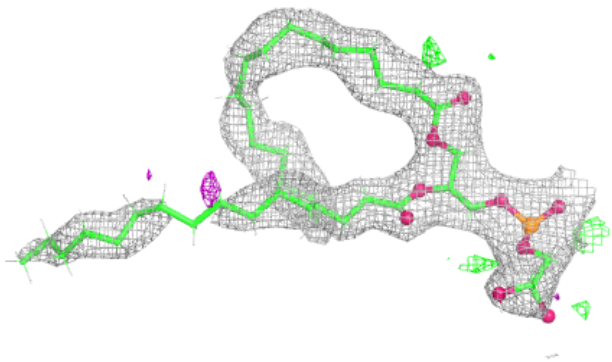


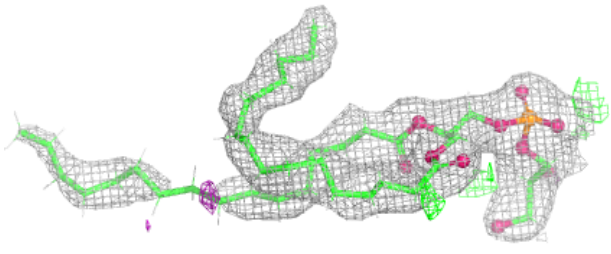


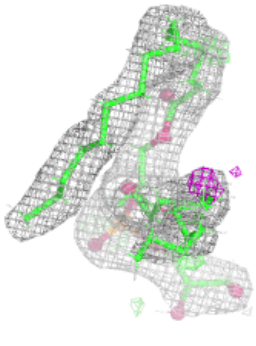


Electron density around LHG a 412:

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

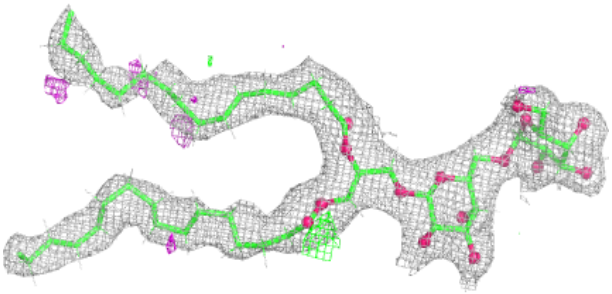


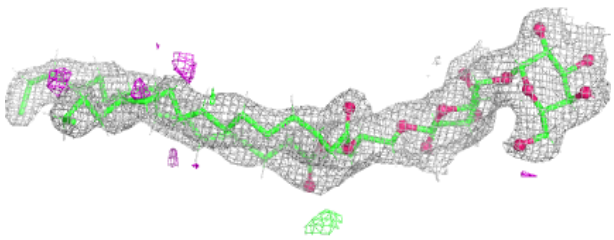




Electron density around DGD C 519:

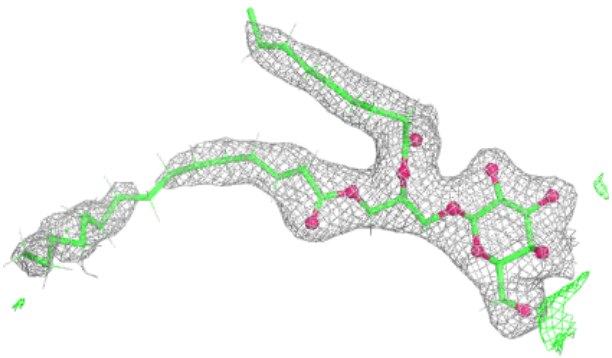
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

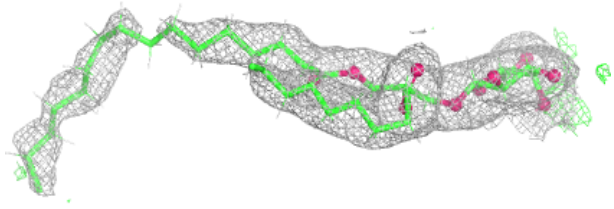


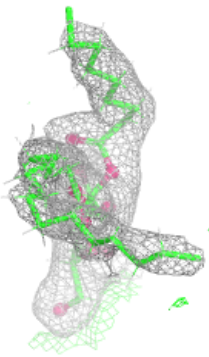


Electron density around LMG d 408:

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

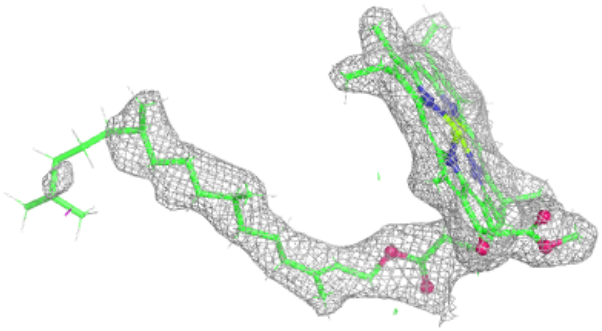


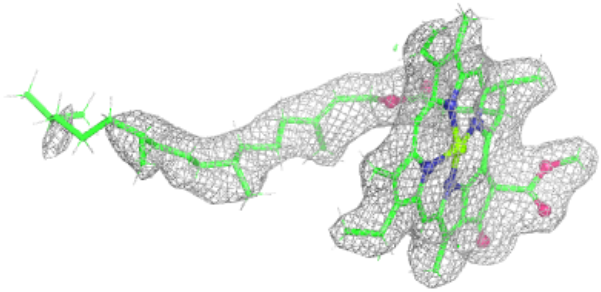


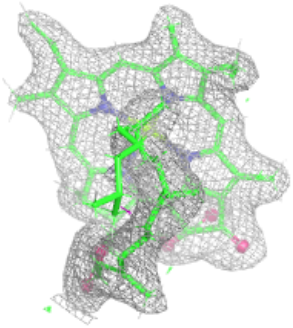


Electron density around CLA C 509:

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

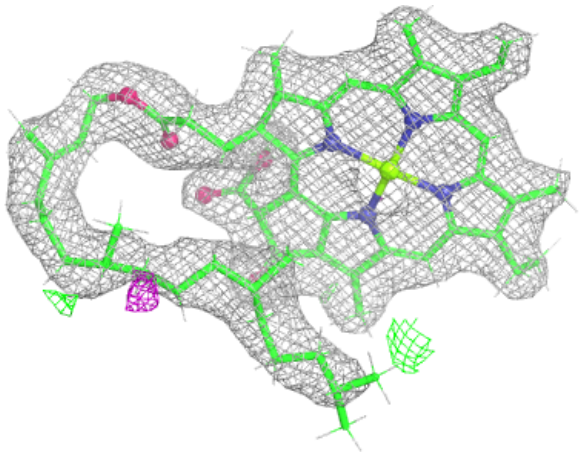


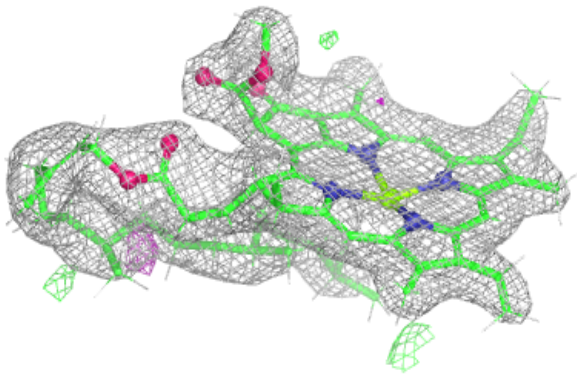


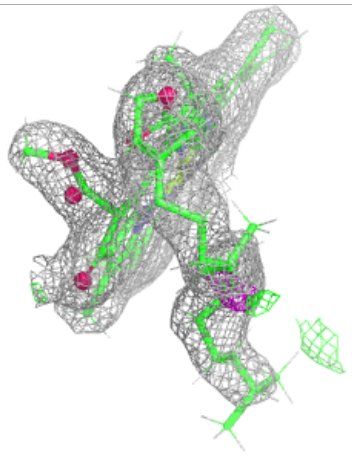


Electron density around CLA C 510:

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

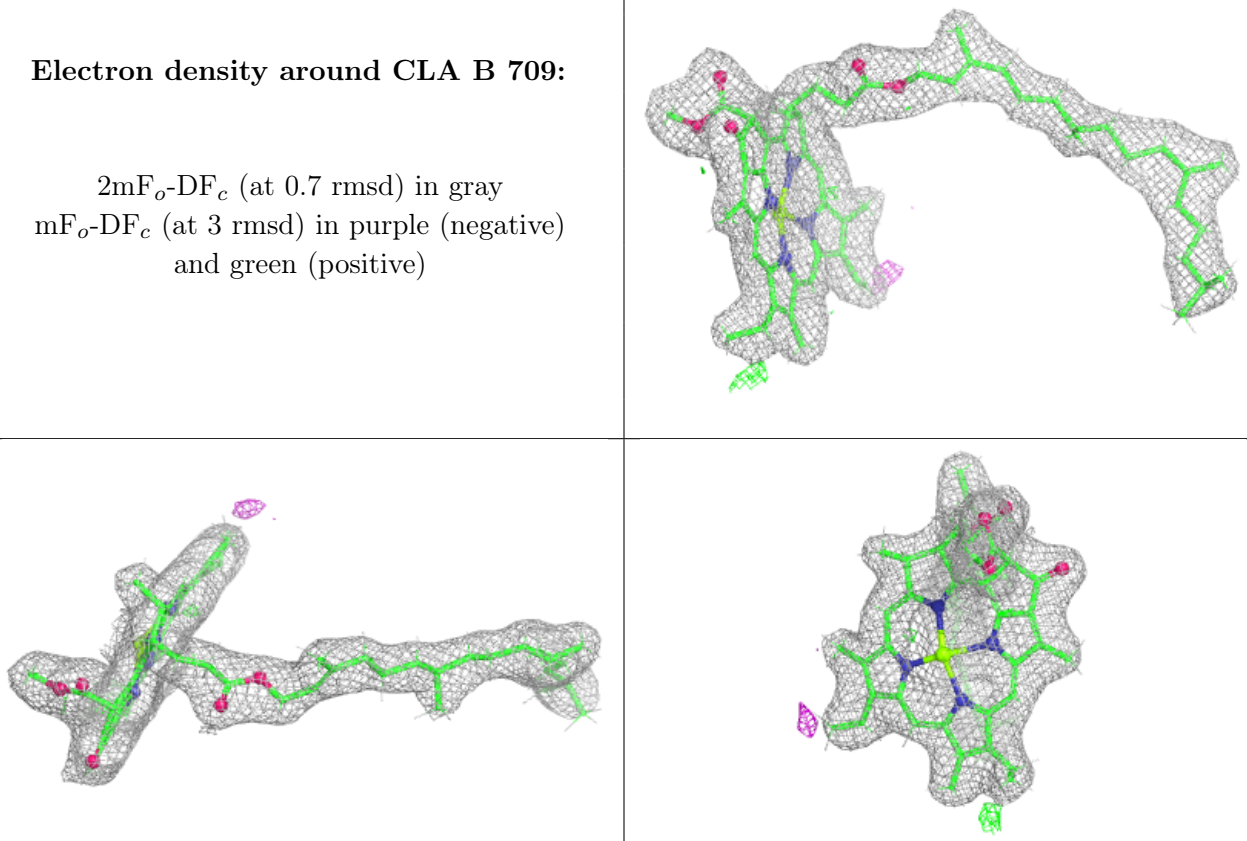






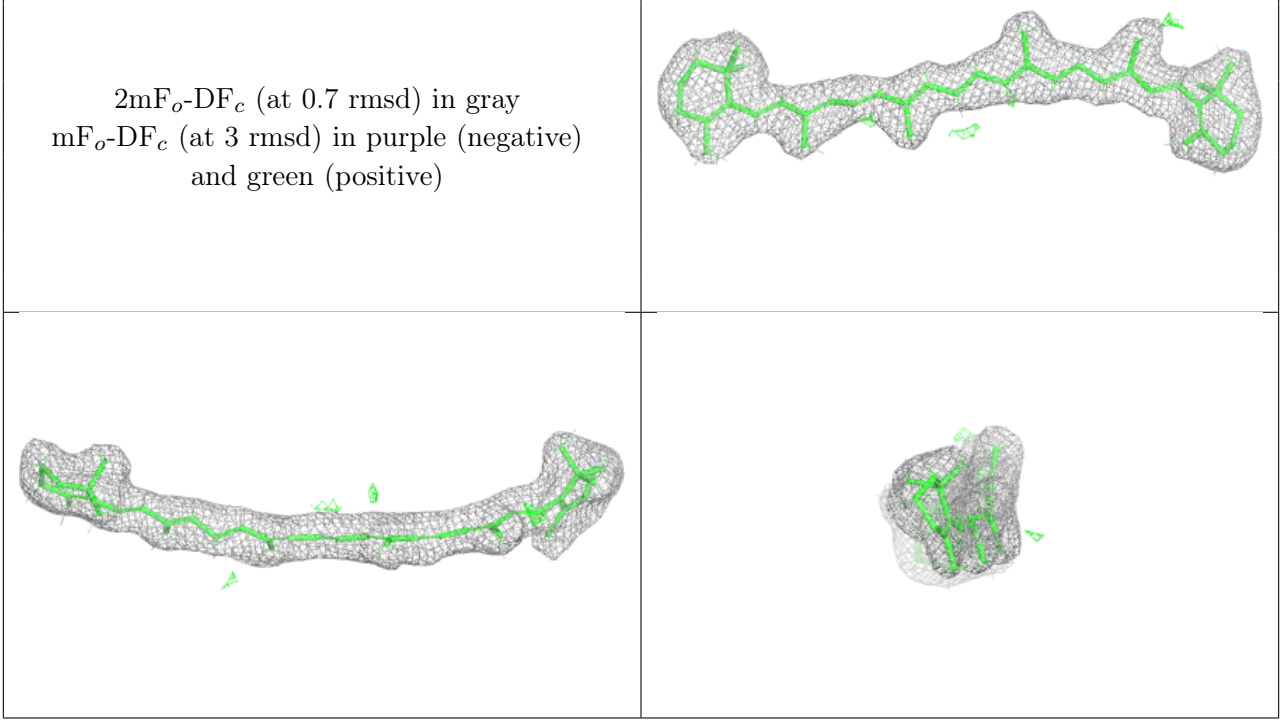
Electron density around CLA B 709:

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



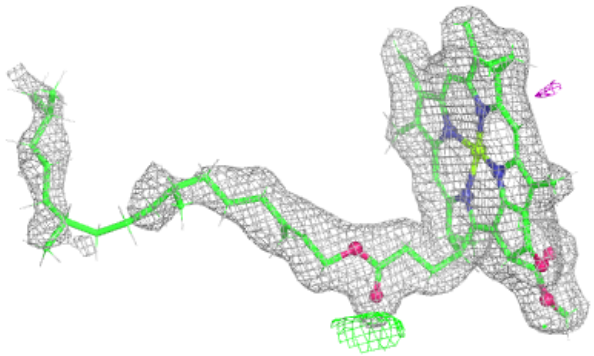
Electron density around BCR t 701:

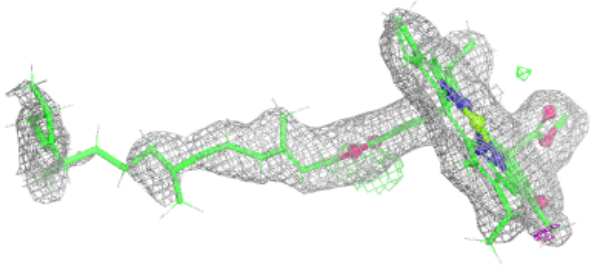
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

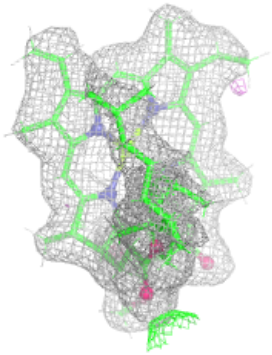


Electron density around CLA d 402:

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

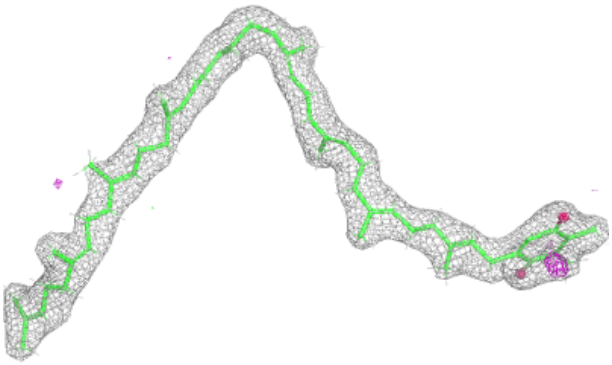


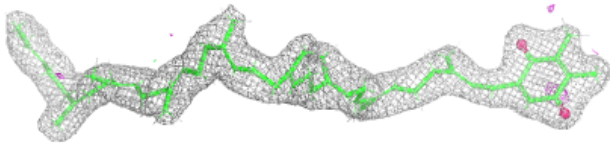


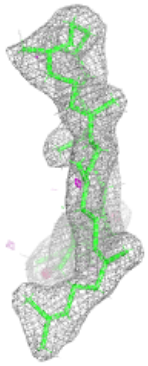


Electron density around PL9 D 405:

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

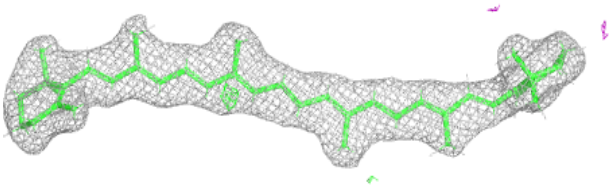


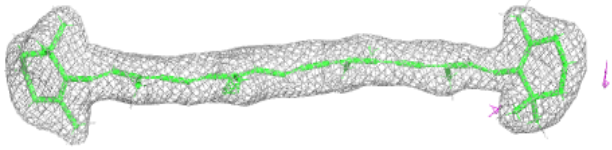


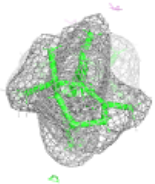


Electron density around BCR A 405:

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

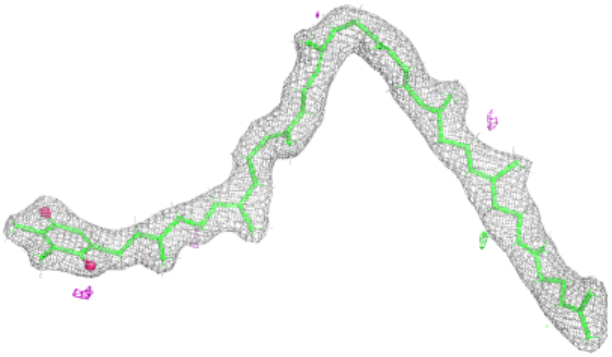


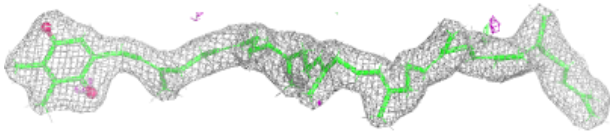


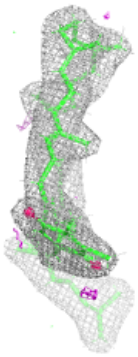


Electron density around PL9 d 404:

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

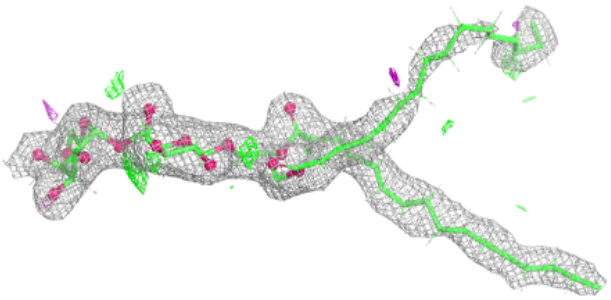


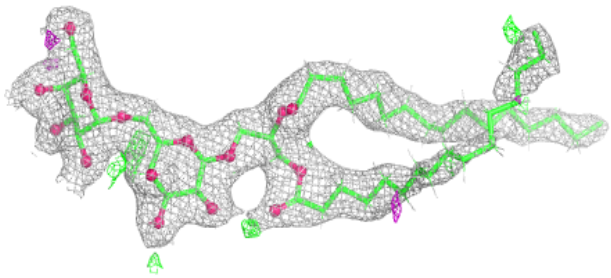


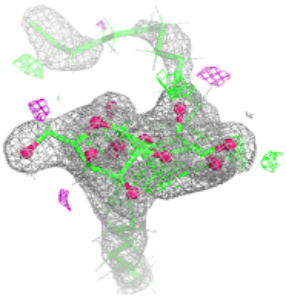


Electron density around DGD C 517:

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

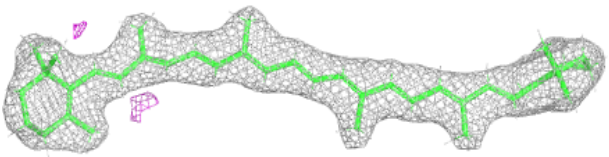


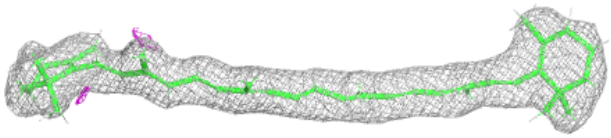


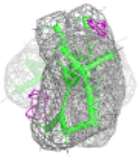


Electron density around BCR B 717:

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

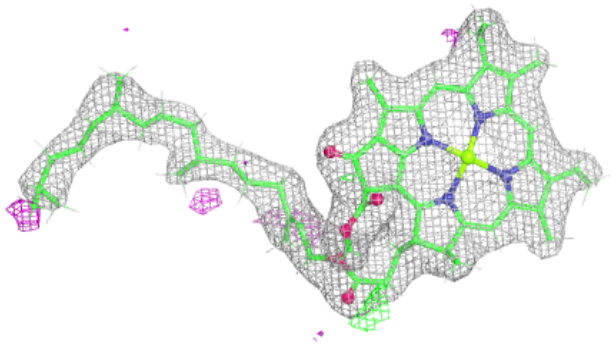


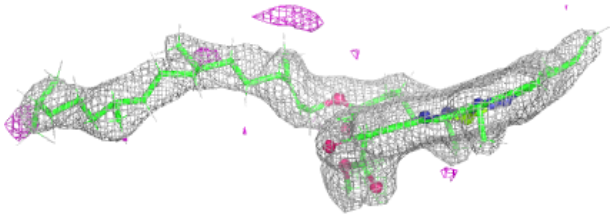


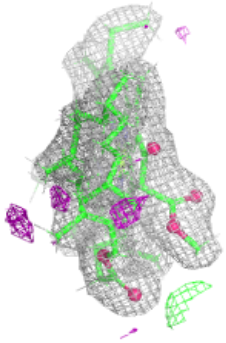


Electron density around CLA b 702:

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

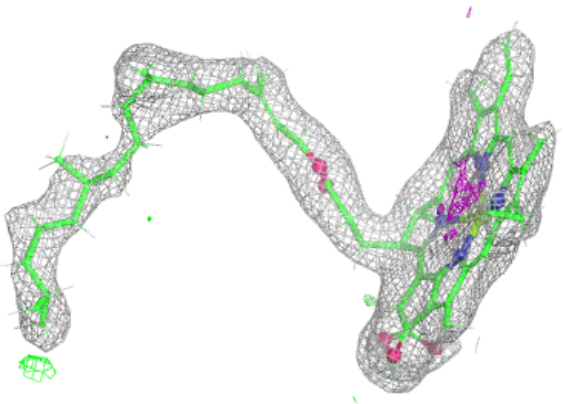


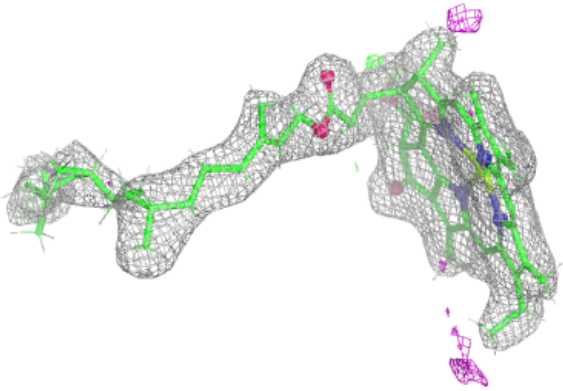


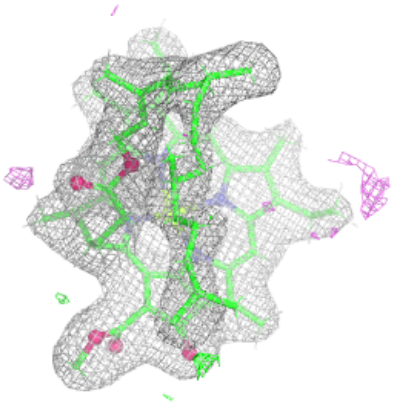


Electron density around CLA b 706:

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

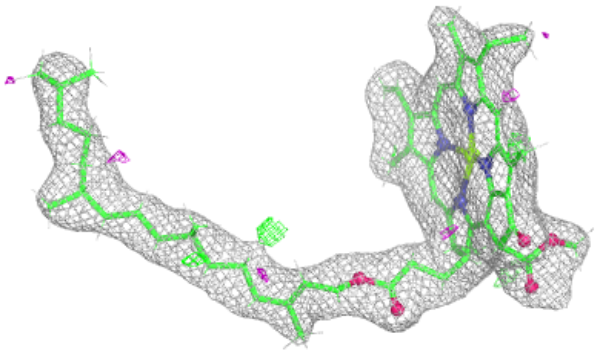


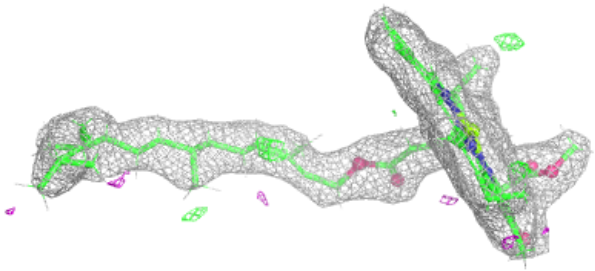


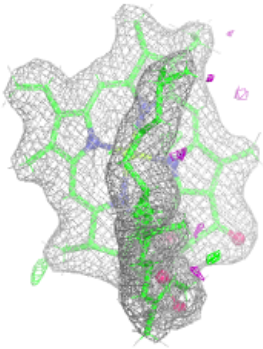


Electron density around CLA b 709:

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

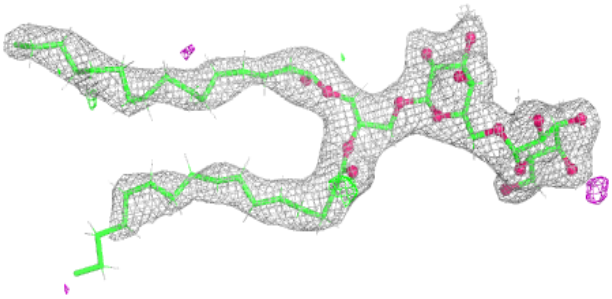


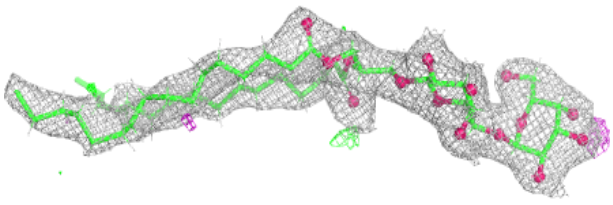


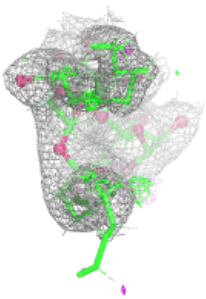


Electron density around DGD c 519:

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

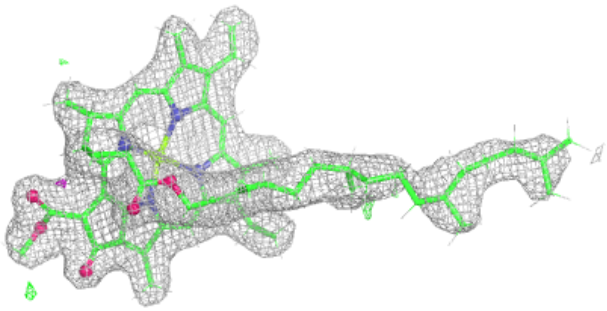


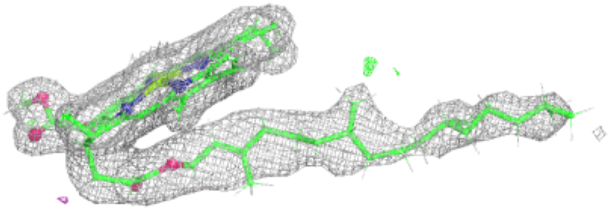


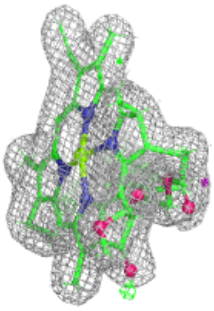


Electron density around CLA b 714:

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

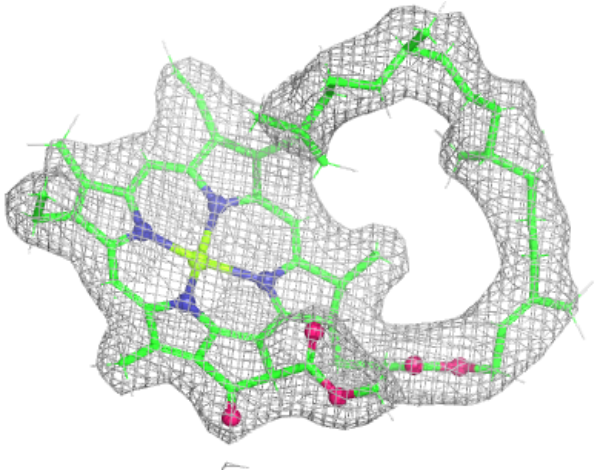


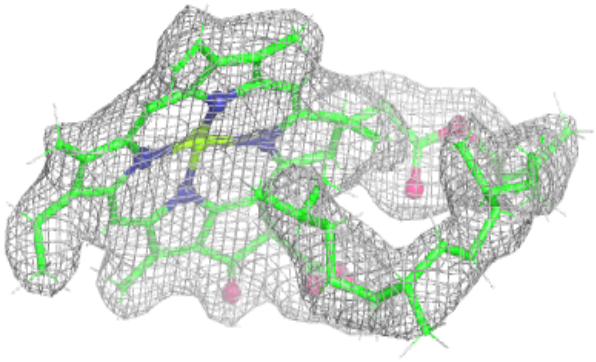


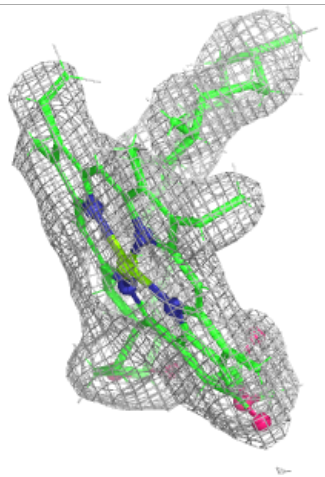


Electron density around CLA b 715:

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

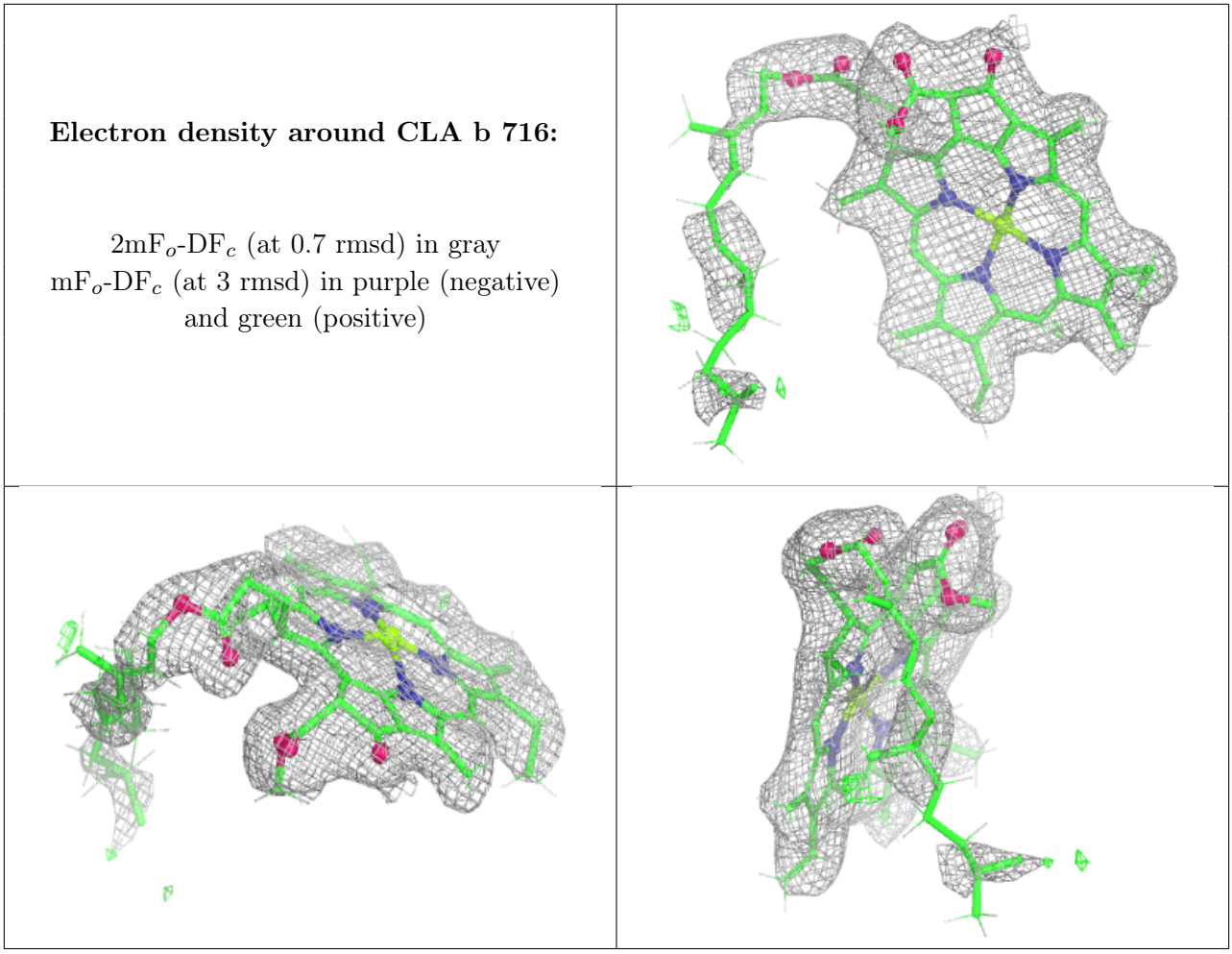






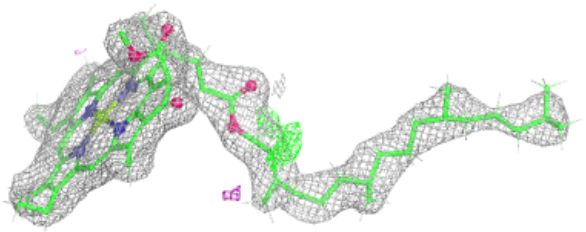
Electron density around CLA b 716:

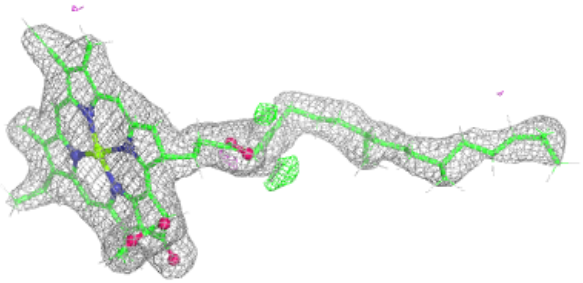
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

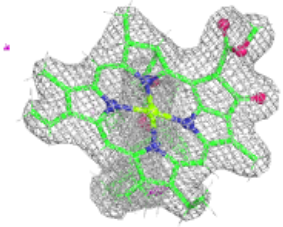


Electron density around CLA c 503:

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

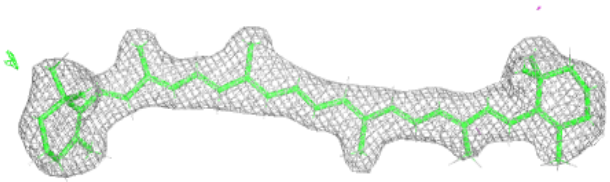


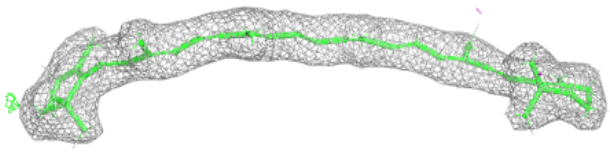


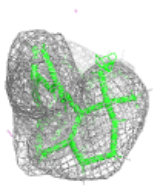


Electron density around BCR T 701:

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

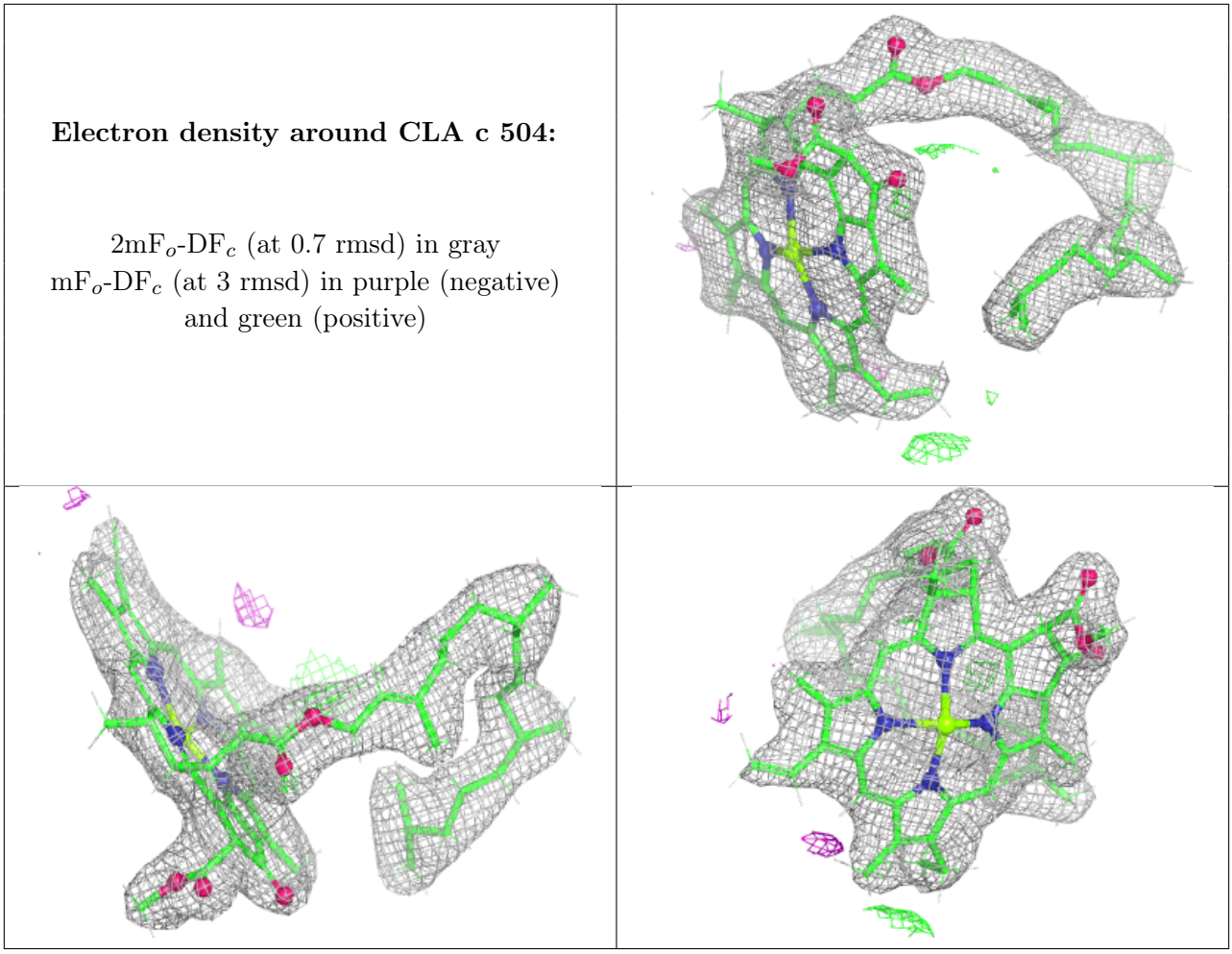






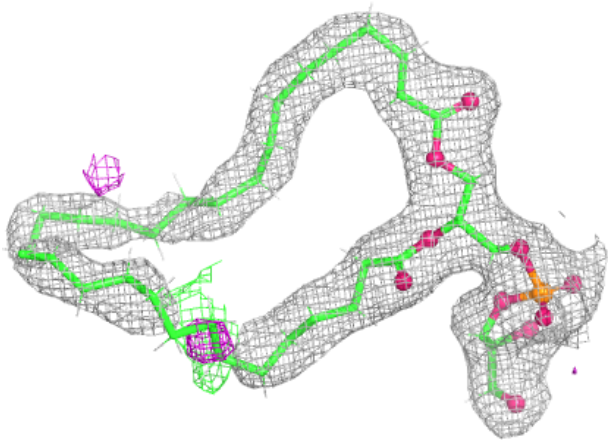
Electron density around CLA c 504:

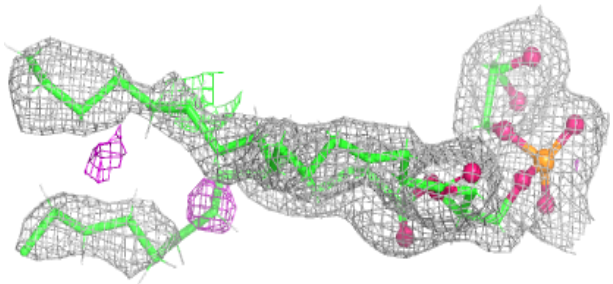
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

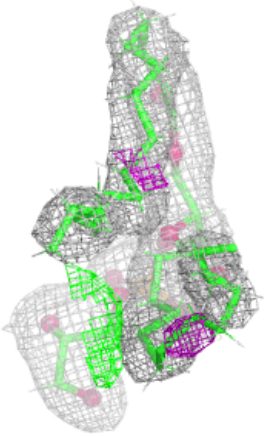


Electron density around LHG D 411:

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

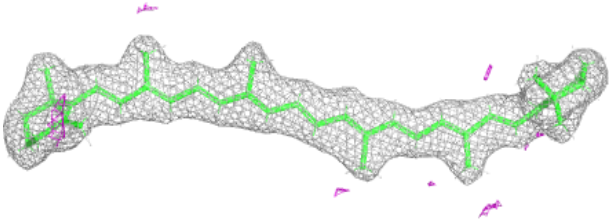


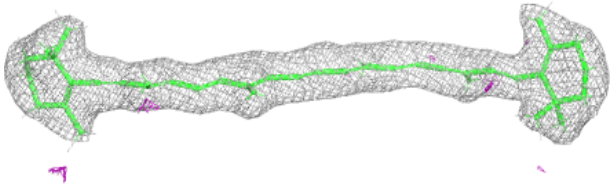


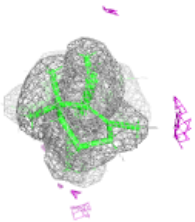


Electron density around BCR a 407:

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

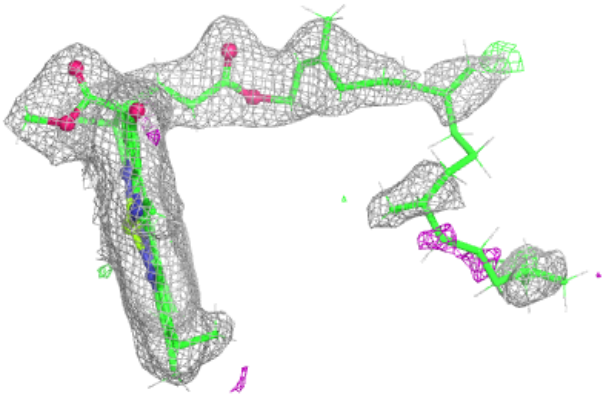


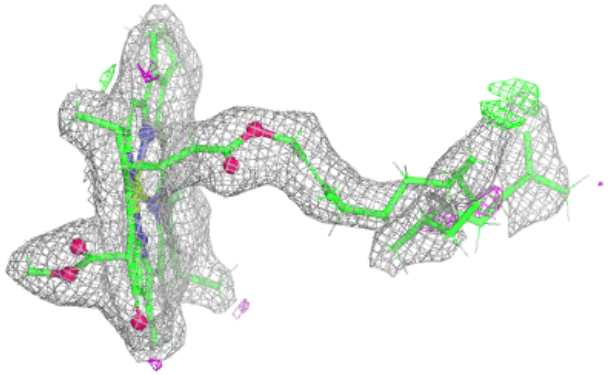


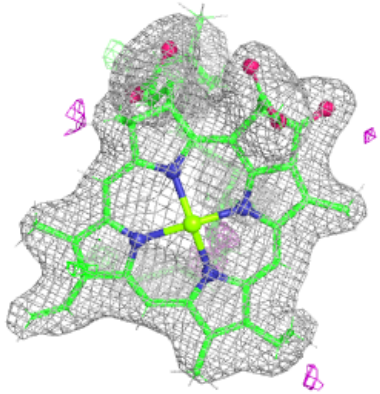


Electron density around CLA c 507:

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

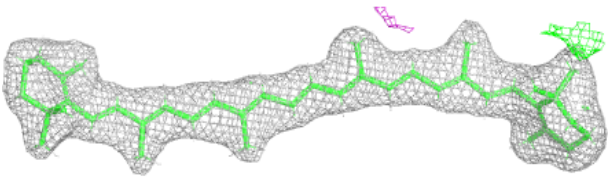


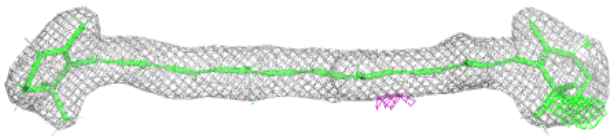


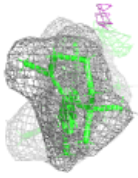


Electron density around BCR b 718:

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

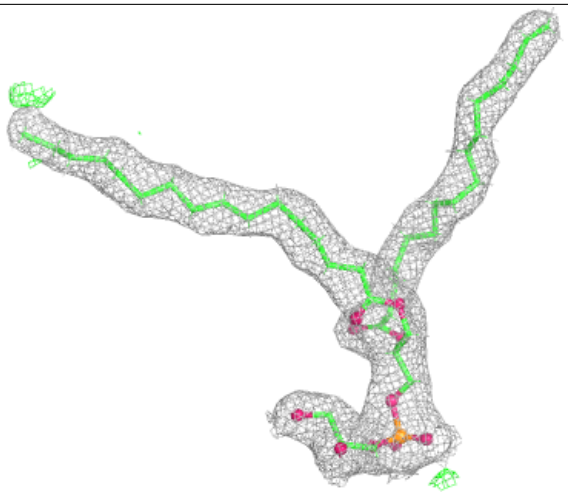


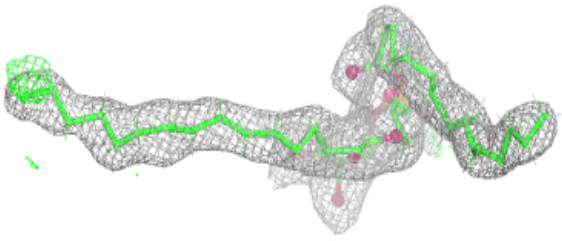


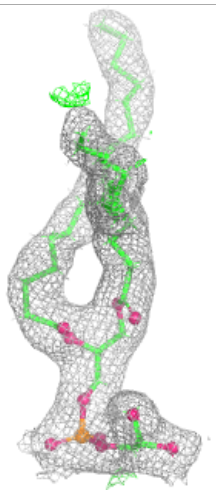


Electron density around LHG l 101:

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

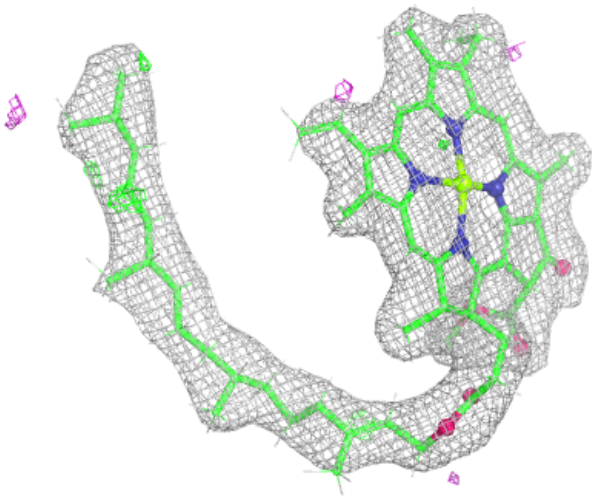


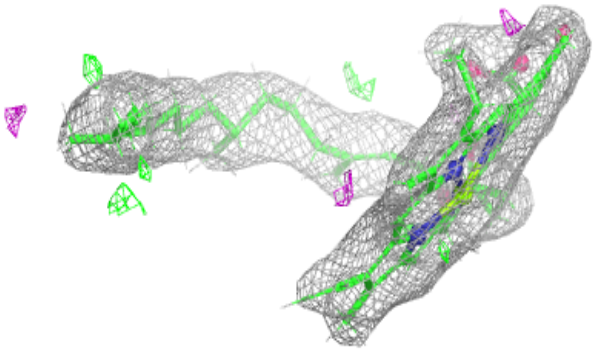




Electron density around CLA c 508:

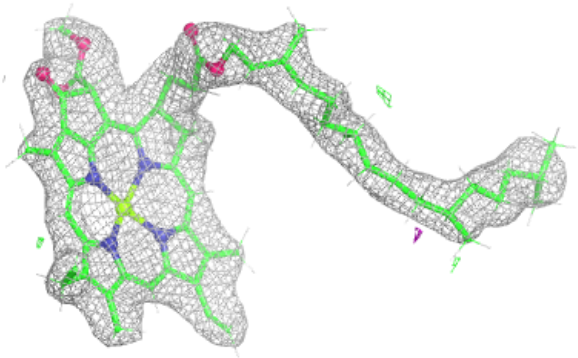
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

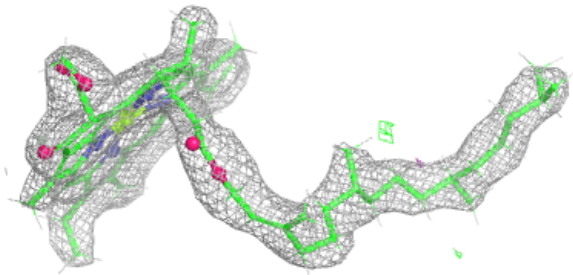


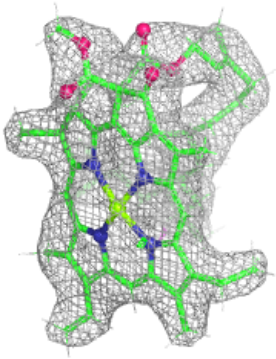


Electron density around CLA C 512:

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

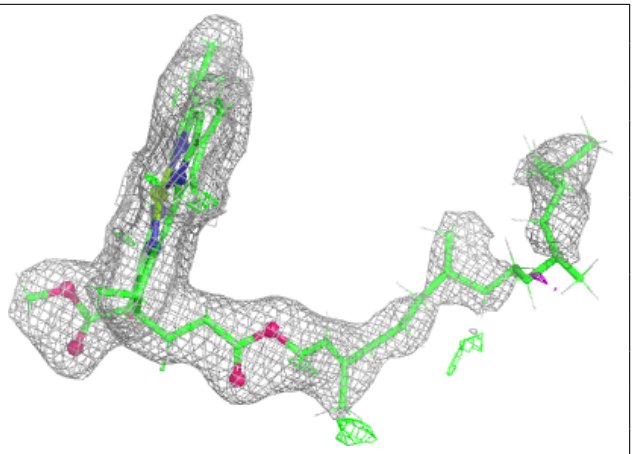


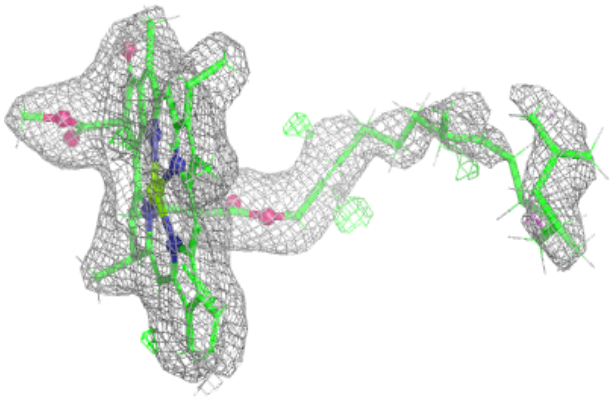


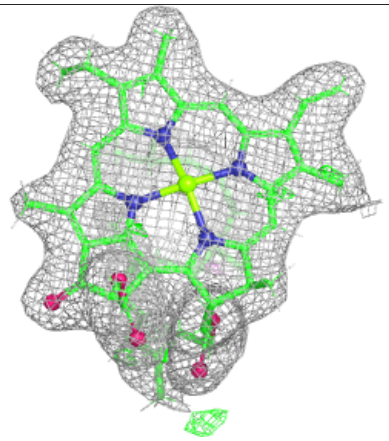


Electron density around CLA C 507:

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

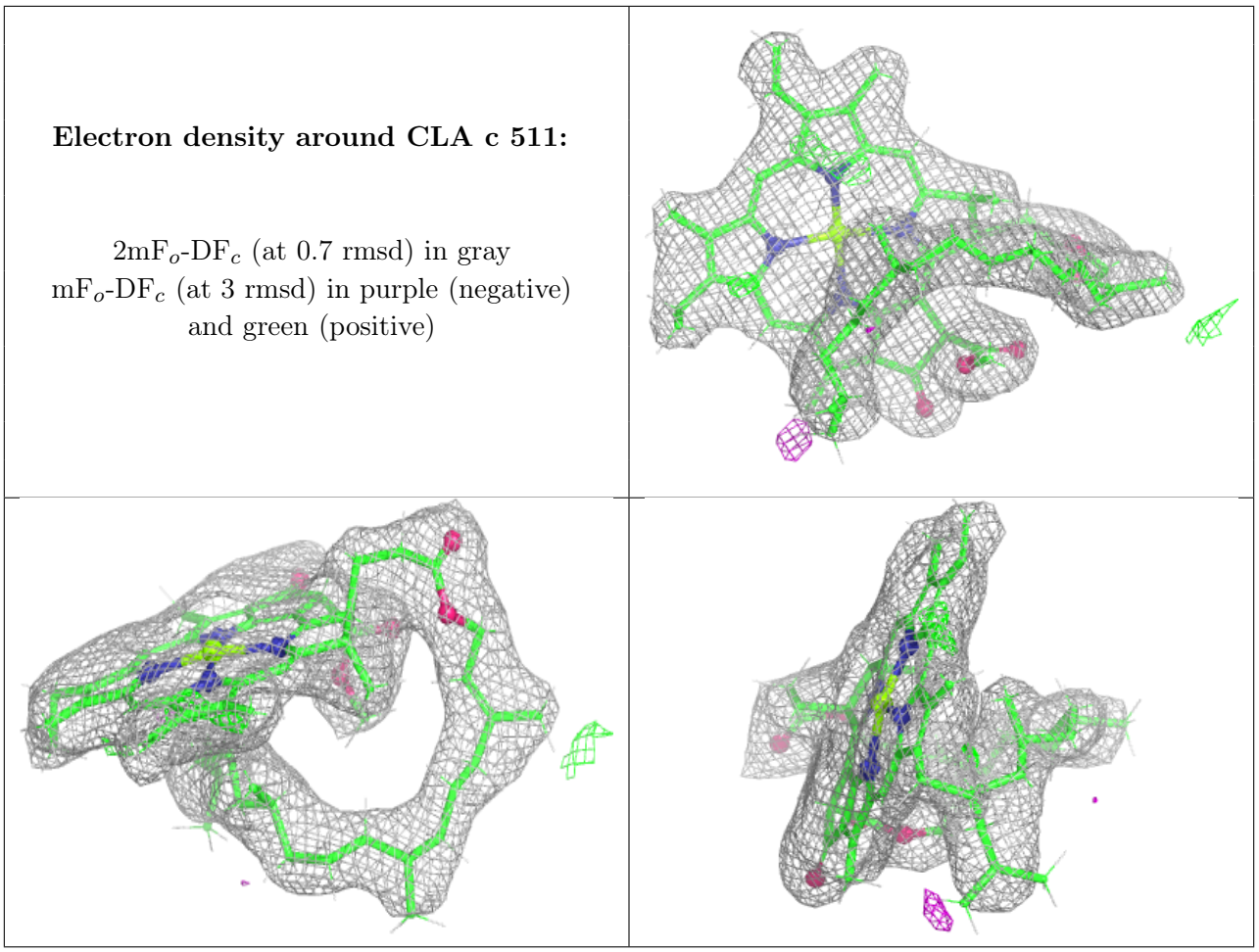






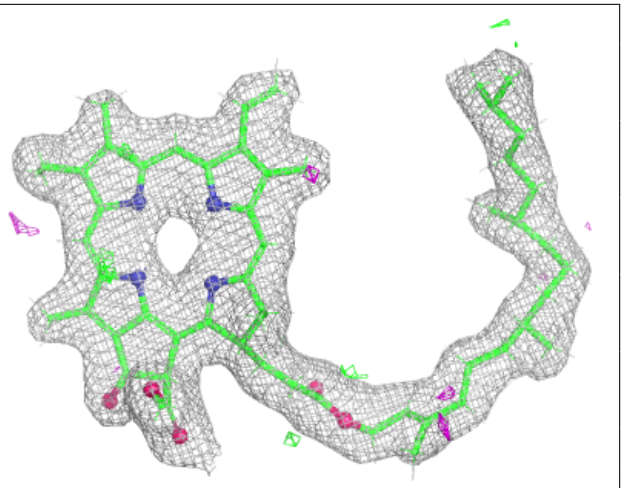
Electron density around CLA c 511:

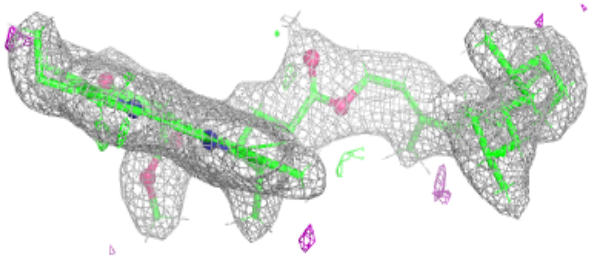
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

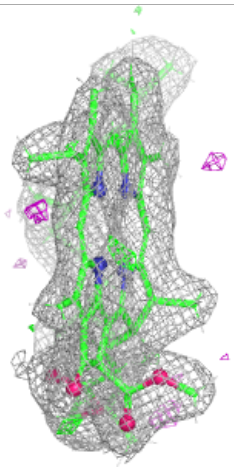


Electron density around PHO a 405:

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

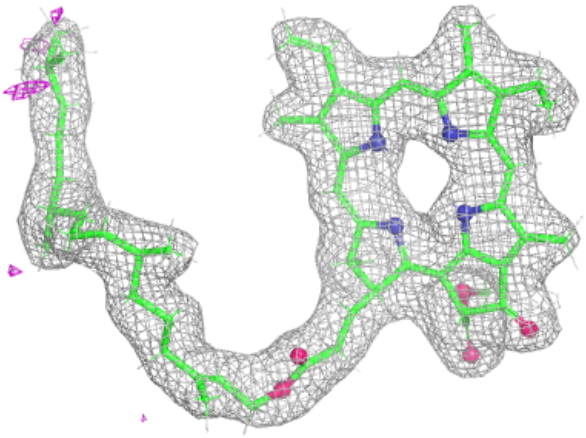


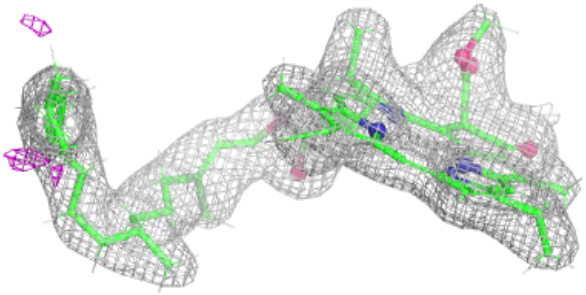


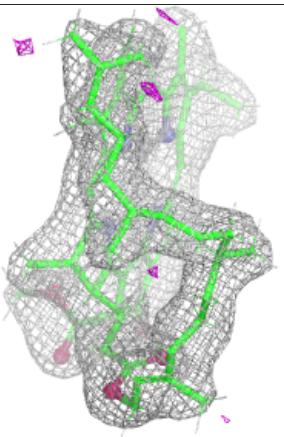


Electron density around PHO d 405:

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

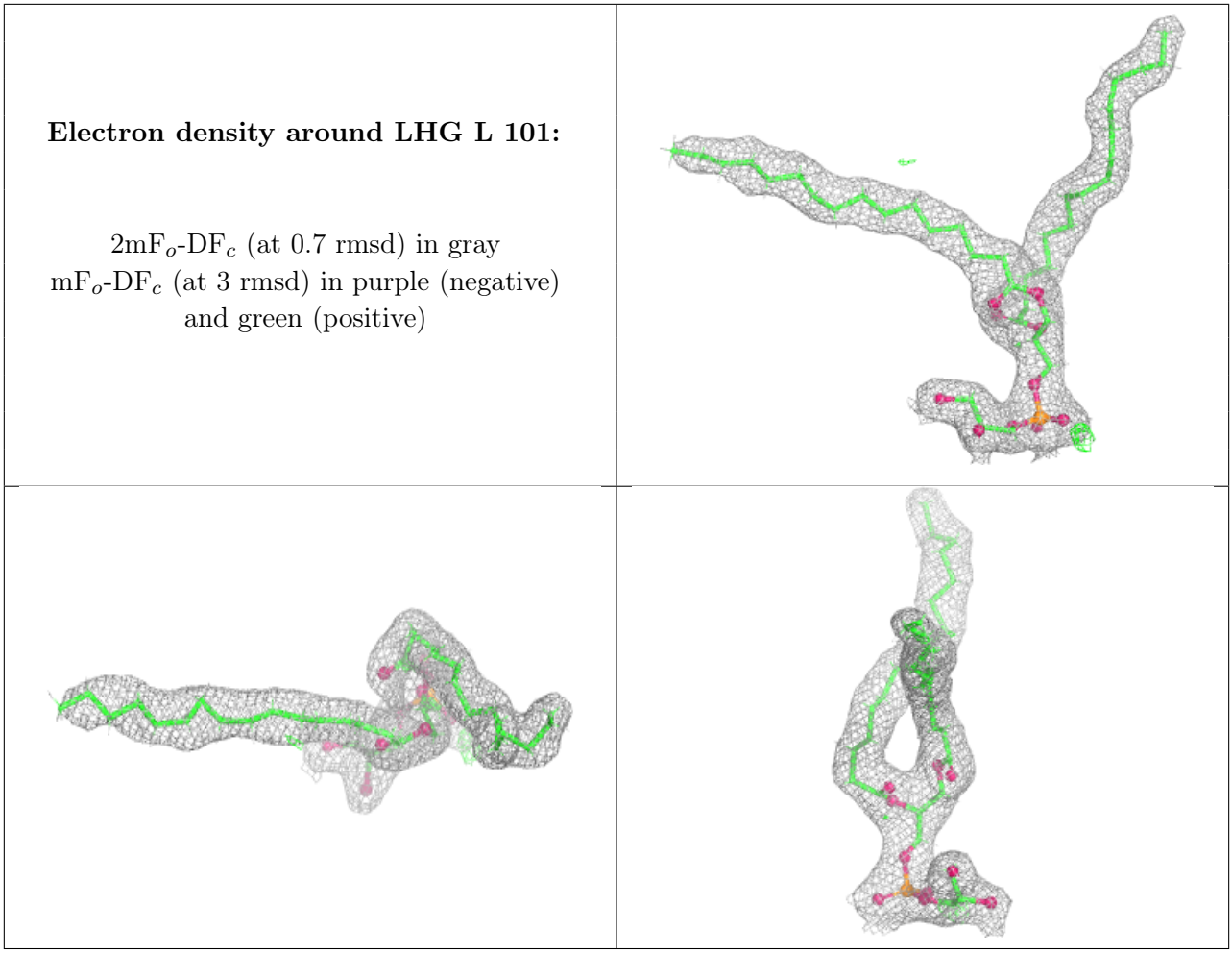






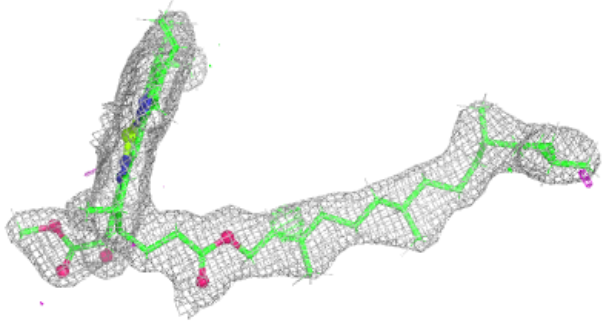
Electron density around LHG L 101:

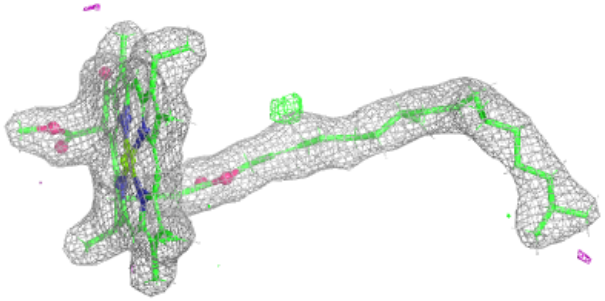
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

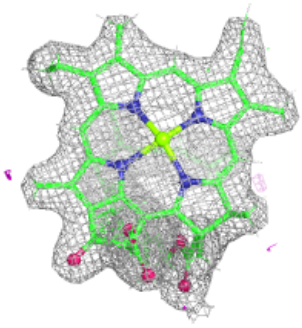


Electron density around CLA b 705:

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

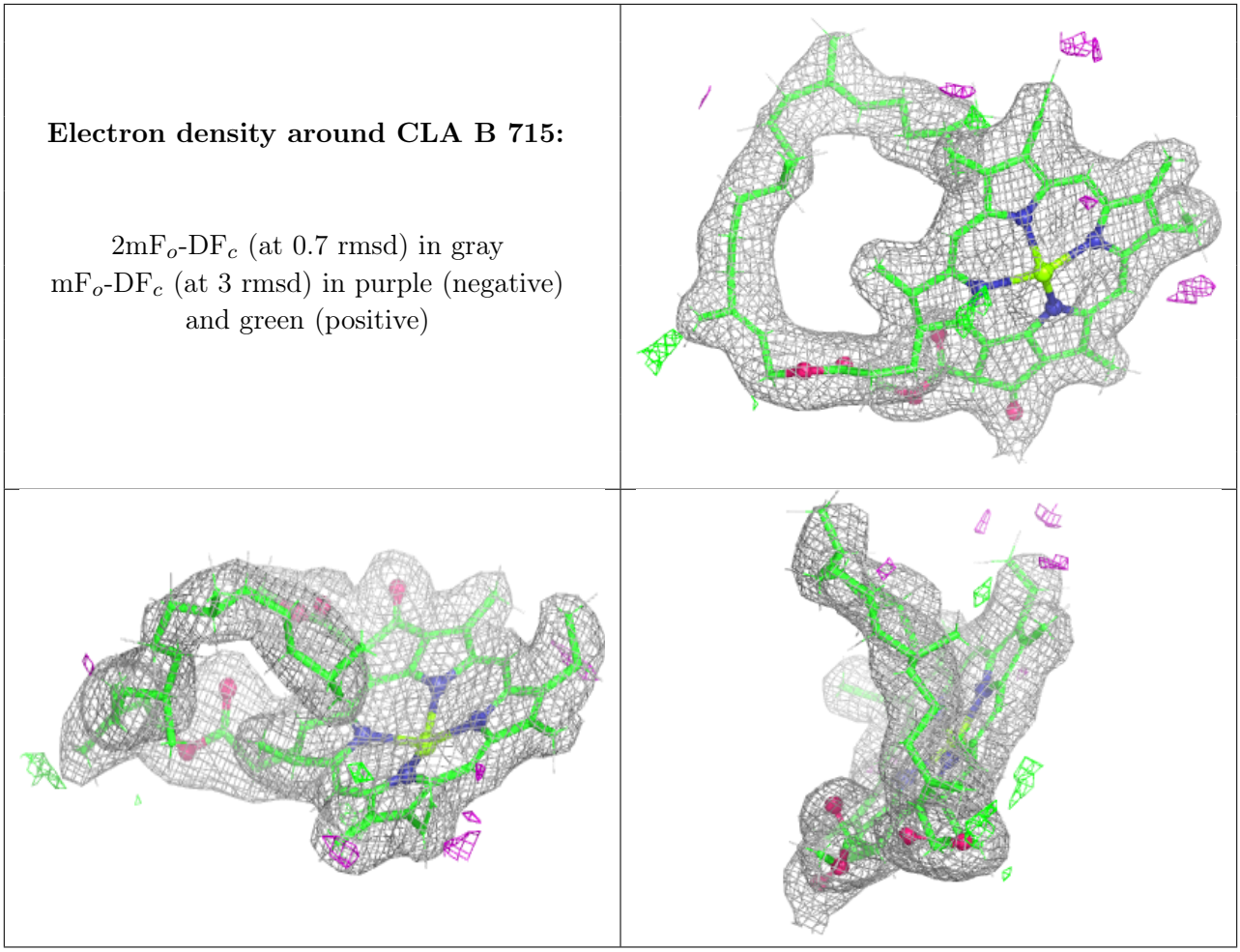






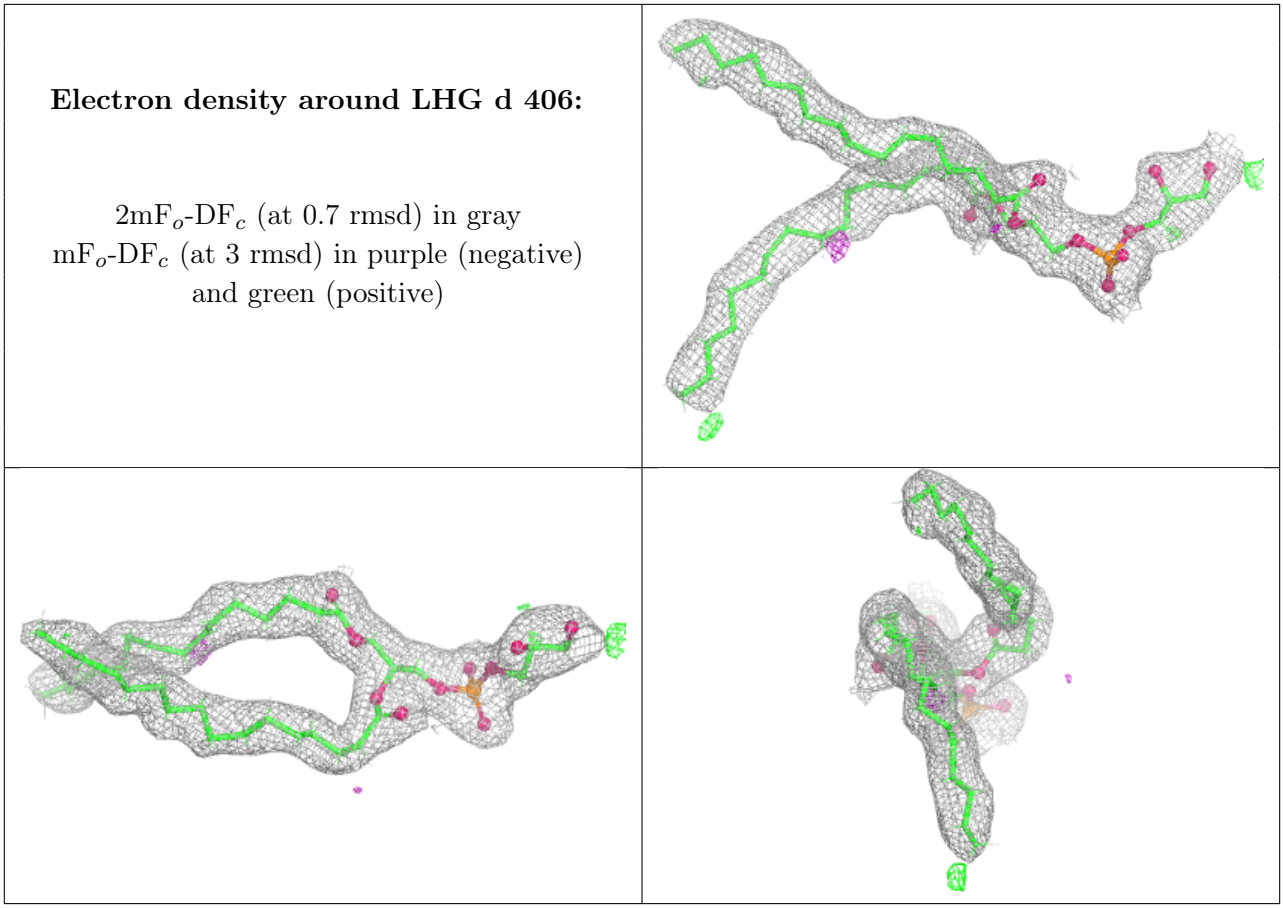
Electron density around CLA B 715:

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



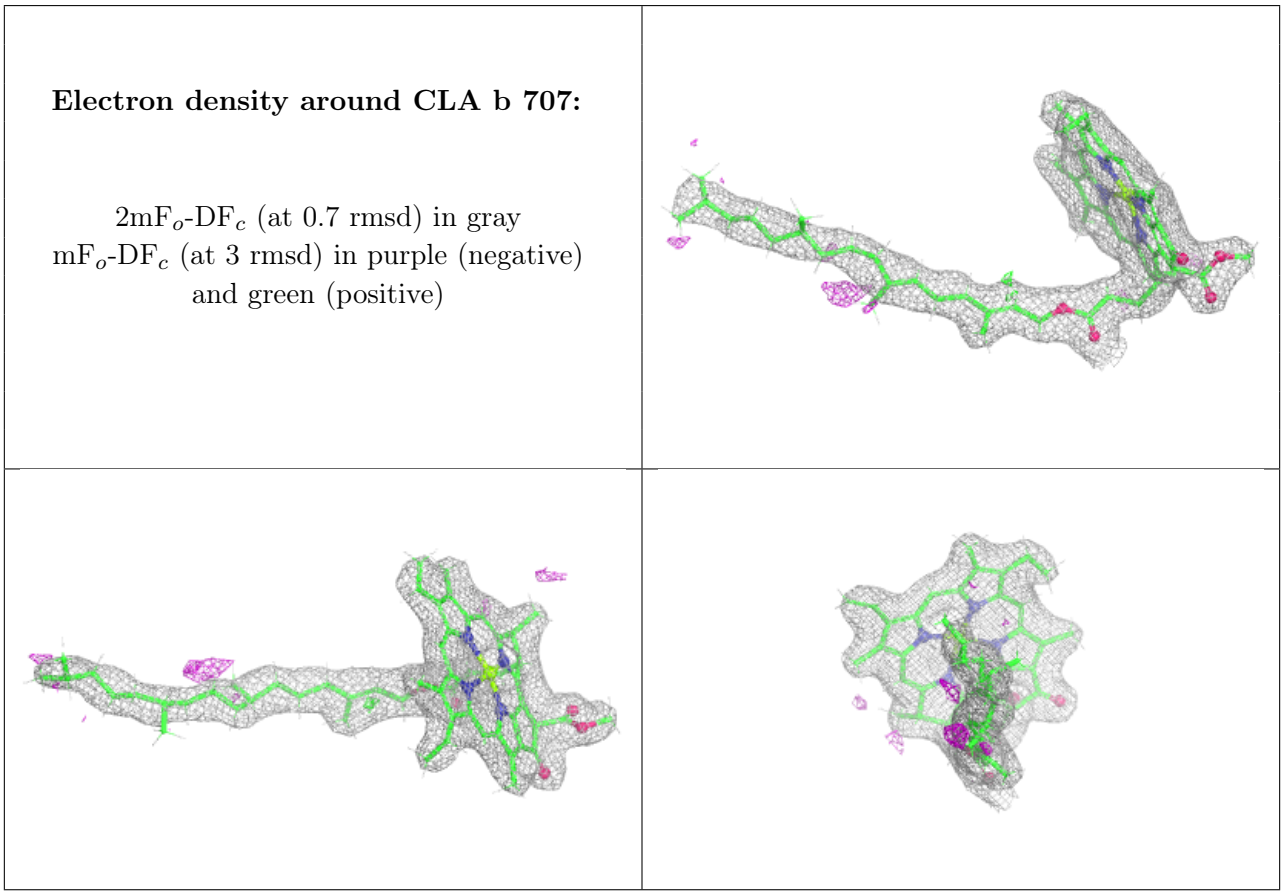
Electron density around LHG d 406:

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



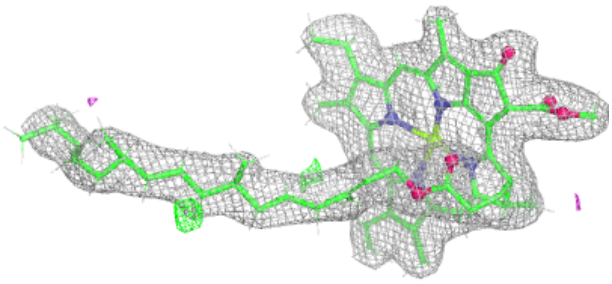
Electron density around CLA b 707:

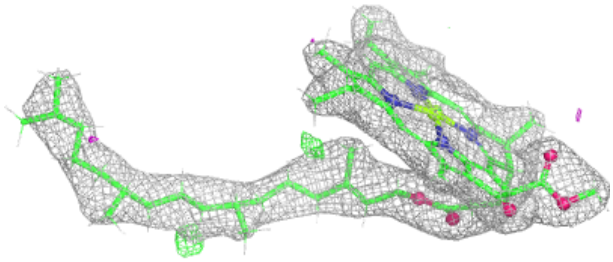
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

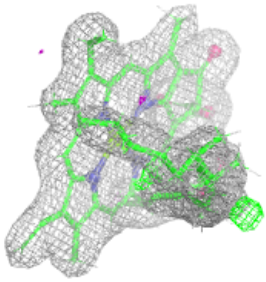


Electron density around CLA b 708:

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

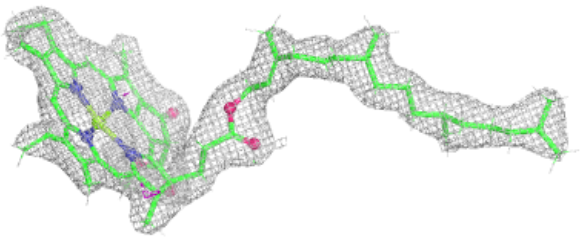


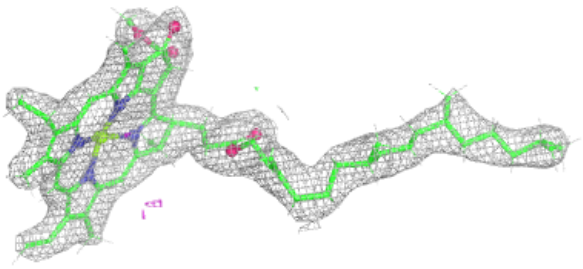


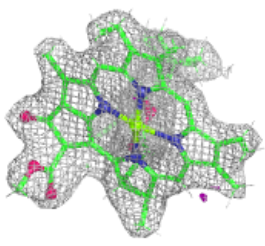


Electron density around CLA C 503:

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

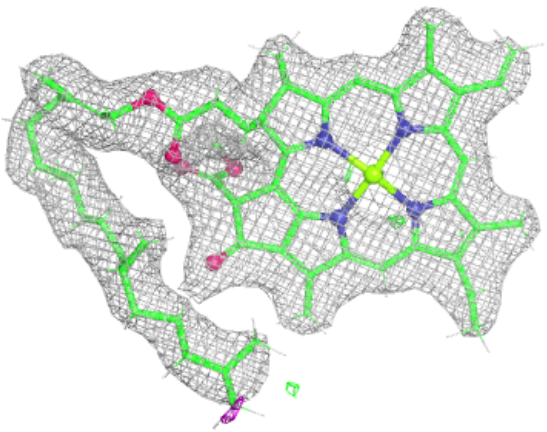


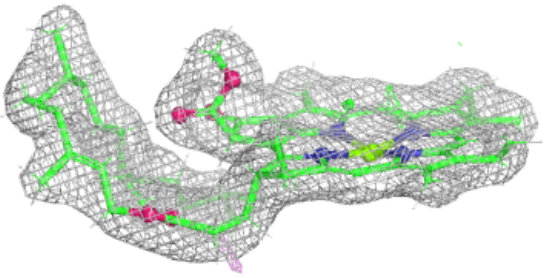




Electron density around CLA b 710:

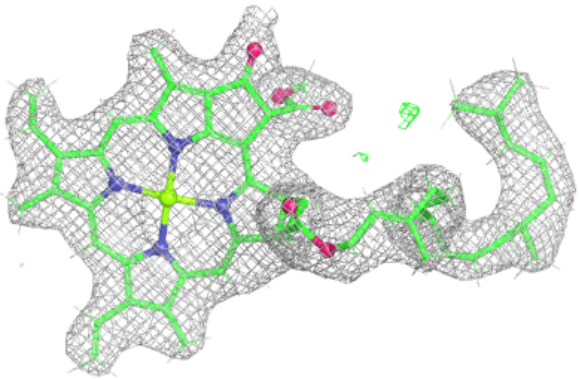
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

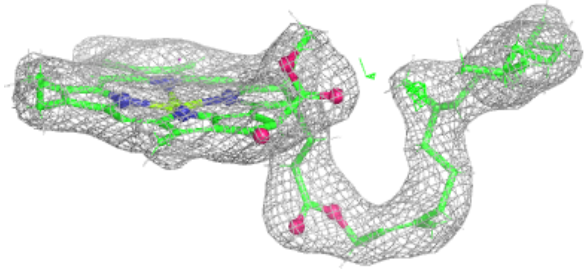


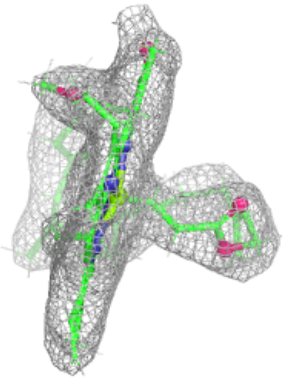


Electron density around CLA b 712:

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

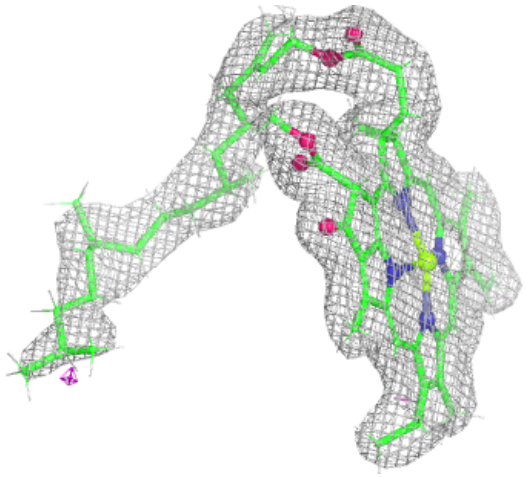


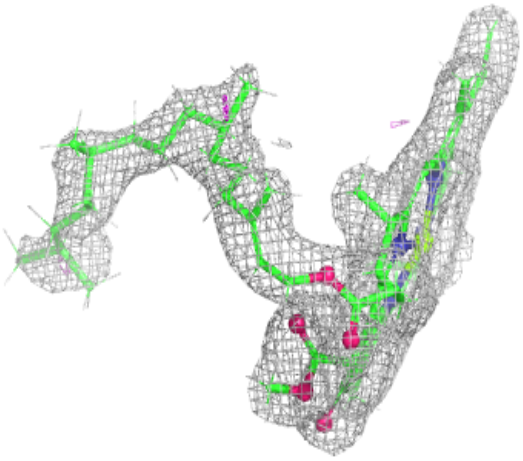


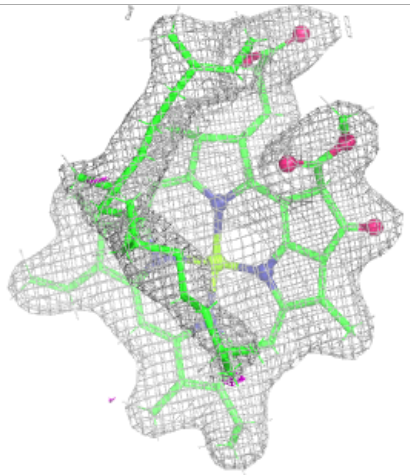


Electron density around CLA b 713:

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

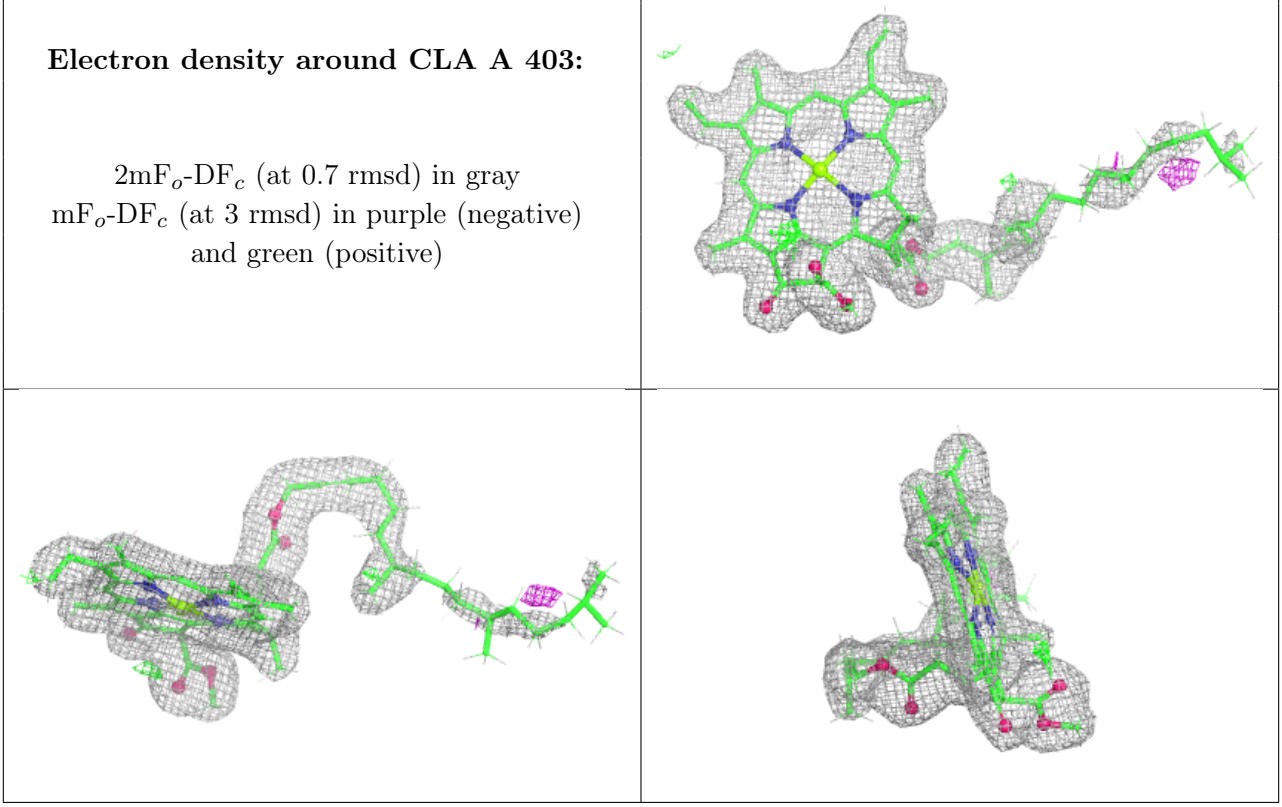






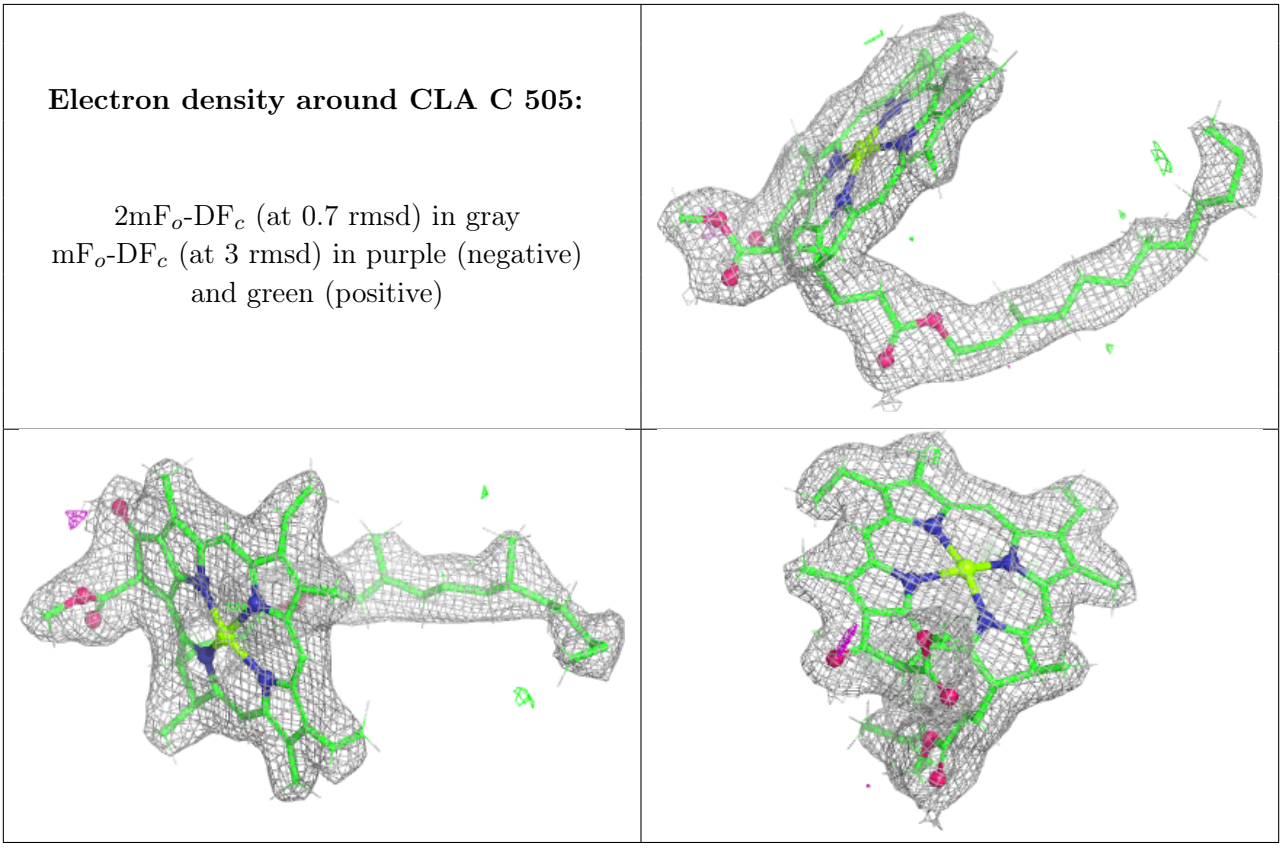
Electron density around CLA A 403:

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



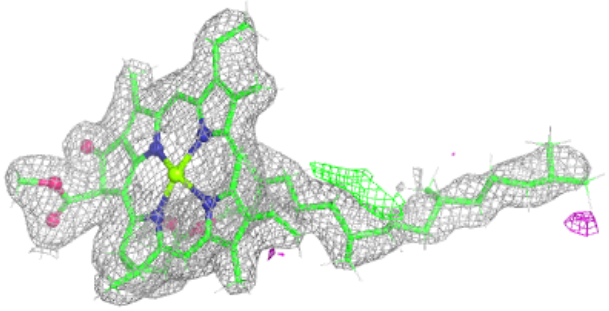
Electron density around CLA C 505:

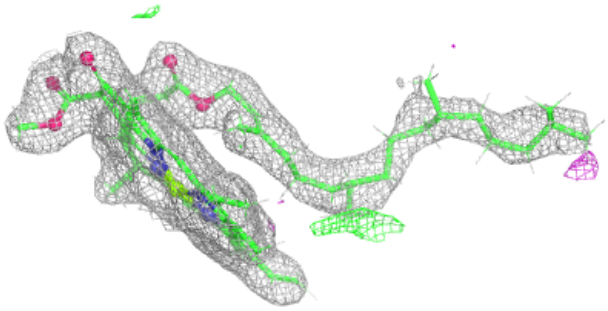
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

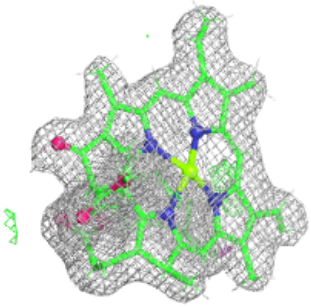


Electron density around CLA C 506:

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

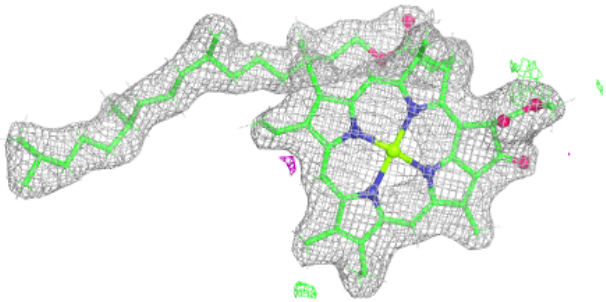


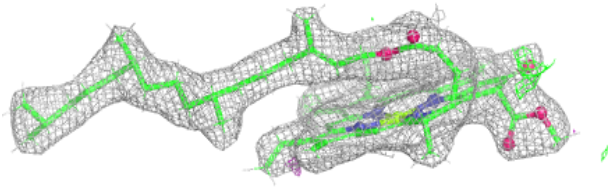


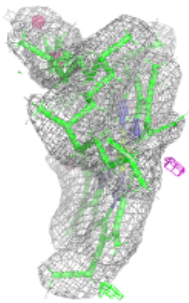


Electron density around CLA c 502:

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

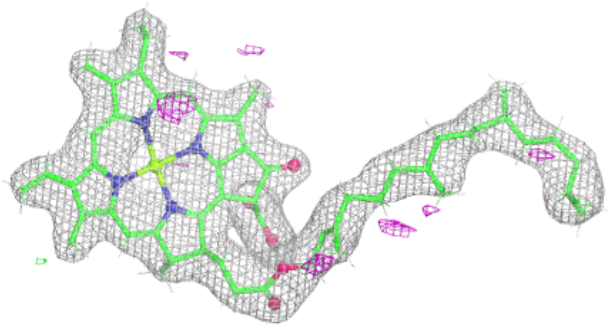


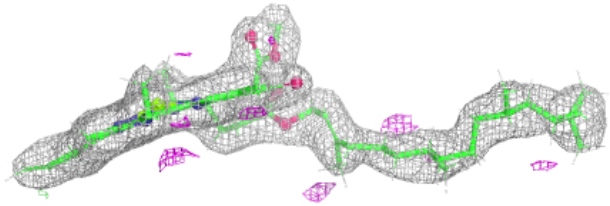


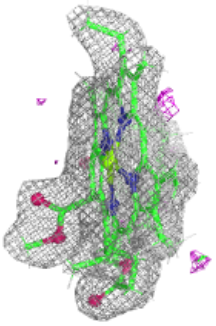


Electron density around CLA B 702:

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

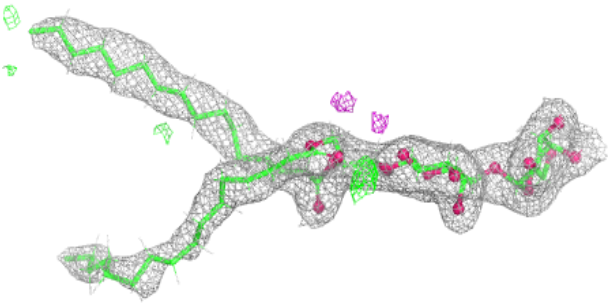


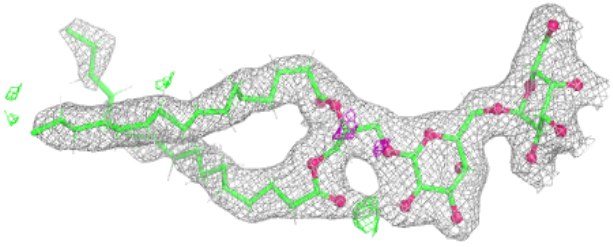


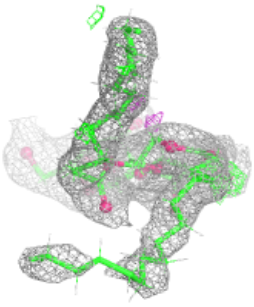


Electron density around DGD c 517:

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

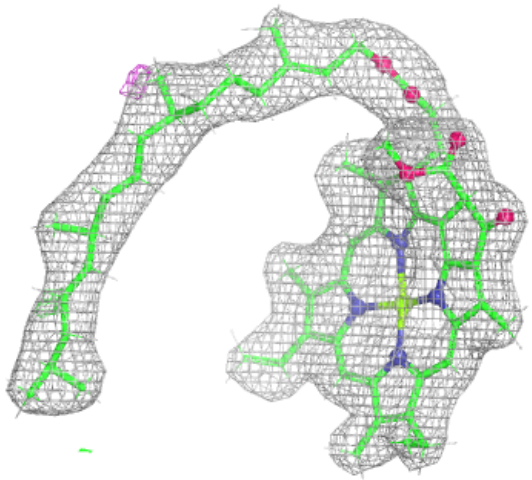


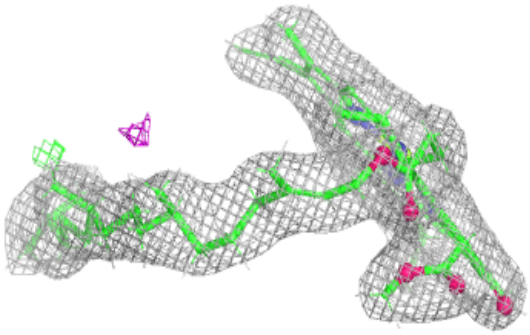


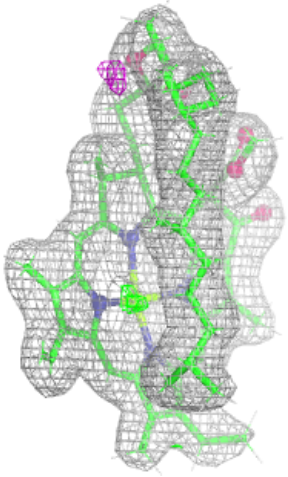


Electron density around CLA C 508:

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

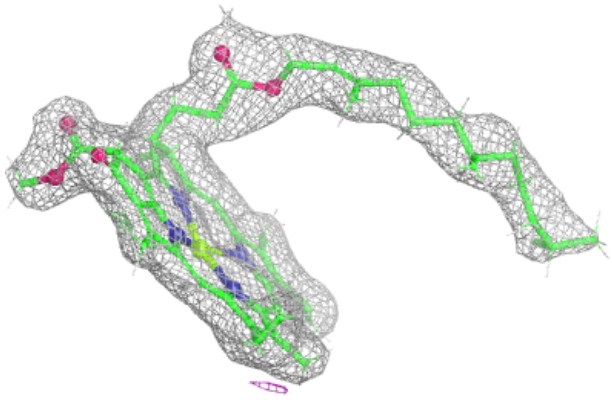


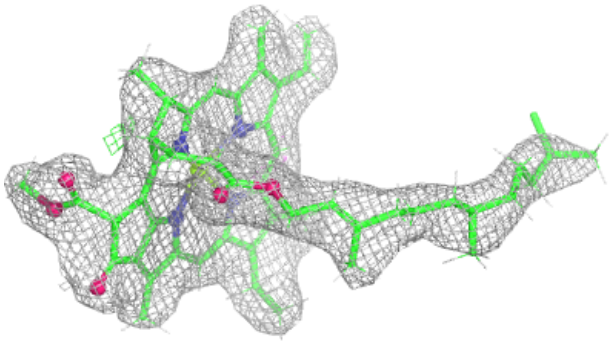


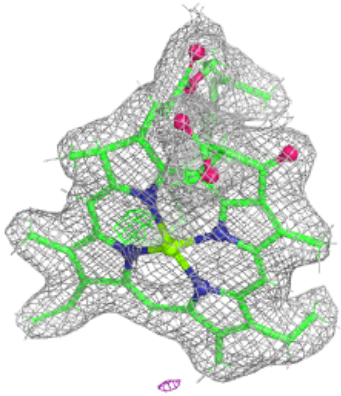


Electron density around CLA c 505:

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

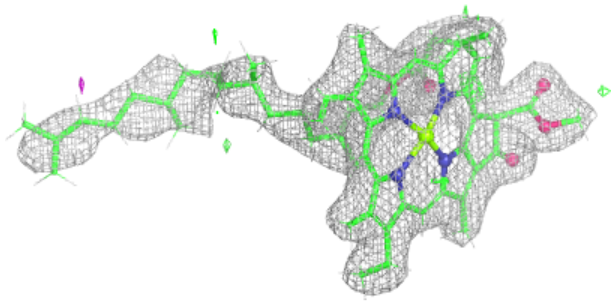


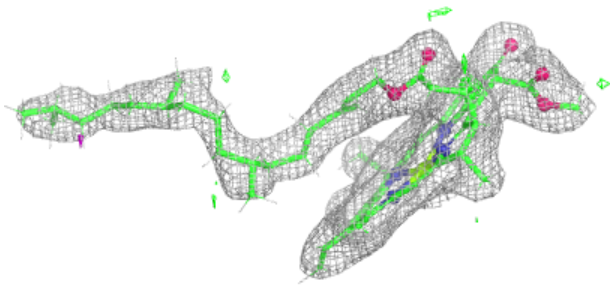


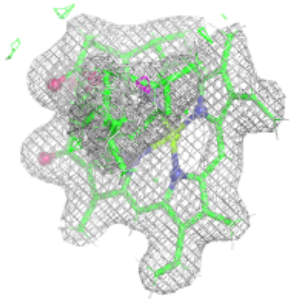


Electron density around CLA c 506:

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

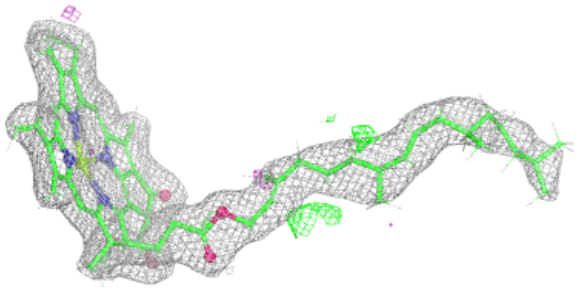


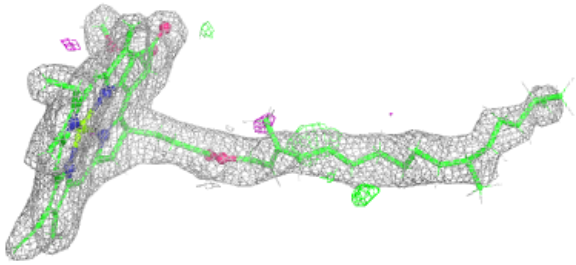


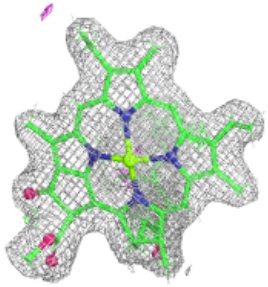


Electron density around CLA B 704:

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

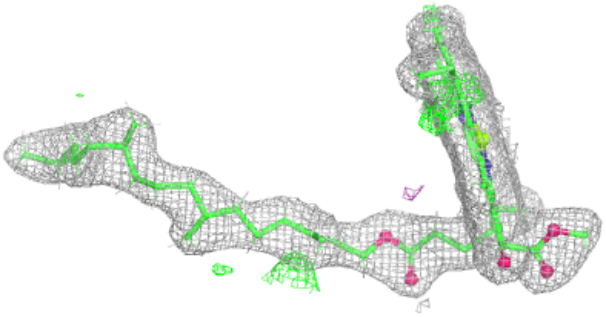


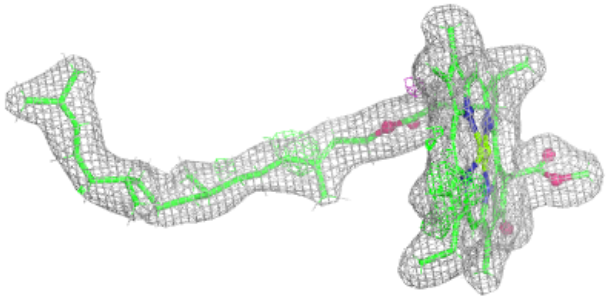


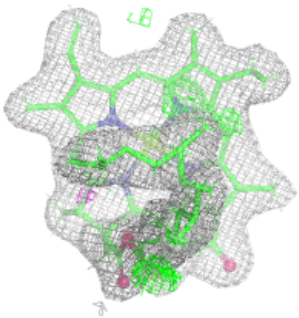


Electron density around CLA B 705:

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

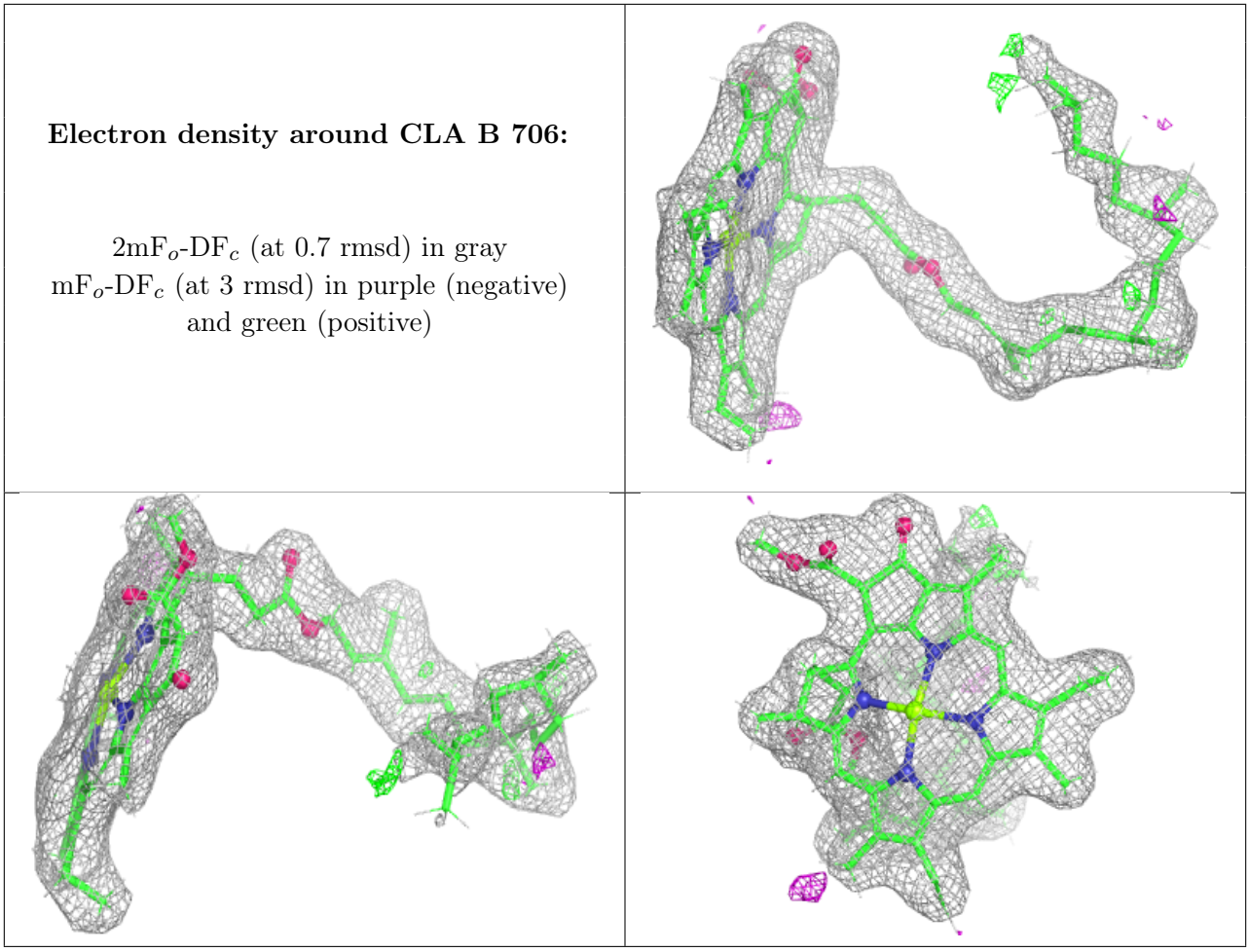






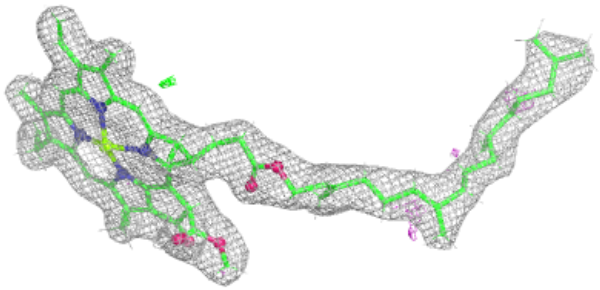
Electron density around CLA B 706:

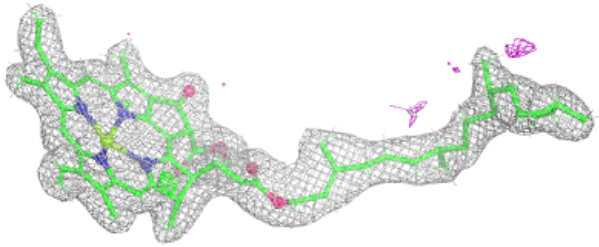
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

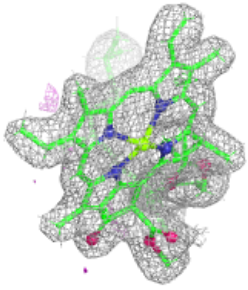


Electron density around CLA A 402:

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

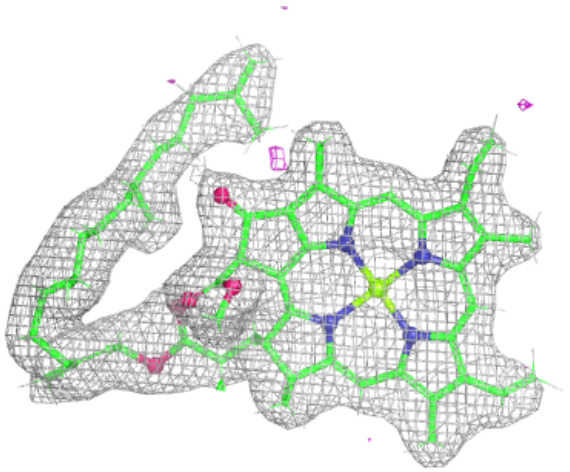


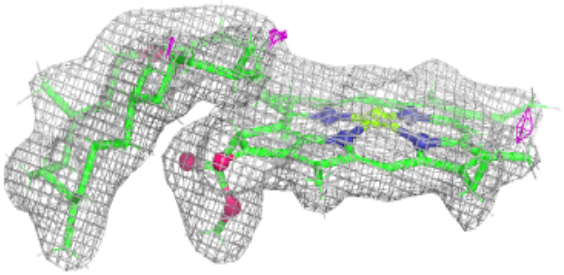




Electron density around CLA B 710:

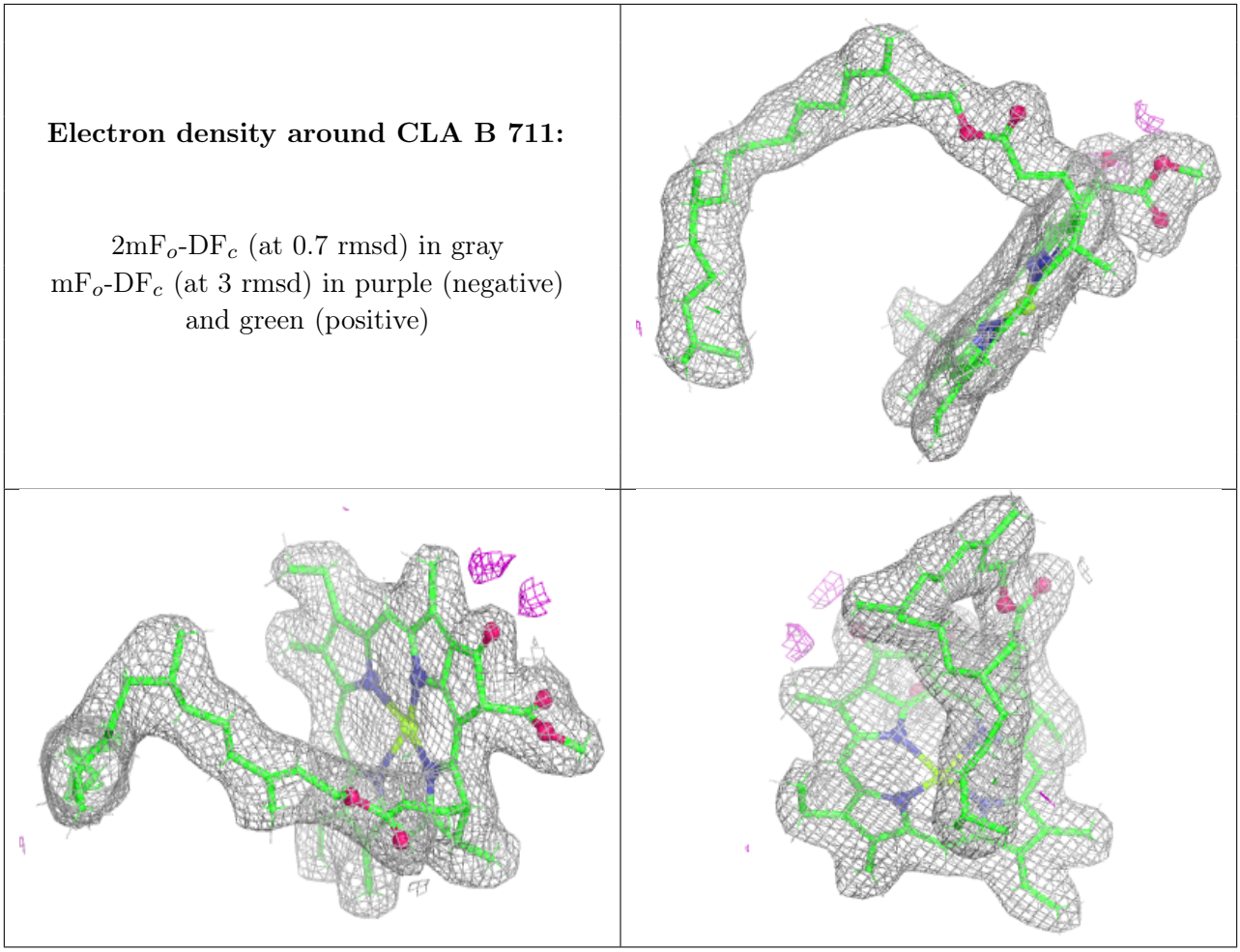
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





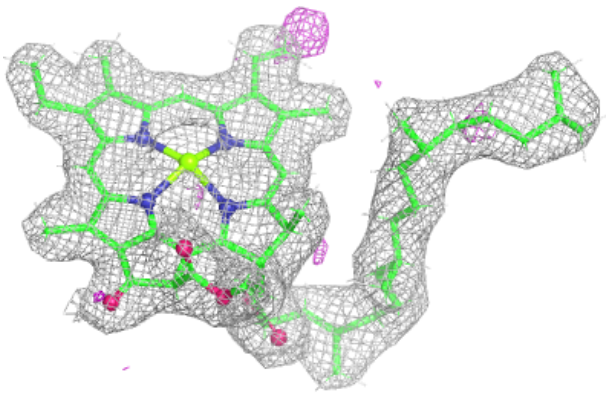
Electron density around CLA B 711:

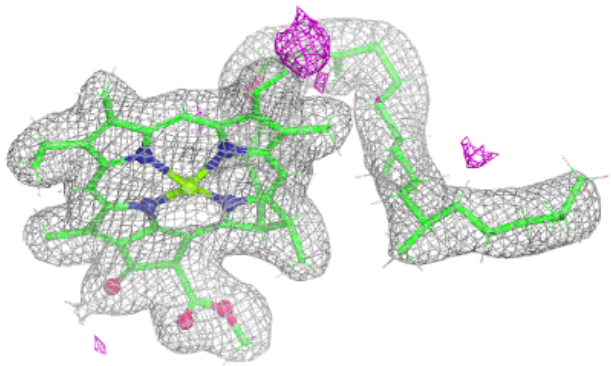
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

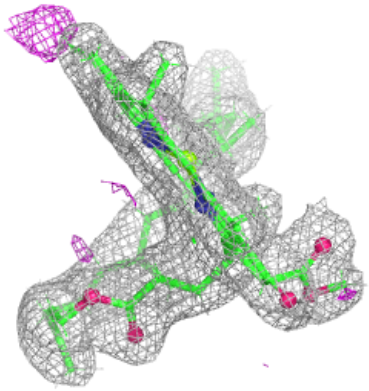


Electron density around CLA D 402:

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

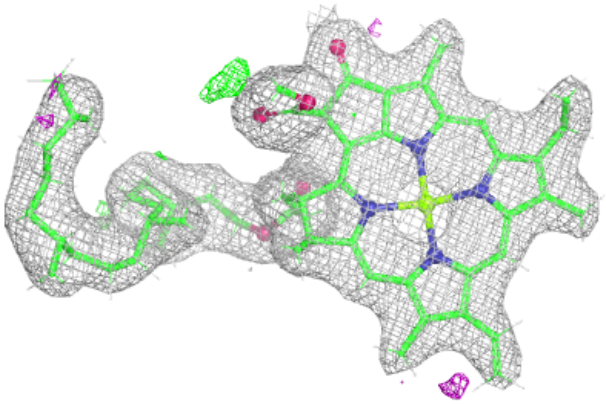


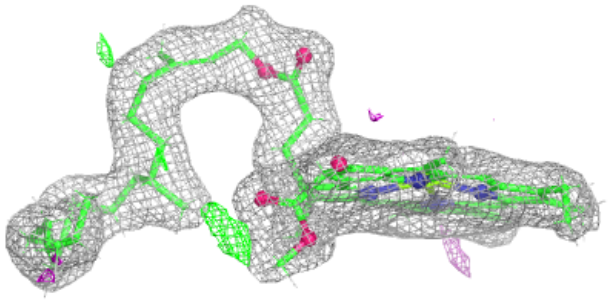


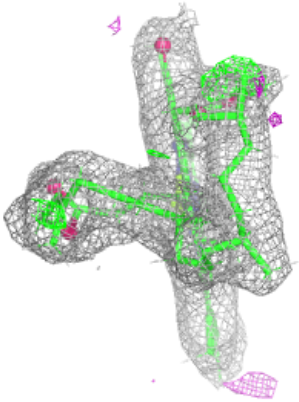


Electron density around CLA B 712:

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

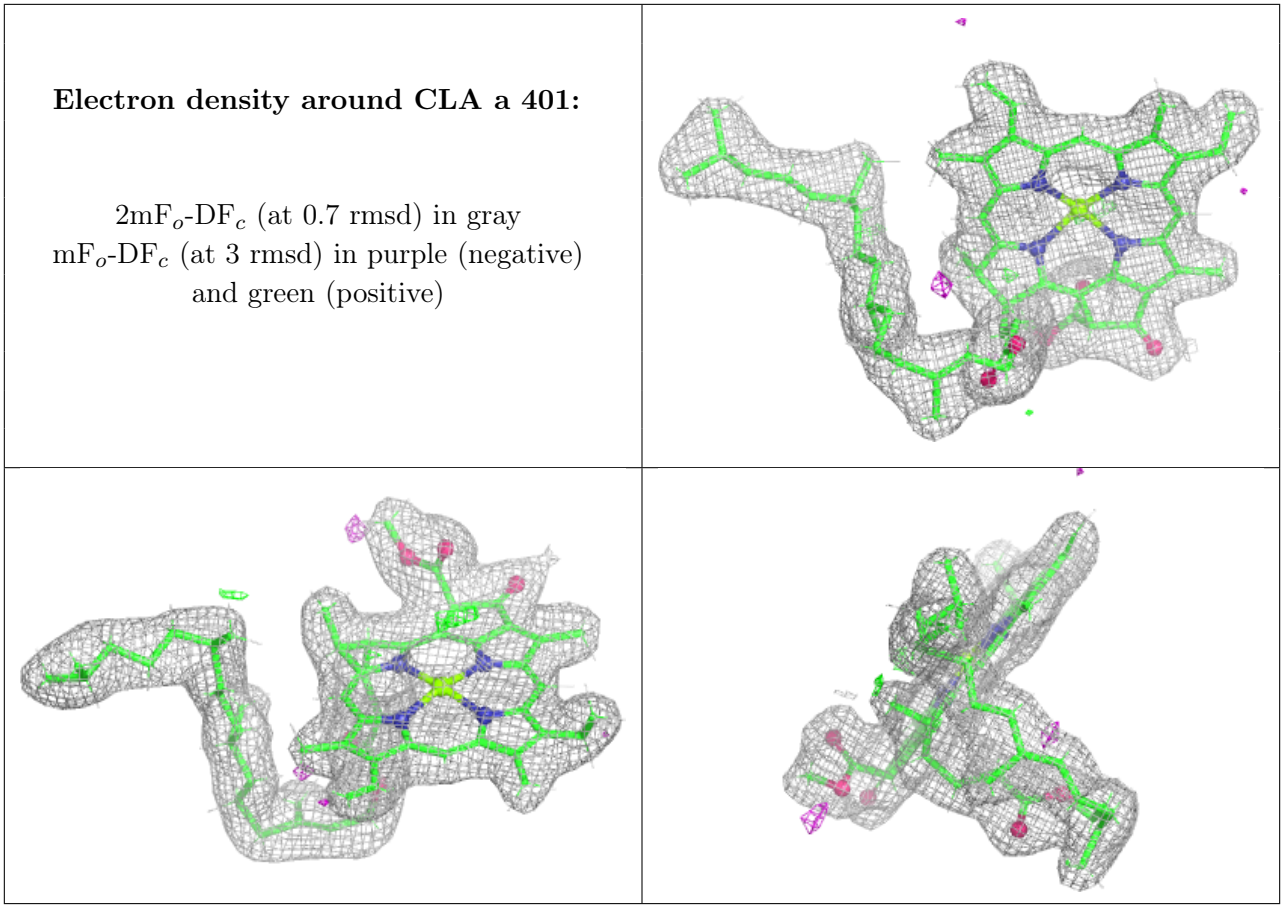






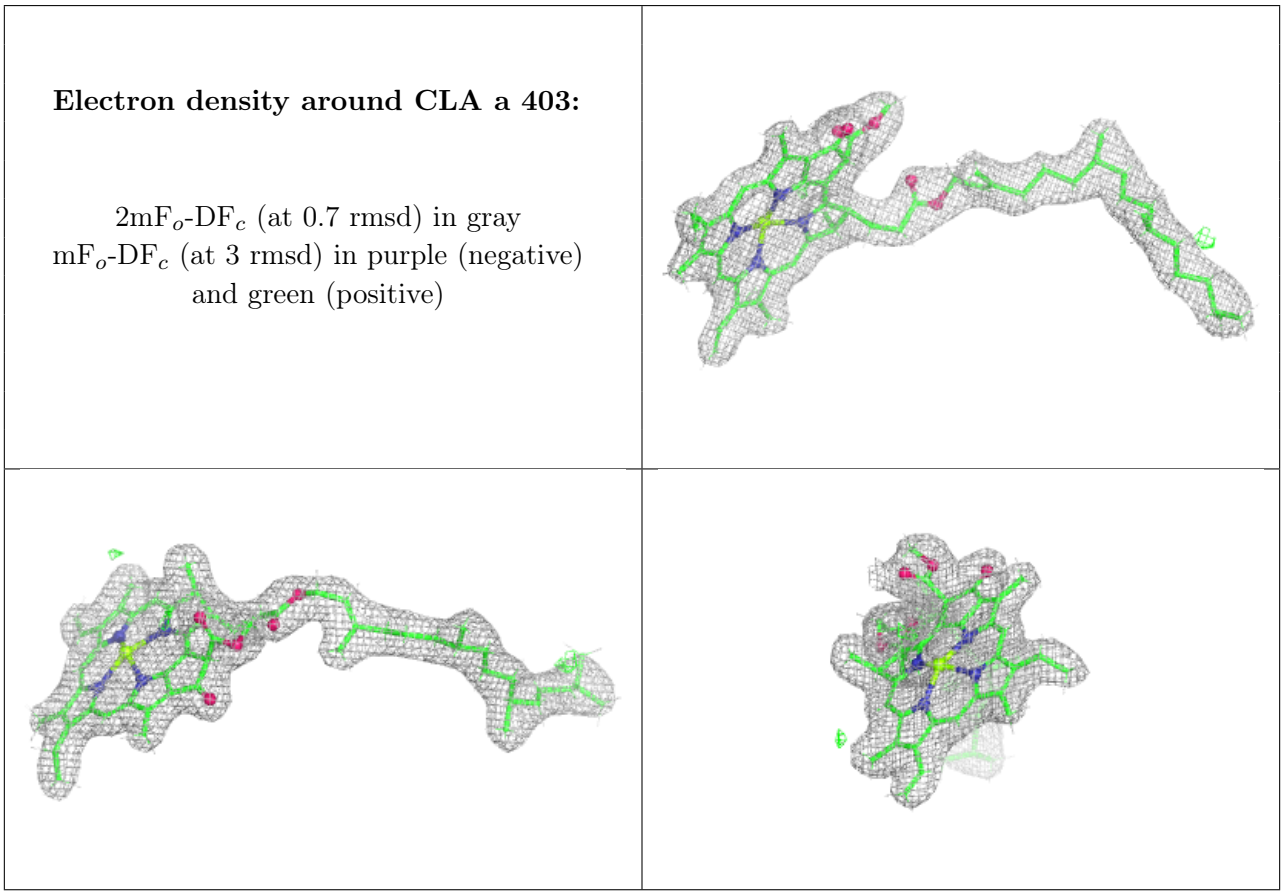
Electron density around CLA a 401:

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



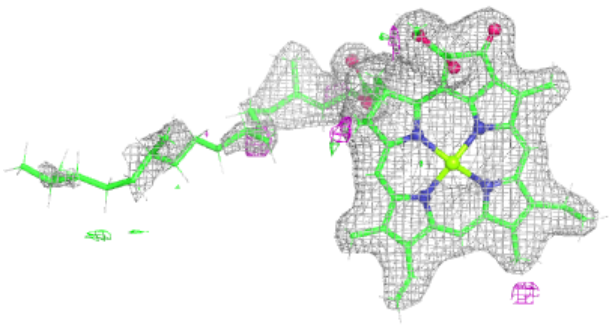
Electron density around CLA a 403:

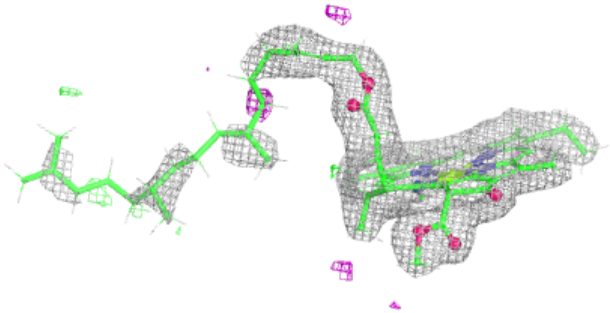
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

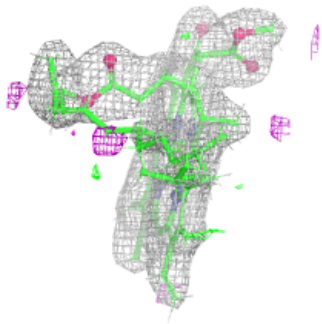


Electron density around CLA a 404:

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

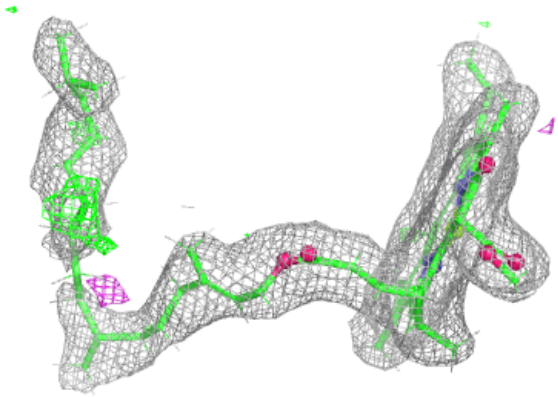


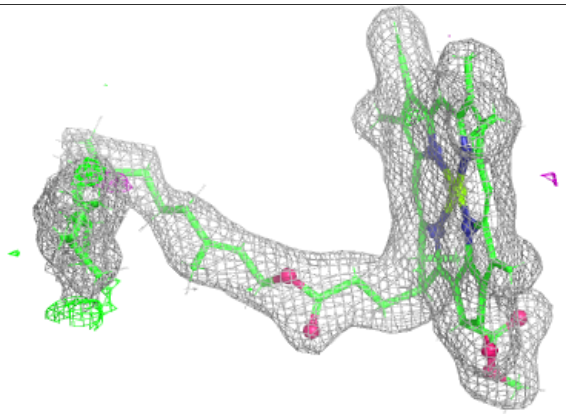


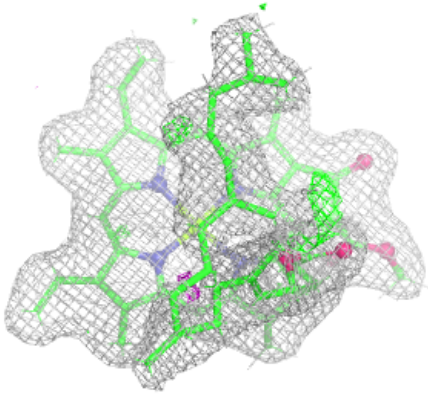


Electron density around CLA a 406:

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

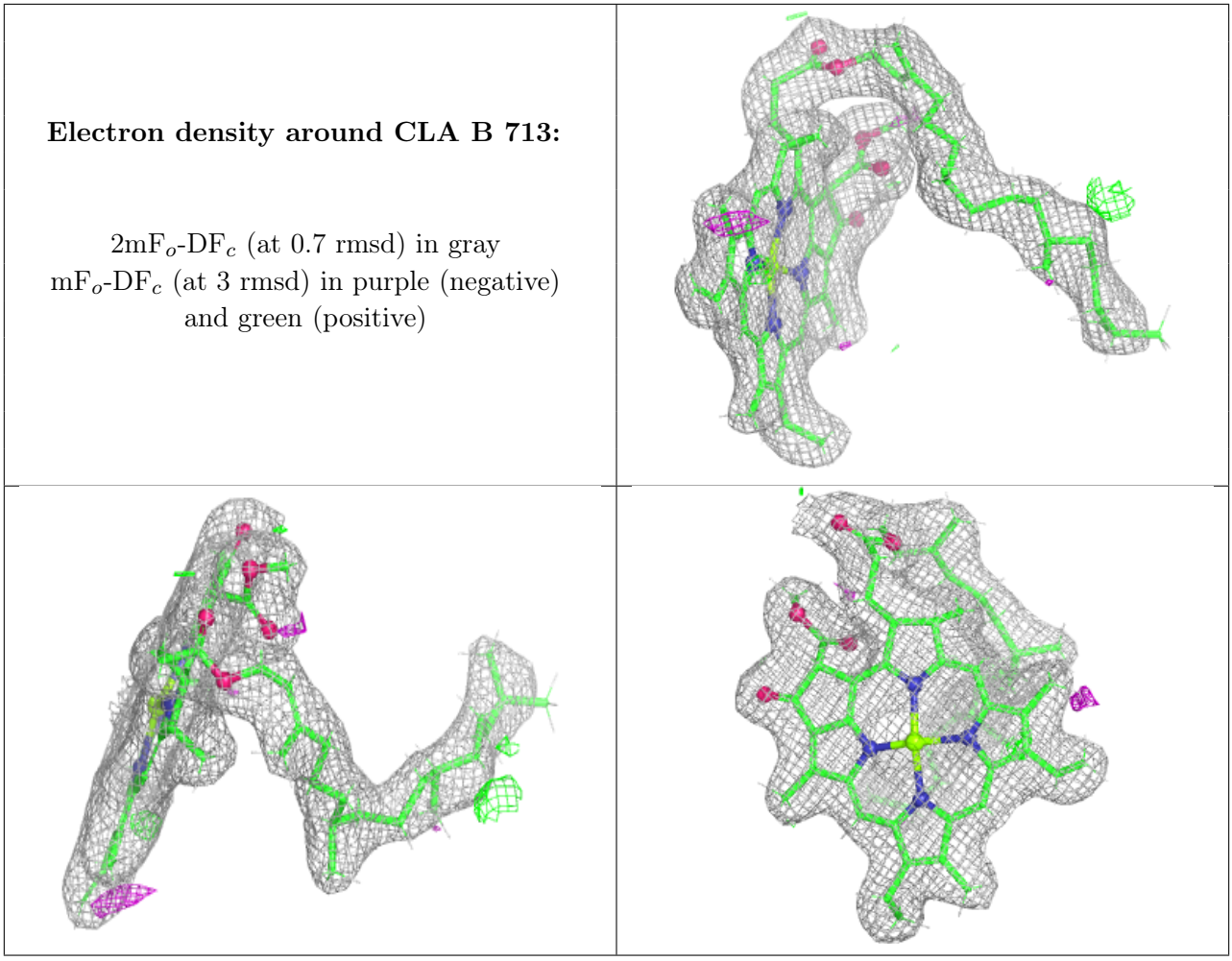






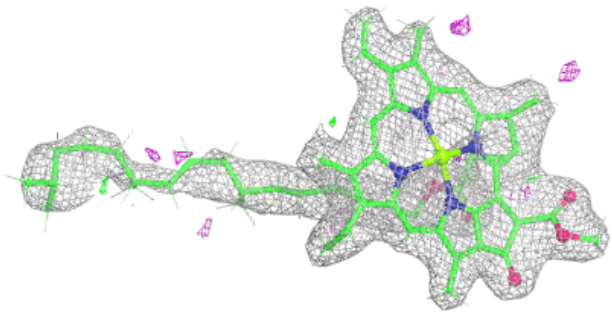
Electron density around CLA B 713:

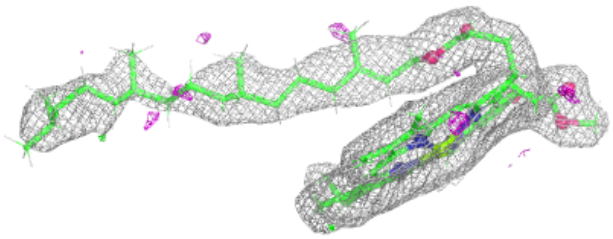
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

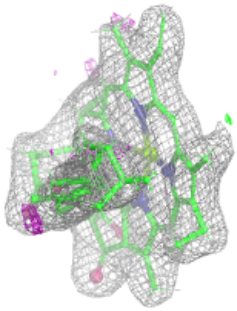


Electron density around CLA B 714:

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

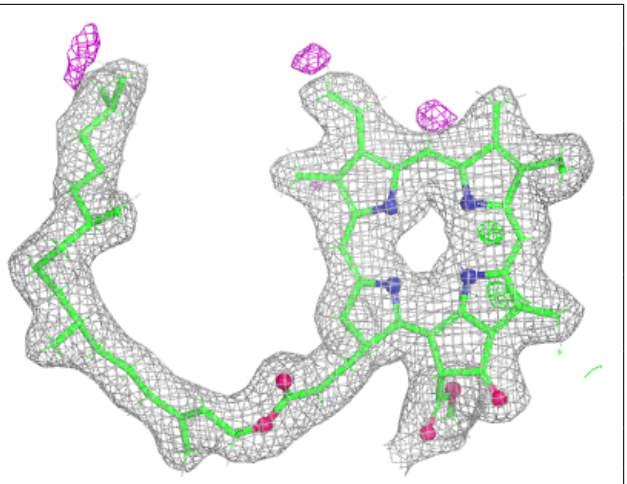


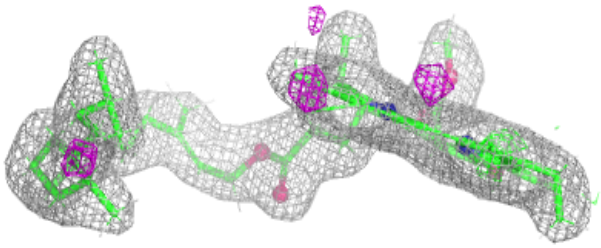


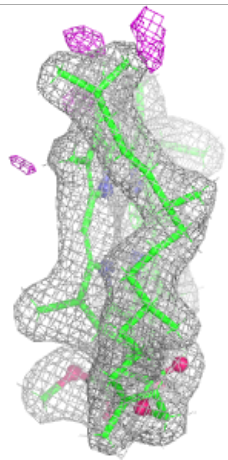


Electron density around PHO D 406:

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

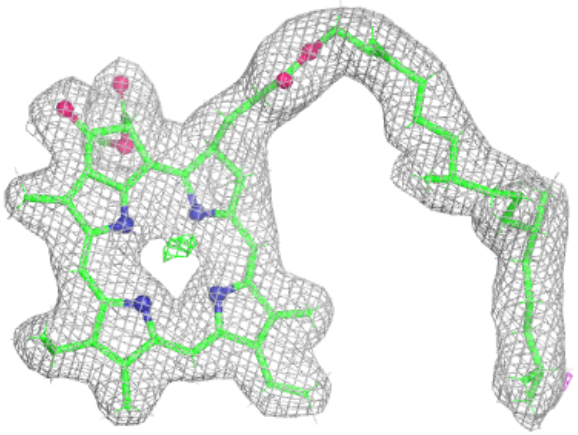


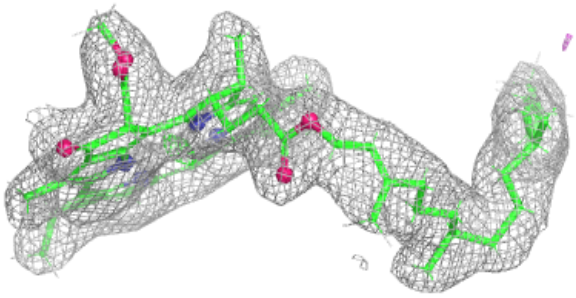


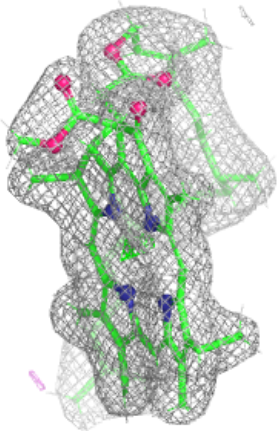


Electron density around PHO D 407:

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

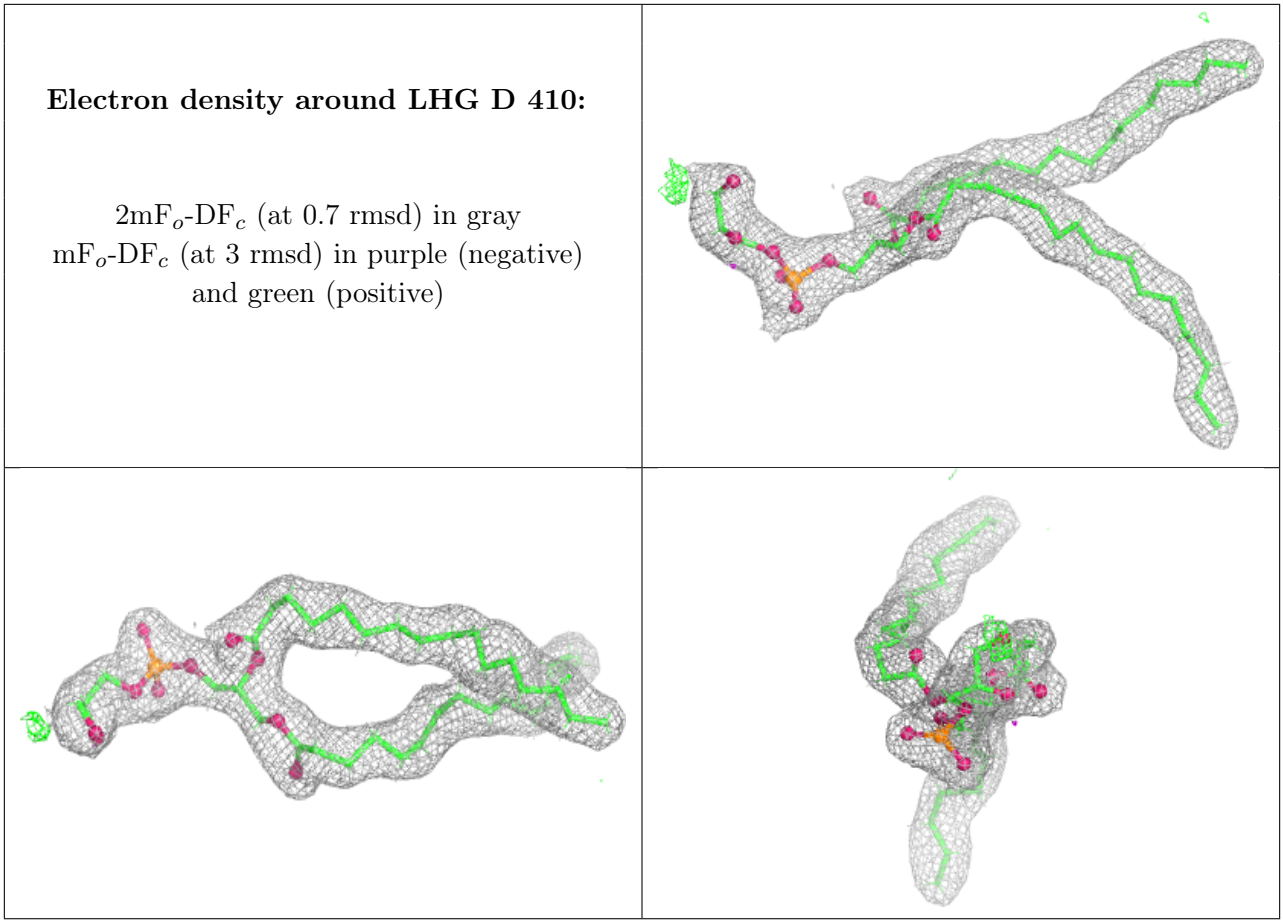






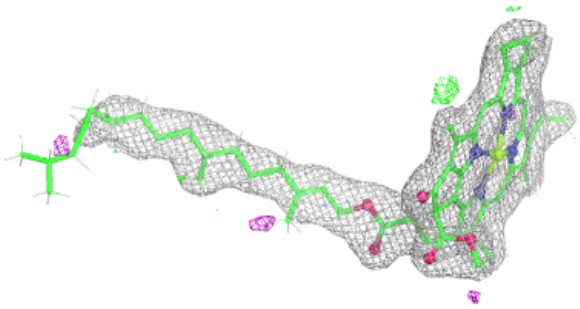
Electron density around LHG D 410:

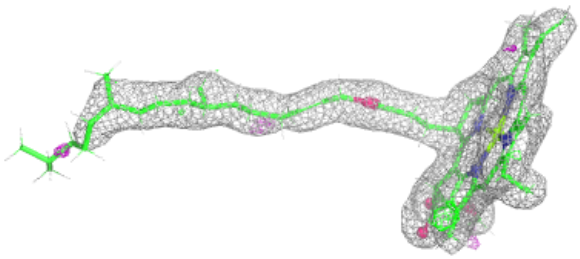
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

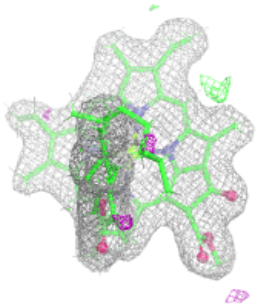


Electron density around CLA b 704:

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

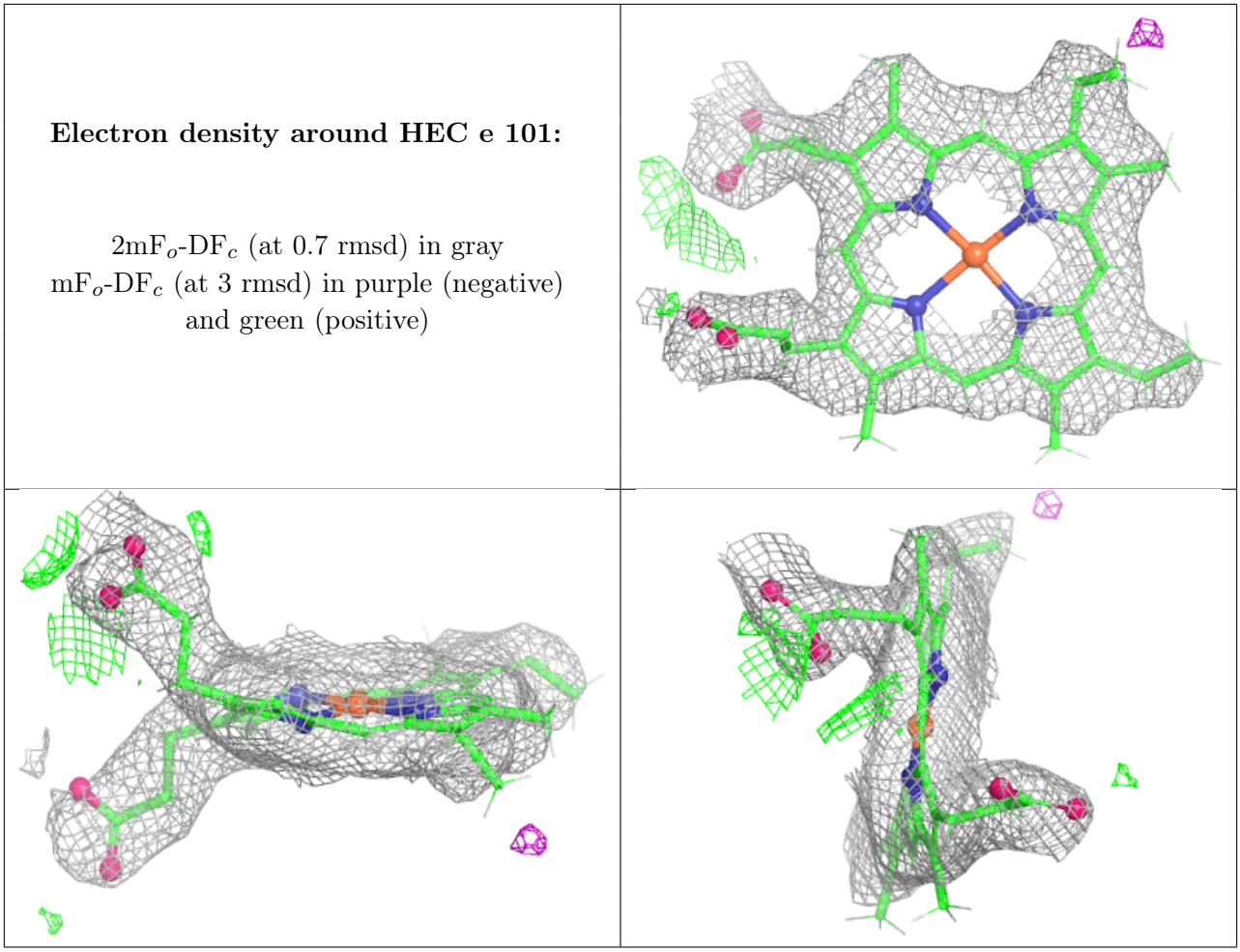






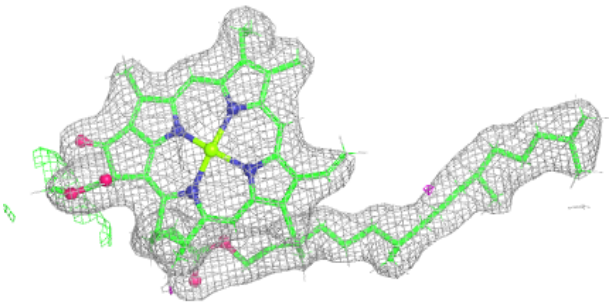
Electron density around HEC e 101:

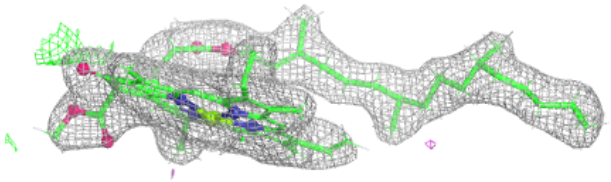
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

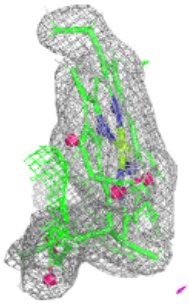


Electron density around CLA C 502:

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

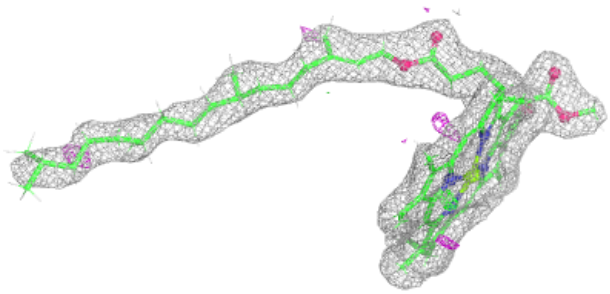


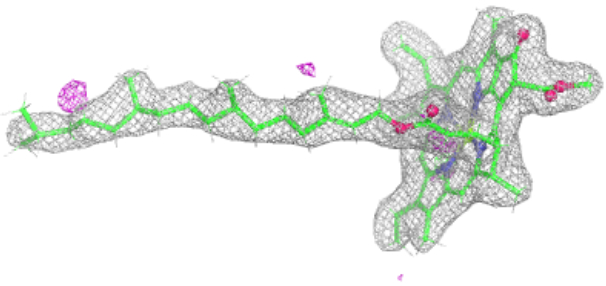


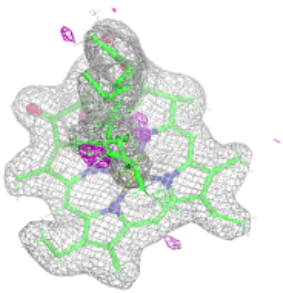


Electron density around CLA B 707:

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

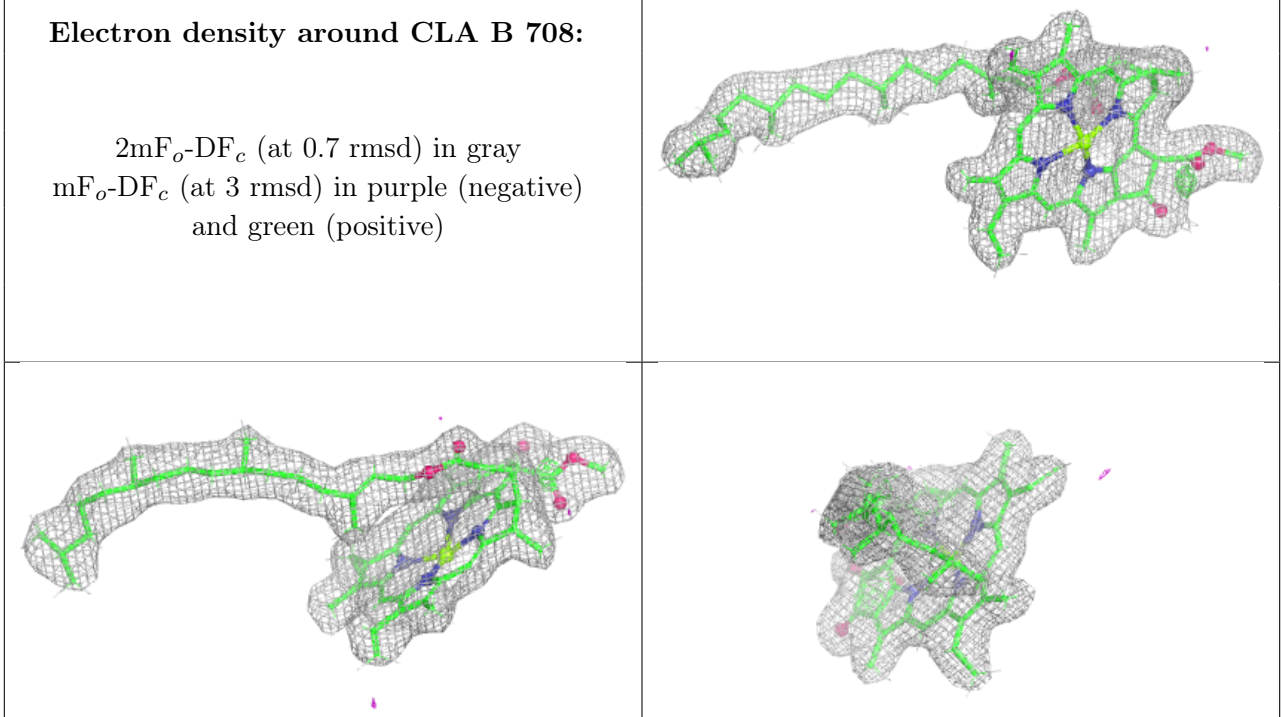






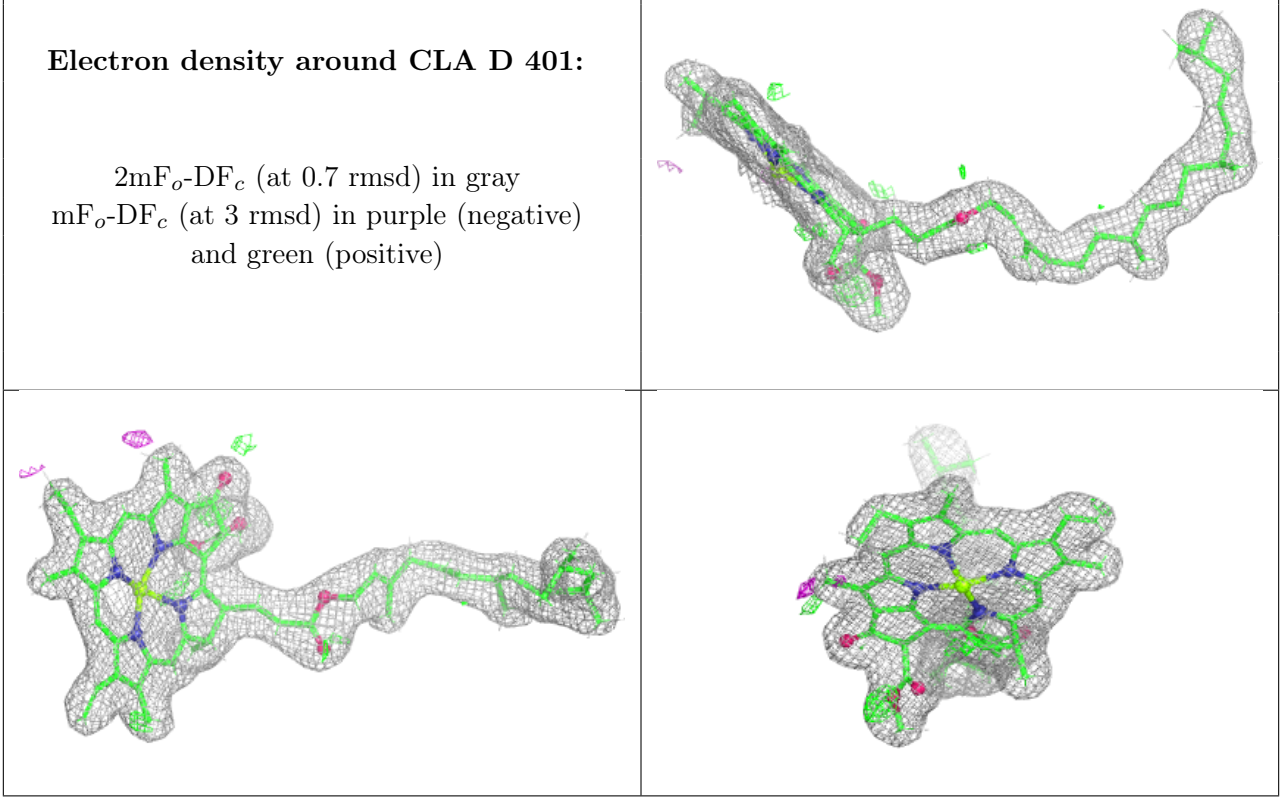
Electron density around CLA B 708:

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



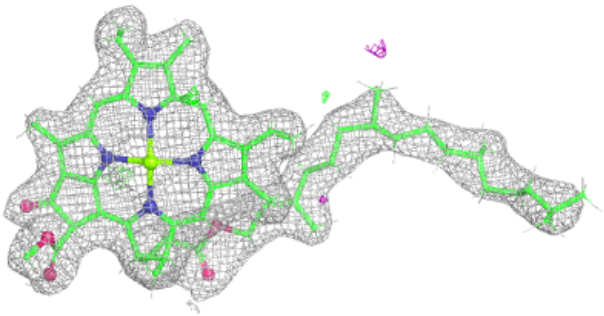
Electron density around CLA D 401:

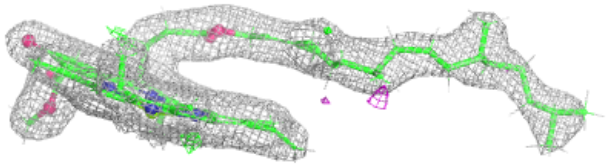
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

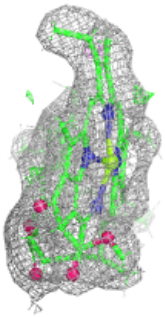


Electron density around CLA B 703:

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

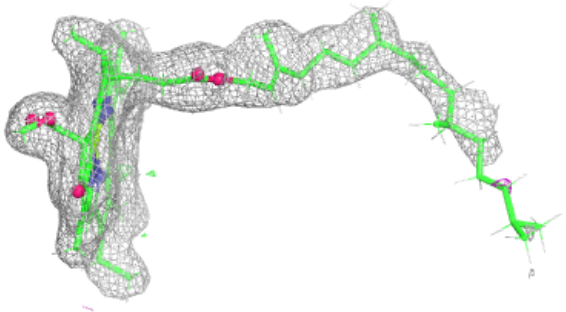


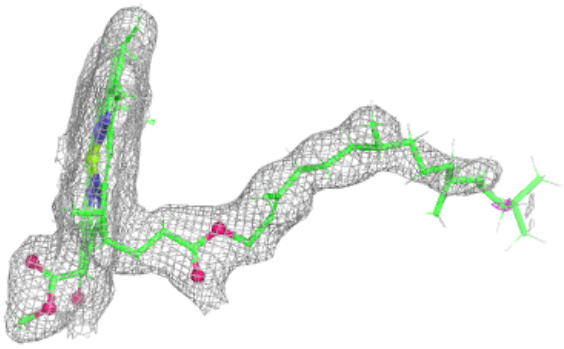


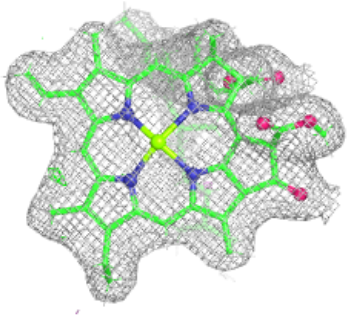


Electron density around CLA D 403:

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

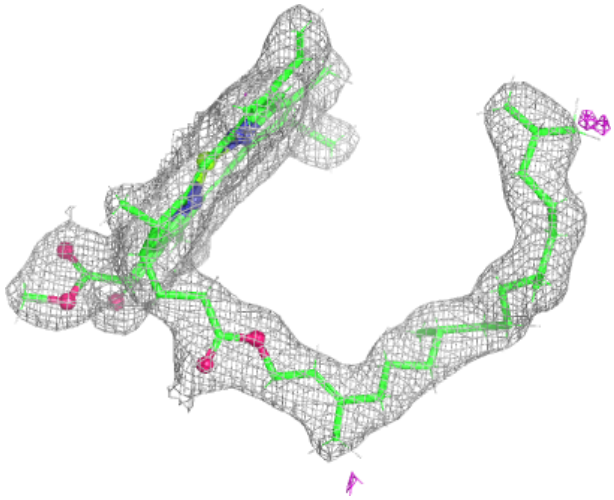


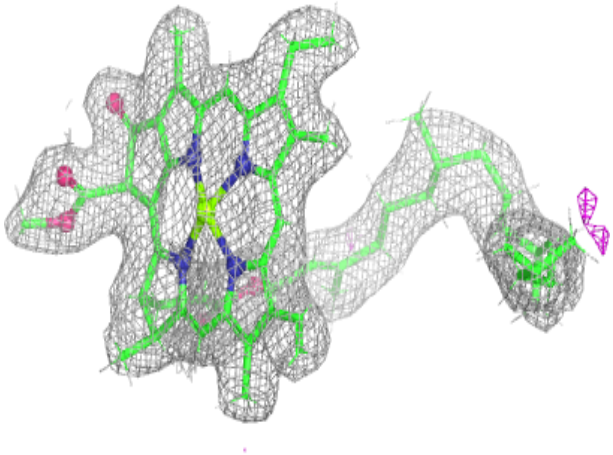


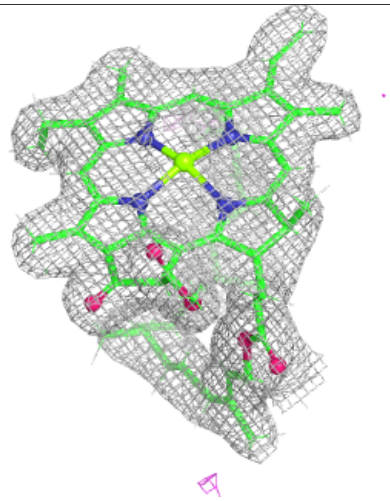


Electron density around CLA b 711:

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

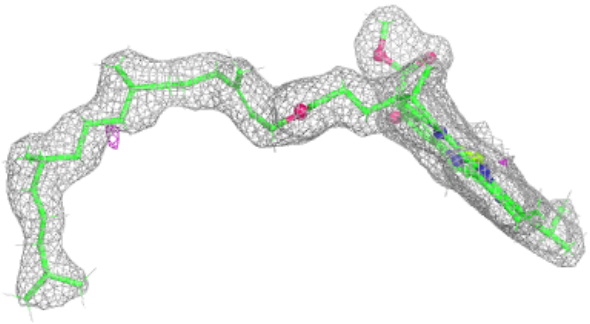


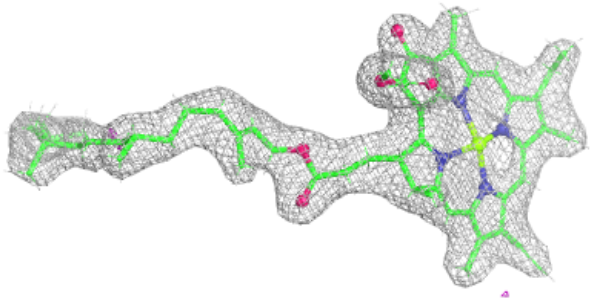


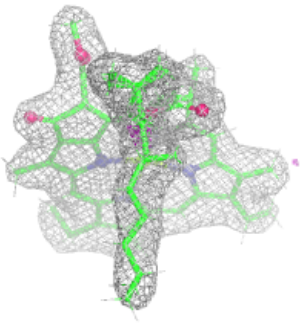


Electron density around CLA d 401:

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

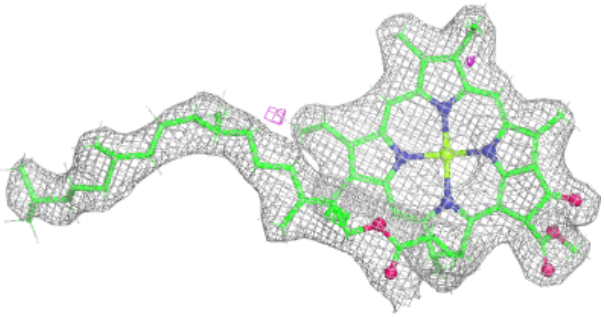


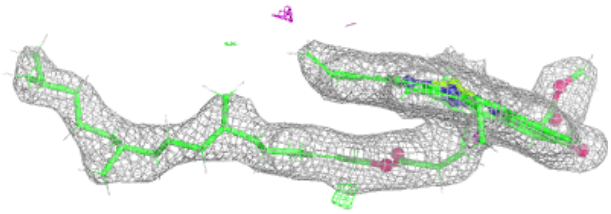


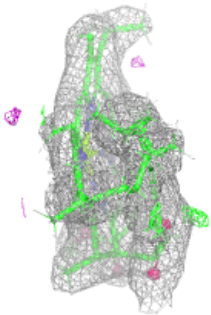


Electron density around CLA b 703:

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

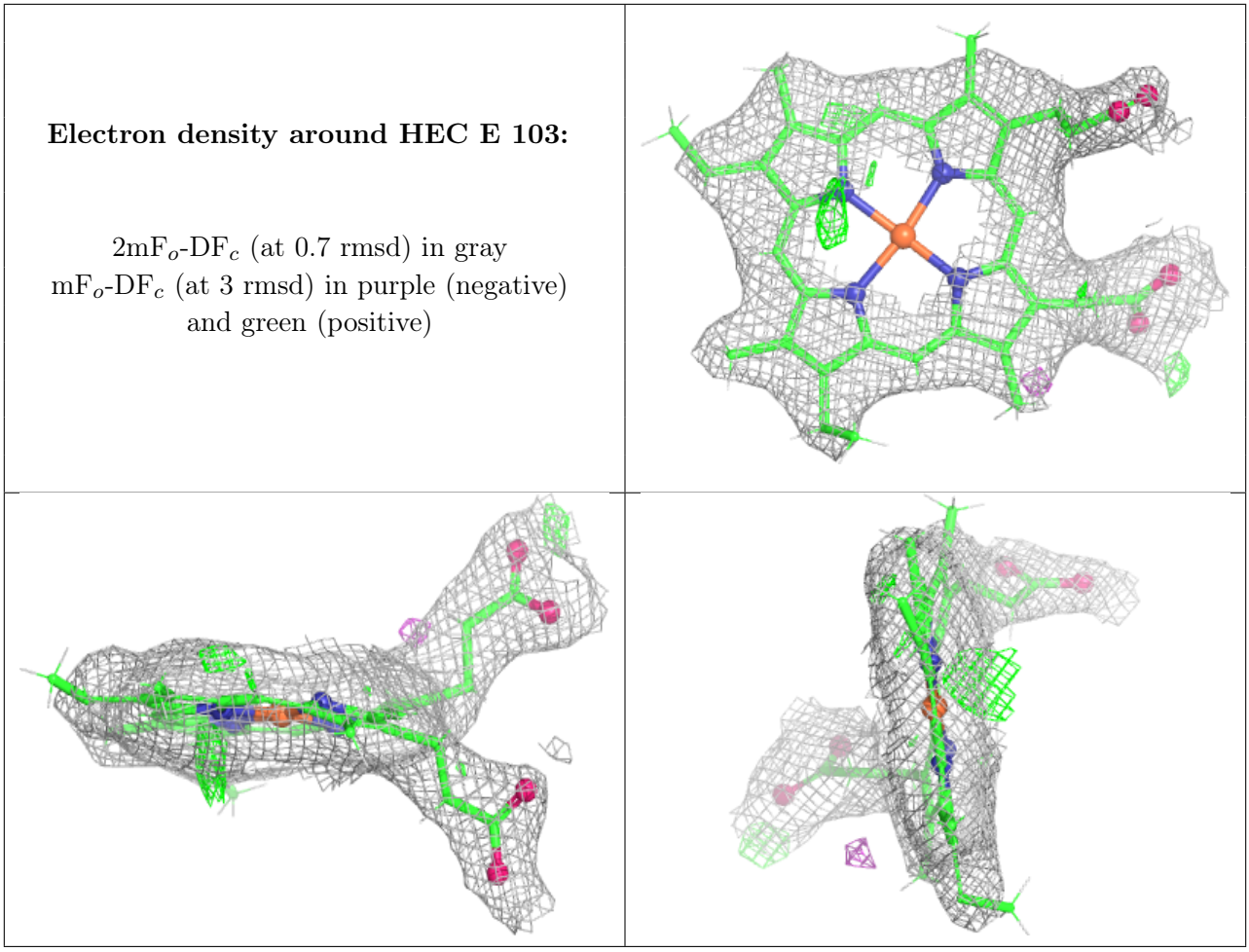






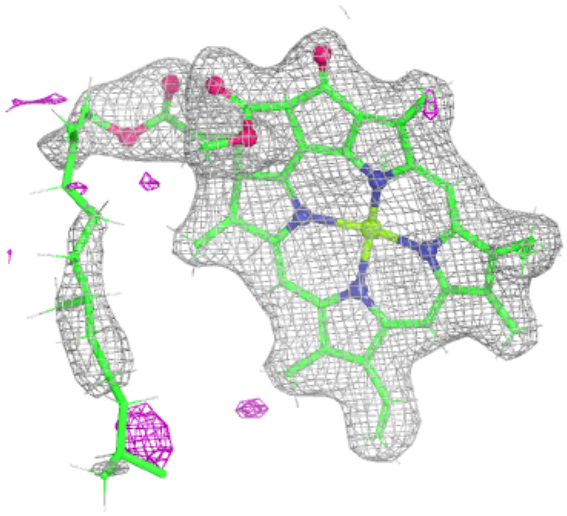
Electron density around HEC E 103:

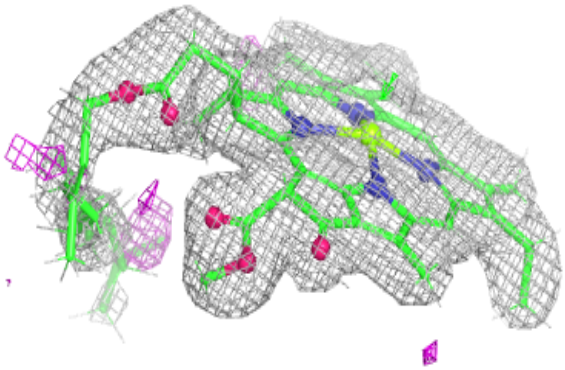
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

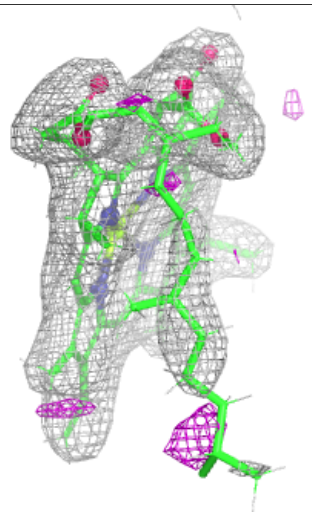


Electron density around CLA B 716:

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

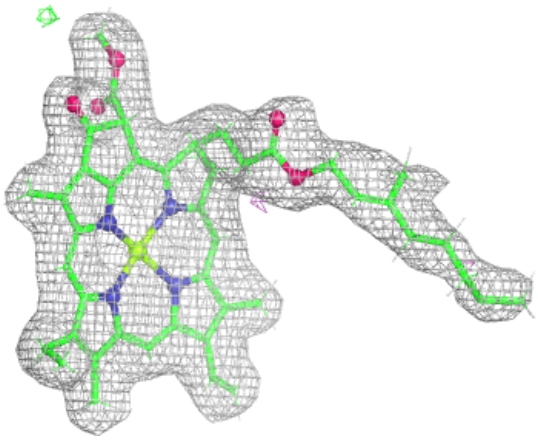


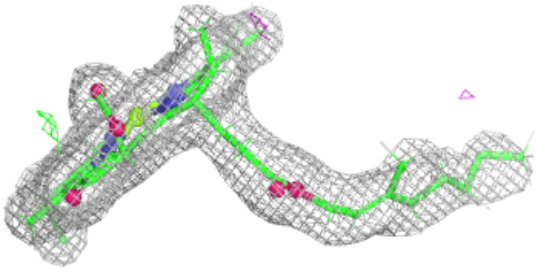


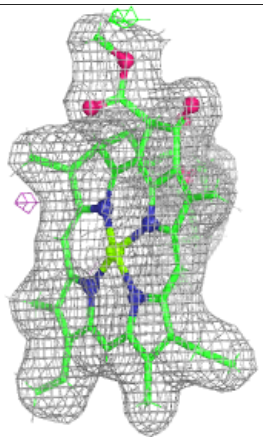


Electron density around CLA A 404:

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

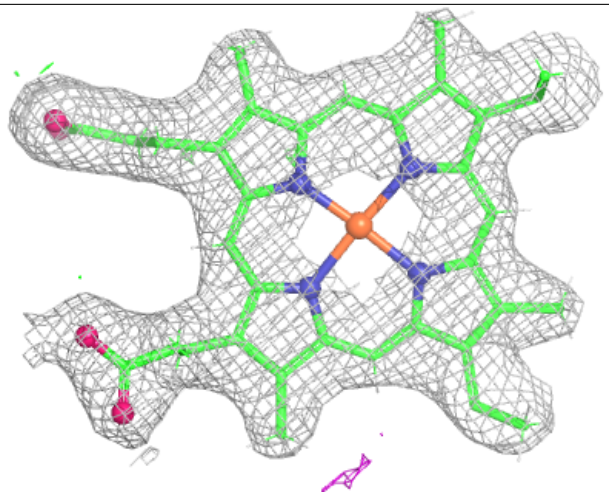


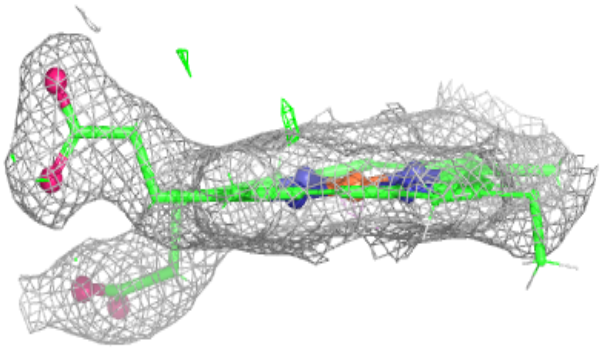


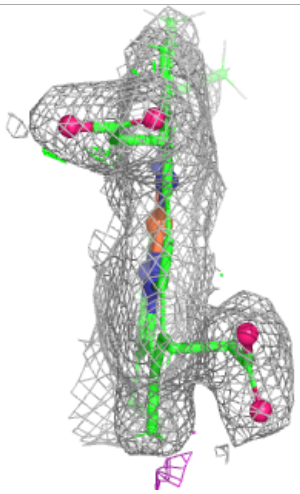


Electron density around HEC V 201:

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

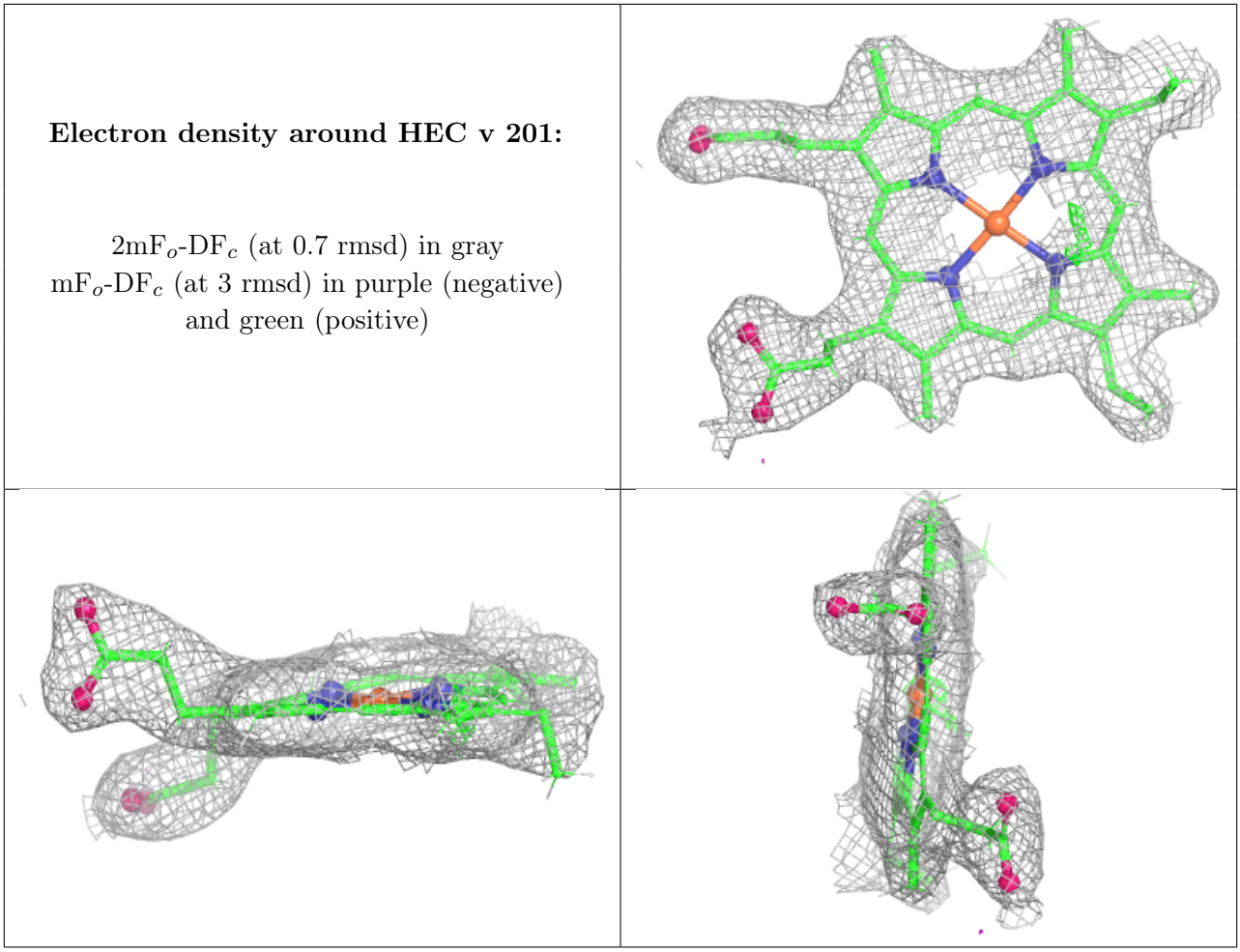






Electron density around HEC v 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.