Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2026 – 02:42 PM UTC

PDB ID	:	6W1U / pdb_00006w1u
Title	:	RT XFEL structure of Photosystem II 400 microseconds after the second illumination at 2.09 Angstrom resolution
Authors	:	Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovski, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on	:	2020-03-04
Resolution	:	2.09 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:

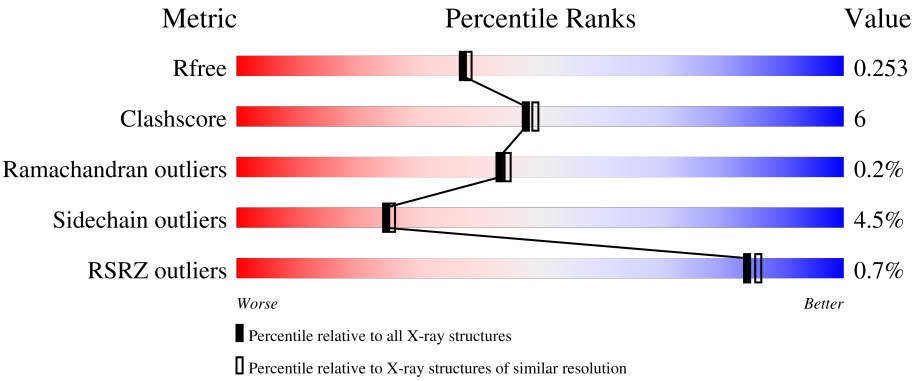
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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	86% 10%
1	a	344	% 81% 15%

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CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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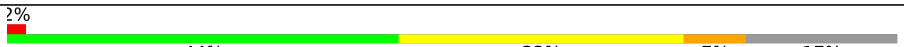
Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	

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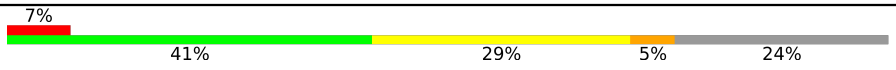
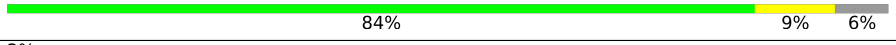
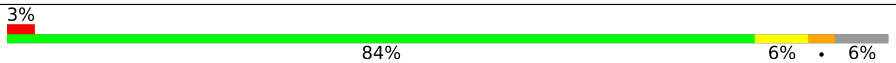
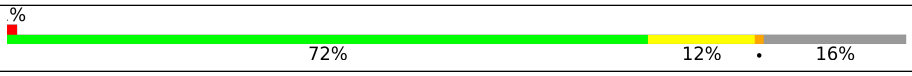
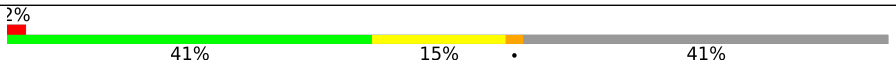
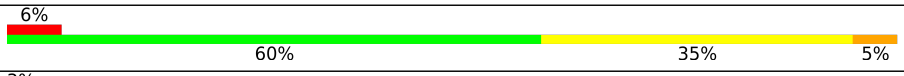
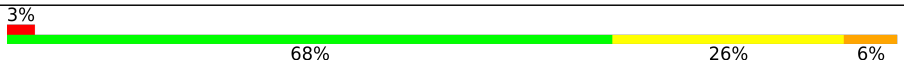
Mol	Chain	Length	Quality of chain
14	r	41	
15	T	32	
15	t	32	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	617	X	-	-	-
22	CLA	C	503	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	D	402	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	411	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	c	515	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	h	101	X	-	-	-
32	OEY	A	417[B]	-	-	X	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 105950 atoms, of which 52556 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	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	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	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	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	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

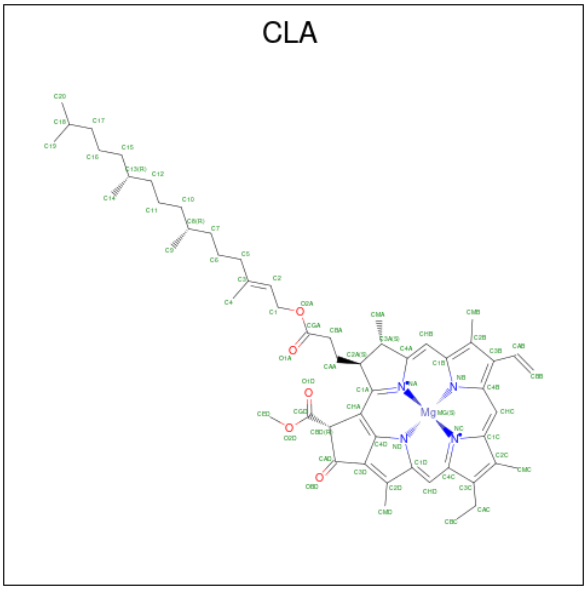
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (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	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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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
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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

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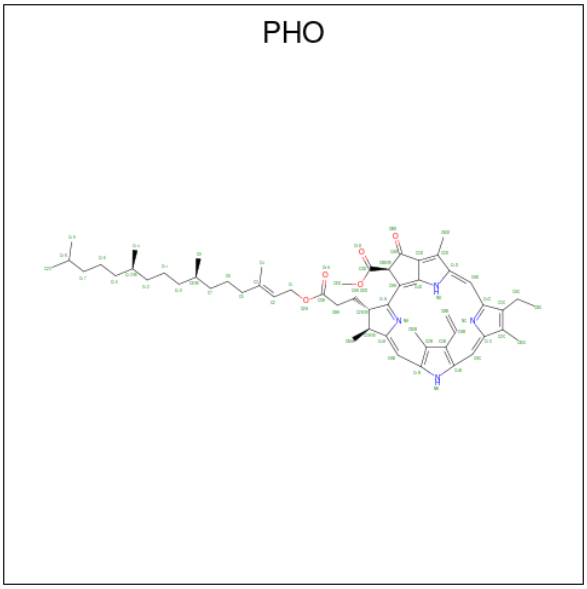
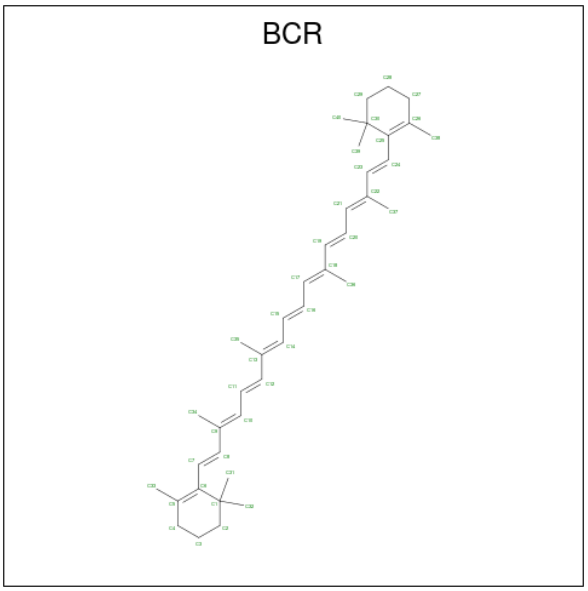
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	h	1	Total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

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



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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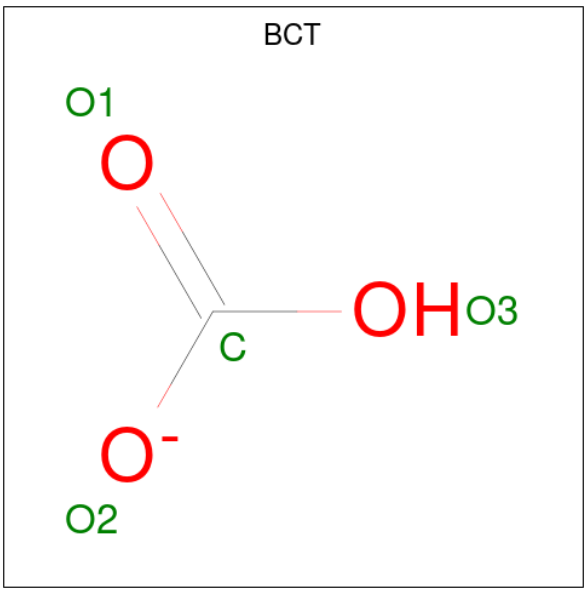
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C H 96 40 56	0	0
24	c	1	Total C H 96 40 56	0	0
24	c	1	Total C H 96 40 56	0	0
24	c	1	Total C H 96 40 56	0	0
24	d	1	Total C H 96 40 56	0	0
24	t	1	Total C H 96 40 56	0	0
24	x	1	Total C H 96 40 56	0	0
24	y	1	Total C H 96 40 56	0	0

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

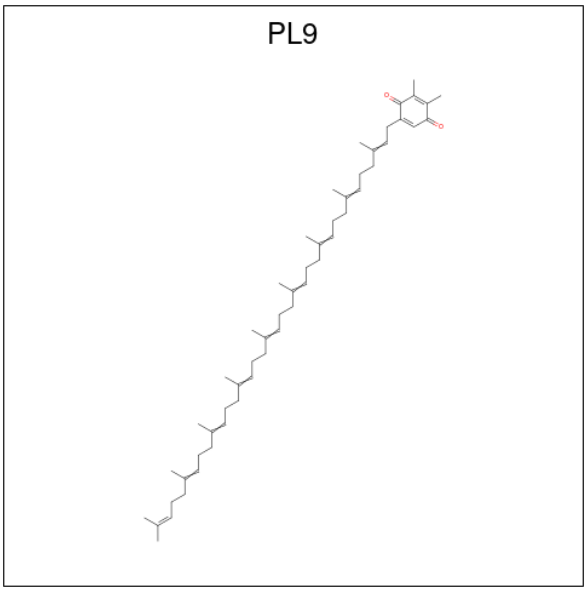
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	2	Total Cl 2 2	0	0
25	a	2	Total Cl 2 2	0	0

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



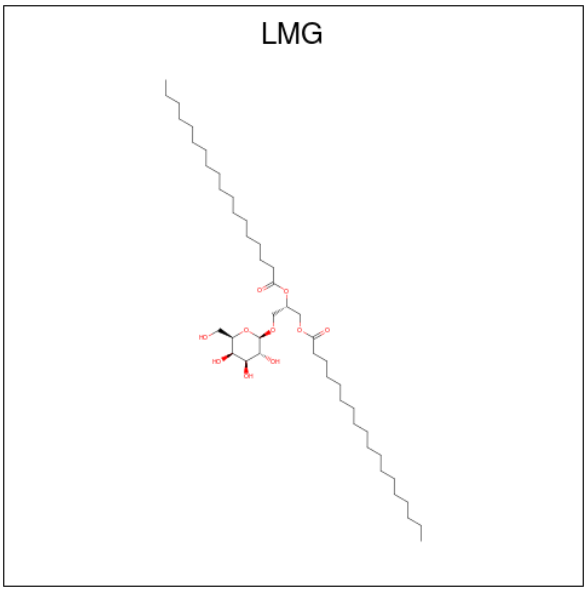
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			5	1	1	3		
26	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

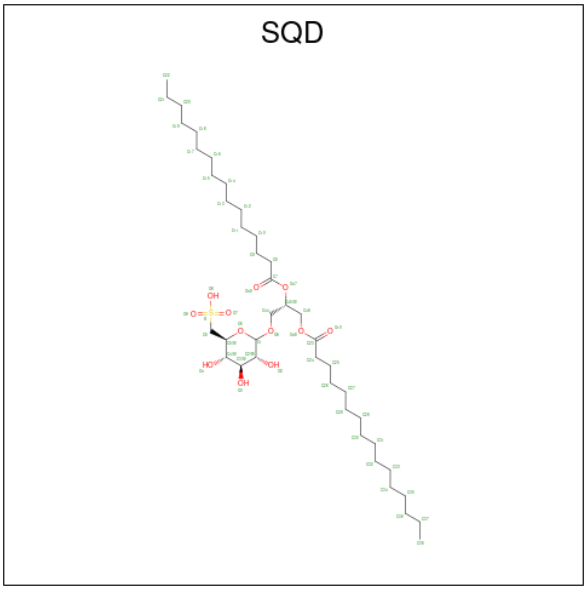
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			114	38	66	10		
28	B	1	Total	C	H	O	0	0
			141	45	86	10		
28	C	1	Total	C	H	O	0	0
			111	38	63	10		
28	D	1	Total	C	H	O	0	0
			121	41	70	10		
28	D	1	Total	C	H	O	0	0
			78	27	45	6		
28	D	1	Total	C	H	O	0	0
			68	24	40	4		
28	M	1	Total	C	H	O	0	0
			121	41	70	10		
28	b	1	Total	C	H	O	0	0
			122	41	71	10		
28	b	1	Total	C	H	O	0	0
			141	45	86	10		
28	c	1	Total	C	H	O	0	0
			80	27	43	10		
28	c	1	Total	C	H	O	0	0
			116	38	68	10		
28	c	1	Total	C	H	O	0	0
			117	39	68	10		
28	d	1	Total	C	H	O	0	0
			102	34	58	10		

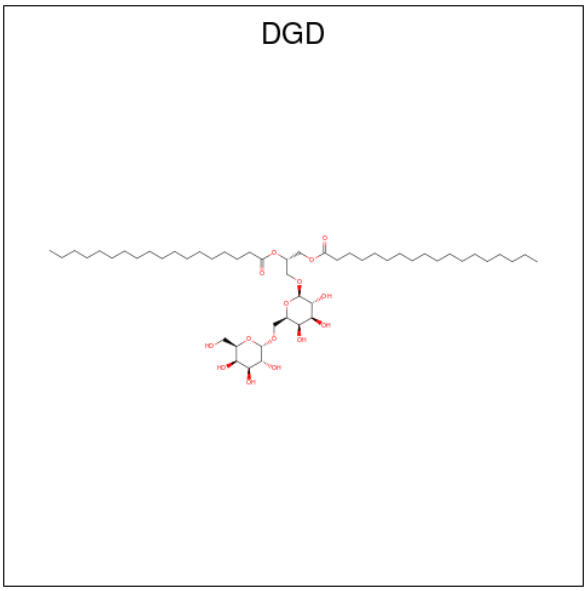
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



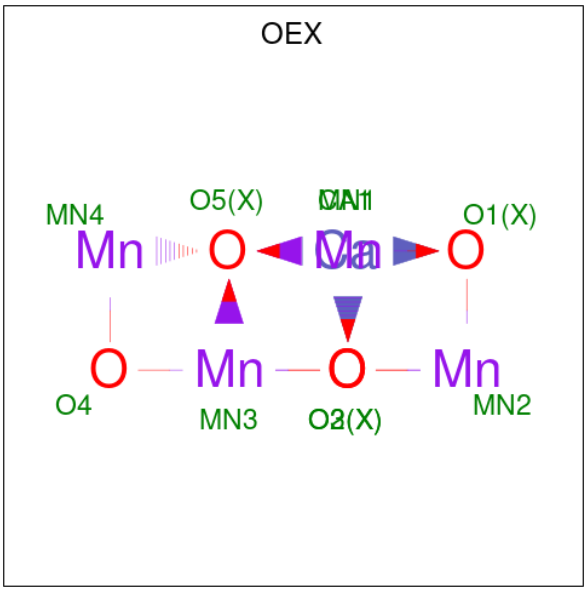
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C H O S 122 39 70 12 1	0	0
29	A	1	Total C H O 104 35 65 4	0	0
29	B	1	Total C H O S 131 41 77 12 1	0	0
29	D	1	Total C H O S 81 25 45 10 1	0	0
29	a	1	Total C H O S 131 41 77 12 1	0	0
29	a	1	Total C H O 92 31 56 5	0	0
29	b	1	Total C H O S 114 36 65 12 1	0	0
29	f	1	Total C H O S 87 28 46 12 1	0	0

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



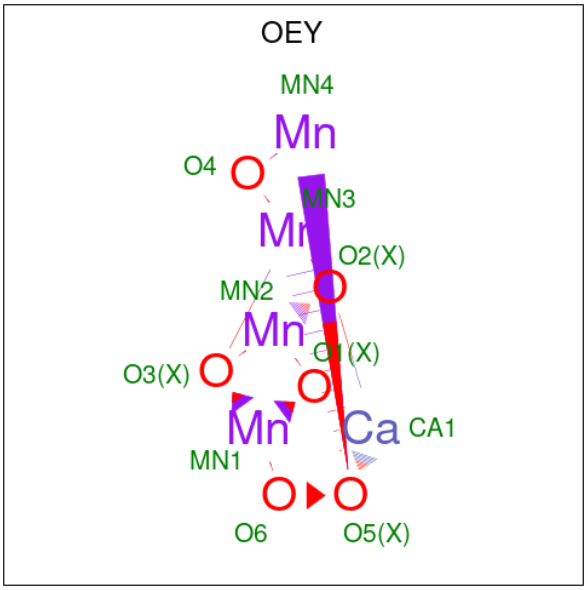
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			159	51	93	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			140	47	78	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	H	1	Total	C	H	O	0	0
			142	47	80	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	c	1	Total	C	H	O	0	0
			141	47	79	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	h	1	Total	C	H	O	0	0
			140	47	78	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



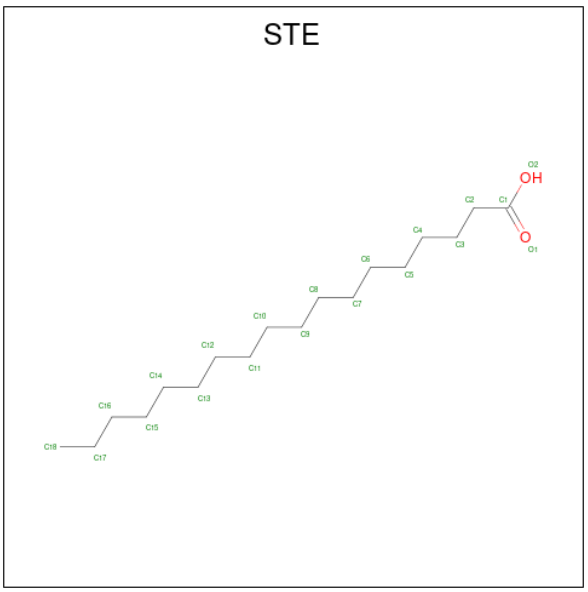
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: $CaMn_4O_6$).



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

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C H O 28 10 16 2	0	0
33	B	1	Total C H O 43 15 26 2	0	0
33	B	1	Total C H O 34 12 20 2	0	0
33	B	1	Total C H O 28 10 16 2	0	0
33	B	1	Total C H O 46 16 28 2	0	0
33	B	1	Total C H 47 16 31	0	0
33	B	1	Total C H 41 15 26	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	C	1	Total C H 47 16 31	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	E	1	Total C H O 28 10 16 2	0	0
33	H	1	Total C H 53 18 35	0	0
33	I	1	Total C H 41 15 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	1	Total C H O 28 10 16 2	0	0
33	L	1	Total C H O 28 10 16 2	0	0
33	M	1	Total C H O 37 13 22 2	0	0
33	M	1	Total C H 26 10 16	0	0
33	T	1	Total C H 44 15 29	0	0
33	X	1	Total C H O 55 18 35 2	0	0
33	Z	1	Total C H 20 8 12	0	0
33	a	1	Total C H 26 10 16	0	0
33	a	1	Total C H O 28 10 16 2	0	0
33	b	1	Total C H 47 16 31	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H O 40 14 24 2	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H 26 10 16	0	0
33	c	1	Total C H O 28 10 16 2	0	0
33	c	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 43 15 26 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	h	1	Total C H 41 14 27	0	0
33	j	1	Total C H O 28 10 16 2	0	0

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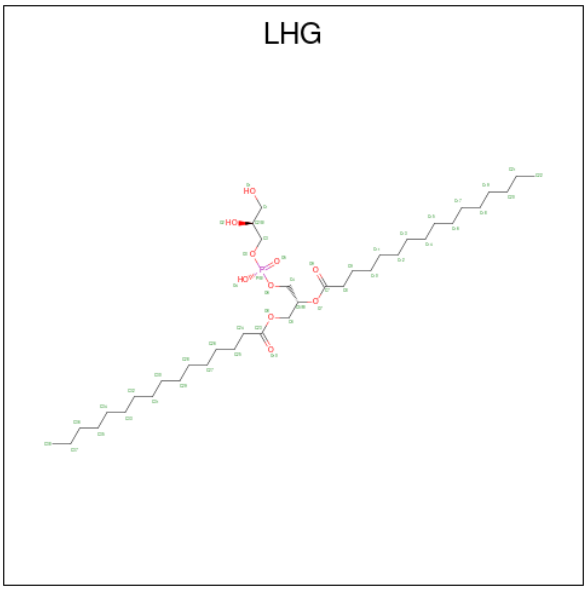
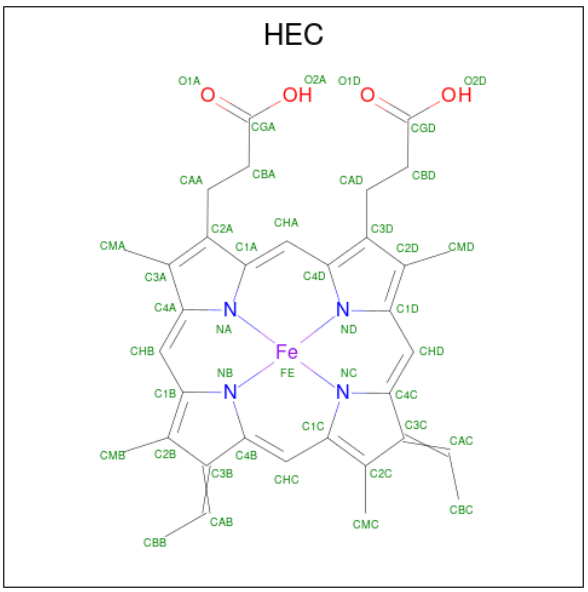
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	l	1	Total C H 53 18 35	0	0

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C H O P 122 38 73 10 1	0	0
34	D	1	Total C H O P 122 38 73 10 1	0	0
34	D	1	Total C H O P 112 36 65 10 1	0	0
34	D	1	Total C H O P 121 38 72 10 1	0	0
34	E	1	Total C H O P 121 38 72 10 1	0	0
34	d	1	Total C H O P 121 38 72 10 1	0	0
34	d	1	Total C H O P 121 38 72 10 1	0	0
34	d	1	Total C H O P 88 28 49 10 1	0	0
34	e	1	Total C H O P 97 31 55 10 1	0	0
34	l	1	Total C H O P 122 38 73 10 1	0	0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	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	153	Total	O	0	8
			153	153		
36	B	216	Total	O	0	0
			216	216		
36	C	179	Total	O	0	0
			179	179		
36	D	131	Total	O	0	0
			131	131		
36	E	39	Total	O	0	0
			39	39		
36	F	7	Total	O	0	0
			7	7		
36	H	23	Total	O	0	0
			23	23		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	I	17	Total O 17 17	0	0
36	J	19	Total O 19 19	0	0
36	K	16	Total O 16 16	0	0
36	L	9	Total O 9 9	0	0
36	M	7	Total O 7 7	0	0
36	O	101	Total O 101 101	0	0
36	R	6	Total O 6 6	0	0
36	T	10	Total O 10 10	0	0
36	U	43	Total O 43 43	0	0
36	V	62	Total O 62 62	0	0
36	X	11	Total O 11 11	0	0
36	Y	5	Total O 5 5	0	0
36	Z	10	Total O 10 10	0	0
36	a	137	Total O 137 137	0	8
36	b	186	Total O 186 186	0	0
36	c	179	Total O 179 179	0	0
36	d	110	Total O 110 110	0	0
36	e	29	Total O 29 29	0	0
36	f	7	Total O 7 7	0	0
36	h	31	Total O 31 31	0	0
36	i	8	Total O 8 8	0	0

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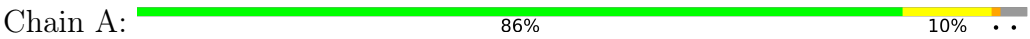
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	j	16	Total O 16 16	0	0
36	k	7	Total O 7 7	0	0
36	l	9	Total O 9 9	0	0
36	m	7	Total O 7 7	0	0
36	o	106	Total O 106 106	0	0
36	r	6	Total O 6 6	0	0
36	t	6	Total O 6 6	0	0
36	u	56	Total O 56 56	0	0
36	v	75	Total O 75 75	0	0
36	x	12	Total O 12 12	0	0
36	y	4	Total O 4 4	0	0
36	z	11	Total O 11 11	0	0

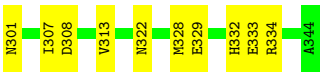
3 Residue-property plots (i)

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:



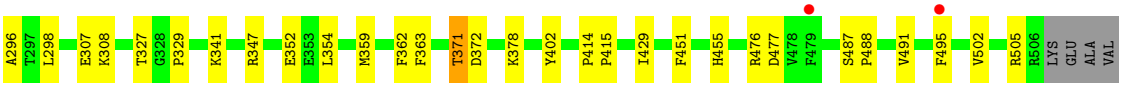


• Molecule 1: Photosystem II protein D1 1

Chain a:

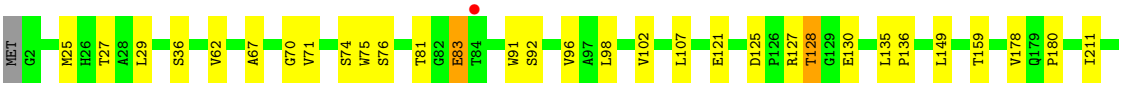
• Molecule 2: Photosystem II CP47 reaction center protein

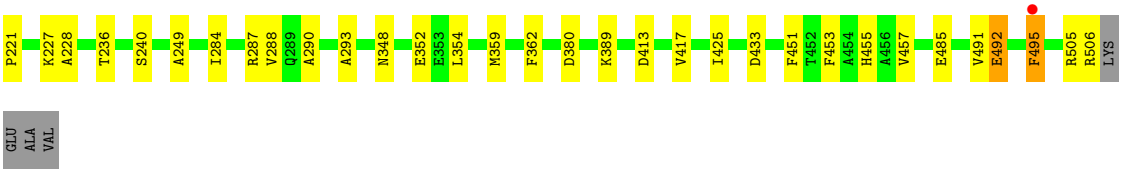
Chain B:



• Molecule 2: Photosystem II CP47 reaction center protein

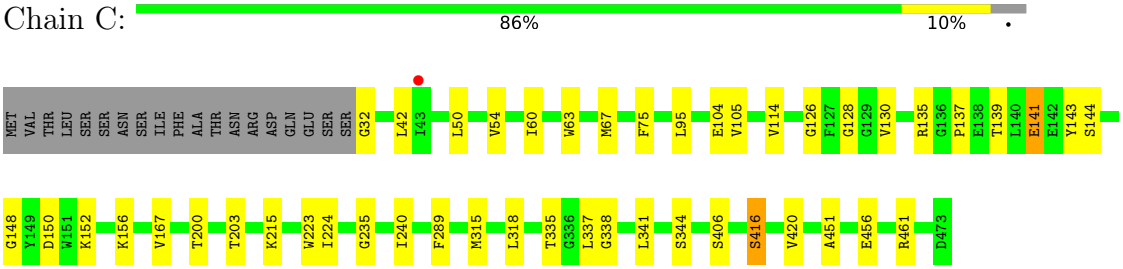
Chain b:





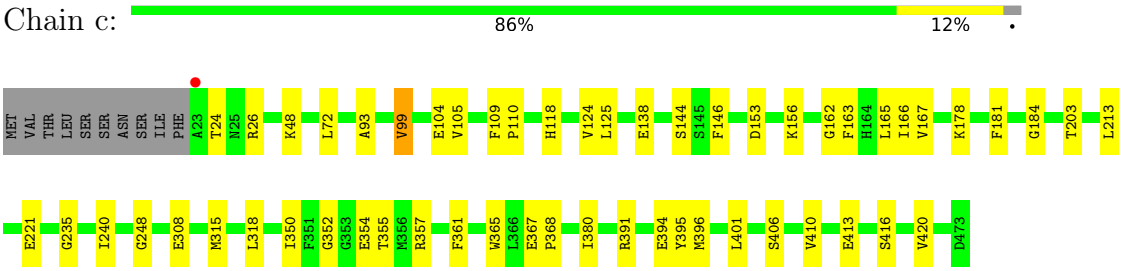
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



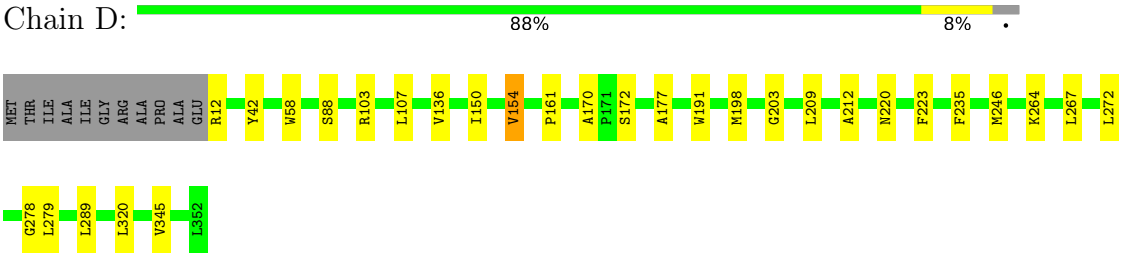
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



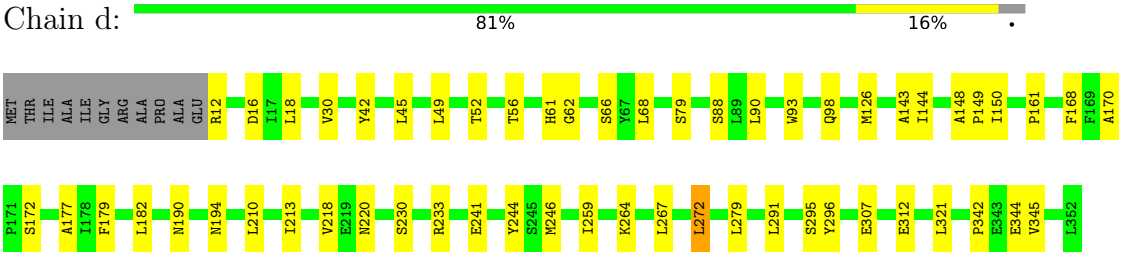
• Molecule 4: Photosystem II D2 protein

Chain D:



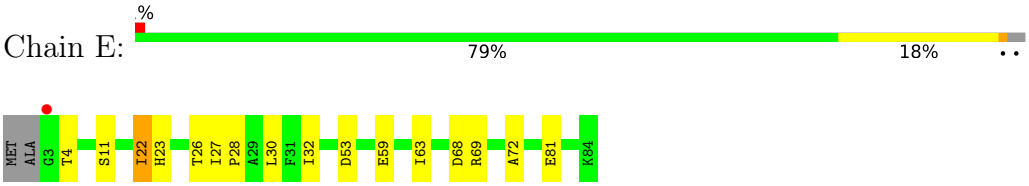
• Molecule 4: Photosystem II D2 protein

Chain d:



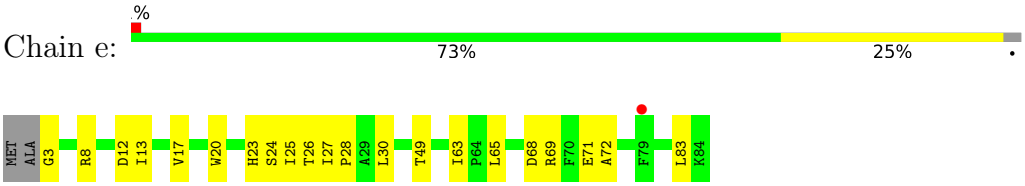
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



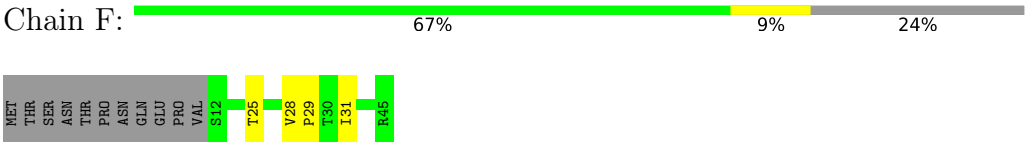
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



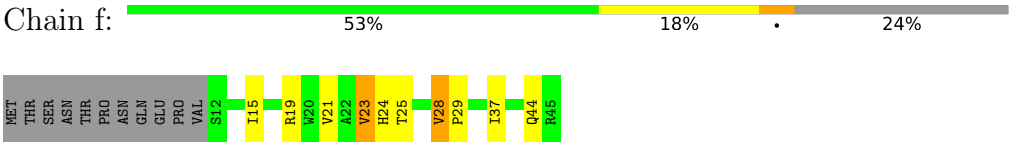
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



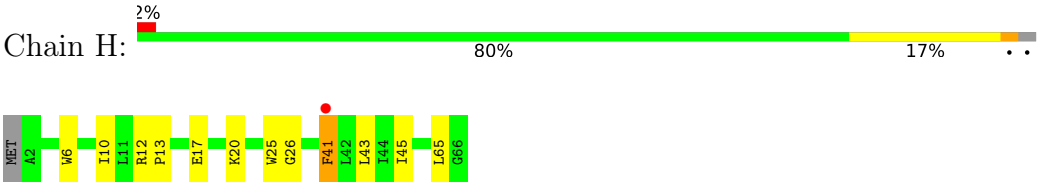
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



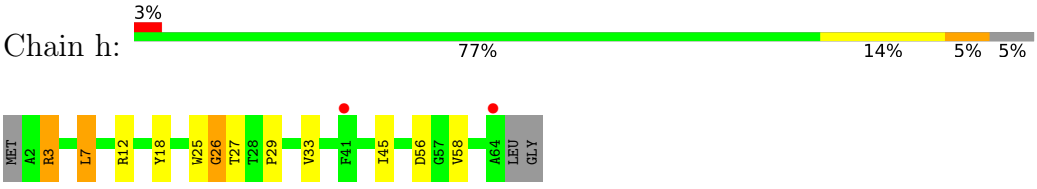
• Molecule 7: Photosystem II reaction center protein H

Chain H:



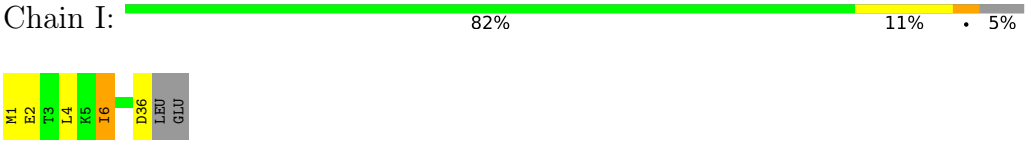
• Molecule 7: Photosystem II reaction center protein H

Chain h:



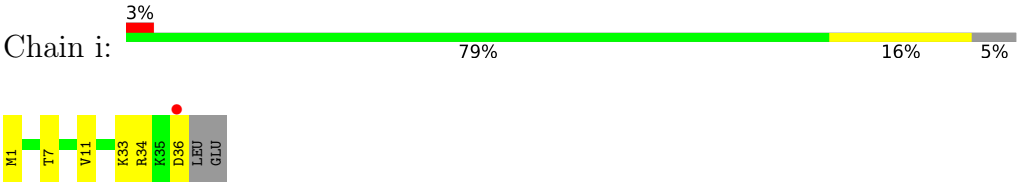
• Molecule 8: Photosystem II reaction center protein I

Chain I:



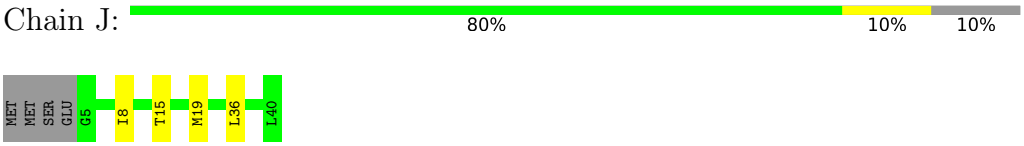
• Molecule 8: Photosystem II reaction center protein I

Chain i:



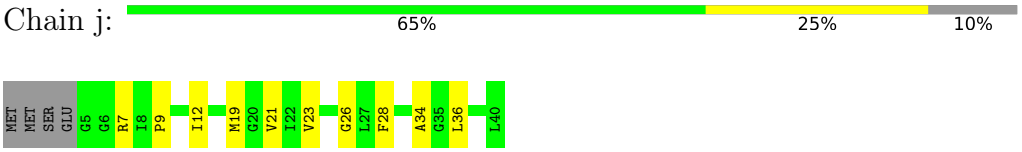
• Molecule 9: Photosystem II reaction center protein J

Chain J:



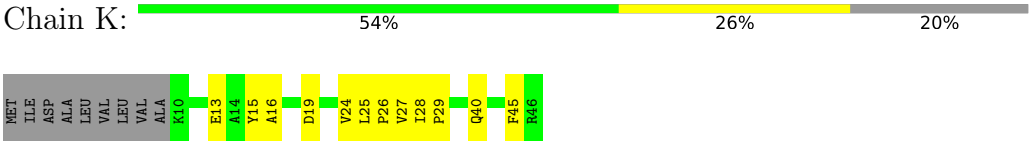
• Molecule 9: Photosystem II reaction center protein J

Chain j:



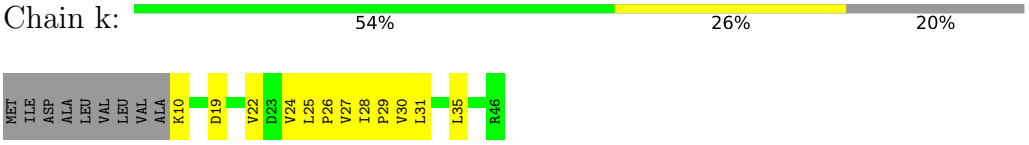
• Molecule 10: Photosystem II reaction center protein K

Chain K:



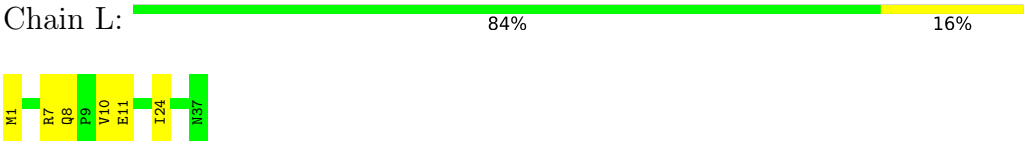
• Molecule 10: Photosystem II reaction center protein K

Chain k:



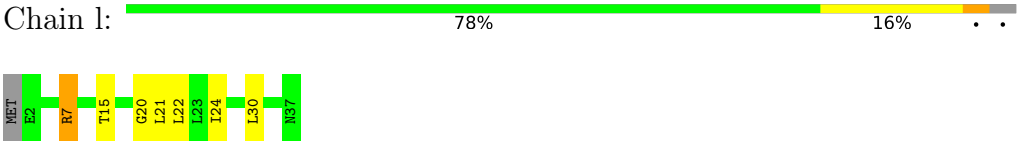
• Molecule 11: Photosystem II reaction center protein L

Chain L:



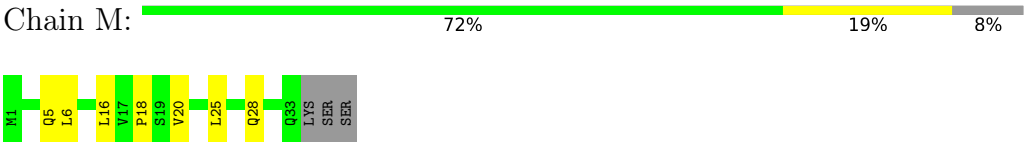
• Molecule 11: Photosystem II reaction center protein L

Chain l:



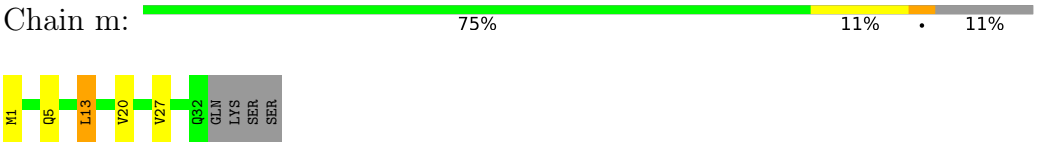
• Molecule 12: Photosystem II reaction center protein M

Chain M:



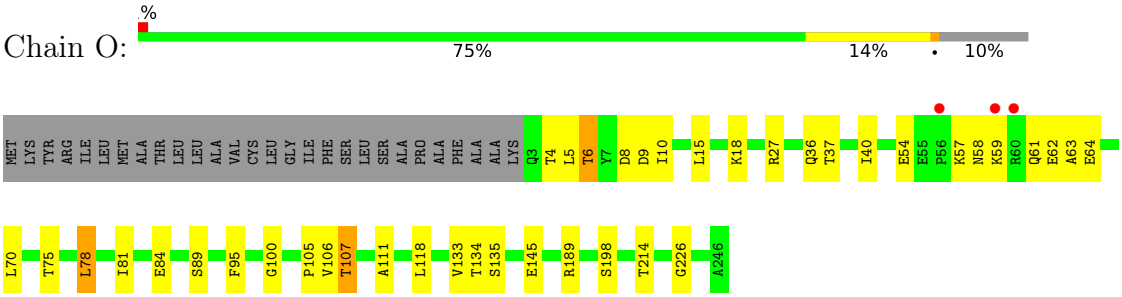
• Molecule 12: Photosystem II reaction center protein M

Chain m:



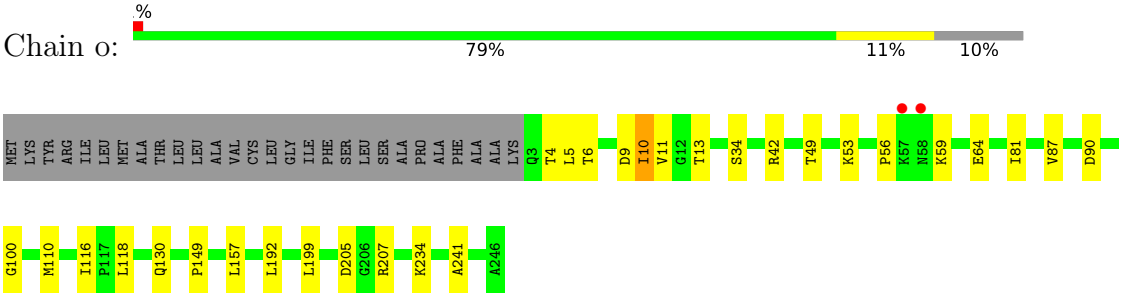
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



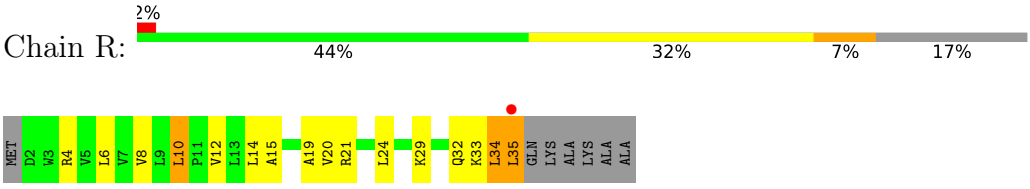
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



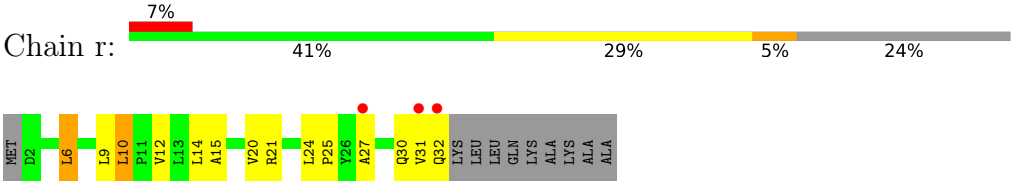
• Molecule 14: Photosystem II protein Y

Chain R:



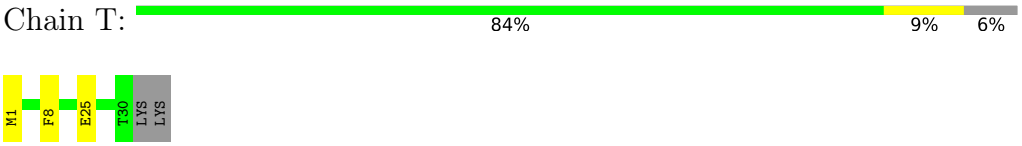
• Molecule 14: Photosystem II protein Y

Chain r:



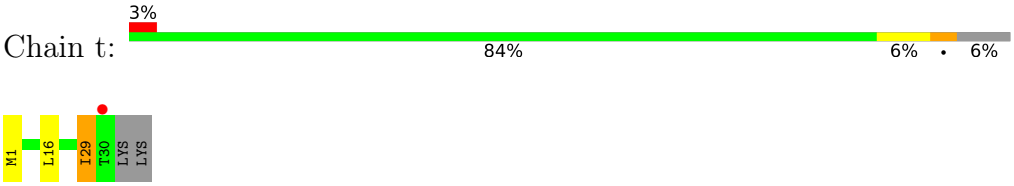
• Molecule 15: Photosystem II reaction center protein T

Chain T:



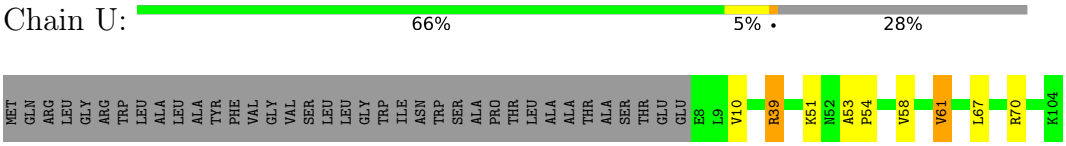
• Molecule 15: Photosystem II reaction center protein T

Chain t:



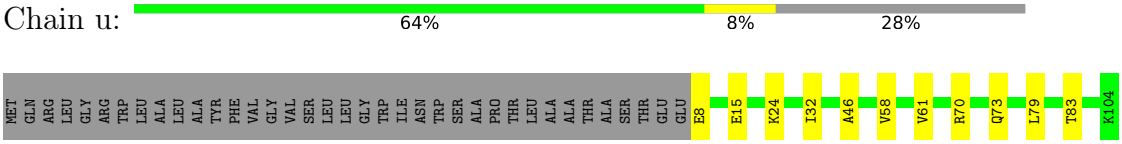
• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:



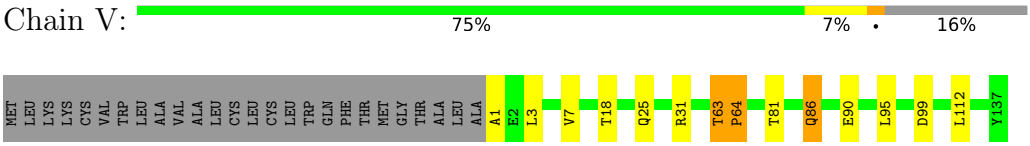
• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:



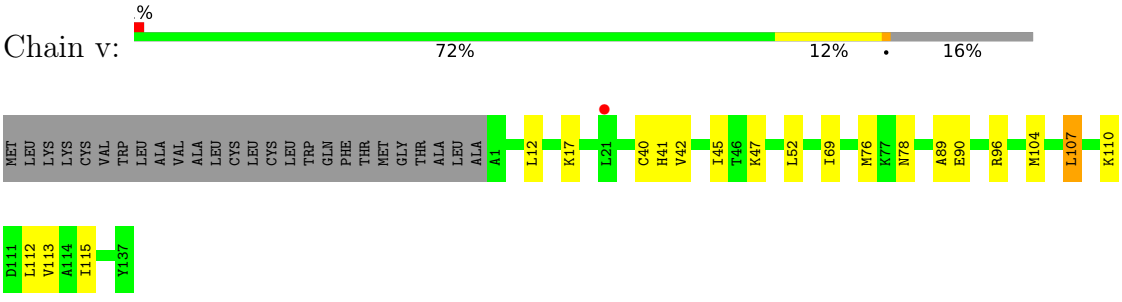
• Molecule 17: Cytochrome c-550

Chain V:



• Molecule 17: Cytochrome c-550

Chain v:

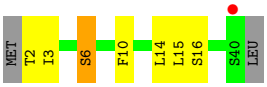


• Molecule 18: Photosystem II reaction center X protein

Chain X:

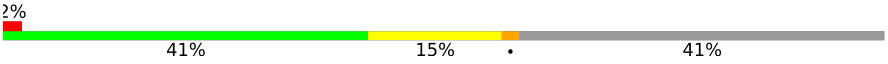
• Molecule 18: Photosystem II reaction center X protein

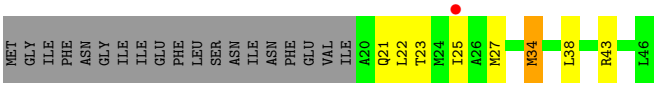
Chain x:



• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:





• Molecule 19: Photosystem II reaction center protein Ycf12

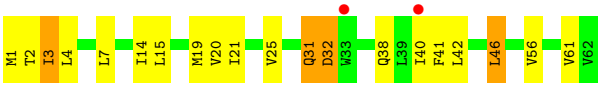
Chain y:

• Molecule 20: Photosystem II reaction center protein Z

Chain Z:

• Molecule 20: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.97Å 221.71Å 308.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.65-2.09) 85.9 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.72 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.180 , 0.239 0.199 , 0.253	Depositor DCC
R_{free} test set	4171 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.5	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	0.96	EDS
Total number of atoms	105950	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: OEY, BCR, FME, STE, LMG, PHO, OEX, BCT, CL, DGD, HEC, PL9, CLA, SQD, 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	0.55	0/3187	0.68	1/4342 (0.0%)
1	a	0.54	0/3184	0.63	0/4338
2	B	0.60	0/4161	0.69	0/5669
2	b	0.58	0/4118	0.67	0/5611
3	C	0.58	0/3621	0.68	0/4930
3	c	0.54	0/3693	0.65	0/5026
4	D	0.64	0/2820	0.70	0/3840
4	d	0.61	0/2829	0.69	0/3852
5	E	0.52	0/688	0.64	0/940
5	e	0.47	0/683	0.64	0/932
6	F	0.53	0/284	0.55	0/387
6	f	0.44	0/284	0.61	0/387
7	H	0.59	0/523	0.71	0/713
7	h	0.51	0/511	0.62	0/697
8	I	0.56	0/293	0.64	0/396
8	i	0.56	0/293	0.62	0/396
9	J	0.49	0/263	0.58	0/356
9	j	0.48	0/263	0.62	0/356
10	K	0.50	0/303	0.61	0/416
10	k	0.43	0/303	0.56	0/416
11	L	0.63	0/311	0.66	0/422
11	l	0.63	0/303	0.60	0/412
12	M	0.57	0/249	0.70	0/341
12	m	0.67	0/244	0.69	0/334
13	O	0.57	0/1904	0.71	0/2585
13	o	0.58	0/1905	0.70	0/2583
14	R	0.41	0/277	0.57	0/380
14	r	0.36	0/245	0.45	0/336
15	T	0.62	0/257	0.77	0/349
15	t	0.61	0/255	0.59	0/346
16	U	0.53	0/785	0.65	0/1064
16	u	0.58	0/785	0.69	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	V	0.56	0/1085	0.66	0/1473
17	v	0.55	0/1085	0.67	0/1473
18	X	0.53	0/284	0.70	0/384
18	x	0.45	0/289	0.58	0/391
19	Y	0.46	0/197	0.57	0/264
19	y	0.40	0/219	0.53	0/294
20	Z	0.40	0/490	0.55	0/669
20	z	0.39	0/488	0.52	0/666
All	All	0.56	0/43961	0.66	1/59830 (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
1	A	0	1
1	a	0	1
17	V	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	TRP	CA-CB-CG	-5.12	103.88	113.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
17	V	63	THR	Peptide
1	a	339[B]	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3089	2942	2956	27	0
1	a	3086	2933	2947	36	0
2	B	4005	3859	3867	34	0
2	b	3978	3822	3836	44	0
3	C	3479	3397	3383	29	0
3	c	3553	3468	3466	37	0
4	D	2726	2624	2632	26	0
4	d	2732	2630	2638	35	0
5	E	666	650	651	11	0
5	e	664	647	648	18	0
6	F	275	281	282	5	0
6	f	275	281	282	9	0
7	H	510	532	532	12	0
7	h	498	518	518	11	0
8	I	296	311	311	2	0
8	i	296	311	311	2	0
9	J	257	268	268	2	0
9	j	257	268	268	8	0
10	K	293	305	305	10	0
10	k	293	305	305	4	0
11	L	304	316	316	5	0
11	l	296	304	304	4	0
12	M	256	269	269	7	0
12	m	251	267	267	5	0
13	O	1870	1828	1830	24	0
13	o	1874	1844	1846	15	0
14	R	271	298	298	8	0
14	r	240	253	249	8	0
15	T	258	261	261	2	0
15	t	256	256	256	2	0
16	U	774	772	773	6	0
16	u	774	772	773	6	0
17	V	1064	1068	1073	8	0
17	v	1064	1068	1074	13	0
18	X	281	312	312	5	0
18	x	286	316	314	4	0
19	Y	196	217	217	8	0
19	y	218	241	241	3	0
20	Z	479	516	516	14	0
20	z	477	509	509	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	249	264	264	5	0
22	B	1035	1139	1139	23	0
22	C	839	922	922	15	0
22	D	130	144	144	4	0
22	a	260	288	288	4	0
22	b	970	1067	1067	28	0
22	c	839	919	919	6	0
22	d	130	144	144	2	0
22	h	65	72	72	1	0
23	A	64	74	74	0	0
23	D	64	74	74	1	0
23	a	64	74	74	1	0
23	d	64	74	74	2	0
24	A	40	56	56	2	0
24	B	120	168	168	6	0
24	C	40	56	56	1	0
24	D	40	56	56	5	0
24	H	40	56	56	3	0
24	K	40	56	56	0	0
24	T	40	56	56	3	0
24	Y	40	56	56	2	0
24	Z	40	56	56	3	0
24	a	40	56	56	0	0
24	b	120	168	168	9	0
24	c	120	168	168	2	0
24	d	40	56	56	2	0
24	t	40	56	56	6	0
24	x	40	56	56	1	0
24	y	40	56	56	1	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	4	1	1	0	0
26	a	4	1	1	0	0
27	A	55	80	80	4	0
27	D	55	80	80	0	0
27	a	55	80	80	7	0
27	d	55	80	80	0	0
28	A	48	66	66	0	0
28	B	55	86	86	2	0
28	C	48	63	66	2	0
28	D	112	155	156	5	0
28	M	51	70	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	106	157	158	1	0
28	c	134	179	181	1	0
28	d	44	58	58	0	0
29	A	91	135	135	6	0
29	B	54	77	78	2	0
29	D	36	45	45	1	0
29	a	90	133	133	0	0
29	b	49	65	65	3	0
29	f	41	46	48	0	0
30	A	66	93	96	1	0
30	C	186	240	244	1	0
30	H	62	80	82	0	0
30	c	186	235	245	0	0
30	h	62	78	81	0	0
31	A	10	0	0	1	0
31	a	10	0	0	1	0
32	A	11	0	0	5	0
32	a	11	0	0	0	0
33	B	104	163	163	4	0
33	C	40	63	63	1	0
33	E	12	16	16	0	0
33	H	18	35	35	0	0
33	I	15	26	26	0	0
33	J	12	16	16	0	0
33	L	12	16	16	0	0
33	M	25	38	38	1	0
33	T	15	29	29	3	0
33	X	20	35	35	2	0
33	Z	8	12	12	1	0
33	a	22	32	32	1	0
33	b	82	141	141	3	0
33	c	32	51	51	1	0
33	d	57	96	96	5	0
33	h	14	27	27	2	0
33	j	12	16	16	1	0
33	l	18	35	35	1	0
34	B	49	73	74	1	0
34	D	145	210	215	4	0
34	E	49	72	74	0	0
34	d	137	193	199	3	0
34	e	42	55	57	0	0
34	l	49	73	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	F	43	32	32	3	0
35	V	43	30	31	1	0
35	e	43	32	32	7	0
35	v	43	30	31	5	0
36	A	153	0	0	3	0
36	B	216	0	0	0	0
36	C	179	0	0	1	0
36	D	131	0	0	4	0
36	E	39	0	0	0	0
36	F	7	0	0	0	0
36	H	23	0	0	1	0
36	I	17	0	0	1	0
36	J	19	0	0	1	0
36	K	16	0	0	0	0
36	L	9	0	0	1	0
36	M	7	0	0	3	0
36	O	101	0	0	7	0
36	R	6	0	0	1	0
36	T	10	0	0	0	0
36	U	43	0	0	3	0
36	V	62	0	0	3	0
36	X	11	0	0	1	0
36	Y	5	0	0	0	0
36	Z	10	0	0	1	0
36	a	137	0	0	4	0
36	b	186	0	0	5	0
36	c	179	0	0	8	0
36	d	110	0	0	0	0
36	e	29	0	0	3	0
36	f	7	0	0	1	0
36	h	31	0	0	4	0
36	i	8	0	0	0	0
36	j	16	0	0	2	0
36	k	7	0	0	0	0
36	l	9	0	0	0	0
36	m	7	0	0	1	0
36	o	106	0	0	4	0
36	r	6	0	0	2	0
36	t	6	0	0	0	0
36	u	56	0	0	1	0
36	v	75	0	0	1	0
36	x	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	y	4	0	0	0	0
36	z	11	0	0	1	0
All	All	53394	52556	52674	586	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (586) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:40:CYS:SG	35:v:201:HEC:CAC	2.06	1.44
17:v:40:CYS:SG	35:v:201:HEC:HAC	1.97	1.03
13:o:9:ASP:OD2	36:o:301:HOH:O	1.76	1.02
14:r:32:GLN:O	36:r:101:HOH:O	1.79	0.97
3:c:315:MET:SD	36:c:751:HOH:O	2.21	0.97
29:A:414:SQD:H383	22:b:605:CLA:H93	1.53	0.89
33:a:415:STE:O1	36:a:1701:HOH:O	1.89	0.89
13:O:27:ARG:NH1	36:O:301:HOH:O	2.06	0.88
4:D:12:ARG:O	36:D:501:HOH:O	1.90	0.87
3:C:32:GLY:N	36:C:601:HOH:O	2.09	0.85
17:v:40:CYS:SG	35:v:201:HEC:C3C	2.69	0.80
14:r:21:ARG:NH1	36:r:102:HOH:O	2.16	0.78
5:e:30:LEU:HD11	35:e:101:HEC:CBB	2.14	0.77
8:I:2:GLU:OE1	36:I:201:HOH:O	2.03	0.77
35:F:101:HEC:HBC3	35:F:101:HEC:HHD	1.66	0.76
17:V:18:THR:OG1	36:V:301:HOH:O	2.02	0.76
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.18	0.76
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.68	0.76
35:v:201:HEC:HBC3	35:v:201:HEC:HMC3	1.67	0.76
27:A:410:PL9:H361	6:F:25:THR:HG21	1.68	0.75
14:r:27:ALA:O	14:r:31:VAL:N	2.20	0.75
5:e:71:GLU:OE1	36:e:201:HOH:O	2.03	0.75
7:h:3:ARG:NH1	36:h:202:HOH:O	2.19	0.74
32:A:417[B]:OEY:O5	32:A:417[B]:OEY:O6	2.06	0.73
9:j:9:PRO:HG2	9:j:12:ILE:HD12	1.71	0.73
24:t:101:BCR:HC8	24:t:101:BCR:H311	1.71	0.73
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.24	0.73
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.70	0.72
22:C:510:CLA:H91	22:C:513:CLA:HAA2	1.71	0.72
1:A:189[B]:GLU:OE2	32:A:417[B]:OEY:O6	2.08	0.72
3:c:394:GLU:OE1	36:c:601:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:t:101:BCR:H23C	24:t:101:BCR:H382	1.73	0.71
20:z:32:ASP:N	20:z:32:ASP:OD1	2.24	0.71
36:A:565:HOH:O	13:O:107:THR:HG21	1.90	0.70
13:O:57:LYS:NZ	36:O:304:HOH:O	2.25	0.70
9:J:36:LEU:O	36:J:201:HOH:O	2.09	0.69
2:b:227:LYS:NZ	36:b:704:HOH:O	2.26	0.69
3:c:221:GLU:OE2	36:c:602:HOH:O	2.09	0.69
9:J:15:THR:HG22	9:J:19:MET:CE	2.23	0.69
24:d:404:BCR:H331	24:d:404:BCR:C8	2.21	0.69
33:M:102:STE:O1	36:M:201:HOH:O	2.10	0.68
18:x:10:PHE:CE2	18:x:14:LEU:HD22	2.29	0.68
35:e:101:HEC:HMC1	35:e:101:HEC:HBC2	1.75	0.68
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.30	0.67
17:V:90:GLU:OE2	36:V:302:HOH:O	2.12	0.67
1:A:189[A]:GLU:OE2	31:A:416[A]:OEX:MN1	1.52	0.67
9:j:36:LEU:O	36:j:201:HOH:O	2.12	0.67
1:a:189[A]:GLU:OE2	31:a:416[A]:OEX:MN1	1.51	0.67
2:b:127:ARG:NH1	7:h:18:TYR:O	2.29	0.66
18:X:3:ILE:HD12	18:X:7:LEU:HD23	1.76	0.66
9:j:34:ALA:O	36:j:201:HOH:O	2.13	0.65
22:B:605:CLA:H42	22:B:606:CLA:H42	1.77	0.64
2:b:221:PRO:HA	22:b:608:CLA:HED3	1.78	0.64
33:X:101:STE:O1	36:X:201:HOH:O	2.14	0.64
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.79	0.64
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.62	0.64
4:d:246:MET:HE3	4:d:264:LYS:CG	2.27	0.64
2:B:117:TYR:HA	11:L:1:MET:HE1	1.79	0.64
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.33	0.64
32:A:417[B]:OEY:O6	32:A:417[B]:OEY:MN1	1.56	0.64
19:Y:34:MET:HE2	19:Y:38:LEU:HD21	1.80	0.64
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.14	0.63
13:o:6:THR:N	36:o:301:HOH:O	2.07	0.63
2:b:36:SER:OG	24:b:617:BCR:H362	1.98	0.63
10:K:15:TYR:OH	20:Z:58:ASN:OD1	2.08	0.63
16:U:54:PRO:O	36:U:201:HOH:O	2.15	0.63
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.79	0.63
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.33	0.63
24:T:101:BCR:H321	24:T:101:BCR:HC8	1.80	0.62
3:C:148:GLY:O	3:C:156:LYS:NZ	2.30	0.62
5:e:30:LEU:HD11	35:e:101:HEC:HBB3	1.82	0.62
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:503:CLA:H61	22:C:513:CLA:H42	1.80	0.62
4:d:126:MET:HE3	4:d:143:ALA:O	1.98	0.62
24:D:404:BCR:H331	24:D:404:BCR:C8	2.30	0.62
22:C:506:CLA:HBC2	24:C:515:BCR:H341	1.80	0.61
16:U:58:VAL:O	16:U:61:VAL:HG22	2.00	0.61
3:C:114:VAL:HG22	33:C:521:STE:H102	1.81	0.61
15:t:29:ILE:HD12	15:t:29:ILE:H	1.64	0.61
22:B:608:CLA:H191	34:D:412:LHG:H142	1.82	0.60
24:b:618:BCR:H331	24:b:618:BCR:C8	2.30	0.60
22:b:601:CLA:H43	7:h:45:ILE:HG22	1.83	0.60
1:A:269:ARG:HD2	4:D:235:PHE:HB2	1.84	0.60
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.84	0.60
2:b:29:LEU:HD23	29:b:619:SQD:C22	2.31	0.60
22:a:411:CLA:O1A	22:a:411:CLA:H43	2.01	0.60
4:d:12:ARG:NH2	4:d:16:ASP:HB3	2.16	0.60
3:c:406:SER:HA	3:c:420:VAL:HG23	1.84	0.59
2:B:193:TYR:O	7:H:65:LEU:HD23	2.01	0.59
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.85	0.59
20:z:38:GLN:O	20:z:42:LEU:HD13	2.03	0.59
16:u:70:ARG:NH1	16:u:73:GLN:OE1	2.35	0.59
22:B:609:CLA:H193	7:H:43:LEU:HD21	1.85	0.59
5:e:26:THR:HB	35:e:101:HEC:HBB2	1.85	0.59
16:u:24:LYS:HB2	16:u:83:THR:HG22	1.84	0.59
13:O:111:ALA:O	36:O:302:HOH:O	2.17	0.59
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.84	0.59
4:D:264:LYS:NZ	36:D:504:HOH:O	2.35	0.59
5:e:8:ARG:NH2	5:e:12:ASP:OD2	2.29	0.59
5:e:20:TRP:O	5:e:24:SER:OG	2.10	0.58
13:o:34:SER:N	36:o:307:HOH:O	2.35	0.58
19:Y:23:THR:CG2	19:Y:27:MET:HE3	2.34	0.58
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.86	0.58
18:X:17:GLY:HA2	33:X:101:STE:H142	1.86	0.58
13:o:149:PRO:HA	13:o:192:LEU:HD12	1.84	0.58
20:Z:54:VAL:O	24:Z:101:BCR:H332	2.04	0.58
2:B:218:LEU:HD12	33:B:601:STE:H21	1.85	0.57
5:e:17:VAL:HG23	9:j:7:ARG:HD3	1.86	0.57
19:y:19:ILE:O	19:y:23:THR:HG22	2.04	0.57
10:K:24:VAL:HG13	19:Y:25:ILE:HD13	1.85	0.57
13:O:189:ARG:NH2	13:O:226:GLY:O	2.36	0.57
5:e:68:ASP:O	5:e:72:ALA:HB2	2.03	0.57
2:b:249:ALA:HB2	22:b:603:CLA:HBC3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.20	0.57
24:Z:101:BCR:H331	24:Z:101:BCR:C8	2.34	0.57
17:v:40:CYS:SG	35:v:201:HEC:CBC	2.91	0.57
28:C:519:LMG:H192	10:K:27:VAL:HG11	1.87	0.57
24:H:101:BCR:H331	24:H:101:BCR:C8	2.34	0.56
2:b:102:VAL:HG11	22:b:605:CLA:H142	1.86	0.56
3:c:413[A]:GLU:OE2	17:v:47:LYS:NZ	2.35	0.56
13:O:5:LEU:HD13	13:O:10:ILE:HD11	1.86	0.56
3:C:406:SER:HA	3:C:420:VAL:HG23	1.86	0.56
22:c:506:CLA:H91	22:c:510:CLA:C17	2.35	0.56
3:C:143:TYR:CE1	22:C:514:CLA:HED3	2.41	0.55
19:Y:22:LEU:HA	19:Y:25:ILE:HG22	1.88	0.55
24:B:620:BCR:H331	24:B:620:BCR:C8	2.36	0.55
13:O:107:THR:HG22	36:O:344:HOH:O	2.05	0.55
17:v:78:ASN:OD1	17:v:96:ARG:NH1	2.38	0.55
2:b:249:ALA:CB	22:b:603:CLA:HBC3	2.36	0.55
3:c:391[A]:ARG:HD2	3:c:395:TYR:CZ	2.42	0.55
2:b:453:PHE:O	2:b:457:VAL:HG23	2.06	0.55
6:f:44:GLN:NE2	36:f:201:HOH:O	2.39	0.55
12:m:5:GLN:NE2	36:m:103:HOH:O	2.38	0.55
15:T:8:PHE:CE2	33:T:102:STE:H183	2.42	0.55
7:h:56:ASP:O	36:h:201:HOH:O	2.18	0.55
17:v:104:MET:HA	17:v:107:LEU:HD22	1.88	0.55
24:y:101:BCR:H321	24:y:101:BCR:HC8	1.88	0.55
24:x:101:BCR:H331	24:x:101:BCR:C8	2.35	0.55
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.08	0.54
2:B:298:LEU:HD23	2:B:402:TYR:CE1	2.42	0.54
22:c:503:CLA:H192	22:c:509:CLA:HBB1	1.89	0.54
3:c:153:ASP:OD2	36:c:603:HOH:O	2.19	0.54
6:f:21:VAL:O	6:f:25:THR:OG1	2.25	0.54
35:F:101:HEC:HHD	35:F:101:HEC:CBC	2.37	0.54
2:b:354:LEU:O	36:b:702:HOH:O	2.19	0.54
22:b:603:CLA:H143	22:b:614:CLA:HMA3	1.88	0.54
24:b:617:BCR:H331	24:b:617:BCR:C8	2.37	0.54
4:d:267:LEU:C	4:d:267:LEU:HD23	2.33	0.54
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.44	0.53
34:d:407:LHG:HC62	11:l:15:THR:HG23	1.90	0.53
5:e:25:ILE:HD12	5:e:25:ILE:N	2.22	0.53
33:d:412:STE:H92	33:h:103:STE:H61	1.91	0.53
7:H:20:LYS:NZ	36:H:201:HOH:O	2.40	0.53
22:B:604:CLA:CMD	22:B:607:CLA:HMB1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:92:SER:O	2:b:96:VAL:HG23	2.07	0.53
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.89	0.53
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.43	0.53
22:A:411:CLA:HMB1	22:A:411:CLA:HBB1	1.91	0.53
12:M:28:GLN:HB3	12:m:27:VAL:HG12	1.90	0.53
2:b:102:VAL:HG21	22:b:605:CLA:H141	1.89	0.53
2:b:352:GLU:C	36:b:716:HOH:O	2.52	0.53
11:l:20:GLY:O	11:l:24:ILE:HD12	2.09	0.53
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.90	0.53
4:D:279:LEU:HD22	23:D:401:PHO:HBC3	1.90	0.53
6:f:24:HIS:O	6:f:28:VAL:HG13	2.09	0.53
29:A:414:SQD:H383	22:b:605:CLA:C9	2.34	0.52
10:K:13:GLU:OE2	10:K:13:GLU:N	2.42	0.52
20:z:1:MET:O	20:z:4:LEU:N	2.41	0.52
22:B:603:CLA:H43	7:H:45:ILE:HG22	1.90	0.52
22:B:605:CLA:C4	22:B:606:CLA:H42	2.40	0.52
2:B:210:ILE:HD13	33:B:627:STE:H172	1.91	0.52
22:C:505:CLA:H143	22:C:509:CLA:H141	1.91	0.52
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.92	0.52
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.52
10:k:24:VAL:O	10:k:27:VAL:HG22	2.10	0.51
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.91	0.51
20:Z:23:VAL:HG22	20:Z:40:ILE:HD12	1.92	0.51
20:Z:51:VAL:O	20:Z:54:VAL:O	2.26	0.51
2:B:36:SER:OG	24:B:619:BCR:H362	2.10	0.51
13:O:27:ARG:HG3	36:O:301:HOH:O	2.10	0.51
13:o:205:ASP:OD1	13:o:207:ARG:NE	2.43	0.51
4:d:16:ASP:OD1	33:d:412:STE:H183	2.10	0.51
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.45	0.51
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.93	0.51
2:b:211:ILE:HG23	33:b:626:STE:H22	1.92	0.51
23:d:401:PHO:HBC2	23:d:401:PHO:HHD	1.93	0.51
1:a:201:GLY:HA3	1:a:286:THR:HB	1.92	0.51
14:R:35:LEU:HG	36:R:101:HOH:O	2.10	0.51
22:b:613:CLA:OBD	22:b:613:CLA:HED3	2.11	0.51
13:o:5:LEU:HA	36:o:301:HOH:O	2.10	0.51
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.11	0.50
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.93	0.50
3:c:391[A]:ARG:NE	36:c:608:HOH:O	2.42	0.50
9:j:19:MET:O	9:j:23:VAL:HG23	2.10	0.50
4:D:272:LEU:C	4:D:272:LEU:HD23	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:58:VAL:O	16:U:61:VAL:CG2	2.59	0.50
1:a:84:PRO:HA	1:a:112:TYR:CG	2.47	0.50
4:d:194:ASN:HA	4:d:295:SER:OG	2.12	0.50
17:v:41:HIS:HA	17:v:45:ILE:O	2.12	0.50
2:B:502:VAL:HG22	2:B:502:VAL:O	2.11	0.50
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.94	0.50
14:r:24:LEU:HD13	14:r:24:LEU:C	2.37	0.50
3:C:150:ASP:OD1	3:C:152:LYS:N	2.37	0.50
7:h:58:VAL:HB	36:h:212:HOH:O	2.12	0.50
13:o:10:ILE:O	13:o:13:THR:HG23	2.12	0.50
1:A:210:LEU:HD23	1:A:214:MET:HG2	1.94	0.50
22:h:101:CLA:H193	22:h:101:CLA:HMB2	1.94	0.50
14:R:33:LYS:O	14:R:35:LEU:N	2.45	0.50
1:a:187[B]:GLN:NE2	1:a:191[B]:ASN:OD1	2.44	0.50
2:b:29:LEU:HD23	29:b:619:SQD:H222	1.92	0.50
22:b:613:CLA:H191	24:b:616:BCR:H331	1.93	0.50
5:e:26:THR:HA	14:r:15:ALA:HB1	1.93	0.50
1:A:11:ALA:O	1:A:16:ARG:NH2	2.45	0.49
1:a:229:GLU:OE1	36:a:1702:HOH:O	2.20	0.49
3:C:137:PRO:HD3	22:C:514:CLA:HED2	1.94	0.49
2:b:221:PRO:CA	22:b:608:CLA:HED3	2.41	0.49
2:B:327:THR:HG21	28:M:101:LMG:H291	1.94	0.49
5:E:68:ASP:O	5:E:72:ALA:HB2	2.12	0.49
2:b:228:ALA:HB2	33:h:103:STE:H62	1.94	0.49
2:b:27:THR:HG22	2:b:107:LEU:HD13	1.94	0.49
24:t:101:BCR:C23	24:t:101:BCR:C38	2.89	0.49
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.48	0.49
12:M:5:GLN:HA	36:M:202:HOH:O	2.12	0.49
1:a:82:VAL:HB	1:a:174[A]:LEU:HB2	1.95	0.49
11:l:22:LEU:HB2	15:t:16:LEU:HD21	1.94	0.49
2:B:221:PRO:HA	22:B:610:CLA:HED3	1.94	0.49
3:C:318:LEU:C	3:C:318:LEU:HD23	2.38	0.49
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.94	0.49
24:D:404:BCR:H372	28:D:406:LMG:H292	1.93	0.49
13:o:110:MET:HE2	13:o:116:ILE:CG1	2.43	0.49
29:D:407:SQD:H341	18:X:23:LEU:HD22	1.93	0.49
12:M:6:LEU:HD12	28:M:101:LMG:HC92	1.95	0.49
17:V:99:ASP:OD1	17:V:99:ASP:N	2.46	0.49
24:D:404:BCR:H392	24:D:404:BCR:H23C	1.95	0.49
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.27	0.49
22:b:605:CLA:HMB1	22:b:605:CLA:HBB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:623:SQD:H382	24:t:101:BCR:C18	2.44	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.95	0.48
24:B:619:BCR:H331	24:B:619:BCR:C8	2.43	0.48
13:O:189:ARG:NH2	36:O:305:HOH:O	2.26	0.48
22:c:508:CLA:C2	22:c:508:CLA:O1A	2.61	0.48
1:A:63[A]:ILE:HB	3:C:335:THR:HG21	1.95	0.48
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.48
20:Z:32:ASP:O	20:Z:36:SER:OG	2.30	0.48
3:c:178:LYS:NZ	3:c:184:GLY:O	2.46	0.48
3:c:391[A]:ARG:NH2	36:c:608:HOH:O	2.45	0.48
7:h:25:TRP:O	7:h:26:GLY:C	2.57	0.48
9:j:9:PRO:CG	9:j:12:ILE:HD12	2.42	0.48
2:B:307:GLU:OE1	13:o:59:LYS:HD3	2.13	0.48
2:B:359:MET:HE2	2:B:363:PHE:O	2.14	0.48
22:C:510:CLA:HMB1	22:C:510:CLA:HBB1	1.96	0.48
4:d:79:SER:HA	4:d:172:SER:HB3	1.96	0.48
35:e:101:HEC:HBB3	35:e:101:HEC:HHC	1.96	0.48
1:A:329[B]:GLU:O	1:A:332[B]:HIS:ND1	2.42	0.48
2:B:291:SER:O	2:B:296:ALA:HB3	2.14	0.48
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.95	0.48
3:c:352:GLY:O	3:c:355[A]:THR:HG22	2.13	0.48
10:K:25:LEU:HD22	24:Y:101:BCR:H332	1.95	0.48
3:c:367:GLU:N	3:c:368:PRO:CD	2.76	0.48
4:d:279:LEU:HD22	23:d:401:PHO:HBC3	1.96	0.48
24:t:101:BCR:H382	24:t:101:BCR:C23	2.43	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.48
14:r:20:VAL:O	14:r:24:LEU:HB2	2.14	0.48
1:a:65[B]:GLU:OE2	4:d:312:GLU:OE1	2.32	0.48
2:b:62:VAL:HB	22:b:604:CLA:HED3	1.95	0.48
13:o:4:THR:HG22	13:o:4:THR:O	2.14	0.48
19:Y:34:MET:O	19:Y:38:LEU:HG	2.14	0.47
22:b:613:CLA:C12	22:b:613:CLA:H91	2.43	0.47
24:t:101:BCR:H23C	24:t:101:BCR:C38	2.42	0.47
3:C:63:TRP:CZ2	3:C:67:MET:HG2	2.50	0.47
4:D:42:TYR:CE1	6:F:25:THR:HG22	2.49	0.47
22:b:613:CLA:H91	22:b:613:CLA:H122	1.95	0.47
10:k:26:PRO:O	10:k:29:PRO:HD2	2.15	0.47
20:z:2:THR:O	20:z:2:THR:HG22	2.14	0.47
2:B:487:SER:OG	2:B:488:PRO:HD2	2.15	0.47
27:a:410:PL9:H302	4:d:45:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:25:MET:HG2	24:b:616:BCR:H23C	1.96	0.47
2:b:287:ARG:HD3	36:b:701:HOH:O	2.15	0.47
2:b:359:MET:HB2	2:b:425:ILE:HD12	1.97	0.47
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.45	0.47
20:z:40:ILE:HG13	20:z:41:PHE:N	2.29	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
1:a:183[B]:MET:HA	22:a:402:CLA:HMD1	1.97	0.47
3:c:315:MET:HE3	3:c:365:TRP:CZ3	2.50	0.47
2:B:67:ALA:HA	2:B:71:VAL:O	2.14	0.47
8:I:6:ILE:HD13	8:I:6:ILE:HA	1.84	0.47
22:c:507:CLA:H93	28:c:525:LMG:C23	2.45	0.47
13:O:133:VAL:C	13:O:134:THR:HG23	2.40	0.46
18:X:38:GLN:NE2	18:X:38:GLN:HA	2.30	0.46
27:A:410:PL9:C11	27:A:410:PL9:H153	2.45	0.46
3:C:50:LEU:O	3:C:54:VAL:HG23	2.15	0.46
14:R:4:ARG:O	14:R:8:VAL:HG23	2.15	0.46
20:Z:61:VAL:O	36:Z:201:HOH:O	2.20	0.46
2:B:371:THR:HG23	2:B:372:ASP:O	2.14	0.46
22:D:403:CLA:H142	18:X:14:LEU:HG	1.97	0.46
5:E:59:GLU:OE1	5:E:59:GLU:HA	2.15	0.46
13:O:81:ILE:HA	13:O:100:GLY:HA3	1.98	0.46
20:Z:47:TRP:CE3	33:Z:102:STE:H142	2.49	0.46
2:B:414:PRO:N	2:B:415:PRO:HD2	2.31	0.46
4:d:98:GLN:HA	33:d:411:STE:H183	1.97	0.46
5:e:23:HIS:HA	5:e:26:THR:OG1	2.16	0.46
16:u:8:GLU:OE1	36:u:201:HOH:O	2.21	0.46
17:v:89:ALA:HB2	36:v:333:HOH:O	2.14	0.46
3:C:95:LEU:HD21	22:C:502:CLA:OBD	2.16	0.46
2:b:125:ASP:OD2	2:b:128:THR:HG23	2.16	0.46
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.98	0.46
20:z:31:GLN:NE2	36:z:102:HOH:O	2.48	0.46
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.96	0.46
24:D:404:BCR:H382	28:D:406:LMG:H171	1.98	0.46
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.46	0.46
1:a:289:GLY:O	1:a:293:MET:HE3	2.14	0.46
22:b:614:CLA:H161	7:h:7:LEU:HD11	1.98	0.46
4:d:342:PRO:O	4:d:345:VAL:HG22	2.16	0.46
33:d:411:STE:H71	18:x:16:SER:HB3	1.97	0.46
13:o:42:ARG:O	13:o:241:ALA:HA	2.15	0.46
1:a:307:ILE:HG22	1:a:313:VAL:HA	1.98	0.46
3:c:213:LEU:HD21	24:c:517:BCR:C20	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HG21	11:L:8:GLN:NE2	2.31	0.46
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.97	0.46
2:B:477:ASP:OD1	2:B:477:ASP:N	2.49	0.46
17:V:63:THR:HG22	17:V:64:PRO:CD	2.45	0.46
7:h:3:ARG:NH1	36:h:205:HOH:O	2.49	0.46
24:A:406:BCR:H24C	24:A:406:BCR:H371	1.76	0.45
1:a:334[A]:ARG:NH2	36:a:1714:HOH:O	2.48	0.45
24:b:617:BCR:H383	24:b:617:BCR:H23C	1.97	0.45
4:d:272:LEU:C	4:d:272:LEU:HD23	2.40	0.45
29:A:414:SQD:C38	22:b:605:CLA:H93	2.38	0.45
36:a:1826:HOH:O	3:c:410:VAL:HB	2.15	0.45
3:c:166:ILE:HG21	22:c:514:CLA:H202	1.99	0.45
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.98	0.45
18:x:6:SER:O	18:x:10:PHE:N	2.38	0.45
13:O:36:GLN:HG3	13:O:37:THR:N	2.30	0.45
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.98	0.45
10:k:25:LEU:N	10:k:26:PRO:CD	2.80	0.45
19:y:34:MET:O	19:y:38:LEU:HG	2.16	0.45
29:A:414:SQD:H341	22:b:615:CLA:H91	1.97	0.45
3:C:167:VAL:HG13	22:C:513:CLA:H93	1.99	0.45
27:a:410:PL9:C25	22:d:402:CLA:H141	2.46	0.45
2:b:290:ALA:O	2:b:293:ALA:HB3	2.15	0.45
2:b:413:ASP:O	2:b:417:VAL:HG23	2.17	0.45
20:z:3:ILE:O	20:z:7:LEU:HD23	2.16	0.45
2:B:141:ILE:O	2:B:145:LEU:HG	2.15	0.45
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.05	0.45
10:K:28:ILE:N	10:K:29:PRO:CD	2.80	0.45
24:T:101:BCR:H15C	24:T:101:BCR:H351	1.84	0.45
22:B:603:CLA:H141	22:B:603:CLA:H161	1.80	0.45
28:B:629:LMG:O10	28:B:629:LMG:C10	2.65	0.45
27:a:410:PL9:H251	22:d:402:CLA:H141	1.98	0.45
4:d:56:THR:HG22	36:e:212:HOH:O	2.16	0.45
6:f:19:ARG:O	6:f:23:VAL:HG13	2.17	0.45
2:B:185:TRP:HB3	22:B:602:CLA:HMA3	1.99	0.45
2:b:67:ALA:HA	2:b:71:VAL:O	2.17	0.45
2:b:81:THR:OG1	2:b:83:GLU:HG3	2.16	0.45
2:b:287:ARG:NH1	36:b:701:HOH:O	2.18	0.45
34:D:412:LHG:O2	36:D:502:HOH:O	2.17	0.44
2:b:91:TRP:CD1	33:b:622:STE:H162	2.53	0.44
2:b:492:GLU:OE1	5:e:3:GLY:N	2.50	0.44
28:b:621:LMG:H391	12:m:13:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.44
4:D:150:ILE:O	4:D:154:VAL:HG13	2.16	0.44
10:K:24:VAL:CG1	19:Y:25:ILE:HD13	2.47	0.44
1:a:229:GLU:CD	1:a:229:GLU:H	2.25	0.44
2:b:29:LEU:HD23	29:b:619:SQD:H223	1.98	0.44
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.04	0.44
22:B:612:CLA:HBB1	22:B:612:CLA:HMB3	1.99	0.44
3:C:135:ARG:O	3:C:135:ARG:HD3	2.17	0.44
3:c:181:PHE:HB3	36:c:621:HOH:O	2.17	0.44
30:A:415:DGD:HD5	2:b:75:TRP:HB3	1.98	0.44
6:F:31:ILE:HG13	35:F:101:HEC:HMC1	2.00	0.44
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.52	0.44
3:c:391[B]:ARG:NH2	36:c:614:HOH:O	2.49	0.44
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	2.00	0.44
3:C:344:SER:O	13:O:75:THR:HG22	2.18	0.44
4:D:267:LEU:C	4:D:267:LEU:HD23	2.43	0.44
14:R:10:LEU:O	14:R:14:LEU:HG	2.17	0.44
3:c:93:ALA:HB1	3:c:99:VAL:HG21	1.99	0.44
24:c:517:BCR:C8	24:c:517:BCR:H331	2.47	0.44
5:e:8:ARG:HG2	5:e:13:ILE:HG13	1.98	0.44
20:z:21:ILE:O	20:z:25:VAL:HG23	2.18	0.44
3:C:141:GLU:H	3:C:141:GLU:CD	2.26	0.44
22:b:614:CLA:HHC	22:b:614:CLA:HBB1	1.99	0.44
18:x:3:ILE:N	18:x:3:ILE:HD12	2.33	0.44
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.53	0.44
29:A:413:SQD:H291	34:D:409:LHG:H151	2.00	0.44
1:a:249:VAL:HG12	2:b:491:VAL:HG21	2.00	0.44
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.00	0.44
4:d:241:GLU:CD	4:d:241:GLU:H	2.24	0.44
14:r:24:LEU:N	14:r:25:PRO:HD2	2.33	0.44
19:y:41:VAL:C	19:y:43:ARG:H	2.25	0.44
5:E:22[A]:ILE:HD12	5:E:23:HIS:CE1	2.52	0.44
11:L:24:ILE:CD1	12:M:18:PRO:HB2	2.48	0.44
15:T:8:PHE:CD2	33:T:102:STE:H183	2.53	0.44
8:i:7:THR:O	8:i:11:VAL:HG23	2.18	0.44
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.00	0.43
1:a:321:ILE:HD11	4:d:179:PHE:HB2	1.99	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.43
5:E:26:THR:HA	14:R:15:ALA:HB1	2.00	0.43
1:a:296:ASN:HB3	3:c:401:LEU:HA	1.99	0.43
2:b:130:GLU:HA	2:b:130:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:284:ILE:O	2:b:288:VAL:HG23	2.17	0.43
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.00	0.43
28:B:629:LMG:O10	28:B:629:LMG:C11	2.66	0.43
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	2.00	0.43
1:a:219:VAL:O	1:a:223:LEU:HD13	2.19	0.43
29:B:623:SQD:H383	29:B:623:SQD:H352	1.83	0.43
24:T:101:BCR:H24C	24:T:101:BCR:H371	1.84	0.43
5:e:8:ARG:NH1	36:e:202:HOH:O	2.51	0.43
4:D:103:ARG:O	4:D:107:LEU:HG	2.19	0.43
24:H:101:BCR:H15C	24:H:101:BCR:H351	1.93	0.43
3:c:318:LEU:HD21	3:c:380:ILE:CG2	2.49	0.43
1:A:40:THR:O	1:A:118:HIS:HB3	2.17	0.43
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.49	0.43
1:A:334[B]:ARG:HD3	4:D:320:LEU:HD13	2.01	0.43
27:A:410:PL9:C25	22:D:402:CLA:H141	2.48	0.43
30:C:517:DGD:O1A	30:C:517:DGD:HA41	2.18	0.43
4:D:209:LEU:HD23	4:D:209:LEU:C	2.43	0.43
1:a:157:VAL:HB	1:a:172[B]:MET:HB2	2.01	0.43
1:A:308:ASP:OD1	1:A:308:ASP:C	2.62	0.43
1:A:332[B]:HIS:O	1:A:333[B]:GLU:C	2.61	0.43
2:B:347:ARG:HA	2:B:352:GLU:O	2.19	0.43
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.52	0.43
1:a:183[B]:MET:HE3	22:a:411:CLA:HAC1	2.01	0.43
1:a:215:HIS:ND1	27:a:410:PL9:O1	2.41	0.43
1:A:270:SER:HB3	29:A:413:SQD:O49	2.18	0.43
13:O:189:ARG:NE	36:O:305:HOH:O	2.36	0.43
1:a:87:ASN:OD1	3:c:357[A]:ARG:NE	2.45	0.43
1:A:189[B]:GLU:CD	32:A:417[B]:OEY:O6	2.61	0.43
2:B:91:TRP:HE1	33:B:621:STE:H32	1.84	0.43
22:C:511:CLA:HBB1	22:C:511:CLA:HMB3	2.00	0.43
22:b:614:CLA:H2	22:b:615:CLA:HBB2	2.01	0.43
24:b:616:BCR:H11C	24:b:616:BCR:H341	1.92	0.43
16:u:32:ILE:HG13	16:u:46:ALA:HB1	2.00	0.43
32:A:417[B]:OEY:O6	32:A:417[B]:OEY:O1	2.36	0.43
3:C:95:LEU:HD13	22:C:503:CLA:H143	2.01	0.43
3:C:128:GLY:HA3	22:C:514:CLA:C3C	2.49	0.43
5:E:30:LEU:HD23	14:R:12:VAL:HG22	2.01	0.43
33:T:102:STE:H162	22:b:613:CLA:H202	2.01	0.43
1:A:301:ASN:OD1	1:A:301:ASN:C	2.62	0.42
22:A:411:CLA:HED2	4:D:198:MET:SD	2.59	0.42
22:B:603:CLA:C4	7:H:45:ILE:HG22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:15:LEU:HD12	20:Z:50:LEU:HD23	2.00	0.42
4:d:49:LEU:HD13	24:d:404:BCR:C15	2.49	0.42
22:B:609:CLA:C19	7:H:43:LEU:HD21	2.49	0.42
5:E:53:ASP:O	17:V:1:ALA:N	2.52	0.42
35:e:101:HEC:HAA1	6:f:15:ILE:HG23	2.00	0.42
2:B:37:MET:O	2:B:41:GLU:HG3	2.18	0.42
4:D:42:TYR:CE1	6:F:25:THR:CG2	3.03	0.42
1:a:162[B]:PRO:HB3	1:a:168[B]:PHE:HA	2.02	0.42
13:o:90:ASP:OD1	13:o:90:ASP:C	2.62	0.42
24:A:406:BCR:H351	24:A:406:BCR:H15C	1.77	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.42
20:Z:61:VAL:O	20:Z:61:VAL:HG23	2.18	0.42
22:b:612:CLA:H203	34:d:406:LHG:H212	2.02	0.42
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.54	0.42
13:o:10:ILE:O	13:o:11:VAL:C	2.62	0.42
22:A:403:CLA:H91	28:D:406:LMG:C25	2.50	0.42
22:B:615:CLA:H141	22:B:615:CLA:H161	1.84	0.42
16:U:70:ARG:NH2	36:U:203:HOH:O	2.32	0.42
1:a:334[A]:ARG:HG3	13:o:157:LEU:HB2	2.01	0.42
2:b:121:GLU:OE1	7:h:12:ARG:NH1	2.50	0.42
22:b:601:CLA:C4	7:h:45:ILE:HG22	2.49	0.42
22:b:606:CLA:H191	34:d:406:LHG:H141	2.00	0.42
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.02	0.42
22:B:609:CLA:C1A	22:B:609:CLA:CGA	2.98	0.42
22:B:609:CLA:H43	22:B:610:CLA:H101	2.02	0.42
28:C:519:LMG:C19	10:K:27:VAL:HG11	2.48	0.42
2:b:91:TRP:HE1	33:b:622:STE:H141	1.85	0.42
7:h:29:PRO:O	7:h:33:VAL:HG23	2.20	0.42
22:C:513:CLA:H122	22:C:513:CLA:H91	2.02	0.42
10:K:40:GLN:HB3	10:K:45:PHE:CD1	2.55	0.42
11:L:7:ARG:HD3	36:L:203:HOH:O	2.20	0.42
13:O:15:LEU:HA	13:O:18:LYS:HD2	2.02	0.42
16:U:39:ARG:HG2	36:U:231:HOH:O	2.20	0.42
20:Z:36:SER:O	20:Z:37:LYS:C	2.63	0.42
4:d:62:GLY:HA2	5:e:63:ILE:HG21	2.02	0.42
35:e:101:HEC:CBB	35:e:101:HEC:HHC	2.49	0.42
16:u:24:LYS:HB2	16:u:83:THR:CG2	2.49	0.42
3:C:42:LEU:HD21	22:C:512:CLA:H2A	2.01	0.42
22:D:402:CLA:H192	28:D:406:LMG:C25	2.49	0.42
1:A:235:TYR:OH	11:L:11:GLU:OE1	2.33	0.42
1:A:322:ASN:OD1	36:A:501:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:PHE:HD1	2:B:505:ARG:NH1	2.18	0.42
17:V:95:LEU:HD11	17:V:112:LEU:HD11	2.01	0.42
1:a:193:LEU:HD23	1:a:193:LEU:HA	1.88	0.42
17:v:12:LEU:HD23	17:v:17:LYS:HD3	2.01	0.42
20:z:15:LEU:O	20:z:19:MET:HG2	2.20	0.42
22:B:606:CLA:H41	22:B:613:CLA:H161	2.02	0.42
3:C:338:GLY:HA3	3:C:341:LEU:O	2.19	0.42
28:D:406:LMG:H112	36:D:515:HOH:O	2.19	0.42
20:Z:38:GLN:O	20:Z:42:LEU:HG	2.19	0.42
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.01	0.42
3:c:315:MET:CE	3:c:365:TRP:HZ3	2.33	0.42
27:A:410:PL9:H33	4:D:42:TYR:HB2	2.02	0.41
3:C:126:GLY:O	3:C:130:VAL:HG13	2.20	0.41
3:C:451:ALA:HA	3:C:456:GLU:OE2	2.20	0.41
17:V:81:THR:HG23	17:V:86:GLN:HG2	2.01	0.41
27:a:410:PL9:H452	4:d:30:VAL:CG1	2.50	0.41
4:d:68:LEU:HD23	5:e:49:THR:HG21	2.02	0.41
22:A:411:CLA:C4A	22:A:411:CLA:HBA1	2.50	0.41
13:O:70:LEU:CD1	13:O:106:VAL:HG13	2.50	0.41
20:Z:27:TYR:HE1	20:Z:33:TRP:CH2	2.38	0.41
3:c:109:PHE:N	3:c:110:PRO:CD	2.83	0.41
3:c:163:PHE:O	3:c:167:VAL:HG23	2.20	0.41
22:c:506:CLA:H62	22:c:506:CLA:H92	1.86	0.41
1:A:307:ILE:HG22	1:A:313:VAL:HA	2.02	0.41
3:C:60:ILE:HG22	22:C:504:CLA:HMD3	2.03	0.41
24:D:404:BCR:H20C	24:D:404:BCR:H361	1.71	0.41
13:O:6:THR:HG23	13:O:8:ASP:H	1.86	0.41
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.02	0.41
3:c:318:LEU:HD21	3:c:380:ILE:HG23	2.03	0.41
9:j:26:GLY:HA2	33:j:101:STE:H71	2.02	0.41
1:A:153:SER:HB3	22:A:402:CLA:HED1	2.02	0.41
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.56	0.41
22:B:616:CLA:H201	22:B:616:CLA:C1B	2.50	0.41
7:H:17:GLU:OE2	7:H:20:LYS:HE2	2.20	0.41
22:b:605:CLA:HBB1	22:b:605:CLA:CMB	2.50	0.41
10:k:28:ILE:HA	10:k:31:LEU:HD12	2.01	0.41
22:B:607:CLA:H72	24:B:620:BCR:H311	2.03	0.41
12:M:5:GLN:C	36:M:202:HOH:O	2.63	0.41
22:b:613:CLA:H93	22:b:613:CLA:H61	1.86	0.41
11:l:7:ARG:NH1	33:l:102:STE:C1	2.84	0.41
34:B:622:LHG:H292	34:D:412:LHG:H161	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:53:ALA:HB1	16:U:54:PRO:HA	2.03	0.41
27:a:410:PL9:H351	27:a:410:PL9:H371	1.87	0.41
2:b:159:THR:O	2:b:180:PRO:HB3	2.20	0.41
22:b:613:CLA:H41	22:b:613:CLA:H62	1.77	0.41
3:c:48:LYS:HG3	3:c:138:GLU:HA	2.02	0.41
3:c:118:HIS:CE1	33:c:523:STE:H142	2.56	0.41
4:d:52:THR:O	4:d:66:SER:HA	2.21	0.41
17:v:69:ILE:HD12	17:v:69:ILE:N	2.36	0.41
5:E:22[A]:ILE:HG13	14:R:19:ALA:CB	2.51	0.41
14:R:34:LEU:O	14:R:35:LEU:O	2.39	0.41
4:d:93:TRP:CZ3	33:d:411:STE:H62	2.56	0.41
6:f:37:ILE:HG22	9:j:28:PHE:CE1	2.55	0.41
3:C:337:LEU:HD23	13:O:105:PRO:CG	2.51	0.41
2:b:380:ASP:OD1	4:d:344:GLU:OE1	2.38	0.41
2:B:354:LEU:HD22	2:B:378:LYS:HB2	2.03	0.41
22:B:602:CLA:H62	22:B:602:CLA:H93	1.87	0.41
22:B:608:CLA:H142	22:B:614:CLA:H172	2.03	0.41
3:C:139:THR:HB	3:C:141:GLU:OE1	2.21	0.41
4:D:203:GLY:HA3	4:D:278:GLY:HA3	2.03	0.41
7:H:25:TRP:O	7:H:26:GLY:C	2.63	0.41
35:V:201:HEC:CMC	35:V:201:HEC:HBC3	2.51	0.41
24:Z:101:BCR:H20C	24:Z:101:BCR:H361	1.92	0.41
1:a:215:HIS:HA	27:a:410:PL9:O1	2.20	0.41
3:c:315:MET:HE3	3:c:365:TRP:HZ3	1.85	0.41
20:z:15:LEU:HD21	20:z:46:LEU:HB3	2.02	0.41
2:B:247:PHE:HE1	22:B:604:CLA:H41	1.86	0.41
4:D:136:VAL:O	4:D:136:VAL:CG1	2.68	0.41
22:D:403:CLA:H42	7:H:43:LEU:HD11	2.02	0.41
17:V:25:GLN:HG2	36:V:340:HOH:O	2.21	0.41
2:b:135:LEU:N	2:b:136:PRO:CD	2.84	0.41
24:b:617:BCR:H331	24:b:617:BCR:HC8	2.02	0.41
4:d:61:HIS:CE1	4:d:168:PHE:CE1	3.09	0.41
14:r:6:LEU:O	14:r:10:LEU:HD23	2.21	0.41
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.03	0.40
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.40
24:B:618:BCR:H24C	24:B:618:BCR:H371	1.90	0.40
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.40
12:M:20:VAL:HG13	12:m:20:VAL:HG13	2.03	0.40
20:Z:49:ALA:O	20:Z:53:VAL:HG23	2.22	0.40
1:a:237:TYR:HB2	1:a:245:THR:HG21	2.02	0.40
8:i:34:ARG:C	8:i:36:ASP:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:76:MET:HE1	17:v:115:ILE:HD12	2.03	0.40
1:A:334[B]:ARG:HD3	36:A:594:HOH:O	2.21	0.40
22:B:605:CLA:H142	33:B:621:STE:H142	2.03	0.40
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.86	0.40
13:O:54:GLU:O	13:O:63:ALA:HB3	2.21	0.40
23:a:404:PHO:ND	23:a:404:PHO:NC	2.69	0.40
2:b:492:GLU:OE2	2:b:495:PHE:CD1	2.74	0.40
4:D:58:TRP:CH2	5:E:63:ILE:HD12	2.57	0.40
24:H:101:BCR:H20C	24:H:101:BCR:H361	1.95	0.40
19:Y:34:MET:HE2	19:Y:38:LEU:CD2	2.50	0.40
24:B:619:BCR:H361	24:B:619:BCR:H20C	1.82	0.40
3:C:461:ARG:HG2	4:D:223:PHE:CD1	2.56	0.40
13:O:5:LEU:CD1	13:O:10:ILE:HD11	2.50	0.40
20:Z:44:SER:O	20:Z:48:ILE:HG13	2.20	0.40
24:b:617:BCR:H15C	24:b:617:BCR:H351	1.84	0.40
1:A:60[B]:ILE:HB	1:A:83:VAL:CG1	2.52	0.40
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.04	0.40
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.03	0.40
1:a:93:PHE:HZ	22:a:405:CLA:HAA1	1.86	0.40
3:c:146:PHE:O	3:c:156:LYS:NZ	2.42	0.40

There are no symmetry-related clashes.

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	391/344 (114%)	385 (98%)	6 (2%)	0	100	100
1	a	391/344 (114%)	381 (97%)	10 (3%)	0	100	100
2	B	508/510 (100%)	501 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	450/461 (98%)	440 (98%)	8 (2%)	2 (0%)	30 28
3	c	459/461 (100%)	445 (97%)	13 (3%)	1 (0%)	43 44
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100 100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100 100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100 100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100 100
6	F	32/45 (71%)	32 (100%)	0	0	100 100
6	f	32/45 (71%)	32 (100%)	0	0	100 100
7	H	63/66 (96%)	55 (87%)	8 (13%)	0	100 100
7	h	61/66 (92%)	56 (92%)	4 (7%)	1 (2%)	7 4
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100 100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100 100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100 100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100 100
10	K	35/46 (76%)	34 (97%)	0	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%)	29 (97%)	1 (3%)	0	100 100
13	O	243/272 (89%)	227 (93%)	14 (6%)	2 (1%)	16 12
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30 28
14	R	32/41 (78%)	29 (91%)	2 (6%)	1 (3%)	3 1
14	r	27/41 (66%)	27 (100%)	0	0	100 100
15	T	28/32 (88%)	28 (100%)	0	0	100 100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100 100
16	U	95/134 (71%)	93 (98%)	2 (2%)	0	100 100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100 100
17	V	135/163 (83%)	127 (94%)	7 (5%)	1 (1%)	18 15
17	v	135/163 (83%)	128 (95%)	7 (5%)	0	100 100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	x	37/41 (90%)	35 (95%)	2 (5%)	0	100 100
19	Y	25/46 (54%)	22 (88%)	2 (8%)	1 (4%)	2 0
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2 1
20	Z	60/62 (97%)	55 (92%)	5 (8%)	0	100 100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	7 3
All	All	5372/5700 (94%)	5201 (97%)	158 (3%)	13 (0%)	43 44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
17	V	64	PRO
3	c	416	SER
14	R	34	LEU
13	O	62	GLU
19	Y	43	ARG
19	y	41	VAL
20	z	61	VAL
10	K	16	ALA
3	C	144	SER
7	h	26	GLY
13	o	56	PRO

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	320/280 (114%)	313 (98%)	7 (2%)	45 53
1	a	319/280 (114%)	303 (95%)	16 (5%)	22 22
2	B	408/407 (100%)	399 (98%)	9 (2%)	45 53
2	b	402/407 (99%)	386 (96%)	16 (4%)	28 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	353/362 (98%)	345 (98%)	8 (2%)	44 51
3	c	361/362 (100%)	347 (96%)	14 (4%)	28 31
4	D	277/283 (98%)	275 (99%)	2 (1%)	76 83
4	d	278/283 (98%)	266 (96%)	12 (4%)	26 27
5	E	72/73 (99%)	66 (92%)	6 (8%)	10 8
5	e	71/73 (97%)	69 (97%)	2 (3%)	38 43
6	F	28/39 (72%)	28 (100%)	0	100 100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13 11
7	H	54/55 (98%)	53 (98%)	1 (2%)	50 58
7	h	53/55 (96%)	50 (94%)	3 (6%)	18 17
8	I	32/34 (94%)	29 (91%)	3 (9%)	8 6
8	i	32/34 (94%)	31 (97%)	1 (3%)	35 39
9	J	24/28 (86%)	23 (96%)	1 (4%)	26 28
9	j	24/28 (86%)	23 (96%)	1 (4%)	26 28
10	K	30/37 (81%)	29 (97%)	1 (3%)	33 37
10	k	30/37 (81%)	25 (83%)	5 (17%)	2 1
11	L	35/35 (100%)	34 (97%)	1 (3%)	37 42
11	l	34/35 (97%)	31 (91%)	3 (9%)	9 7
12	M	28/32 (88%)	26 (93%)	2 (7%)	13 11
12	m	28/32 (88%)	27 (96%)	1 (4%)	31 34
13	O	206/228 (90%)	194 (94%)	12 (6%)	18 16
13	o	207/228 (91%)	198 (96%)	9 (4%)	26 27
14	R	28/33 (85%)	20 (71%)	8 (29%)	0 0
14	r	23/33 (70%)	17 (74%)	6 (26%)	0 0
15	T	26/28 (93%)	25 (96%)	1 (4%)	29 32
15	t	25/28 (89%)	24 (96%)	1 (4%)	28 29
16	U	84/112 (75%)	79 (94%)	5 (6%)	17 15
16	u	84/112 (75%)	82 (98%)	2 (2%)	43 49
17	V	117/138 (85%)	113 (97%)	4 (3%)	32 35
17	v	117/138 (85%)	111 (95%)	6 (5%)	21 21
18	X	31/34 (91%)	29 (94%)	2 (6%)	15 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	x	31/34 (91%)	28 (90%)	3 (10%)	8 5
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6 4
19	y	22/37 (60%)	19 (86%)	3 (14%)	3 2
20	Z	52/52 (100%)	44 (85%)	8 (15%)	2 1
20	z	51/52 (98%)	44 (86%)	7 (14%)	3 2
All	All	4444/4654 (96%)	4248 (96%)	196 (4%)	24 26

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	229	GLU
1	A	243	GLU
1	A	270	SER
1	A	286	THR
2	B	76	SER
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	130	GLU
2	B	161	LEU
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	141	GLU
3	C	200	THR
3	C	215	LYS
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	154	VAL
4	D	345	VAL
5	E	4	THR
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE

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Mol	Chain	Res	Type
5	E	32	ILE
5	E	81	GLU
7	H	41	PHE
8	I	4	LEU
8	I	6	ILE
8	I	36	ASP
9	J	8	ILE
10	K	19	ASP
11	L	10	VAL
12	M	16	LEU
12	M	25	LEU
13	O	4	THR
13	O	6	THR
13	O	64	GLU
13	O	78	LEU
13	O	84	GLU
13	O	89	SER
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	145	GLU
13	O	198	SER
13	O	214	THR
14	R	6	LEU
14	R	10	LEU
14	R	20	VAL
14	R	21	ARG
14	R	24	LEU
14	R	29	LYS
14	R	32	GLN
14	R	35	LEU
15	T	25	GLU
16	U	10	VAL
16	U	39	ARG
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	31	ARG
17	V	86	GLN
18	X	3	ILE

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Mol	Chain	Res	Type
18	X	15	LEU
19	Y	21	GLN
19	Y	34	MET
20	Z	2	THR
20	Z	6	GLN
20	Z	15	LEU
20	Z	17	PHE
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
20	Z	61	VAL
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	134	SER
1	a	159	LEU
1	a	200	LEU
1	a	210	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	231	GLU
1	a	245	THR
1	a	266	ASN
1	a	271	LEU
1	a	288	LEU
2	b	74	SER
2	b	76	SER
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	240	SER
2	b	362	PHE
2	b	389	LYS
2	b	433	ASP
2	b	485	GLU
2	b	492	GLU
2	b	495	PHE
2	b	505	ARG

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Mol	Chain	Res	Type
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	72	LEU
3	c	99	VAL
3	c	104	GLU
3	c	105	VAL
3	c	124	VAL
3	c	125	LEU
3	c	144	SER
3	c	165	LEU
3	c	240	ILE
3	c	354[A]	GLU
3	c	354[B]	GLU
3	c	396	MET
4	d	18	LEU
4	d	90	LEU
4	d	144	ILE
4	d	150	ILE
4	d	182	LEU
4	d	230	SER
4	d	233	ARG
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	307	GLU
4	d	321	LEU
5	e	65	LEU
5	e	83	LEU
6	f	23	VAL
6	f	28	VAL
7	h	3	ARG
7	h	7	LEU
7	h	27	THR
8	i	33	LYS
9	j	21	VAL
10	k	10	LYS
10	k	19	ASP
10	k	22	VAL
10	k	30	VAL
10	k	35	LEU
11	l	7	ARG

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Mol	Chain	Res	Type
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	10	ILE
13	o	49	THR
13	o	53	LYS
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	199	LEU
13	o	234	LYS
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
14	r	14	LEU
14	r	30	GLN
15	t	29	ILE
16	u	15	GLU
16	u	61	VAL
17	v	42	VAL
17	v	52	LEU
17	v	90	GLU
17	v	107	LEU
17	v	110	LYS
17	v	113	VAL
18	x	2	THR
18	x	6	SER
18	x	15	LEU
19	y	19	ILE
19	y	45	ASN
19	y	46	LEU
20	z	3	ILE
20	z	14	ILE
20	z	20	VAL
20	z	31	GLN
20	z	32	ASP
20	z	46	LEU
20	z	56	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	394	GLN
2	B	409	GLN
3	C	327	ASN
3	C	385	GLN
4	D	61	HIS
4	D	301	GLN
11	L	8	GLN
12	M	32	GLN
13	O	88	ASN
13	O	132	ASN
13	O	155	ASN
14	R	22	ASN
16	U	37	GLN
16	U	78	ASN
17	V	86	GLN
18	X	38	GLN
19	Y	45	ASN
20	Z	6	GLN
1	a	234	ASN
1	a	266	ASN
2	b	179	GLN
2	b	409	GLN
3	c	28	GLN
3	c	201	ASN
3	c	311	GLN
3	c	322	GLN
3	c	378	ASN
4	d	350	ASN
7	h	59	ASN
13	o	61	GLN
13	o	132	ASN
13	o	155	ASN
18	x	33	GLN
20	z	31	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	1.18	1 (12%)	8,9,11	1.31	1 (12%)
12	FME	m	1	12	8,9,10	1.07	1 (12%)	8,9,11	1.30	1 (12%)
8	FME	i	1	8	8,9,10	0.91	0	8,9,11	1.44	2 (25%)
15	FME	t	1	15	8,9,10	1.22	1 (12%)	8,9,11	1.08	0
15	FME	T	1	15	8,9,10	1.01	1 (12%)	8,9,11	1.37	1 (12%)
12	FME	M	1	12	8,9,10	0.89	0	8,9,11	1.02	0

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.07	1.42	1.46
8	I	1	FME	CA-N	-2.92	1.42	1.46
12	m	1	FME	CA-N	-2.32	1.43	1.46
15	T	1	FME	CA-N	-2.11	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	CA-N-CN	-2.75	118.60	122.82
15	T	1	FME	O1-CN-N	-2.68	118.39	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	CA-N-CN	-2.18	119.46	122.82
8	i	1	FME	C-CA-N	2.03	113.41	109.50
12	m	1	FME	CA-N-CN	-2.02	119.72	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	c	511	-	69,73,73	1.42	7 (10%)	82,113,113	1.43	9 (10%)
22	CLA	a	405	-	69,73,73	1.49	9 (13%)	82,113,113	1.38	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	610	-	69,73,73	1.14	5 (7%)	82,113,113	1.41	12 (14%)
22	CLA	c	504	-	69,73,73	1.33	8 (11%)	82,113,113	1.39	7 (8%)
22	CLA	B	607	-	69,73,73	1.35	7 (10%)	82,113,113	1.30	8 (9%)
28	LMG	d	409	-	44,44,55	1.02	4 (9%)	52,52,63	1.41	7 (13%)
34	LHG	D	412	-	48,48,48	0.97	2 (4%)	51,54,54	1.45	8 (15%)
29	SQD	b	619	-	47,49,54	0.95	2 (4%)	57,60,65	2.07	14 (24%)
33	STE	I	101	-	14,14,19	0.51	0	13,13,19	0.62	0
22	CLA	c	506	36	64,68,73	1.21	6 (9%)	76,107,113	1.38	14 (18%)
22	CLA	b	603	-	69,73,73	1.13	8 (11%)	82,113,113	1.57	15 (18%)
30	DGD	c	520	-	63,63,67	1.07	4 (6%)	77,77,81	1.42	10 (12%)
33	STE	c	523	-	19,19,19	0.82	0	19,19,19	0.82	0
34	LHG	d	407	-	48,48,48	1.07	3 (6%)	51,54,54	1.26	6 (11%)
33	STE	E	102	-	11,11,19	0.87	0	11,11,19	1.24	1 (9%)
33	STE	d	412	-	19,19,19	0.64	0	19,19,19	1.02	1 (5%)
24	BCR	T	101	-	41,41,41	1.09	4 (9%)	56,56,56	1.37	6 (10%)
33	STE	B	625	-	11,11,19	0.97	1 (9%)	11,11,19	1.06	0
24	BCR	Y	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.28	8 (14%)
22	CLA	b	606	36	69,73,73	1.21	7 (10%)	82,113,113	1.45	8 (9%)
22	CLA	b	611	-	69,73,73	1.08	8 (11%)	82,113,113	1.29	8 (9%)
22	CLA	b	608	-	69,73,73	1.23	6 (8%)	82,113,113	1.28	12 (14%)
28	LMG	c	524	-	48,48,55	1.13	3 (6%)	56,56,63	1.33	7 (12%)
22	CLA	C	513	-	69,73,73	1.25	11 (15%)	82,113,113	1.33	12 (14%)
34	LHG	d	406	-	48,48,48	1.04	3 (6%)	51,54,54	1.39	6 (11%)
22	CLA	C	507	-	69,73,73	1.40	11 (15%)	82,113,113	1.17	5 (6%)
22	CLA	B	611	36	69,73,73	1.28	8 (11%)	82,113,113	1.65	12 (14%)
24	BCR	C	515	-	41,41,41	1.32	4 (9%)	56,56,56	1.32	8 (14%)
34	LHG	D	409	-	46,46,48	1.01	2 (4%)	49,52,54	1.36	2 (4%)
22	CLA	C	510	-	69,73,73	1.14	7 (10%)	82,113,113	1.49	7 (8%)
22	CLA	B	608	36	69,73,73	1.32	9 (13%)	82,113,113	1.42	8 (9%)
22	CLA	C	502	-	69,73,73	1.43	10 (14%)	82,113,113	1.43	7 (8%)
24	BCR	y	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.12	3 (5%)
24	BCR	a	406	-	41,41,41	1.09	3 (7%)	56,56,56	1.45	8 (14%)
33	STE	T	102	-	14,14,19	0.48	0	13,13,19	0.68	0
22	CLA	B	617	-	64,68,73	1.33	6 (9%)	76,107,113	1.73	16 (21%)
33	STE	b	625	-	19,19,19	0.81	0	19,19,19	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	613	-	69,73,73	1.15	7 (10%)	82,113,113	1.43	8 (9%)
33	STE	M	103	-	9,9,19	0.45	0	8,8,19	0.59	0
33	STE	j	101	-	11,11,19	0.86	0	11,11,19	1.34	1 (9%)
28	LMG	B	629	-	55,55,55	1.48	6 (10%)	63,63,63	1.48	7 (11%)
24	BCR	K	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	5 (8%)
34	LHG	B	622	-	48,48,48	1.06	2 (4%)	51,54,54	1.10	2 (3%)
28	LMG	D	411	-	26,26,55	0.76	1 (3%)	26,26,63	1.20	3 (11%)
22	CLA	d	403	-	69,73,73	1.52	11 (15%)	82,113,113	1.31	9 (10%)
22	CLA	A	402	-	69,73,73	1.23	7 (10%)	82,113,113	1.40	11 (13%)
33	STE	a	414	-	9,9,19	0.54	0	8,8,19	0.43	0
33	STE	a	415	-	11,11,19	0.83	0	11,11,19	1.13	1 (9%)
22	CLA	c	507	-	69,73,73	1.20	7 (10%)	82,113,113	1.15	6 (7%)
22	CLA	b	614	-	69,73,73	1.73	8 (11%)	82,113,113	1.52	12 (14%)
22	CLA	C	512	3	69,73,73	1.64	11 (15%)	82,113,113	1.34	6 (7%)
28	LMG	D	406	-	51,51,55	0.89	3 (5%)	59,59,63	1.48	9 (15%)
22	CLA	C	509	-	69,73,73	1.30	10 (14%)	82,113,113	1.60	12 (14%)
22	CLA	c	505	-	69,73,73	1.36	7 (10%)	82,113,113	1.43	8 (9%)
22	CLA	c	510	-	68,72,73	1.39	9 (13%)	80,111,113	1.36	10 (12%)
33	STE	B	621	-	16,16,19	0.63	0	16,16,19	1.31	2 (12%)
22	CLA	B	614	-	69,73,73	1.47	9 (13%)	82,113,113	1.33	13 (15%)
22	CLA	c	514	-	69,73,73	1.26	10 (14%)	82,113,113	1.46	7 (8%)
24	BCR	c	518	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	8 (14%)
29	SQD	B	623	-	52,54,54	0.98	3 (5%)	62,65,65	1.79	10 (16%)
24	BCR	c	517	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	6 (10%)
22	CLA	c	509	36	69,73,73	1.22	7 (10%)	82,113,113	1.35	8 (9%)
22	CLA	b	609	36	69,73,73	1.45	5 (7%)	82,113,113	1.55	14 (17%)
30	DGD	c	519	-	63,63,67	1.37	8 (12%)	77,77,81	1.43	15 (19%)
22	CLA	C	508	36	69,73,73	1.42	7 (10%)	82,113,113	1.61	13 (15%)
34	LHG	E	101	-	48,48,48	0.97	4 (8%)	51,54,54	1.21	5 (9%)
22	CLA	b	601	-	69,73,73	1.11	8 (11%)	82,113,113	1.54	7 (8%)
30	DGD	c	521	-	63,63,67	1.09	4 (6%)	77,77,81	1.38	10 (12%)
28	LMG	c	525	-	49,49,55	1.03	5 (10%)	57,57,63	1.34	5 (8%)
33	STE	d	410	-	16,16,19	0.57	0	16,16,19	1.38	2 (12%)
22	CLA	A	411	36	69,73,73	1.29	9 (13%)	82,113,113	1.21	7 (8%)
29	SQD	a	413	-	35,35,54	1.27	2 (5%)	37,37,65	1.51	6 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	STE	C	522	-	11,11,19	0.74	0	11,11,19	1.31	2 (18%)
22	CLA	c	515	-	69,73,73	1.34	10 (14%)	82,113,113	1.04	7 (8%)
22	CLA	C	503	-	69,73,73	1.24	5 (7%)	82,113,113	1.56	11 (13%)
29	SQD	f	101	-	39,41,54	1.10	5 (12%)	49,52,65	1.91	12 (24%)
24	BCR	H	101	-	41,41,41	1.12	1 (2%)	56,56,56	1.49	10 (17%)
22	CLA	b	612	-	69,73,73	1.21	9 (13%)	82,113,113	1.45	11 (13%)
33	STE	l	102	-	17,17,19	0.37	0	16,16,19	0.87	0
23	PHO	d	401	-	58,69,69	1.97	11 (18%)	55,99,99	1.51	10 (18%)
24	BCR	c	516	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	8 (14%)
26	BCT	A	409	21	3,3,3	1.12	0	2,3,3	3.38	2 (100%)
35	HEC	e	101	5,6	46,50,50	1.86	9 (19%)	58,82,82	2.06	10 (17%)
22	CLA	B	610	-	69,73,73	1.25	10 (14%)	82,113,113	1.35	10 (12%)
33	STE	B	624	-	13,13,19	0.68	0	13,13,19	1.39	2 (15%)
30	DGD	C	516	-	63,63,67	1.17	6 (9%)	77,77,81	1.41	17 (22%)
33	STE	B	626	-	17,17,19	0.67	0	17,17,19	1.08	0
22	CLA	c	512	-	69,73,73	1.23	6 (8%)	82,113,113	1.21	7 (8%)
33	STE	C	520	-	11,11,19	0.88	0	11,11,19	1.01	0
35	HEC	V	201	17	46,50,50	1.86	6 (13%)	58,82,82	2.03	11 (18%)
30	DGD	A	415	-	67,67,67	1.41	10 (14%)	81,81,81	1.44	12 (14%)
30	DGD	h	102	-	63,63,67	1.15	7 (11%)	77,77,81	1.51	14 (18%)
22	CLA	a	403	36	69,73,73	1.25	7 (10%)	82,113,113	1.21	8 (9%)
22	CLA	a	411	36	69,73,73	1.65	6 (8%)	82,113,113	1.24	6 (7%)
32	OEY	a	417[B]	1,36,3	0,16,16	-	-	-		
24	BCR	d	404	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	6 (10%)
22	CLA	C	514	-	69,73,73	1.28	7 (10%)	82,113,113	1.22	6 (7%)
22	CLA	C	505	36	63,67,73	1.32	7 (11%)	74,105,113	1.44	11 (14%)
33	STE	b	624	-	15,15,19	0.86	0	15,15,19	0.81	0
24	BCR	A	406	-	41,41,41	1.06	2 (4%)	56,56,56	1.48	8 (14%)
35	HEC	F	101	5,6	46,50,50	1.84	7 (15%)	58,82,82	1.80	9 (15%)
30	DGD	C	518	-	63,63,67	0.97	5 (7%)	77,77,81	1.31	7 (9%)
35	HEC	v	201	17	46,50,50	1.87	5 (10%)	58,82,82	2.20	12 (20%)
22	CLA	c	503	-	69,73,73	1.02	5 (7%)	82,113,113	1.53	10 (12%)
22	CLA	d	402	-	69,73,73	1.45	9 (13%)	82,113,113	1.26	10 (12%)
33	STE	h	103	-	13,13,19	0.44	0	12,12,19	0.64	0
22	CLA	b	604	-	69,73,73	1.14	5 (7%)	82,113,113	1.56	12 (14%)
28	LMG	D	410	-	31,31,55	1.14	3 (9%)	33,33,63	1.17	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	605	-	69,73,73	1.41	7 (10%)	82,113,113	1.72	9 (10%)
33	STE	J	101	-	11,11,19	0.73	0	11,11,19	1.11	1 (9%)
33	STE	C	521	-	15,15,19	0.48	0	14,14,19	0.67	0
33	STE	b	626	-	9,9,19	0.59	0	8,8,19	0.44	0
23	PHO	A	404	-	58,69,69	1.84	9 (15%)	55,99,99	1.84	12 (21%)
34	LHG	e	102	-	41,41,48	1.05	3 (7%)	44,47,54	1.40	5 (11%)
24	BCR	b	616	-	41,41,41	1.23	5 (12%)	56,56,56	1.46	12 (21%)
27	PL9	a	410	-	55,55,55	1.13	5 (9%)	68,69,69	1.53	9 (13%)
22	CLA	b	605	-	69,73,73	1.62	10 (14%)	82,113,113	1.78	18 (21%)
24	BCR	Z	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.35	6 (10%)
28	LMG	A	412	-	48,48,55	1.05	2 (4%)	56,56,63	1.44	7 (12%)
29	SQD	A	413	-	50,52,54	0.94	4 (8%)	60,63,65	1.94	10 (16%)
30	DGD	H	102	-	63,63,67	1.40	11 (17%)	77,77,81	1.46	15 (19%)
28	LMG	b	623	-	55,55,55	0.94	1 (1%)	63,63,63	1.50	10 (15%)
22	CLA	h	101	36	69,73,73	1.38	9 (13%)	82,113,113	1.59	6 (7%)
28	LMG	C	519	-	48,48,55	1.14	4 (8%)	56,56,63	1.37	7 (12%)
33	STE	d	411	-	19,19,19	0.74	0	19,19,19	0.98	2 (10%)
24	BCR	t	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.36	6 (10%)
22	CLA	B	606	-	69,73,73	1.13	7 (10%)	82,113,113	1.35	11 (13%)
27	PL9	d	405	-	55,55,55	1.65	7 (12%)	68,69,69	1.62	15 (22%)
33	STE	B	628	-	14,14,19	0.43	0	13,13,19	0.88	0
31	OEX	A	416[A]	1,36,3	0,15,15	-	-	-		
27	PL9	A	410	-	55,55,55	1.10	5 (9%)	68,69,69	1.70	14 (20%)
26	BCT	a	409	21	3,3,3	1.09	0	2,3,3	2.73	2 (100%)
23	PHO	D	401	-	58,69,69	1.91	8 (13%)	55,99,99	1.36	9 (16%)
22	CLA	B	602	36	69,73,73	1.34	8 (11%)	82,113,113	1.85	12 (14%)
22	CLA	B	616	-	69,73,73	1.22	9 (13%)	82,113,113	1.29	10 (12%)
31	OEX	a	416[A]	1,36,3	0,15,15	-	-	-		
22	CLA	B	612	-	69,73,73	1.45	9 (13%)	82,113,113	1.45	10 (12%)
32	OEY	A	417[B]	1,36,3	0,16,16	-	-	-		
28	LMG	c	522	-	37,37,55	1.33	6 (16%)	45,45,63	1.27	6 (13%)
34	LHG	D	408	-	48,48,48	1.13	4 (8%)	51,54,54	1.23	5 (9%)
24	BCR	b	617	-	41,41,41	1.29	4 (9%)	56,56,56	1.30	7 (12%)
22	CLA	A	403	36	69,73,73	1.30	10 (14%)	82,113,113	1.21	9 (10%)
29	SQD	D	407	-	34,36,54	0.96	1 (2%)	42,45,65	2.25	13 (30%)
29	SQD	a	412	-	52,54,54	0.98	4 (7%)	62,65,65	1.82	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	STE	M	102	-	14,14,19	0.86	0	14,14,19	0.98	1 (7%)
24	BCR	x	101	-	41,41,41	1.13	4 (9%)	56,56,56	1.36	8 (14%)
29	SQD	A	414	-	38,38,54	1.08	3 (7%)	40,40,65	1.36	5 (12%)
22	CLA	a	402	-	69,73,73	1.32	8 (11%)	82,113,113	1.39	12 (14%)
33	STE	B	627	-	15,15,19	0.52	0	14,14,19	0.69	0
24	BCR	B	620	-	41,41,41	1.13	3 (7%)	56,56,56	1.36	8 (14%)
33	STE	b	620	-	15,15,19	0.47	0	14,14,19	0.71	0
22	CLA	C	506	-	69,73,73	1.24	7 (10%)	82,113,113	1.19	5 (6%)
22	CLA	D	402	-	69,73,73	1.18	5 (7%)	82,113,113	1.32	6 (7%)
22	CLA	b	602	-	69,73,73	1.32	9 (13%)	82,113,113	1.60	19 (23%)
33	STE	c	501	-	11,11,19	0.83	0	11,11,19	0.92	0
22	CLA	D	403	-	69,73,73	1.58	12 (17%)	82,113,113	1.26	8 (9%)
24	BCR	B	619	-	41,41,41	1.03	2 (4%)	56,56,56	1.42	11 (19%)
22	CLA	A	405	-	58,62,73	1.27	5 (8%)	68,99,113	1.32	11 (16%)
34	LHG	d	408	-	38,38,48	0.80	1 (2%)	41,44,54	1.11	3 (7%)
33	STE	X	101	-	19,19,19	0.67	0	19,19,19	1.31	3 (15%)
22	CLA	b	615	-	64,68,73	1.44	10 (15%)	76,107,113	1.51	8 (10%)
27	PL9	D	405	-	55,55,55	1.65	10 (18%)	68,69,69	1.71	13 (19%)
23	PHO	a	404	-	58,69,69	1.88	10 (17%)	55,99,99	1.80	13 (23%)
33	STE	Z	102	-	7,7,19	0.31	0	6,6,19	0.77	0
22	CLA	B	615	-	69,73,73	1.44	10 (14%)	82,113,113	1.45	15 (18%)
33	STE	L	101	-	11,11,19	0.79	0	11,11,19	1.51	2 (18%)
28	LMG	b	621	-	51,51,55	0.98	3 (5%)	59,59,63	1.47	10 (16%)
22	CLA	c	508	-	69,73,73	1.58	11 (15%)	82,113,113	1.36	9 (10%)
33	STE	b	622	-	19,19,19	0.68	0	19,19,19	1.11	1 (5%)
22	CLA	b	613	-	69,73,73	1.13	6 (8%)	82,113,113	1.23	10 (12%)
24	BCR	b	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	10 (17%)
34	LHG	l	101	-	48,48,48	0.76	1 (2%)	51,54,54	1.15	4 (7%)
24	BCR	D	404	-	41,41,41	1.20	2 (4%)	56,56,56	1.26	5 (8%)
22	CLA	B	603	-	69,73,73	1.22	8 (11%)	82,113,113	1.40	9 (10%)
24	BCR	B	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.23	7 (12%)
22	CLA	C	511	-	69,73,73	1.23	10 (14%)	82,113,113	1.23	4 (4%)
22	CLA	C	504	-	69,73,73	1.47	9 (13%)	82,113,113	1.63	9 (10%)
22	CLA	c	513	3	69,73,73	1.33	8 (11%)	82,113,113	1.36	5 (6%)
22	CLA	B	604	-	69,73,73	1.29	7 (10%)	82,113,113	1.41	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	DGD	C	517	-	63,63,67	1.33	8 (12%)	77,77,81	1.34	10 (12%)
28	LMG	M	101	-	51,51,55	0.96	3 (5%)	59,59,63	1.41	12 (20%)
33	STE	B	601	-	11,11,19	0.64	0	11,11,19	1.30	2 (18%)
22	CLA	B	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.43	12 (14%)
33	STE	H	103	-	17,17,19	0.51	0	16,16,19	0.62	0
22	CLA	b	607	-	69,73,73	1.30	9 (13%)	82,113,113	1.34	10 (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
22	CLA	c	511	-	1/1/20/20	9/39/115/115	-
22	CLA	a	405	-	1/1/20/20	7/39/115/115	-
22	CLA	b	610	-	-	6/39/115/115	-
22	CLA	c	504	-	-	5/39/115/115	-
22	CLA	B	607	-	1/1/20/20	8/39/115/115	-
28	LMG	d	409	-	-	12/39/59/70	0/1/1/1
34	LHG	D	412	-	-	17/53/53/53	-
29	SQD	b	619	-	-	19/44/64/69	0/1/1/1
33	STE	I	101	-	-	4/12/12/17	-
22	CLA	c	506	36	1/1/19/20	10/33/109/115	-
22	CLA	b	603	-	1/1/20/20	5/39/115/115	-
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
33	STE	c	523	-	-	10/17/17/17	-
34	LHG	d	407	-	-	19/53/53/53	-
33	STE	E	102	-	-	3/9/9/17	-
33	STE	d	412	-	-	7/17/17/17	-
24	BCR	T	101	-	-	6/29/63/63	0/2/2/2
33	STE	B	625	-	-	5/9/9/17	-
24	BCR	Y	101	-	-	10/29/63/63	0/2/2/2
22	CLA	b	606	36	1/1/20/20	12/39/115/115	-
22	CLA	b	611	-	1/1/20/20	6/39/115/115	-
22	CLA	b	608	-	-	7/39/115/115	-
28	LMG	c	524	-	-	23/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	513	-	1/1/20/20	17/39/115/115	-
34	LHG	d	406	-	-	22/53/53/53	-
22	CLA	C	507	-	1/1/20/20	11/39/115/115	-
22	CLA	B	611	36	1/1/20/20	5/39/115/115	-
24	BCR	C	515	-	-	3/29/63/63	0/2/2/2
34	LHG	D	409	-	-	26/51/51/53	-
22	CLA	C	510	-	1/1/20/20	6/39/115/115	-
22	CLA	B	608	36	1/1/20/20	9/39/115/115	-
22	CLA	C	502	-	-	2/39/115/115	-
24	BCR	y	101	-	-	11/29/63/63	0/2/2/2
24	BCR	a	406	-	-	6/29/63/63	0/2/2/2
33	STE	T	102	-	-	7/12/12/17	-
22	CLA	B	617	-	1/1/19/20	7/33/109/115	-
33	STE	b	625	-	-	6/17/17/17	-
22	CLA	B	613	-	1/1/20/20	7/39/115/115	-
33	STE	M	103	-	-	2/7/7/17	-
33	STE	j	101	-	-	4/9/9/17	-
28	LMG	B	629	-	-	29/50/70/70	0/1/1/1
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2
34	LHG	B	622	-	-	20/53/53/53	-
28	LMG	D	411	-	-	10/22/22/70	-
22	CLA	d	403	-	1/1/20/20	7/39/115/115	-
22	CLA	A	402	-	1/1/20/20	3/39/115/115	-
33	STE	a	414	-	-	3/7/7/17	-
33	STE	a	415	-	-	3/9/9/17	-
22	CLA	c	507	-	1/1/20/20	6/39/115/115	-
22	CLA	b	614	-	1/1/20/20	9/39/115/115	-
22	CLA	C	512	3	1/1/20/20	9/39/115/115	-
28	LMG	D	406	-	-	17/46/66/70	0/1/1/1
22	CLA	C	509	-	-	4/39/115/115	-
22	CLA	c	505	-	-	2/39/115/115	-
22	CLA	c	510	-	-	9/38/114/115	-
33	STE	B	621	-	-	6/14/14/17	-
22	CLA	B	614	-	1/1/20/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	514	-	1/1/20/20	22/39/115/115	-
24	BCR	c	518	-	-	8/29/63/63	0/2/2/2
29	SQD	B	623	-	-	21/49/69/69	0/1/1/1
24	BCR	c	517	-	-	9/29/63/63	0/2/2/2
22	CLA	c	509	36	1/1/20/20	7/39/115/115	-
22	CLA	b	609	36	1/1/20/20	6/39/115/115	-
30	DGD	c	519	-	-	23/51/91/95	0/2/2/2
22	CLA	C	508	36	1/1/20/20	10/39/115/115	-
34	LHG	E	101	-	-	27/53/53/53	-
22	CLA	b	601	-	1/1/20/20	5/39/115/115	-
30	DGD	c	521	-	-	13/51/91/95	0/2/2/2
28	LMG	c	525	-	-	18/44/64/70	0/1/1/1
33	STE	d	410	-	-	9/14/14/17	-
22	CLA	A	411	36	-	9/39/115/115	-
29	SQD	a	413	-	-	21/37/37/69	-
33	STE	C	522	-	-	3/9/9/17	-
22	CLA	c	515	-	1/1/20/20	6/39/115/115	-
22	CLA	C	503	-	1/1/20/20	7/39/115/115	-
29	SQD	f	101	-	-	13/36/56/69	0/1/1/1
24	BCR	H	101	-	-	1/29/63/63	0/2/2/2
22	CLA	b	612	-	1/1/20/20	4/39/115/115	-
33	STE	l	102	-	-	7/15/15/17	-
23	PHO	d	401	-	-	6/37/103/103	0/5/6/6
24	BCR	c	516	-	-	13/29/63/63	0/2/2/2
35	HEC	e	101	5,6	-	5/14/54/54	-
22	CLA	B	610	-	-	6/39/115/115	-
33	STE	B	624	-	-	3/11/11/17	-
30	DGD	C	516	-	-	18/51/91/95	0/2/2/2
33	STE	B	626	-	-	8/15/15/17	-
22	CLA	c	512	-	1/1/20/20	11/39/115/115	-
33	STE	C	520	-	-	3/9/9/17	-
35	HEC	V	201	17	-	6/14/54/54	-
30	DGD	A	415	-	-	21/55/95/95	0/2/2/2
30	DGD	h	102	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	403	36	-	14/39/115/115	-
22	CLA	a	411	36	1/1/20/20	2/39/115/115	-
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
22	CLA	C	514	-	-	11/39/115/115	-
22	CLA	C	505	36	1/1/18/20	8/32/108/115	-
33	STE	b	624	-	-	8/13/13/17	-
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
35	HEC	F	101	5,6	-	6/14/54/54	-
30	DGD	C	518	-	-	15/51/91/95	0/2/2/2
35	HEC	v	201	17	-	6/14/54/54	-
22	CLA	c	503	-	1/1/20/20	5/39/115/115	-
22	CLA	d	402	-	1/1/20/20	9/39/115/115	-
33	STE	h	103	-	-	5/11/11/17	-
22	CLA	b	604	-	1/1/20/20	8/39/115/115	-
28	LMG	D	410	-	-	15/33/33/70	-
22	CLA	B	605	-	1/1/20/20	11/39/115/115	-
33	STE	J	101	-	-	3/9/9/17	-
33	STE	C	521	-	-	5/13/13/17	-
33	STE	b	626	-	-	5/7/7/17	-
23	PHO	A	404	-	-	4/37/103/103	0/5/6/6
34	LHG	e	102	-	-	23/46/46/53	-
24	BCR	b	616	-	-	5/29/63/63	0/2/2/2
27	PL9	a	410	-	-	17/53/73/73	0/1/1/1
22	CLA	b	605	-	1/1/20/20	9/39/115/115	-
24	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
28	LMG	A	412	-	-	12/43/63/70	0/1/1/1
29	SQD	A	413	-	-	17/47/67/69	0/1/1/1
30	DGD	H	102	-	-	20/51/91/95	0/2/2/2
28	LMG	b	623	-	-	20/50/70/70	0/1/1/1
22	CLA	h	101	36	1/1/20/20	18/39/115/115	-
28	LMG	C	519	-	-	19/43/63/70	0/1/1/1
33	STE	d	411	-	-	10/17/17/17	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/20/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PL9	d	405	-	-	13/53/73/73	0/1/1/1
33	STE	B	628	-	-	7/12/12/17	-
27	PL9	A	410	-	-	19/53/73/73	0/1/1/1
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
22	CLA	B	602	36	1/1/20/20	17/39/115/115	-
22	CLA	B	616	-	1/1/20/20	7/39/115/115	-
34	LHG	D	408	-	-	21/53/53/53	-
22	CLA	B	612	-	1/1/20/20	10/39/115/115	-
28	LMG	c	522	-	-	9/31/51/70	0/1/1/1
24	BCR	b	617	-	-	3/29/63/63	0/2/2/2
22	CLA	A	403	36	1/1/20/20	9/39/115/115	-
29	SQD	D	407	-	-	10/28/48/69	0/1/1/1
29	SQD	a	412	-	-	29/49/69/69	0/1/1/1
33	STE	M	102	-	-	5/12/12/17	-
24	BCR	x	101	-	-	4/29/63/63	0/2/2/2
29	SQD	A	414	-	-	14/39/39/69	-
22	CLA	a	402	-	1/1/20/20	6/39/115/115	-
33	STE	B	627	-	-	6/13/13/17	-
24	BCR	B	620	-	-	4/29/63/63	0/2/2/2
33	STE	b	620	-	-	6/13/13/17	-
22	CLA	C	506	-	1/1/20/20	13/39/115/115	-
22	CLA	D	402	-	1/1/20/20	7/39/115/115	-
22	CLA	b	602	-	1/1/20/20	7/39/115/115	-
33	STE	c	501	-	-	5/9/9/17	-
22	CLA	D	403	-	-	7/39/115/115	-
24	BCR	B	619	-	-	8/29/63/63	0/2/2/2
22	CLA	A	405	-	1/1/17/20	6/26/102/115	-
34	LHG	d	408	-	-	15/43/43/53	-
33	STE	X	101	-	-	10/17/17/17	-
22	CLA	b	615	-	1/1/19/20	9/33/109/115	-
27	PL9	D	405	-	-	9/53/73/73	0/1/1/1
23	PHO	a	404	-	-	2/37/103/103	0/5/6/6
33	STE	Z	102	-	-	2/5/5/17	-
22	CLA	B	615	-	1/1/20/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	L	101	-	-	5/9/9/17	-
28	LMG	b	621	-	-	21/46/66/70	0/1/1/1
22	CLA	c	508	-	1/1/20/20	15/39/115/115	-
33	STE	b	622	-	-	11/17/17/17	-
22	CLA	b	613	-	1/1/20/20	19/39/115/115	-
24	BCR	b	618	-	-	3/29/63/63	0/2/2/2
34	LHG	l	101	-	-	20/53/53/53	-
24	BCR	D	404	-	-	4/29/63/63	0/2/2/2
22	CLA	B	603	-	-	4/39/115/115	-
24	BCR	B	618	-	-	8/29/63/63	0/2/2/2
22	CLA	C	511	-	1/1/20/20	8/39/115/115	-
22	CLA	c	513	3	1/1/20/20	11/39/115/115	-
22	CLA	C	504	-	-	3/39/115/115	-
22	CLA	B	604	-	1/1/20/20	8/39/115/115	-
30	DGD	C	517	-	-	18/51/91/95	0/2/2/2
28	LMG	M	101	-	-	19/46/66/70	0/1/1/1
33	STE	B	601	-	-	1/9/9/17	-
22	CLA	B	609	-	-	2/39/115/115	-
33	STE	H	103	-	-	8/15/15/17	-
22	CLA	b	607	-	1/1/20/20	10/39/115/115	-

All (871) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	MG-NB	9.21	2.24	2.05
22	a	411	CLA	MG-NA	8.98	2.27	2.06
22	C	512	CLA	MG-NA	8.92	2.27	2.06
22	b	605	CLA	MG-NA	8.78	2.27	2.06
23	d	401	PHO	C1B-C2B	8.65	1.49	1.39
23	a	404	PHO	C1B-C2B	8.39	1.48	1.39
23	D	401	PHO	C1B-C2B	7.90	1.48	1.39
23	d	401	PHO	C3B-C4B	7.49	1.49	1.41
23	D	401	PHO	C3B-C4B	7.38	1.49	1.41
22	B	605	CLA	MG-NA	7.25	2.23	2.06
22	C	504	CLA	MG-NA	7.15	2.23	2.06
22	b	609	CLA	MG-NB	-7.09	1.91	2.05
23	A	404	PHO	C3B-C4B	6.95	1.48	1.41
35	V	201	HEC	CAC-C3C	6.87	1.57	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	PHO	C3B-C4B	6.74	1.48	1.41
22	B	612	CLA	MG-NA	6.71	2.22	2.06
23	A	404	PHO	C1B-C2B	6.69	1.46	1.39
22	c	508	CLA	MG-ND	-6.68	1.92	2.05
35	v	201	HEC	CAC-C3C	6.56	1.56	1.35
27	d	405	PL9	C6-C1	-6.40	1.37	1.48
22	C	508	CLA	MG-NA	6.39	2.21	2.06
22	c	508	CLA	MG-NB	6.36	2.18	2.05
22	B	607	CLA	MG-NA	6.34	2.21	2.06
28	B	629	LMG	C4-C5	6.19	1.66	1.53
35	F	101	HEC	CAB-C3B	6.18	1.55	1.35
35	V	201	HEC	CAB-C3B	6.13	1.54	1.35
22	d	403	CLA	MG-ND	-6.10	1.93	2.05
22	B	604	CLA	MG-NA	6.10	2.20	2.06
22	c	505	CLA	MG-NC	6.09	2.20	2.06
35	e	101	HEC	CAC-C3C	6.05	1.54	1.35
22	b	614	CLA	MG-NA	6.01	2.20	2.06
35	e	101	HEC	CAB-C3B	5.98	1.54	1.35
22	d	402	CLA	MG-ND	-5.97	1.94	2.05
35	v	201	HEC	CAB-C3B	5.90	1.54	1.35
35	F	101	HEC	CAC-C3C	5.87	1.54	1.35
22	C	502	CLA	MG-NA	5.79	2.20	2.06
22	D	403	CLA	MG-ND	-5.68	1.94	2.05
22	h	101	CLA	MG-NA	5.53	2.19	2.06
22	C	514	CLA	MG-NA	5.51	2.19	2.06
22	a	403	CLA	MG-NC	5.45	2.19	2.06
22	D	403	CLA	MG-NB	-5.37	1.95	2.05
27	d	405	PL9	C3-C4	-5.32	1.41	1.49
22	a	405	CLA	MG-NB	-5.30	1.95	2.05
22	B	615	CLA	MG-ND	-5.26	1.95	2.05
22	c	513	CLA	MG-NA	5.24	2.18	2.06
22	c	509	CLA	MG-NB	-5.24	1.95	2.05
22	c	511	CLA	MG-NB	-5.23	1.95	2.05
22	c	510	CLA	MG-NA	5.10	2.18	2.06
24	H	101	BCR	C30-C25	-5.06	1.47	1.53
24	C	515	BCR	C1-C6	-5.06	1.47	1.53
22	c	504	CLA	MG-NA	5.05	2.18	2.06
22	c	515	CLA	MG-ND	-5.01	1.95	2.05
34	B	622	LHG	O7-C5	-5.00	1.34	1.46
35	F	101	HEC	C3D-C2D	4.95	1.51	1.38
24	Y	101	BCR	C30-C25	-4.87	1.47	1.53
35	v	201	HEC	C3D-C2D	4.86	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	MG-NA	4.84	2.17	2.06
22	B	617	CLA	MG-NA	4.82	2.17	2.06
35	e	101	HEC	C3D-C2D	4.82	1.51	1.38
22	C	503	CLA	MG-ND	4.81	2.15	2.05
22	b	615	CLA	MG-ND	-4.79	1.96	2.05
34	D	408	LHG	O8-C6	-4.79	1.34	1.45
22	A	411	CLA	MG-NA	4.78	2.17	2.06
35	V	201	HEC	C3D-C2D	4.77	1.51	1.38
22	C	507	CLA	MG-NA	4.71	2.17	2.06
22	c	511	CLA	MG-NC	4.70	2.17	2.06
22	B	614	CLA	MG-NB	-4.69	1.96	2.05
30	c	519	DGD	C4D-C3D	4.63	1.64	1.52
22	a	402	CLA	MG-NA	4.61	2.17	2.06
22	b	615	CLA	MG-NB	4.59	2.14	2.05
24	D	404	BCR	C30-C25	-4.54	1.48	1.53
27	D	405	PL9	C7-C3	-4.51	1.45	1.51
22	D	403	CLA	C1D-ND	4.51	1.43	1.37
22	b	605	CLA	C1D-ND	4.47	1.43	1.37
22	A	405	CLA	MG-ND	-4.47	1.96	2.05
22	a	405	CLA	MG-NA	4.41	2.16	2.06
22	b	612	CLA	MG-NA	4.39	2.16	2.06
22	b	609	CLA	MG-NC	4.36	2.16	2.06
24	b	616	BCR	C1-C6	-4.36	1.48	1.53
22	c	507	CLA	MG-NB	-4.36	1.97	2.05
22	B	614	CLA	MG-NC	4.35	2.16	2.06
22	C	508	CLA	MG-NB	-4.34	1.97	2.05
22	b	602	CLA	MG-NA	4.31	2.16	2.06
22	A	403	CLA	MG-NB	-4.31	1.97	2.05
22	b	607	CLA	MG-ND	4.28	2.14	2.05
30	A	415	DGD	C3G-C2G	4.27	1.64	1.50
22	a	405	CLA	C1D-ND	4.27	1.43	1.37
22	C	505	CLA	MG-NA	4.26	2.16	2.06
22	d	403	CLA	MG-NB	-4.25	1.97	2.05
30	H	102	DGD	C4E-C5E	4.19	1.62	1.53
22	c	510	CLA	C1D-ND	4.19	1.43	1.37
22	b	606	CLA	MG-NA	4.19	2.16	2.06
27	D	405	PL9	C52-C5	-4.16	1.42	1.50
22	B	608	CLA	MG-ND	-4.15	1.97	2.05
22	D	402	CLA	C1D-ND	4.15	1.43	1.37
27	D	405	PL9	C6-C1	-4.11	1.41	1.48
28	B	629	LMG	C4-C3	4.11	1.63	1.52
22	d	403	CLA	C1D-ND	4.11	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	411	CLA	MG-ND	-4.11	1.97	2.05
22	C	507	CLA	MG-ND	-4.10	1.97	2.05
22	b	608	CLA	MG-NA	4.09	2.16	2.06
22	C	506	CLA	MG-NA	4.08	2.16	2.06
24	c	517	BCR	C1-C6	-4.06	1.48	1.53
22	A	402	CLA	C1D-ND	4.05	1.43	1.37
23	A	404	PHO	C4D-ND	-4.03	1.32	1.38
24	c	516	BCR	C1-C6	-4.03	1.48	1.53
22	b	609	CLA	C1D-ND	4.01	1.43	1.37
30	C	517	DGD	O5D-C1E	4.01	1.46	1.40
24	x	101	BCR	C30-C25	-4.00	1.48	1.53
24	d	404	BCR	C1-C6	-3.97	1.48	1.53
22	B	602	CLA	MG-NA	3.97	2.15	2.06
28	C	519	LMG	C4-C5	3.96	1.61	1.53
22	b	615	CLA	C1D-ND	3.95	1.43	1.37
24	A	406	BCR	C1-C6	-3.93	1.48	1.53
22	B	602	CLA	C1D-ND	3.93	1.43	1.37
22	c	511	CLA	C1D-ND	3.90	1.43	1.37
22	c	506	CLA	MG-ND	-3.89	1.98	2.05
30	c	521	DGD	O2G-C2G	-3.89	1.37	1.46
22	C	503	CLA	MG-NA	3.87	2.15	2.06
24	b	617	BCR	C30-C25	-3.87	1.48	1.53
27	D	405	PL9	C41-C39	-3.86	1.43	1.51
22	B	615	CLA	MG-NA	3.85	2.15	2.06
22	C	509	CLA	MG-NA	3.85	2.15	2.06
22	D	403	CLA	MG-NA	3.83	2.15	2.06
22	B	615	CLA	MG-NB	3.80	2.13	2.05
22	B	614	CLA	MG-ND	-3.78	1.98	2.05
24	B	618	BCR	C1-C6	-3.74	1.49	1.53
22	B	616	CLA	C1D-ND	3.74	1.42	1.37
22	D	402	CLA	MG-ND	-3.73	1.98	2.05
30	c	519	DGD	O5D-C6D	3.72	1.50	1.43
24	b	618	BCR	C1-C6	-3.71	1.49	1.53
27	a	410	PL9	C6-C1	-3.71	1.42	1.48
34	D	412	LHG	O7-C5	-3.69	1.37	1.46
34	d	407	LHG	O7-C5	-3.68	1.37	1.46
22	c	509	CLA	C1D-ND	3.67	1.42	1.37
22	a	411	CLA	C1D-ND	3.66	1.42	1.37
22	B	612	CLA	MG-ND	-3.64	1.98	2.05
24	Z	101	BCR	C30-C25	-3.63	1.49	1.53
22	d	402	CLA	MG-NA	3.61	2.14	2.06
24	y	101	BCR	C30-C25	-3.61	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	C1D-ND	3.61	1.42	1.37
22	C	513	CLA	MG-NA	3.60	2.14	2.06
29	a	413	SQD	O47-C7	3.60	1.44	1.34
29	B	623	SQD	O47-C7	3.60	1.44	1.34
30	C	517	DGD	C4D-C3D	3.59	1.61	1.52
22	a	405	CLA	MG-NC	-3.57	1.97	2.06
23	D	401	PHO	C4D-ND	-3.57	1.33	1.38
22	A	411	CLA	C1D-ND	3.57	1.42	1.37
22	B	611	CLA	C4B-NB	3.57	1.42	1.37
28	A	412	LMG	O1-C7	-3.56	1.37	1.43
22	C	505	CLA	C4B-NB	3.55	1.42	1.37
27	d	405	PL9	C53-C6	-3.55	1.43	1.50
23	D	401	PHO	C1D-C2D	3.55	1.43	1.39
23	D	401	PHO	CMB-C2B	-3.55	1.44	1.51
22	B	603	CLA	C1D-ND	3.54	1.42	1.37
29	a	413	SQD	O48-C23	3.52	1.43	1.33
22	B	614	CLA	MG-NA	3.52	2.14	2.06
27	A	410	PL9	C7-C3	-3.50	1.46	1.51
24	d	404	BCR	C30-C25	-3.49	1.49	1.53
27	d	405	PL9	C46-C44	-3.47	1.44	1.51
29	A	414	SQD	O48-C23	3.46	1.43	1.33
24	y	101	BCR	C1-C6	-3.46	1.49	1.53
30	c	520	DGD	O3G-C3G	-3.45	1.37	1.43
24	b	617	BCR	C1-C6	-3.44	1.49	1.53
23	A	404	PHO	CMC-C2C	-3.43	1.45	1.50
24	B	618	BCR	C30-C25	-3.42	1.49	1.53
30	A	415	DGD	C4D-C3D	3.40	1.61	1.52
23	d	401	PHO	C1D-C2D	3.38	1.43	1.39
27	D	405	PL9	C11-C9	-3.37	1.44	1.51
22	B	614	CLA	C4B-NB	3.36	1.42	1.37
29	a	412	SQD	O48-C23	3.34	1.43	1.33
22	B	617	CLA	MG-NB	3.33	2.12	2.05
22	B	608	CLA	MG-NC	3.33	2.14	2.06
24	Y	101	BCR	C1-C6	-3.31	1.49	1.53
29	b	619	SQD	O48-C23	3.31	1.43	1.33
34	d	407	LHG	C1-C2	-3.31	1.39	1.51
22	C	510	CLA	C1D-ND	3.30	1.42	1.37
34	d	406	LHG	O7-C5	-3.30	1.38	1.46
28	c	524	LMG	C3-C2	3.30	1.60	1.52
22	B	615	CLA	C4B-NB	3.30	1.42	1.37
22	h	101	CLA	C1D-ND	3.29	1.42	1.37
22	b	613	CLA	C4B-NB	3.29	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	C1D-ND	3.29	1.42	1.37
30	C	518	DGD	O2G-C2G	-3.28	1.38	1.46
22	c	510	CLA	MG-NB	3.28	2.12	2.05
29	A	414	SQD	O47-C7	3.27	1.43	1.34
24	K	101	BCR	C30-C25	-3.27	1.49	1.53
22	C	504	CLA	C4B-NB	3.27	1.42	1.37
22	c	515	CLA	C1D-ND	3.26	1.42	1.37
22	h	101	CLA	C1B-C2B	3.26	1.50	1.43
22	c	511	CLA	C4B-NB	3.26	1.42	1.37
22	B	602	CLA	C4B-NB	3.26	1.42	1.37
28	D	410	LMG	C7-C8	3.26	1.58	1.51
22	C	502	CLA	C1D-ND	3.26	1.42	1.37
22	c	513	CLA	MG-NB	3.26	2.12	2.05
22	a	411	CLA	C4B-NB	3.25	1.42	1.37
34	D	409	LHG	P-O6	3.25	1.72	1.59
24	B	620	BCR	C1-C6	-3.25	1.49	1.53
22	c	504	CLA	CMD-C2D	-3.24	1.44	1.50
22	B	608	CLA	C1D-ND	3.24	1.42	1.37
24	B	620	BCR	C30-C25	-3.24	1.49	1.53
22	C	506	CLA	C1B-C2B	3.23	1.50	1.43
23	D	401	PHO	CAC-C3C	-3.23	1.46	1.51
24	B	619	BCR	C30-C25	-3.23	1.49	1.53
22	C	502	CLA	C1B-C2B	3.22	1.50	1.43
30	C	517	DGD	C6E-C5E	3.22	1.62	1.51
22	C	511	CLA	C1B-C2B	3.20	1.50	1.43
24	Z	101	BCR	C1-C6	-3.19	1.49	1.53
28	c	525	LMG	O7-C8	-3.19	1.39	1.46
22	C	514	CLA	C4B-NB	3.19	1.42	1.37
28	c	522	LMG	O1-C1	3.19	1.45	1.40
29	f	101	SQD	O47-C7	3.19	1.43	1.34
22	c	504	CLA	C4B-NB	3.19	1.42	1.37
22	B	617	CLA	CMC-C2C	-3.18	1.44	1.50
28	B	629	LMG	O8-C9	-3.16	1.38	1.45
22	a	402	CLA	C1D-ND	3.16	1.42	1.37
22	d	403	CLA	C4B-NB	3.16	1.42	1.37
34	e	102	LHG	P-O6	3.16	1.71	1.59
22	c	514	CLA	MG-NC	3.15	2.13	2.06
23	A	404	PHO	C1D-C2D	3.13	1.43	1.39
30	A	415	DGD	C4E-C5E	3.13	1.59	1.53
23	d	401	PHO	CAC-C3C	-3.13	1.46	1.51
24	c	518	BCR	C1-C6	-3.13	1.49	1.53
22	C	512	CLA	MG-ND	-3.12	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	517	DGD	O3E-C3E	-3.12	1.35	1.43
22	B	603	CLA	MG-NA	3.12	2.13	2.06
29	D	407	SQD	O48-C23	3.11	1.42	1.33
22	B	602	CLA	MG-NC	3.11	2.13	2.06
22	C	508	CLA	C1B-NB	-3.10	1.33	1.37
22	C	514	CLA	C1D-ND	3.10	1.41	1.37
22	B	611	CLA	MG-NC	3.10	2.13	2.06
23	a	404	PHO	C3D-C4D	3.10	1.45	1.41
24	b	618	BCR	C30-C25	-3.09	1.49	1.53
22	B	613	CLA	C4B-NB	3.08	1.41	1.37
22	c	515	CLA	MG-NB	3.08	2.11	2.05
22	B	611	CLA	C1D-ND	3.08	1.41	1.37
22	d	403	CLA	CMD-C2D	-3.07	1.44	1.50
28	b	623	LMG	C3-C2	3.07	1.60	1.52
24	b	616	BCR	C30-C25	-3.07	1.49	1.53
22	C	511	CLA	C1D-ND	3.07	1.41	1.37
22	C	512	CLA	C1B-C2B	3.06	1.50	1.43
22	C	506	CLA	CHC-C1C	3.06	1.44	1.38
22	b	613	CLA	CMC-C2C	-3.05	1.44	1.50
30	c	519	DGD	O3G-C1D	-3.05	1.35	1.40
22	a	405	CLA	C1B-C2B	3.05	1.50	1.43
28	C	519	LMG	O7-C8	-3.05	1.39	1.46
28	D	410	LMG	C9-C8	3.05	1.60	1.50
23	a	404	PHO	C4D-ND	-3.05	1.34	1.38
22	c	507	CLA	C3B-C4B	3.05	1.51	1.42
24	c	518	BCR	C30-C25	-3.05	1.49	1.53
22	C	511	CLA	CMC-C2C	-3.04	1.44	1.50
22	b	612	CLA	MG-NC	-3.04	1.99	2.06
22	c	514	CLA	C1D-ND	3.04	1.41	1.37
30	H	102	DGD	O5D-C1E	3.04	1.45	1.40
22	C	502	CLA	C3B-C4B	3.04	1.51	1.42
24	C	515	BCR	C30-C25	-3.03	1.49	1.53
22	c	506	CLA	MG-NA	-3.03	1.99	2.06
22	C	513	CLA	C1D-ND	3.03	1.41	1.37
22	C	507	CLA	C4B-NB	3.03	1.41	1.37
22	A	405	CLA	MG-NB	-3.03	1.99	2.05
22	B	609	CLA	C1B-C2B	3.02	1.50	1.43
22	b	602	CLA	C1B-NB	-3.02	1.33	1.37
22	B	612	CLA	C1D-ND	3.02	1.41	1.37
34	E	101	LHG	P-O6	3.02	1.71	1.59
22	C	512	CLA	C4B-NB	3.02	1.41	1.37
22	c	510	CLA	CHC-C1C	3.01	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	514	CLA	C4B-NB	3.01	1.41	1.37
22	d	402	CLA	MG-NB	-3.01	1.99	2.05
22	C	504	CLA	C1B-C2B	3.01	1.50	1.43
30	c	520	DGD	O2G-C2G	-3.01	1.39	1.46
22	c	506	CLA	C4B-NB	3.01	1.41	1.37
22	b	602	CLA	MG-NC	3.00	2.13	2.06
27	D	405	PL9	C36-C34	-3.00	1.45	1.51
22	c	508	CLA	CMD-C2D	-3.00	1.44	1.50
22	A	402	CLA	C1B-C2B	3.00	1.50	1.43
22	a	405	CLA	CMC-C2C	-3.00	1.44	1.50
22	B	615	CLA	C1D-ND	3.00	1.41	1.37
28	c	522	LMG	C1-C2	2.99	1.61	1.52
30	C	516	DGD	C4D-C3D	2.99	1.60	1.52
22	A	403	CLA	MG-NC	2.99	2.13	2.06
22	A	411	CLA	C4B-NB	2.99	1.41	1.37
30	h	102	DGD	C4E-C5E	2.99	1.59	1.53
28	c	522	LMG	C3-C2	2.99	1.60	1.52
22	C	509	CLA	C1B-C2B	2.98	1.50	1.43
30	A	415	DGD	C1E-C2E	2.98	1.61	1.52
23	A	404	PHO	C3D-C4D	2.98	1.45	1.41
22	A	411	CLA	C1B-C2B	2.98	1.50	1.43
22	B	605	CLA	C1D-ND	2.97	1.41	1.37
34	d	407	LHG	O8-C6	-2.97	1.38	1.45
22	b	614	CLA	CMD-C2D	-2.97	1.44	1.50
22	b	614	CLA	C3B-C4B	2.96	1.51	1.42
22	b	608	CLA	C1D-ND	2.96	1.41	1.37
22	B	609	CLA	CMD-C2D	-2.96	1.44	1.50
22	b	606	CLA	CHD-C1D	-2.96	1.32	1.38
28	b	621	LMG	C4-C3	2.96	1.60	1.52
29	a	412	SQD	O47-C7	2.95	1.42	1.34
22	C	507	CLA	C1B-NB	-2.94	1.34	1.37
29	b	619	SQD	O47-C7	2.94	1.42	1.34
22	C	506	CLA	C4B-NB	2.94	1.41	1.37
24	T	101	BCR	C1-C6	-2.93	1.50	1.53
22	B	610	CLA	CMD-C2D	-2.93	1.44	1.50
22	a	403	CLA	C1D-ND	2.93	1.41	1.37
22	d	402	CLA	C1D-ND	2.93	1.41	1.37
22	B	604	CLA	MG-ND	2.93	2.11	2.05
22	C	509	CLA	C3B-C4B	2.93	1.51	1.42
35	e	101	HEC	C3B-C2B	-2.92	1.31	1.41
22	A	403	CLA	C4B-NB	2.92	1.41	1.37
22	B	614	CLA	CMD-C2D	-2.92	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	CHC-C1C	2.91	1.44	1.38
22	c	504	CLA	C1D-ND	2.91	1.41	1.37
34	E	101	LHG	C24-C23	2.91	1.59	1.50
22	C	508	CLA	C1B-C2B	2.91	1.49	1.43
30	C	516	DGD	O2E-C2E	-2.90	1.35	1.43
22	b	601	CLA	C1D-ND	2.90	1.41	1.37
29	A	414	SQD	O47-C45	-2.90	1.42	1.47
22	b	608	CLA	C4B-NB	2.90	1.41	1.37
30	A	415	DGD	C4D-C5D	2.90	1.59	1.53
22	d	402	CLA	C4B-NB	2.90	1.41	1.37
22	c	514	CLA	MG-NB	2.90	2.11	2.05
34	E	101	LHG	O7-C5	-2.89	1.39	1.46
28	c	525	LMG	C4-C5	2.89	1.59	1.53
22	A	402	CLA	C4B-NB	2.89	1.41	1.37
30	A	415	DGD	C3D-C2D	2.89	1.59	1.52
29	B	623	SQD	O48-C23	2.89	1.41	1.33
24	a	406	BCR	C1-C6	-2.88	1.50	1.53
22	b	604	CLA	CMD-C2D	-2.88	1.44	1.50
22	C	507	CLA	C1D-ND	2.88	1.41	1.37
22	c	510	CLA	C3B-C4B	2.87	1.51	1.42
22	B	602	CLA	C1B-C2B	2.87	1.49	1.43
22	c	504	CLA	C1B-C2B	2.87	1.49	1.43
34	d	406	LHG	C24-C23	2.86	1.59	1.50
22	B	607	CLA	C1D-ND	2.86	1.41	1.37
22	C	505	CLA	C1D-ND	2.86	1.41	1.37
22	b	610	CLA	C1D-ND	2.85	1.41	1.37
22	b	606	CLA	C1D-ND	2.85	1.41	1.37
28	A	412	LMG	C4-C3	2.85	1.59	1.52
22	B	603	CLA	C4B-NB	2.85	1.41	1.37
22	C	502	CLA	C4B-NB	2.85	1.41	1.37
29	f	101	SQD	O48-C23	2.84	1.41	1.33
23	a	404	PHO	C4D-CHA	2.84	1.43	1.39
22	b	608	CLA	CMB-C2B	-2.84	1.45	1.50
22	b	602	CLA	C1D-ND	2.84	1.41	1.37
22	B	616	CLA	C4B-NB	2.84	1.41	1.37
22	B	613	CLA	C1B-C2B	2.84	1.49	1.43
22	b	604	CLA	C1B-C2B	2.83	1.49	1.43
24	C	515	BCR	C36-C18	-2.83	1.45	1.50
30	A	415	DGD	O2G-C1B	2.83	1.42	1.34
24	T	101	BCR	C30-C25	-2.82	1.50	1.53
22	B	610	CLA	C1D-ND	2.82	1.41	1.37
22	b	602	CLA	CMD-C2D	-2.81	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	C4B-NB	2.81	1.41	1.37
34	e	102	LHG	O8-C23	2.80	1.41	1.33
22	b	607	CLA	CMD-C2D	-2.80	1.45	1.50
30	C	516	DGD	C2A-C1A	-2.80	1.42	1.50
22	b	603	CLA	CMC-C2C	-2.79	1.45	1.50
30	C	518	DGD	O3G-C3G	-2.79	1.38	1.43
28	c	524	LMG	C4-C3	2.79	1.59	1.52
22	c	506	CLA	CAC-C3C	-2.79	1.44	1.51
22	a	402	CLA	C1B-C2B	2.78	1.49	1.43
30	c	521	DGD	O3D-C3D	-2.78	1.36	1.43
27	a	410	PL9	C30-C29	-2.78	1.43	1.50
22	C	508	CLA	C4B-NB	2.78	1.41	1.37
22	c	512	CLA	C1B-C2B	2.78	1.49	1.43
28	c	522	LMG	C4-C5	2.77	1.58	1.53
30	H	102	DGD	O6E-C1E	2.77	1.49	1.41
22	B	611	CLA	CMB-C2B	-2.77	1.45	1.50
22	B	613	CLA	MG-NA	2.77	2.12	2.06
22	b	603	CLA	C4B-NB	2.77	1.41	1.37
22	B	611	CLA	MG-ND	2.76	2.11	2.05
22	c	507	CLA	MG-NC	2.76	2.12	2.06
22	a	411	CLA	CMB-C2B	-2.76	1.45	1.50
22	b	609	CLA	C1B-C2B	2.76	1.49	1.43
22	a	403	CLA	C1B-NB	-2.76	1.34	1.37
24	c	516	BCR	C30-C25	-2.75	1.50	1.53
30	H	102	DGD	O1G-C1G	-2.75	1.39	1.45
22	a	402	CLA	MG-NB	2.75	2.11	2.05
24	c	517	BCR	C30-C25	-2.74	1.50	1.53
22	d	403	CLA	CMC-C2C	-2.74	1.45	1.50
22	B	606	CLA	C1B-NB	-2.73	1.34	1.37
22	A	403	CLA	C1D-ND	2.73	1.41	1.37
22	B	609	CLA	C1D-ND	2.73	1.41	1.37
22	b	607	CLA	C3B-C4B	2.72	1.50	1.42
27	a	410	PL9	C3-C4	-2.71	1.45	1.49
22	C	514	CLA	C1B-C2B	2.71	1.49	1.43
22	C	504	CLA	C1D-ND	2.71	1.41	1.37
22	B	613	CLA	C1D-ND	2.71	1.41	1.37
22	C	508	CLA	C1D-ND	2.71	1.41	1.37
22	b	603	CLA	C1D-ND	2.71	1.41	1.37
22	d	402	CLA	CMD-C2D	-2.71	1.45	1.50
22	c	511	CLA	MG-ND	2.70	2.11	2.05
22	C	506	CLA	CMC-C2C	-2.70	1.45	1.50
22	b	611	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	CLA	C1B-C2B	2.69	1.49	1.43
22	B	615	CLA	CMC-C2C	-2.69	1.45	1.50
22	C	505	CLA	CMD-C2D	-2.69	1.45	1.50
27	d	405	PL9	C25-C24	-2.69	1.44	1.50
27	A	410	PL9	C3-C4	-2.69	1.45	1.49
30	H	102	DGD	C3D-C2D	2.69	1.59	1.52
22	C	505	CLA	C3B-C4B	2.68	1.50	1.42
22	C	507	CLA	C1B-C2B	2.68	1.49	1.43
22	C	505	CLA	CHC-C1C	2.68	1.43	1.38
22	b	610	CLA	CMD-C2D	-2.68	1.45	1.50
30	h	102	DGD	O2G-C1B	2.68	1.41	1.34
22	b	601	CLA	C1B-C2B	2.68	1.49	1.43
22	b	614	CLA	CHC-C1C	2.67	1.43	1.38
22	b	607	CLA	C1B-C2B	2.67	1.49	1.43
22	c	508	CLA	C1B-C2B	2.67	1.49	1.43
22	A	405	CLA	C4B-NB	2.67	1.41	1.37
22	B	607	CLA	C1B-C2B	2.67	1.49	1.43
22	C	502	CLA	CMD-C2D	-2.66	1.45	1.50
22	b	612	CLA	CMD-C2D	-2.66	1.45	1.50
22	c	514	CLA	C1B-C2B	2.66	1.49	1.43
22	C	509	CLA	C4B-NB	2.65	1.41	1.37
22	c	505	CLA	C4B-NB	2.65	1.41	1.37
22	c	515	CLA	C3B-C4B	2.65	1.50	1.42
22	B	611	CLA	C3B-C4B	2.65	1.50	1.42
22	B	612	CLA	C1B-C2B	2.64	1.49	1.43
22	c	515	CLA	C4B-NB	2.64	1.41	1.37
22	B	606	CLA	C3B-C4B	2.64	1.50	1.42
22	C	504	CLA	CHC-C1C	2.64	1.43	1.38
22	B	610	CLA	C4B-NB	2.64	1.41	1.37
22	B	612	CLA	MG-NC	-2.64	2.00	2.06
30	c	521	DGD	C1D-C2D	2.63	1.60	1.52
22	B	605	CLA	C3B-C4B	2.63	1.50	1.42
22	a	402	CLA	C4B-NB	2.63	1.41	1.37
24	b	617	BCR	C38-C26	-2.63	1.46	1.50
34	D	409	LHG	O3-C3	-2.62	1.34	1.44
22	C	513	CLA	CAA-C2A	-2.62	1.49	1.54
22	B	614	CLA	C1D-ND	2.62	1.41	1.37
22	A	405	CLA	CMD-C2D	-2.62	1.45	1.50
22	B	610	CLA	MG-NA	2.62	2.12	2.06
22	C	503	CLA	C1B-C2B	2.62	1.49	1.43
22	a	402	CLA	C3B-C4B	2.62	1.50	1.42
22	C	510	CLA	CMD-C2D	-2.61	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	C4B-NB	2.61	1.41	1.37
28	d	409	LMG	O1-C7	-2.61	1.39	1.43
22	b	605	CLA	MG-ND	-2.61	2.00	2.05
22	C	513	CLA	CMD-C2D	-2.61	1.45	1.50
22	b	604	CLA	CHC-C1C	2.61	1.43	1.38
22	b	604	CLA	C1D-ND	2.61	1.41	1.37
22	C	504	CLA	CMD-C2D	-2.61	1.45	1.50
23	D	401	PHO	C3B-C2B	-2.61	1.36	1.40
22	C	509	CLA	MG-NB	2.60	2.10	2.05
22	C	513	CLA	C3B-C4B	2.60	1.50	1.42
22	h	101	CLA	CHC-C1C	2.60	1.43	1.38
22	c	507	CLA	CMB-C2B	-2.60	1.45	1.50
22	b	611	CLA	MG-NA	2.60	2.12	2.06
22	b	607	CLA	CHC-C1C	2.59	1.43	1.38
22	C	506	CLA	C1D-ND	2.59	1.41	1.37
22	B	609	CLA	C1B-NB	-2.59	1.34	1.37
22	b	601	CLA	C4B-NB	2.59	1.41	1.37
22	b	605	CLA	MG-NC	2.59	2.12	2.06
22	c	511	CLA	C1B-C2B	2.59	1.49	1.43
22	c	513	CLA	C1B-C2B	2.59	1.49	1.43
22	B	604	CLA	C1B-C2B	2.59	1.49	1.43
22	c	509	CLA	C1B-C2B	2.59	1.49	1.43
30	H	102	DGD	C6E-C5E	2.58	1.60	1.51
24	T	101	BCR	C38-C26	-2.58	1.46	1.50
22	C	509	CLA	CMD-C2D	-2.58	1.45	1.50
24	D	404	BCR	C1-C6	-2.58	1.50	1.53
22	a	402	CLA	CHC-C1C	2.57	1.43	1.38
22	B	610	CLA	C1B-NB	-2.57	1.34	1.37
22	h	101	CLA	C4B-NB	2.57	1.41	1.37
22	b	604	CLA	C3B-C4B	2.57	1.50	1.42
23	d	401	PHO	C4D-ND	-2.56	1.34	1.38
22	d	402	CLA	CMB-C2B	-2.56	1.45	1.50
22	c	514	CLA	CHC-C1C	2.56	1.43	1.38
22	C	513	CLA	CMB-C2B	-2.55	1.45	1.50
22	b	605	CLA	CMD-C2D	-2.55	1.45	1.50
23	a	404	PHO	C1D-C2D	2.54	1.42	1.39
22	B	611	CLA	MG-NB	-2.54	2.00	2.05
22	B	616	CLA	C1B-C2B	2.54	1.49	1.43
34	B	622	LHG	O8-C6	-2.54	1.39	1.45
22	a	405	CLA	C4B-NB	2.54	1.41	1.37
22	b	608	CLA	CAC-C3C	-2.54	1.44	1.51
23	a	404	PHO	C3B-C2B	-2.53	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	CHC-C1C	2.53	1.43	1.38
22	b	615	CLA	CMB-C2B	-2.53	1.45	1.50
22	d	403	CLA	CMB-C2B	-2.52	1.45	1.50
22	b	611	CLA	CMC-C2C	-2.52	1.45	1.50
22	D	403	CLA	CMC-C2C	-2.51	1.45	1.50
22	b	607	CLA	CMB-C2B	-2.51	1.45	1.50
22	C	509	CLA	C1D-C2D	2.51	1.50	1.45
35	v	201	HEC	CMA-C3A	2.51	1.55	1.50
22	b	612	CLA	C1B-NB	-2.50	1.34	1.37
22	c	513	CLA	C1D-ND	2.50	1.41	1.37
22	B	615	CLA	C1B-NB	-2.50	1.34	1.37
22	C	510	CLA	CMC-C2C	-2.50	1.45	1.50
24	T	101	BCR	C27-C26	-2.50	1.46	1.51
22	d	402	CLA	CMC-C2C	-2.50	1.45	1.50
35	V	201	HEC	C3C-C4C	-2.50	1.41	1.46
22	b	615	CLA	CMC-C2C	-2.50	1.45	1.50
22	c	511	CLA	CMB-C2B	-2.50	1.45	1.50
22	b	610	CLA	C1B-C2B	2.49	1.49	1.43
30	H	102	DGD	C1G-C2G	2.49	1.58	1.50
30	h	102	DGD	O1G-C1G	-2.49	1.39	1.45
22	C	514	CLA	C3B-C4B	2.49	1.50	1.42
22	b	606	CLA	MG-ND	-2.49	2.00	2.05
22	c	505	CLA	C1B-C2B	2.48	1.49	1.43
22	C	513	CLA	C1B-C2B	2.48	1.49	1.43
22	c	503	CLA	CAC-C3C	-2.48	1.44	1.51
22	a	411	CLA	C1B-C2B	2.48	1.48	1.43
23	d	401	PHO	CMD-C2D	-2.48	1.46	1.51
22	A	402	CLA	MG-ND	-2.47	2.00	2.05
22	c	515	CLA	C1B-C2B	2.47	1.48	1.43
22	c	508	CLA	CAC-C3C	-2.47	1.44	1.51
22	D	403	CLA	CMD-C2D	-2.47	1.45	1.50
22	B	616	CLA	CHC-C1C	2.47	1.43	1.38
22	c	507	CLA	CHC-C1C	2.47	1.43	1.38
22	D	403	CLA	C1B-C2B	2.46	1.48	1.43
30	H	102	DGD	C4D-C5D	2.46	1.58	1.53
22	b	611	CLA	CMD-C2D	-2.46	1.45	1.50
22	a	402	CLA	CMB-C2B	-2.46	1.45	1.50
22	c	512	CLA	CMB-C2B	-2.46	1.45	1.50
24	b	616	BCR	C4-C5	-2.46	1.46	1.51
22	c	504	CLA	CHC-C1C	2.45	1.43	1.38
22	B	608	CLA	CMC-C2C	-2.45	1.45	1.50
22	c	510	CLA	C1B-C2B	2.45	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C1B-C2B	2.45	1.48	1.43
22	B	604	CLA	C3B-C4B	2.45	1.49	1.42
22	b	602	CLA	MG-NB	-2.45	2.00	2.05
22	C	507	CLA	CMA-C3A	-2.44	1.48	1.53
28	C	519	LMG	O8-C9	-2.44	1.39	1.45
28	D	410	LMG	O8-C28	2.43	1.40	1.33
22	c	514	CLA	CMB-C2B	-2.43	1.45	1.50
22	b	612	CLA	C1D-ND	2.43	1.41	1.37
28	D	406	LMG	C6-C5	2.42	1.59	1.51
22	B	616	CLA	CMB-C2B	-2.42	1.45	1.50
30	H	102	DGD	O3E-C3E	-2.42	1.37	1.43
22	c	513	CLA	C3B-C4B	2.42	1.49	1.42
22	A	411	CLA	CAC-C3C	-2.41	1.44	1.51
34	D	412	LHG	C24-C23	2.41	1.57	1.50
22	B	608	CLA	CMB-C2B	-2.41	1.45	1.50
22	A	411	CLA	C1B-NB	-2.41	1.34	1.37
22	b	601	CLA	CAC-C3C	-2.41	1.44	1.51
22	c	515	CLA	CMB-C2B	-2.41	1.45	1.50
23	a	404	PHO	CBD-CGD	-2.41	1.49	1.52
29	A	413	SQD	O48-C23	2.40	1.40	1.33
22	B	612	CLA	MG-NB	2.40	2.10	2.05
28	C	519	LMG	C4-C3	2.40	1.58	1.52
22	B	616	CLA	MG-NA	2.40	2.12	2.06
22	B	603	CLA	C1B-C2B	2.40	1.48	1.43
23	d	401	PHO	CMC-C2C	-2.40	1.46	1.50
22	b	605	CLA	C1B-C2B	2.40	1.48	1.43
30	c	519	DGD	C3E-C2E	2.39	1.58	1.52
22	B	610	CLA	C1B-C2B	2.39	1.48	1.43
27	D	405	PL9	C3-C4	-2.39	1.45	1.49
22	c	513	CLA	CHC-C1C	2.38	1.43	1.38
22	A	402	CLA	C1D-C2D	2.38	1.50	1.45
28	b	621	LMG	O6-C1	2.38	1.48	1.41
30	C	517	DGD	O3D-C3D	-2.38	1.37	1.43
22	B	612	CLA	CMB-C2B	-2.38	1.45	1.50
22	C	512	CLA	CMB-C2B	-2.38	1.45	1.50
22	d	403	CLA	MG-NC	2.38	2.11	2.06
22	D	403	CLA	CHC-C4B	-2.38	1.34	1.39
22	B	608	CLA	MG-NA	2.38	2.11	2.06
35	v	201	HEC	C3B-C2B	-2.38	1.33	1.41
22	C	511	CLA	CHC-C1C	2.38	1.43	1.38
23	d	401	PHO	CMB-C2B	-2.38	1.46	1.51
30	A	415	DGD	O1G-C1G	-2.37	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	CHC-C1C	2.37	1.43	1.38
22	B	605	CLA	O2D-CGD	2.37	1.39	1.33
22	c	510	CLA	C4B-NB	2.37	1.41	1.37
22	B	607	CLA	CMD-C2D	-2.37	1.45	1.50
22	c	504	CLA	CMC-C2C	-2.36	1.45	1.50
22	b	614	CLA	C1B-C2B	2.36	1.48	1.43
24	K	101	BCR	C1-C6	-2.36	1.50	1.53
22	D	403	CLA	C4B-NB	2.36	1.41	1.37
22	c	505	CLA	CMC-C2C	-2.36	1.45	1.50
22	d	403	CLA	C1B-C2B	2.36	1.48	1.43
22	C	511	CLA	C1B-NB	-2.36	1.34	1.37
23	d	401	PHO	C1D-ND	2.36	1.42	1.38
22	C	504	CLA	C3B-C4B	2.36	1.49	1.42
22	c	515	CLA	CHC-C1C	2.35	1.43	1.38
22	c	505	CLA	MG-NB	2.35	2.10	2.05
28	d	409	LMG	O7-C8	-2.35	1.41	1.46
23	a	404	PHO	O2D-CGD	2.35	1.39	1.33
22	B	606	CLA	CMD-C2D	-2.35	1.46	1.50
22	h	101	CLA	CMC-C2C	-2.35	1.46	1.50
27	D	405	PL9	C46-C44	-2.34	1.46	1.51
28	D	406	LMG	C4-C3	2.34	1.58	1.52
22	C	511	CLA	CMD-C2D	-2.34	1.46	1.50
29	A	413	SQD	O47-C7	2.34	1.40	1.34
22	C	507	CLA	CAC-C3C	-2.34	1.45	1.51
22	b	605	CLA	C3B-C4B	2.34	1.49	1.42
22	B	614	CLA	C1B-C2B	2.34	1.48	1.43
22	C	513	CLA	CMC-C2C	-2.33	1.46	1.50
34	D	408	LHG	C3-C2	2.33	1.59	1.51
30	A	415	DGD	C3E-C2E	2.33	1.58	1.52
22	B	604	CLA	CMD-C2D	-2.33	1.46	1.50
22	A	402	CLA	O2D-CED	-2.33	1.40	1.45
30	C	517	DGD	O5D-C6D	-2.33	1.39	1.43
30	C	516	DGD	O6E-C1E	2.32	1.47	1.41
22	D	402	CLA	CAA-C2A	-2.32	1.49	1.54
22	b	603	CLA	C1B-C2B	2.32	1.48	1.43
22	C	507	CLA	C3B-C4B	2.32	1.49	1.42
30	C	517	DGD	O2G-C2G	-2.32	1.41	1.46
28	M	101	LMG	C9-C8	2.32	1.58	1.50
30	h	102	DGD	C4D-C3D	2.32	1.58	1.52
22	C	511	CLA	C3B-C4B	2.32	1.49	1.42
22	B	617	CLA	C1D-ND	2.32	1.40	1.37
22	C	514	CLA	CMB-C2B	-2.31	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	CMB-C2B	-2.31	1.46	1.50
22	C	512	CLA	CMC-C2C	-2.31	1.46	1.50
22	b	613	CLA	C1D-ND	2.31	1.40	1.37
22	C	513	CLA	C4B-NB	2.31	1.40	1.37
22	C	502	CLA	CMC-C2C	-2.31	1.46	1.50
22	C	512	CLA	C3B-C4B	2.31	1.49	1.42
28	B	629	LMG	O8-C28	2.31	1.40	1.33
22	c	514	CLA	C3D-C4D	2.31	1.49	1.44
22	B	603	CLA	CHC-C1C	2.30	1.43	1.38
22	D	402	CLA	C1B-C2B	2.30	1.48	1.43
34	D	408	LHG	C4-C5	2.30	1.58	1.50
22	B	608	CLA	C4B-NB	2.30	1.40	1.37
30	H	102	DGD	C1E-C2E	2.30	1.59	1.52
30	C	517	DGD	C1E-C2E	2.30	1.59	1.52
24	t	101	BCR	C30-C25	-2.30	1.50	1.53
22	b	615	CLA	C1B-C2B	2.30	1.48	1.43
22	b	613	CLA	C3B-C4B	2.30	1.49	1.42
27	d	405	PL9	C16-C14	-2.29	1.46	1.51
22	B	604	CLA	CHC-C1C	2.29	1.43	1.38
30	C	516	DGD	C3D-C2D	2.29	1.58	1.52
22	c	503	CLA	C4B-NB	2.29	1.40	1.37
35	F	101	HEC	C3B-C2B	-2.29	1.33	1.41
22	b	605	CLA	CHC-C4B	-2.29	1.34	1.39
22	c	509	CLA	C4B-NB	2.29	1.40	1.37
22	D	402	CLA	C4B-NB	2.29	1.40	1.37
22	b	614	CLA	MG-ND	-2.29	2.01	2.05
22	b	610	CLA	C3B-C4B	2.29	1.49	1.42
22	B	616	CLA	C3D-C4D	2.28	1.49	1.44
28	c	525	LMG	C1-C2	2.28	1.59	1.52
24	B	620	BCR	C38-C26	-2.28	1.47	1.50
22	B	609	CLA	C3B-C4B	2.28	1.49	1.42
22	B	602	CLA	CMC-C2C	-2.28	1.46	1.50
29	f	101	SQD	O3-C3	-2.28	1.37	1.43
22	B	610	CLA	MG-NB	-2.28	2.01	2.05
23	d	401	PHO	C3D-C4D	2.27	1.44	1.41
27	a	410	PL9	C25-C24	-2.27	1.45	1.50
22	B	608	CLA	C3B-C4B	2.27	1.49	1.42
24	a	406	BCR	C38-C26	-2.27	1.47	1.50
24	x	101	BCR	C1-C6	-2.27	1.50	1.53
22	C	512	CLA	CHC-C1C	2.27	1.43	1.38
22	C	509	CLA	MG-ND	2.27	2.10	2.05
34	d	408	LHG	P-O6	2.27	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	101	CLA	O2A-CGA	2.27	1.40	1.33
22	b	612	CLA	MG-ND	-2.27	2.01	2.05
22	C	503	CLA	CHC-C1C	2.27	1.43	1.38
30	C	518	DGD	O1G-C1G	-2.26	1.40	1.45
22	c	506	CLA	CMD-C2D	-2.26	1.46	1.50
22	c	503	CLA	CMD-C2D	-2.26	1.46	1.50
22	A	403	CLA	C1B-C2B	2.26	1.48	1.43
22	c	508	CLA	C1B-NB	-2.26	1.34	1.37
24	C	515	BCR	C27-C26	-2.26	1.46	1.51
29	A	413	SQD	O2-C2	-2.26	1.37	1.43
22	c	514	CLA	C1B-NB	-2.25	1.34	1.37
22	b	615	CLA	CAB-C3B	-2.25	1.41	1.47
22	A	403	CLA	CHC-C4B	-2.25	1.34	1.39
27	A	410	PL9	C37-C38	2.25	1.57	1.50
24	b	616	BCR	C33-C5	-2.25	1.47	1.50
22	A	405	CLA	C1B-NB	-2.25	1.34	1.37
22	c	506	CLA	C3B-C4B	2.25	1.49	1.42
24	x	101	BCR	C33-C5	-2.25	1.47	1.50
22	c	515	CLA	MG-NA	-2.24	2.00	2.06
35	e	101	HEC	CMB-C2B	2.24	1.55	1.50
27	d	405	PL9	C51-C49	-2.24	1.44	1.50
22	b	606	CLA	CMC-C2C	-2.24	1.46	1.50
27	D	405	PL9	C26-C24	-2.24	1.46	1.51
22	B	614	CLA	CHC-C1C	2.24	1.43	1.38
22	C	505	CLA	C1B-C2B	2.24	1.48	1.43
28	B	629	LMG	O7-C10	2.24	1.40	1.34
22	B	615	CLA	CMB-C2B	-2.24	1.46	1.50
28	c	525	LMG	O1-C7	-2.23	1.39	1.43
22	B	612	CLA	CMD-C2D	-2.23	1.46	1.50
22	c	509	CLA	CMB-C2B	-2.23	1.46	1.50
22	b	606	CLA	C1B-NB	-2.23	1.34	1.37
30	c	519	DGD	C1D-C2D	2.23	1.59	1.52
34	D	408	LHG	O7-C5	-2.22	1.41	1.46
22	B	616	CLA	CHC-C4B	-2.22	1.34	1.39
22	D	403	CLA	CMB-C2B	-2.22	1.46	1.50
22	B	604	CLA	CAB-C3B	-2.22	1.41	1.47
22	C	512	CLA	C1B-NB	-2.22	1.34	1.37
28	c	522	LMG	O2-C2	-2.21	1.37	1.43
22	B	607	CLA	CHC-C1C	2.21	1.42	1.38
22	b	607	CLA	MG-NB	-2.21	2.01	2.05
28	c	524	LMG	C1-C2	2.21	1.59	1.52
27	a	410	PL9	C10-C9	-2.21	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	403	CLA	C4B-NB	2.21	1.40	1.37
22	B	606	CLA	MG-NB	2.21	2.10	2.05
22	C	509	CLA	CHC-C1C	2.21	1.42	1.38
22	C	503	CLA	C3B-C4B	2.20	1.49	1.42
34	l	101	LHG	P-O6	2.20	1.68	1.59
30	H	102	DGD	C6D-C5D	2.20	1.58	1.51
22	B	608	CLA	C1B-C2B	2.20	1.48	1.43
22	b	614	CLA	CMC-C2C	-2.20	1.46	1.50
22	c	508	CLA	C1D-ND	2.20	1.40	1.37
24	b	616	BCR	C38-C26	-2.19	1.47	1.50
24	x	101	BCR	C36-C18	-2.19	1.46	1.50
22	B	606	CLA	CMC-C2C	-2.19	1.46	1.50
22	B	610	CLA	CAB-C3B	-2.19	1.41	1.47
22	B	613	CLA	C3B-C4B	2.19	1.49	1.42
22	c	512	CLA	C3B-C4B	2.19	1.49	1.42
22	a	403	CLA	CHC-C1C	2.19	1.42	1.38
22	b	601	CLA	CMD-C2D	-2.19	1.46	1.50
22	c	515	CLA	CMC-C2C	-2.19	1.46	1.50
22	A	411	CLA	C3B-C4B	2.19	1.49	1.42
22	b	610	CLA	MG-NA	2.19	2.11	2.06
22	B	615	CLA	C1B-C2B	2.19	1.48	1.43
22	C	510	CLA	C1B-C2B	2.19	1.48	1.43
35	e	101	HEC	CMC-C2C	2.19	1.55	1.50
22	b	602	CLA	C1B-C2B	2.18	1.48	1.43
30	h	102	DGD	O2D-C2D	-2.18	1.37	1.43
22	C	504	CLA	CMB-C2B	-2.18	1.46	1.50
22	b	612	CLA	C3C-C2C	2.17	1.41	1.36
24	B	619	BCR	C1-C6	-2.17	1.51	1.53
22	c	503	CLA	C1D-ND	2.17	1.40	1.37
23	a	404	PHO	CMD-C2D	-2.17	1.47	1.51
22	b	611	CLA	C4B-NB	2.17	1.40	1.37
22	A	411	CLA	CMD-C2D	-2.17	1.46	1.50
22	b	615	CLA	C3D-C4D	2.17	1.49	1.44
22	A	403	CLA	CMB-C2B	-2.17	1.46	1.50
22	h	101	CLA	C3B-C4B	2.17	1.49	1.42
22	D	403	CLA	C3D-C4D	2.17	1.49	1.44
22	C	504	CLA	CMC-C2C	-2.16	1.46	1.50
35	F	101	HEC	CMC-C2C	2.16	1.55	1.50
22	c	512	CLA	C4B-NB	2.16	1.40	1.37
22	C	507	CLA	CHC-C1C	2.16	1.42	1.38
22	b	611	CLA	C3B-C4B	2.16	1.49	1.42
22	a	405	CLA	CAC-C3C	-2.16	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	CMC-C2C	-2.16	1.46	1.50
22	D	403	CLA	C3B-C4B	2.16	1.49	1.42
22	b	601	CLA	CHC-C4B	-2.16	1.34	1.39
22	B	607	CLA	MG-NC	-2.16	2.01	2.06
22	B	609	CLA	C1D-C2D	2.15	1.49	1.45
22	B	602	CLA	MG-ND	-2.15	2.01	2.05
30	C	518	DGD	C6E-C5E	2.15	1.59	1.51
22	B	613	CLA	C1B-NB	-2.15	1.35	1.37
23	A	404	PHO	CMB-C2B	-2.15	1.47	1.51
28	D	411	LMG	O8-C28	2.15	1.37	1.30
28	M	101	LMG	O6-C1	2.15	1.47	1.41
27	D	405	PL9	C31-C29	-2.15	1.46	1.51
24	A	406	BCR	C33-C5	-2.14	1.47	1.50
23	D	401	PHO	CMD-C2D	-2.14	1.47	1.51
22	B	605	CLA	MG-NB	2.14	2.10	2.05
34	e	102	LHG	O7-C5	-2.14	1.41	1.46
27	A	410	PL9	C25-C24	-2.14	1.45	1.50
30	c	520	DGD	C4D-C5D	2.14	1.57	1.53
30	c	521	DGD	C6D-C5D	2.14	1.58	1.51
30	h	102	DGD	C1E-C2E	2.14	1.58	1.52
22	B	615	CLA	CHC-C1C	2.14	1.42	1.38
22	A	411	CLA	CMB-C2B	-2.14	1.46	1.50
22	C	502	CLA	MG-NC	2.14	2.11	2.06
22	b	602	CLA	C1A-CHA	-2.14	1.34	1.43
22	d	402	CLA	C1B-C2B	2.14	1.48	1.43
22	c	510	CLA	CMC-C2C	-2.13	1.46	1.50
22	c	513	CLA	C4B-NB	2.13	1.40	1.37
22	C	511	CLA	MG-NC	2.13	2.11	2.06
22	B	610	CLA	MG-ND	2.13	2.10	2.05
29	f	101	SQD	O2-C2	-2.13	1.37	1.43
22	b	605	CLA	CAC-C3C	-2.13	1.45	1.51
22	c	505	CLA	C3D-C4D	2.13	1.49	1.44
22	C	509	CLA	CMB-C2B	-2.13	1.46	1.50
22	c	503	CLA	C1B-C2B	2.13	1.48	1.43
22	b	606	CLA	C1B-C2B	2.12	1.48	1.43
22	b	601	CLA	CMB-C2B	-2.12	1.46	1.50
29	A	413	SQD	O47-C45	-2.12	1.41	1.46
22	B	605	CLA	MG-NC	2.12	2.11	2.06
22	a	403	CLA	CMB-C2B	-2.11	1.46	1.50
30	c	519	DGD	C3G-C2G	2.11	1.57	1.50
22	c	508	CLA	CHC-C1C	2.11	1.42	1.38
22	d	403	CLA	O1D-CGD	2.11	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	C3B-C4B	2.10	1.48	1.42
22	B	611	CLA	CHC-C1C	2.10	1.42	1.38
28	c	522	LMG	C7-C8	2.10	1.57	1.50
22	b	608	CLA	C1B-C2B	2.10	1.48	1.43
22	c	507	CLA	C1B-C2B	2.10	1.48	1.43
22	B	605	CLA	MG-ND	-2.10	2.01	2.05
29	f	101	SQD	O4-C4	-2.10	1.37	1.43
22	c	507	CLA	CMC-C2C	-2.10	1.46	1.50
22	d	403	CLA	CHC-C4B	-2.10	1.34	1.39
22	B	616	CLA	C1B-NB	-2.10	1.35	1.37
22	C	502	CLA	CAA-C2A	2.09	1.57	1.54
22	b	607	CLA	C1D-ND	2.09	1.40	1.37
35	e	101	HEC	C2A-C3A	-2.09	1.32	1.36
35	F	101	HEC	C3C-C2C	-2.09	1.34	1.41
28	B	629	LMG	C7-C8	2.09	1.57	1.50
30	h	102	DGD	C4E-C3E	2.09	1.57	1.52
22	b	603	CLA	C3B-C4B	2.09	1.48	1.42
22	c	513	CLA	C1D-C2D	2.09	1.49	1.45
22	b	615	CLA	CMD-C2D	-2.09	1.46	1.50
29	a	412	SQD	O3-C3	-2.09	1.37	1.43
22	a	405	CLA	CHC-C4B	-2.09	1.34	1.39
30	C	516	DGD	C4D-C5D	2.09	1.57	1.53
35	e	101	HEC	CMA-C3A	2.08	1.55	1.50
23	A	404	PHO	C3B-C2B	-2.08	1.37	1.40
22	b	601	CLA	CMC-C2C	-2.08	1.46	1.50
22	b	612	CLA	CMB-C2B	-2.08	1.46	1.50
28	d	409	LMG	C4-C5	2.08	1.57	1.53
22	B	612	CLA	C3B-C4B	2.08	1.48	1.42
22	C	513	CLA	CHC-C1C	2.07	1.42	1.38
22	b	609	CLA	CMB-C2B	-2.07	1.46	1.50
22	c	514	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	609	CLA	CMC-C2C	-2.07	1.46	1.50
22	b	603	CLA	CHC-C1C	2.07	1.42	1.38
22	C	512	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	610	CLA	CMC-C2C	-2.07	1.46	1.50
22	B	609	CLA	MG-NC	-2.07	2.01	2.06
22	b	605	CLA	C4D-CHA	2.07	1.45	1.38
34	E	101	LHG	O8-C23	2.07	1.39	1.33
22	b	613	CLA	C1B-C2B	2.07	1.48	1.43
22	C	510	CLA	O2D-CGD	2.07	1.38	1.33
22	b	602	CLA	CMC-C2C	-2.06	1.46	1.50
28	b	621	LMG	C6-C5	2.06	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	510	CLA	CMB-C2B	-2.06	1.46	1.50
24	B	618	BCR	C33-C5	-2.06	1.47	1.50
22	B	603	CLA	C1D-C2D	2.06	1.49	1.45
22	A	403	CLA	CHC-C1C	2.06	1.42	1.38
28	D	406	LMG	O7-C8	-2.06	1.41	1.46
22	B	603	CLA	C3C-C2C	2.05	1.41	1.36
22	C	511	CLA	CAA-C2A	-2.05	1.50	1.54
24	y	101	BCR	C38-C26	-2.05	1.47	1.50
30	C	518	DGD	C4D-C3D	2.05	1.57	1.52
22	B	613	CLA	C3D-C4D	2.05	1.48	1.44
24	b	617	BCR	C36-C18	-2.05	1.46	1.50
22	h	101	CLA	CMD-C2D	-2.05	1.46	1.50
23	d	401	PHO	CBD-CGD	-2.05	1.49	1.52
35	V	201	HEC	C3B-C2B	-2.05	1.34	1.41
30	c	519	DGD	O1A-C1A	2.05	1.28	1.22
22	c	508	CLA	C4B-NB	2.04	1.40	1.37
27	A	410	PL9	C7-C8	-2.04	1.47	1.50
22	a	403	CLA	C1B-C2B	2.04	1.47	1.43
22	C	514	CLA	CHC-C1C	2.04	1.42	1.38
22	b	603	CLA	MG-ND	-2.04	2.01	2.05
35	V	201	HEC	C3C-C2C	-2.04	1.34	1.41
22	b	615	CLA	CMA-C3A	-2.04	1.48	1.53
22	b	603	CLA	CAC-C3C	-2.04	1.45	1.51
22	c	509	CLA	C3D-C4D	2.04	1.48	1.44
22	C	513	CLA	C1A-CHA	-2.04	1.34	1.43
24	a	406	BCR	C30-C25	-2.04	1.51	1.53
22	c	509	CLA	CMC-C2C	-2.04	1.46	1.50
24	Y	101	BCR	C38-C26	-2.04	1.47	1.50
29	a	412	SQD	O4-C4	-2.03	1.37	1.43
28	M	101	LMG	O1-C7	-2.03	1.40	1.43
35	F	101	HEC	CMA-C3A	2.03	1.54	1.50
30	c	519	DGD	O1G-C1A	2.03	1.39	1.33
22	b	611	CLA	CHC-C1C	2.03	1.42	1.38
22	B	609	CLA	CMA-C3A	-2.02	1.48	1.53
22	A	403	CLA	MG-NA	-2.02	2.01	2.06
23	A	404	PHO	CMD-C2D	-2.02	1.47	1.51
22	B	617	CLA	CHC-C1C	2.02	1.42	1.38
24	Z	101	BCR	C33-C5	-2.02	1.47	1.50
22	C	510	CLA	CHC-C1C	2.02	1.42	1.38
22	A	403	CLA	CMC-C2C	-2.02	1.46	1.50
22	b	611	CLA	C1B-NB	-2.02	1.35	1.37
22	C	510	CLA	O2A-CGA	2.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	e	101	HEC	CHA-C4D	-2.01	1.34	1.39
34	d	406	LHG	C4-C5	2.01	1.57	1.50
29	B	623	SQD	O2-C2	-2.01	1.38	1.43
22	C	508	CLA	C3B-C4B	2.01	1.48	1.42
22	B	607	CLA	CHC-C4B	-2.01	1.34	1.39
22	c	512	CLA	CHC-C1C	2.01	1.42	1.38
33	B	625	STE	O1-C1	2.01	1.28	1.22
22	A	402	CLA	C3B-C4B	2.01	1.48	1.42
22	C	507	CLA	C3D-C4D	2.01	1.48	1.44
28	d	409	LMG	O8-C9	-2.01	1.40	1.45
22	C	506	CLA	C3B-C4B	2.01	1.48	1.42
22	c	508	CLA	MG-NC	2.01	2.11	2.06
22	c	508	CLA	C3B-C4B	2.01	1.48	1.42
28	c	525	LMG	O6-C5	-2.00	1.39	1.44
22	B	602	CLA	CMB-C2B	-2.00	1.46	1.50
30	A	415	DGD	O5D-C6D	-2.00	1.40	1.43
30	c	520	DGD	C6E-C5E	2.00	1.58	1.51

All (1334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	C4A-NA-C1A	11.43	111.89	106.68
22	B	605	CLA	C4A-NA-C1A	10.71	111.56	106.68
35	v	201	HEC	CBB-CAB-C3B	-10.06	107.32	127.43
22	b	605	CLA	C4A-NA-C1A	9.73	111.12	106.68
22	h	101	CLA	C4A-NA-C1A	9.72	111.11	106.68
22	C	504	CLA	C4A-NA-C1A	9.57	111.05	106.68
29	D	407	SQD	O6-C1-C2	9.27	122.35	108.27
29	b	619	SQD	O6-C1-C2	9.22	122.27	108.27
35	v	201	HEC	CBC-CAC-C3C	-8.99	109.47	127.43
22	C	508	CLA	C4A-NA-C1A	8.69	110.64	106.68
35	e	101	HEC	CBB-CAB-C3B	-8.51	110.42	127.43
22	C	509	CLA	C4A-NA-C1A	8.49	110.55	106.68
29	a	412	SQD	O6-C1-C2	8.31	120.90	108.27
22	b	606	CLA	C4A-NA-C1A	8.13	110.39	106.68
35	V	201	HEC	CBC-CAC-C3C	-8.07	111.31	127.43
29	A	413	SQD	O6-C1-C2	8.07	120.52	108.27
22	B	617	CLA	C4A-NA-C1A	7.72	110.20	106.68
29	B	623	SQD	O6-C1-C2	7.52	119.70	108.27
22	C	503	CLA	C4A-NA-C1A	7.49	110.10	106.68
22	b	601	CLA	C4A-NA-C1A	7.45	110.08	106.68
22	b	603	CLA	C4A-NA-C1A	7.40	110.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	505	CLA	C4A-NA-C1A	7.27	110.00	106.68
22	c	513	CLA	C4A-NA-C1A	7.27	110.00	106.68
22	a	405	CLA	C4A-NA-C1A	7.24	109.98	106.68
22	C	512	CLA	C4A-NA-C1A	7.11	109.92	106.68
22	c	511	CLA	C4A-NA-C1A	7.09	109.92	106.68
35	F	101	HEC	CBC-CAC-C3C	-6.90	113.65	127.43
22	C	510	CLA	C4A-NA-C1A	6.85	109.80	106.68
35	e	101	HEC	CBC-CAC-C3C	-6.84	113.75	127.43
22	B	608	CLA	C4A-NA-C1A	6.79	109.78	106.68
22	c	504	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	C	511	CLA	C4A-NA-C1A	6.49	109.64	106.68
35	V	201	HEC	CBB-CAB-C3B	-6.46	114.53	127.43
22	c	514	CLA	C4A-NA-C1A	6.36	109.58	106.68
22	b	614	CLA	C4A-NA-C1A	6.33	109.57	106.68
22	B	611	CLA	C4A-NA-C1A	6.28	109.54	106.68
22	B	611	CLA	O2D-CGD-O1D	-6.26	111.67	123.85
35	F	101	HEC	CBB-CAB-C3B	-6.25	114.94	127.43
22	B	610	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	C	502	CLA	C4A-NA-C1A	6.12	109.47	106.68
23	a	404	PHO	C4D-CHA-CBD	-6.11	105.52	108.45
23	A	404	PHO	C4D-CHA-CBD	-6.08	105.54	108.45
22	b	615	CLA	C4A-NA-C1A	6.03	109.43	106.68
22	B	613	CLA	C4A-NA-C1A	6.02	109.43	106.68
22	a	411	CLA	C4A-NA-C1A	5.98	109.41	106.68
27	D	405	PL9	C7-C3-C4	5.88	121.76	116.91
22	c	503	CLA	O2D-CGD-O1D	-5.88	112.39	123.85
29	f	101	SQD	O7-S-C6	5.88	115.54	106.76
22	c	510	CLA	C4A-NA-C1A	5.87	109.36	106.68
22	B	603	CLA	O2D-CGD-CBD	5.85	121.45	111.23
22	b	609	CLA	C4A-NA-C1A	5.77	109.31	106.68
27	A	410	PL9	C7-C3-C4	5.65	121.56	116.91
22	A	411	CLA	C4A-NA-C1A	5.64	109.25	106.68
22	D	402	CLA	C4A-NA-C1A	5.63	109.25	106.68
22	B	607	CLA	C4A-NA-C1A	5.63	109.25	106.68
22	c	503	CLA	C4A-NA-C1A	5.53	109.20	106.68
22	c	509	CLA	C4A-NA-C1A	5.52	109.20	106.68
27	a	410	PL9	C7-C3-C4	5.49	121.43	116.91
22	B	612	CLA	C4A-NA-C1A	5.47	109.18	106.68
22	b	612	CLA	C1-C2-C3	-5.46	117.24	126.20
22	b	615	CLA	O2D-CGD-O1D	-5.36	113.42	123.85
22	b	614	CLA	C3B-C4B-NB	-5.33	105.77	110.53
22	B	603	CLA	O2D-CGD-O1D	-5.26	113.60	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	f	101	SQD	O6-C1-C2	5.19	116.16	108.27
28	b	623	LMG	C1-O6-C5	-5.16	103.64	113.72
22	C	505	CLA	C4A-NA-C1A	5.14	109.02	106.68
22	B	615	CLA	C4A-NA-C1A	5.13	109.02	106.68
22	b	604	CLA	C4A-NA-C1A	5.12	109.01	106.68
22	B	604	CLA	C3B-C4B-NB	-5.10	105.98	110.53
22	C	514	CLA	C4A-NA-C1A	5.04	108.98	106.68
35	V	201	HEC	CHD-C4C-NC	5.00	129.90	124.45
29	D	407	SQD	O9-S-C6	4.95	114.15	106.76
34	D	409	LHG	O4-P-O5	4.92	135.35	112.44
22	c	503	CLA	O2D-CGD-CBD	4.81	119.63	111.23
27	d	405	PL9	C7-C3-C4	4.79	120.86	116.91
22	C	502	CLA	O2D-CGD-O1D	-4.78	114.54	123.85
22	C	507	CLA	C4A-NA-C1A	4.77	108.86	106.68
22	c	512	CLA	C4A-NA-C1A	4.76	108.85	106.68
22	a	402	CLA	C4A-NA-C1A	4.75	108.85	106.68
29	a	413	SQD	O48-C23-O10	-4.75	111.75	123.63
22	b	610	CLA	O2D-CGD-CBD	4.74	119.52	111.23
22	b	602	CLA	O2D-CGD-O1D	-4.73	114.65	123.85
22	b	610	CLA	O2D-CGD-O1D	-4.61	114.88	123.85
35	e	101	HEC	CBD-CAD-C3D	-4.55	99.95	112.53
22	D	403	CLA	C4A-NA-C1A	4.55	108.75	106.68
29	A	413	SQD	C1-C2-C3	-4.54	100.45	110.01
27	A	410	PL9	C7-C3-C2	-4.51	118.08	123.39
22	h	101	CLA	O2D-CGD-O1D	-4.49	115.10	123.85
22	b	607	CLA	C3B-C4B-NB	-4.49	106.52	110.53
23	a	404	PHO	CBC-CAC-C3C	4.46	119.26	112.87
29	A	413	SQD	O47-C7-C8	4.45	121.11	111.48
29	f	101	SQD	O9-S-O7	-4.42	99.44	113.82
22	B	611	CLA	C3B-C4B-NB	-4.37	106.63	110.53
22	c	514	CLA	C3B-C4B-NB	-4.35	106.65	110.53
34	E	101	LHG	O4-P-O5	4.34	132.62	112.44
26	A	409	BCT	O2-C-O1	4.33	130.76	119.68
29	A	414	SQD	C45-O47-C7	4.33	124.03	117.78
30	c	521	DGD	O3G-C3G-C2G	-4.32	100.32	110.82
22	B	616	CLA	C4A-NA-C1A	4.31	108.65	106.68
30	C	517	DGD	O3G-C3G-C2G	-4.30	100.35	110.82
22	C	509	CLA	O2D-CGD-O1D	-4.28	115.51	123.85
34	e	102	LHG	O4-P-O5	4.27	132.32	112.44
28	B	629	LMG	C1-O6-C5	-4.27	105.38	113.72
30	C	518	DGD	O3G-C3G-C2G	-4.27	100.44	110.82
34	D	412	LHG	O4-P-O5	4.25	132.24	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	619	SQD	O7-S-C6	4.23	113.08	106.76
22	b	609	CLA	O2D-CGD-O1D	-4.23	115.62	123.85
29	a	413	SQD	O47-C7-C8	4.21	120.59	111.48
28	B	629	LMG	C1-C2-C3	-4.21	101.16	110.01
34	l	101	LHG	O4-P-O5	4.20	131.99	112.44
29	A	413	SQD	C1-O5-C5	-4.20	105.52	113.72
22	c	514	CLA	C1-C2-C3	-4.19	119.33	126.20
29	B	623	SQD	O47-C7-C8	4.18	120.53	111.48
22	C	510	CLA	C3B-C4B-NB	-4.17	106.80	110.53
30	H	102	DGD	O3G-C3G-C2G	-4.17	100.67	110.82
22	b	601	CLA	O2D-CGD-CBD	4.16	118.51	111.23
34	B	622	LHG	O4-P-O5	4.16	131.80	112.44
24	H	101	BCR	C16-C15-C14	-4.16	115.01	123.52
22	B	609	CLA	O2D-CGD-O1D	-4.15	115.78	123.85
23	A	404	PHO	CMB-C2B-C3B	4.14	132.96	124.68
27	a	410	PL9	C7-C3-C2	-4.14	118.51	123.39
22	B	615	CLA	C3B-C4B-NB	-4.14	106.84	110.53
29	A	413	SQD	O9-S-O7	-4.10	100.47	113.82
34	D	412	LHG	O8-C23-C24	4.10	124.35	111.83
29	b	619	SQD	C1-C2-C3	-4.10	101.38	110.01
28	d	409	LMG	O1-C1-C2	-4.10	102.05	108.27
22	A	402	CLA	C4A-NA-C1A	4.09	108.55	106.68
22	B	612	CLA	O2D-CGD-O1D	-4.09	115.89	123.85
22	C	504	CLA	C7-C6-C5	-4.09	102.37	113.26
23	d	401	PHO	O1D-CGD-CBD	4.08	130.91	124.72
22	b	601	CLA	O2D-CGD-O1D	-4.08	115.91	123.85
22	b	602	CLA	C4A-NA-C1A	4.07	108.54	106.68
29	B	623	SQD	O7-S-C6	4.07	112.83	106.76
22	B	606	CLA	C3B-C4B-NB	-4.04	106.92	110.53
22	A	402	CLA	C3B-C4B-NB	-4.04	106.93	110.53
23	A	404	PHO	C3B-C4B-NB	-4.03	104.84	107.46
34	d	406	LHG	O8-C23-C24	4.02	124.09	111.83
22	B	602	CLA	CAA-CBA-CGA	-4.02	101.81	113.21
29	a	412	SQD	O7-S-C6	4.01	112.74	106.76
23	d	401	PHO	C4D-CHA-CBD	-3.98	106.54	108.45
34	d	406	LHG	O4-P-O5	3.98	130.95	112.44
27	d	405	PL9	C37-C38-C39	-3.97	118.54	127.62
23	a	404	PHO	OBD-CAD-CBD	-3.96	120.02	125.82
22	c	510	CLA	C3B-C4B-NB	-3.96	107.00	110.53
22	C	510	CLA	CHB-C4A-NA	3.95	130.10	124.40
22	B	614	CLA	C1-C2-C3	-3.95	119.73	126.20
29	a	412	SQD	O9-S-O7	-3.95	100.98	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	C1-C2-C3	-3.94	119.74	126.20
22	b	615	CLA	CHB-C4A-NA	3.92	130.06	124.40
22	b	613	CLA	C4A-NA-C1A	3.91	108.47	106.68
22	c	511	CLA	O2A-CGA-O1A	-3.89	113.89	123.63
22	B	602	CLA	CAA-C2A-C3A	-3.89	102.49	113.00
22	b	604	CLA	O2D-CGD-O1D	-3.89	116.28	123.85
24	A	406	BCR	C35-C13-C14	-3.88	116.53	122.82
23	D	401	PHO	C2B-C1B-NB	-3.88	106.63	109.43
22	D	402	CLA	CED-O2D-CGD	3.87	124.70	115.92
22	c	504	CLA	C3B-C4B-NB	-3.87	107.08	110.53
34	d	408	LHG	O4-P-O5	3.86	130.39	112.44
34	D	408	LHG	O4-P-O5	3.85	130.34	112.44
27	D	405	PL9	C7-C3-C2	-3.82	118.88	123.39
22	C	513	CLA	C3B-C4B-NB	-3.82	107.12	110.53
22	B	609	CLA	O2D-CGD-CBD	3.81	117.89	111.23
24	t	101	BCR	C3-C4-C5	-3.80	107.27	114.06
34	d	407	LHG	O4-P-O5	3.80	130.13	112.44
28	b	623	LMG	O2-C2-C1	-3.80	101.02	110.08
29	a	412	SQD	O9-S-C6	3.78	112.41	106.76
30	A	415	DGD	O5D-C1E-C2E	3.78	114.01	108.27
22	B	611	CLA	O2A-CGA-O1A	-3.78	114.18	123.63
22	b	612	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
24	b	616	BCR	C2-C1-C6	3.75	115.89	110.44
23	a	404	PHO	OBD-CAD-C3D	3.74	133.73	127.89
34	e	102	LHG	O8-C23-C24	3.74	123.24	111.83
22	B	612	CLA	O2D-CGD-CBD	3.74	117.76	111.23
22	C	503	CLA	C3B-C4B-NB	-3.74	107.19	110.53
35	e	101	HEC	CHD-C4C-NC	3.73	128.51	124.45
23	A	404	PHO	C2D-C1D-ND	3.72	112.12	109.43
35	F	101	HEC	CBA-CAA-C2A	-3.72	102.26	112.53
22	B	608	CLA	CED-O2D-CGD	3.71	124.33	115.92
27	a	410	PL9	C35-C34-C36	3.71	121.67	115.23
22	c	508	CLA	C4-C3-C5	3.70	121.64	115.23
22	B	605	CLA	C3B-C4B-NB	-3.69	107.23	110.53
22	C	506	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
22	b	611	CLA	C4A-NA-C1A	3.67	108.35	106.68
23	A	404	PHO	CBC-CAC-C3C	3.65	118.10	112.87
22	B	611	CLA	O2D-CGD-CBD	3.65	117.61	111.23
27	D	405	PL9	C22-C23-C24	-3.65	119.28	127.62
22	C	502	CLA	O2D-CGD-CBD	3.64	117.60	111.23
22	B	617	CLA	C1-O2A-CGA	3.64	125.46	116.65
30	c	520	DGD	O3G-C3G-C2G	-3.64	101.97	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	CLA	C4A-NA-C1A	3.63	108.34	106.68
22	b	604	CLA	C4-C3-C5	3.63	121.52	115.23
27	A	410	PL9	O2-C1-C6	3.61	126.22	120.48
24	Y	101	BCR	C27-C26-C25	3.61	127.58	122.70
30	A	415	DGD	C4E-C3E-C2E	-3.60	104.52	110.83
22	d	402	CLA	C4A-NA-C1A	3.59	108.32	106.68
22	c	504	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
22	c	508	CLA	CBC-CAC-C3C	-3.59	102.70	112.42
30	c	520	DGD	O2D-C2D-C1D	-3.58	101.54	110.08
27	d	405	PL9	C40-C39-C41	3.57	121.43	115.23
22	C	503	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
22	C	502	CLA	C3B-C4B-NB	-3.57	107.34	110.53
23	d	401	PHO	C2B-C1B-NB	-3.57	106.85	109.43
34	d	406	LHG	O8-C23-O10	-3.56	114.72	123.63
30	h	102	DGD	O3G-C3G-C2G	-3.56	102.16	110.82
22	c	505	CLA	C3B-C4B-NB	-3.56	107.35	110.53
24	C	515	BCR	C15-C16-C17	-3.56	116.25	123.52
24	T	101	BCR	C7-C8-C9	-3.55	120.98	126.23
22	b	606	CLA	C3B-C4B-NB	-3.55	107.36	110.53
35	v	201	HEC	CBD-CAD-C3D	-3.55	102.72	112.53
35	e	101	HEC	CMD-C2D-C1D	3.54	130.81	125.42
29	D	407	SQD	O8-S-C6	3.54	112.81	105.97
22	B	617	CLA	C1D-ND-C4D	3.53	108.79	106.31
29	A	413	SQD	O7-S-C6	3.52	112.01	106.76
24	c	518	BCR	C16-C15-C14	-3.52	116.33	123.52
22	a	402	CLA	CMB-C2B-C1B	-3.51	120.07	125.42
33	L	101	STE	O2-C1-C2	3.51	125.10	114.00
28	A	412	LMG	O6-C1-O1	-3.51	101.75	110.04
22	B	609	CLA	C4A-NA-C1A	3.50	108.27	106.68
24	D	404	BCR	C24-C23-C22	-3.50	121.06	126.23
24	Z	101	BCR	C33-C5-C6	-3.49	120.67	124.48
28	b	621	LMG	O1-C1-C2	-3.49	102.97	108.27
22	A	403	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
22	b	609	CLA	CAC-C3C-C4C	3.48	129.32	124.79
28	b	621	LMG	O3-C3-C2	-3.48	102.17	110.38
29	A	414	SQD	O48-C23-C24	3.48	122.43	111.83
27	D	405	PL9	C42-C43-C44	-3.47	119.67	127.62
22	a	402	CLA	CAC-C3C-C4C	3.47	129.31	124.79
30	h	102	DGD	C1D-C2D-C3D	-3.46	102.72	110.01
22	B	615	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
23	D	401	PHO	O2D-CGD-O1D	-3.46	117.12	123.85
27	d	405	PL9	C22-C23-C24	-3.45	119.72	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	F	101	HEC	CBD-CAD-C3D	-3.44	103.03	112.53
22	b	613	CLA	C3B-C4B-NB	-3.44	107.46	110.53
22	C	503	CLA	O1D-CGD-CBD	3.43	131.28	124.52
22	C	504	CLA	C3B-C4B-NB	-3.42	107.48	110.53
30	C	516	DGD	O3G-C3G-C2G	-3.42	102.50	110.82
22	C	505	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
27	A	410	PL9	C22-C23-C24	-3.41	119.82	127.62
22	B	607	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
24	B	620	BCR	C2-C1-C6	3.41	115.39	110.44
22	B	617	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
35	e	101	HEC	CBA-CAA-C2A	-3.40	103.12	112.53
27	D	405	PL9	C37-C38-C39	-3.39	119.85	127.62
22	B	613	CLA	O2A-CGA-O1A	-3.39	115.16	123.63
22	C	506	CLA	CAC-C3C-C4C	3.38	129.19	124.79
22	C	508	CLA	C1-C2-C3	-3.38	120.66	126.20
22	B	608	CLA	CMB-C2B-C1B	-3.38	120.27	125.42
22	c	506	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
30	H	102	DGD	O2D-C2D-C1D	-3.38	102.03	110.08
22	d	403	CLA	CMB-C2B-C1B	-3.38	120.28	125.42
22	d	403	CLA	CAC-C3C-C4C	3.37	129.18	124.79
23	a	404	PHO	C3B-C4B-NB	-3.37	105.27	107.46
24	Z	101	BCR	C11-C10-C9	-3.37	122.56	127.28
24	a	406	BCR	C27-C26-C25	3.36	127.25	122.70
29	a	412	SQD	O48-C23-C24	3.35	122.05	111.83
22	B	605	CLA	O2D-CGD-CBD	3.35	117.08	111.23
22	B	602	CLA	O2D-CGD-O1D	-3.35	117.34	123.85
22	c	507	CLA	C3B-C4B-NB	-3.34	107.55	110.53
22	c	508	CLA	C4A-NA-C1A	3.34	108.20	106.68
22	c	514	CLA	O2A-CGA-O1A	-3.33	115.30	123.63
22	C	503	CLA	C4D-CHA-C1A	3.33	125.21	121.24
22	C	513	CLA	O2D-CGD-CBD	3.32	117.04	111.23
22	b	612	CLA	CED-O2D-CGD	3.32	123.45	115.92
22	B	613	CLA	CHB-C4A-NA	3.32	129.19	124.40
22	h	101	CLA	CHB-C4A-NA	3.32	129.19	124.40
22	B	604	CLA	C4A-NA-C1A	3.32	108.19	106.68
24	B	619	BCR	C40-C30-C25	3.32	115.45	110.24
22	b	613	CLA	CHD-C1D-ND	-3.32	120.14	124.80
24	x	101	BCR	C33-C5-C6	-3.31	120.87	124.48
22	D	403	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
33	j	101	STE	O2-C1-C2	3.30	124.43	114.00
22	A	402	CLA	C1D-ND-C4D	-3.30	104.00	106.31
22	c	505	CLA	C7-C6-C5	-3.29	104.48	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	605	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
22	h	101	CLA	O2D-CGD-CBD	3.29	116.98	111.23
30	C	517	DGD	O2D-C2D-C1D	-3.28	102.25	110.08
22	B	603	CLA	CHB-C4A-NA	3.28	129.14	124.40
28	D	406	LMG	O1-C7-C8	-3.28	102.84	110.82
23	D	401	PHO	O1D-CGD-CBD	3.28	129.70	124.72
26	a	409	BCT	O2-C-O1	3.28	128.06	119.68
34	D	409	LHG	O8-C23-C24	3.28	121.82	111.83
22	b	610	CLA	CHB-C4A-NA	3.27	129.12	124.40
30	C	517	DGD	O6D-C1D-O3G	-3.27	102.32	110.04
22	b	604	CLA	C3B-C4B-NB	-3.26	107.62	110.53
22	C	503	CLA	CHD-C1D-ND	-3.25	120.23	124.80
29	B	623	SQD	C1-O5-C5	-3.24	107.39	113.72
22	b	602	CLA	C7-C6-C5	-3.24	104.63	113.26
22	B	614	CLA	C3B-C4B-NB	-3.24	107.64	110.53
22	a	403	CLA	C3B-C4B-NB	-3.23	107.64	110.53
22	d	402	CLA	O2A-CGA-O1A	-3.23	115.55	123.63
22	B	606	CLA	CHB-C4A-NA	3.22	129.05	124.40
29	f	101	SQD	C1-C2-C3	-3.22	103.24	110.01
29	D	407	SQD	O5-C1-C2	-3.22	103.76	110.37
29	a	412	SQD	C1-O5-C5	-3.22	107.44	113.72
22	c	514	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
22	c	512	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
22	C	505	CLA	C4-C3-C5	3.21	120.80	115.23
24	c	518	BCR	C11-C10-C9	-3.21	122.78	127.28
22	B	609	CLA	CHD-C1D-ND	-3.21	120.29	124.80
24	t	101	BCR	C7-C8-C9	-3.20	121.50	126.23
29	a	412	SQD	C1-C2-C3	-3.20	103.28	110.01
22	c	514	CLA	CHB-C4A-NA	3.20	129.01	124.40
29	D	407	SQD	C1-C2-C3	-3.20	103.29	110.01
22	b	602	CLA	C3B-C4B-NB	-3.19	107.68	110.53
29	a	413	SQD	O48-C23-C24	3.19	121.57	111.83
22	A	402	CLA	CHB-C4A-NA	3.19	129.00	124.40
24	B	620	BCR	C29-C30-C25	3.18	115.06	110.44
22	b	609	CLA	C1-C2-C3	-3.18	120.99	126.20
27	d	405	PL9	C7-C3-C2	-3.18	119.64	123.39
22	c	510	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
24	H	101	BCR	C27-C26-C25	3.18	127.00	122.70
24	x	101	BCR	C27-C26-C25	3.18	127.00	122.70
22	B	606	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
22	C	510	CLA	C1-C2-C3	-3.17	121.00	126.20
22	b	607	CLA	C4A-NA-C1A	3.17	108.13	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	619	SQD	O9-S-O7	-3.17	103.52	113.82
22	c	509	CLA	O2A-CGA-O1A	-3.16	115.71	123.63
22	C	511	CLA	CHB-C4A-NA	3.16	128.96	124.40
28	b	623	LMG	O1-C1-C2	-3.16	103.48	108.27
35	V	201	HEC	CBD-CAD-C3D	-3.15	103.82	112.53
24	a	406	BCR	C29-C30-C25	3.15	115.01	110.44
22	b	607	CLA	O2A-CGA-O1A	-3.15	115.76	123.63
22	b	608	CLA	C3B-C4B-NB	-3.15	107.72	110.53
22	B	611	CLA	O1D-CGD-CBD	3.14	130.72	124.52
29	b	619	SQD	O47-C7-C8	3.14	118.28	111.48
22	b	604	CLA	O1D-CGD-CBD	3.14	130.71	124.52
22	b	613	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
22	a	405	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
23	d	401	PHO	CMB-C2B-C3B	3.13	130.93	124.68
27	a	410	PL9	C22-C23-C24	-3.13	120.47	127.62
22	a	403	CLA	C4A-NA-C1A	3.12	108.10	106.68
35	e	101	HEC	CHC-C4B-C3B	3.12	130.47	125.21
22	B	602	CLA	C3B-C4B-NB	-3.12	107.75	110.53
22	C	508	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
22	b	612	CLA	C4A-NA-C1A	3.11	108.10	106.68
30	C	518	DGD	O6D-C1D-O3G	-3.11	102.70	110.04
23	a	404	PHO	C2B-C1B-NB	-3.10	107.19	109.43
22	C	513	CLA	C4A-NA-C1A	3.10	108.09	106.68
24	H	101	BCR	C2-C1-C6	3.10	114.94	110.44
29	B	623	SQD	O48-C23-C24	3.10	121.27	111.83
24	b	617	BCR	C27-C26-C25	3.09	126.89	122.70
29	A	413	SQD	O9-S-C6	3.09	111.37	106.76
22	C	514	CLA	C3B-C4B-NB	-3.09	107.77	110.53
24	x	101	BCR	C37-C22-C21	-3.09	117.81	122.82
34	D	412	LHG	O3-P-O5	-3.09	96.70	108.94
24	a	406	BCR	C30-C25-C26	-3.08	118.43	122.64
22	b	608	CLA	C4A-NA-C1A	3.08	108.08	106.68
28	c	525	LMG	O6-C1-O1	-3.07	102.79	110.04
28	A	412	LMG	C1-O6-C5	-3.06	107.74	113.72
22	d	403	CLA	O2A-CGA-O1A	-3.06	115.96	123.63
24	T	101	BCR	C27-C26-C25	3.06	126.83	122.70
22	B	606	CLA	CHD-C1D-ND	-3.06	120.50	124.80
24	b	617	BCR	C15-C14-C13	-3.05	123.00	127.28
30	c	520	DGD	O3G-C1D-C2D	-3.05	103.64	108.27
22	C	513	CLA	C1-C2-C3	-3.05	121.20	126.20
24	b	618	BCR	C2-C1-C6	3.05	114.87	110.44
30	c	519	DGD	O2G-C1B-O1B	-3.04	116.60	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	606	CLA	C1D-ND-C4D	-3.04	104.18	106.31
22	b	605	CLA	CGD-CBD-CAD	-3.03	101.02	110.85
24	C	515	BCR	C36-C18-C17	-3.03	117.90	122.82
22	C	514	CLA	O2A-CGA-O1A	-3.03	116.04	123.63
22	b	611	CLA	O2A-CGA-O1A	-3.03	116.05	123.63
22	b	612	CLA	CHB-C4A-NA	3.03	128.77	124.40
22	B	614	CLA	OBD-CAD-C3D	3.02	135.49	128.42
28	C	519	LMG	O1-C7-C8	-3.02	103.48	110.82
22	A	402	CLA	O1D-CGD-CBD	3.02	130.47	124.52
34	D	408	LHG	O8-C23-C24	3.01	121.00	111.83
35	v	201	HEC	CHB-C1B-NB	3.00	129.31	123.86
29	D	407	SQD	O48-C23-C24	3.00	120.99	111.83
27	A	410	PL9	O2-C1-C2	-3.00	115.02	121.83
30	A	415	DGD	O2D-C2D-C1D	-2.99	102.94	110.08
22	C	505	CLA	C3B-C4B-NB	-2.99	107.86	110.53
22	b	601	CLA	CHB-C4A-NA	2.99	128.72	124.40
22	C	506	CLA	C3B-C4B-NB	-2.99	107.86	110.53
27	D	405	PL9	C7-C8-C9	-2.99	121.69	126.83
35	V	201	HEC	CMC-C2C-C1C	-2.98	120.88	125.42
22	A	402	CLA	CHD-C1D-ND	-2.98	120.61	124.80
24	b	617	BCR	C30-C25-C26	-2.98	118.56	122.64
22	C	508	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	A	403	CLA	CED-O2D-CGD	-2.98	109.16	115.92
29	b	619	SQD	O5-C5-C4	2.98	115.06	109.70
22	b	609	CLA	CHC-C4B-NB	2.98	128.51	124.05
34	D	408	LHG	O8-C23-O10	-2.98	116.19	123.63
28	B	629	LMG	O6-C1-C2	-2.97	104.26	110.37
22	b	615	CLA	O2D-CGD-CBD	2.97	116.43	111.23
22	B	616	CLA	CHB-C4A-NA	2.97	128.69	124.40
22	b	602	CLA	CMB-C2B-C1B	-2.97	120.89	125.42
22	b	604	CLA	C1-C2-C3	-2.97	121.33	126.20
22	b	606	CLA	C6-C7-C8	-2.97	106.09	115.97
28	b	621	LMG	O7-C10-O9	-2.97	116.76	123.70
24	c	518	BCR	C27-C26-C25	2.97	126.71	122.70
22	b	611	CLA	C11-C12-C13	-2.97	106.10	115.97
22	C	508	CLA	C4-C3-C5	2.97	120.38	115.23
24	Y	101	BCR	C30-C25-C26	-2.97	118.58	122.64
22	B	604	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
22	B	607	CLA	C3B-C4B-NB	-2.96	107.89	110.53
22	b	605	CLA	C1C-C2C-C3C	-2.95	103.87	106.98
22	b	614	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
24	c	517	BCR	C35-C13-C14	-2.95	118.04	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	505	CLA	CMB-C2B-C1B	-2.94	120.94	125.42
22	D	403	CLA	CHB-C1B-NB	2.94	128.46	124.05
24	y	101	BCR	C33-C5-C6	-2.94	121.28	124.48
30	C	516	DGD	O1G-C1A-C2A	-2.94	102.88	111.83
35	V	201	HEC	CHD-C4C-C3C	-2.93	120.27	125.21
22	C	511	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	Z	101	BCR	C24-C23-C22	-2.93	121.90	126.23
22	C	509	CLA	C1D-ND-C4D	2.92	108.36	106.31
30	c	521	DGD	C3D-C4D-C5D	-2.92	104.93	110.23
22	B	606	CLA	C7-C6-C5	-2.92	105.47	113.26
22	c	513	CLA	C3B-C4B-NB	-2.92	107.92	110.53
29	D	407	SQD	C1-O5-C5	-2.92	108.02	113.72
22	c	508	CLA	C3B-C4B-NB	-2.92	107.92	110.53
29	A	413	SQD	O47-C7-O49	-2.92	116.88	123.70
28	d	409	LMG	O6-C1-O1	-2.92	103.15	110.04
22	B	605	CLA	C11-C12-C13	-2.92	106.28	115.97
27	a	410	PL9	C20-C19-C21	2.91	120.28	115.23
28	b	621	LMG	C38-C37-C36	-2.91	99.66	114.37
22	d	403	CLA	CMB-C2B-C3B	2.91	133.39	126.55
28	d	409	LMG	O2-C2-C1	-2.91	103.15	110.08
22	b	605	CLA	O1D-CGD-CBD	2.90	130.24	124.52
30	c	519	DGD	O6E-C5E-C4E	2.90	114.93	109.70
29	a	413	SQD	O49-C7-C8	-2.90	112.44	123.78
24	A	406	BCR	C38-C26-C25	-2.90	121.32	124.48
30	c	519	DGD	O6D-C1D-O3G	-2.90	103.19	110.04
29	B	623	SQD	O9-S-O7	-2.90	104.39	113.82
30	A	415	DGD	C3G-C2G-C1G	-2.90	105.03	111.78
23	A	404	PHO	C4D-ND-C1D	-2.90	105.40	108.87
33	d	410	STE	O2-C1-C2	2.89	123.13	114.00
22	A	403	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
22	B	602	CLA	C1-C2-C3	-2.89	121.47	126.20
28	c	524	LMG	O7-C10-O9	-2.88	116.96	123.70
27	A	410	PL9	C27-C28-C29	-2.88	121.03	127.62
24	b	616	BCR	C3-C4-C5	-2.88	108.92	114.06
22	b	605	CLA	C2D-C1D-ND	-2.88	107.28	110.13
22	A	405	CLA	O2D-CGD-CBD	2.87	116.25	111.23
30	h	102	DGD	C3D-C4D-C5D	-2.87	105.03	110.23
24	T	101	BCR	C28-C27-C26	-2.87	108.94	114.06
24	d	404	BCR	C24-C23-C22	-2.87	121.99	126.23
22	c	513	CLA	CHB-C4A-NA	2.87	128.54	124.40
22	b	602	CLA	CHB-C1B-NB	2.87	128.35	124.05
27	D	405	PL9	C12-C13-C14	-2.87	121.07	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	O2D-CGD-CBD	2.86	116.24	111.23
28	b	623	LMG	C3-C4-C5	-2.86	105.04	110.23
22	b	604	CLA	C1D-ND-C4D	2.86	108.32	106.31
22	c	515	CLA	CHB-C4A-NA	2.86	128.53	124.40
28	b	621	LMG	C1-O6-C5	-2.86	108.13	113.72
28	D	406	LMG	C3-C4-C5	-2.85	105.06	110.23
22	b	615	CLA	O1D-CGD-CBD	2.85	130.15	124.52
22	B	604	CLA	O2A-CGA-O1A	-2.85	116.49	123.63
24	c	516	BCR	C11-C10-C9	-2.85	123.28	127.28
22	a	403	CLA	CHB-C4A-NA	2.85	128.51	124.40
22	B	613	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
22	C	507	CLA	CHA-C1A-NA	-2.85	119.95	126.39
27	d	405	PL9	C36-C34-C33	-2.84	114.78	121.17
22	b	605	CLA	C1D-ND-C4D	2.83	108.30	106.31
22	B	614	CLA	CHA-C1A-NA	-2.83	119.98	126.39
22	A	402	CLA	CMD-C2D-C1D	2.83	129.71	124.73
24	A	406	BCR	C27-C26-C25	2.83	126.52	122.70
22	B	617	CLA	C5-C3-C2	2.82	127.50	121.17
22	a	403	CLA	O2D-CGD-CBD	2.82	116.16	111.23
27	D	405	PL9	C32-C33-C34	-2.82	121.17	127.62
34	d	407	LHG	C20-C19-C18	-2.82	100.11	114.37
22	B	605	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
29	b	619	SQD	O2-C2-C1	2.82	116.79	110.08
24	x	101	BCR	C2-C1-C6	2.82	114.53	110.44
29	B	623	SQD	O5-C5-C4	2.81	114.77	109.70
24	c	516	BCR	C33-C5-C6	-2.81	121.42	124.48
22	b	608	CLA	CHD-C1D-ND	-2.81	120.85	124.80
24	b	618	BCR	C29-C30-C25	2.81	114.52	110.44
22	c	506	CLA	O2D-CGD-CBD	2.81	116.14	111.23
24	b	616	BCR	C8-C7-C6	-2.80	119.51	127.00
22	b	609	CLA	C2C-C1C-NC	2.80	112.92	109.98
22	B	617	CLA	CHB-C4A-NA	2.80	128.44	124.40
30	c	521	DGD	O6D-C1D-O3G	-2.80	103.44	110.04
22	C	506	CLA	O1D-CGD-CBD	2.80	130.03	124.52
22	B	612	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
22	B	615	CLA	CHA-C1A-NA	-2.79	120.07	126.39
24	c	517	BCR	C27-C26-C25	2.79	126.47	122.70
22	C	507	CLA	CHB-C4A-NA	2.79	128.42	124.40
22	b	601	CLA	CAC-C3C-C4C	2.79	128.42	124.79
22	A	411	CLA	C2C-C1C-NC	2.79	112.91	109.98
22	B	608	CLA	CMB-C2B-C3B	2.78	133.09	126.55
28	D	406	LMG	O6-C1-O1	-2.78	103.47	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	415	DGD	O1G-C1A-O1A	-2.78	116.67	123.63
22	B	607	CLA	C6-C5-C3	-2.78	106.70	113.47
28	C	519	LMG	O1-C1-C2	-2.78	104.06	108.27
24	B	619	BCR	C29-C30-C25	2.77	114.47	110.44
24	B	618	BCR	C2-C1-C6	2.77	114.47	110.44
24	B	618	BCR	C15-C16-C17	-2.77	117.85	123.52
22	b	604	CLA	C2D-C1D-ND	-2.77	107.38	110.13
30	h	102	DGD	O6E-C5E-C6E	-2.77	99.57	106.44
22	B	602	CLA	CHB-C4A-NA	2.77	128.39	124.40
22	C	513	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
22	B	615	CLA	CHB-C4A-NA	2.76	128.38	124.40
29	b	619	SQD	O48-C23-C24	2.75	120.22	111.83
27	A	410	PL9	C35-C34-C36	2.75	120.00	115.23
24	b	616	BCR	C15-C14-C13	-2.75	123.42	127.28
22	B	613	CLA	C11-C12-C13	-2.75	106.84	115.97
22	B	608	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
22	B	615	CLA	CMD-C2D-C3D	2.74	133.97	127.69
22	b	611	CLA	CHB-C4A-NA	2.74	128.35	124.40
23	d	401	PHO	C3D-C4D-ND	2.74	111.22	107.71
28	M	101	LMG	C1-C2-C3	-2.74	104.26	110.01
28	A	412	LMG	O8-C28-O10	-2.73	116.79	123.63
22	c	506	CLA	C7-C6-C5	-2.73	105.97	113.26
30	h	102	DGD	O3E-C3E-C2E	-2.73	103.94	110.38
33	E	102	STE	O2-C1-C2	2.73	122.61	114.00
30	C	516	DGD	C3G-C2G-C1G	-2.73	105.43	111.78
22	C	505	CLA	CHB-C1B-NB	2.73	128.14	124.05
22	c	503	CLA	CED-O2D-CGD	-2.72	109.74	115.92
22	B	609	CLA	CHD-C4C-NC	2.71	128.44	124.23
24	D	404	BCR	C27-C26-C25	2.71	126.36	122.70
22	D	403	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
33	b	622	STE	O2-C1-C2	2.71	122.55	114.00
22	B	602	CLA	C2A-C1A-CHA	2.71	128.56	123.87
24	b	616	BCR	C11-C10-C9	-2.71	123.48	127.28
22	B	617	CLA	C1-C2-C3	2.70	130.63	126.20
30	c	520	DGD	C3G-O3G-C1D	2.70	119.59	113.80
22	b	612	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
30	C	516	DGD	CDB-CCB-CBB	-2.70	100.71	114.37
24	T	101	BCR	C35-C13-C14	-2.70	118.44	122.82
22	B	608	CLA	C3B-C4B-NB	-2.70	108.12	110.53
22	b	602	CLA	CMB-C2B-C3B	2.70	132.90	126.55
22	B	612	CLA	C7-C6-C5	-2.70	106.07	113.26
34	d	406	LHG	C11-C10-C9	-2.69	100.75	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404	PHO	CMB-C2B-C3B	2.69	130.06	124.68
22	D	402	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	C	503	CLA	C1D-ND-C4D	2.69	108.20	106.31
22	C	509	CLA	C3B-C4B-NB	-2.69	108.13	110.53
28	c	525	LMG	C1-O6-C5	-2.69	108.47	113.72
28	B	629	LMG	O6-C5-C4	2.69	114.54	109.70
24	H	101	BCR	C35-C13-C14	-2.69	118.47	122.82
22	c	512	CLA	C3B-C4B-NB	-2.68	108.13	110.53
22	b	610	CLA	C7-C6-C5	-2.68	106.11	113.26
33	X	101	STE	C3-C2-C1	-2.68	107.51	114.51
23	A	404	PHO	C3D-C4D-ND	2.68	111.14	107.71
22	b	614	CLA	CHB-C4A-NA	2.68	128.26	124.40
30	c	519	DGD	C4D-C3D-C2D	-2.68	106.13	110.83
29	b	619	SQD	O8-S-C6	2.67	111.14	105.97
22	C	510	CLA	C2A-C1A-CHA	2.67	128.51	123.87
22	d	403	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
27	A	410	PL9	C30-C29-C31	-2.67	110.59	115.23
24	b	618	BCR	C15-C16-C17	-2.67	118.06	123.52
30	h	102	DGD	C3G-C2G-C1G	-2.67	105.56	111.78
30	c	519	DGD	CDB-CCB-CBB	-2.67	100.88	114.37
30	H	102	DGD	O2G-C1B-O1B	-2.67	117.47	123.70
22	A	411	CLA	C3B-C4B-NB	-2.66	108.16	110.53
22	b	602	CLA	C4-C3-C5	2.66	119.84	115.23
22	B	617	CLA	O1D-CGD-CBD	2.65	129.75	124.52
22	b	602	CLA	O2D-CGD-CBD	2.65	115.87	111.23
22	b	603	CLA	CHD-C1D-ND	-2.65	121.07	124.80
28	c	525	LMG	O7-C10-O9	-2.65	117.50	123.70
24	b	617	BCR	C31-C1-C6	2.65	114.40	110.24
22	D	403	CLA	O1D-CGD-CBD	2.65	129.75	124.52
22	B	612	CLA	CHD-C4C-NC	2.65	128.34	124.23
29	B	623	SQD	C3-C4-C5	2.65	115.03	110.23
24	b	616	BCR	C29-C30-C25	2.65	114.29	110.44
22	a	405	CLA	C4-C3-C5	2.65	119.82	115.23
22	b	613	CLA	CHB-C4A-NA	2.65	128.22	124.40
22	b	613	CLA	O2D-CGD-CBD	2.65	115.86	111.23
24	Z	101	BCR	C28-C27-C26	-2.64	109.34	114.06
28	c	524	LMG	C1-O6-C5	-2.64	108.56	113.72
22	B	609	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
22	C	512	CLA	CHA-C4D-ND	2.64	138.00	132.55
30	H	102	DGD	C3D-C4D-C5D	-2.64	105.45	110.23
28	c	524	LMG	O3-C3-C2	-2.64	104.15	110.38
22	B	610	CLA	O2D-CGD-CBD	2.64	115.84	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	413	SQD	C45-O47-C7	2.64	124.11	117.80
30	c	519	DGD	O6D-C1D-C2D	2.64	115.79	110.37
22	C	504	CLA	CHD-C1D-ND	-2.64	121.09	124.80
29	D	407	SQD	O8-S-O9	-2.63	104.81	111.40
22	b	614	CLA	CHB-C1B-NB	2.63	128.00	124.05
22	B	617	CLA	C2D-C1D-ND	-2.63	107.52	110.13
22	a	402	CLA	CMB-C2B-C3B	2.63	132.75	126.55
22	b	614	CLA	C1-O2A-CGA	2.63	123.02	116.65
33	B	624	STE	C3-C2-C1	-2.63	107.64	114.51
30	C	517	DGD	C1D-C2D-C3D	-2.63	104.48	110.01
22	B	615	CLA	C4-C3-C5	2.63	119.79	115.23
22	A	403	CLA	CMB-C2B-C3B	2.62	132.72	126.55
22	c	508	CLA	CMC-C2C-C1C	2.62	129.13	125.03
22	c	506	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
22	b	603	CLA	C3B-C4B-NB	-2.62	108.19	110.53
22	b	609	CLA	O2D-CGD-CBD	2.62	115.81	111.23
24	d	404	BCR	C33-C5-C6	-2.62	121.63	124.48
24	Y	101	BCR	C39-C30-C25	-2.62	106.14	110.24
22	b	604	CLA	CHC-C1C-NC	2.62	128.25	124.31
24	b	616	BCR	C35-C13-C12	2.62	122.08	118.09
29	f	101	SQD	O48-C23-O10	-2.61	117.09	123.63
22	b	608	CLA	CMB-C2B-C1B	-2.61	121.44	125.42
28	b	623	LMG	O6-C5-C6	2.61	112.91	106.44
29	b	619	SQD	O5-C1-C2	-2.61	105.00	110.37
22	B	605	CLA	CHB-C4A-NA	2.61	128.17	124.40
22	B	602	CLA	O2D-CGD-CBD	2.61	115.79	111.23
22	a	403	CLA	CHC-C4B-NB	2.61	127.97	124.05
34	E	101	LHG	O8-C23-C24	2.61	119.79	111.83
22	B	608	CLA	CHB-C1B-NB	2.61	127.96	124.05
29	f	101	SQD	O47-C7-C8	2.61	120.51	110.93
23	A	404	PHO	C2B-C1B-NB	-2.60	107.55	109.43
24	b	618	BCR	C32-C1-C6	-2.60	106.16	110.24
22	B	604	CLA	CHB-C4A-NA	2.60	128.16	124.40
35	V	201	HEC	CHB-C4A-NA	2.60	127.28	124.45
23	D	401	PHO	CMB-C2B-C3B	2.60	129.88	124.68
24	c	517	BCR	C11-C10-C9	-2.60	123.63	127.28
22	c	513	CLA	CHD-C1D-ND	-2.60	121.14	124.80
24	d	404	BCR	C16-C15-C14	-2.60	118.20	123.52
35	v	201	HEC	C4D-ND-C1D	2.60	110.06	105.82
24	B	619	BCR	C39-C30-C25	-2.60	106.17	110.24
30	H	102	DGD	C3E-C4E-C5E	-2.60	105.52	110.23
22	c	503	CLA	CHB-C4A-NA	2.60	128.15	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	618	BCR	C27-C26-C25	2.60	126.21	122.70
33	B	601	STE	O2-C1-C2	2.59	122.19	114.00
22	b	602	CLA	CMD-C2D-C1D	2.59	129.29	124.73
22	C	509	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
24	a	406	BCR	C7-C8-C9	-2.59	122.41	126.23
23	d	401	PHO	C1-C2-C3	-2.59	121.96	126.20
22	A	405	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
30	H	102	DGD	C1D-C2D-C3D	-2.59	104.57	110.01
24	B	619	BCR	C15-C14-C13	-2.59	123.65	127.28
22	B	609	CLA	C1D-ND-C4D	-2.59	104.50	106.31
22	B	609	CLA	CHB-C4A-NA	2.58	128.13	124.40
24	c	517	BCR	C15-C16-C17	-2.58	118.24	123.52
24	H	101	BCR	C29-C30-C25	2.58	114.18	110.44
23	a	404	PHO	O2A-CGA-O1A	-2.58	117.18	123.63
22	h	101	CLA	C3B-C4B-NB	-2.58	108.23	110.53
28	D	406	LMG	O3-C3-C2	-2.57	104.32	110.38
22	B	604	CLA	C3B-C2B-C1B	-2.57	104.14	107.17
28	c	524	LMG	O2-C2-C1	-2.57	103.95	110.08
28	c	522	LMG	O7-C10-O9	-2.57	118.03	122.99
22	c	506	CLA	CMB-C2B-C1B	-2.57	121.51	125.42
34	e	102	LHG	C20-C19-C18	-2.57	101.40	114.37
22	B	611	CLA	CHB-C4A-NA	2.57	128.10	124.40
23	a	404	PHO	CMA-C3A-C4A	-2.56	109.08	114.61
22	h	101	CLA	CHD-C1D-ND	-2.56	121.20	124.80
22	d	403	CLA	O1D-CGD-CBD	2.56	129.57	124.52
22	d	403	CLA	C1-C2-C3	-2.56	122.00	126.20
22	b	602	CLA	CHC-C4B-NB	2.56	127.89	124.05
33	d	411	STE	O2-C1-O1	-2.56	116.75	123.33
23	d	401	PHO	C6-C7-C8	-2.56	107.47	115.97
22	C	509	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	C	514	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
29	b	619	SQD	C3-C4-C5	2.55	114.86	110.23
24	A	406	BCR	C15-C14-C13	-2.55	123.70	127.28
22	B	609	CLA	C3D-C4D-ND	2.55	114.13	109.99
27	A	410	PL9	C36-C34-C33	-2.55	115.45	121.17
27	D	405	PL9	C50-C49-C48	-2.55	115.01	122.66
24	C	515	BCR	C33-C5-C6	-2.55	121.71	124.48
30	c	519	DGD	O5E-C6E-C5E	-2.55	102.67	111.33
33	d	411	STE	O2-C1-C2	2.54	122.03	114.00
22	c	506	CLA	CHB-C4A-NA	2.54	128.07	124.40
22	B	613	CLA	CHD-C1D-ND	-2.53	121.23	124.80
22	b	605	CLA	C2A-C1A-CHA	2.53	128.26	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	508	CLA	C4-C3-C2	-2.53	117.12	123.63
22	B	616	CLA	C14-C13-C15	-2.53	102.25	111.27
22	C	509	CLA	C2D-C1D-ND	-2.53	107.62	110.13
28	d	409	LMG	C9-C8-C7	-2.53	105.88	111.78
22	b	605	CLA	CHB-C1B-C2B	-2.53	120.09	127.43
22	c	506	CLA	C3B-C4B-NB	-2.53	108.28	110.53
22	c	506	CLA	CHD-C4C-NC	2.53	128.15	124.23
24	c	518	BCR	C8-C7-C6	-2.52	120.26	127.00
22	b	602	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
22	d	402	CLA	C4-C3-C5	2.52	119.61	115.23
30	C	516	DGD	O2G-C1B-C2B	-2.52	106.02	111.48
22	b	603	CLA	C2A-C1A-CHA	2.52	128.24	123.87
22	B	614	CLA	O1D-CGD-CBD	2.52	129.49	124.52
24	T	101	BCR	C39-C30-C25	2.52	114.20	110.24
22	C	502	CLA	C2D-C1D-ND	-2.52	107.63	110.13
22	c	510	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
34	D	412	LHG	O8-C23-O10	-2.52	117.33	123.63
35	V	201	HEC	C1D-C2D-C3D	-2.52	103.93	106.82
22	C	513	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	A	405	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
24	d	404	BCR	C2-C1-C6	2.51	114.09	110.44
28	B	629	LMG	O5-C6-C5	-2.51	102.77	111.33
22	B	617	CLA	O2A-C1-C2	2.51	117.78	108.11
22	C	503	CLA	C4D-C3D-CAD	-2.51	105.38	108.11
22	B	611	CLA	CHD-C1D-ND	-2.51	121.27	124.80
35	F	101	HEC	CHA-C1A-NA	2.51	127.19	124.45
24	B	619	BCR	C11-C10-C9	-2.51	123.76	127.28
22	c	505	CLA	C3A-C2A-C1A	2.51	105.10	101.34
22	a	402	CLA	C7-C6-C5	-2.51	106.57	113.26
24	B	619	BCR	C7-C8-C9	-2.51	122.52	126.23
22	C	504	CLA	O1D-CGD-CBD	2.51	129.47	124.52
22	B	603	CLA	C1-C2-C3	-2.51	122.09	126.20
24	a	406	BCR	C2-C1-C6	2.51	114.08	110.44
22	C	502	CLA	O2A-CGA-O1A	-2.51	117.36	123.63
22	C	504	CLA	C1-O2A-CGA	2.51	122.72	116.65
22	C	508	CLA	C2A-C1A-CHA	2.51	128.22	123.87
28	A	412	LMG	C38-C37-C36	-2.50	101.71	114.37
22	b	610	CLA	CED-O2D-CGD	-2.50	110.24	115.92
22	d	402	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	B	616	CLA	C3B-C4B-NB	-2.50	108.30	110.53
33	B	624	STE	O2-C1-C2	2.50	121.90	114.00
34	d	408	LHG	O8-C23-O10	-2.50	117.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	PHO	O2A-CGA-O1A	-2.50	117.38	123.63
28	D	406	LMG	C1-C2-C3	-2.50	104.76	110.01
22	c	504	CLA	C1-C2-C3	-2.50	122.11	126.20
22	a	402	CLA	C3B-C4B-NB	-2.49	108.30	110.53
22	B	602	CLA	CHC-C4B-NB	2.49	127.79	124.05
22	C	509	CLA	CHD-C1D-C2D	2.49	130.67	125.49
28	c	525	LMG	C40-C39-C38	-2.49	101.78	114.37
28	B	629	LMG	O7-C10-O9	-2.49	117.89	123.70
29	b	619	SQD	C45-O47-C7	2.49	123.75	117.80
33	L	101	STE	O1-C1-C2	-2.49	115.21	123.09
30	C	516	DGD	O6D-C1D-O3G	-2.48	104.18	110.04
30	H	102	DGD	C7B-C6B-C5B	-2.48	101.83	114.37
22	B	602	CLA	C3A-C2A-C1A	2.48	105.05	101.34
30	c	519	DGD	O1G-C1A-C2A	-2.48	104.28	111.83
30	C	518	DGD	O3E-C3E-C2E	-2.48	104.54	110.38
22	B	602	CLA	C4-C3-C5	2.47	119.52	115.23
22	C	512	CLA	C4-C3-C5	2.47	119.52	115.23
24	x	101	BCR	C38-C26-C25	-2.47	121.78	124.48
22	B	615	CLA	C2A-C1A-CHA	2.47	128.16	123.87
22	C	508	CLA	CHB-C4A-NA	2.47	127.97	124.40
33	C	522	STE	C3-C2-C1	-2.47	108.06	114.51
27	d	405	PL9	C15-C14-C13	-2.47	117.28	123.63
27	d	405	PL9	C12-C13-C14	-2.47	121.97	127.62
28	c	522	LMG	O6-C1-O1	-2.47	104.21	110.04
22	B	607	CLA	O2D-CGD-CBD	2.47	115.55	111.23
22	c	507	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
22	C	505	CLA	C6-C5-C3	2.47	119.48	113.47
22	b	602	CLA	O1D-CGD-CBD	2.47	129.38	124.52
24	A	406	BCR	C24-C23-C22	-2.47	122.59	126.23
22	c	507	CLA	CHB-C1B-NB	2.47	127.75	124.05
35	V	201	HEC	C4D-ND-C1D	2.46	109.84	105.82
22	B	605	CLA	C1-O2A-CGA	-2.46	110.69	116.65
22	B	617	CLA	C3B-C4B-NB	-2.46	108.33	110.53
35	F	101	HEC	C4D-C3D-C2D	-2.46	103.06	106.87
22	a	411	CLA	C3B-C4B-NB	-2.46	108.33	110.53
28	B	629	LMG	C9-C8-C7	-2.46	106.05	111.78
22	c	514	CLA	O1D-CGD-CBD	2.46	129.37	124.52
30	H	102	DGD	C1E-O6E-C5E	2.46	118.52	113.72
22	B	605	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
22	B	604	CLA	C2D-C1D-ND	-2.46	107.69	110.13
28	C	519	LMG	O2-C2-C1	-2.46	104.22	110.08
22	C	508	CLA	C1C-C2C-C3C	-2.45	104.40	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	604	CLA	CHD-C1D-C2D	2.45	130.59	125.49
30	C	516	DGD	C3D-C4D-C5D	-2.45	105.79	110.23
27	a	410	PL9	C7-C8-C9	-2.45	122.61	126.83
22	B	615	CLA	C4D-C3D-CAD	-2.45	105.44	108.11
22	b	607	CLA	CHB-C4A-NA	2.45	127.93	124.40
22	a	405	CLA	O2D-CGD-CBD	2.45	115.51	111.23
24	t	101	BCR	C15-C16-C17	-2.45	118.51	123.52
22	A	405	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
29	D	407	SQD	C44-O6-C1	2.44	117.85	113.68
22	b	602	CLA	C5-C3-C2	-2.44	115.69	121.17
33	B	621	STE	C3-C2-C1	-2.44	108.14	114.51
23	D	401	PHO	C3D-C4D-ND	2.44	110.83	107.71
29	f	101	SQD	O5-C1-O6	2.44	115.81	110.04
22	B	606	CLA	CHD-C4C-C3C	-2.44	121.22	124.77
29	f	101	SQD	C1-O5-C5	-2.43	108.97	113.72
22	D	402	CLA	CHB-C4A-NA	2.43	127.91	124.40
22	c	509	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
22	C	508	CLA	C4-C3-C2	-2.43	117.38	123.63
30	H	102	DGD	O6D-C1D-O3G	-2.43	104.30	110.04
24	A	406	BCR	C35-C13-C12	2.43	121.80	118.09
27	a	410	PL9	C42-C43-C44	-2.43	122.06	127.62
34	B	622	LHG	C27-C26-C25	-2.43	102.09	114.37
22	c	511	CLA	O1D-CGD-CBD	2.43	129.31	124.52
24	a	406	BCR	C15-C16-C17	-2.43	118.55	123.52
28	b	623	LMG	O5-C6-C5	-2.43	103.07	111.33
24	t	101	BCR	C29-C30-C25	2.43	113.96	110.44
30	c	519	DGD	O2D-C2D-C1D	-2.43	104.30	110.08
24	b	616	BCR	C24-C23-C22	-2.42	122.65	126.23
24	b	616	BCR	C15-C16-C17	-2.42	118.57	123.52
22	A	403	CLA	C4A-NA-C1A	2.42	107.78	106.68
22	b	609	CLA	C11-C12-C13	-2.42	107.93	115.97
24	b	618	BCR	C31-C1-C6	2.42	114.03	110.24
24	H	101	BCR	C38-C26-C25	-2.42	121.85	124.48
27	A	410	PL9	C40-C39-C41	2.42	119.42	115.23
27	D	405	PL9	C8-C7-C3	2.42	118.28	112.03
22	B	606	CLA	C3D-C4D-ND	2.41	113.91	109.99
22	c	507	CLA	CMB-C2B-C1B	-2.41	121.74	125.42
29	f	101	SQD	O5-C5-C4	2.41	114.05	109.70
24	y	101	BCR	C27-C26-C25	2.41	125.96	122.70
24	B	619	BCR	C2-C1-C6	2.41	113.94	110.44
33	X	101	STE	C12-C11-C10	-2.41	102.18	114.37
23	d	401	PHO	O2D-CGD-O1D	-2.41	119.16	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	v	201	HEC	CMD-C2D-C1D	2.41	129.09	125.42
22	b	605	CLA	CHB-C1B-NB	2.41	127.66	124.05
22	d	403	CLA	CHD-C4C-C3C	2.41	128.28	124.77
22	b	607	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
22	c	503	CLA	CBC-CAC-C3C	-2.40	105.90	112.42
24	K	101	BCR	C29-C30-C25	2.40	113.93	110.44
22	b	608	CLA	CED-O2D-CGD	2.40	121.37	115.92
30	h	102	DGD	C4D-C3D-C2D	-2.40	106.61	110.83
22	A	402	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
22	c	506	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
22	b	609	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	C	513	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
22	D	402	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
22	b	614	CLA	CMB-C2B-C3B	2.40	132.19	126.55
30	c	520	DGD	O5D-C6D-C5D	-2.39	104.02	109.42
33	C	522	STE	C4-C3-C2	-2.39	104.34	113.13
29	A	414	SQD	O48-C23-O10	-2.39	117.64	123.63
22	B	607	CLA	CHB-C4A-NA	2.39	127.85	124.40
28	D	406	LMG	O2-C2-C1	-2.39	104.38	110.08
24	B	620	BCR	C28-C27-C26	-2.39	109.80	114.06
22	A	411	CLA	C1C-C2C-C3C	-2.39	104.47	106.98
34	D	408	LHG	C29-C28-C27	-2.39	102.30	114.37
24	b	616	BCR	C38-C26-C25	-2.39	121.88	124.48
22	A	403	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	c	506	CLA	CMC-C2C-C1C	2.38	128.76	125.03
30	C	516	DGD	C7B-C6B-C5B	-2.38	102.32	114.37
27	d	405	PL9	C42-C43-C44	-2.38	122.17	127.62
34	e	102	LHG	C11-C10-C9	-2.38	102.33	114.37
22	b	603	CLA	C4D-CHA-C1A	2.38	124.08	121.24
22	c	505	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
22	c	511	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
22	b	609	CLA	O2A-CGA-O1A	-2.38	117.69	123.63
22	b	602	CLA	C2D-C1D-ND	-2.38	107.78	110.13
22	B	615	CLA	C2B-C1B-NB	-2.37	107.87	110.33
22	B	604	CLA	CMB-C2B-C3B	2.37	132.13	126.55
23	a	404	PHO	CMD-C2D-C3D	2.37	129.42	124.68
24	K	101	BCR	C3-C4-C5	-2.37	109.83	114.06
24	B	620	BCR	C30-C25-C26	-2.37	119.40	122.64
30	C	517	DGD	O5D-C6D-C5D	-2.37	104.08	109.42
28	D	410	LMG	O8-C28-O10	-2.37	117.71	123.63
30	c	519	DGD	O3G-C3G-C2G	-2.37	105.06	110.82
29	b	619	SQD	O47-C45-C46	2.36	116.83	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404	PHO	C1-C2-C3	-2.36	122.32	126.20
22	c	511	CLA	C3B-C4B-NB	-2.36	108.42	110.53
34	D	412	LHG	C20-C19-C18	-2.36	102.42	114.37
22	C	508	CLA	CHC-C4B-NB	2.36	127.59	124.05
22	B	609	CLA	C6-C7-C8	-2.36	108.11	115.97
22	b	612	CLA	O1D-CGD-CBD	2.36	129.17	124.52
22	C	512	CLA	C1D-ND-C4D	2.36	107.97	106.31
34	e	102	LHG	C15-C14-C13	-2.36	102.45	114.37
22	B	616	CLA	C5-C3-C2	-2.36	115.88	121.17
22	b	606	CLA	CHD-C1D-ND	-2.35	121.49	124.80
22	C	509	CLA	O1D-CGD-CBD	2.35	129.16	124.52
22	b	608	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
22	B	604	CLA	CAC-C3C-C4C	2.35	127.85	124.79
22	d	402	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
22	d	402	CLA	C6-C5-C3	2.35	119.19	113.47
22	b	607	CLA	CHC-C1C-NC	2.35	127.85	124.31
22	A	411	CLA	CHB-C4A-NA	2.35	127.78	124.40
22	c	511	CLA	CHB-C4A-NA	2.35	127.78	124.40
22	c	512	CLA	CHB-C4A-NA	2.35	127.78	124.40
22	b	613	CLA	C1-C2-C3	-2.34	122.36	126.20
23	A	404	PHO	OBD-CAD-C3D	2.34	131.55	127.89
22	C	513	CLA	CAA-CBA-CGA	-2.34	106.56	113.21
22	a	402	CLA	C3A-C2A-C1A	2.34	104.85	101.34
30	c	520	DGD	O6D-C1D-O3G	-2.34	104.51	110.04
30	H	102	DGD	O3E-C3E-C2E	-2.34	104.86	110.38
24	K	101	BCR	C7-C8-C9	-2.34	122.77	126.23
22	c	515	CLA	CHD-C1D-ND	-2.34	121.51	124.80
28	A	412	LMG	C35-C34-C33	-2.34	102.55	114.37
22	C	504	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
22	B	617	CLA	CAC-C3C-C4C	2.34	127.83	124.79
28	d	409	LMG	O3-C3-C2	-2.34	104.87	110.38
24	B	620	BCR	C1-C6-C5	-2.34	119.44	122.64
22	d	402	CLA	O2D-CGD-O1D	-2.33	119.30	123.85
22	b	605	CLA	CHB-C4A-NA	2.33	127.77	124.40
35	v	201	HEC	CHD-C4C-NC	2.33	126.99	124.45
22	c	515	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
22	B	616	CLA	C6-C7-C8	-2.33	108.22	115.97
24	b	616	BCR	C36-C18-C17	-2.33	119.04	122.82
28	D	406	LMG	O1-C1-C2	-2.33	104.74	108.27
24	T	101	BCR	C38-C26-C27	-2.33	108.63	113.60
22	a	403	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
22	D	403	CLA	CHB-C1B-C2B	-2.33	120.67	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	511	CLA	CHC-C4B-NB	2.33	127.54	124.05
22	c	515	CLA	C3B-C4B-NB	-2.33	108.45	110.53
34	l	101	LHG	C11-C10-C9	-2.33	102.61	114.37
22	b	603	CLA	C6-C7-C8	-2.33	108.23	115.97
22	C	514	CLA	O1D-CGD-CBD	2.33	129.10	124.52
22	A	405	CLA	C1D-ND-C4D	-2.32	104.68	106.31
22	B	604	CLA	CHB-C1B-NB	2.32	127.54	124.05
22	b	612	CLA	CHA-C1A-NA	-2.32	121.13	126.39
28	A	412	LMG	C1-C2-C3	-2.32	105.12	110.01
30	c	520	DGD	O3D-C3D-C4D	-2.32	104.91	110.38
24	d	404	BCR	C38-C26-C25	-2.32	121.95	124.48
27	A	410	PL9	C12-C13-C14	-2.32	122.31	127.62
29	b	619	SQD	O48-C23-O10	-2.32	117.83	123.63
22	B	606	CLA	CHD-C4C-NC	2.32	127.83	124.23
22	b	610	CLA	CHA-C1A-NA	-2.32	121.14	126.39
22	b	611	CLA	CMC-C2C-C1C	-2.32	121.41	125.03
22	b	615	CLA	C3B-C4B-NB	-2.32	108.46	110.53
22	a	403	CLA	CAC-C3C-C4C	2.32	127.80	124.79
28	C	519	LMG	C38-C37-C36	-2.31	102.67	114.37
30	C	517	DGD	CDB-CCB-CBB	-2.31	102.67	114.37
22	B	617	CLA	CHD-C1D-C2D	2.31	130.30	125.49
28	M	101	LMG	C1-O6-C5	-2.31	109.20	113.72
28	b	621	LMG	C9-C8-C7	-2.31	106.39	111.78
34	l	101	LHG	O8-C23-C24	2.31	118.89	111.83
22	b	615	CLA	CMB-C2B-C3B	2.31	131.99	126.55
34	d	407	LHG	O7-C7-C8	-2.31	106.49	111.48
24	c	518	BCR	C37-C22-C21	-2.31	119.08	122.82
35	F	101	HEC	O2D-CGD-CBD	2.31	121.28	114.00
22	b	607	CLA	O2D-CGD-CBD	2.30	115.26	111.23
29	D	407	SQD	O5-C5-C4	2.30	113.85	109.70
22	a	411	CLA	O2D-CGD-CBD	2.30	115.25	111.23
24	Z	101	BCR	C2-C1-C6	2.30	113.78	110.44
22	B	612	CLA	C2C-C1C-NC	2.30	112.40	109.98
27	a	410	PL9	C36-C34-C33	-2.30	116.01	121.17
24	c	516	BCR	C27-C26-C25	2.30	125.81	122.70
28	b	621	LMG	O2-C2-C1	-2.30	104.60	110.08
22	c	508	CLA	CHB-C4A-NA	2.30	127.71	124.40
22	c	515	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
28	C	519	LMG	O3-C3-C2	-2.29	104.97	110.38
22	C	503	CLA	CHD-C4C-NC	2.29	127.78	124.23
28	M	101	LMG	C4-C3-C2	-2.29	106.81	110.83
34	d	406	LHG	C27-C26-C25	-2.29	102.80	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	603	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
22	b	610	CLA	C4A-NA-C1A	2.29	107.72	106.68
22	a	402	CLA	CGD-CBD-CAD	-2.29	103.44	110.85
22	B	616	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
34	d	407	LHG	C18-C17-C16	-2.28	102.82	114.37
30	C	516	DGD	C9B-C8B-C7B	-2.28	102.84	114.37
35	F	101	HEC	CMC-C2C-C1C	-2.28	121.95	125.42
30	c	521	DGD	O5D-C6D-C5D	-2.28	104.29	109.42
28	b	621	LMG	O1-C7-C8	-2.27	105.29	110.82
22	c	505	CLA	C11-C12-C13	-2.27	108.41	115.97
22	A	405	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
34	D	412	LHG	C11-C10-C9	-2.27	102.88	114.37
24	b	617	BCR	C8-C7-C6	-2.27	120.92	127.00
22	c	509	CLA	C1C-C2C-C3C	-2.27	104.59	106.98
22	B	610	CLA	CHA-C1A-NA	-2.27	121.24	126.39
27	d	405	PL9	C20-C19-C21	2.27	119.17	115.23
34	d	407	LHG	C11-C10-C9	-2.27	102.89	114.37
27	A	410	PL9	C15-C14-C16	-2.27	111.29	115.23
30	C	516	DGD	C6B-C5B-C4B	-2.27	102.89	114.37
22	C	509	CLA	O2D-CGD-CBD	2.27	115.19	111.23
24	a	406	BCR	C11-C10-C9	-2.27	124.10	127.28
22	A	402	CLA	CHC-C4B-NB	2.27	127.45	124.05
30	c	521	DGD	CAB-C9B-C8B	-2.27	102.91	114.37
35	v	201	HEC	C1D-C2D-C3D	-2.26	104.22	106.82
28	b	621	LMG	O8-C28-O10	-2.26	117.97	123.63
22	B	603	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
22	d	402	CLA	C6-C7-C8	-2.26	108.45	115.97
30	C	516	DGD	CCB-CBB-CAB	-2.26	102.94	114.37
22	B	615	CLA	CHC-C4B-NB	2.26	127.44	124.05
27	A	410	PL9	C20-C19-C21	2.26	119.15	115.23
24	t	101	BCR	C35-C13-C14	-2.26	119.16	122.82
22	B	605	CLA	OBD-CAD-C3D	2.26	133.69	128.42
22	c	504	CLA	O2D-CGD-CBD	2.26	115.17	111.23
28	D	406	LMG	O8-C28-O10	-2.26	117.98	123.63
30	C	518	DGD	CDB-CCB-CBB	-2.26	102.97	114.37
22	d	402	CLA	C1-C2-C3	-2.25	122.50	126.20
28	M	101	LMG	O6-C1-O1	-2.25	104.72	110.04
29	f	101	SQD	C46-C45-C44	-2.25	106.54	111.78
24	d	404	BCR	C27-C26-C25	2.25	125.74	122.70
34	l	101	LHG	O8-C23-O10	-2.25	118.00	123.63
24	B	619	BCR	C15-C16-C17	-2.25	118.92	123.52
24	K	101	BCR	C15-C16-C17	-2.25	118.92	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	CLA	O2D-CGD-CBD	-2.25	107.30	111.23
24	a	406	BCR	C38-C26-C27	-2.25	108.81	113.60
22	c	513	CLA	O2D-CGD-O1D	-2.25	119.48	123.85
22	B	603	CLA	C3B-C4B-NB	-2.25	108.53	110.53
22	a	402	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
22	A	405	CLA	CHA-C1A-NA	-2.25	121.31	126.39
22	B	608	CLA	C6-C5-C3	-2.24	108.00	113.47
24	b	616	BCR	C27-C26-C25	2.24	125.74	122.70
28	b	623	LMG	C40-C39-C38	-2.24	103.03	114.37
28	D	411	LMG	O8-C28-O10	-2.24	117.56	123.33
28	c	525	LMG	C38-C37-C36	-2.24	103.03	114.37
24	b	618	BCR	C33-C5-C6	-2.24	122.04	124.48
27	a	410	PL9	C27-C28-C29	-2.24	122.49	127.62
22	b	603	CLA	OBD-CAD-C3D	2.24	133.66	128.42
22	c	503	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
29	D	407	SQD	O2-C2-C1	2.24	115.41	110.08
22	C	508	CLA	CHD-C1D-ND	-2.24	121.66	124.80
22	A	403	CLA	O1D-CGD-CBD	2.24	128.93	124.52
30	c	519	DGD	O3E-C3E-C2E	-2.24	105.11	110.38
24	c	516	BCR	C12-C13-C14	-2.24	115.49	119.01
22	c	508	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
22	b	607	CLA	CHD-C1D-ND	-2.23	121.66	124.80
29	D	407	SQD	O48-C23-O10	-2.23	118.04	123.63
22	B	611	CLA	C3A-C2A-C1A	2.23	104.68	101.34
24	c	516	BCR	C7-C8-C9	-2.23	122.93	126.23
29	B	623	SQD	O8-S-C6	2.23	110.28	105.97
29	a	412	SQD	O47-C7-C8	2.23	116.31	111.48
28	C	519	LMG	C40-C39-C38	-2.23	103.09	114.37
30	c	521	DGD	C1D-C2D-C3D	-2.23	105.32	110.01
28	c	524	LMG	C3-C4-C5	-2.23	106.19	110.23
30	A	415	DGD	CDB-CCB-CBB	-2.23	103.09	114.37
22	b	611	CLA	CMD-C2D-C3D	2.23	132.80	127.69
22	b	601	CLA	CHC-C1C-NC	2.23	127.67	124.31
22	B	609	CLA	CMB-C2B-C3B	2.23	131.79	126.55
24	B	618	BCR	C11-C10-C9	-2.23	124.15	127.28
27	A	410	PL9	C32-C33-C34	-2.23	122.52	127.62
23	A	404	PHO	O2D-CGD-CBD	2.23	113.39	110.95
22	b	610	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
22	c	506	CLA	CMB-C2B-C3B	2.23	131.79	126.55
30	H	102	DGD	CCB-CBB-CAB	-2.23	103.11	114.37
28	c	522	LMG	O2-C2-C1	-2.23	104.77	110.08
22	a	411	CLA	O2D-CGD-O1D	-2.23	119.51	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	403	CLA	CMB-C2B-C3B	2.23	131.79	126.55
28	c	524	LMG	O6-C1-O1	-2.23	104.78	110.04
24	C	515	BCR	C27-C26-C25	2.23	125.71	122.70
28	c	524	LMG	O1-C1-C2	-2.23	104.89	108.27
30	C	516	DGD	O3E-C3E-C2E	-2.23	105.13	110.38
22	B	607	CLA	C2A-C1A-CHA	2.23	127.73	123.87
30	h	102	DGD	C7B-C6B-C5B	-2.22	103.12	114.37
29	D	407	SQD	O9-S-O7	-2.22	106.60	113.82
35	v	201	HEC	CHA-C1A-C2A	2.22	128.37	124.86
35	e	101	HEC	CHB-C1B-NB	2.22	127.89	123.86
22	b	610	CLA	CHD-C1D-ND	-2.22	121.68	124.80
24	C	515	BCR	C10-C11-C12	-2.22	116.77	123.20
29	A	413	SQD	O5-C1-O6	2.22	115.29	110.04
22	b	609	CLA	C2A-C1A-CHA	2.22	127.72	123.87
30	A	415	DGD	O6D-C1D-O3G	-2.22	104.80	110.04
22	c	509	CLA	C2C-C1C-NC	2.22	112.31	109.98
22	b	605	CLA	CHA-C1A-NA	-2.22	121.37	126.39
35	e	101	HEC	O1A-CGA-CBA	-2.22	116.06	123.09
22	C	513	CLA	O2A-CGA-O1A	-2.22	118.09	123.63
24	b	617	BCR	C39-C30-C25	2.21	113.72	110.24
22	b	602	CLA	CMA-C3A-C4A	2.21	117.72	111.77
22	c	510	CLA	C7-C6-C5	-2.21	107.36	113.26
22	B	610	CLA	C2A-C3A-C4A	2.21	105.44	101.87
30	C	516	DGD	O2D-C2D-C1D	-2.21	104.80	110.08
22	A	411	CLA	C2A-C1A-CHA	2.21	127.70	123.87
22	C	508	CLA	O2D-CGD-CBD	2.21	115.10	111.23
30	c	521	DGD	O3E-C3E-C2E	-2.21	105.16	110.38
24	B	618	BCR	C8-C7-C6	-2.21	121.09	127.00
30	c	521	DGD	O2D-C2D-C1D	-2.21	104.81	110.08
22	a	402	CLA	CHB-C4A-NA	2.21	127.59	124.40
22	B	614	CLA	C2A-C1A-CHA	2.21	127.70	123.87
22	B	603	CLA	CMB-C2B-C3B	2.21	131.75	126.55
22	b	613	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
27	D	405	PL9	C41-C39-C38	-2.21	116.21	121.17
22	C	504	CLA	C6-C7-C8	-2.21	108.63	115.97
22	B	616	CLA	CHD-C1D-ND	-2.21	121.70	124.80
22	B	615	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
22	a	405	CLA	C3B-C4B-NB	-2.20	108.56	110.53
30	c	519	DGD	C3D-C4D-C5D	-2.20	106.23	110.23
30	c	520	DGD	C1D-O6D-C5D	-2.20	109.42	113.72
30	C	517	DGD	O3D-C3D-C4D	-2.20	105.18	110.38
22	B	614	CLA	CMA-C3A-C4A	-2.20	105.86	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	510	CLA	CHD-C1D-ND	-2.20	121.70	124.80
28	b	621	LMG	C36-C35-C34	-2.20	103.24	114.37
22	c	509	CLA	CHC-C4B-NB	2.20	127.35	124.05
30	C	516	DGD	CBB-CAB-C9B	-2.20	103.25	114.37
22	b	603	CLA	CHD-C4C-NC	2.20	127.64	124.23
24	B	618	BCR	C33-C5-C6	-2.20	122.08	124.48
22	C	509	CLA	CHD-C1D-ND	-2.20	121.71	124.80
24	D	404	BCR	C30-C25-C26	-2.20	119.63	122.64
24	c	516	BCR	C28-C27-C26	-2.20	110.14	114.06
22	b	602	CLA	CHA-C4D-ND	2.20	137.08	132.55
22	d	403	CLA	CHA-C1A-NA	-2.19	121.42	126.39
22	C	505	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
33	B	621	STE	C6-C5-C4	-2.19	103.28	114.37
28	c	522	LMG	C40-C39-C38	-2.19	103.29	114.37
30	C	518	DGD	O3D-C3D-C4D	-2.19	105.21	110.38
22	C	506	CLA	CGD-CBD-CAD	-2.19	103.75	110.85
22	b	603	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
24	B	619	BCR	C27-C26-C25	2.19	125.66	122.70
33	J	101	STE	C4-C3-C2	-2.19	105.09	113.13
34	E	101	LHG	C20-C19-C18	-2.19	103.31	114.37
28	M	101	LMG	C22-C21-C20	-2.19	103.31	114.37
24	c	518	BCR	C15-C16-C17	-2.19	119.04	123.52
22	B	610	CLA	CHB-C4A-NA	2.19	127.55	124.40
22	b	604	CLA	CBC-CAC-C3C	-2.18	106.50	112.42
22	B	607	CLA	CHA-C1A-NA	-2.18	121.44	126.39
24	H	101	BCR	C16-C17-C18	-2.18	124.22	127.28
35	F	101	HEC	C4D-ND-C1D	2.18	109.38	105.82
22	b	611	CLA	CMD-C2D-C1D	-2.18	120.89	124.73
22	c	503	CLA	C2C-C1C-NC	2.18	112.27	109.98
22	b	614	CLA	C14-C13-C15	-2.18	103.50	111.27
22	b	603	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
22	c	504	CLA	CHB-C1B-NB	2.18	127.32	124.05
24	B	619	BCR	C40-C30-C29	-2.18	100.58	108.95
22	c	505	CLA	CMA-C3A-C4A	2.18	117.63	111.77
22	B	612	CLA	CHD-C4C-C3C	-2.18	121.60	124.77
23	D	401	PHO	OBD-CAD-CBD	-2.18	122.63	125.82
22	d	402	CLA	O1D-CGD-CBD	2.18	128.81	124.52
30	A	415	DGD	O6E-C5E-C4E	2.18	113.62	109.70
22	C	513	CLA	CMA-C3A-C2A	-2.18	105.57	113.98
22	B	610	CLA	C2C-C1C-NC	2.18	112.27	109.98
22	C	503	CLA	C1-C2-C3	-2.18	122.63	126.20
22	b	608	CLA	CHD-C4C-NC	2.18	127.61	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	B	601	STE	O1-C1-C2	-2.17	116.20	123.09
22	C	512	CLA	CHA-C1A-NA	-2.17	121.47	126.39
29	A	413	SQD	O48-C23-O10	-2.17	118.19	123.63
22	b	603	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
22	b	610	CLA	C11-C10-C8	-2.17	108.75	115.97
28	d	409	LMG	C38-C37-C36	-2.17	103.39	114.37
24	Y	101	BCR	C16-C15-C14	-2.17	119.08	123.52
34	E	101	LHG	C11-C10-C9	-2.17	103.40	114.37
22	b	609	CLA	CAA-CBA-CGA	-2.17	107.06	113.21
22	A	402	CLA	CAA-CBA-CGA	-2.17	107.06	113.21
30	h	102	DGD	C1E-O6E-C5E	2.17	117.95	113.72
22	c	512	CLA	O1D-CGD-CBD	2.16	128.79	124.52
28	M	101	LMG	C37-C36-C35	-2.16	103.42	114.37
29	B	623	SQD	C1-C2-C3	-2.16	105.46	110.01
22	B	606	CLA	O1D-CGD-CBD	2.16	128.79	124.52
24	C	515	BCR	C32-C1-C6	-2.16	106.85	110.24
22	a	402	CLA	CHA-C4D-ND	2.16	137.01	132.55
22	A	411	CLA	CHA-C1A-NA	-2.16	121.49	126.39
23	d	401	PHO	C4D-ND-C1D	-2.16	106.28	108.87
22	b	605	CLA	C7-C6-C5	-2.16	107.50	113.26
29	a	412	SQD	C45-O47-C7	2.16	122.97	117.80
24	C	515	BCR	C15-C14-C13	-2.16	124.25	127.28
28	M	101	LMG	O8-C28-O10	-2.16	118.23	123.63
34	D	408	LHG	C27-C26-C25	-2.16	103.46	114.37
22	c	504	CLA	C4D-CHA-C1A	2.16	123.82	121.24
24	x	101	BCR	C15-C16-C17	-2.16	119.11	123.52
22	C	510	CLA	CHA-C1A-NA	-2.16	121.51	126.39
22	c	508	CLA	CHA-C1A-NA	-2.16	121.51	126.39
22	b	602	CLA	CHD-C1D-C2D	2.16	129.97	125.49
22	b	614	CLA	O2D-CGD-CBD	2.16	115.00	111.23
22	b	603	CLA	CHA-C1A-NA	-2.15	121.52	126.39
30	h	102	DGD	C4E-C3E-C2E	-2.15	107.06	110.83
22	C	505	CLA	O1A-CGA-CBA	2.15	132.19	123.78
22	D	402	CLA	C1D-CHD-C4C	-2.15	121.45	126.02
24	b	617	BCR	C15-C16-C17	-2.15	119.12	123.52
28	b	623	LMG	O7-C10-O9	-2.15	118.68	123.70
24	c	517	BCR	C2-C1-C6	2.15	113.56	110.44
35	v	201	HEC	CHD-C1D-ND	2.15	127.75	123.86
23	D	401	PHO	O2A-CGA-O1A	-2.14	118.27	123.63
24	D	404	BCR	C3-C4-C5	-2.14	110.23	114.06
28	b	623	LMG	C38-C37-C36	-2.14	103.54	114.37
33	d	412	STE	O2-C1-C2	2.14	120.77	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	405	CLA	C3D-C4D-ND	2.14	113.47	109.99
23	a	404	PHO	C7-C6-C5	-2.14	107.56	113.26
27	D	405	PL9	C36-C34-C33	-2.14	116.36	121.17
29	a	412	SQD	C9-C8-C7	-2.14	105.86	113.69
22	a	402	CLA	O1D-CGD-CBD	2.14	128.74	124.52
22	B	610	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
22	a	405	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
28	M	101	LMG	C38-C37-C36	-2.13	103.58	114.37
22	C	503	CLA	CHD-C1D-C2D	2.13	129.93	125.49
27	d	405	PL9	C35-C34-C36	2.13	118.93	115.23
22	B	615	CLA	O1D-CGD-CBD	2.13	128.72	124.52
22	c	510	CLA	CHB-C4A-NA	2.13	127.48	124.40
28	M	101	LMG	O3-C3-C2	-2.13	105.35	110.38
30	h	102	DGD	O6D-C1D-O3G	-2.13	105.01	110.04
22	C	505	CLA	CHD-C1D-ND	-2.13	121.81	124.80
24	x	101	BCR	C8-C9-C10	2.13	122.36	119.01
22	b	608	CLA	CHB-C4A-NA	2.13	127.47	124.40
22	B	606	CLA	CHD-C1D-C2D	2.13	129.91	125.49
22	b	605	CLA	CMB-C2B-C3B	2.13	131.55	126.55
22	c	509	CLA	CHB-C4A-NA	2.13	127.47	124.40
24	H	101	BCR	C35-C13-C12	2.13	121.34	118.09
22	B	616	CLA	C2B-C1B-NB	-2.13	108.12	110.33
28	M	101	LMG	C40-C39-C38	-2.12	103.63	114.37
27	d	405	PL9	C7-C8-C9	-2.12	123.17	126.83
22	A	405	CLA	C2C-C1C-NC	2.12	112.21	109.98
22	b	614	CLA	C16-C15-C13	-2.12	108.91	115.97
23	d	401	PHO	CMA-C3A-C2A	-2.12	105.94	114.13
28	D	411	LMG	O7-C10-O9	-2.12	117.88	123.33
22	B	612	CLA	C17-C16-C15	-2.12	103.78	113.28
22	b	605	CLA	CHC-C1C-C2C	-2.12	120.93	126.95
24	b	618	BCR	C27-C26-C25	2.12	125.56	122.70
29	f	101	SQD	O5-C1-C2	-2.12	106.02	110.37
22	c	510	CLA	O2D-CGD-CBD	2.11	114.93	111.23
30	c	520	DGD	C4E-C3E-C2E	-2.11	107.12	110.83
24	c	518	BCR	C38-C26-C25	-2.11	122.18	124.48
22	C	513	CLA	CHB-C1B-NB	2.11	127.22	124.05
24	c	518	BCR	C29-C30-C25	2.11	113.51	110.44
22	c	512	CLA	CHD-C1D-ND	-2.11	121.83	124.80
22	b	608	CLA	CMB-C2B-C3B	2.11	131.51	126.55
22	b	615	CLA	CED-O2D-CGD	-2.11	111.13	115.92
28	A	412	LMG	O1-C7-C8	-2.11	105.69	110.82
24	K	101	BCR	C38-C26-C25	-2.11	122.19	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	102	DGD	O6E-C1E-O5D	-2.11	105.07	110.04
22	b	614	CLA	CHD-C4C-NC	2.10	127.50	124.23
22	c	506	CLA	C4A-NA-C1A	2.10	107.64	106.68
22	D	403	CLA	CHA-C1A-NA	-2.10	121.63	126.39
22	b	605	CLA	CHA-C4D-ND	2.10	136.89	132.55
22	B	614	CLA	CHB-C1B-NB	2.10	127.20	124.05
22	C	507	CLA	O1D-CGD-CBD	2.10	128.66	124.52
28	c	522	LMG	C1-O6-C5	-2.10	109.62	113.72
22	b	609	CLA	CHA-C1A-NA	-2.10	121.64	126.39
22	C	512	CLA	C2D-C1D-ND	-2.10	108.05	110.13
30	c	519	DGD	C4E-C3E-C2E	-2.10	107.15	110.83
22	C	504	CLA	CHC-C4B-NB	2.10	127.20	124.05
30	C	516	DGD	C4E-C3E-C2E	-2.10	107.15	110.83
22	c	506	CLA	CHB-C1B-NB	2.10	127.19	124.05
30	C	517	DGD	C7B-C6B-C5B	-2.09	103.78	114.37
30	c	521	DGD	CDB-CCB-CBB	-2.09	103.78	114.37
22	C	502	CLA	CHB-C1B-NB	2.09	127.19	124.05
22	b	605	CLA	C2C-C1C-NC	2.09	112.18	109.98
23	A	404	PHO	O2D-CGD-O1D	-2.09	119.77	123.85
30	C	517	DGD	O3G-C1D-C2D	-2.09	105.09	108.27
22	c	510	CLA	CHD-C4C-NC	2.09	127.48	124.23
22	b	605	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
22	b	608	CLA	O1D-CGD-CBD	2.09	128.65	124.52
24	c	517	BCR	C34-C9-C10	-2.09	119.43	122.82
22	C	511	CLA	CHA-C1A-NA	-2.09	121.66	126.39
22	B	614	CLA	CED-O2D-CGD	2.09	120.66	115.92
33	a	415	STE	O2-C1-C2	2.09	120.60	114.00
35	V	201	HEC	C2C-C1C-NC	-2.09	106.80	110.14
24	Y	101	BCR	C15-C16-C17	-2.09	119.25	123.52
22	c	507	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
24	B	618	BCR	C3-C4-C5	-2.09	110.33	114.06
22	B	611	CLA	C4D-CHA-C1A	2.09	123.73	121.24
22	c	512	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	B	615	CLA	C1-C2-C3	-2.08	122.78	126.20
27	d	405	PL9	C27-C28-C29	-2.08	122.86	127.62
24	B	620	BCR	C2-C3-C4	-2.08	106.70	111.28
22	a	411	CLA	CHC-C4B-NB	2.08	127.17	124.05
30	C	516	DGD	O6E-C5E-C4E	2.08	113.45	109.70
22	B	610	CLA	CHD-C4C-NC	2.08	127.46	124.23
22	B	614	CLA	CAC-C3C-C4C	2.08	127.50	124.79
22	b	612	CLA	C7-C6-C5	-2.08	107.72	113.26
24	A	406	BCR	C33-C5-C6	-2.08	122.22	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	H	102	DGD	C4D-C3D-C2D	-2.08	107.18	110.83
27	D	405	PL9	C20-C19-C21	2.08	118.83	115.23
24	Y	101	BCR	C8-C7-C6	-2.08	121.45	127.00
28	D	406	LMG	C38-C37-C36	-2.08	103.87	114.37
24	A	406	BCR	C2-C1-C6	2.08	113.45	110.44
22	C	507	CLA	C3B-C4B-NB	-2.07	108.68	110.53
30	H	102	DGD	CAB-C9B-C8B	-2.07	103.88	114.37
22	B	616	CLA	CHC-C4B-NB	2.07	127.16	124.05
22	B	610	CLA	CHC-C4B-NB	2.07	127.16	124.05
22	b	612	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
22	C	514	CLA	CHB-C4A-NA	2.07	127.39	124.40
22	b	614	CLA	CHD-C4C-C3C	-2.07	121.75	124.77
29	f	101	SQD	C45-O47-C7	2.07	122.75	117.80
22	D	403	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
22	c	515	CLA	CMB-C2B-C3B	2.07	131.42	126.55
22	c	511	CLA	C3A-C2A-C1A	2.07	104.44	101.34
22	A	403	CLA	C3B-C4B-NB	-2.07	108.68	110.53
22	B	604	CLA	CHD-C1D-C2D	2.07	129.79	125.49
34	d	408	LHG	C26-C25-C24	2.07	120.73	113.13
22	B	617	CLA	CAA-CBA-CGA	-2.07	107.34	113.21
24	H	101	BCR	C34-C9-C8	-2.07	114.93	118.09
24	C	515	BCR	C2-C1-C6	2.07	113.44	110.44
30	A	415	DGD	O5E-C6E-C5E	-2.07	104.30	111.33
22	b	608	CLA	CHD-C1D-C2D	2.06	129.78	125.49
24	b	618	BCR	C16-C15-C14	-2.06	119.30	123.52
34	d	407	LHG	O8-C23-C24	2.06	118.13	111.83
28	M	101	LMG	O7-C10-O9	-2.06	118.88	123.70
22	B	613	CLA	CMB-C2B-C3B	2.06	131.40	126.55
22	c	503	CLA	C3B-C4B-NB	-2.06	108.69	110.53
35	v	201	HEC	CHA-C4D-ND	2.06	127.60	123.86
30	c	520	DGD	C3E-C4E-C5E	-2.06	106.49	110.23
30	C	516	DGD	C5B-C4B-C3B	-2.06	103.96	114.37
27	d	405	PL9	C8-C7-C3	2.06	117.36	112.03
24	B	620	BCR	C38-C26-C25	-2.06	122.24	124.48
22	C	508	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
24	x	101	BCR	C35-C13-C12	2.06	121.23	118.09
22	B	603	CLA	C4A-NA-C1A	2.06	107.62	106.68
22	c	507	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
30	H	102	DGD	C1D-O6D-C5D	-2.06	109.70	113.72
22	C	509	CLA	C3A-C2A-C1A	2.06	104.42	101.34
27	d	405	PL9	C47-C48-C49	-2.06	120.79	127.64
30	c	519	DGD	C3G-C2G-C1G	-2.06	106.99	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	X	101	STE	C10-C9-C8	-2.05	103.99	114.37
22	B	615	CLA	CHB-C1B-NB	2.05	127.13	124.05
29	a	413	SQD	C46-O48-C23	2.05	124.62	117.12
24	t	101	BCR	C2-C1-C6	2.05	113.42	110.44
22	b	610	CLA	CMB-C2B-C3B	2.05	131.38	126.55
22	b	603	CLA	C1-O2A-CGA	-2.05	111.68	116.65
22	b	613	CLA	CHD-C1D-C2D	2.05	129.75	125.49
24	H	101	BCR	C1-C6-C5	-2.05	119.83	122.64
30	A	415	DGD	O4D-C4D-C3D	2.05	115.21	110.38
22	a	405	CLA	CHD-C1D-ND	-2.05	121.92	124.80
23	a	404	PHO	C3D-C4D-ND	2.05	110.33	107.71
22	B	610	CLA	CMC-C2C-C1C	2.05	128.24	125.03
22	b	606	CLA	CHB-C4A-NA	2.05	127.36	124.40
22	B	612	CLA	CHB-C4A-NA	2.05	127.35	124.40
22	b	606	CLA	C2D-C1D-ND	2.05	112.15	110.13
22	C	510	CLA	CMB-C2B-C3B	2.05	131.36	126.55
22	A	405	CLA	CMB-C2B-C3B	2.05	131.36	126.55
28	d	409	LMG	C3-C4-C5	-2.04	106.53	110.23
24	b	618	BCR	C36-C18-C19	2.04	121.21	118.09
30	c	519	DGD	CBB-CAB-C9B	-2.04	104.04	114.37
22	b	610	CLA	CHD-C1D-C2D	2.04	129.74	125.49
28	D	410	LMG	O1-C7-C8	-2.04	106.52	111.77
22	b	601	CLA	C2D-C1D-ND	-2.04	108.10	110.13
22	b	606	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
24	Z	101	BCR	C7-C8-C9	-2.04	123.21	126.23
34	E	101	LHG	O8-C23-O10	-2.04	118.52	123.63
35	V	201	HEC	O1A-CGA-CBA	-2.04	116.62	123.09
22	b	603	CLA	CHB-C4A-NA	2.04	127.35	124.40
22	B	617	CLA	C4D-CHA-C1A	2.04	123.68	121.24
22	c	510	CLA	CAC-C3C-C4C	-2.04	122.14	124.79
30	h	102	DGD	C1D-O6D-C5D	-2.04	109.74	113.72
22	C	513	CLA	C6-C5-C3	-2.04	108.51	113.47
33	d	410	STE	C3-C2-C1	-2.04	109.19	114.51
24	y	101	BCR	C4-C5-C6	2.04	125.45	122.70
24	c	516	BCR	C15-C16-C17	-2.04	119.35	123.52
23	D	401	PHO	O2D-CGD-CBD	2.03	113.18	110.95
22	b	607	CLA	CHD-C1D-C2D	2.03	129.72	125.49
26	a	409	BCT	O3-C-O1	-2.03	114.47	119.68
22	b	604	CLA	C4-C3-C2	-2.03	118.41	123.63
22	B	614	CLA	C4D-CHA-C1A	2.03	123.67	121.24
29	A	414	SQD	O48-C46-C45	2.03	114.14	108.35
24	Y	101	BCR	C38-C26-C27	-2.03	109.27	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	O1A-CGA-CBA	2.03	131.72	123.78
22	b	607	CLA	C11-C10-C8	-2.03	109.22	115.97
22	b	612	CLA	C16-C15-C13	-2.03	109.22	115.97
30	c	521	DGD	C6B-C5B-C4B	-2.03	104.12	114.37
28	D	411	LMG	C36-C35-C34	-2.03	104.12	114.37
24	c	516	BCR	C20-C21-C22	-2.03	124.44	127.28
30	C	518	DGD	C6B-C5B-C4B	-2.03	104.13	114.37
22	b	613	CLA	CMD-C2D-C1D	2.02	128.29	124.73
28	M	101	LMG	C33-C32-C31	-2.02	104.14	114.37
24	b	618	BCR	C30-C25-C26	-2.02	119.87	122.64
22	A	402	CLA	CED-O2D-CGD	2.02	120.50	115.92
22	b	609	CLA	C3B-C4B-NB	-2.02	108.73	110.53
34	d	406	LHG	C20-C19-C18	-2.02	104.16	114.37
22	b	611	CLA	CMC-C2C-C3C	2.02	131.61	126.15
22	B	613	CLA	CAA-CBA-CGA	-2.02	107.48	113.21
35	v	201	HEC	CHA-C1A-NA	-2.02	122.25	124.45
33	M	102	STE	C3-C2-C1	-2.02	109.24	114.51
22	B	611	CLA	O1A-CGA-CBA	2.02	131.67	123.78
28	b	623	LMG	C8-O7-C10	2.02	122.62	117.80
34	D	412	LHG	C27-C26-C25	-2.02	104.17	114.37
24	D	404	BCR	C8-C7-C6	-2.02	121.61	127.00
22	c	506	CLA	O1A-CGA-CBA	2.01	131.66	123.78
22	b	602	CLA	CMD-C2D-C3D	-2.01	123.07	127.69
22	c	505	CLA	CHC-C4B-NB	2.01	127.07	124.05
22	c	509	CLA	C3B-C4B-NB	-2.01	108.73	110.53
22	B	606	CLA	CHA-C1A-NA	-2.01	121.83	126.39
24	Y	101	BCR	C33-C5-C6	-2.01	122.29	124.48
28	C	519	LMG	O7-C10-O9	-2.01	119.00	123.70
22	b	608	CLA	C6-C5-C3	2.01	118.37	113.47
34	D	412	LHG	C18-C17-C16	-2.01	104.20	114.37
30	C	517	DGD	CBB-CAB-C9B	-2.01	104.20	114.37
28	c	522	LMG	C3-C4-C5	-2.01	106.58	110.23
22	c	511	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
35	e	101	HEC	CHC-C4B-NB	-2.01	122.26	124.45
22	B	611	CLA	C1-C2-C3	-2.01	122.90	126.20
22	c	503	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
26	A	409	BCT	O3-C-O1	-2.01	114.54	119.68
22	A	405	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	B	619	BCR	C33-C5-C6	-2.01	122.30	124.48
22	C	505	CLA	O1D-CGD-CBD	2.01	128.47	124.52
24	B	620	BCR	C33-C5-C6	-2.01	122.30	124.48
22	A	403	CLA	O1A-CGA-CBA	2.00	131.62	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	415	DGD	CBB-CAB-C9B	-2.00	104.24	114.37
30	h	102	DGD	C3E-C4E-C5E	-2.00	106.60	110.23
22	a	411	CLA	CMB-C2B-C1B	-2.00	122.37	125.42
23	D	401	PHO	CBA-CAA-C2A	-2.00	107.88	113.78
22	B	617	CLA	C4-C3-C2	-2.00	118.48	123.63
30	A	415	DGD	CAB-C9B-C8B	-2.00	104.25	114.37
30	H	102	DGD	CBB-CAB-C9B	-2.00	104.25	114.37
29	A	414	SQD	O47-C45-C44	2.00	112.44	107.96
22	c	515	CLA	C3D-C4D-ND	2.00	113.24	109.99
30	C	518	DGD	C5B-C4B-C3B	-2.00	104.25	114.37
22	B	609	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (55) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	602	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	B	617	CLA	ND
22	C	503	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	D	402	CLA	ND
22	a	402	CLA	ND

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Mol	Chain	Res	Type	Atom
22	a	405	CLA	ND
22	a	411	CLA	ND
22	b	601	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	609	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	c	503	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	c	514	CLA	ND
22	c	515	CLA	ND
22	d	402	CLA	ND
22	d	403	CLA	ND
22	h	101	CLA	ND

All (1750) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C11-C12-C13-C14
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C2B-C3B-CAB-CBB
22	C	513	CLA	C4B-C3B-CAB-CBB
22	a	403	CLA	C2B-C3B-CAB-CBB
22	a	403	CLA	C4B-C3B-CAB-CBB
22	b	608	CLA	C4B-C3B-CAB-CBB
22	b	613	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	b	613	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	C12-C13-C15-C16
22	c	513	CLA	C14-C13-C15-C16
22	c	514	CLA	C2B-C3B-CAB-CBB
22	c	514	CLA	C4B-C3B-CAB-CBB
24	A	406	BCR	C20-C21-C22-C37
24	B	619	BCR	C11-C10-C9-C34
24	C	515	BCR	C20-C21-C22-C37
24	D	404	BCR	C23-C24-C25-C26
24	D	404	BCR	C23-C24-C25-C30
24	K	101	BCR	C17-C18-C19-C20
24	T	101	BCR	C18-C19-C20-C21
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
24	Z	101	BCR	C11-C12-C13-C35
24	Z	101	BCR	C35-C13-C14-C15
24	Z	101	BCR	C16-C17-C18-C19
24	Z	101	BCR	C16-C17-C18-C36
24	Z	101	BCR	C17-C18-C19-C20
24	Z	101	BCR	C21-C22-C23-C24
24	a	406	BCR	C11-C10-C9-C34
24	a	406	BCR	C35-C13-C14-C15
24	a	406	BCR	C20-C21-C22-C37
24	c	516	BCR	C7-C8-C9-C10
24	c	516	BCR	C7-C8-C9-C34
24	c	516	BCR	C12-C13-C14-C15
24	c	516	BCR	C35-C13-C14-C15
24	c	516	BCR	C18-C19-C20-C21
24	c	517	BCR	C35-C13-C14-C15
24	c	517	BCR	C18-C19-C20-C21
24	c	517	BCR	C20-C21-C22-C37
24	c	518	BCR	C35-C13-C14-C15
24	t	101	BCR	C17-C18-C19-C20
24	t	101	BCR	C36-C18-C19-C20
24	y	101	BCR	C1-C6-C7-C8
24	y	101	BCR	C5-C6-C7-C8
27	A	410	PL9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	A	410	PL9	C12-C13-C14-C16
27	A	410	PL9	C17-C18-C19-C21
27	A	410	PL9	C37-C38-C39-C40
27	A	410	PL9	C37-C38-C39-C41
27	D	405	PL9	C32-C33-C34-C35
27	D	405	PL9	C32-C33-C34-C36
27	a	410	PL9	C17-C18-C19-C21
27	a	410	PL9	C22-C23-C24-C25
27	a	410	PL9	C22-C23-C24-C26
27	a	410	PL9	C42-C43-C44-C45
27	d	405	PL9	C32-C33-C34-C36
27	d	405	PL9	C42-C43-C44-C45
27	d	405	PL9	C42-C43-C44-C46
28	A	412	LMG	O9-C10-O7-C8
28	D	410	LMG	O1-C7-C8-C9
28	D	410	LMG	O1-C7-C8-O7
28	D	410	LMG	C11-C10-O7-C8
28	b	623	LMG	O9-C10-O7-C8
28	b	623	LMG	C11-C10-O7-C8
28	c	524	LMG	C11-C10-O7-C8
28	c	525	LMG	O6-C1-O1-C7
29	A	414	SQD	C46-C45-O47-C7
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
29	B	623	SQD	C8-C7-O47-C45
29	D	407	SQD	O5-C1-O6-C44
29	a	412	SQD	O6-C44-C45-O47
29	a	412	SQD	C5-C6-S-O7
29	a	412	SQD	C5-C6-S-O8
29	a	412	SQD	C5-C6-S-O9
29	a	413	SQD	O6-C44-C45-C46
29	a	413	SQD	O6-C44-C45-O47
29	a	413	SQD	C8-C7-O47-C45
29	f	101	SQD	C2-C1-O6-C44
29	f	101	SQD	O5-C1-O6-C44
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
34	B	622	LHG	C3-O3-P-O4
34	B	622	LHG	C4-O6-P-O3
34	B	622	LHG	C4-O6-P-O4
34	B	622	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
34	D	408	LHG	O1-C1-C2-C3
34	D	408	LHG	C1-C2-C3-O3
34	D	408	LHG	O2-C2-C3-O3
34	D	408	LHG	C3-O3-P-O4
34	D	408	LHG	C3-O3-P-O6
34	D	408	LHG	C4-O6-P-O3
34	D	408	LHG	C4-O6-P-O4
34	D	409	LHG	C3-O3-P-O6
34	D	412	LHG	O1-C1-C2-O2
34	D	412	LHG	O1-C1-C2-C3
34	E	101	LHG	O1-C1-C2-C3
34	E	101	LHG	C4-O6-P-O3
34	E	101	LHG	C4-O6-P-O4
34	d	406	LHG	O1-C1-C2-C3
34	d	406	LHG	C4-O6-P-O5
34	d	407	LHG	O1-C1-C2-C3
34	d	407	LHG	C3-O3-P-O4
34	d	407	LHG	C3-O3-P-O6
34	d	407	LHG	C4-O6-P-O3
34	d	407	LHG	C4-O6-P-O4
34	d	407	LHG	C4-O6-P-O5
34	e	102	LHG	C3-O3-P-O5
34	e	102	LHG	O10-C23-O8-C6
34	e	102	LHG	C24-C23-O8-C6
34	l	101	LHG	C4-O6-P-O3
34	l	101	LHG	C4-O6-P-O4
34	l	101	LHG	C4-O6-P-O5
35	F	101	HEC	C2B-C3B-CAB-CBB
35	F	101	HEC	C4B-C3B-CAB-CBB
35	F	101	HEC	C2C-C3C-CAC-CBC
35	F	101	HEC	C4C-C3C-CAC-CBC
35	V	201	HEC	C2B-C3B-CAB-CBB
35	V	201	HEC	C4B-C3B-CAB-CBB
35	V	201	HEC	C2C-C3C-CAC-CBC
35	V	201	HEC	C4C-C3C-CAC-CBC
35	e	101	HEC	C2C-C3C-CAC-CBC
35	e	101	HEC	C4C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
35	v	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
22	b	613	CLA	O1D-CGD-O2D-CED
28	M	101	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	c	524	LMG	O10-C28-O8-C9
28	c	525	LMG	O10-C28-O8-C9
34	E	101	LHG	O10-C23-O8-C6
29	D	407	SQD	C24-C23-O48-C46
34	E	101	LHG	C24-C23-O8-C6
29	D	407	SQD	O10-C23-O48-C46
29	a	413	SQD	O10-C23-O48-C46
29	b	619	SQD	O10-C23-O48-C46
28	D	410	LMG	O9-C10-O7-C8
28	c	524	LMG	O9-C10-O7-C8
29	a	413	SQD	O49-C7-O47-C45
22	A	405	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	b	613	CLA	C3-C5-C6-C7
28	c	524	LMG	C29-C28-O8-C9
28	c	525	LMG	C29-C28-O8-C9
29	a	413	SQD	C24-C23-O48-C46
29	b	619	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
22	B	602	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
28	A	412	LMG	C11-C10-O7-C8
29	B	623	SQD	O10-C23-O48-C46
22	A	405	CLA	C4-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
22	b	615	CLA	C4-C3-C5-C6
22	c	509	CLA	C4-C3-C5-C6
27	a	410	PL9	C35-C34-C36-C37
22	A	405	CLA	C2-C3-C5-C6
22	C	505	CLA	C2-C3-C5-C6
22	b	615	CLA	C2-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
27	d	405	PL9	C38-C39-C41-C42
22	B	602	CLA	CBA-CGA-O2A-C1
28	M	101	LMG	C29-C28-O8-C9
28	b	621	LMG	C29-C28-O8-C9
29	B	623	SQD	C24-C23-O48-C46
30	A	415	DGD	O6E-C5E-C6E-O5E
27	d	405	PL9	C12-C13-C14-C15
27	a	410	PL9	C42-C43-C44-C46

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Mol	Chain	Res	Type	Atoms
29	f	101	SQD	O10-C23-O48-C46
33	C	522	STE	C4-C5-C6-C7
22	B	606	CLA	C3-C5-C6-C7
22	B	604	CLA	CBD-CGD-O2D-CED
34	d	406	LHG	O2-C2-C3-O3
34	e	102	LHG	O2-C2-C3-O3
30	C	516	DGD	C1B-C2B-C3B-C4B
28	c	522	LMG	O9-C10-O7-C8
29	b	619	SQD	C8-C7-O47-C45
28	d	409	LMG	C10-C11-C12-C13
22	a	402	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	B	615	CLA	C4-C3-C5-C6
22	b	602	CLA	C4-C3-C5-C6
22	c	508	CLA	C4-C3-C5-C6
27	A	410	PL9	C20-C19-C21-C22
22	B	615	CLA	C2-C3-C5-C6
22	b	602	CLA	C2-C3-C5-C6
22	B	602	CLA	O1A-CGA-O2A-C1
27	A	410	PL9	C9-C11-C12-C13
27	A	410	PL9	C39-C41-C42-C43
27	a	410	PL9	C19-C21-C22-C23
27	a	410	PL9	C24-C26-C27-C28
27	a	410	PL9	C34-C36-C37-C38
22	c	514	CLA	CBD-CGD-O2D-CED
30	A	415	DGD	C4E-C5E-C6E-O5E
22	B	605	CLA	C3-C5-C6-C7
22	d	402	CLA	C3-C5-C6-C7
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
27	D	405	PL9	C27-C28-C29-C30
27	a	410	PL9	C7-C8-C9-C10
27	a	410	PL9	C17-C18-C19-C20
30	H	102	DGD	C4E-C5E-C6E-O5E
22	C	513	CLA	CBD-CGD-O2D-CED
34	d	406	LHG	C1-C2-C3-O3
34	e	102	LHG	C1-C2-C3-O3
22	c	508	CLA	CBA-CGA-O2A-C1
22	h	101	CLA	CBA-CGA-O2A-C1
28	B	629	LMG	C29-C28-O8-C9
30	A	415	DGD	C2A-C1A-O1G-C1G
22	h	101	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	B	622	LHG	C7-C8-C9-C10
33	X	101	STE	C13-C14-C15-C16
22	C	508	CLA	C4-C3-C5-C6
22	C	508	CLA	C2-C3-C5-C6
22	b	604	CLA	C2-C3-C5-C6
22	b	613	CLA	C2-C3-C5-C6
27	a	410	PL9	C33-C34-C36-C37
22	B	617	CLA	C3-C5-C6-C7
22	c	511	CLA	C3-C5-C6-C7
22	A	403	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C12-C13-C14
22	B	617	CLA	C11-C10-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	D	402	CLA	C11-C10-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C10-C8-C9
22	b	610	CLA	C14-C13-C15-C16
22	b	615	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	h	101	CLA	C14-C13-C15-C16
23	A	404	PHO	C14-C13-C15-C16
29	A	413	SQD	C7-C8-C9-C10
22	B	602	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
24	B	619	BCR	C37-C22-C23-C24
24	C	515	BCR	C36-C18-C19-C20
24	K	101	BCR	C36-C18-C19-C20
24	K	101	BCR	C37-C22-C23-C24
24	b	616	BCR	C36-C18-C19-C20
24	b	618	BCR	C37-C22-C23-C24
24	c	516	BCR	C11-C12-C13-C35
24	c	518	BCR	C36-C18-C19-C20
24	c	518	BCR	C37-C22-C23-C24
24	d	404	BCR	C37-C22-C23-C24
24	y	101	BCR	C36-C18-C19-C20
33	b	622	STE	C1-C2-C3-C4
29	A	413	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	d	401	PHO	CBD-CGD-O2D-CED
30	H	102	DGD	O6E-C5E-C6E-O5E
22	b	606	CLA	C10-C11-C12-C13
27	d	405	PL9	C32-C33-C34-C35
22	B	603	CLA	C13-C15-C16-C17
22	B	612	CLA	C8-C10-C11-C12
22	B	616	CLA	C5-C6-C7-C8
22	C	507	CLA	C5-C6-C7-C8
22	D	402	CLA	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
27	D	405	PL9	C47-C48-C49-C51
28	b	623	LMG	O6-C5-C6-O5
28	D	406	LMG	C10-C11-C12-C13
22	B	608	CLA	C10-C11-C12-C13
22	C	507	CLA	C13-C15-C16-C17
22	C	512	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
28	c	524	LMG	C4-C5-C6-O5
28	D	411	LMG	C28-C29-C30-C31
28	M	101	LMG	C28-C29-C30-C31
28	d	409	LMG	C28-C29-C30-C31
33	B	621	STE	C1-C2-C3-C4
27	A	410	PL9	C29-C31-C32-C33
27	A	410	PL9	C34-C36-C37-C38
27	d	405	PL9	C34-C36-C37-C38
28	c	522	LMG	C11-C10-O7-C8
28	M	101	LMG	C10-C11-C12-C13
29	B	623	SQD	C23-C24-C25-C26
30	c	521	DGD	C1A-C2A-C3A-C4A
33	L	101	STE	C1-C2-C3-C4
34	d	406	LHG	C23-C24-C25-C26
22	c	508	CLA	O1A-CGA-O2A-C1
28	B	629	LMG	O10-C28-O8-C9
28	D	410	LMG	O10-C28-O8-C9
22	B	606	CLA	C8-C10-C11-C12
22	B	615	CLA	C8-C10-C11-C12
22	C	514	CLA	C15-C16-C17-C18
22	c	508	CLA	C15-C16-C17-C18
22	c	514	CLA	C5-C6-C7-C8
22	c	514	CLA	C2A-CAA-CBA-CGA
24	d	404	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	503	CLA	C15-C16-C17-C18
22	C	504	CLA	C5-C6-C7-C8
22	C	510	CLA	C10-C11-C12-C13
22	c	505	CLA	C8-C10-C11-C12
22	c	508	CLA	C13-C15-C16-C17
22	c	514	CLA	C13-C15-C16-C17
28	C	519	LMG	C28-C29-C30-C31
28	c	522	LMG	C28-C29-C30-C31
33	b	624	STE	C1-C2-C3-C4
33	j	101	STE	C1-C2-C3-C4
34	D	409	LHG	C7-C8-C9-C10
34	E	101	LHG	C7-C8-C9-C10
22	h	101	CLA	O1A-CGA-O2A-C1
28	C	519	LMG	O10-C28-O8-C9
22	B	614	CLA	C8-C10-C11-C12
22	C	508	CLA	C10-C11-C12-C13
22	C	511	CLA	C15-C16-C17-C18
22	a	402	CLA	C15-C16-C17-C18
22	b	602	CLA	C5-C6-C7-C8
22	b	603	CLA	C15-C16-C17-C18
22	b	608	CLA	C15-C16-C17-C18
22	b	610	CLA	C13-C15-C16-C17
22	b	614	CLA	C10-C11-C12-C13
22	c	511	CLA	C13-C15-C16-C17
28	b	623	LMG	C28-C29-C30-C31
22	B	604	CLA	O1D-CGD-O2D-CED
30	c	520	DGD	C4E-C5E-C6E-O5E
22	C	505	CLA	C8-C10-C11-C12
22	C	506	CLA	C10-C11-C12-C13
22	c	513	CLA	C15-C16-C17-C18
22	c	514	CLA	C8-C10-C11-C12
22	B	608	CLA	C5-C6-C7-C8
22	C	514	CLA	CBA-CGA-O2A-C1
22	c	514	CLA	CBA-CGA-O2A-C1
28	C	519	LMG	C29-C28-O8-C9
28	C	519	LMG	C11-C10-O7-C8
28	D	410	LMG	C10-C11-C12-C13
22	B	606	CLA	C13-C15-C16-C17
22	c	513	CLA	C13-C15-C16-C17
22	A	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	a	412	SQD	C7-C8-C9-C10
22	B	607	CLA	C2A-CAA-CBA-CGA
24	B	619	BCR	C14-C15-C16-C17
22	B	603	CLA	C8-C10-C11-C12
22	B	608	CLA	C8-C10-C11-C12
22	B	613	CLA	C10-C11-C12-C13
22	B	616	CLA	C13-C15-C16-C17
22	C	510	CLA	C13-C15-C16-C17
22	b	603	CLA	C10-C11-C12-C13
22	c	508	CLA	C8-C10-C11-C12
22	a	402	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	C13-C15-C16-C17
22	c	505	CLA	C5-C6-C7-C8
22	h	101	CLA	C8-C10-C11-C12
29	A	413	SQD	C30-C31-C32-C33
22	C	509	CLA	C15-C16-C17-C18
22	b	610	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	c	511	CLA	C8-C10-C11-C12
22	c	512	CLA	C8-C10-C11-C12
34	l	101	LHG	C7-C8-C9-C10
22	b	613	CLA	C4-C3-C5-C6
22	c	508	CLA	C2-C3-C5-C6
22	B	607	CLA	C15-C16-C17-C18
22	d	403	CLA	C15-C16-C17-C18
28	B	629	LMG	C11-C10-O7-C8
22	b	613	CLA	C6-C7-C8-C9
29	B	623	SQD	C2-C1-O6-C44
30	C	517	DGD	C2E-C1E-O5D-C6D
30	c	520	DGD	C2E-C1E-O5D-C6D
22	b	601	CLA	C16-C17-C18-C20
24	A	406	BCR	C35-C13-C14-C15
24	B	618	BCR	C11-C10-C9-C34
24	B	618	BCR	C35-C13-C14-C15
24	B	618	BCR	C16-C17-C18-C36
24	B	619	BCR	C16-C17-C18-C36
24	B	619	BCR	C20-C21-C22-C37
24	B	620	BCR	C11-C10-C9-C34
24	B	620	BCR	C20-C21-C22-C37
24	D	404	BCR	C20-C21-C22-C37
24	Y	101	BCR	C11-C10-C9-C34
24	Y	101	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
24	Z	101	BCR	C20-C21-C22-C37
24	b	616	BCR	C16-C17-C18-C36
24	b	616	BCR	C20-C21-C22-C37
24	b	617	BCR	C16-C17-C18-C36
24	b	617	BCR	C20-C21-C22-C37
24	b	618	BCR	C35-C13-C14-C15
24	c	518	BCR	C20-C21-C22-C37
24	t	101	BCR	C20-C21-C22-C37
24	x	101	BCR	C11-C10-C9-C34
24	x	101	BCR	C20-C21-C22-C37
24	T	101	BCR	C36-C18-C19-C20
24	d	404	BCR	C21-C22-C23-C24
22	C	514	CLA	O1A-CGA-O2A-C1
28	b	621	LMG	O10-C28-O8-C9
30	A	415	DGD	CEB-CFB-CGB-CHB
22	b	605	CLA	C2A-CAA-CBA-CGA
34	D	409	LHG	O1-C1-C2-C3
34	d	408	LHG	O1-C1-C2-C3
30	c	520	DGD	O6E-C5E-C6E-O5E
29	b	619	SQD	C46-C45-O47-C7
22	c	512	CLA	C16-C17-C18-C20
22	d	402	CLA	C16-C17-C18-C19
22	c	514	CLA	O1A-CGA-O2A-C1
30	c	521	DGD	O1A-C1A-O1G-C1G
22	b	612	CLA	C13-C15-C16-C17
22	c	507	CLA	C15-C16-C17-C18
24	Z	101	BCR	C12-C13-C14-C15
24	a	406	BCR	C20-C21-C22-C23
24	c	516	BCR	C20-C21-C22-C23
24	c	517	BCR	C20-C21-C22-C23
24	c	518	BCR	C16-C17-C18-C19
24	t	101	BCR	C20-C21-C22-C23
24	x	101	BCR	C11-C10-C9-C8
24	y	101	BCR	C20-C21-C22-C23
30	c	520	DGD	O6E-C1E-O5D-C6D
22	c	514	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C13-C15-C16-C17
22	b	606	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	C2-C1-O2A-CGA
22	B	607	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	C16-C17-C18-C19
22	C	511	CLA	C16-C17-C18-C20
22	c	506	CLA	C11-C12-C13-C14
22	c	514	CLA	C16-C17-C18-C19
22	B	604	CLA	C15-C16-C17-C18
28	D	411	LMG	C30-C31-C32-C33
28	c	522	LMG	C36-C37-C38-C39
28	c	524	LMG	C34-C35-C36-C37
34	D	412	LHG	C12-C13-C14-C15
34	l	101	LHG	C17-C18-C19-C20
22	C	502	CLA	CBD-CGD-O2D-CED
24	A	406	BCR	C14-C15-C16-C17
24	c	517	BCR	C14-C15-C16-C17
28	B	629	LMG	C36-C37-C38-C39
29	a	413	SQD	C11-C10-C9-C8
30	C	518	DGD	C6A-C7A-C8A-C9A
30	c	519	DGD	C6B-C7B-C8B-C9B
33	b	620	STE	C6-C7-C8-C9
33	b	622	STE	C7-C8-C9-C10
33	b	625	STE	C12-C13-C14-C15
33	h	103	STE	C9-C10-C11-C12
34	B	622	LHG	C31-C32-C33-C34
34	E	101	LHG	C11-C12-C13-C14
34	e	102	LHG	C14-C15-C16-C17
29	a	412	SQD	C15-C16-C17-C18
29	a	413	SQD	C10-C11-C12-C13
33	B	624	STE	C11-C10-C9-C8
33	d	410	STE	C5-C6-C7-C8
34	D	409	LHG	C25-C26-C27-C28
34	D	412	LHG	C29-C30-C31-C32
34	d	406	LHG	C32-C33-C34-C35
30	c	519	DGD	O6D-C5D-C6D-O5D
28	D	406	LMG	C21-C22-C23-C24
30	A	415	DGD	CBB-CCB-CDB-CEB
30	C	516	DGD	C5A-C6A-C7A-C8A
30	c	519	DGD	C4B-C5B-C6B-C7B
33	B	627	STE	C11-C12-C13-C14
33	E	102	STE	C3-C4-C5-C6
33	b	620	STE	C7-C8-C9-C10
33	b	625	STE	C14-C15-C16-C17
34	D	408	LHG	C11-C12-C13-C14
34	D	412	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	O1-C1-C2-O2
34	d	406	LHG	O1-C1-C2-O2
34	d	407	LHG	O1-C1-C2-O2
28	D	406	LMG	C35-C36-C37-C38
29	A	413	SQD	C13-C14-C15-C16
29	B	623	SQD	C33-C34-C35-C36
34	B	622	LHG	C29-C30-C31-C32
34	D	408	LHG	C10-C11-C12-C13
22	b	609	CLA	C4B-C3B-CAB-CBB
22	d	402	CLA	C4B-C3B-CAB-CBB
28	A	412	LMG	C28-C29-C30-C31
29	D	407	SQD	C31-C32-C33-C34
30	A	415	DGD	CBA-CCA-CDA-CEA
30	C	517	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	C2B-C3B-C4B-C5B
22	B	606	CLA	C16-C17-C18-C19
22	a	402	CLA	C16-C17-C18-C19
22	c	514	CLA	C16-C17-C18-C20
22	d	402	CLA	C16-C17-C18-C20
28	C	519	LMG	C32-C33-C34-C35
28	c	525	LMG	C15-C16-C17-C18
30	H	102	DGD	C7A-C8A-C9A-CAA
33	c	523	STE	C9-C10-C11-C12
22	b	605	CLA	C15-C16-C17-C18
22	c	511	CLA	C10-C11-C12-C13
28	B	629	LMG	C12-C13-C14-C15
22	b	614	CLA	C11-C12-C13-C15
22	d	403	CLA	C12-C13-C15-C16
29	f	101	SQD	C32-C33-C34-C35
33	d	412	STE	C14-C15-C16-C17
34	D	412	LHG	C18-C19-C20-C21
34	d	407	LHG	C29-C30-C31-C32
34	D	409	LHG	O2-C2-C3-O3
34	E	101	LHG	C23-C24-C25-C26
28	A	412	LMG	C38-C39-C40-C41
28	b	623	LMG	C30-C31-C32-C33
28	c	525	LMG	C13-C14-C15-C16
33	l	102	STE	C14-C15-C16-C17
30	C	518	DGD	O1A-C1A-O1G-C1G
22	C	513	CLA	C3A-C2A-CAA-CBA
22	c	514	CLA	C3A-C2A-CAA-CBA
22	C	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
34	d	406	LHG	C10-C11-C12-C13
28	A	412	LMG	C16-C17-C18-C19
22	C	507	CLA	C8-C10-C11-C12
22	c	515	CLA	C5-C6-C7-C8
28	c	524	LMG	C28-C29-C30-C31
22	C	505	CLA	C11-C12-C13-C14
22	a	402	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C19
28	B	629	LMG	C11-C12-C13-C14
28	d	409	LMG	C32-C33-C34-C35
28	b	623	LMG	C32-C33-C34-C35
29	f	101	SQD	C29-C30-C31-C32
33	B	627	STE	C4-C5-C6-C7
33	b	622	STE	C14-C15-C16-C17
33	d	412	STE	C9-C10-C11-C12
28	c	524	LMG	C16-C17-C18-C19
29	B	623	SQD	C13-C14-C15-C16
33	H	103	STE	C13-C14-C15-C16
34	d	408	LHG	C32-C33-C34-C35
28	b	621	LMG	C28-C29-C30-C31
33	B	625	STE	C1-C2-C3-C4
34	d	406	LHG	C7-C8-C9-C10
34	d	408	LHG	C23-C24-C25-C26
28	c	524	LMG	C31-C32-C33-C34
30	H	102	DGD	C5B-C6B-C7B-C8B
30	c	519	DGD	C5B-C6B-C7B-C8B
33	b	626	STE	C6-C7-C8-C9
34	B	622	LHG	C17-C18-C19-C20
34	E	101	LHG	C34-C35-C36-C37
29	A	413	SQD	C16-C17-C18-C19
29	B	623	SQD	C11-C12-C13-C14
29	a	413	SQD	C11-C12-C13-C14
30	A	415	DGD	C4B-C5B-C6B-C7B
30	A	415	DGD	C6B-C7B-C8B-C9B
30	h	102	DGD	C9A-CAA-CBA-CCA
34	B	622	LHG	C12-C13-C14-C15
34	e	102	LHG	C16-C17-C18-C19
30	C	517	DGD	C5A-C6A-C7A-C8A
34	l	101	LHG	C32-C33-C34-C35
28	b	621	LMG	C32-C33-C34-C35
29	b	619	SQD	C26-C27-C28-C29
30	c	521	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C32-C33-C34-C35
22	b	608	CLA	C2B-C3B-CAB-CBB
24	T	101	BCR	C1-C6-C7-C8
24	c	516	BCR	C1-C6-C7-C8
24	c	516	BCR	C5-C6-C7-C8
28	M	101	LMG	C16-C17-C18-C19
34	D	408	LHG	C12-C13-C14-C15
34	D	408	LHG	C30-C31-C32-C33
34	D	409	LHG	C9-C10-C11-C12
34	l	101	LHG	C27-C28-C29-C30
28	D	410	LMG	C28-C29-C30-C31
33	E	102	STE	C1-C2-C3-C4
28	d	409	LMG	C33-C34-C35-C36
30	C	517	DGD	C7B-C8B-C9B-CAB
30	c	520	DGD	C6B-C7B-C8B-C9B
33	c	523	STE	C11-C12-C13-C14
33	d	410	STE	C10-C11-C12-C13
33	h	103	STE	C11-C12-C13-C14
33	l	102	STE	C10-C11-C12-C13
34	D	409	LHG	C11-C10-C9-C8
28	b	621	LMG	O9-C10-O7-C8
29	b	619	SQD	O49-C7-O47-C45
28	D	411	LMG	C32-C33-C34-C35
28	M	101	LMG	C36-C37-C38-C39
24	B	618	BCR	C10-C11-C12-C13
24	B	620	BCR	C10-C11-C12-C13
24	a	406	BCR	C18-C19-C20-C21
22	C	506	CLA	C5-C6-C7-C8
27	A	410	PL9	C23-C24-C26-C27
22	B	607	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C19
22	b	601	CLA	C16-C17-C18-C19
28	A	412	LMG	C12-C13-C14-C15
29	A	413	SQD	C28-C29-C30-C31
30	c	520	DGD	C5B-C6B-C7B-C8B
33	b	622	STE	C2-C3-C4-C5
28	c	525	LMG	C30-C31-C32-C33
30	c	520	DGD	CAB-CBB-CCB-CDB
33	h	103	STE	C7-C8-C9-C10
28	B	629	LMG	C16-C17-C18-C19
28	c	522	LMG	C33-C34-C35-C36
28	c	525	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	c	525	LMG	C17-C18-C19-C20
29	a	412	SQD	C29-C30-C31-C32
33	l	102	STE	C4-C5-C6-C7
34	d	407	LHG	C11-C12-C13-C14
30	C	517	DGD	O6E-C1E-O5D-C6D
28	D	411	LMG	C14-C15-C16-C17
28	c	524	LMG	O6-C5-C6-O5
22	A	411	CLA	C15-C16-C17-C18
30	c	519	DGD	C3B-C4B-C5B-C6B
33	b	625	STE	C4-C5-C6-C7
33	b	626	STE	C2-C3-C4-C5
34	D	408	LHG	C34-C35-C36-C37
28	c	525	LMG	C39-C40-C41-C42
29	a	413	SQD	C15-C16-C17-C18
33	H	103	STE	C7-C8-C9-C10
33	L	101	STE	C4-C5-C6-C7
34	D	409	LHG	C32-C33-C34-C35
22	c	513	CLA	C16-C17-C18-C19
33	d	410	STE	C1-C2-C3-C4
33	T	102	STE	C12-C13-C14-C15
22	b	613	CLA	C5-C6-C7-C8
34	B	622	LHG	O9-C7-O7-C5
33	c	523	STE	C2-C3-C4-C5
34	D	409	LHG	C10-C11-C12-C13
22	A	402	CLA	C2C-C3C-CAC-CBC
28	A	412	LMG	C34-C35-C36-C37
28	D	410	LMG	C14-C15-C16-C17
34	d	407	LHG	C12-C13-C14-C15
30	h	102	DGD	CBA-CCA-CDA-CEA
30	c	520	DGD	C1A-C2A-C3A-C4A
30	C	517	DGD	CBA-CCA-CDA-CEA
22	h	101	CLA	C3-C5-C6-C7
28	B	629	LMG	C8-C7-O1-C1
30	C	517	DGD	C5D-C6D-O5D-C1E
30	c	520	DGD	C5D-C6D-O5D-C1E
28	B	629	LMG	C14-C15-C16-C17
33	d	410	STE	C4-C5-C6-C7
22	C	503	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C20
22	c	513	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
28	D	406	LMG	C17-C18-C19-C20
28	D	406	LMG	C39-C40-C41-C42
30	C	518	DGD	C5A-C6A-C7A-C8A
34	D	408	LHG	C32-C33-C34-C35
34	l	101	LHG	C26-C27-C28-C29
33	B	621	STE	C4-C5-C6-C7
33	B	627	STE	C5-C6-C7-C8
34	D	409	LHG	C30-C31-C32-C33
29	B	623	SQD	C35-C36-C37-C38
28	b	621	LMG	C33-C34-C35-C36
33	l	102	STE	C9-C10-C11-C12
34	d	408	LHG	O10-C23-O8-C6
30	c	519	DGD	O6E-C5E-C6E-O5E
22	B	602	CLA	C8-C10-C11-C12
22	B	612	CLA	C13-C15-C16-C17
22	B	617	CLA	C5-C6-C7-C8
22	d	403	CLA	C8-C10-C11-C12
28	D	410	LMG	C29-C28-O8-C9
29	a	412	SQD	O49-C7-O47-C45
30	H	102	DGD	C9A-CAA-CBA-CCA
33	T	102	STE	C13-C14-C15-C16
33	b	622	STE	C10-C11-C12-C13
22	c	509	CLA	C5-C6-C7-C8
33	X	101	STE	C4-C5-C6-C7
34	e	102	LHG	C7-C8-C9-C10
28	D	411	LMG	C31-C32-C33-C34
30	A	415	DGD	O2G-C2G-C3G-O3G
34	d	406	LHG	C34-C35-C36-C37
30	C	516	DGD	CCB-CDB-CEB-CFB
33	B	626	STE	C9-C10-C11-C12
33	C	521	STE	C4-C5-C6-C7
33	b	624	STE	C3-C4-C5-C6
22	A	411	CLA	C13-C15-C16-C17
22	B	610	CLA	C15-C16-C17-C18
30	A	415	DGD	C2B-C3B-C4B-C5B
33	T	102	STE	C5-C6-C7-C8
33	a	414	STE	C2-C3-C4-C5
34	E	101	LHG	C24-C25-C26-C27
28	B	629	LMG	C32-C33-C34-C35
30	c	521	DGD	C9B-CAB-CBB-CCB
34	D	409	LHG	C31-C32-C33-C34
22	c	513	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	C16-C17-C18-C19
30	c	520	DGD	CBB-CCB-CDB-CEB
33	M	102	STE	C11-C10-C9-C8
29	A	414	SQD	C12-C13-C14-C15
30	c	521	DGD	C6A-C7A-C8A-C9A
27	D	405	PL9	C13-C14-C16-C17
28	C	519	LMG	C18-C19-C20-C21
28	b	623	LMG	C11-C12-C13-C14
29	D	407	SQD	C30-C31-C32-C33
33	c	501	STE	C5-C6-C7-C8
28	D	406	LMG	C30-C31-C32-C33
30	c	519	DGD	C4A-C5A-C6A-C7A
34	D	408	LHG	C13-C14-C15-C16
28	b	621	LMG	C37-C38-C39-C40
28	b	623	LMG	C16-C17-C18-C19
33	d	411	STE	C3-C4-C5-C6
22	a	405	CLA	C10-C11-C12-C13
22	h	101	CLA	O1D-CGD-O2D-CED
28	b	623	LMG	C34-C35-C36-C37
33	b	622	STE	C9-C10-C11-C12
33	c	501	STE	C6-C7-C8-C9
34	D	408	LHG	O1-C1-C2-O2
30	c	519	DGD	C7A-C8A-C9A-CAA
34	D	409	LHG	C24-C25-C26-C27
22	c	510	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C1A-C2A-CAA-CBA
28	c	525	LMG	C33-C34-C35-C36
29	A	413	SQD	C9-C10-C11-C12
34	D	408	LHG	C33-C34-C35-C36
30	A	415	DGD	CCA-CDA-CEA-CFA
33	b	626	STE	C5-C6-C7-C8
34	d	406	LHG	C33-C34-C35-C36
27	D	405	PL9	C47-C48-C49-C50
28	B	629	LMG	C30-C31-C32-C33
28	b	621	LMG	C18-C19-C20-C21
29	a	412	SQD	C24-C25-C26-C27
34	d	406	LHG	C31-C32-C33-C34
30	c	519	DGD	O1B-C1B-O2G-C2G
30	h	102	DGD	C6B-C7B-C8B-C9B
33	B	627	STE	C9-C10-C11-C12
33	H	103	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	j	101	STE	C4-C5-C6-C7
22	B	604	CLA	C11-C12-C13-C15
22	B	605	CLA	C12-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C7
22	B	616	CLA	C11-C12-C13-C15
22	C	506	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C12-C13-C15
22	C	514	CLA	C11-C10-C8-C7
22	a	405	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C12-C13-C15
22	c	507	CLA	C6-C7-C8-C10
22	c	515	CLA	C11-C12-C13-C15
22	h	101	CLA	C12-C13-C15-C16
30	A	415	DGD	C4A-C5A-C6A-C7A
22	B	611	CLA	C16-C17-C18-C20
22	h	101	CLA	C16-C17-C18-C20
29	A	413	SQD	C26-C27-C28-C29
34	B	622	LHG	C14-C15-C16-C17
29	A	414	SQD	C7-C8-C9-C10
22	B	610	CLA	C2-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
22	C	511	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
27	A	410	PL9	C28-C29-C31-C32
29	a	412	SQD	C17-C18-C19-C20
28	c	522	LMG	O6-C5-C6-O5
30	C	516	DGD	O6E-C5E-C6E-O5E
29	a	412	SQD	C32-C33-C34-C35
33	E	102	STE	C4-C5-C6-C7
34	l	101	LHG	C29-C30-C31-C32
22	A	403	CLA	C11-C12-C13-C14
22	B	605	CLA	C6-C7-C8-C9
22	B	608	CLA	C11-C10-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
22	c	515	CLA	C11-C12-C13-C14
22	d	403	CLA	C14-C13-C15-C16
33	L	101	STE	C5-C6-C7-C8
28	D	406	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
33	d	410	STE	C11-C12-C13-C14
27	A	410	PL9	C42-C43-C44-C45
33	B	628	STE	C5-C6-C7-C8
28	B	629	LMG	O1-C7-C8-C9
29	B	623	SQD	O6-C44-C45-C46
30	A	415	DGD	C1G-C2G-C3G-O3G
34	d	408	LHG	C4-C5-C6-O8
28	C	519	LMG	C30-C31-C32-C33
28	C	519	LMG	C31-C32-C33-C34
30	C	516	DGD	C9A-CAA-CBA-CCA
30	H	102	DGD	C7B-C8B-C9B-CAB
33	b	622	STE	C13-C14-C15-C16
28	c	524	LMG	C30-C31-C32-C33
30	A	415	DGD	CCB-CDB-CEB-CFB
34	E	101	LHG	C15-C16-C17-C18
34	d	406	LHG	C16-C17-C18-C19
34	e	102	LHG	C24-C25-C26-C27
28	D	406	LMG	O6-C5-C6-O5
29	a	412	SQD	C25-C26-C27-C28
33	H	103	STE	C10-C11-C12-C13
34	B	622	LHG	C18-C19-C20-C21
34	d	407	LHG	C11-C10-C9-C8
33	H	103	STE	C3-C4-C5-C6
28	d	409	LMG	O6-C5-C6-O5
22	b	604	CLA	C15-C16-C17-C18
28	D	411	LMG	C16-C17-C18-C19
34	d	407	LHG	C17-C18-C19-C20
29	A	414	SQD	C18-C19-C20-C21
30	C	517	DGD	C9B-CAB-CBB-CCB
33	d	411	STE	C10-C11-C12-C13
34	D	409	LHG	C27-C28-C29-C30
34	d	406	LHG	C18-C19-C20-C21
22	B	610	CLA	C4-C3-C5-C6
22	C	506	CLA	C4-C3-C5-C6
22	a	403	CLA	C8-C10-C11-C12
22	b	606	CLA	C8-C10-C11-C12
30	h	102	DGD	O6E-C5E-C6E-O5E
24	b	617	BCR	C37-C22-C23-C24
28	A	412	LMG	C33-C34-C35-C36
34	d	407	LHG	C14-C15-C16-C17
28	B	629	LMG	O6-C5-C6-O5
29	a	412	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	C3A-C4A-C5A-C6A
34	D	408	LHG	C9-C10-C11-C12
28	d	409	LMG	C38-C39-C40-C41
29	f	101	SQD	C24-C25-C26-C27
22	B	604	CLA	C5-C6-C7-C8
28	B	629	LMG	C39-C40-C41-C42
28	b	623	LMG	C31-C32-C33-C34
29	b	619	SQD	C25-C26-C27-C28
33	Z	102	STE	C11-C12-C13-C14
33	a	414	STE	C4-C5-C6-C7
34	D	408	LHG	C25-C26-C27-C28
28	D	406	LMG	C12-C13-C14-C15
28	b	621	LMG	C31-C32-C33-C34
30	h	102	DGD	C5B-C6B-C7B-C8B
33	B	628	STE	C10-C11-C12-C13
22	b	607	CLA	CBA-CGA-O2A-C1
22	c	513	CLA	CBA-CGA-O2A-C1
22	C	513	CLA	O2A-C1-C2-C3
22	C	514	CLA	O2A-C1-C2-C3
28	D	410	LMG	C9-C8-O7-C10
29	a	413	SQD	C9-C10-C11-C12
28	b	623	LMG	C17-C18-C19-C20
29	B	623	SQD	C34-C35-C36-C37
30	c	519	DGD	C3A-C4A-C5A-C6A
30	h	102	DGD	C7A-C8A-C9A-CAA
34	B	622	LHG	C34-C35-C36-C37
23	d	401	PHO	C2C-C3C-CAC-CBC
28	b	623	LMG	C40-C41-C42-C43
30	c	520	DGD	C4A-C5A-C6A-C7A
33	M	103	STE	C4-C5-C6-C7
34	D	412	LHG	C24-C25-C26-C27
30	c	519	DGD	C4D-C5D-C6D-O5D
28	d	409	LMG	C14-C15-C16-C17
29	A	414	SQD	C19-C20-C21-C22
29	a	412	SQD	C35-C36-C37-C38
22	C	512	CLA	O1D-CGD-O2D-CED
24	B	619	BCR	C11-C10-C9-C8
24	C	515	BCR	C16-C17-C18-C19
24	b	616	BCR	C20-C21-C22-C23
24	c	516	BCR	C16-C17-C18-C19
29	B	623	SQD	C9-C10-C11-C12
34	D	412	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
34	d	408	LHG	C26-C27-C28-C29
22	c	503	CLA	O1D-CGD-O2D-CED
22	A	405	CLA	CBA-CGA-O2A-C1
22	a	405	CLA	CBA-CGA-O2A-C1
34	l	101	LHG	C34-C35-C36-C37
30	H	102	DGD	CCA-CDA-CEA-CFA
34	d	406	LHG	C25-C26-C27-C28
27	a	410	PL9	C20-C19-C21-C22
27	d	405	PL9	C13-C14-C16-C17
28	b	623	LMG	C42-C43-C44-C45
29	a	413	SQD	C19-C20-C21-C22
28	M	101	LMG	C12-C13-C14-C15
28	b	623	LMG	C18-C19-C20-C21
28	c	524	LMG	C41-C42-C43-C44
29	f	101	SQD	C31-C32-C33-C34
30	H	102	DGD	C3B-C4B-C5B-C6B
33	d	412	STE	C11-C12-C13-C14
22	C	503	CLA	C16-C17-C18-C19
28	B	629	LMG	C33-C34-C35-C36
28	M	101	LMG	C29-C30-C31-C32
29	A	413	SQD	C34-C35-C36-C37
33	B	601	STE	C2-C3-C4-C5
33	b	620	STE	C10-C11-C12-C13
33	d	410	STE	C9-C10-C11-C12
22	c	510	CLA	C16-C17-C18-C19
30	C	517	DGD	CDA-CEA-CFA-CGA
33	C	521	STE	C3-C4-C5-C6
28	B	629	LMG	C37-C38-C39-C40
29	B	623	SQD	C18-C19-C20-C21
30	C	516	DGD	C2A-C3A-C4A-C5A
33	C	520	STE	C2-C3-C4-C5
33	h	103	STE	C6-C7-C8-C9
28	c	524	LMG	O1-C7-C8-O7
28	c	525	LMG	O1-C7-C8-O7
29	A	413	SQD	O6-C44-C45-O47
29	b	619	SQD	O47-C45-C46-O48
29	A	413	SQD	C17-C18-C19-C20
33	d	410	STE	C12-C13-C14-C15
30	c	520	DGD	CBA-CCA-CDA-CEA
33	b	622	STE	C5-C6-C7-C8
34	d	406	LHG	C27-C28-C29-C30
34	d	407	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
34	d	406	LHG	C19-C20-C21-C22
28	M	101	LMG	C14-C15-C16-C17
33	B	628	STE	C11-C10-C9-C8
22	a	403	CLA	C16-C17-C18-C20
30	h	102	DGD	CDB-CEB-CFB-CGB
34	D	412	LHG	C19-C20-C21-C22
33	B	624	STE	C4-C5-C6-C7
33	B	628	STE	C6-C7-C8-C9
33	H	103	STE	C1-C2-C3-C4
28	D	410	LMG	C33-C34-C35-C36
28	b	623	LMG	C4-C5-C6-O5
33	I	101	STE	C1-C2-C3-C4
33	b	626	STE	C1-C2-C3-C4
34	D	409	LHG	C35-C36-C37-C38
27	d	405	PL9	C37-C38-C39-C40
30	H	102	DGD	CAA-CBA-CCA-CDA
33	l	102	STE	C2-C3-C4-C5
22	c	506	CLA	C5-C6-C7-C8
23	d	401	PHO	O1D-CGD-O2D-CED
22	C	506	CLA	C16-C17-C18-C20
22	c	512	CLA	C4-C3-C5-C6
27	D	405	PL9	C30-C29-C31-C32
34	D	409	LHG	C14-C15-C16-C17
33	d	411	STE	C2-C3-C4-C5
28	c	522	LMG	C34-C35-C36-C37
29	a	412	SQD	C10-C11-C12-C13
34	l	101	LHG	C13-C14-C15-C16
34	d	408	LHG	O1-C1-C2-O2
22	B	605	CLA	C14-C13-C15-C16
22	B	606	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C12-C13-C14
22	C	506	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	C	511	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C12-C13-C14
22	C	513	CLA	C14-C13-C15-C16
22	C	514	CLA	C11-C10-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	602	CLA	C11-C10-C8-C9
22	b	606	CLA	C11-C12-C13-C14
22	b	608	CLA	C14-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C6-C7-C8-C9
22	c	514	CLA	C11-C12-C13-C14
30	c	521	DGD	C5A-C6A-C7A-C8A
34	B	622	LHG	C27-C28-C29-C30
30	A	415	DGD	O1A-C1A-O1G-C1G
22	c	506	CLA	C4B-C3B-CAB-CBB
22	c	507	CLA	C4B-C3B-CAB-CBB
22	h	101	CLA	C4B-C3B-CAB-CBB
30	h	102	DGD	CAB-CBB-CCB-CDB
34	e	102	LHG	C27-C28-C29-C30
30	c	519	DGD	CDB-CEB-CFB-CGB
22	a	403	CLA	C16-C17-C18-C19
30	A	415	DGD	CFA-CGA-CHA-CIA
33	X	101	STE	C2-C3-C4-C5
34	e	102	LHG	C11-C10-C9-C8
29	D	407	SQD	C2-C1-O6-C44
28	B	629	LMG	C34-C35-C36-C37
30	C	517	DGD	C5B-C6B-C7B-C8B
33	I	101	STE	C4-C5-C6-C7
34	e	102	LHG	C13-C14-C15-C16
29	a	412	SQD	C19-C20-C21-C22
34	d	407	LHG	O6-C4-C5-C6
34	E	101	LHG	C28-C29-C30-C31
22	A	403	CLA	C11-C12-C13-C15
22	B	605	CLA	C6-C7-C8-C10
22	B	606	CLA	C12-C13-C15-C16
22	B	607	CLA	C11-C12-C13-C15
22	B	608	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	511	CLA	C11-C10-C8-C7
22	C	513	CLA	C12-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C7
22	b	603	CLA	C11-C12-C13-C15
22	b	607	CLA	C11-C12-C13-C15
22	b	608	CLA	C12-C13-C15-C16
22	b	613	CLA	C12-C13-C15-C16
22	c	508	CLA	C11-C12-C13-C15
22	c	511	CLA	C11-C12-C13-C15
22	c	513	CLA	C12-C13-C15-C16
22	c	514	CLA	C11-C12-C13-C15
22	c	514	CLA	C12-C13-C15-C16
33	B	627	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
34	e	102	LHG	C23-C24-C25-C26
22	A	405	CLA	C6-C7-C8-C9
33	L	101	STE	C7-C8-C9-C10
30	c	520	DGD	C7A-C8A-C9A-CAA
22	c	504	CLA	C16-C17-C18-C20
34	D	409	LHG	C26-C27-C28-C29
34	l	101	LHG	C33-C34-C35-C36
22	c	514	CLA	C4-C3-C5-C6
27	a	410	PL9	C40-C39-C41-C42
28	b	621	LMG	C39-C40-C41-C42
33	L	101	STE	C3-C4-C5-C6
33	M	102	STE	C9-C10-C11-C12
22	c	513	CLA	O1A-CGA-O2A-C1
33	B	626	STE	C11-C12-C13-C14
34	l	101	LHG	C15-C16-C17-C18
24	c	518	BCR	C19-C20-C21-C22
24	y	101	BCR	C19-C20-C21-C22
24	y	101	BCR	C7-C8-C9-C34
34	d	408	LHG	C35-C36-C37-C38
34	d	406	LHG	C15-C16-C17-C18
34	B	622	LHG	C19-C20-C21-C22
30	A	415	DGD	CAA-CBA-CCA-CDA
29	a	413	SQD	C31-C32-C33-C34
29	D	407	SQD	C25-C26-C27-C28
30	H	102	DGD	CAB-CBB-CCB-CDB
28	c	524	LMG	O1-C7-C8-C9
28	c	524	LMG	C7-C8-C9-O8
28	c	525	LMG	O1-C7-C8-C9
29	a	412	SQD	O6-C44-C45-C46
30	c	519	DGD	O1G-C1G-C2G-C3G
34	E	101	LHG	C4-C5-C6-O8
33	c	523	STE	C7-C8-C9-C10
34	D	412	LHG	C7-C8-C9-C10
22	B	611	CLA	C16-C17-C18-C19
33	b	625	STE	C11-C10-C9-C8
30	C	518	DGD	CCA-CDA-CEA-CFA
33	b	624	STE	C9-C10-C11-C12
28	A	412	LMG	C40-C41-C42-C43
28	C	519	LMG	C19-C20-C21-C22
28	D	406	LMG	C36-C37-C38-C39
34	D	412	LHG	C28-C29-C30-C31
22	C	511	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	c	521	DGD	C7A-C8A-C9A-CAA
22	c	514	CLA	C2-C3-C5-C6
22	B	606	CLA	C16-C17-C18-C20
22	C	506	CLA	C16-C17-C18-C19
24	T	101	BCR	C5-C6-C7-C8
24	Z	101	BCR	C23-C24-C25-C30
33	c	523	STE	C12-C13-C14-C15
33	X	101	STE	C11-C10-C9-C8
33	c	523	STE	C4-C5-C6-C7
22	c	512	CLA	C5-C6-C7-C8
33	C	521	STE	C12-C13-C14-C15
33	H	103	STE	C12-C13-C14-C15
33	X	101	STE	C10-C11-C12-C13
34	E	101	LHG	C16-C17-C18-C19
33	a	415	STE	C6-C7-C8-C9
22	C	513	CLA	C13-C15-C16-C17
22	c	515	CLA	C13-C15-C16-C17
28	M	101	LMG	O7-C8-C9-O8
28	b	621	LMG	O7-C8-C9-O8
29	a	412	SQD	O47-C45-C46-O48
29	a	413	SQD	O47-C45-C46-O48
27	a	410	PL9	C4-C3-C7-C8
29	a	413	SQD	C14-C15-C16-C17
30	c	521	DGD	C3B-C4B-C5B-C6B
33	d	411	STE	C1-C2-C3-C4
28	C	519	LMG	C15-C16-C17-C18
28	M	101	LMG	C18-C19-C20-C21
34	D	409	LHG	C33-C34-C35-C36
34	d	407	LHG	C25-C26-C27-C28
22	B	602	CLA	C15-C16-C17-C18
22	b	615	CLA	C10-C11-C12-C13
27	D	405	PL9	C28-C29-C31-C32
29	a	413	SQD	C18-C19-C20-C21
28	c	525	LMG	C31-C32-C33-C34
33	d	410	STE	C7-C8-C9-C10
33	d	412	STE	C1-C2-C3-C4
22	B	604	CLA	C11-C12-C13-C14
22	B	614	CLA	C11-C12-C13-C14
22	a	403	CLA	C14-C13-C15-C16
22	b	613	CLA	C14-C13-C15-C16
22	c	514	CLA	C6-C7-C8-C9
22	c	514	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	b	621	LMG	C38-C39-C40-C41
33	d	411	STE	C9-C10-C11-C12
24	y	101	BCR	C22-C23-C24-C25
28	b	621	LMG	C13-C14-C15-C16
34	d	407	LHG	C32-C33-C34-C35
22	B	612	CLA	C16-C17-C18-C20
22	B	614	CLA	C16-C17-C18-C19
22	b	606	CLA	C16-C17-C18-C20
22	c	506	CLA	C11-C12-C13-C15
22	h	101	CLA	C16-C17-C18-C19
29	B	623	SQD	C27-C28-C29-C30
34	e	102	LHG	C10-C11-C12-C13
33	a	414	STE	C7-C8-C9-C10
28	c	525	LMG	C2-C1-O1-C7
33	b	622	STE	C6-C7-C8-C9
33	M	102	STE	C4-C5-C6-C7
28	b	621	LMG	C11-C12-C13-C14
28	b	621	LMG	C14-C15-C16-C17
29	a	412	SQD	O10-C23-O48-C46
22	C	511	CLA	C10-C11-C12-C13
29	a	412	SQD	C24-C23-O48-C46
28	B	629	LMG	O8-C28-C29-C30
30	C	516	DGD	O1G-C1A-C2A-C3A
22	B	614	CLA	C16-C17-C18-C20
33	C	520	STE	C3-C4-C5-C6
22	a	411	CLA	C2C-C3C-CAC-CBC
22	B	615	CLA	C15-C16-C17-C18
30	c	519	DGD	C2A-C3A-C4A-C5A
33	X	101	STE	C3-C4-C5-C6
33	b	624	STE	C11-C10-C9-C8
33	B	628	STE	C2-C3-C4-C5
34	D	412	LHG	O9-C7-O7-C5
28	M	101	LMG	C13-C14-C15-C16
24	B	618	BCR	C20-C21-C22-C37
24	H	101	BCR	C35-C13-C14-C15
24	y	101	BCR	C16-C17-C18-C36
24	y	101	BCR	C20-C21-C22-C37
22	A	405	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	CBA-CGA-O2A-C1
29	A	414	SQD	C30-C31-C32-C33
27	A	410	PL9	C11-C12-C13-C14
22	A	402	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C11-C12-C13-C15
22	B	612	CLA	C6-C7-C8-C10
22	B	617	CLA	C6-C7-C8-C10
22	C	503	CLA	C12-C13-C15-C16
22	a	403	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C7
22	b	606	CLA	C6-C7-C8-C10
22	d	402	CLA	C6-C7-C8-C10
33	J	101	STE	C3-C4-C5-C6
22	c	515	CLA	C3-C5-C6-C7
29	D	407	SQD	O6-C44-C45-C46
24	A	406	BCR	C17-C18-C19-C20
24	B	618	BCR	C11-C12-C13-C14
24	T	101	BCR	C7-C8-C9-C10
24	Y	101	BCR	C11-C12-C13-C14
24	c	518	BCR	C11-C12-C13-C14
28	b	621	LMG	C16-C17-C18-C19
22	a	405	CLA	O1A-CGA-O2A-C1
22	b	607	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	C2G-C3G-O3G-C1D
30	c	520	DGD	C2G-C3G-O3G-C1D
30	c	519	DGD	C1A-C2A-C3A-C4A
28	c	524	LMG	C15-C16-C17-C18
30	C	517	DGD	C6A-C7A-C8A-C9A
34	d	408	LHG	C30-C31-C32-C33
27	A	410	PL9	C13-C14-C16-C17
33	C	522	STE	C5-C6-C7-C8
28	B	629	LMG	C9-C8-O7-C10
29	f	101	SQD	C46-C45-O47-C7
22	B	605	CLA	C2C-C3C-CAC-CBC
28	b	623	LMG	O10-C28-O8-C9
33	c	523	STE	C10-C11-C12-C13
24	c	516	BCR	C13-C14-C15-C16
28	c	525	LMG	C19-C20-C21-C22
30	c	520	DGD	C3A-C4A-C5A-C6A
29	B	623	SQD	C30-C31-C32-C33
22	C	506	CLA	O1A-CGA-O2A-C1
24	Z	101	BCR	C11-C10-C9-C8
30	c	520	DGD	CCA-CDA-CEA-CFA
30	C	518	DGD	C3A-C4A-C5A-C6A
28	b	621	LMG	C7-C8-C9-O8
29	f	101	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	C13-C15-C16-C17
22	c	504	CLA	C16-C17-C18-C19
33	l	102	STE	C15-C16-C17-C18
28	M	101	LMG	C39-C40-C41-C42
27	A	410	PL9	C43-C44-C46-C47
28	d	409	LMG	C30-C31-C32-C33
22	b	608	CLA	C13-C15-C16-C17
22	b	610	CLA	C8-C10-C11-C12
28	c	524	LMG	O7-C8-C9-O8
29	f	101	SQD	O47-C45-C46-O48
34	E	101	LHG	O7-C5-C6-O8
22	B	612	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	604	CLA	C11-C10-C8-C9
22	b	614	CLA	C6-C7-C8-C9
22	C	508	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
30	c	521	DGD	C8B-C9B-CAB-CBB
33	X	101	STE	C12-C13-C14-C15
33	j	101	STE	C5-C6-C7-C8
28	D	406	LMG	C32-C33-C34-C35
30	H	102	DGD	CBA-CCA-CDA-CEA
33	C	521	STE	C7-C8-C9-C10
22	C	512	CLA	C15-C16-C17-C18
22	c	506	CLA	C8-C10-C11-C12
28	D	410	LMG	C13-C14-C15-C16
30	C	518	DGD	C9B-CAB-CBB-CCB
33	d	412	STE	C2-C3-C4-C5
33	l	102	STE	C7-C8-C9-C10
33	I	101	STE	C7-C8-C9-C10
30	C	518	DGD	CAB-CBB-CCB-CDB
29	b	619	SQD	C28-C29-C30-C31
33	h	103	STE	C10-C11-C12-C13
22	A	411	CLA	C16-C17-C18-C19
29	f	101	SQD	C28-C29-C30-C31
28	D	406	LMG	C15-C16-C17-C18
30	c	520	DGD	C9A-CAA-CBA-CCA
34	D	409	LHG	C17-C18-C19-C20
34	E	101	LHG	C19-C20-C21-C22
30	C	516	DGD	CBA-CCA-CDA-CEA
33	T	102	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	B	629	LMG	C38-C39-C40-C41
33	X	101	STE	C7-C8-C9-C10
29	a	413	SQD	C28-C29-C30-C31
28	c	524	LMG	C12-C13-C14-C15
34	e	102	LHG	C28-C29-C30-C31
34	D	409	LHG	O1-C1-C2-O2
22	C	507	CLA	C3-C5-C6-C7
24	B	619	BCR	C11-C12-C13-C35
27	a	410	PL9	C9-C11-C12-C13
22	B	602	CLA	C4B-C3B-CAB-CBB
33	B	621	STE	C7-C8-C9-C10
34	D	412	LHG	C25-C26-C27-C28
34	D	412	LHG	C31-C32-C33-C34
24	b	618	BCR	C6-C7-C8-C9
27	A	410	PL9	C33-C34-C36-C37
28	C	519	LMG	C39-C40-C41-C42
29	D	407	SQD	C32-C33-C34-C35
34	l	101	LHG	O6-C4-C5-C6
28	B	629	LMG	C18-C19-C20-C21
30	H	102	DGD	C6B-C7B-C8B-C9B
22	d	403	CLA	CBD-CGD-O2D-CED
28	C	519	LMG	O9-C10-O7-C8
30	C	517	DGD	CAB-CBB-CCB-CDB
30	c	519	DGD	CBB-CCB-CDB-CEB
34	d	406	LHG	C13-C14-C15-C16
29	a	413	SQD	C12-C13-C14-C15
33	C	520	STE	C4-C5-C6-C7
22	A	411	CLA	C12-C13-C15-C16
22	B	605	CLA	C11-C12-C13-C15
22	B	614	CLA	C6-C7-C8-C10
22	C	506	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	C	513	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C12-C13-C15
23	a	404	PHO	C6-C7-C8-C10
28	B	629	LMG	C23-C24-C25-C26
33	j	101	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C16-C17-C18-C19
22	b	606	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C19
30	C	518	DGD	CDB-CEB-CFB-CGB
33	a	415	STE	C3-C4-C5-C6
34	D	412	LHG	C30-C31-C32-C33
35	v	201	HEC	C4B-C3B-CAB-CBB
28	b	623	LMG	C37-C38-C39-C40
34	l	101	LHG	C14-C15-C16-C17
34	D	409	LHG	O9-C7-O7-C5
34	d	407	LHG	O6-C4-C5-O7
22	B	607	CLA	C5-C6-C7-C8
22	B	617	CLA	C6-C7-C8-C9
22	C	503	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	d	402	CLA	C6-C7-C8-C9
22	C	514	CLA	C10-C11-C12-C13
28	c	522	LMG	C30-C31-C32-C33
24	Z	101	BCR	C9-C10-C11-C12
24	Z	101	BCR	C15-C16-C17-C18
22	b	605	CLA	C5-C6-C7-C8
33	c	523	STE	C3-C4-C5-C6
33	d	410	STE	C6-C7-C8-C9
34	E	101	LHG	C30-C31-C32-C33
28	A	412	LMG	O7-C8-C9-O8
28	B	629	LMG	O1-C7-C8-O7
29	b	619	SQD	O6-C44-C45-O47
30	C	516	DGD	O1G-C1G-C2G-O2G
30	c	519	DGD	O1G-C1G-C2G-O2G
34	d	408	LHG	O7-C5-C6-O8
28	A	412	LMG	C7-C8-C9-O8
28	M	101	LMG	C7-C8-C9-O8
29	A	413	SQD	O6-C44-C45-C46
29	a	413	SQD	C44-C45-C46-O48
29	A	414	SQD	C15-C16-C17-C18
29	a	412	SQD	C11-C12-C13-C14
22	B	608	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	c	508	CLA	CAD-CBD-CGD-O2D
22	h	101	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	C13-C15-C16-C17
28	C	519	LMG	C16-C17-C18-C19
30	h	102	DGD	C7B-C8B-C9B-CAB
33	B	621	STE	C6-C7-C8-C9
22	C	513	CLA	C16-C17-C18-C19
22	C	513	CLA	C2A-CAA-CBA-CGA
33	b	620	STE	C3-C4-C5-C6
30	H	102	DGD	C5A-C6A-C7A-C8A
30	A	415	DGD	C5B-C6B-C7B-C8B
33	d	411	STE	C12-C13-C14-C15
28	d	409	LMG	C36-C37-C38-C39
22	B	608	CLA	CAD-CBD-CGD-O1D
22	B	617	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CAD-CBD-CGD-O1D
22	h	101	CLA	CAD-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
24	c	517	BCR	C11-C10-C9-C34
24	y	101	BCR	C9-C10-C11-C12
34	D	409	LHG	C3-O3-P-O5
34	d	408	LHG	C4-O6-P-O4
34	e	102	LHG	C4-O6-P-O5
34	l	101	LHG	C3-O3-P-O4
22	C	513	CLA	C3-C5-C6-C7
28	c	525	LMG	C35-C36-C37-C38
22	B	602	CLA	C2B-C3B-CAB-CBB
22	b	609	CLA	C2B-C3B-CAB-CBB
22	c	506	CLA	C2B-C3B-CAB-CBB
22	c	507	CLA	C2B-C3B-CAB-CBB
22	d	402	CLA	C2B-C3B-CAB-CBB
22	h	101	CLA	C2B-C3B-CAB-CBB
28	b	621	LMG	C35-C36-C37-C38
24	x	101	BCR	C37-C22-C23-C24
34	D	409	LHG	C2-C3-O3-P
34	E	101	LHG	C2-C3-O3-P
34	d	408	LHG	C2-C3-O3-P
28	D	410	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
34	E	101	LHG	C9-C10-C11-C12
28	c	524	LMG	C13-C14-C15-C16
30	C	516	DGD	C2B-C3B-C4B-C5B
34	B	622	LHG	C32-C33-C34-C35
34	E	101	LHG	C11-C10-C9-C8
30	C	516	DGD	CDB-CEB-CFB-CGB
30	C	516	DGD	C5B-C6B-C7B-C8B
33	T	102	STE	C10-C11-C12-C13
27	A	410	PL9	C4-C3-C7-C8
22	C	508	CLA	C16-C17-C18-C19
29	B	623	SQD	C46-C45-O47-C7
29	a	412	SQD	C44-C45-O47-C7
33	B	628	STE	C4-C5-C6-C7
33	T	102	STE	C14-C15-C16-C17
34	E	101	LHG	C26-C27-C28-C29
30	h	102	DGD	O2G-C1B-C2B-C3B
22	b	614	CLA	C8-C10-C11-C12
22	D	402	CLA	C2C-C3C-CAC-CBC
33	I	101	STE	C11-C10-C9-C8
22	b	604	CLA	C5-C6-C7-C8
22	B	611	CLA	C8-C10-C11-C12
22	d	402	CLA	C2C-C3C-CAC-CBC
22	B	612	CLA	C11-C12-C13-C14
22	a	403	CLA	C11-C12-C13-C14
22	a	405	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C6-C7-C8-C9
22	d	403	CLA	C11-C12-C13-C14
22	h	101	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C10-C8-C7
22	c	508	CLA	C12-C13-C15-C16
24	B	619	BCR	C16-C17-C18-C19
24	B	620	BCR	C11-C10-C9-C8
24	c	517	BCR	C12-C13-C14-C15
24	y	101	BCR	C11-C10-C9-C8
33	M	103	STE	C5-C6-C7-C8
34	l	101	LHG	O6-C4-C5-O7
28	D	406	LMG	C33-C34-C35-C36
30	A	415	DGD	C2A-C3A-C4A-C5A
29	A	414	SQD	C10-C11-C12-C13
33	J	101	STE	C6-C7-C8-C9
30	H	102	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
33	c	501	STE	C7-C8-C9-C10
28	b	621	LMG	C19-C20-C21-C22
23	A	404	PHO	C4-C3-C5-C6
33	Z	102	STE	C14-C15-C16-C17
34	e	102	LHG	O9-C7-O7-C5
34	e	102	LHG	O7-C5-C6-O8
22	a	405	CLA	C15-C16-C17-C18
33	X	101	STE	C6-C7-C8-C9
35	e	101	HEC	C2A-CAA-CBA-CGA
29	a	413	SQD	C24-C25-C26-C27
33	B	625	STE	C6-C7-C8-C9
33	b	625	STE	C2-C3-C4-C5
30	C	518	DGD	O6D-C5D-C6D-O5D
22	B	617	CLA	C2-C1-O2A-CGA
28	C	519	LMG	C14-C15-C16-C17
29	A	414	SQD	C32-C33-C34-C35
33	C	522	STE	C6-C7-C8-C9
28	C	519	LMG	O1-C7-C8-C9
29	a	412	SQD	C28-C29-C30-C31
22	c	511	CLA	CAA-CBA-CGA-O2A
24	T	101	BCR	C7-C8-C9-C34
24	c	517	BCR	C7-C8-C9-C34
28	c	524	LMG	C35-C36-C37-C38
33	a	415	STE	C4-C5-C6-C7
24	Z	101	BCR	C11-C12-C13-C14
22	a	405	CLA	C5-C6-C7-C8
22	c	503	CLA	C2A-CAA-CBA-CGA
24	c	516	BCR	C9-C10-C11-C12
30	c	520	DGD	C4B-C5B-C6B-C7B
30	c	521	DGD	CBA-CCA-CDA-CEA
28	D	410	LMG	C15-C16-C17-C18
30	h	102	DGD	CDA-CEA-CFA-CGA
29	D	407	SQD	C44-C45-C46-O48
30	c	519	DGD	O1G-C1A-C2A-C3A
29	A	413	SQD	C31-C32-C33-C34
30	C	518	DGD	C9A-CAA-CBA-CCA
28	M	101	LMG	C15-C16-C17-C18
28	d	409	LMG	C37-C38-C39-C40
29	A	414	SQD	C28-C29-C30-C31
22	c	510	CLA	C8-C10-C11-C12
34	E	101	LHG	C35-C36-C37-C38
22	B	614	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	c	521	DGD	C2A-C1A-O1G-C1G
33	b	626	STE	C4-C5-C6-C7
22	b	604	CLA	C4B-C3B-CAB-CBB
34	l	101	LHG	C9-C10-C11-C12
33	d	411	STE	C11-C12-C13-C14
30	C	517	DGD	C6B-C7B-C8B-C9B
33	b	620	STE	C15-C16-C17-C18
34	e	102	LHG	O6-C4-C5-O7
34	D	412	LHG	C26-C27-C28-C29
22	b	610	CLA	C10-C11-C12-C13
28	D	406	LMG	C34-C35-C36-C37
22	A	411	CLA	C11-C12-C13-C15
22	B	607	CLA	C6-C7-C8-C10
22	a	403	CLA	C6-C7-C8-C10
29	b	619	SQD	C14-C15-C16-C17
30	C	516	DGD	C6B-C7B-C8B-C9B
28	C	519	LMG	C37-C38-C39-C40
28	D	406	LMG	C37-C38-C39-C40
33	b	624	STE	C6-C7-C8-C9
22	C	509	CLA	C16-C17-C18-C19
27	d	405	PL9	C47-C48-C49-C50
33	B	628	STE	C7-C8-C9-C10
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	608	CLA	C3A-C2A-CAA-CBA
33	d	412	STE	C3-C4-C5-C6
33	B	626	STE	C13-C14-C15-C16
28	C	519	LMG	C4-C5-C6-O5
24	c	516	BCR	C16-C17-C18-C36
33	d	411	STE	C15-C16-C17-C18
22	B	605	CLA	C13-C15-C16-C17
23	d	401	PHO	C5-C6-C7-C8
29	a	412	SQD	C9-C10-C11-C12
24	Y	101	BCR	C13-C14-C15-C16
22	b	608	CLA	C3-C5-C6-C7
33	d	411	STE	C4-C5-C6-C7
34	d	408	LHG	C9-C10-C11-C12
29	b	619	SQD	C13-C14-C15-C16
30	C	516	DGD	C3A-C4A-C5A-C6A
30	c	519	DGD	C6A-C7A-C8A-C9A
34	d	406	LHG	C17-C18-C19-C20
22	D	403	CLA	C4-C3-C5-C6
29	b	619	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C16-C17-C18-C19
30	C	518	DGD	C2A-C3A-C4A-C5A
22	D	402	CLA	C10-C11-C12-C13
30	C	516	DGD	O1G-C1G-C2G-C3G
34	e	102	LHG	C4-C5-C6-O8
33	T	102	STE	C15-C16-C17-C18
24	Z	101	BCR	C14-C15-C16-C17
22	C	514	CLA	C8-C10-C11-C12
34	B	622	LHG	C11-C12-C13-C14
34	l	101	LHG	C18-C19-C20-C21
33	d	412	STE	C15-C16-C17-C18
22	C	512	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	B	610	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C19
22	C	506	CLA	C15-C16-C17-C18
22	b	611	CLA	C8-C10-C11-C12
28	c	522	LMG	C31-C32-C33-C34
30	C	518	DGD	CBA-CCA-CDA-CEA
29	a	412	SQD	C46-C45-O47-C7
22	B	615	CLA	CBD-CGD-O2D-CED
33	c	523	STE	O1-C1-C2-C3
33	c	523	STE	O2-C1-C2-C3
28	B	629	LMG	C21-C22-C23-C24
28	b	623	LMG	C12-C13-C14-C15
27	a	410	PL9	C38-C39-C41-C42
30	C	518	DGD	C4B-C5B-C6B-C7B
22	c	515	CLA	C1A-C2A-CAA-CBA
22	h	101	CLA	C10-C11-C12-C13
24	B	618	BCR	C1-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C30
24	Y	101	BCR	C23-C24-C25-C30
24	Z	101	BCR	C23-C24-C25-C26
24	b	616	BCR	C1-C6-C7-C8
28	D	411	LMG	O8-C28-C29-C30
33	c	501	STE	O1-C1-C2-C3
22	b	602	CLA	C13-C15-C16-C17
28	D	411	LMG	C29-C30-C31-C32
22	C	514	CLA	C4-C3-C5-C6
30	C	517	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
35	e	101	HEC	CAD-CBD-CGD-O1D
22	A	403	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C10-C8-C7
22	C	507	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C7
23	A	404	PHO	C12-C13-C15-C16
22	b	607	CLA	C2C-C3C-CAC-CBC
22	b	613	CLA	C10-C11-C12-C13
28	B	629	LMG	O7-C8-C9-O8
28	M	101	LMG	C11-C12-C13-C14
28	d	409	LMG	C12-C13-C14-C15
30	c	519	DGD	CBA-CCA-CDA-CEA
33	b	622	STE	O2-C1-C2-C3
35	F	101	HEC	CAD-CBD-CGD-O1D
33	H	103	STE	C11-C12-C13-C14
30	c	519	DGD	C8A-C9A-CAA-CBA
28	A	412	LMG	C14-C15-C16-C17
22	b	603	CLA	C4-C3-C5-C6
22	C	514	CLA	C2-C3-C5-C6
34	d	406	LHG	C29-C30-C31-C32
33	B	621	STE	O2-C1-C2-C3
29	a	412	SQD	C11-C10-C9-C8
22	A	411	CLA	C11-C12-C13-C14
22	a	403	CLA	C6-C7-C8-C9
22	b	609	CLA	C14-C13-C15-C16
33	b	620	STE	C12-C13-C14-C15
30	C	518	DGD	C3B-C4B-C5B-C6B
33	B	625	STE	C7-C8-C9-C10
33	B	621	STE	O1-C1-C2-C3
22	D	403	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12
24	D	404	BCR	C22-C23-C24-C25
29	b	619	SQD	O5-C1-O6-C44
22	C	507	CLA	C4-C3-C5-C6
33	B	626	STE	O1-C1-C2-C3
33	B	626	STE	O2-C1-C2-C3
33	C	521	STE	C11-C12-C13-C14
34	D	408	LHG	C29-C30-C31-C32
23	A	404	PHO	C2-C3-C5-C6
22	D	403	CLA	C3-C5-C6-C7
29	b	619	SQD	C10-C11-C12-C13
22	b	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	C16-C17-C18-C20
22	B	615	CLA	C16-C17-C18-C20
30	H	102	DGD	CDA-CEA-CFA-CGA
33	B	627	STE	C7-C8-C9-C10
22	A	411	CLA	C4C-C3C-CAC-CBC
27	d	405	PL9	C40-C39-C41-C42
22	A	411	CLA	C16-C17-C18-C20
22	b	601	CLA	C8-C10-C11-C12
33	b	625	STE	C6-C7-C8-C9
33	B	625	STE	O2-C1-C2-C3
33	c	501	STE	O2-C1-C2-C3
34	D	408	LHG	C17-C18-C19-C20
34	E	101	LHG	C18-C19-C20-C21
28	D	411	LMG	O7-C10-C11-C12
35	F	101	HEC	CAD-CBD-CGD-O2D
35	V	201	HEC	CAD-CBD-CGD-O2D
23	d	401	PHO	CHA-CBD-CGD-O1D
22	b	604	CLA	C10-C11-C12-C13
22	a	411	CLA	C4C-C3C-CAC-CBC
34	e	102	LHG	O6-C4-C5-C6
29	A	413	SQD	C10-C11-C12-C13
22	C	507	CLA	C2-C3-C5-C6
28	b	623	LMG	O6-C1-O1-C7
22	D	403	CLA	C10-C11-C12-C13
22	B	613	CLA	C11-C10-C8-C7
22	b	613	CLA	C11-C10-C8-C7
22	b	615	CLA	C6-C7-C8-C10
22	h	101	CLA	C11-C12-C13-C15
33	b	622	STE	O1-C1-C2-C3
35	e	101	HEC	CAD-CBD-CGD-O2D
28	b	623	LMG	C33-C34-C35-C36
33	B	624	STE	C7-C8-C9-C10
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16
28	c	525	LMG	C28-C29-C30-C31
29	f	101	SQD	C35-C36-C37-C38
28	B	629	LMG	C35-C36-C37-C38
22	B	614	CLA	C2-C1-O2A-CGA
30	C	516	DGD	O6D-C5D-C6D-O5D
22	B	604	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C16-C17-C18-C19
28	M	101	LMG	C22-C23-C24-C25
34	E	101	LHG	C12-C13-C14-C15
22	B	606	CLA	C2-C3-C5-C6
29	b	619	SQD	C19-C20-C21-C22
34	e	102	LHG	C19-C20-C21-C22
33	M	102	STE	C5-C6-C7-C8
22	B	605	CLA	O2A-C1-C2-C3
22	h	101	CLA	O2A-C1-C2-C3
24	d	404	BCR	C18-C19-C20-C21
29	a	412	SQD	C16-C17-C18-C19
34	d	408	LHG	C11-C10-C9-C8
22	B	605	CLA	C4C-C3C-CAC-CBC
28	B	629	LMG	O10-C28-C29-C30
28	b	621	LMG	C12-C13-C14-C15
22	c	514	CLA	C15-C16-C17-C18
34	D	408	LHG	C14-C15-C16-C17
35	v	201	HEC	CAD-CBD-CGD-O2D
33	B	626	STE	C4-C5-C6-C7
22	c	511	CLA	C15-C16-C17-C18
28	D	410	LMG	C37-C38-C39-C40
22	C	512	CLA	CBA-CGA-O2A-C1
28	M	101	LMG	O1-C7-C8-C9
29	b	619	SQD	C44-C45-C46-O48
23	D	401	PHO	O1D-CGD-O2D-CED
28	B	629	LMG	C22-C23-C24-C25
30	h	102	DGD	O1B-C1B-C2B-C3B
33	B	625	STE	O1-C1-C2-C3
28	D	411	LMG	O10-C28-C29-C30
28	c	524	LMG	C36-C37-C38-C39
29	A	414	SQD	C24-C25-C26-C27
30	H	102	DGD	C4A-C5A-C6A-C7A
30	H	102	DGD	CCB-CDB-CEB-CFB
28	C	519	LMG	O1-C7-C8-O7
22	C	514	CLA	C13-C15-C16-C17
22	B	613	CLA	C11-C10-C8-C9
22	C	507	CLA	C6-C7-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	c	503	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
23	a	404	PHO	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	CAA-CBA-CGA-O2A
35	V	201	HEC	CAD-CBD-CGD-O1D
30	C	517	DGD	C8A-C9A-CAA-CBA
22	A	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	B	616	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C10-C8-C7
22	b	610	CLA	C12-C13-C15-C16
22	b	612	CLA	C12-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C10
22	b	614	CLA	C12-C13-C15-C16
22	c	504	CLA	C11-C12-C13-C15
28	C	519	LMG	C11-C12-C13-C14
22	D	402	CLA	C2B-C3B-CAB-CBB
24	B	618	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
24	c	518	BCR	C1-C6-C7-C8
28	D	406	LMG	C38-C39-C40-C41
22	a	402	CLA	C2-C1-O2A-CGA
22	d	402	CLA	C2-C1-O2A-CGA
33	B	626	STE	C7-C8-C9-C10
35	v	201	HEC	CAD-CBD-CGD-O1D
22	B	611	CLA	C15-C16-C17-C18
30	C	518	DGD	C8A-C9A-CAA-CBA
34	B	622	LHG	O7-C7-C8-C9
34	D	409	LHG	O8-C23-C24-C25
33	d	411	STE	C5-C6-C7-C8
22	b	609	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	CAA-CBA-CGA-O2A
22	B	614	CLA	CAA-CBA-CGA-O2A
29	A	414	SQD	C31-C32-C33-C34
34	E	101	LHG	C10-C11-C12-C13
22	b	615	CLA	CBA-CGA-O2A-C1
28	d	409	LMG	O7-C10-C11-C12
30	H	102	DGD	CBB-CCB-CDB-CEB
22	b	609	CLA	O1D-CGD-O2D-CED
29	B	623	SQD	C11-C10-C9-C8
22	b	607	CLA	C4-C3-C5-C6
22	c	510	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C2-C3-C5-C6
27	d	405	PL9	C33-C34-C36-C37
29	a	412	SQD	C34-C35-C36-C37
33	B	626	STE	C11-C10-C9-C8
34	e	102	LHG	C17-C18-C19-C20
22	A	403	CLA	C11-C10-C8-C9
22	A	411	CLA	C14-C13-C15-C16
22	b	605	CLA	C14-C13-C15-C16
28	b	621	LMG	O8-C28-C29-C30
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
22	D	402	CLA	C4B-C3B-CAB-CBB
34	d	408	LHG	C24-C25-C26-C27
33	b	624	STE	C10-C11-C12-C13
27	d	405	PL9	C45-C44-C46-C47
34	B	622	LHG	C30-C31-C32-C33
30	C	517	DGD	O6D-C1D-O3G-C3G
29	A	414	SQD	O48-C23-C24-C25
29	A	413	SQD	O47-C45-C46-O48
24	a	406	BCR	C21-C22-C23-C24
24	c	517	BCR	C21-C22-C23-C24
33	M	102	STE	C1-C2-C3-C4
22	C	512	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	CDB-CEB-CFB-CGB
29	b	619	SQD	C11-C12-C13-C14
30	c	520	DGD	C8B-C9B-CAB-CBB
28	D	406	LMG	C16-C17-C18-C19
30	c	521	DGD	C2B-C3B-C4B-C5B
33	J	101	STE	C5-C6-C7-C8
33	b	624	STE	C7-C8-C9-C10
22	D	402	CLA	C2-C1-O2A-CGA
22	C	510	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C10-C8-C7
22	b	604	CLA	C12-C13-C15-C16
22	b	611	CLA	C6-C7-C8-C10
22	c	509	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
34	D	412	LHG	C10-C11-C12-C13
34	D	409	LHG	C28-C29-C30-C31
29	a	412	SQD	O47-C7-C8-C9
28	c	524	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	C13-C15-C16-C17
27	A	410	PL9	C44-C46-C47-C48
22	B	603	CLA	C3A-C2A-CAA-CBA
22	C	508	CLA	C5-C6-C7-C8
22	b	613	CLA	C13-C15-C16-C17
34	B	622	LHG	C26-C27-C28-C29
28	c	524	LMG	C40-C41-C42-C43
30	H	102	DGD	C8B-C9B-CAB-CBB
30	C	516	DGD	O6E-C1E-O5D-C6D
29	a	413	SQD	C30-C31-C32-C33
22	B	613	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C11-C12-C13-C14
22	B	616	CLA	C11-C10-C8-C9
22	C	505	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	507	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C10-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	504	CLA	C11-C12-C13-C14
22	c	509	CLA	C14-C13-C15-C16
22	C	507	CLA	C15-C16-C17-C18
22	B	602	CLA	CAA-CBA-CGA-O1A
29	B	623	SQD	O10-C23-C24-C25
34	d	407	LHG	C26-C27-C28-C29
22	b	607	CLA	C13-C15-C16-C17
22	b	611	CLA	CAA-CBA-CGA-O2A
29	A	414	SQD	O10-C23-C24-C25
30	c	519	DGD	O1B-C1B-C2B-C3B
34	d	406	LHG	C35-C36-C37-C38
33	b	624	STE	O1-C1-C2-C3
28	c	525	LMG	C8-C9-O8-C28
22	b	605	CLA	C16-C17-C18-C19
22	B	614	CLA	CAA-CBA-CGA-O1A
27	D	405	PL9	C46-C47-C48-C49
22	C	510	CLA	C8-C10-C11-C12
22	b	609	CLA	C15-C16-C17-C18
28	B	629	LMG	O7-C10-C11-C12
30	C	516	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	O1D-CGD-O2D-CED
22	C	502	CLA	O1D-CGD-O2D-CED
22	A	403	CLA	C15-C16-C17-C18
22	B	602	CLA	C2-C1-O2A-CGA
34	D	409	LHG	O10-C23-C24-C25
29	A	413	SQD	O47-C7-C8-C9
22	b	613	CLA	C16-C17-C18-C19
28	M	101	LMG	C34-C35-C36-C37
34	l	101	LHG	O9-C7-C8-C9
30	c	521	DGD	O1G-C1A-C2A-C3A
34	D	409	LHG	C11-C12-C13-C14
22	c	512	CLA	CAA-CBA-CGA-O2A
30	c	519	DGD	O2G-C1B-C2B-C3B
22	C	507	CLA	O1D-CGD-O2D-CED
29	b	619	SQD	C23-C24-C25-C26
30	h	102	DGD	C1A-C2A-C3A-C4A
29	A	413	SQD	O49-C7-C8-C9
33	X	101	STE	C5-C6-C7-C8

There are no ring outliers.

117 monomers are involved in 209 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	405	CLA	1	0
22	B	607	CLA	2	0
34	D	412	LHG	3	0
29	b	619	SQD	3	0
22	c	506	CLA	2	0
22	b	603	CLA	3	0
33	c	523	STE	1	0
34	d	407	LHG	1	0
33	d	412	STE	2	0
24	T	101	BCR	3	0
24	Y	101	BCR	2	0
22	b	606	CLA	1	0
22	b	608	CLA	2	0
22	C	513	CLA	4	0
34	d	406	LHG	2	0
24	C	515	BCR	1	0
34	D	409	LHG	1	0
22	C	510	CLA	2	0
22	B	608	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	502	CLA	1	0
24	y	101	BCR	1	0
33	T	102	STE	3	0
22	B	613	CLA	1	0
33	j	101	STE	1	0
28	B	629	LMG	2	0
34	B	622	LHG	1	0
22	A	402	CLA	1	0
33	a	415	STE	1	0
22	c	507	CLA	1	0
22	b	614	CLA	4	0
22	C	512	CLA	1	0
28	D	406	LMG	5	0
22	C	509	CLA	1	0
22	c	510	CLA	1	0
33	B	621	STE	2	0
22	B	614	CLA	2	0
22	c	514	CLA	1	0
29	B	623	SQD	2	0
24	c	517	BCR	2	0
22	c	509	CLA	1	0
22	b	601	CLA	2	0
28	c	525	LMG	1	0
22	A	411	CLA	3	0
22	C	503	CLA	2	0
24	H	101	BCR	3	0
22	b	612	CLA	1	0
33	l	102	STE	1	0
23	d	401	PHO	2	0
35	e	101	HEC	7	0
22	B	610	CLA	2	0
35	V	201	HEC	1	0
30	A	415	DGD	1	0
22	a	411	CLA	2	0
24	d	404	BCR	2	0
22	C	514	CLA	3	0
22	C	505	CLA	1	0
24	A	406	BCR	2	0
35	F	101	HEC	3	0
35	v	201	HEC	5	0
22	c	503	CLA	1	0
22	d	402	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	h	103	STE	2	0
22	b	604	CLA	1	0
22	B	605	CLA	3	0
33	C	521	STE	1	0
33	b	626	STE	1	0
24	b	616	BCR	3	0
27	a	410	PL9	7	0
22	b	605	CLA	7	0
24	Z	101	BCR	3	0
29	A	413	SQD	2	0
22	h	101	CLA	1	0
28	C	519	LMG	2	0
33	d	411	STE	3	0
24	t	101	BCR	6	0
22	B	606	CLA	3	0
31	A	416[A]	OEX	1	0
27	A	410	PL9	4	0
23	D	401	PHO	1	0
22	B	602	CLA	2	0
22	B	616	CLA	1	0
31	a	416[A]	OEX	1	0
22	B	612	CLA	1	0
32	A	417[B]	OEY	5	0
24	b	617	BCR	5	0
22	A	403	CLA	1	0
29	D	407	SQD	1	0
33	M	102	STE	1	0
24	x	101	BCR	1	0
29	A	414	SQD	4	0
22	a	402	CLA	1	0
33	B	627	STE	1	0
24	B	620	BCR	2	0
22	C	506	CLA	1	0
22	D	402	CLA	2	0
22	D	403	CLA	2	0
24	B	619	BCR	3	0
33	X	101	STE	2	0
22	b	615	CLA	2	0
23	a	404	PHO	1	0
33	Z	102	STE	1	0
22	B	615	CLA	1	0
28	b	621	LMG	1	0

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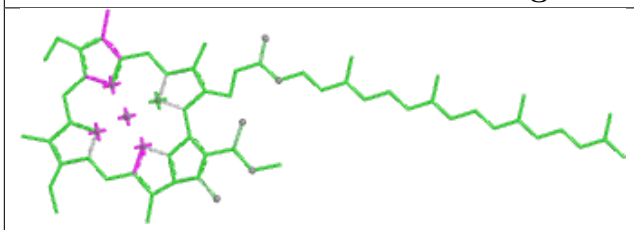
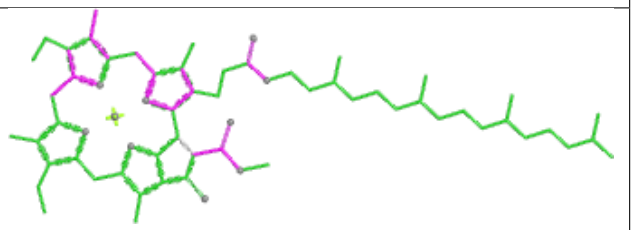
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	508	CLA	1	0
33	b	622	STE	2	0
22	b	613	CLA	7	0
24	b	618	BCR	1	0
24	D	404	BCR	5	0
22	B	603	CLA	3	0
24	B	618	BCR	1	0
22	C	511	CLA	1	0
22	C	504	CLA	1	0
22	B	604	CLA	2	0
30	C	517	DGD	1	0
28	M	101	LMG	2	0
33	B	601	STE	1	0
22	B	609	CLA	4	0

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

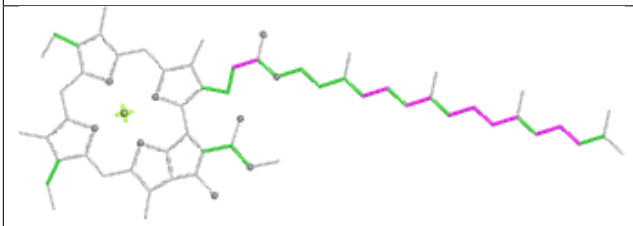
Ligand CLA c 511



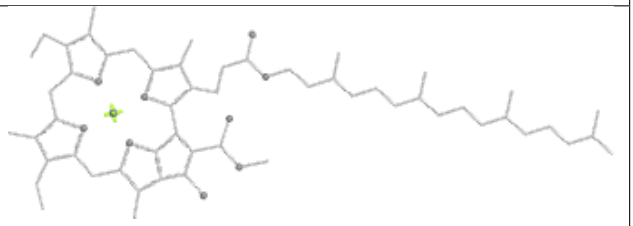
Bond lengths



Bond angles

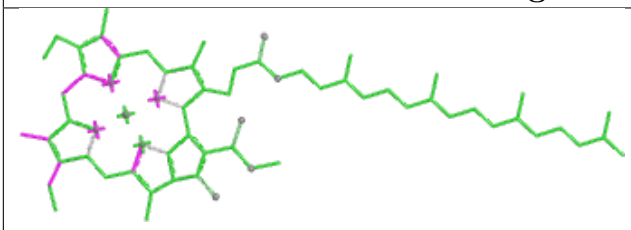


Torsions

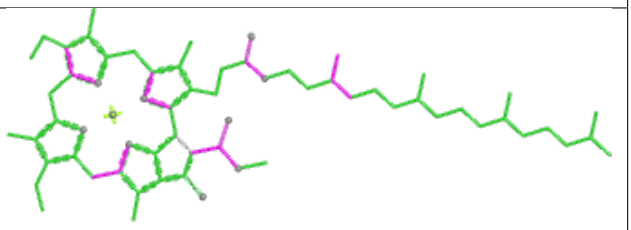


Rings

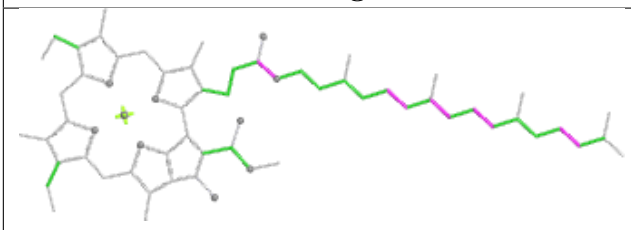
Ligand CLA a 405



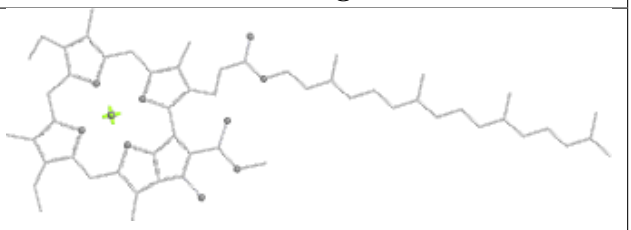
Bond lengths



Bond angles

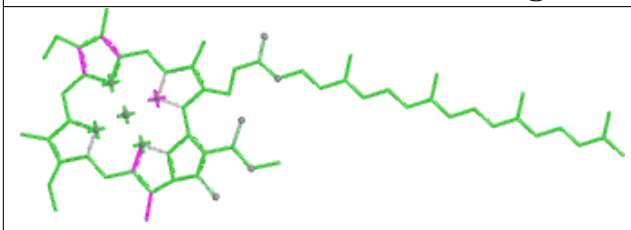


Torsions



Rings

Ligand CLA b 610



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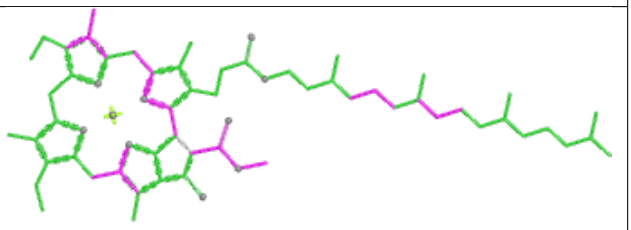
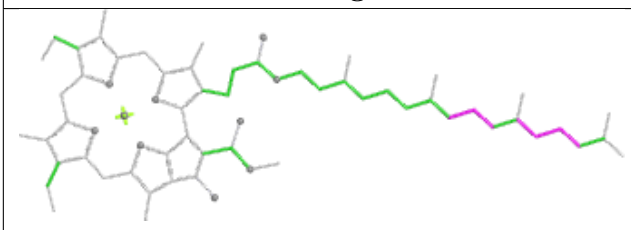
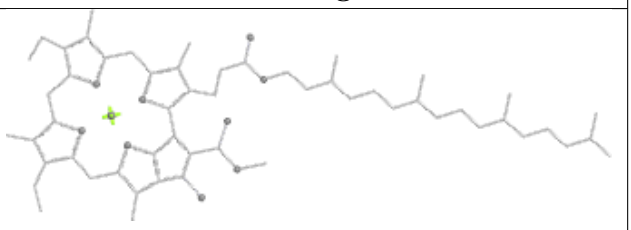


Bond angles

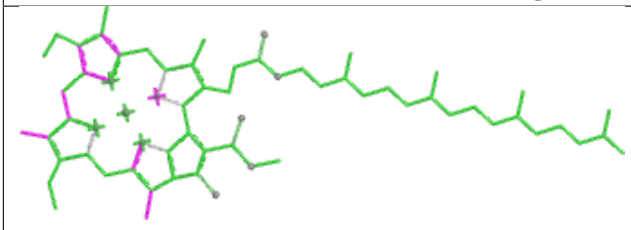


Torsions

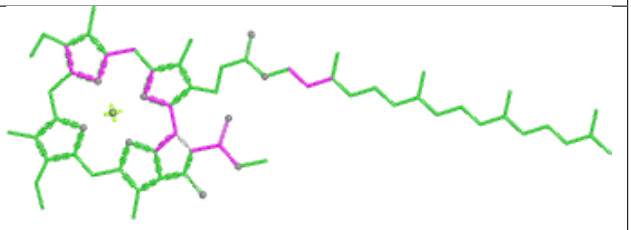


Rings

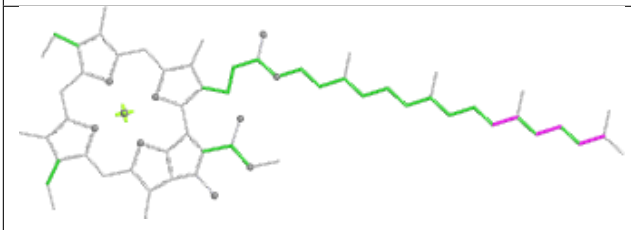
Ligand CLA c 504



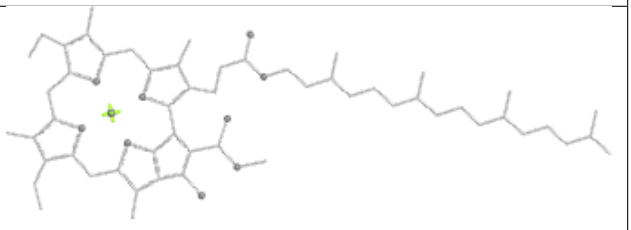
Bond lengths



Bond angles

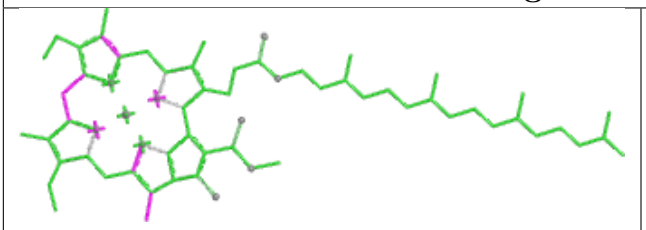


Torsions

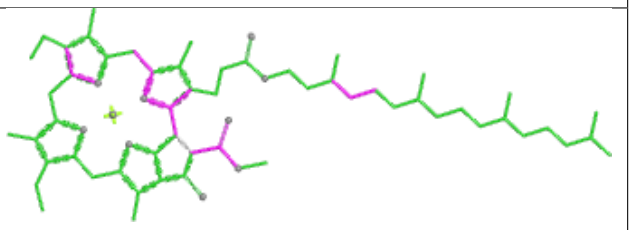


Rings

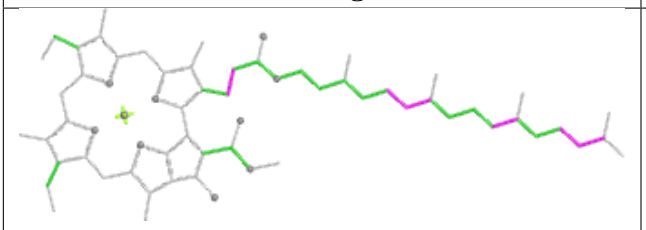
Ligand CLA B 607



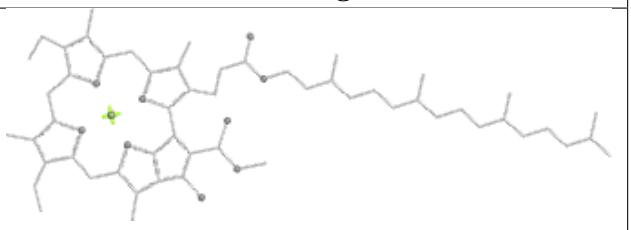
Bond lengths



Bond angles

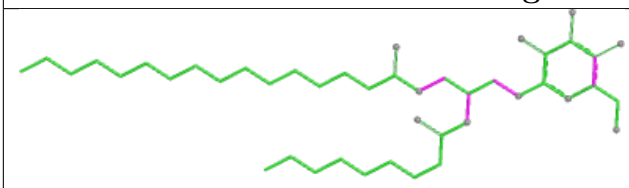


Torsions



Rings

Ligand LMG d 409



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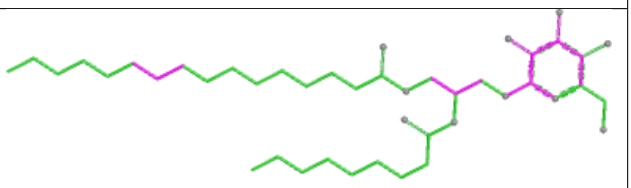
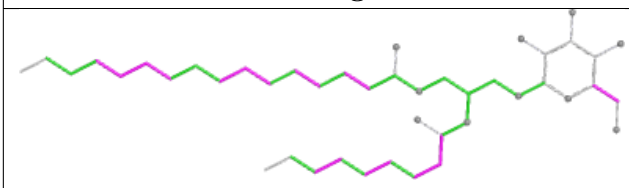
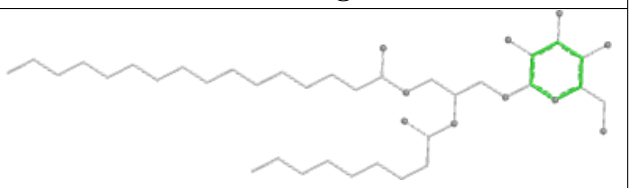


Bond angles

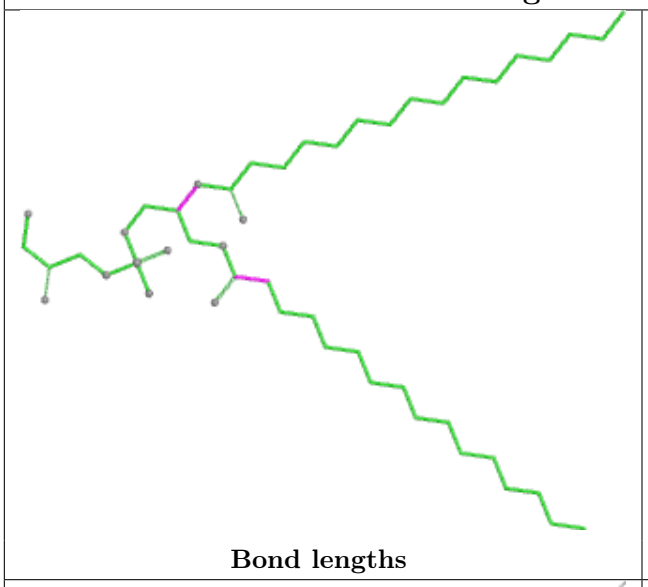


Torsions



Rings

Ligand LHG D 412



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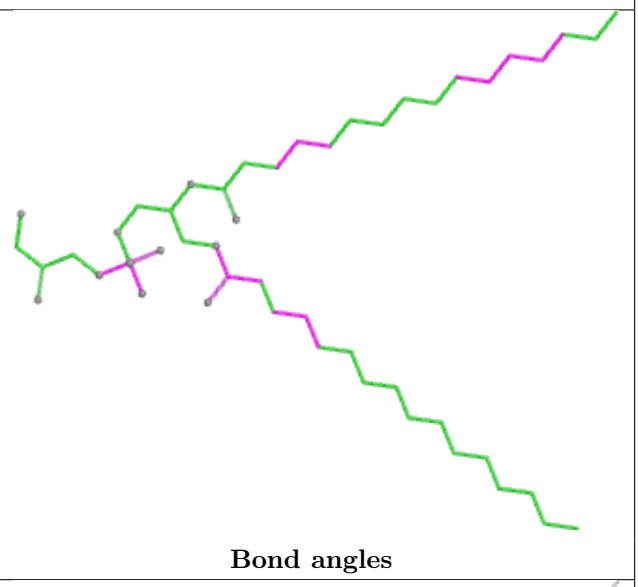
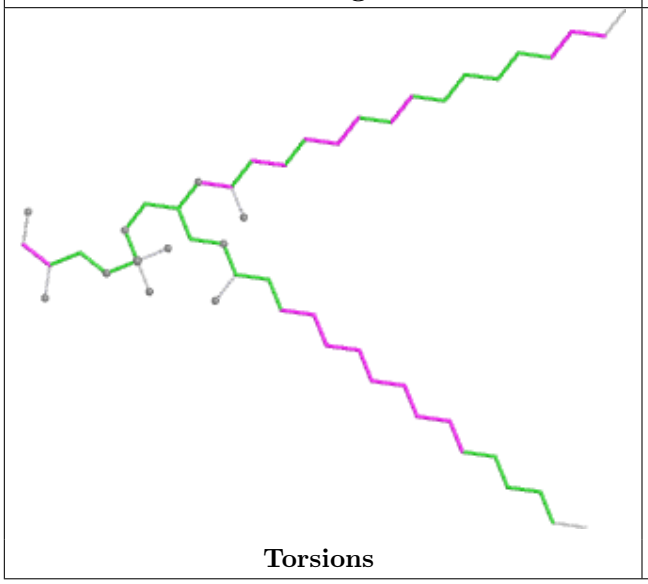
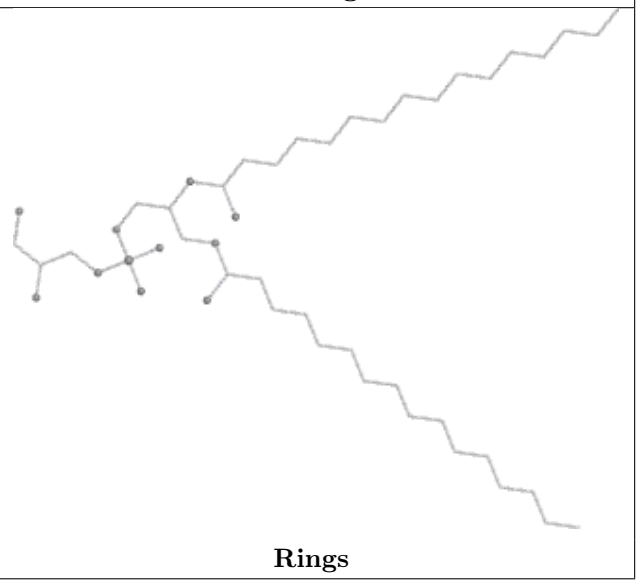


Bond angles

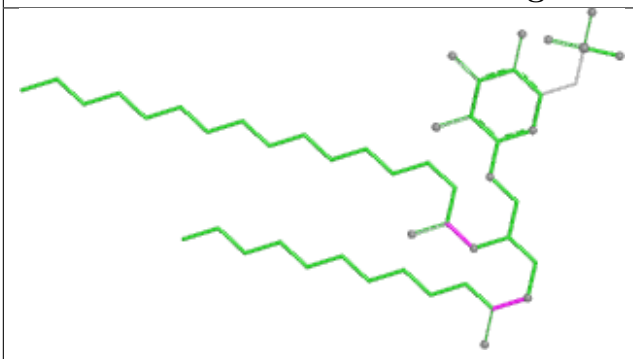


Torsions

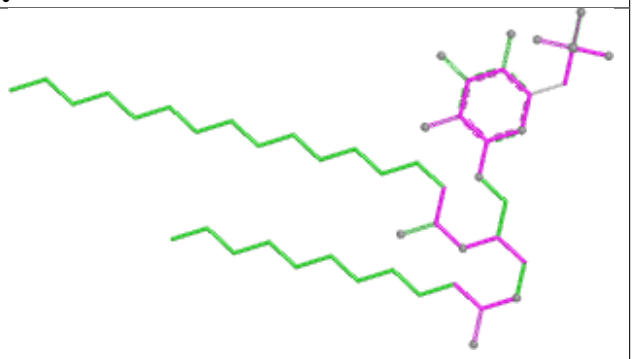


Rings

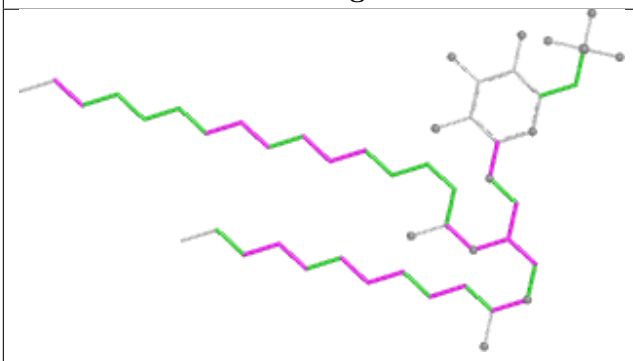
Ligand SQD b 619



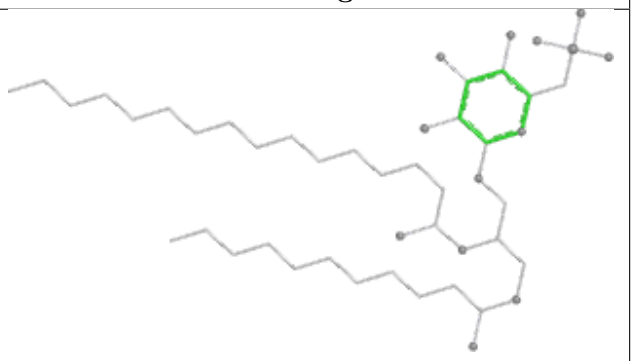
Bond lengths



Bond angles



Torsions



Rings

Ligand STE I 101

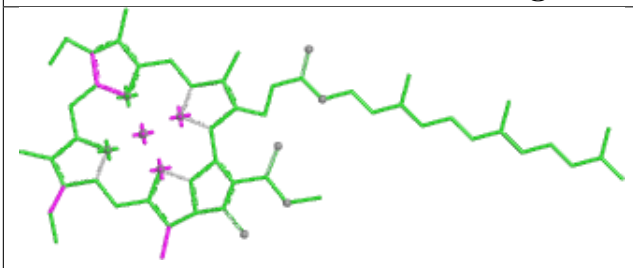
Bond lengths

Bond angles

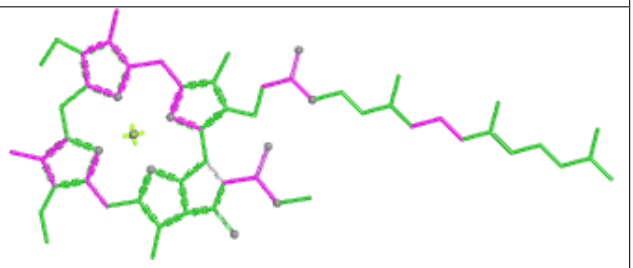
Torsions

Rings

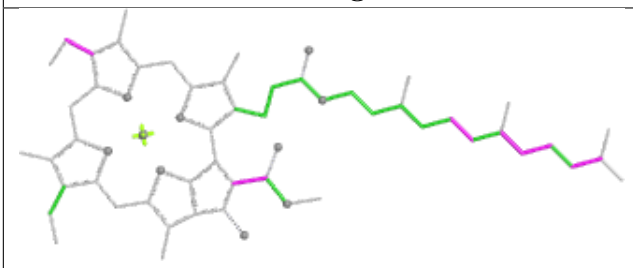
Ligand CLA c 506



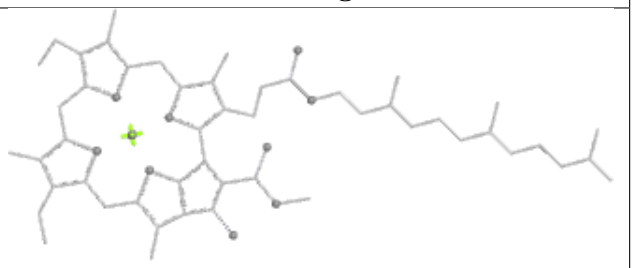
Bond lengths



Bond angles

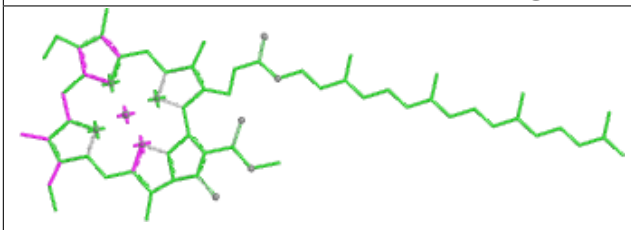


Torsions

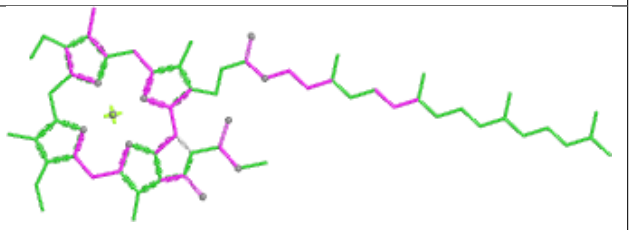


Rings

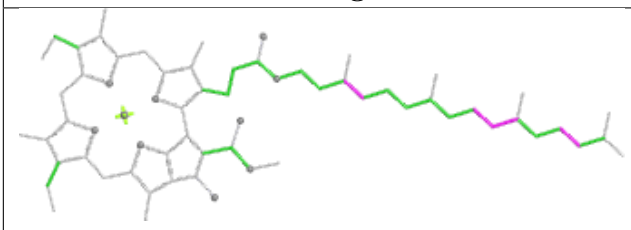
Ligand CLA b 603



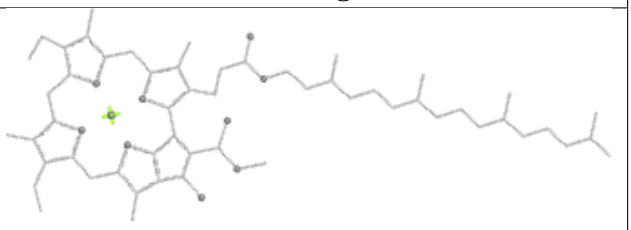
Bond lengths



Bond angles

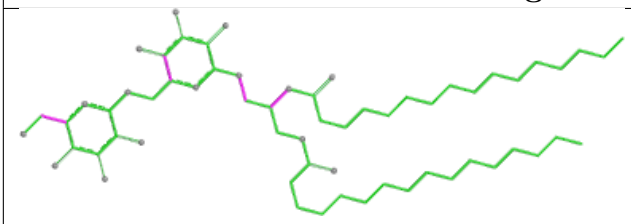


Torsions

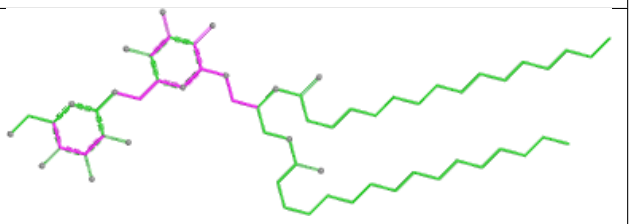


Rings

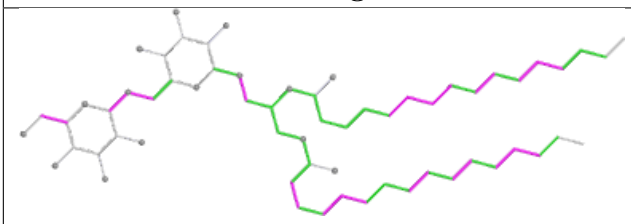
Ligand DGD c 520



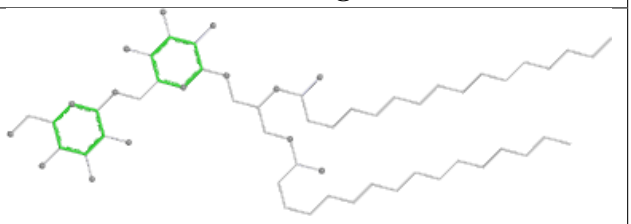
Bond lengths



Bond angles

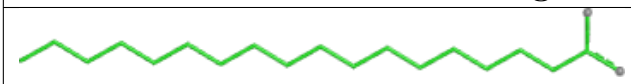


Torsions



Rings

Ligand STE c 523



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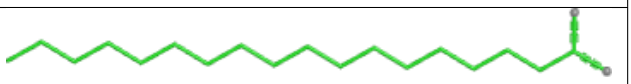
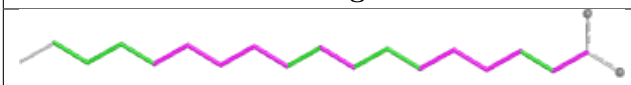
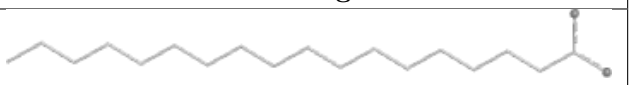


Bond angles

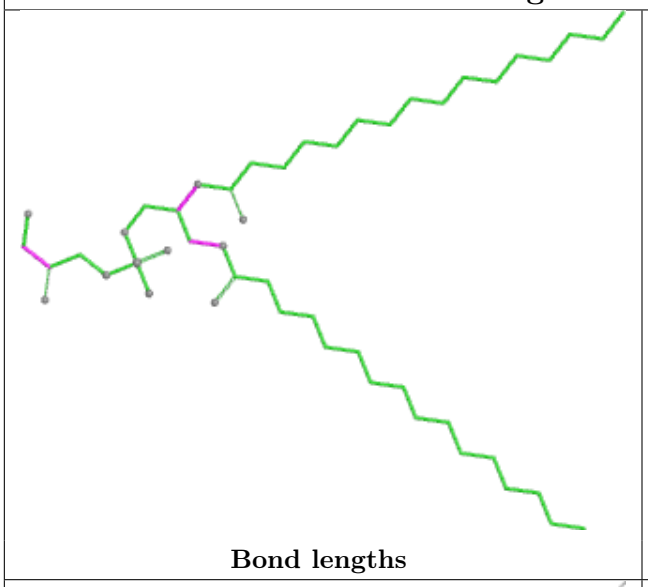


Torsions

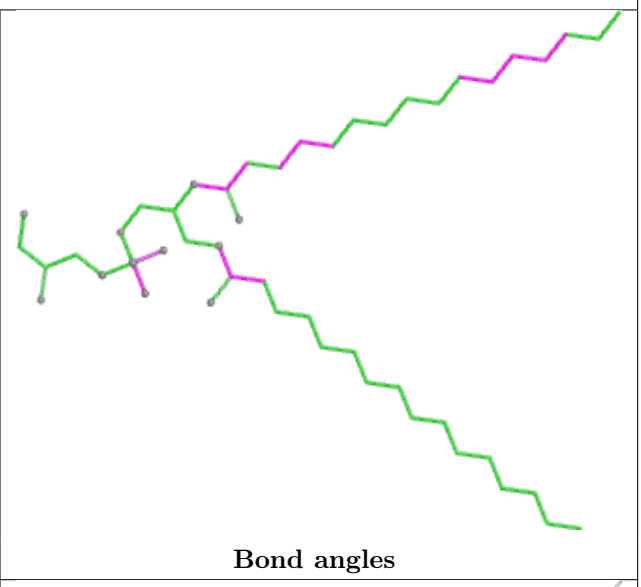


Rings

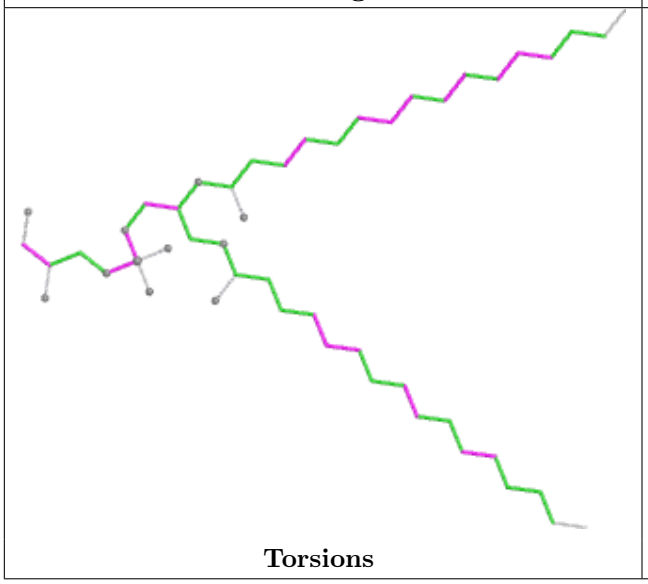
Ligand LHG d 407



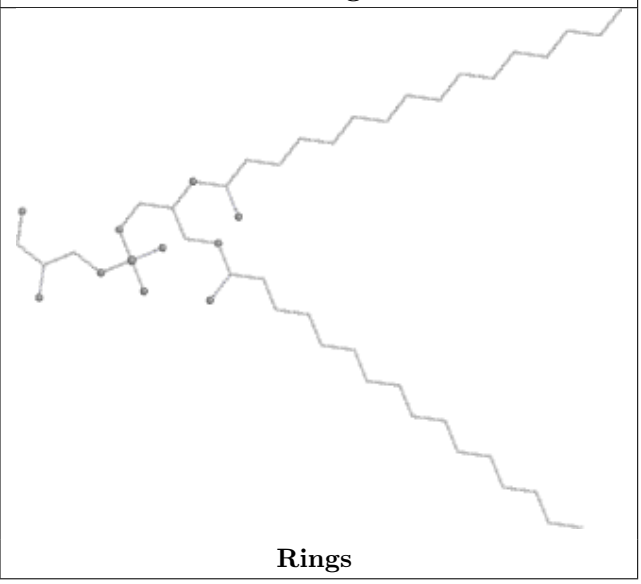
Bond lengths



Bond angles

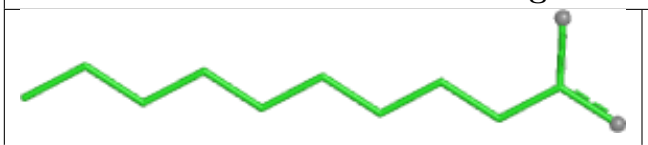


Torsions



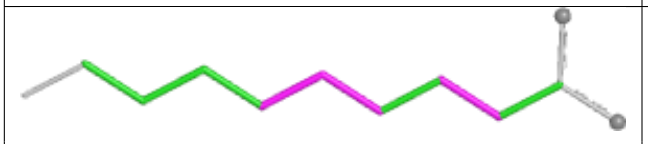
Rings

Ligand STE E 102

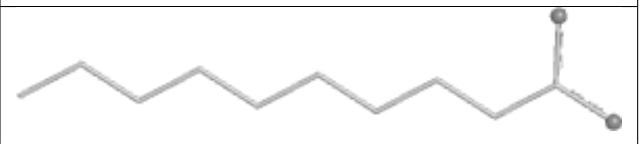


Bond lengths

Bond angles

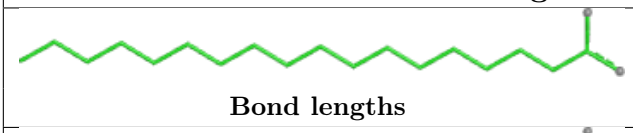


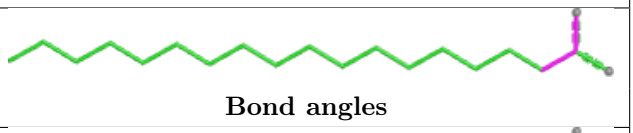
Torsions



Rings

Ligand STE d 412


Bond lengths

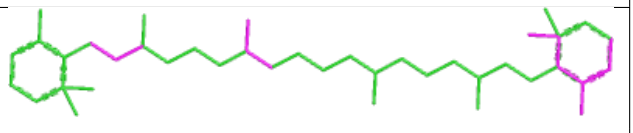

Bond angles

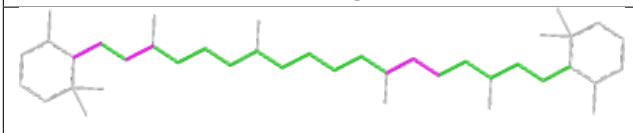
Torsions

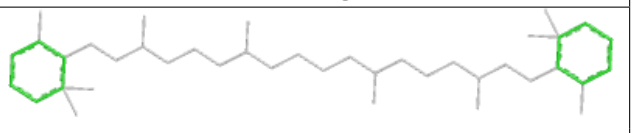
Rings

Ligand BCR T 101

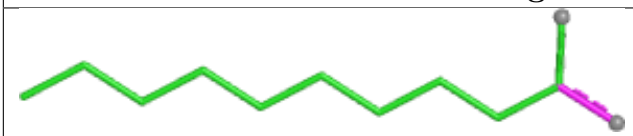
Bond lengths

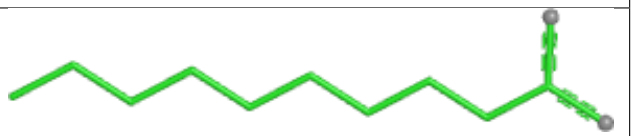

Bond angles

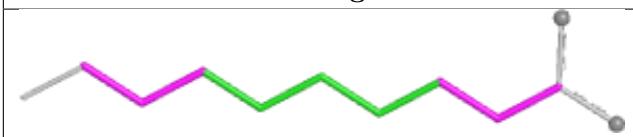

Torsions


Rings

Ligand STE B 625


Bond lengths


Bond angles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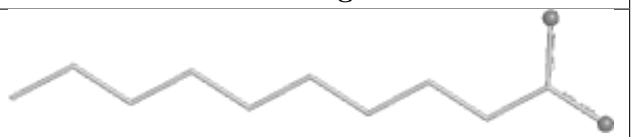
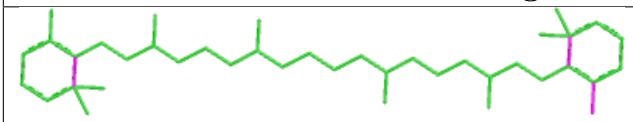

Rings

Ligand BCR Y 101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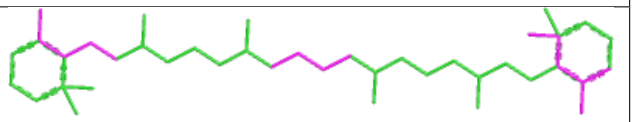
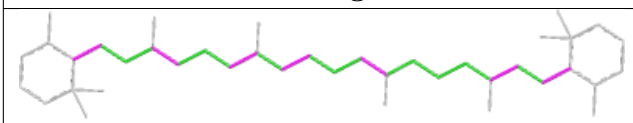
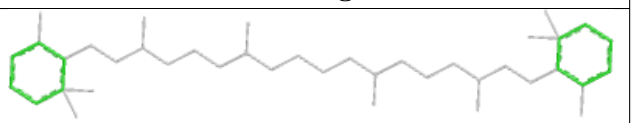
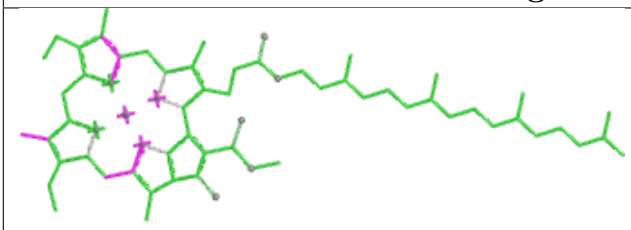

Bond angles


Torsions


Rings

Ligand CLA b 606



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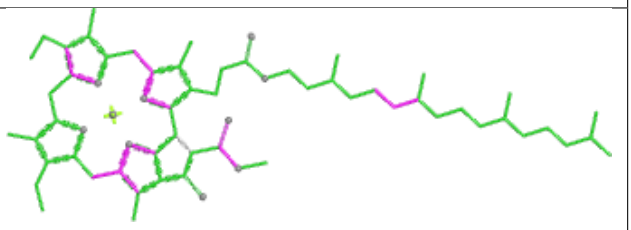
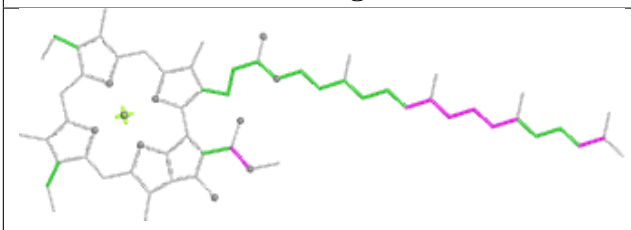


Bond angles



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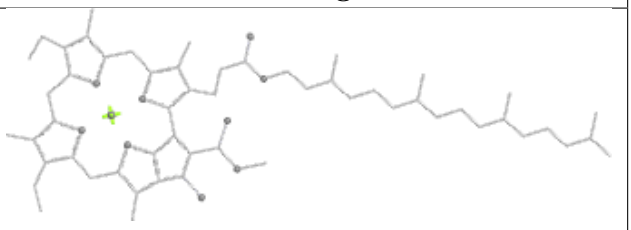
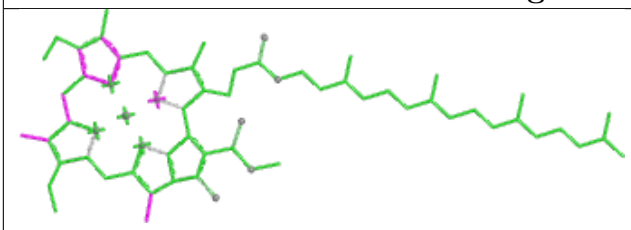


Rings

Ligand CLA b 611



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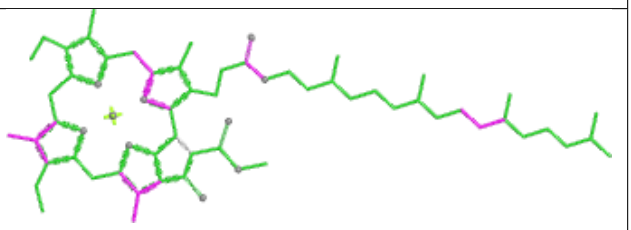
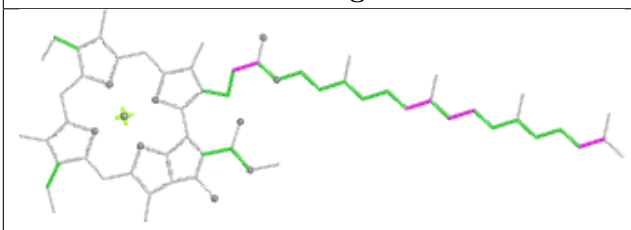


Bond angles



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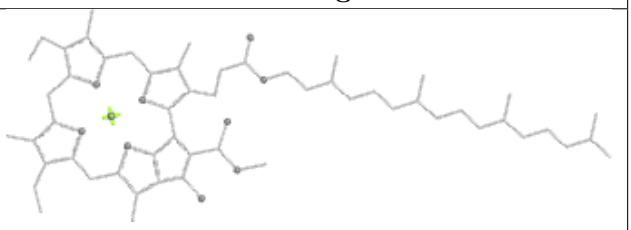
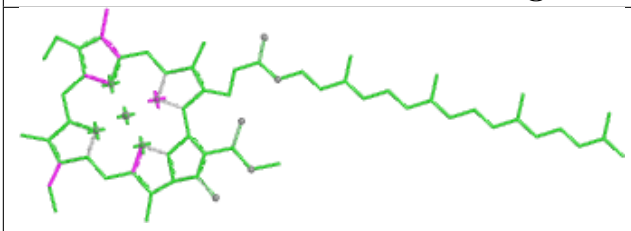


Rings

Ligand CLA b 608



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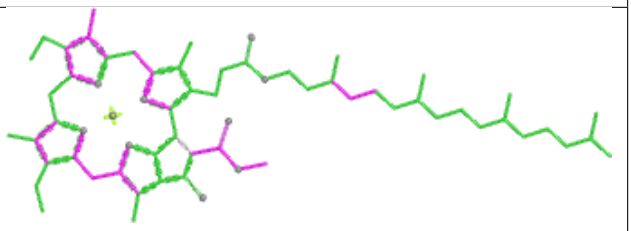
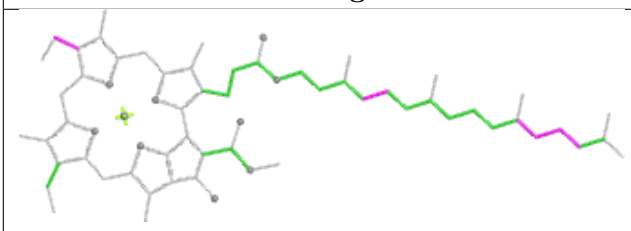


Bond angles



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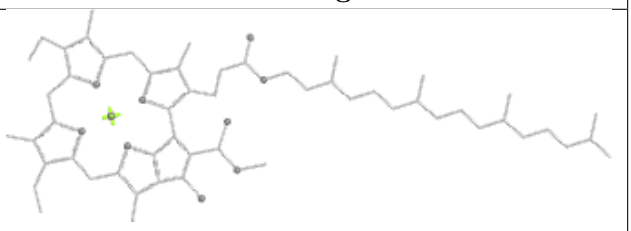
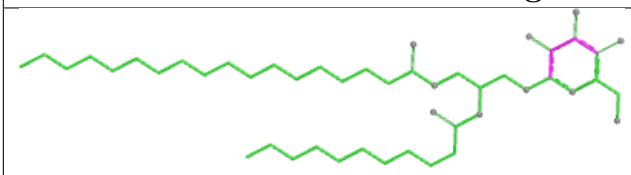


Rings

Ligand LMG c 524



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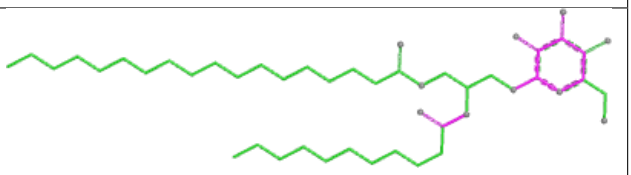
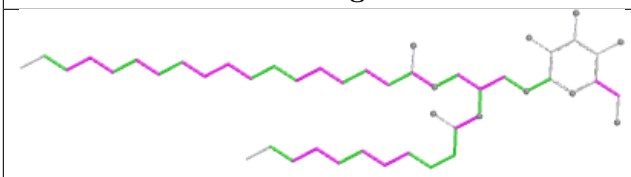


Bond angles



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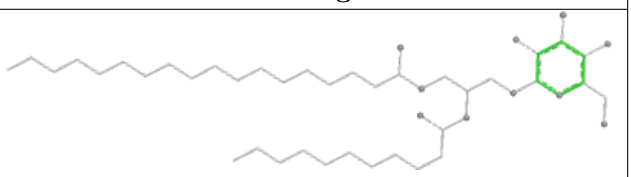
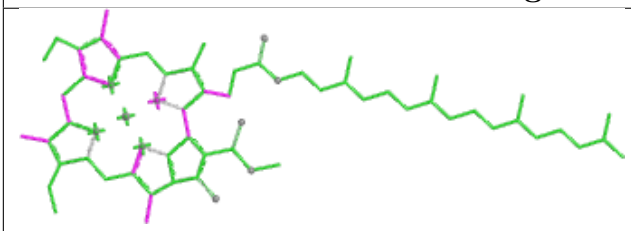


Rings

Ligand CLA C 513



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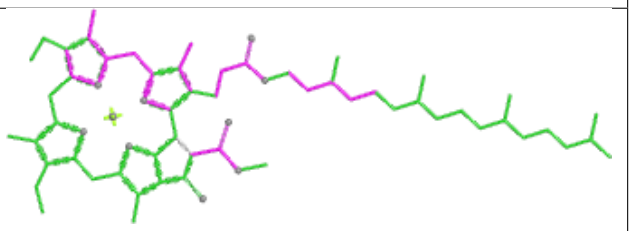
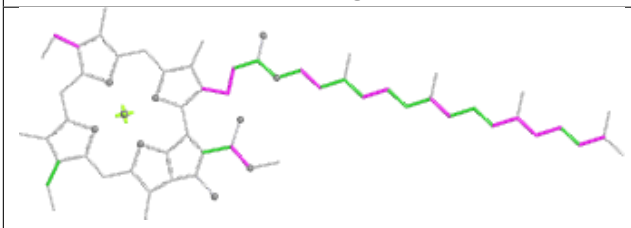


Bond angles



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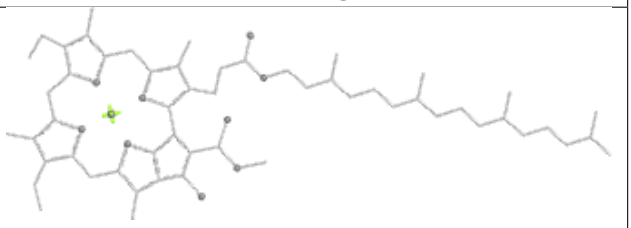
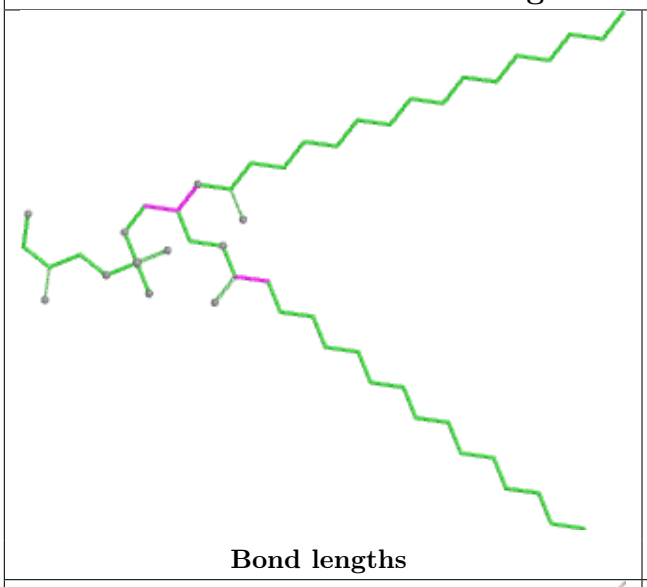


Rings

Ligand LHG d 406



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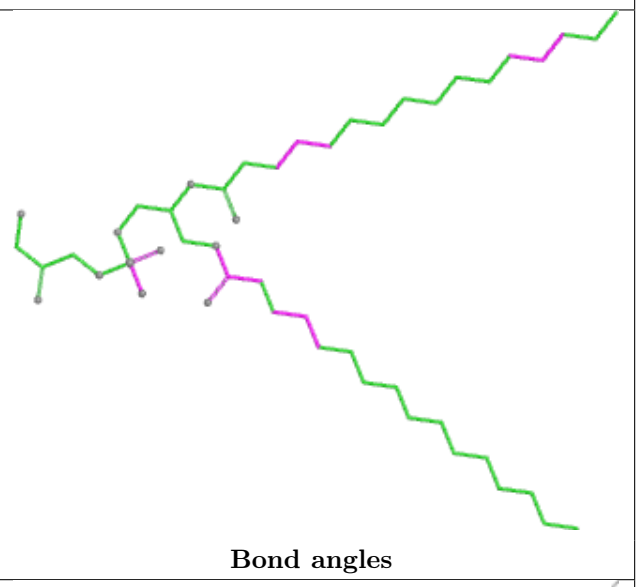
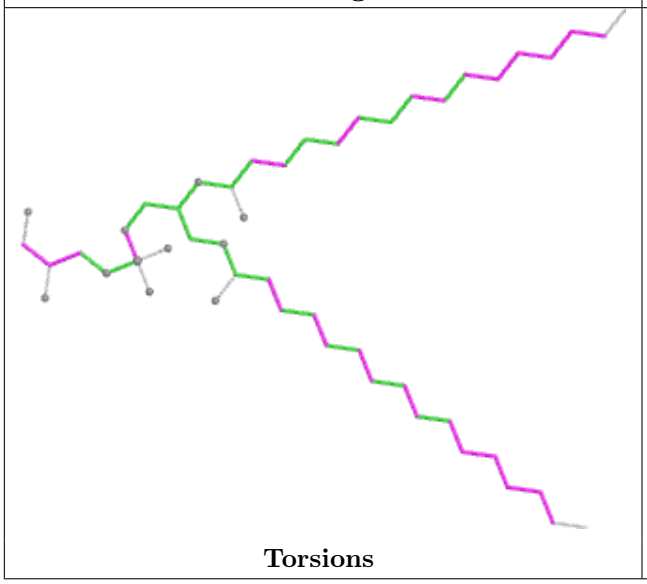


Bond angles



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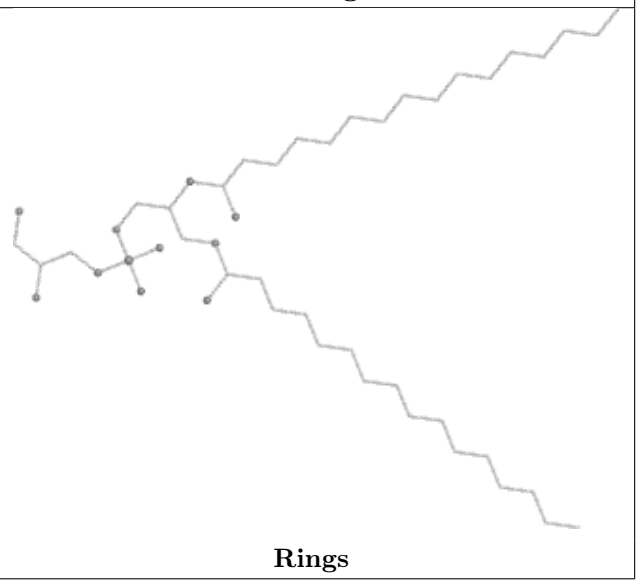
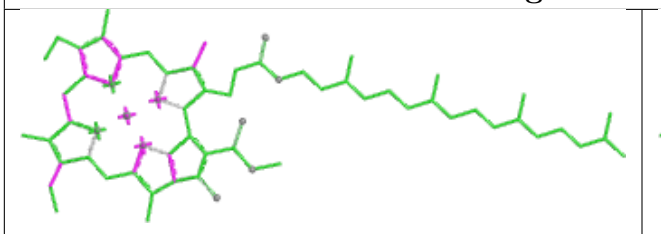


Rings

Ligand CLA C 507



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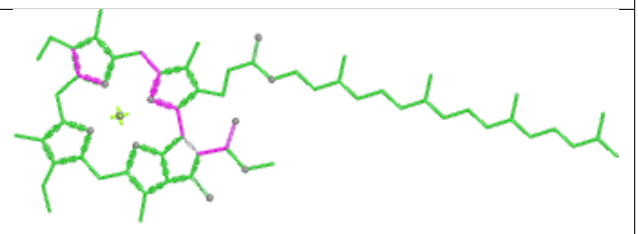

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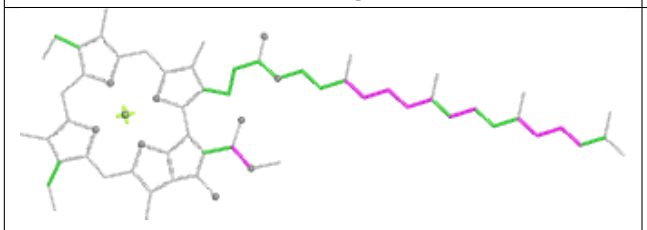

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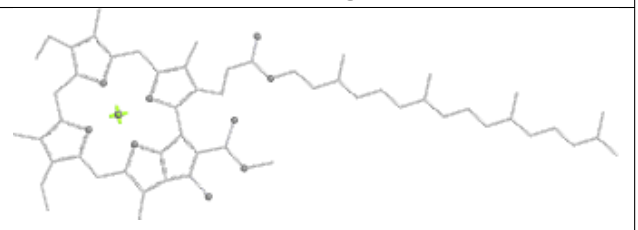
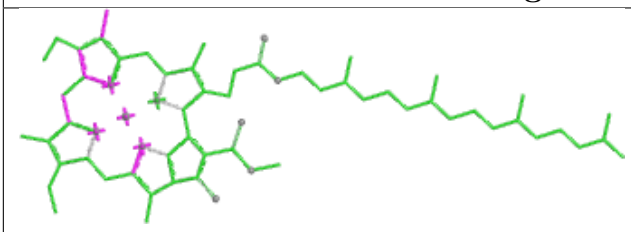


Rings

Ligand CLA B 611



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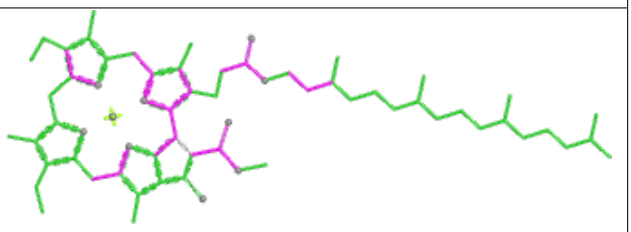
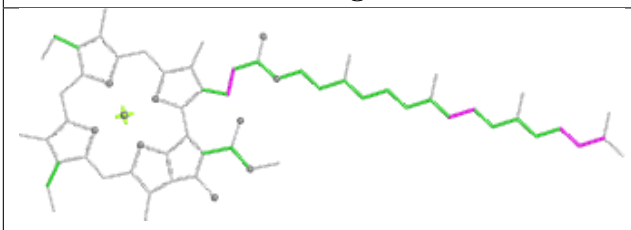


Bond angles



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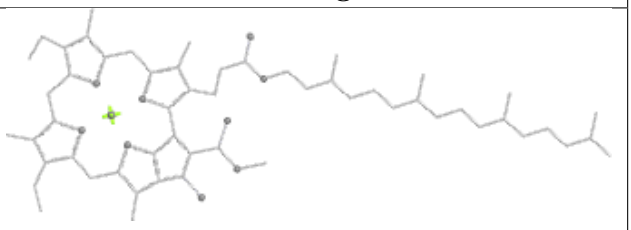
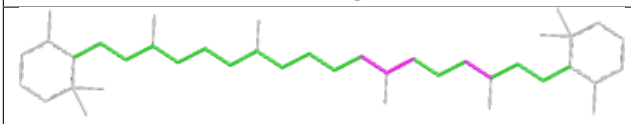


Rings

Ligand BCR C 515

Bond lengths

Bond angles



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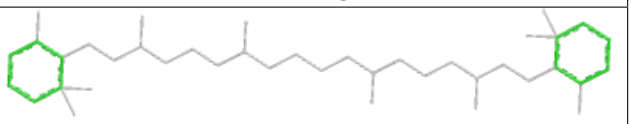
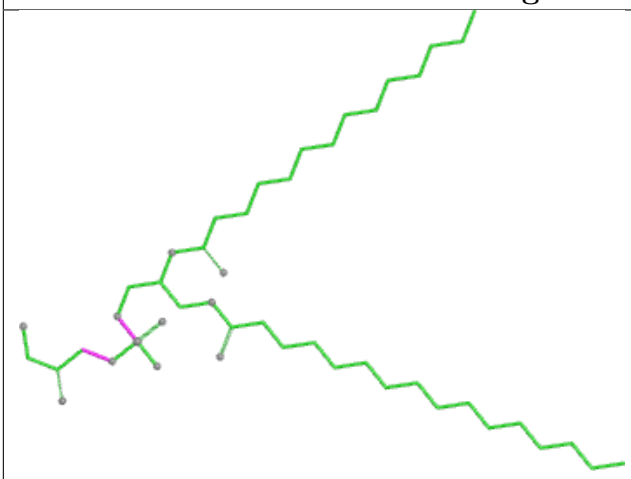


Rings

Ligand LHG D 409



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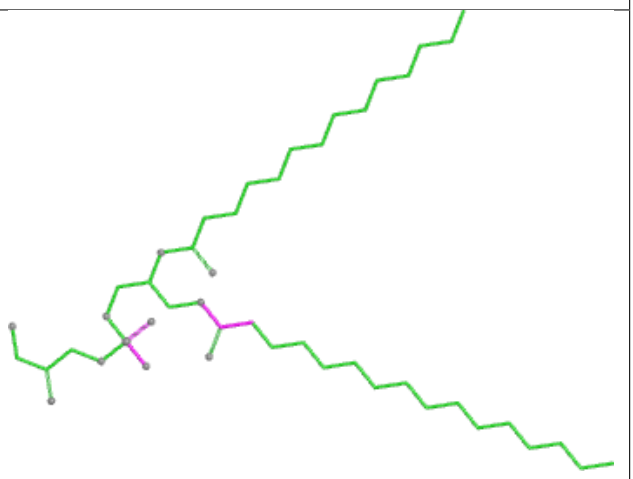
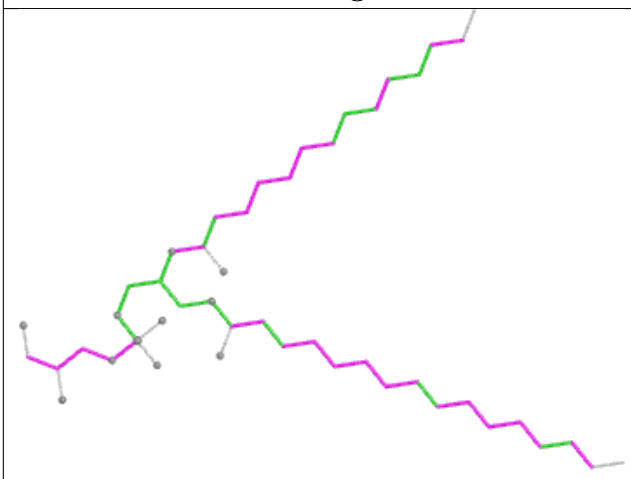


Bond angles



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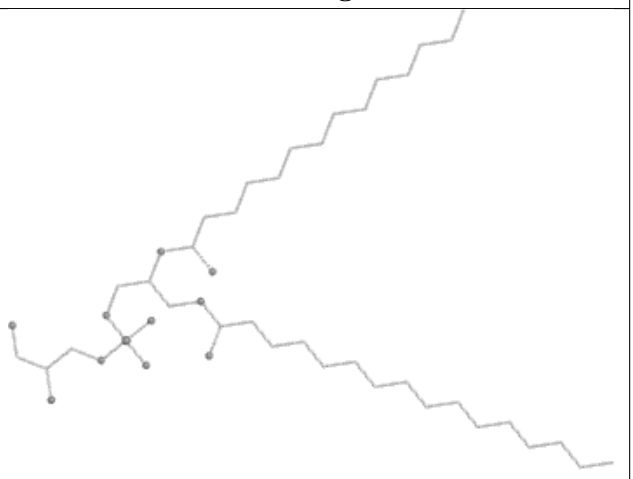
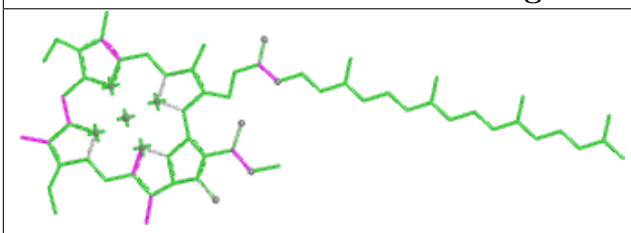


Rings

Ligand CLA C 510



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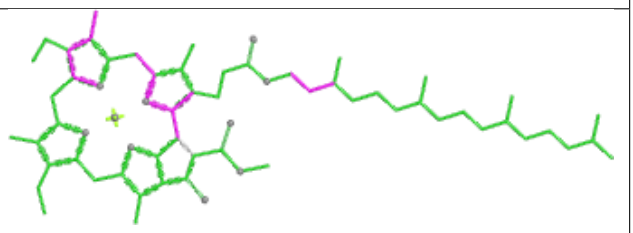
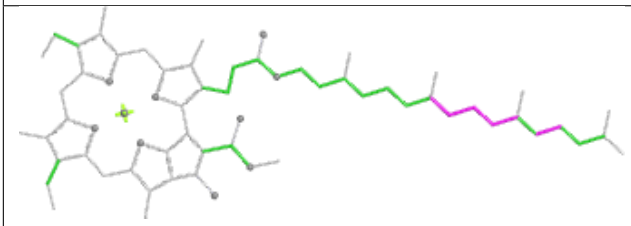


Bond angles



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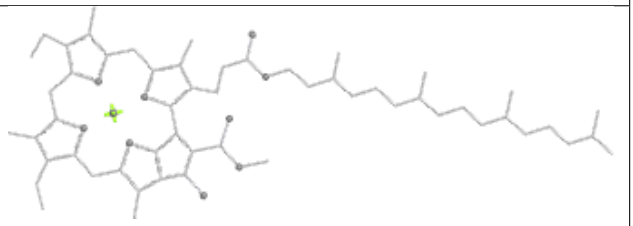
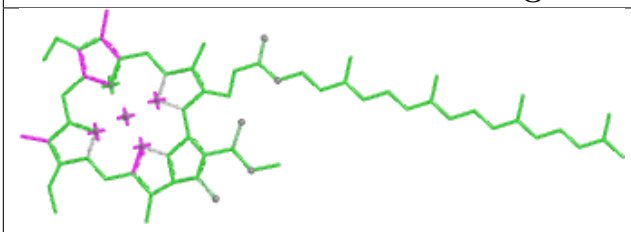
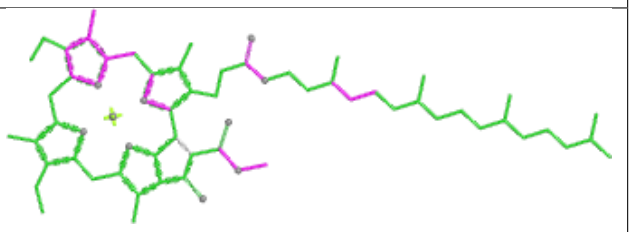


Rings

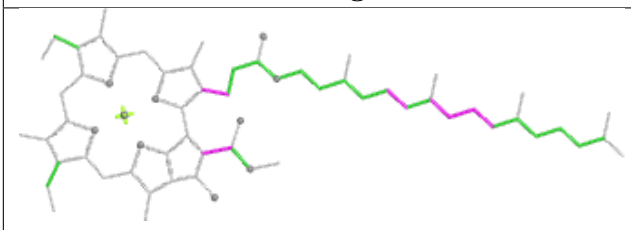
Ligand CLA B 608



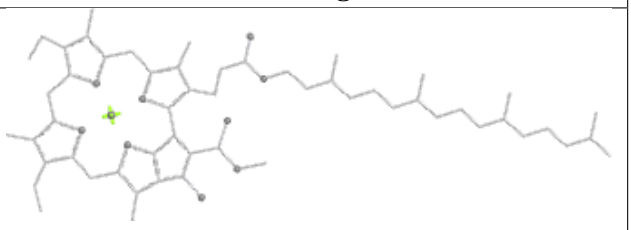
Bond lengths



Bond angles

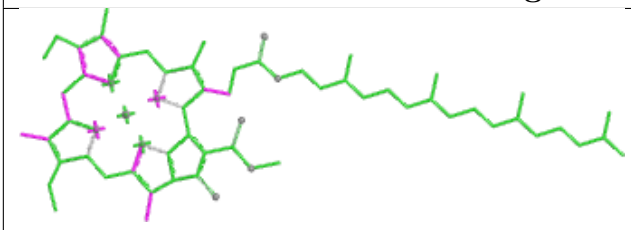


Torsions

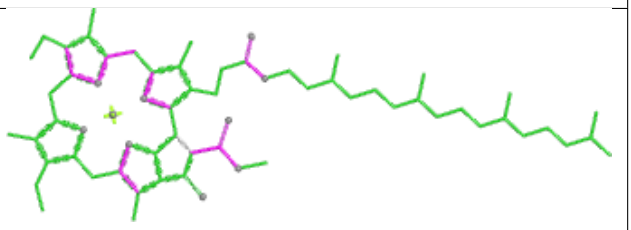


Rings

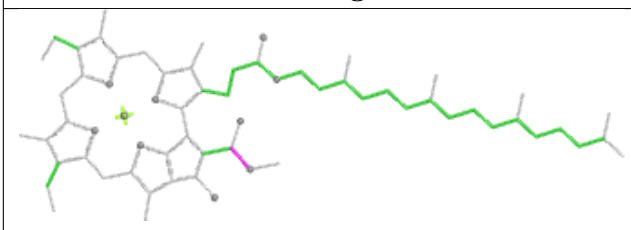
Ligand CLA C 502



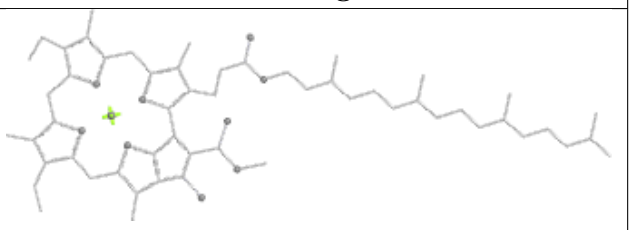
Bond lengths



Bond angles

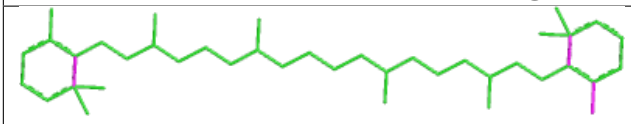


Torsions



Rings

Ligand BCR y 101



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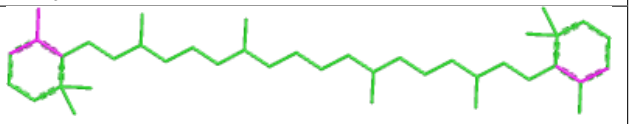
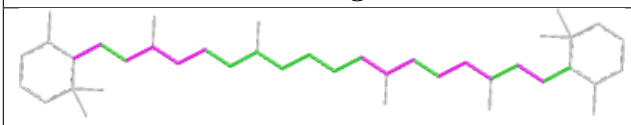
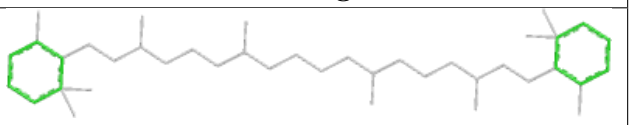


Bond angles

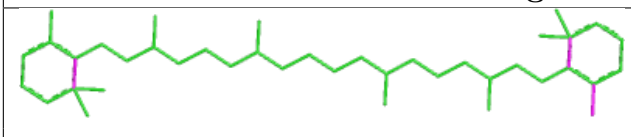


Torsions



Rings

Ligand BCR a 406



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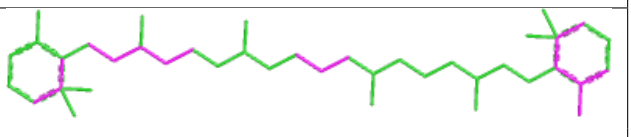
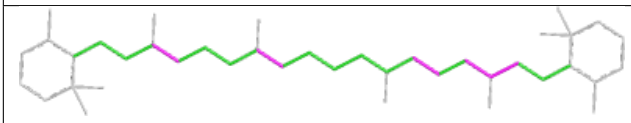
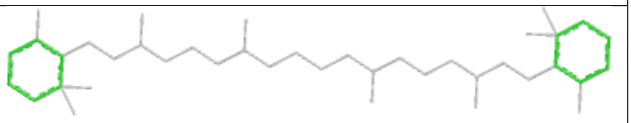


Bond angles



Torsions



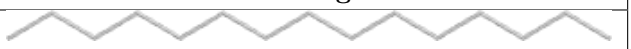
Rings

Ligand STE T 102

Bond lengths

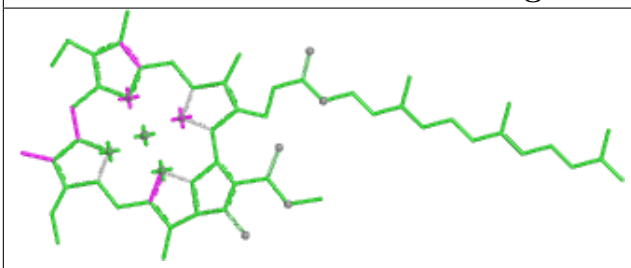
Bond angles

Torsions

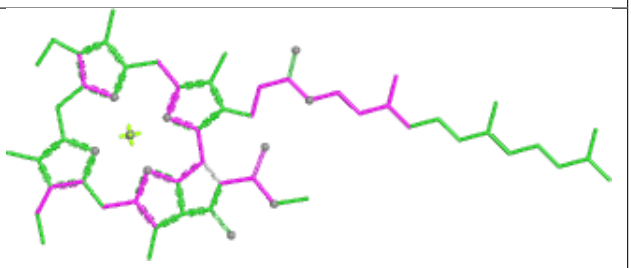


Rings

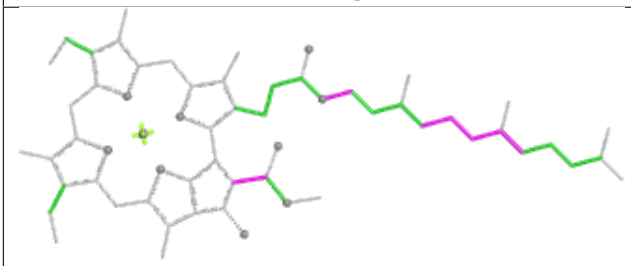
Ligand CLA B 617



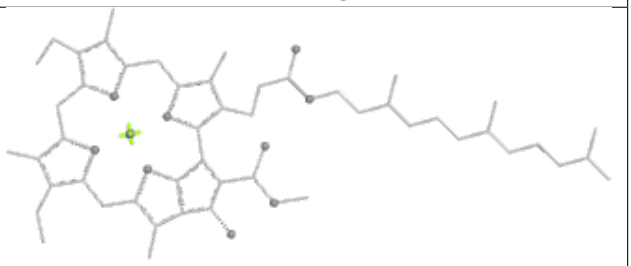
Bond lengths



Bond angles

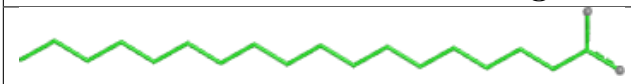


Torsions

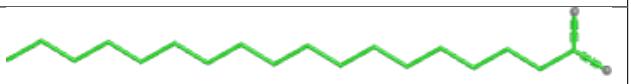


Rings

Ligand STE b 625



Bond lengths

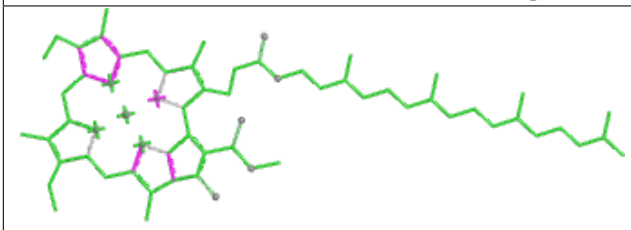


Bond angles

Torsions

Rings

Ligand CLA B 613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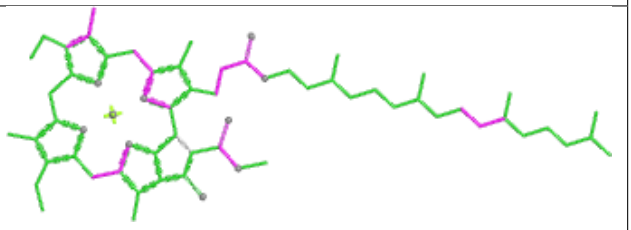
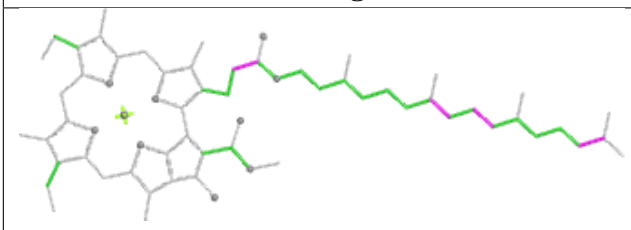

Bond angles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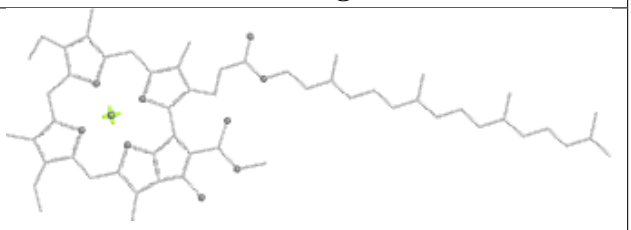

Rings

Ligand STE M 103

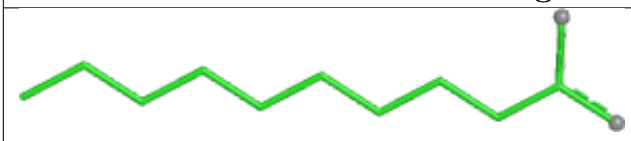
Bond lengths

Bond angles

Torsions

Rings

Ligand STE j 101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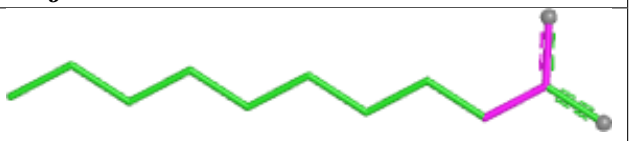
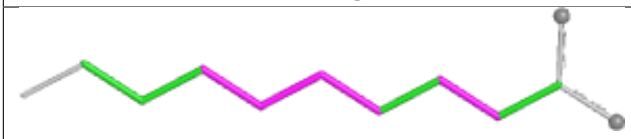
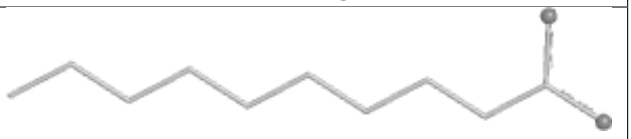
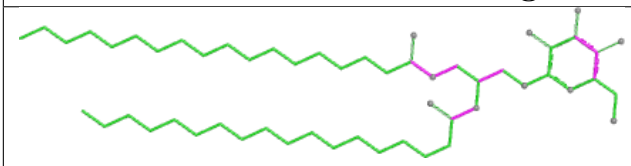
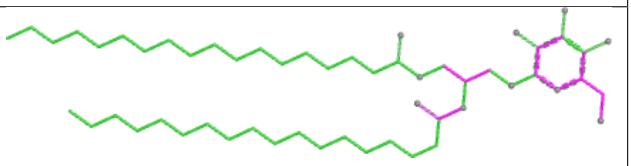

Bond angles

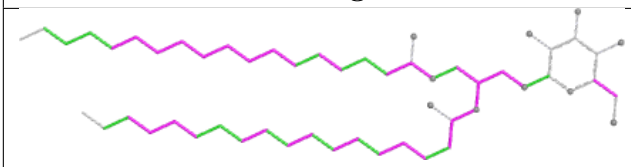

Torsions


Rings

Ligand LMG B 629

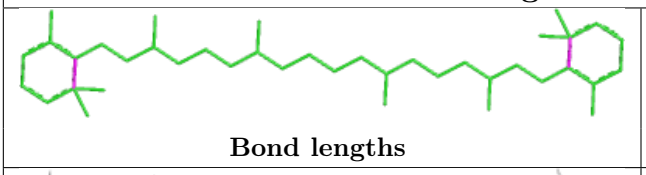

Bond lengths


Bond angles

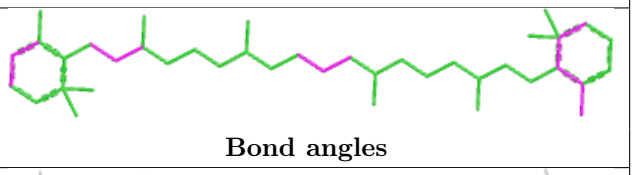

Torsions

Rings

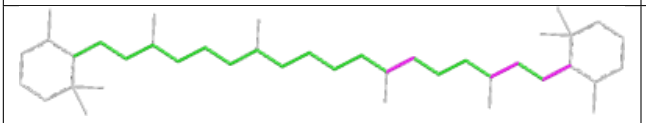
Ligand BCR K 101



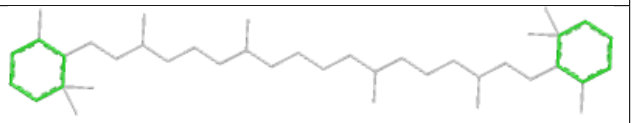
Bond lengths



Bond angles

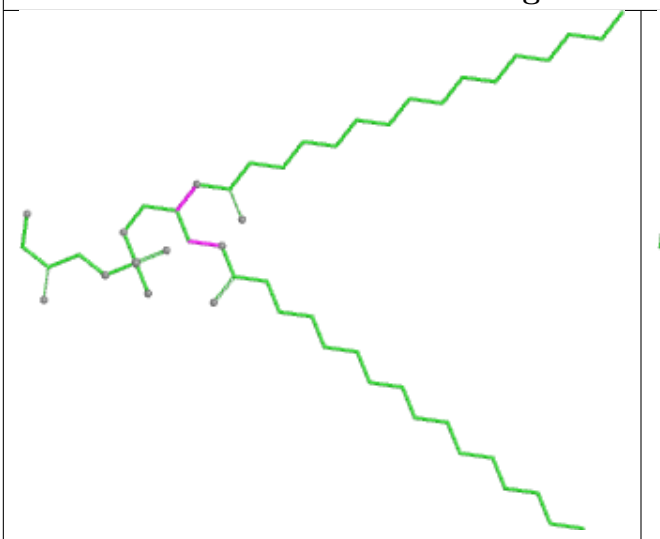


Torsions



Rings

Ligand LHG B 622



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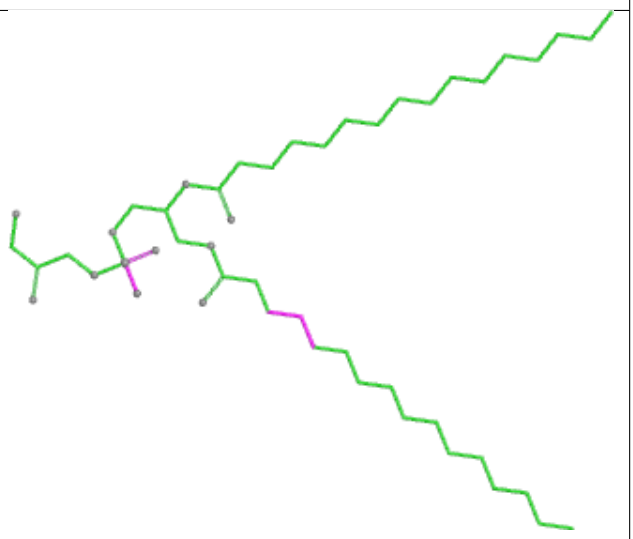
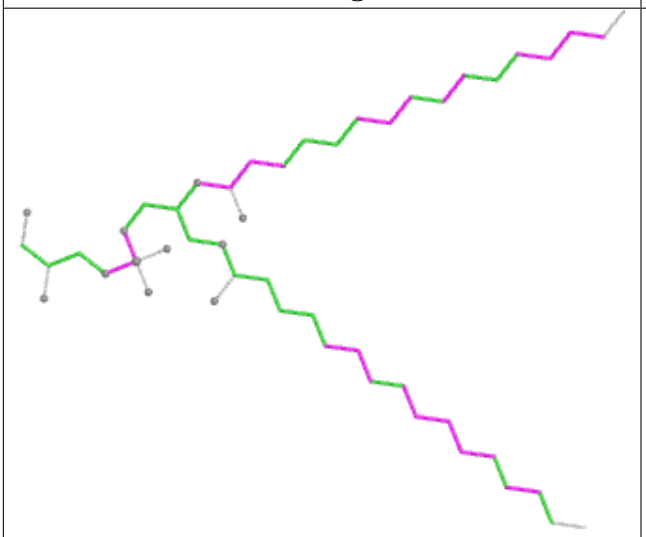


Bond angles



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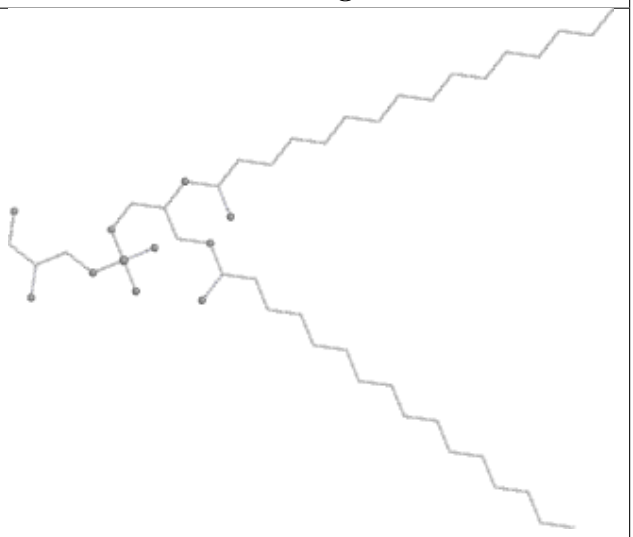
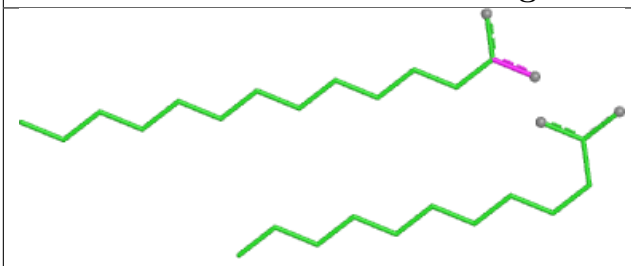


Rings

Ligand LMG D 411



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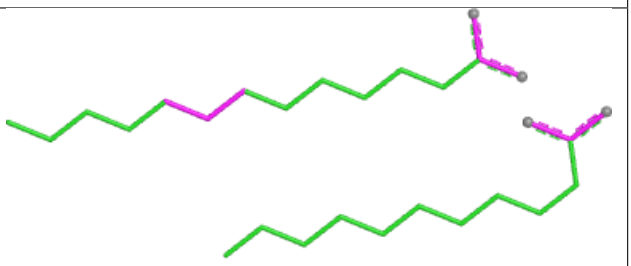
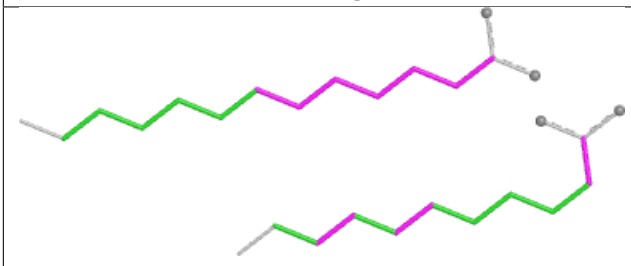
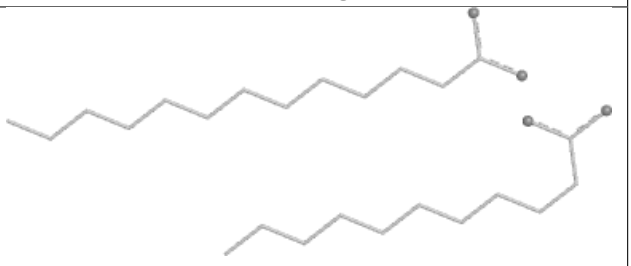


Bond angles

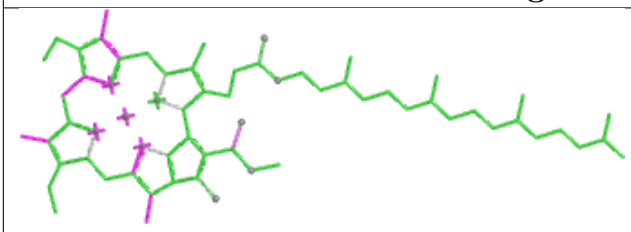


Torsions



Rings

Ligand CLA d 403



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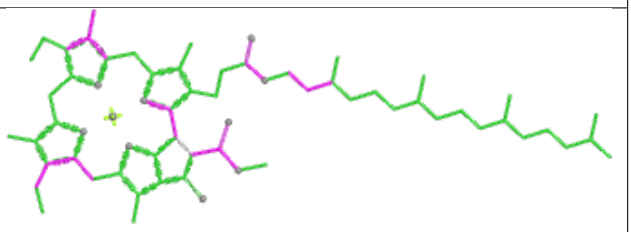
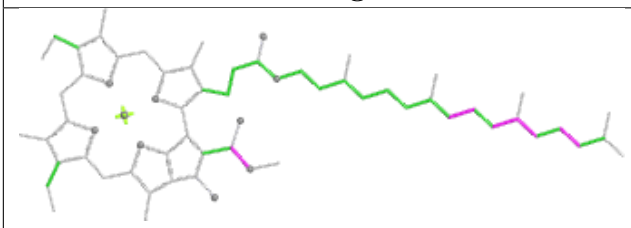
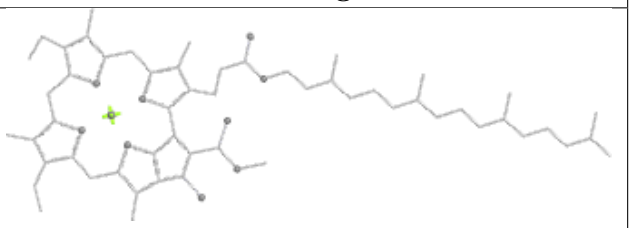


Bond angles

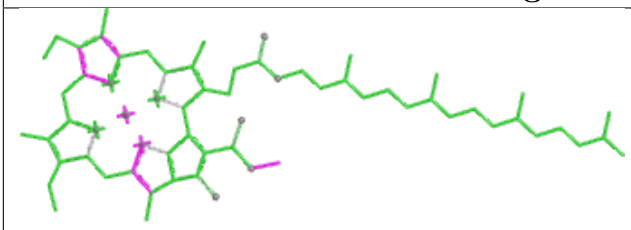


Torsions

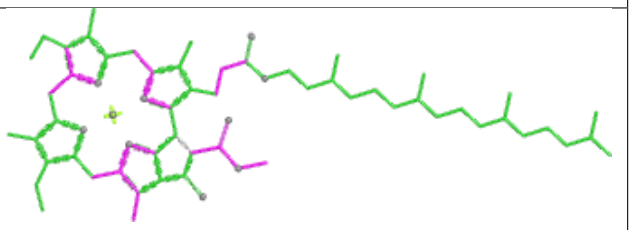


Rings

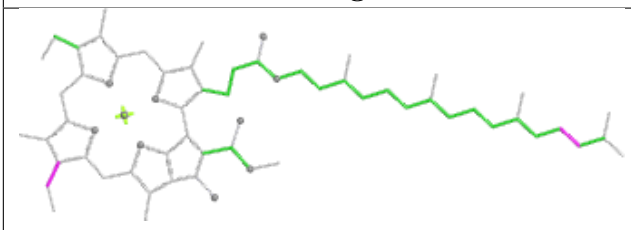
Ligand CLA A 402



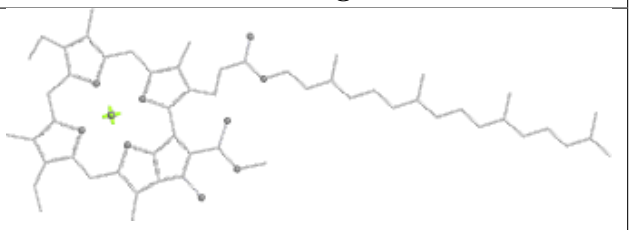
Bond lengths



Bond angles



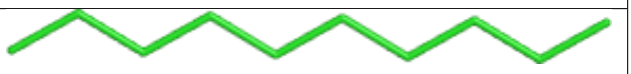
Torsions



Rings

Ligand STE a 414

Bond lengths

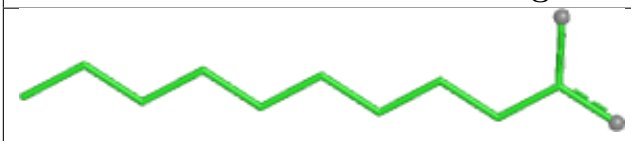


Bond angles

Torsions

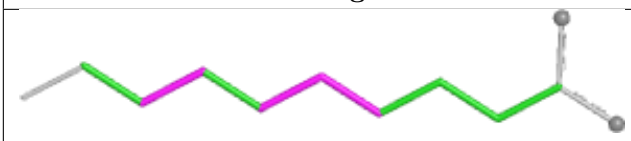
Rings

Ligand STE a 415

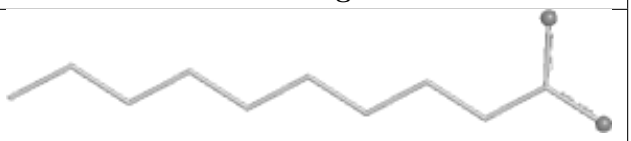


Bond lengths

Bond angles

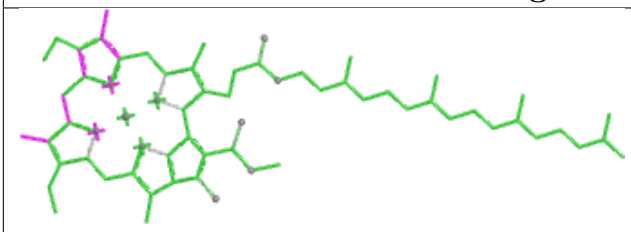


Torsions

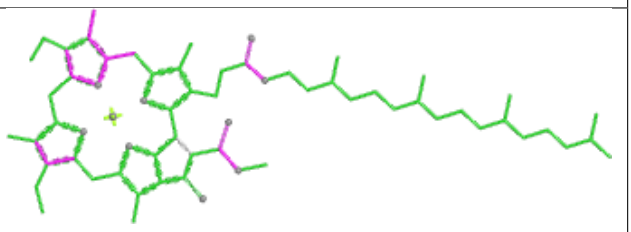


Rings

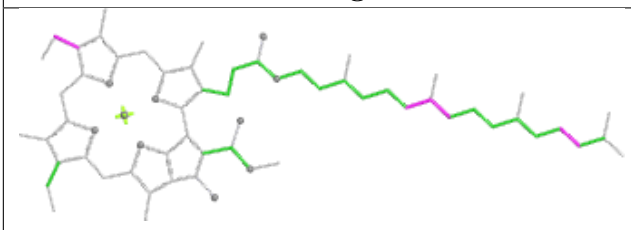
Ligand CLA c 507



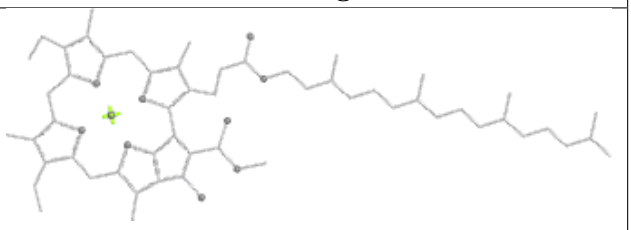
Bond lengths



Bond angles

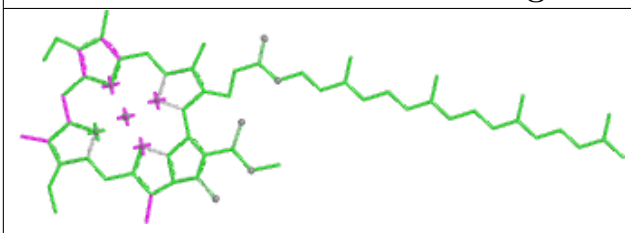


Torsions



Rings

Ligand CLA b 614



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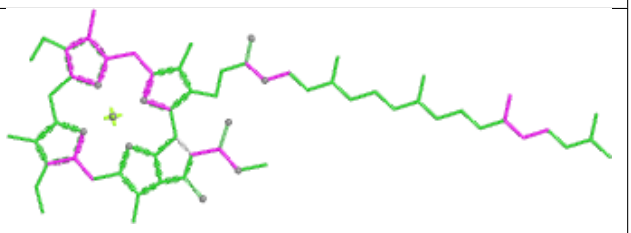
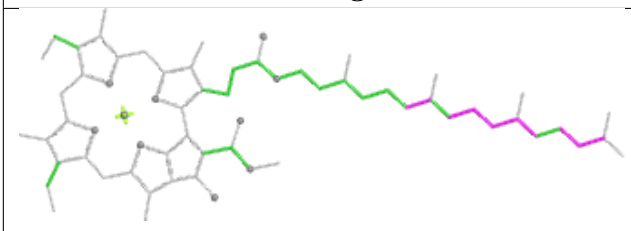
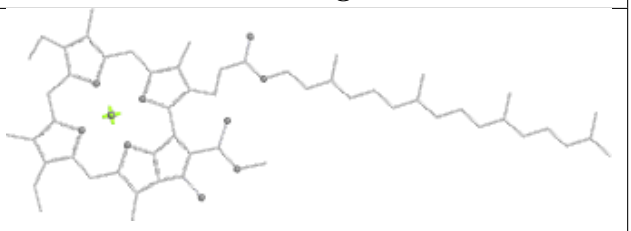


Bond angles

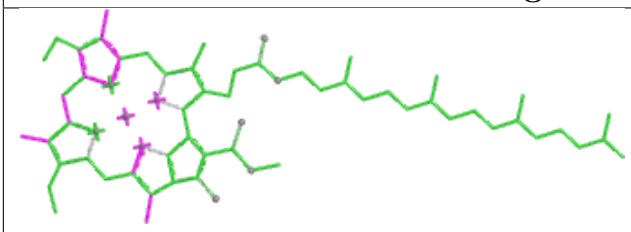


Torsions



Rings

Ligand CLA C 512



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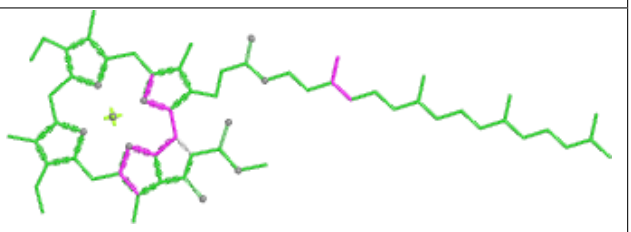
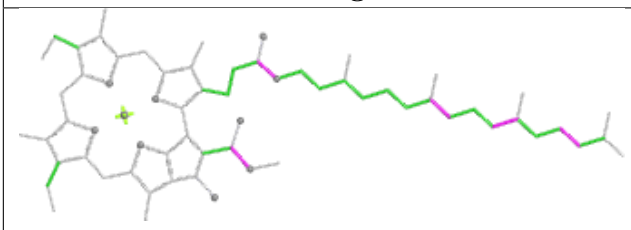
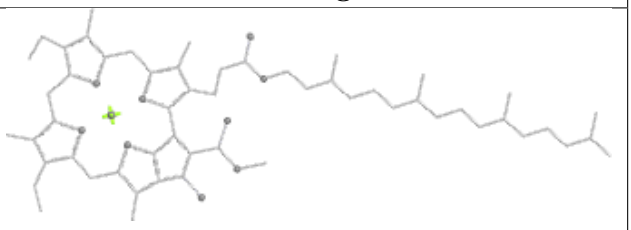


Bond angles

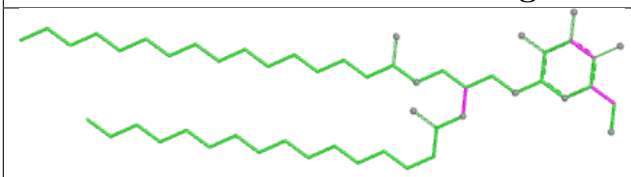


Torsions



Rings

Ligand LMG D 406



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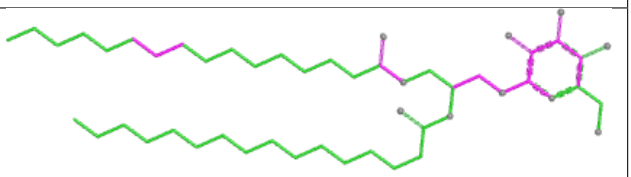
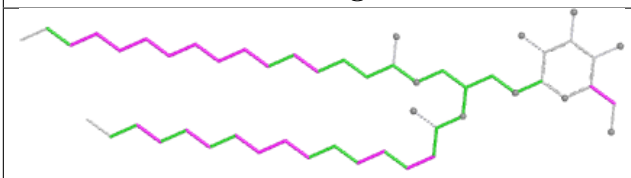
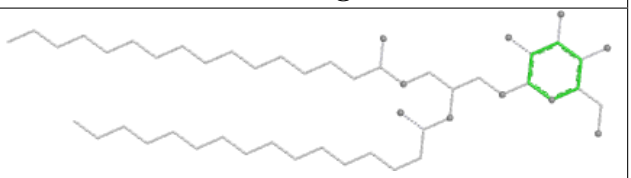


Bond angles

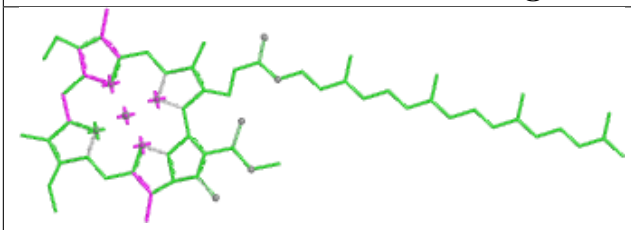


Torsions



Rings

Ligand CLA C 509



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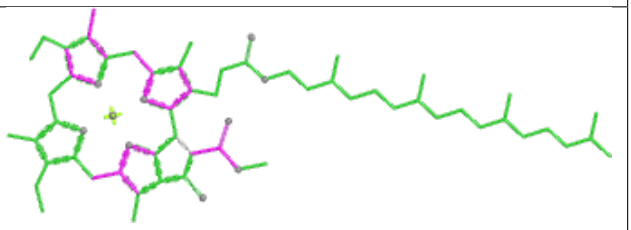
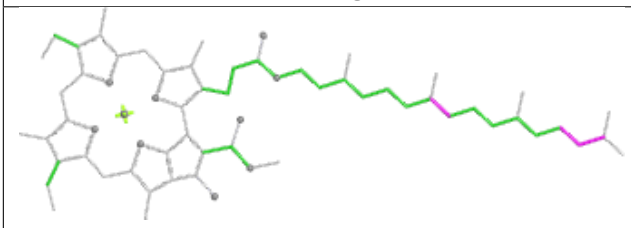
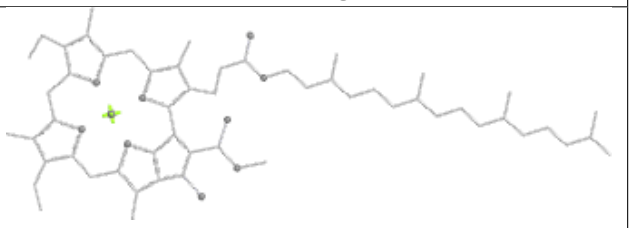


Bond angles

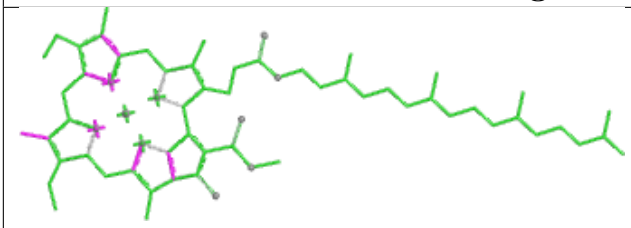


Torsions

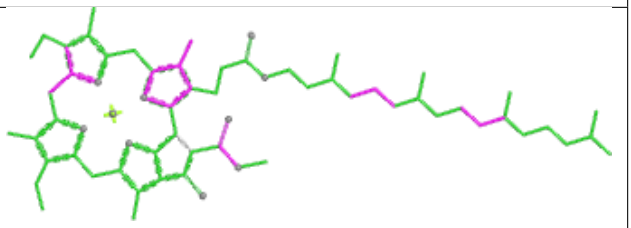


Rings

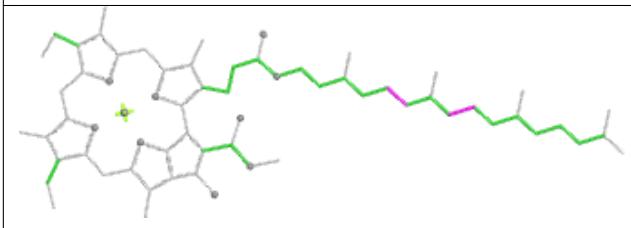
Ligand CLA c 505



Bond lengths



Bond angles



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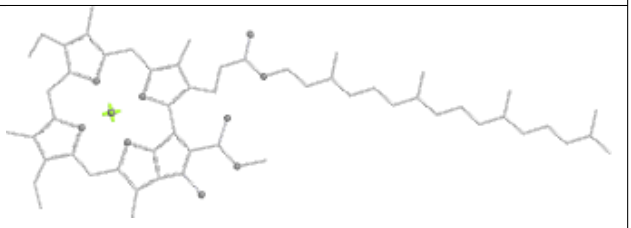
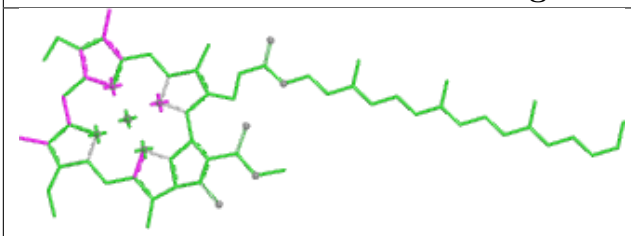
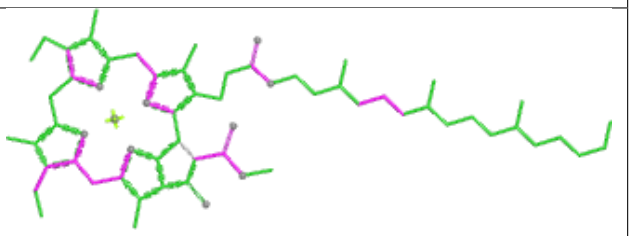


Rings

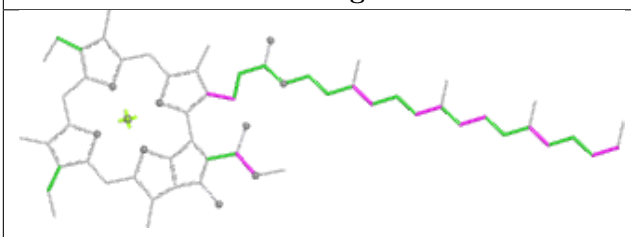
Ligand CLA c 510



Bond lengths



Bond angles



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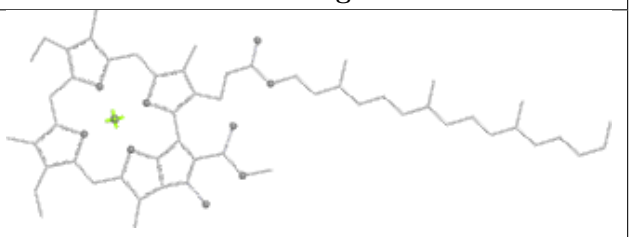
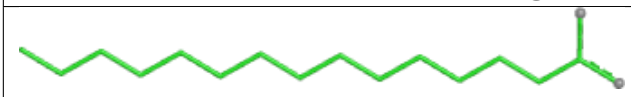
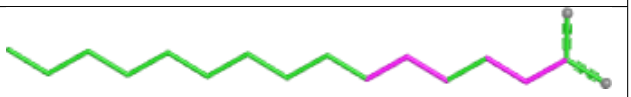


Rings

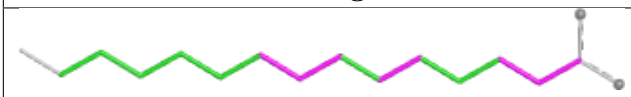
Ligand STE B 621



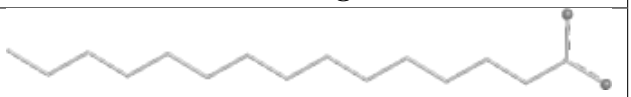
Bond lengths



Bond angles

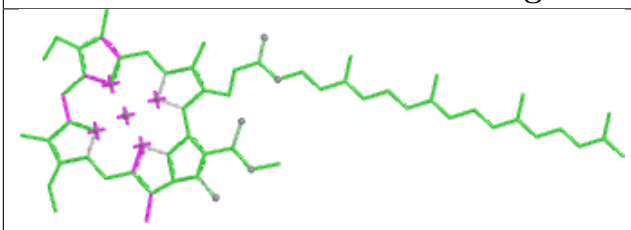


Torsions

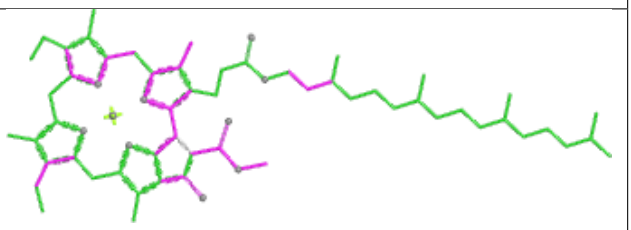


Rings

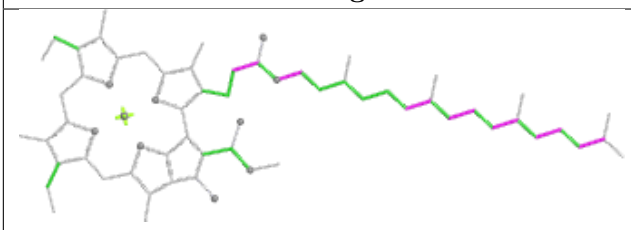
Ligand CLA B 614



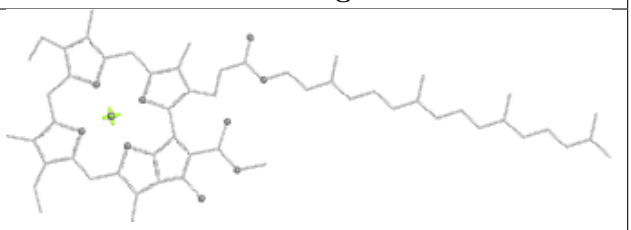
Bond lengths



Bond angles

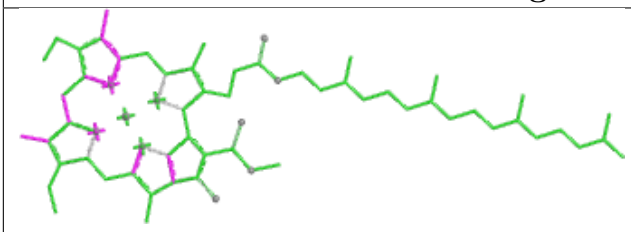


Torsions

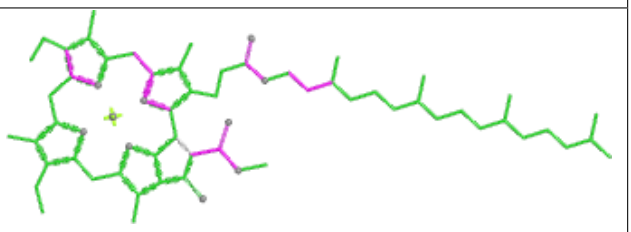


Rings

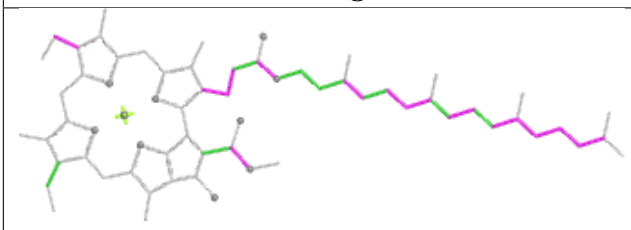
Ligand CLA c 514



Bond lengths



Bond angles



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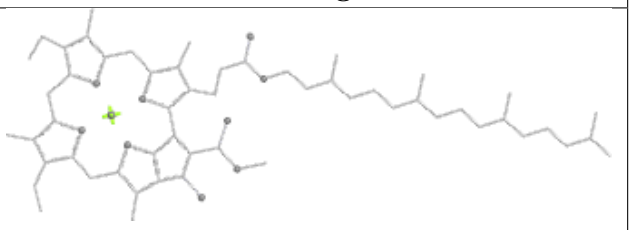
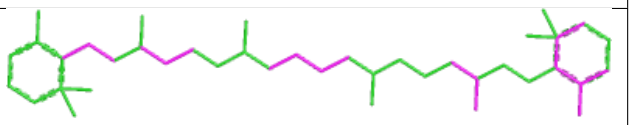


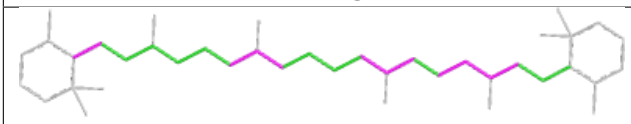
Rings

Ligand BCR c 518

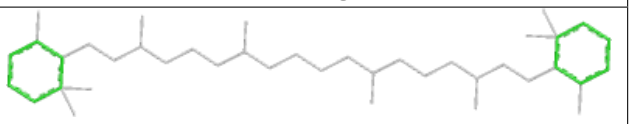
Bond lengths



Bond angles

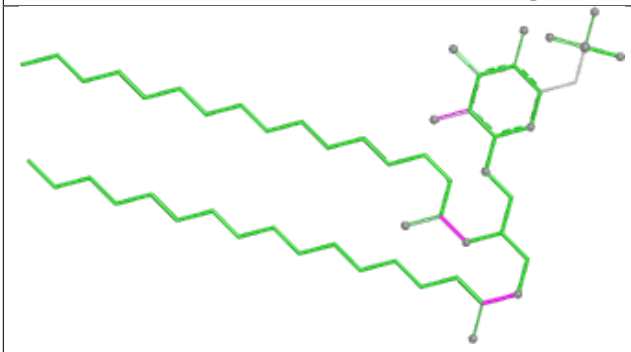


Torsions

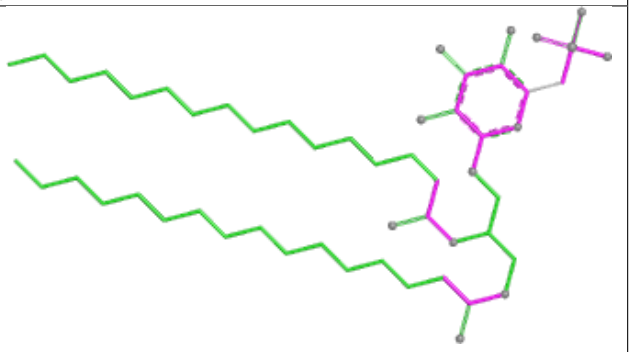


Rings

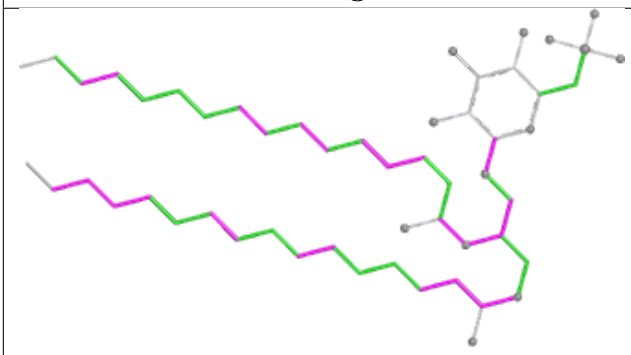
Ligand SQD B 623



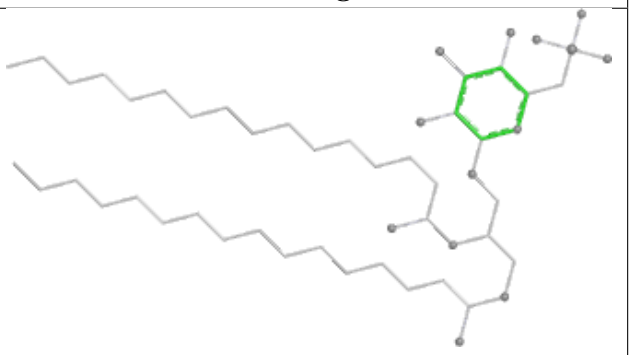
Bond lengths



Bond angles

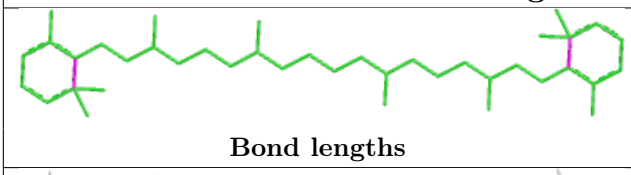


Torsions

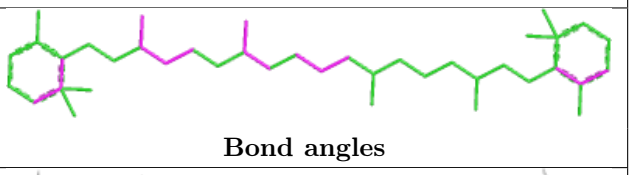


Rings

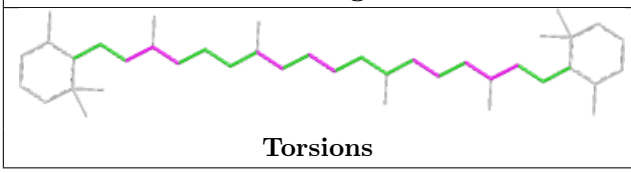
Ligand BCR c 517



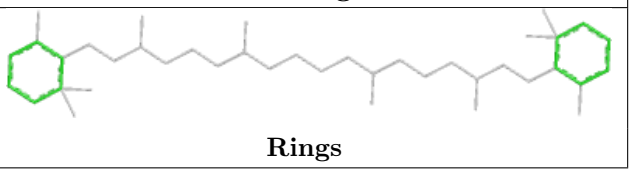
Bond lengths



Bond angles

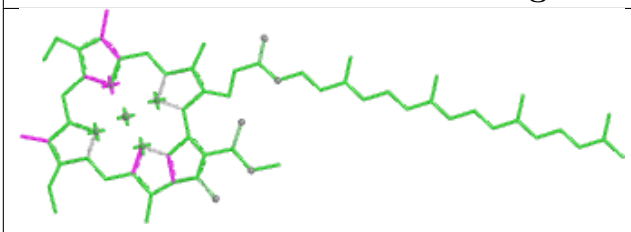


Torsions

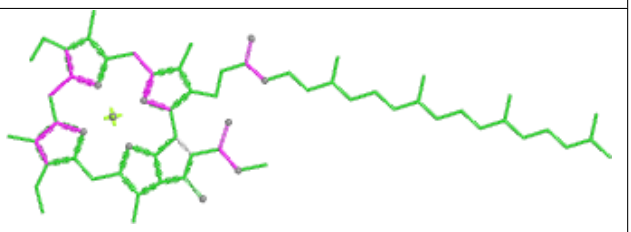


Rings

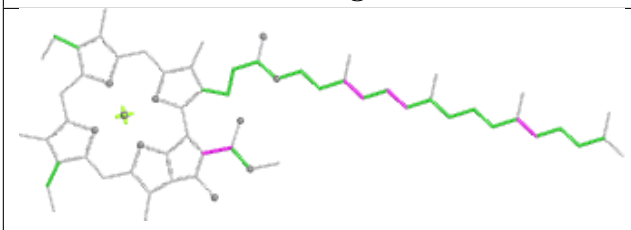
Ligand CLA c 509



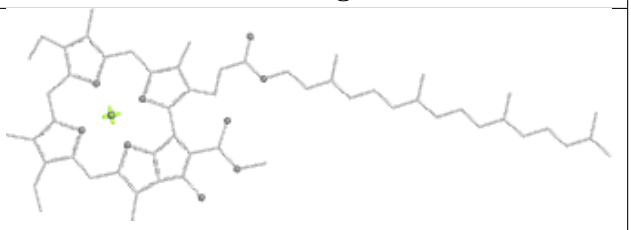
Bond lengths



Bond angles

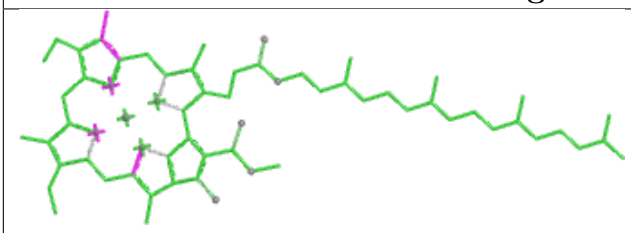


Torsions

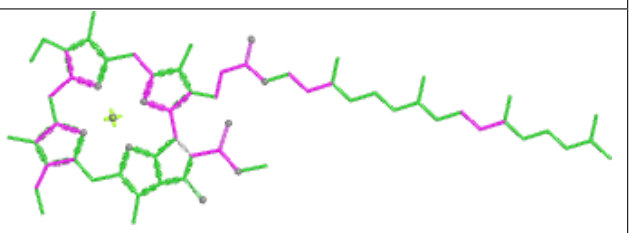


Rings

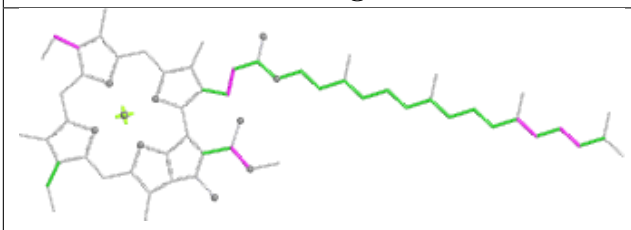
Ligand CLA b 609



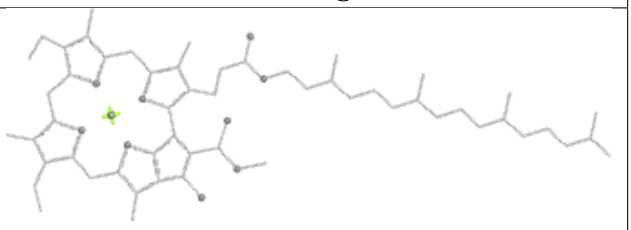
Bond lengths



Bond angles

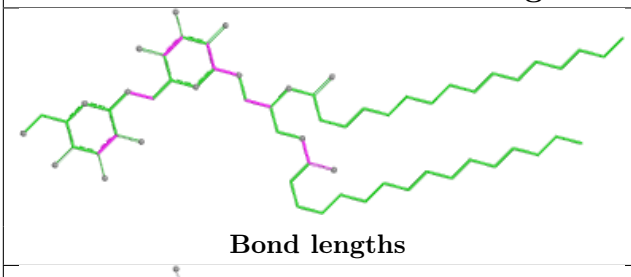


Torsions



Rings

Ligand DGD c 519



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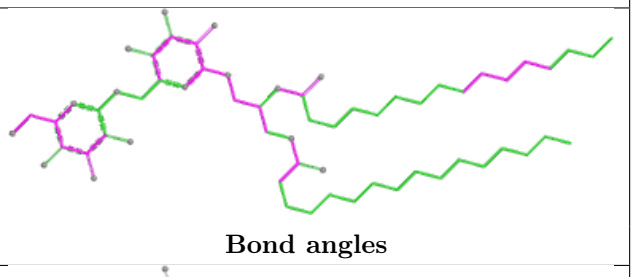
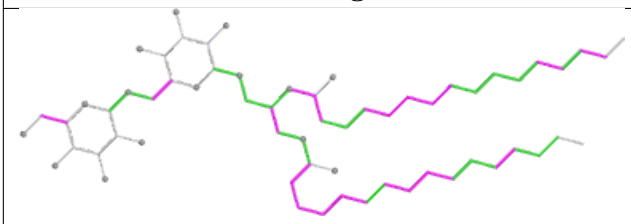
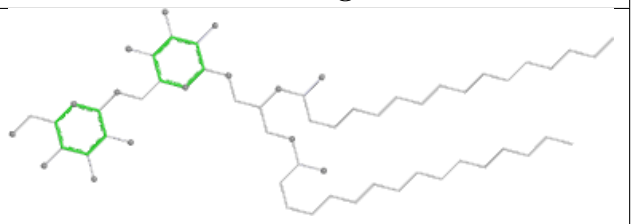


Bond angles

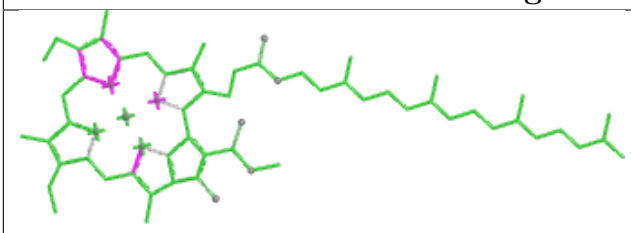


Torsions



Rings

Ligand CLA C 508



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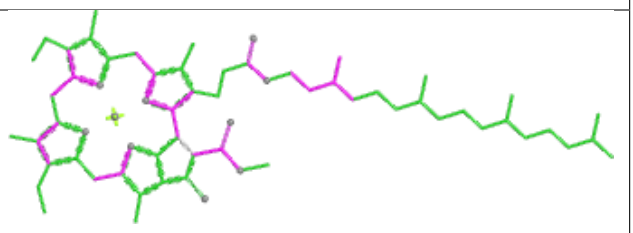
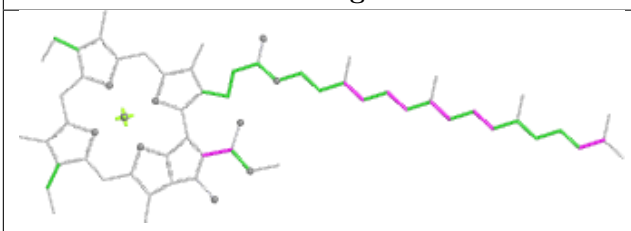
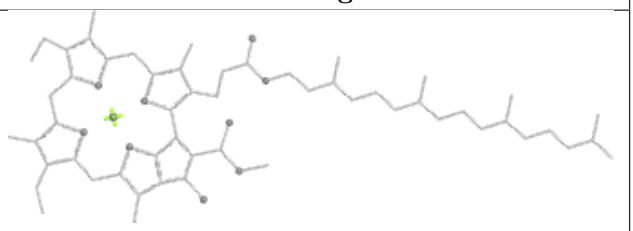


Bond angles

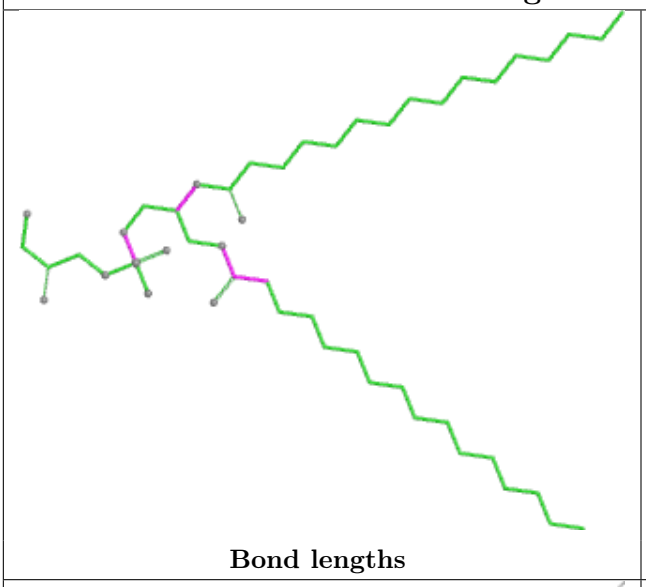


Torsions

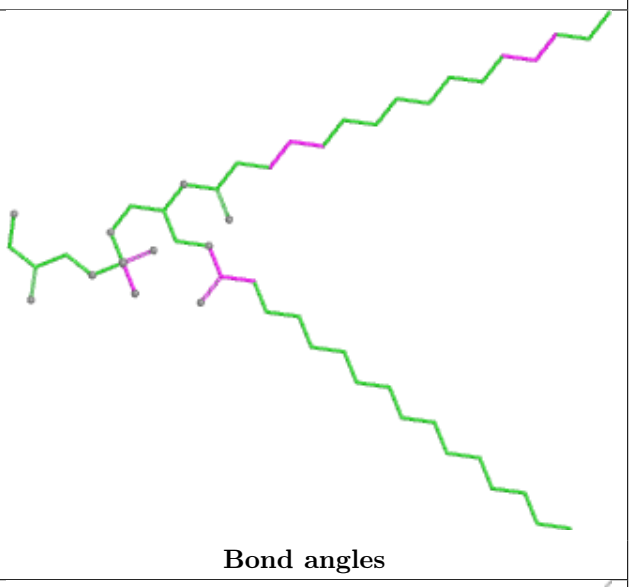


Rings

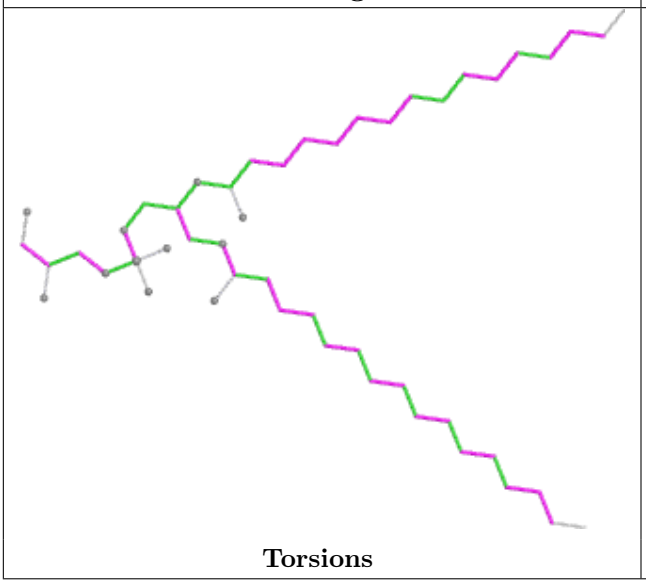
Ligand LHG E 101



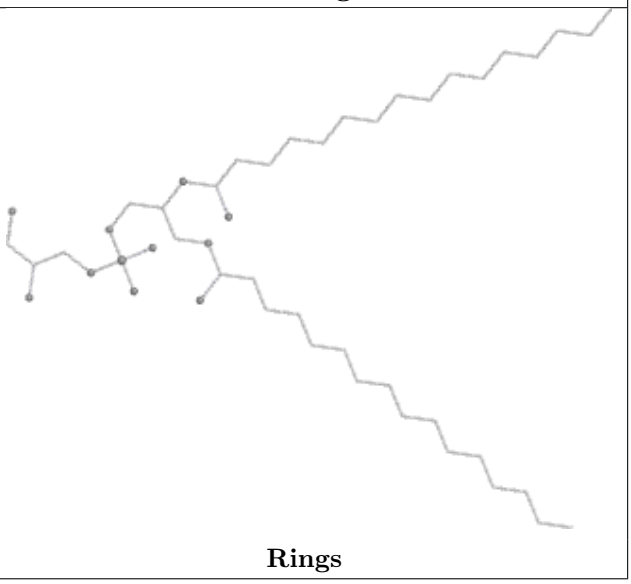
Bond lengths



Bond angles

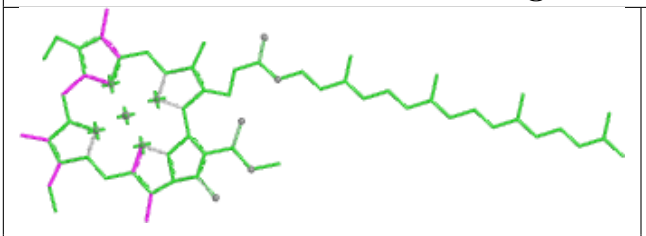


Torsions



Rings

Ligand CLA b 601



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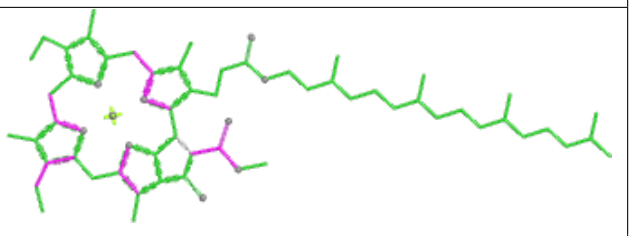
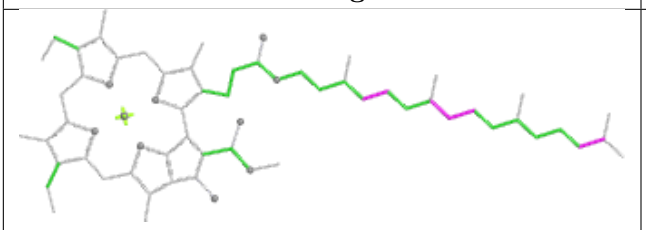


Bond angles



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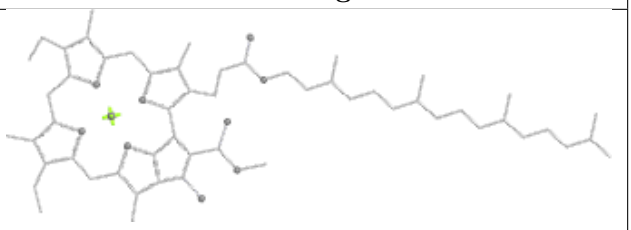
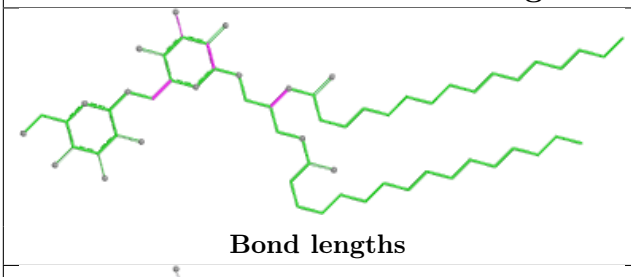


Rings

Ligand DGD c 521



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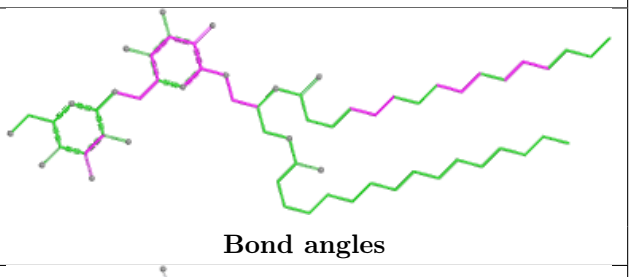
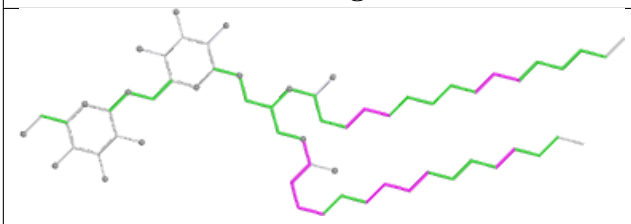
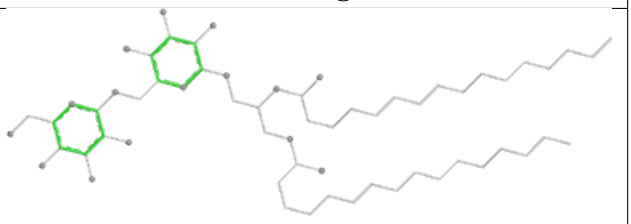


Bond angles

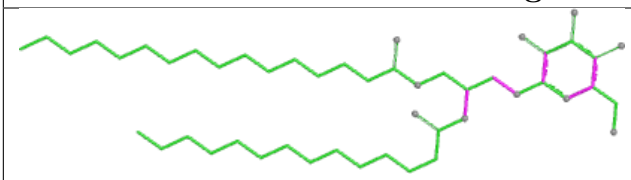


Torsions



Rings

Ligand LMG c 525



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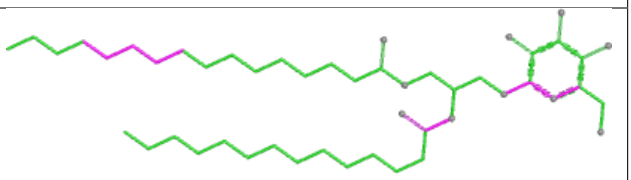
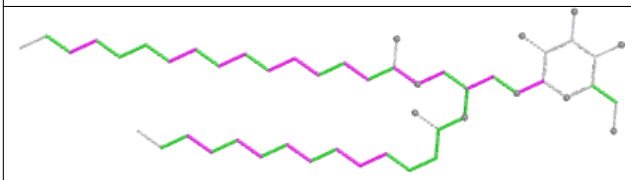
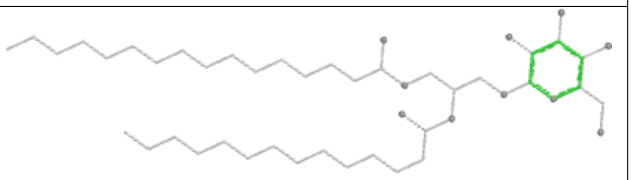


Bond angles

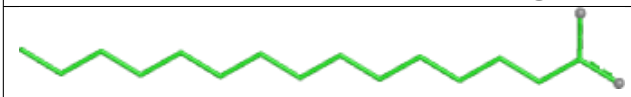


Torsions



Rings

Ligand STE d 410



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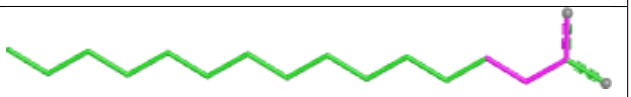
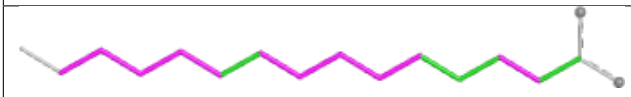
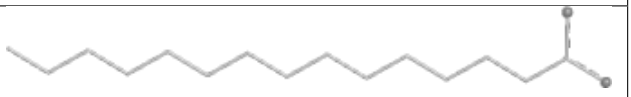


Bond angles

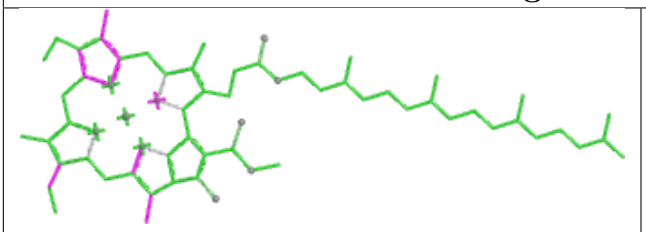


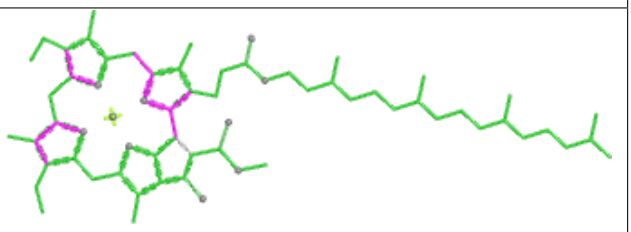
Torsions

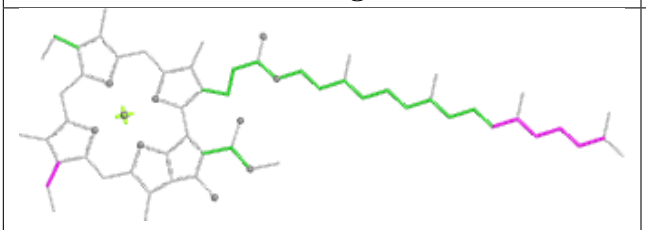


Rings

Ligand CLA A 411


Bond lengths


Bond angles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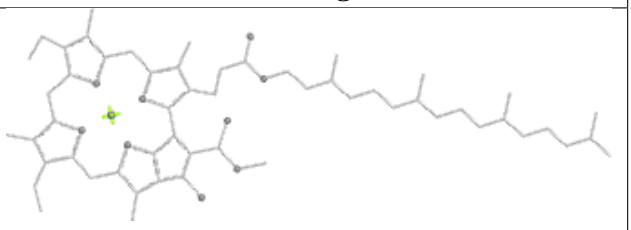
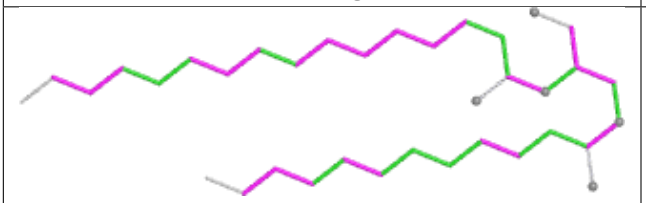

Rings

Ligand SQD a 413

Bond lengths

Bond angles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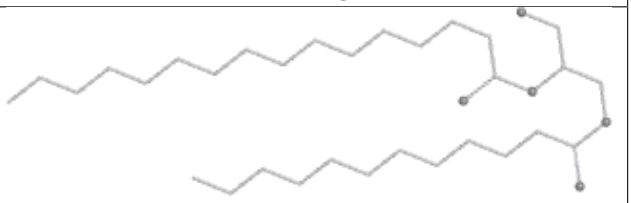
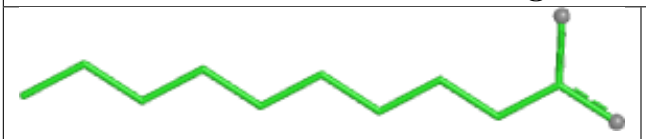
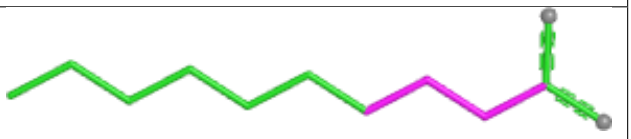
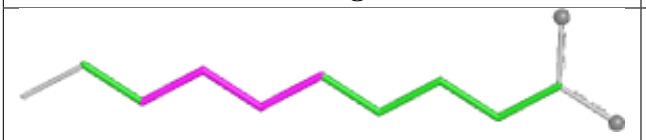
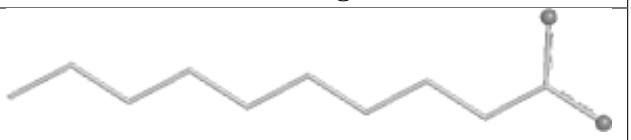

Rings

Ligand STE C 522

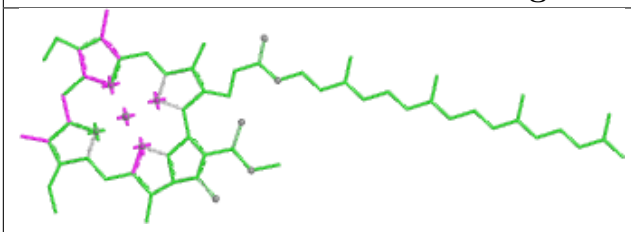

Bond lengths


Bond angles

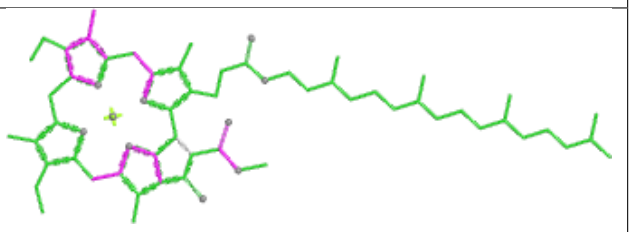

Torsions


Rings

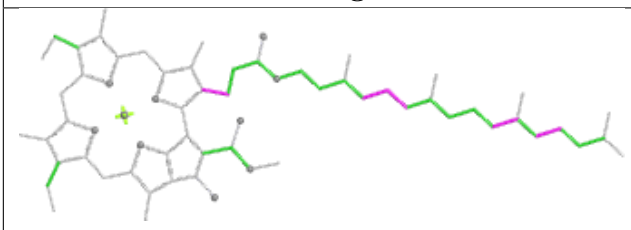
Ligand CLA c 515



Bond lengths



Bond angles



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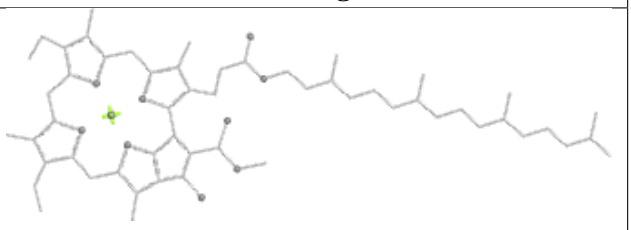
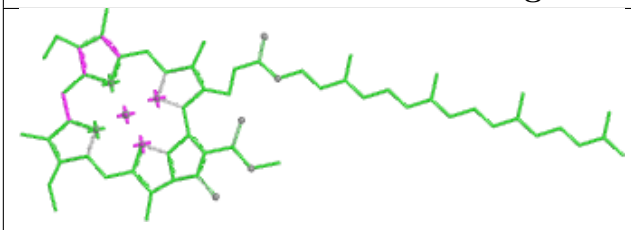
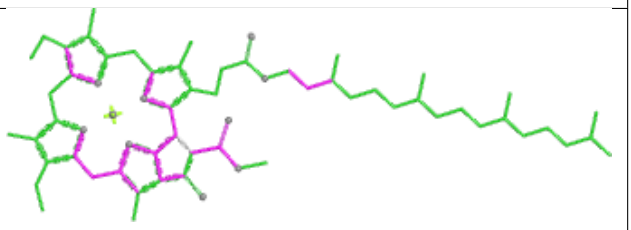


Rings

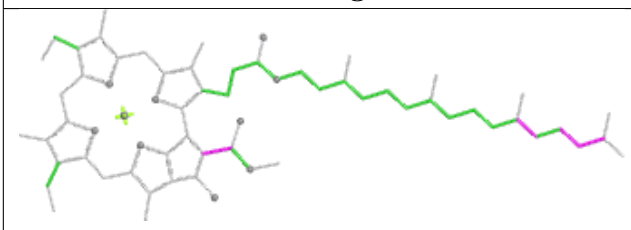
Ligand CLA C 503



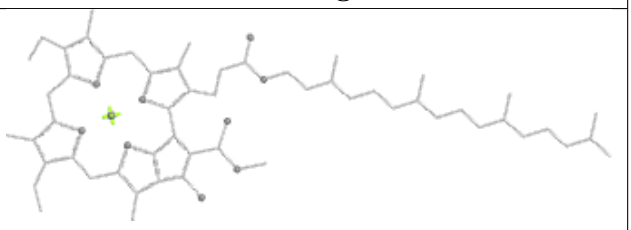
Bond lengths



Bond angles

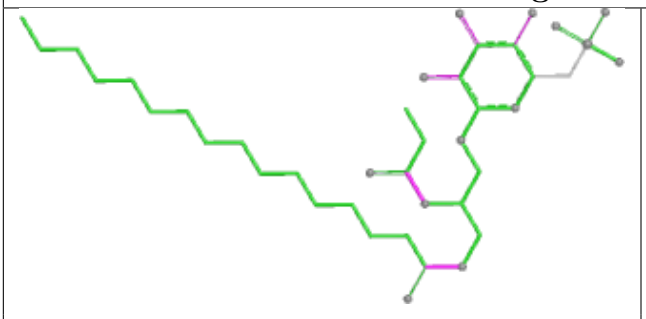


Torsions

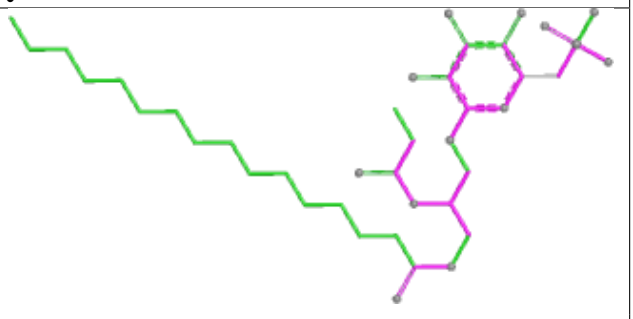


Rings

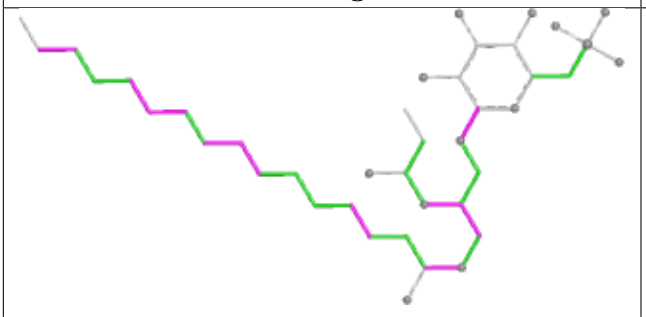
Ligand SQD f 101



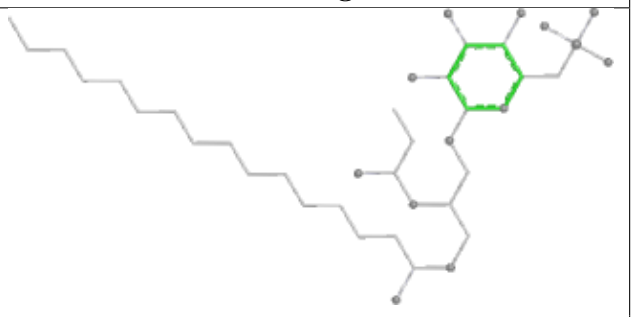
Bond lengths



Bond angles



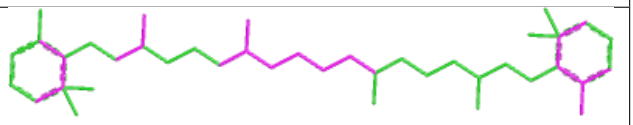
Torsions



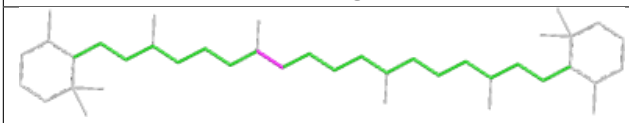
Rings

Ligand BCR H 101

Bond lengths



Bond angles



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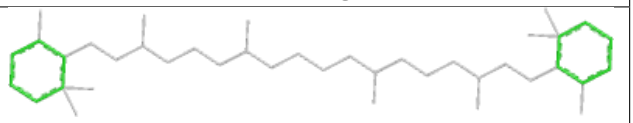
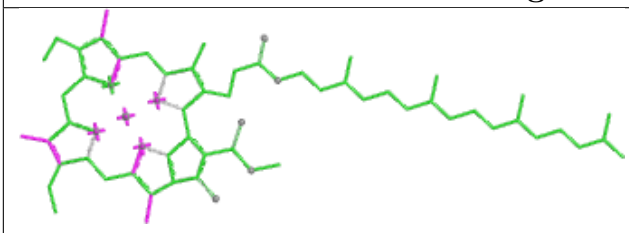


Rings

Ligand CLA b 612



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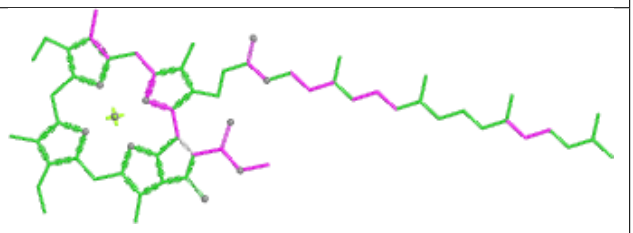
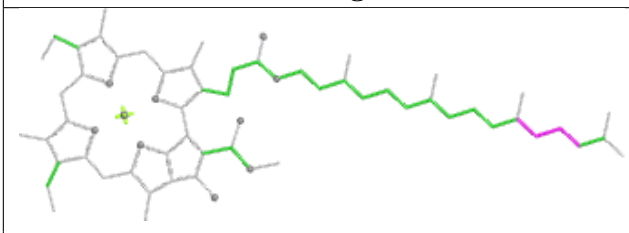


Bond angles



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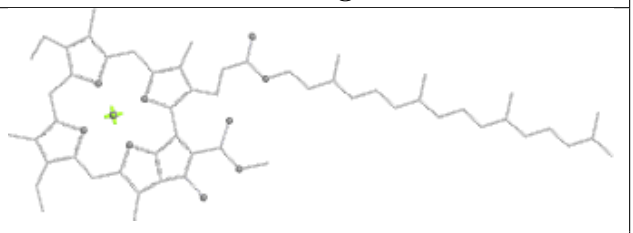
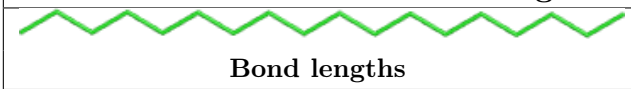


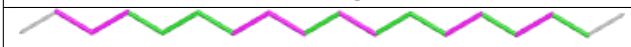
Rings

Ligand STE l 102



Bond lengths

Bond angles



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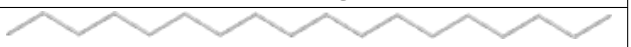
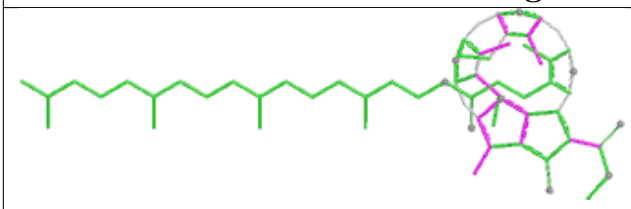


Rings

Ligand PHO d 401



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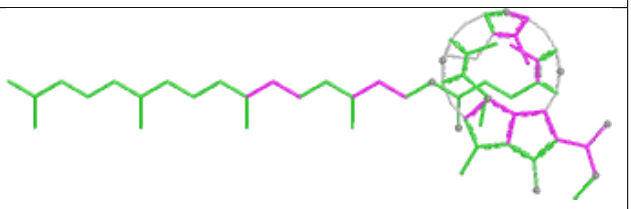
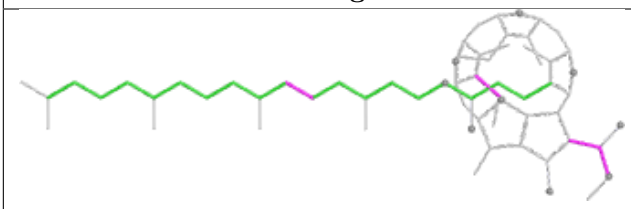


Bond angles



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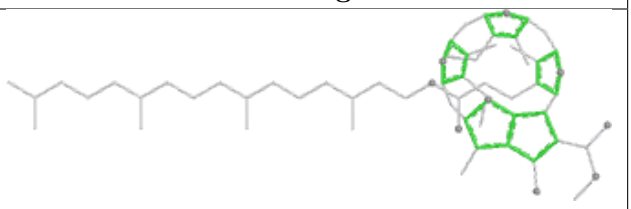
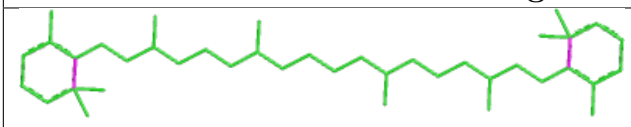


Rings

Ligand BCR c 516



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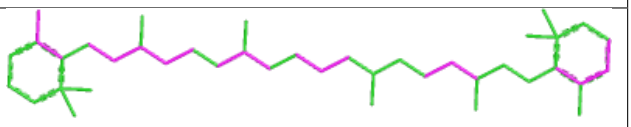
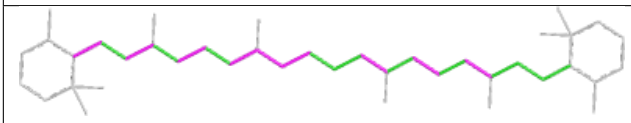


Bond angles



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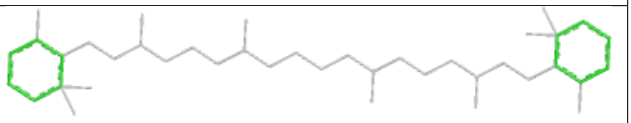
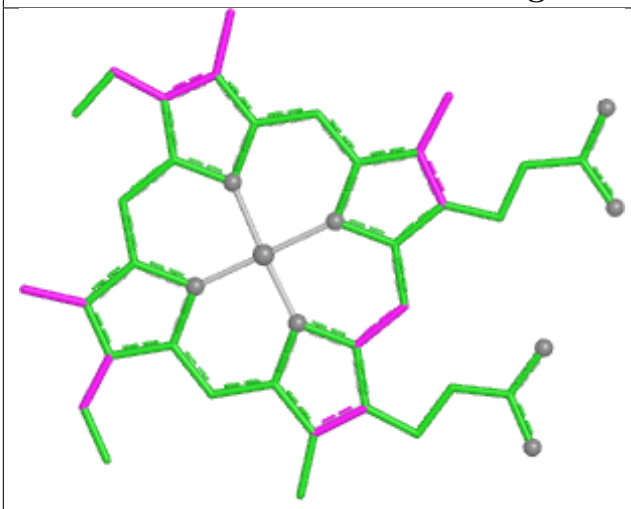
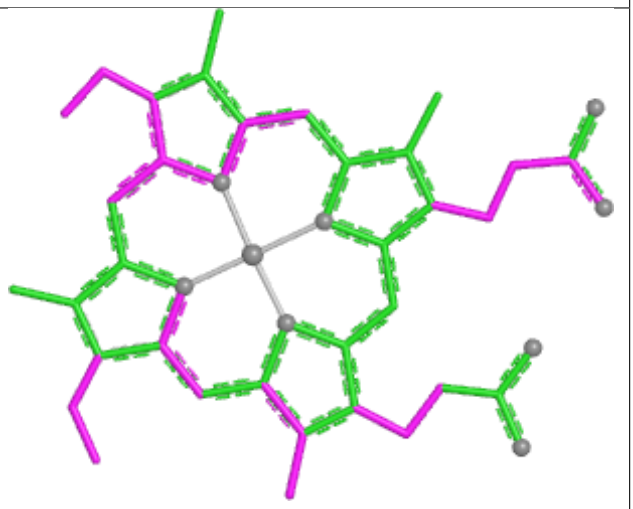


Rings

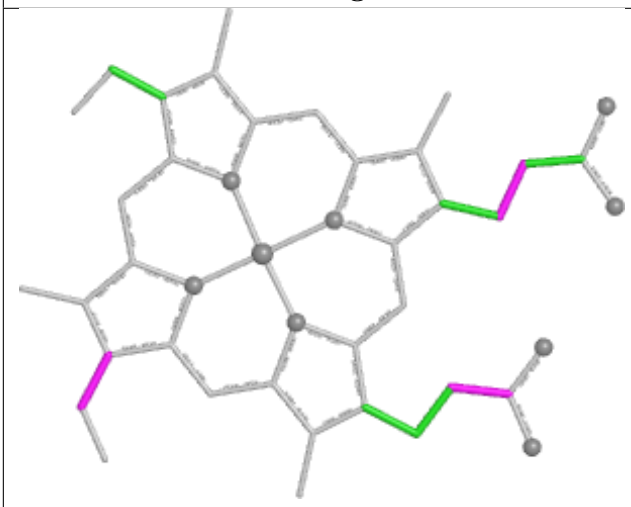
Ligand HEC e 101



Bond lengths



Bond angles



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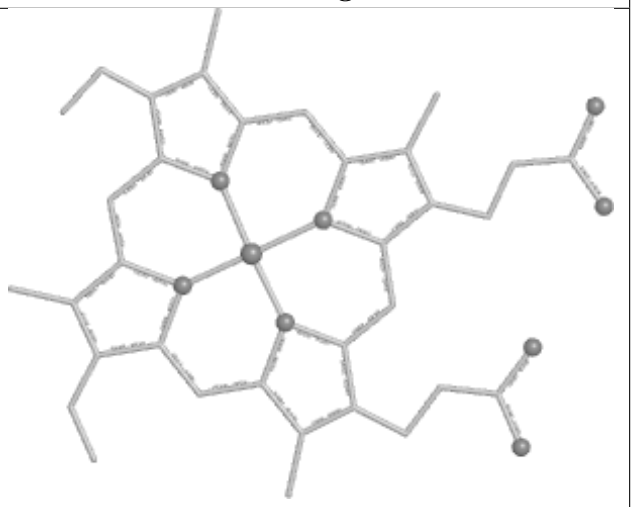
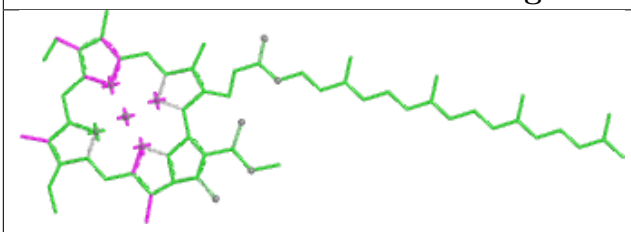


Rings

Ligand CLA B 610



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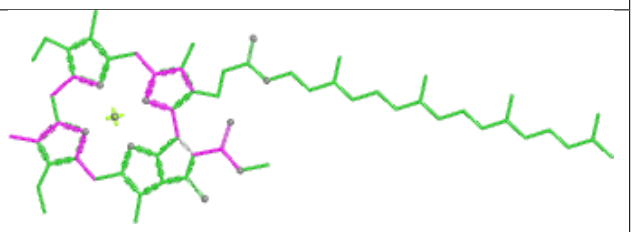
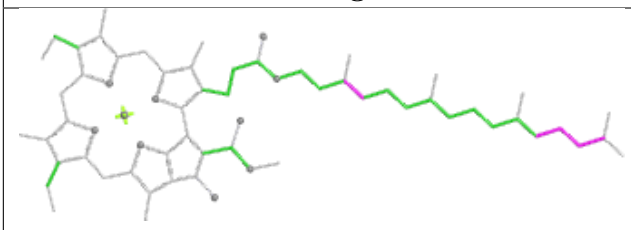


Bond angles



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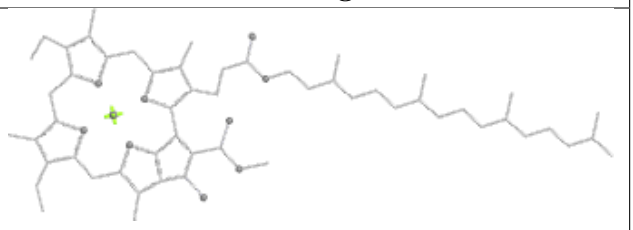
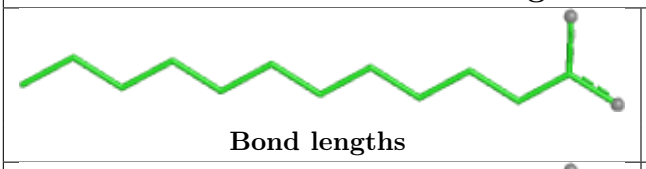


Rings

Ligand STE B 624



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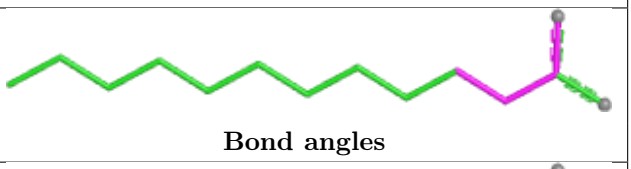
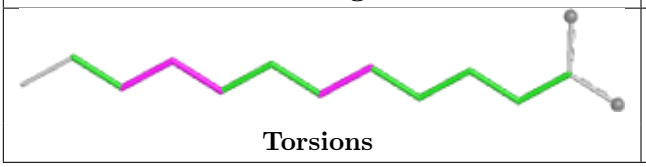


Bond angles



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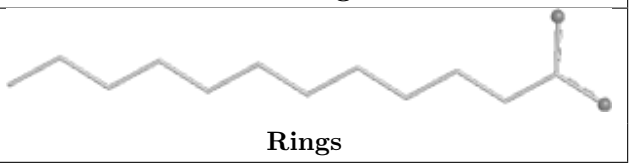
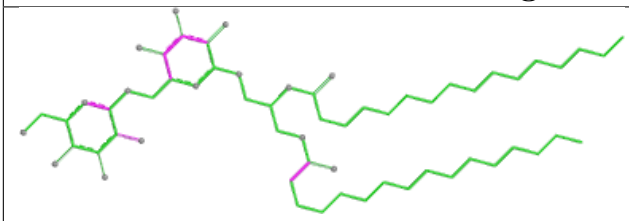
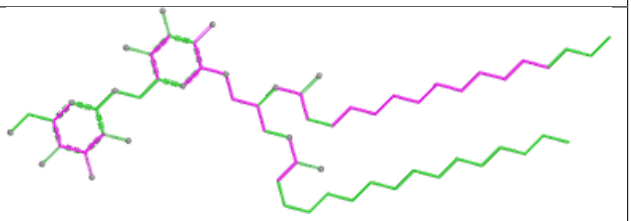


Rings

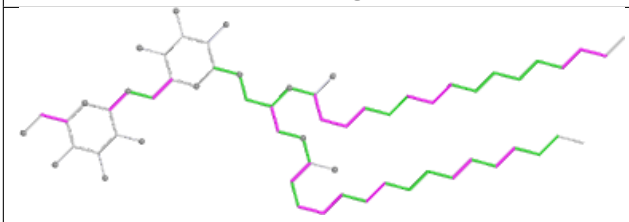
Ligand DGD C 516



Bond lengths



Bond angles



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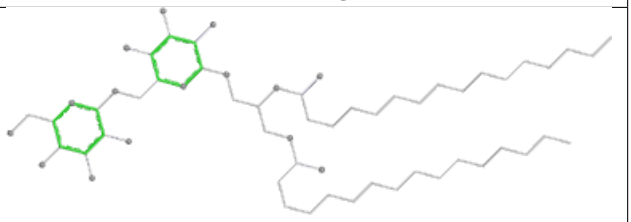
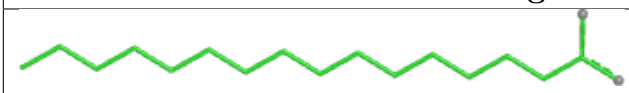


Rings

Ligand STE B 626



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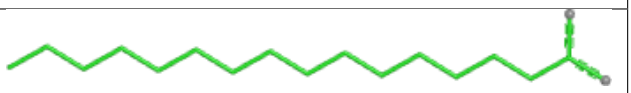
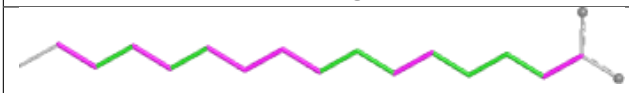


Bond angles



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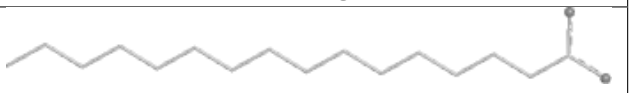
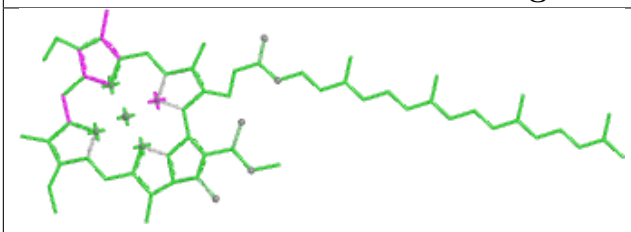


Rings

Ligand CLA c 512



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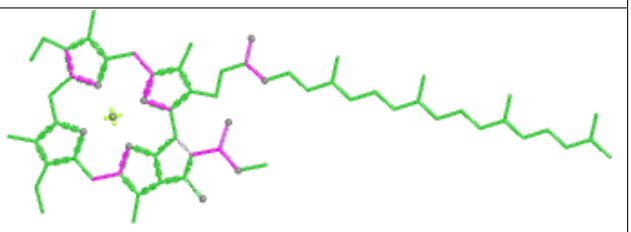
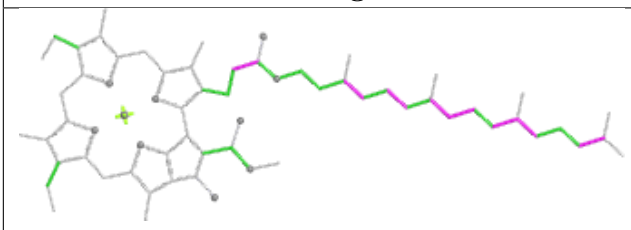


Bond angles



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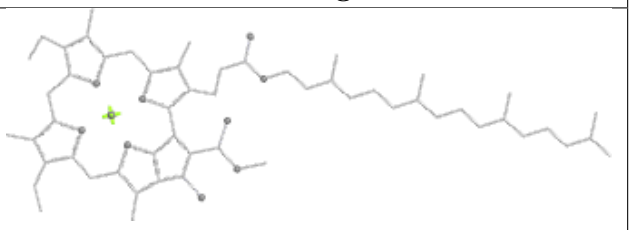
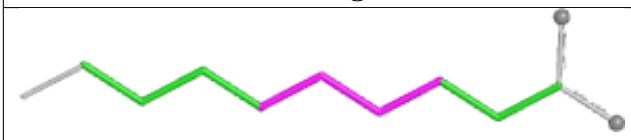


Rings

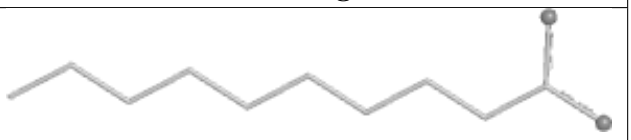
Ligand STE C 520

Bond lengths

Bond angles

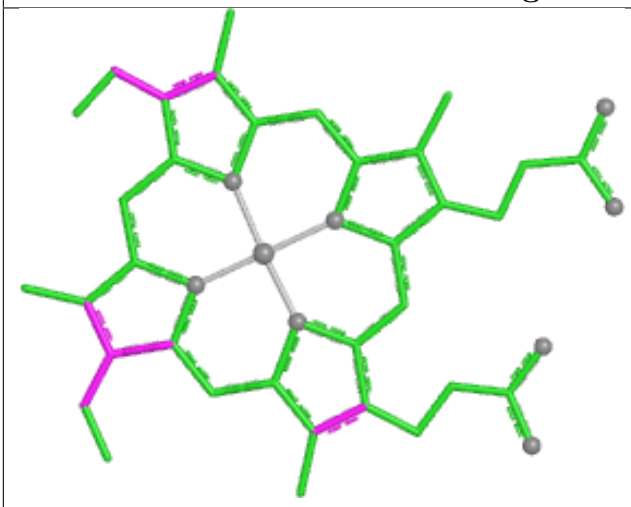


Torsions

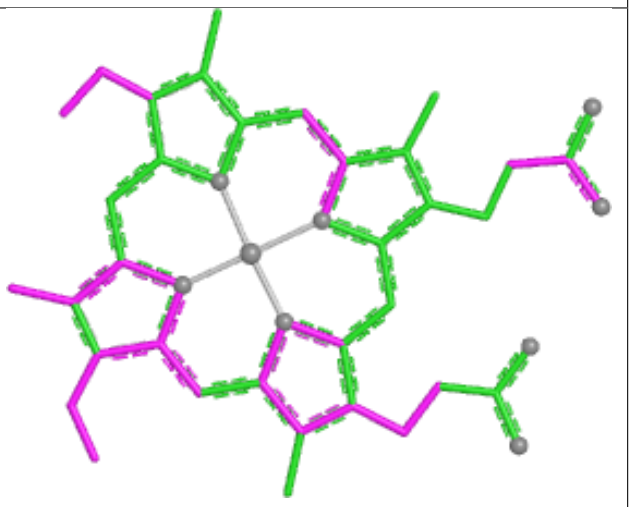


Rings

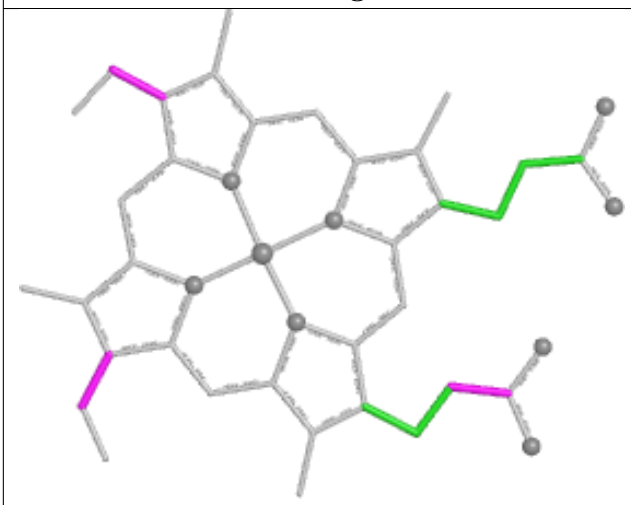
Ligand HEC V 201



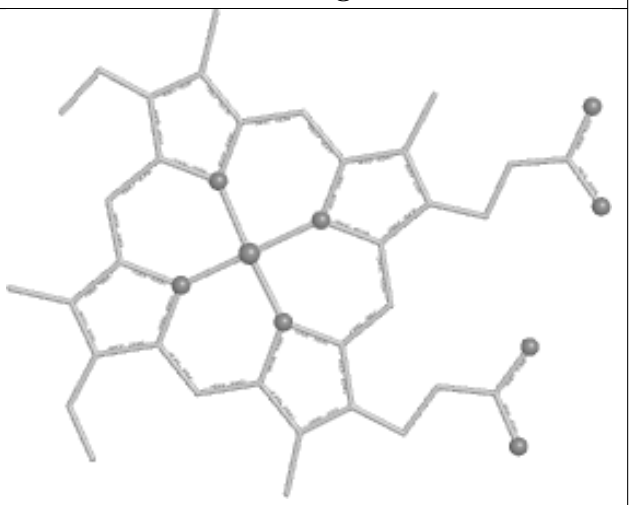
Bond lengths



Bond angles

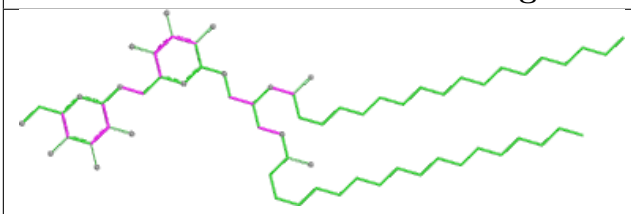


Torsions



Rings

Ligand DGD A 415



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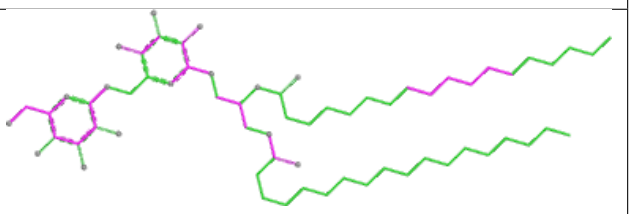
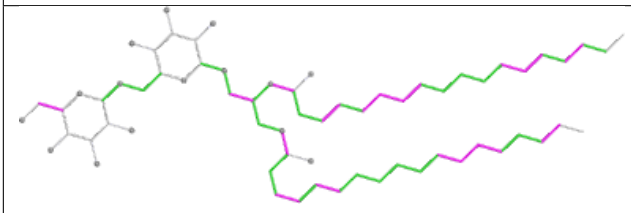


Bond angles



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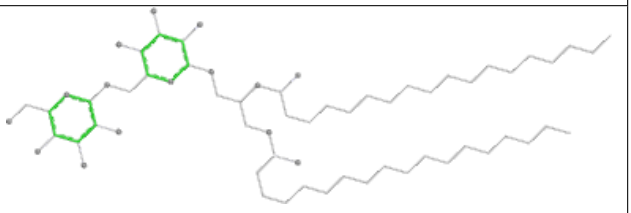
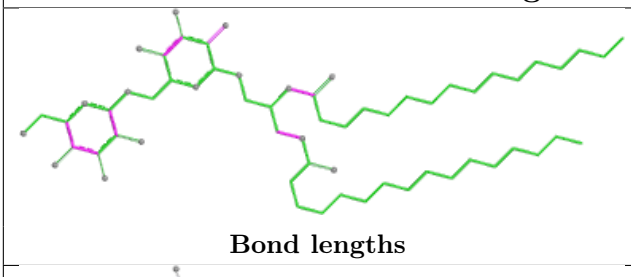
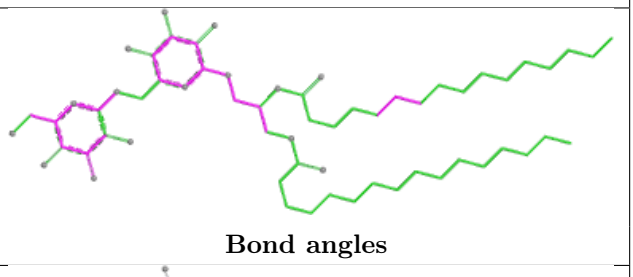


Rings

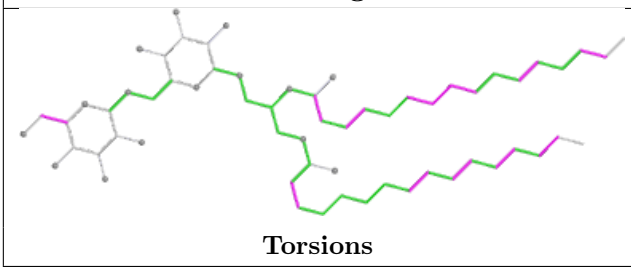
Ligand DGD h 102



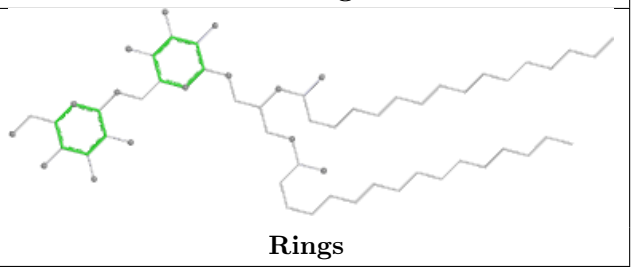
Bond lengths



Bond angles

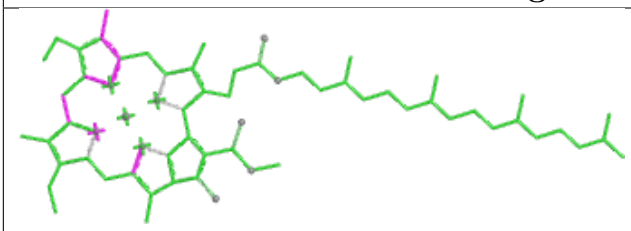


Torsions



Rings

Ligand CLA a 403



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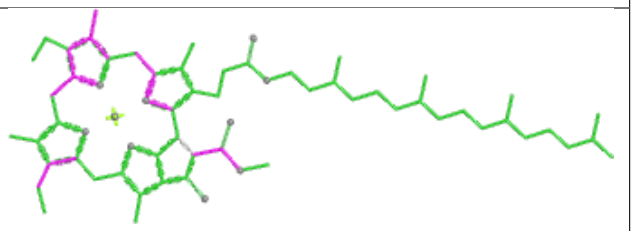
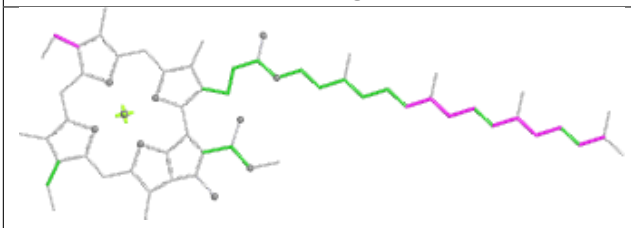
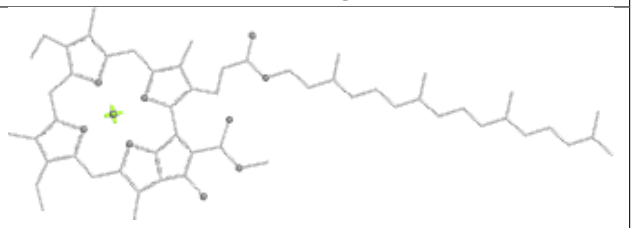


Bond angles

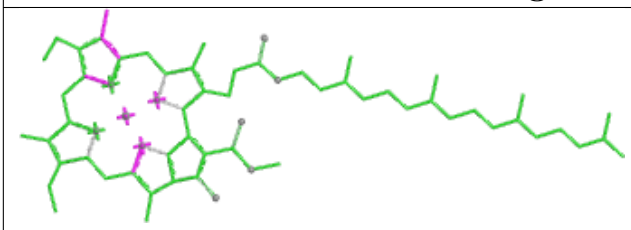


Torsions



Rings

Ligand CLA a 411



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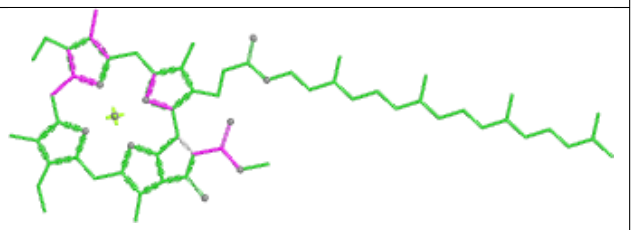
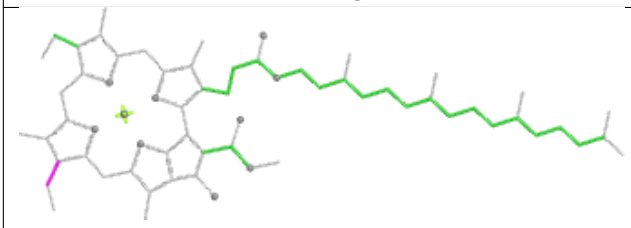


Bond angles



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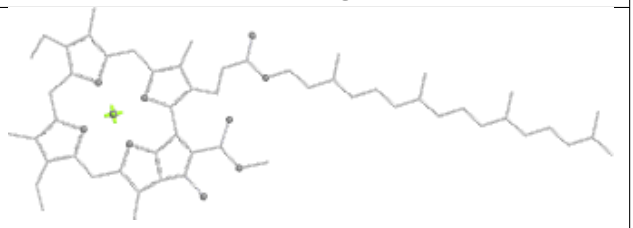
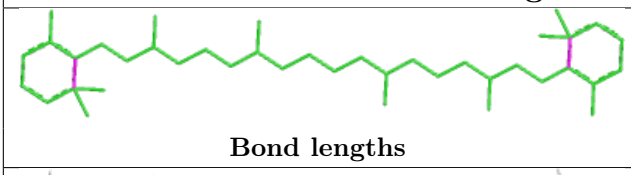


Rings

Ligand BCR d 404



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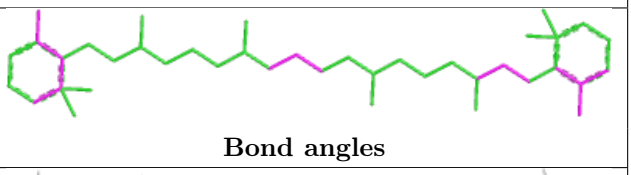
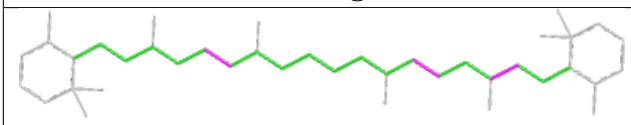


Bond angles



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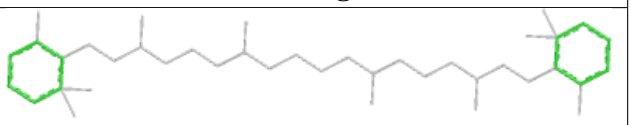
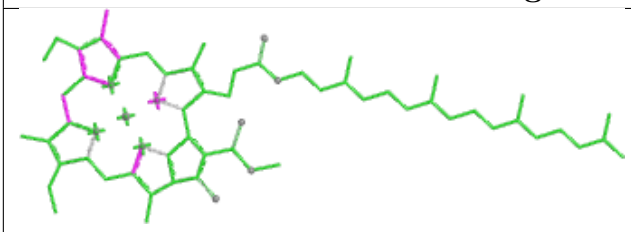


Rings

Ligand CLA C 514



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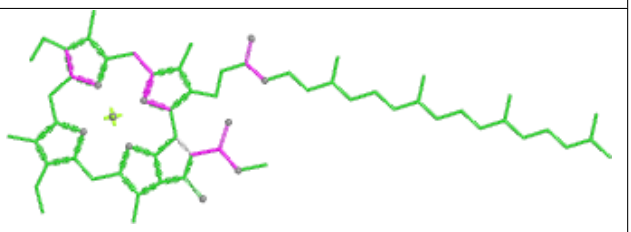
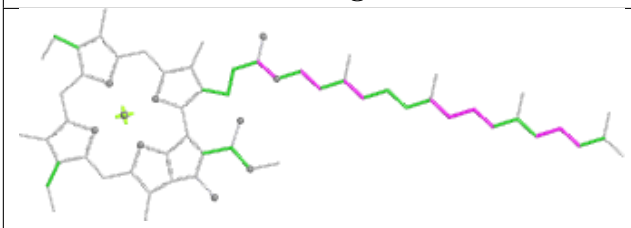


Bond angles



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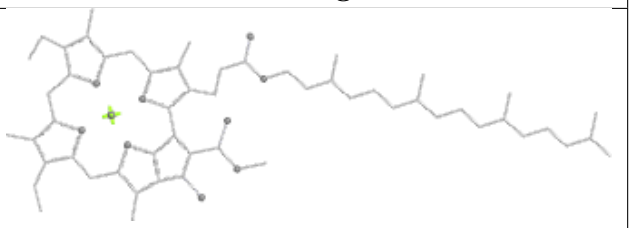
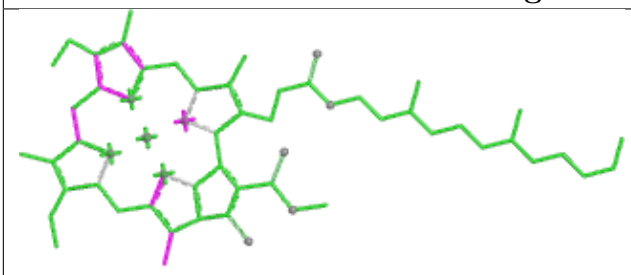


Rings

Ligand CLA C 505



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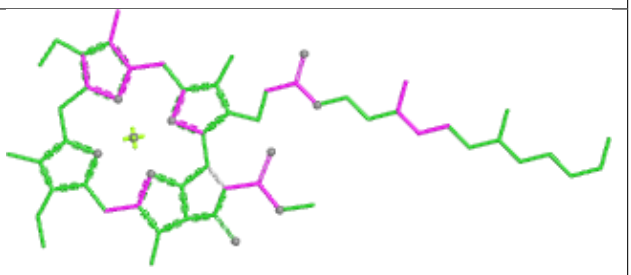
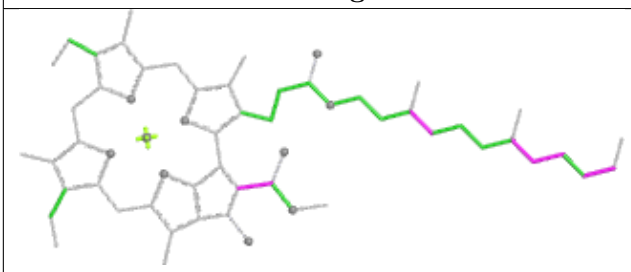


Bond angles



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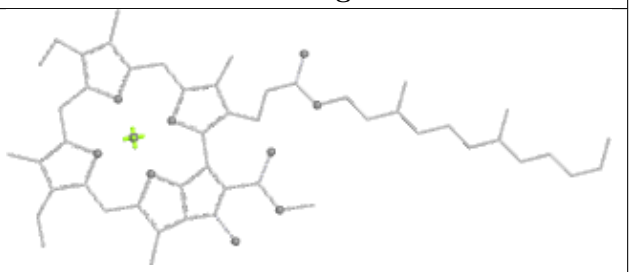
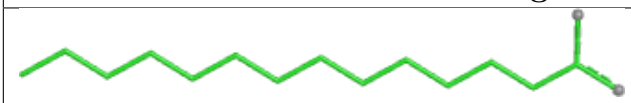
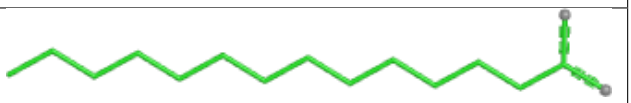
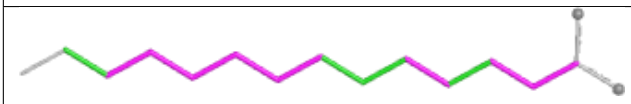
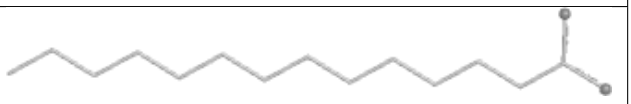
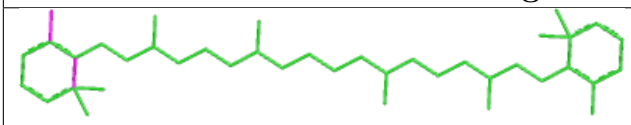
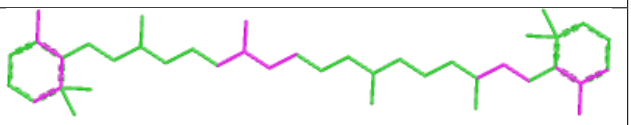
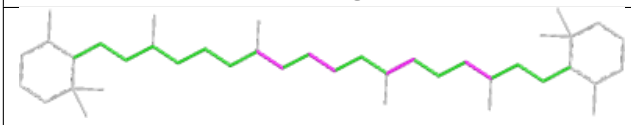
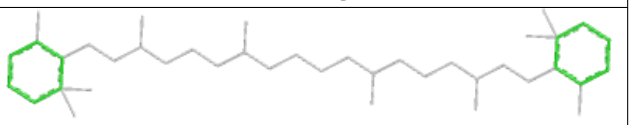
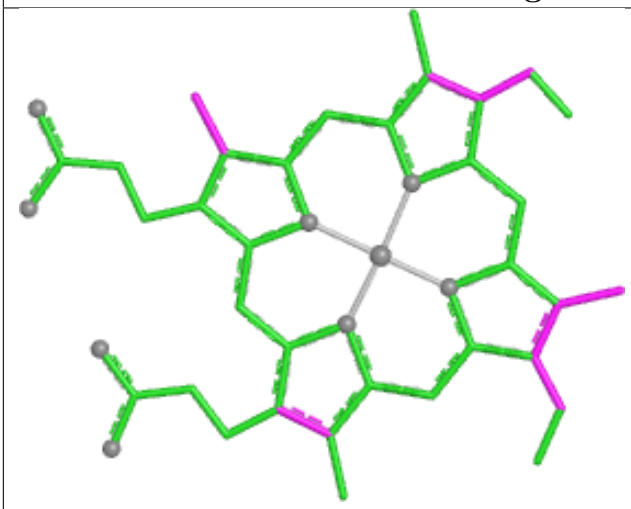


Rings

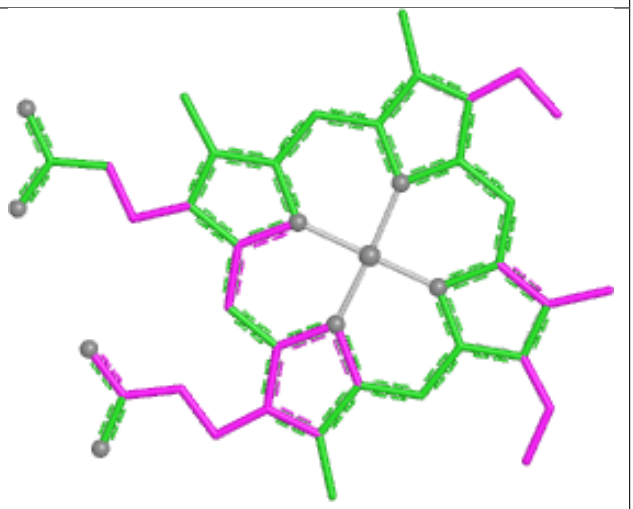
Ligand STE b 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

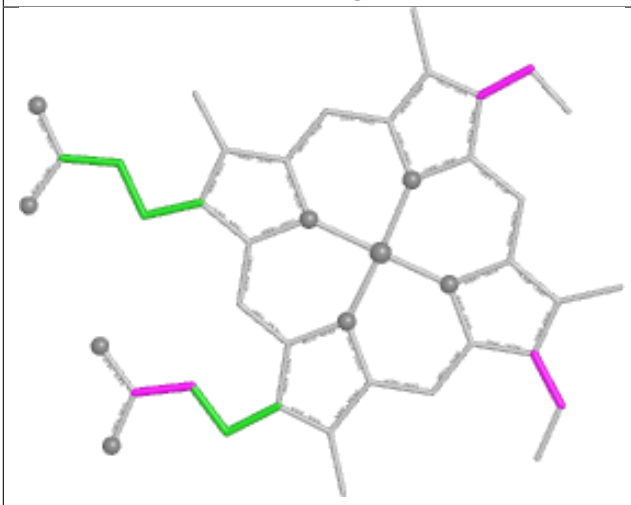
Ligand HEC F 101



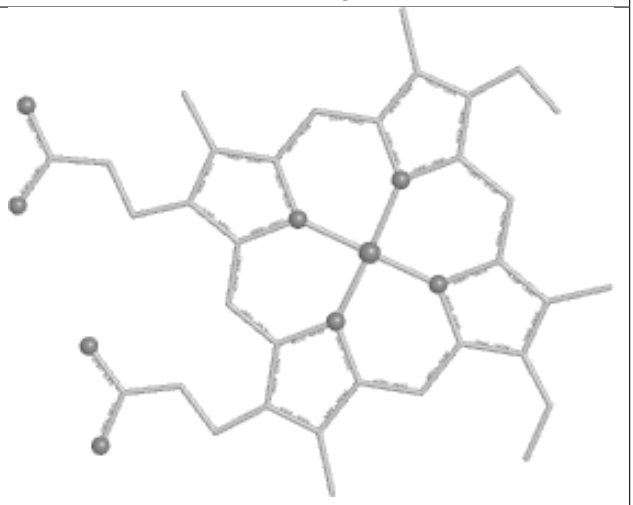
Bond lengths



Bond angles

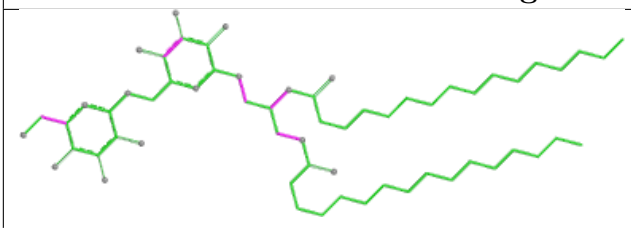


Torsions



Rings

Ligand DGD C 518



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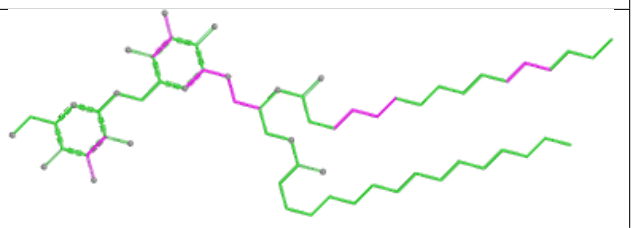
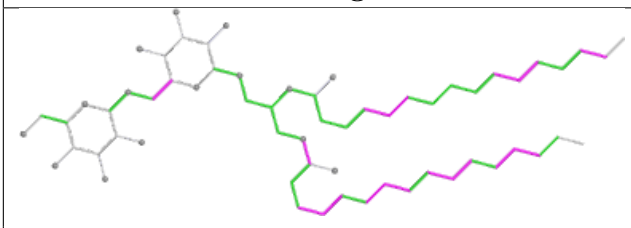


Bond angles



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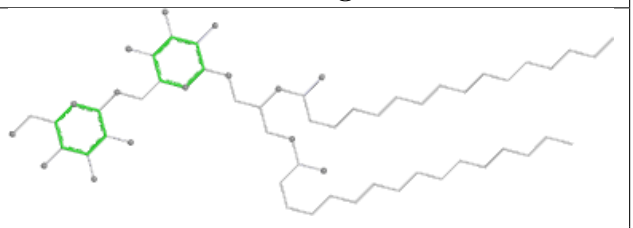
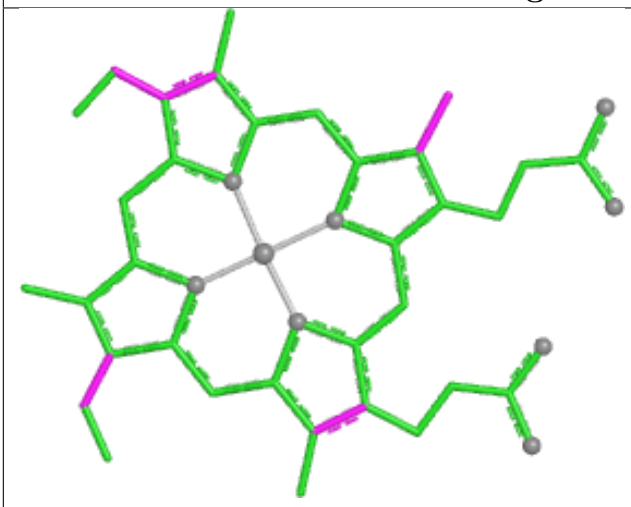


Rings

Ligand HEC v 201



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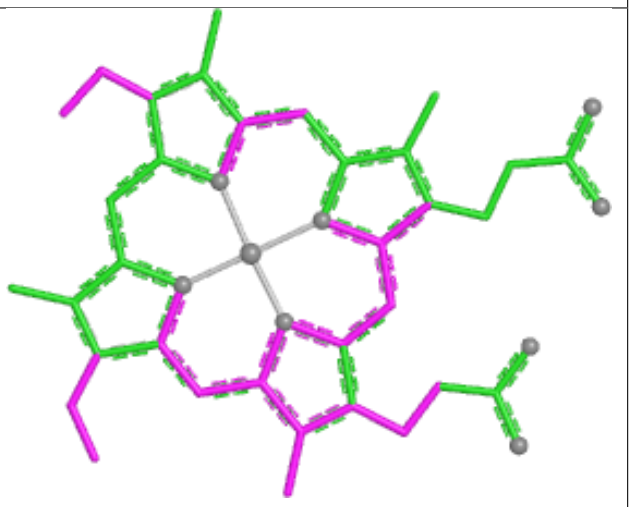
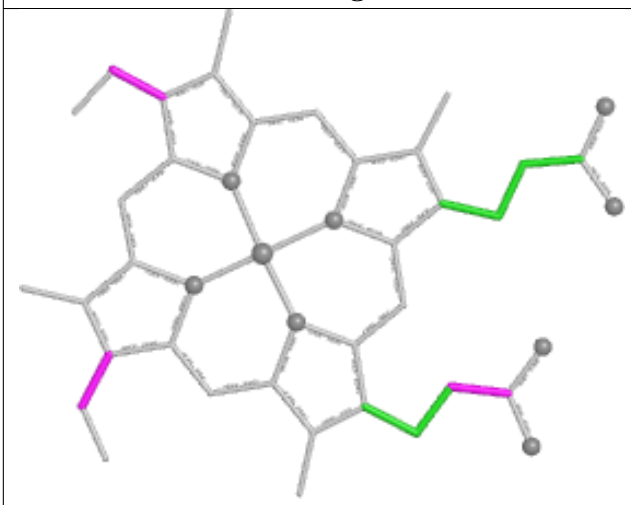


Bond angles



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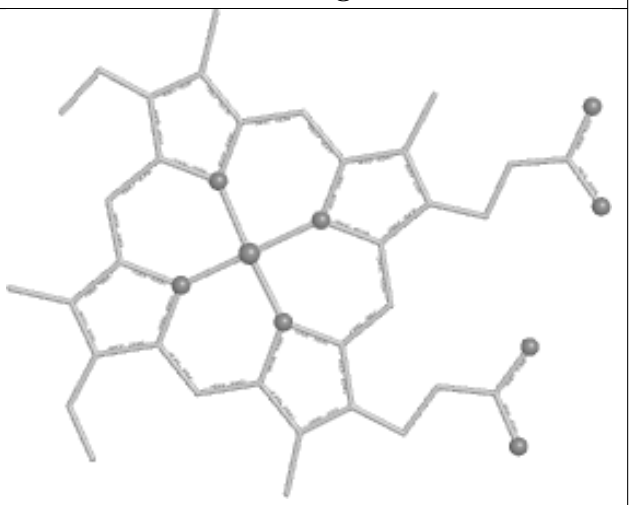
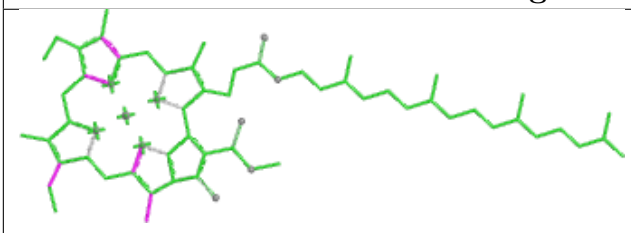
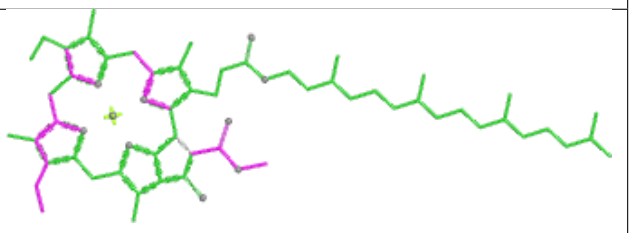


Rings

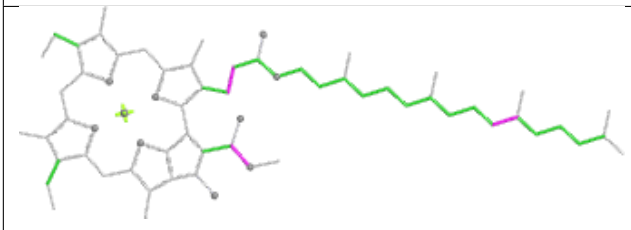
Ligand CLA c 503



Bond lengths



Bond angles



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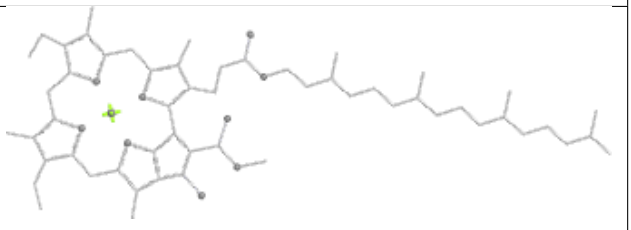
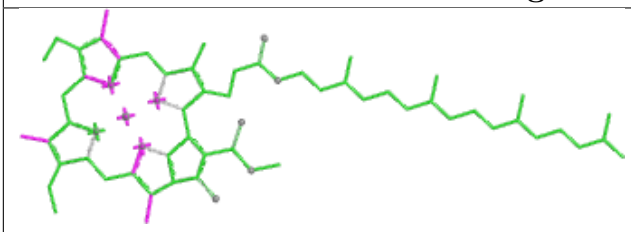
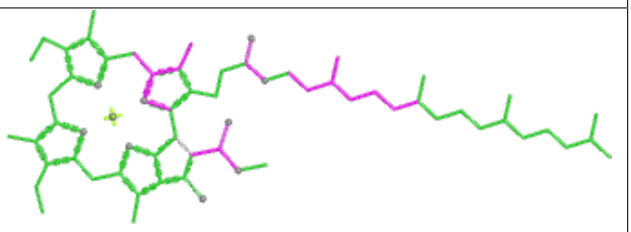


Rings

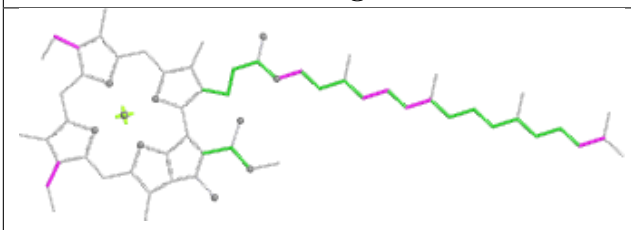
Ligand CLA d 402



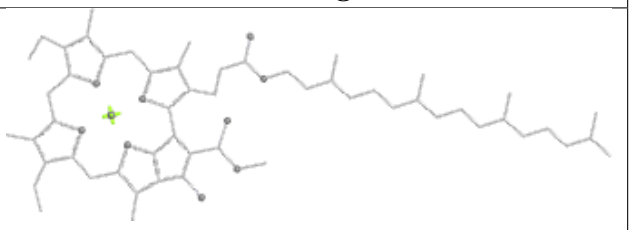
Bond lengths



Bond angles



Torsions



Rings

Ligand STE h 103

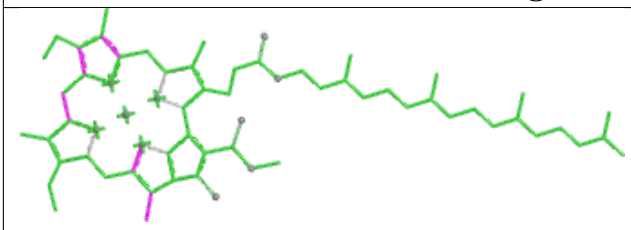
Bond lengths

Bond angles

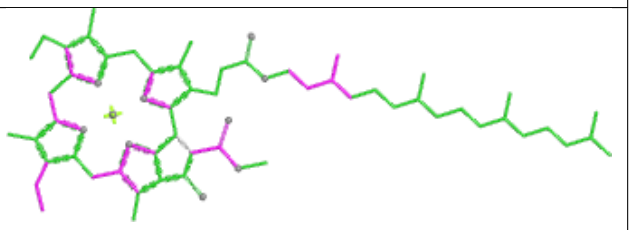
Torsions

Rings

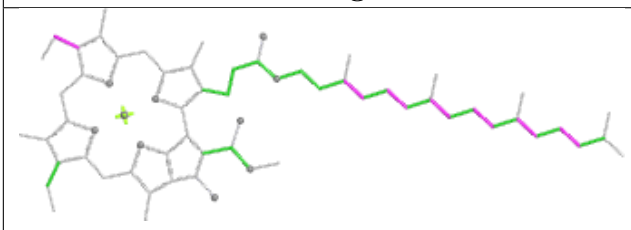
Ligand CLA b 604



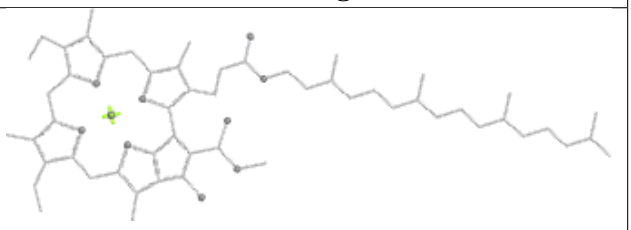
Bond lengths



Bond angles

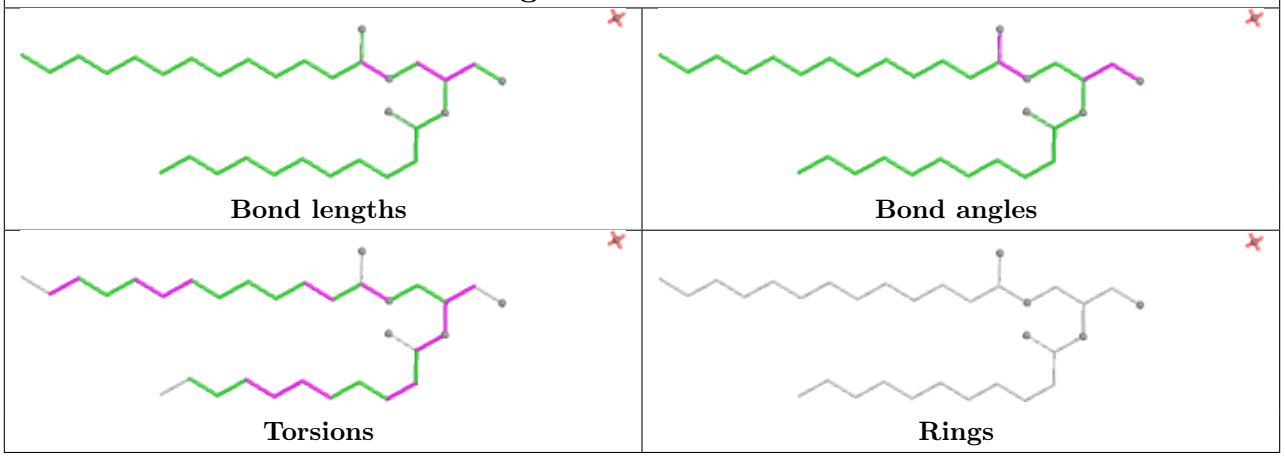


Torsions

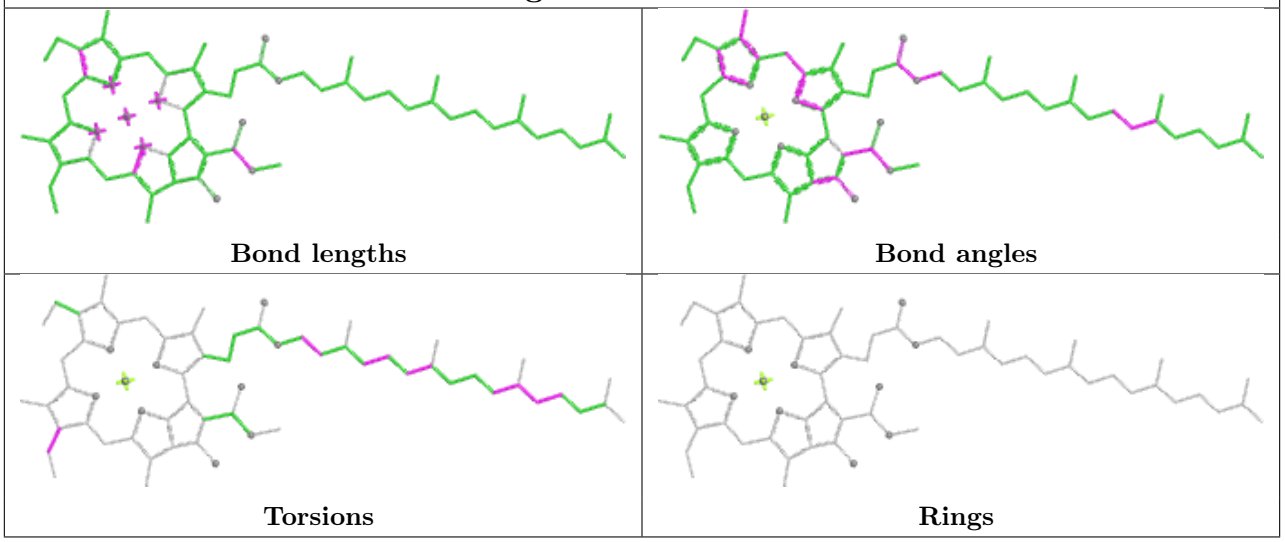


Rings

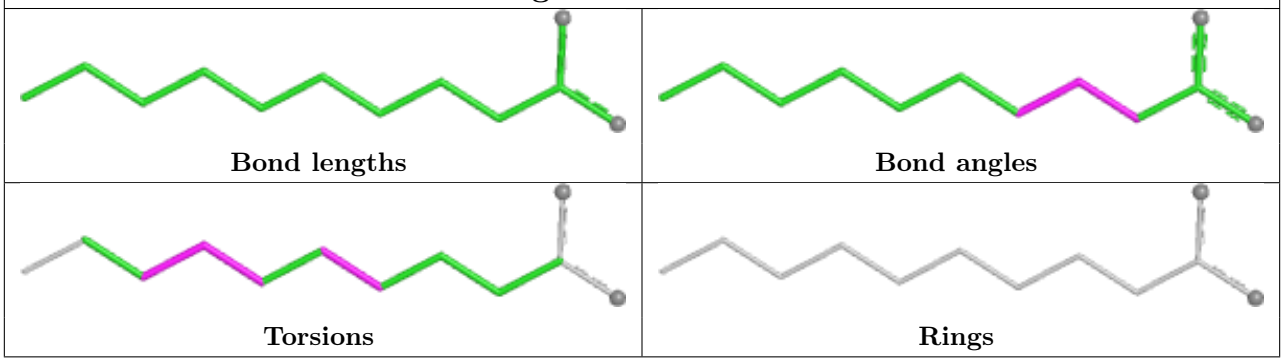
Ligand LMG D 410



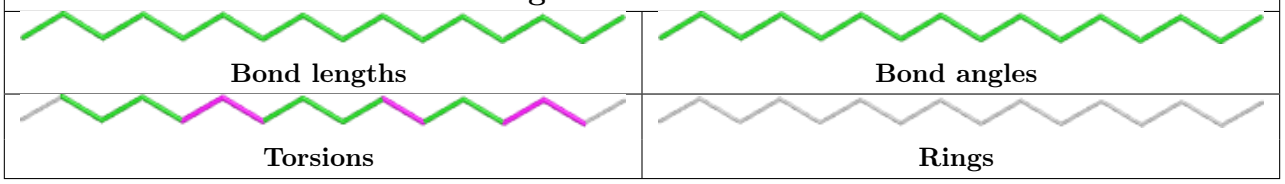
Ligand CLA B 605



Ligand STE J 101



Ligand STE C 521



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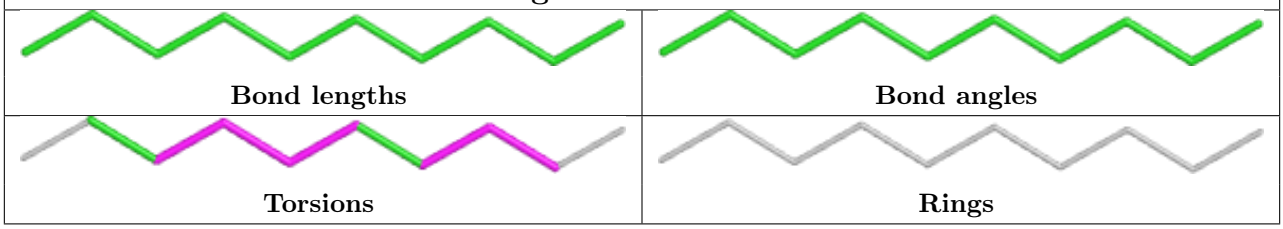

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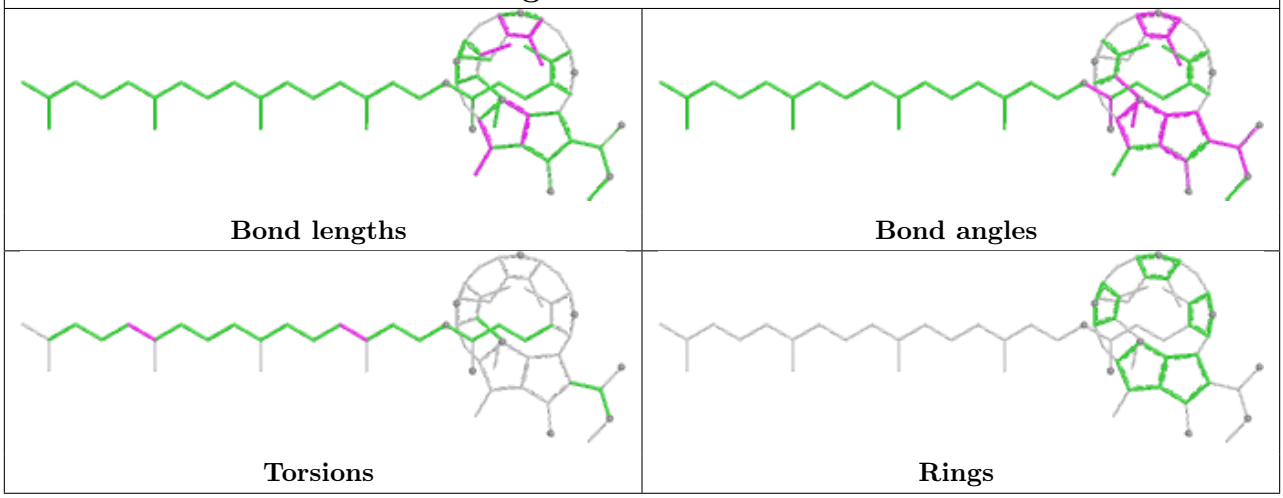
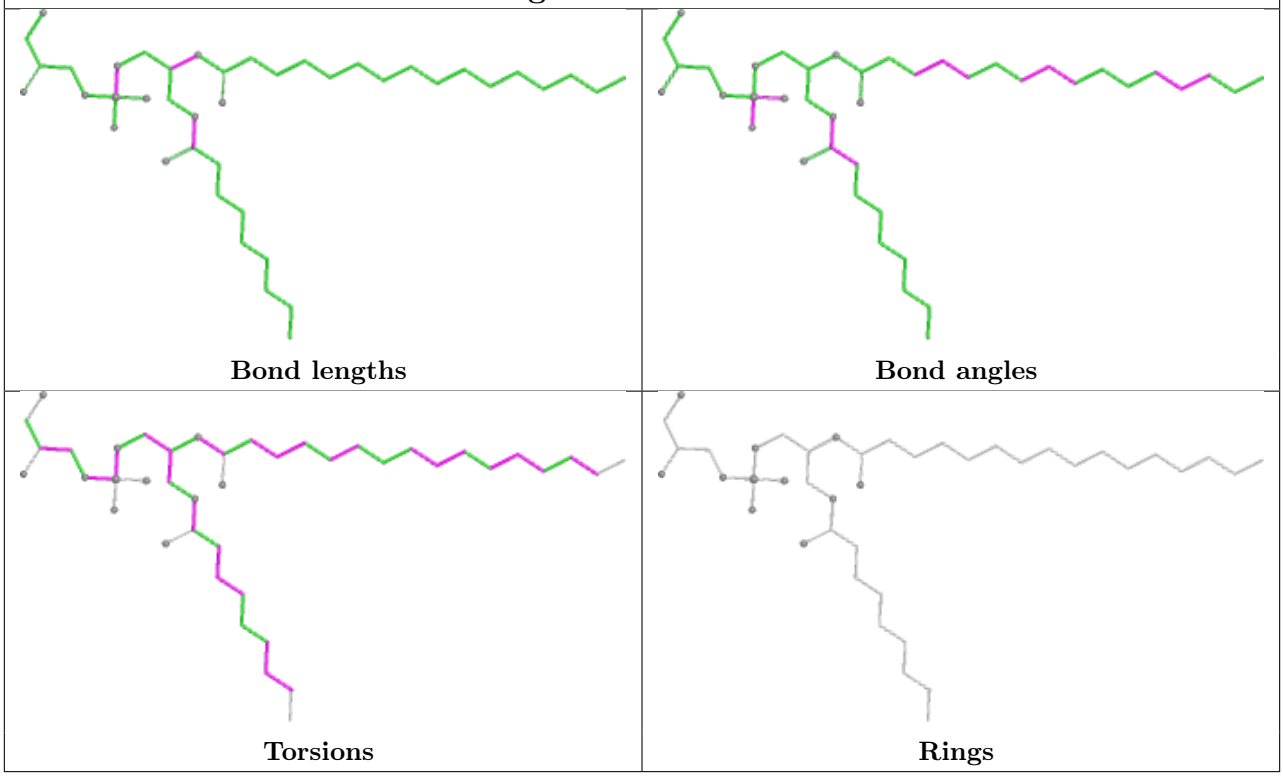
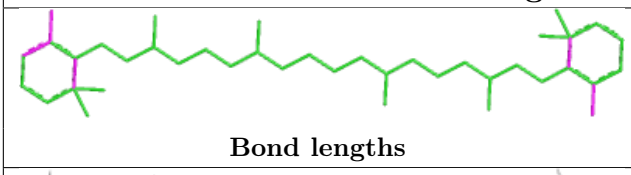
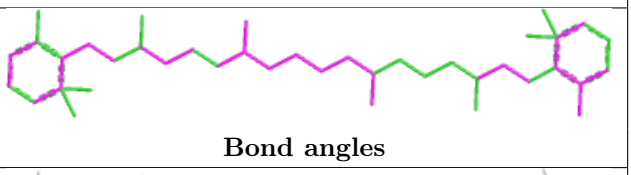


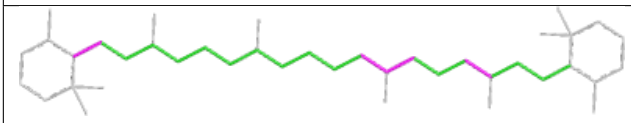
Ligand LHG e 102

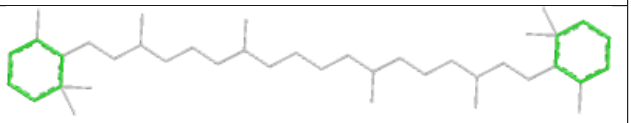


Ligand BCR b 616


Bond lengths


Bond angles

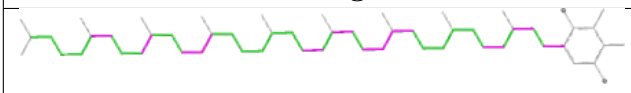

Torsions


Rings

Ligand PL9 a 410

Bond lengths

Bond angles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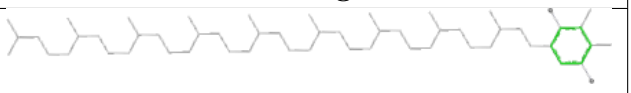
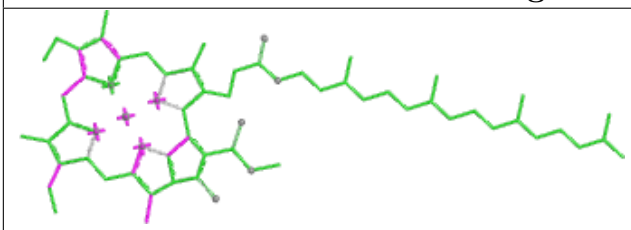
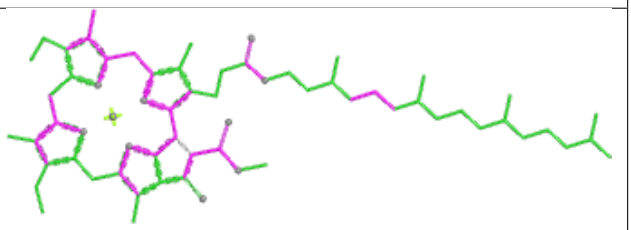
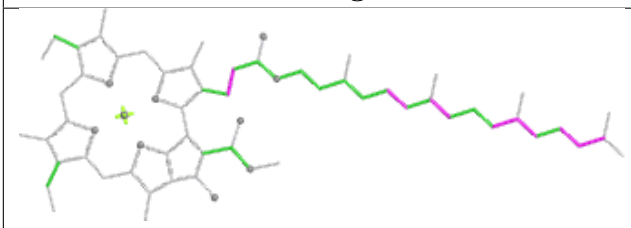

Rings

Ligand CLA b 605


Bond lengths


Bond angles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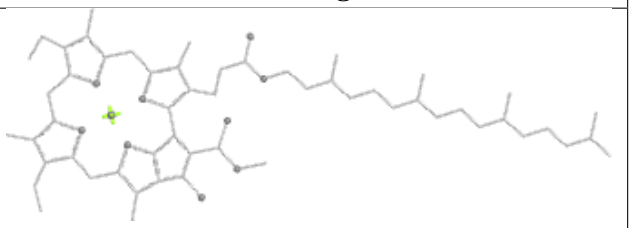
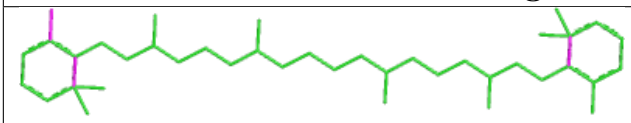

Rings

Ligand BCR Z 101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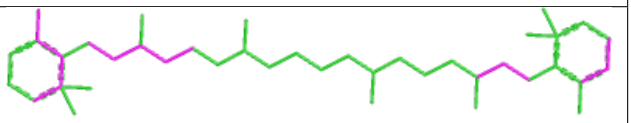
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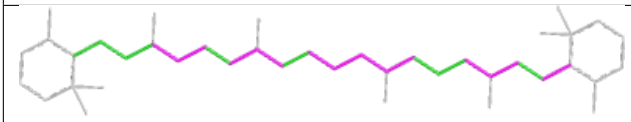
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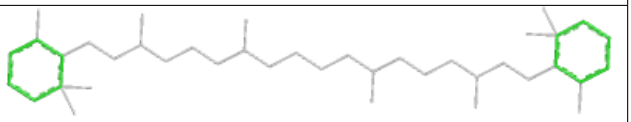
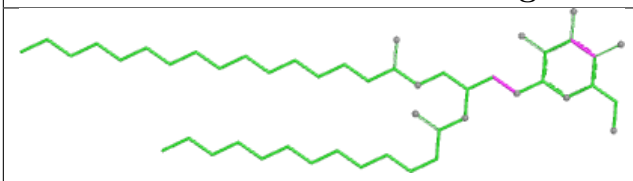

Rings

Ligand LMG A 412



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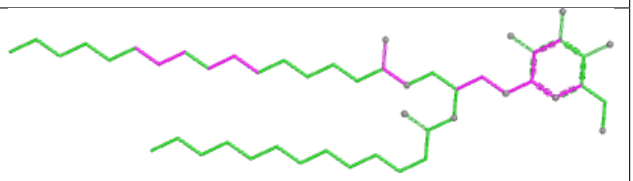
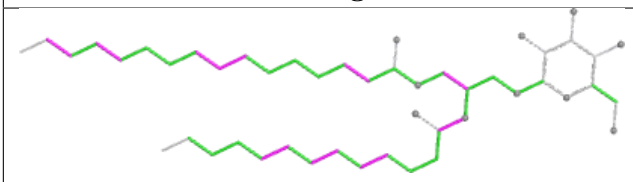


Bond angles



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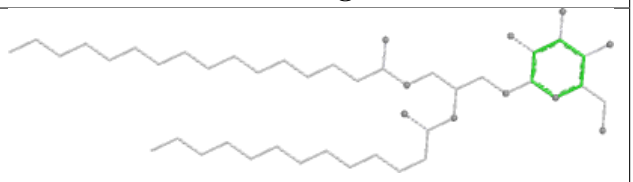
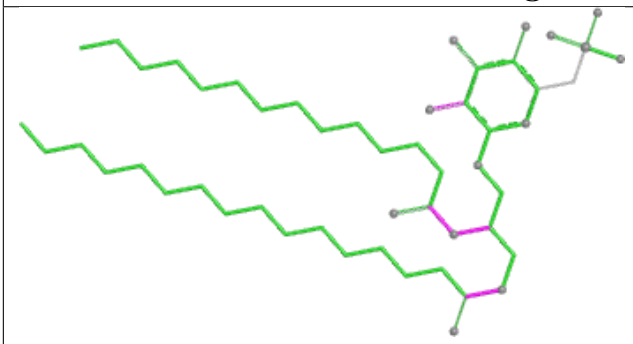


Rings

Ligand SQD A 413



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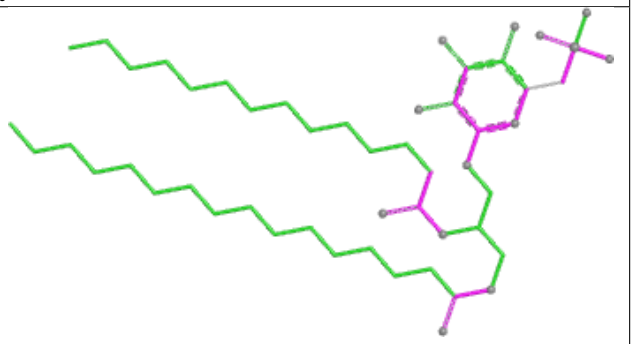
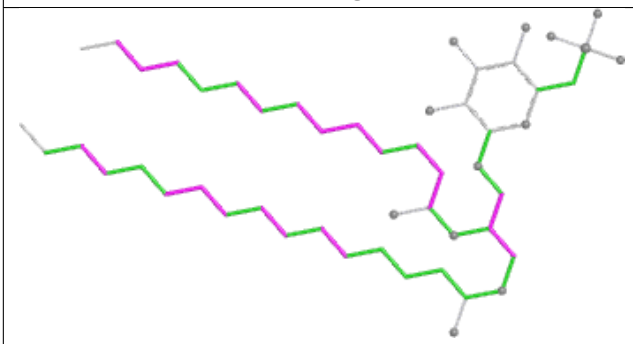


Bond angles



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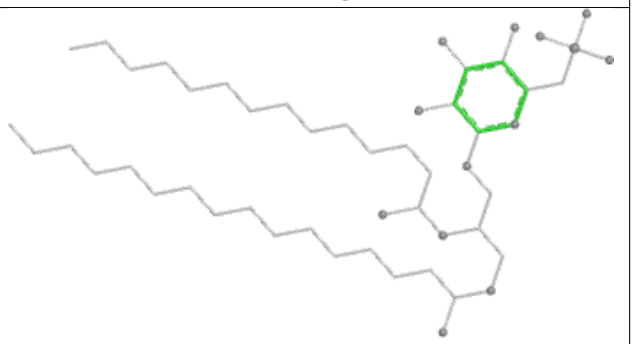
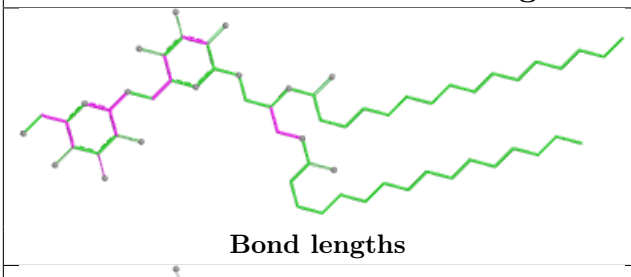


Rings

Ligand DGD H 102



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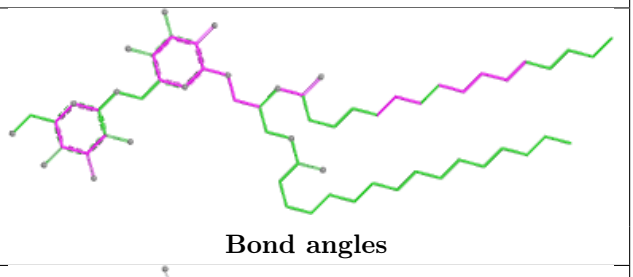
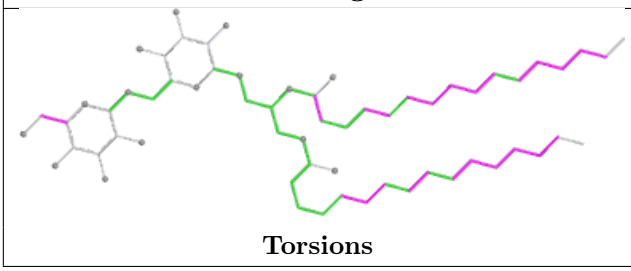


Bond angles



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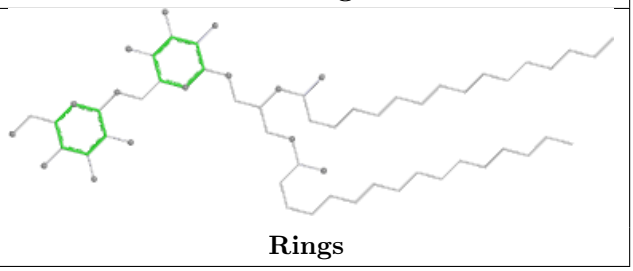
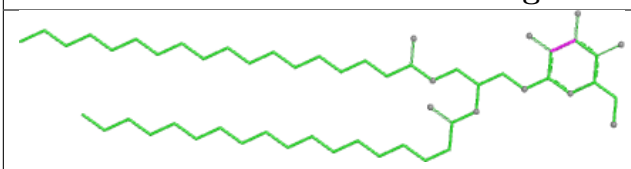


Rings

Ligand LMG b 623



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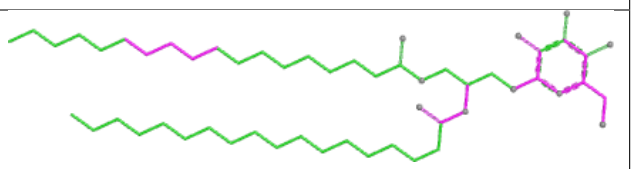

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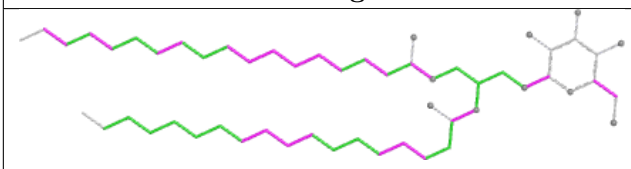

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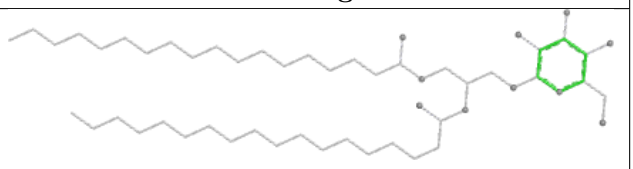
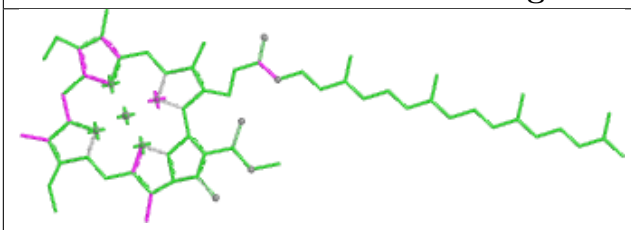


Rings

Ligand CLA h 101



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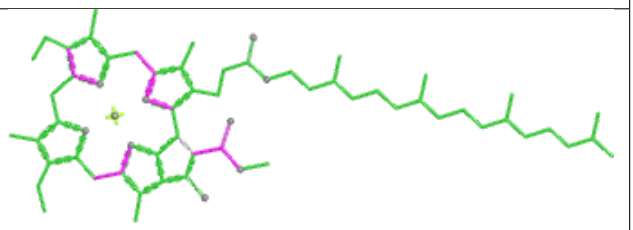
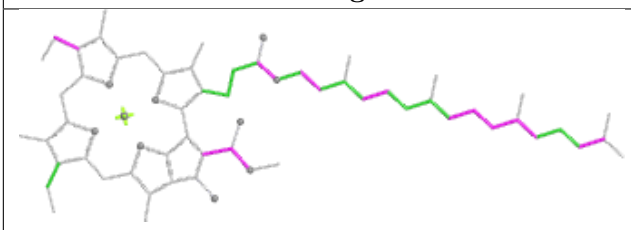


Bond angles



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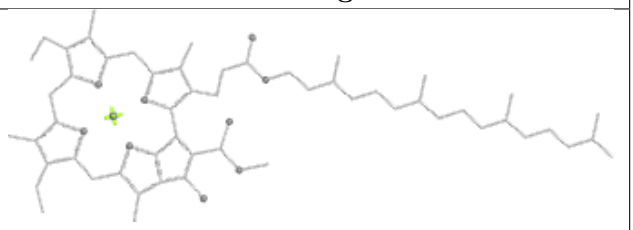
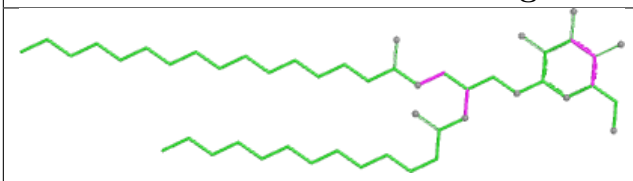
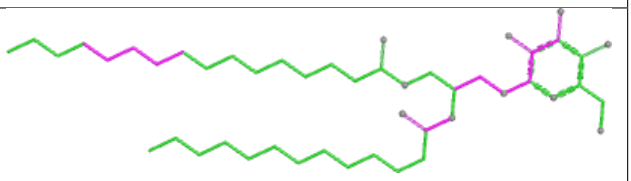


Rings

Ligand LMG C 519


Bond lengths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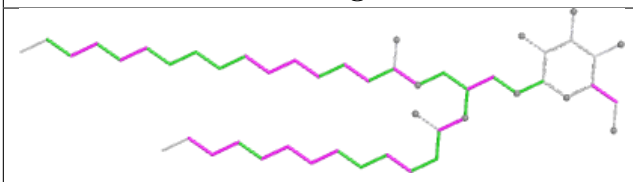
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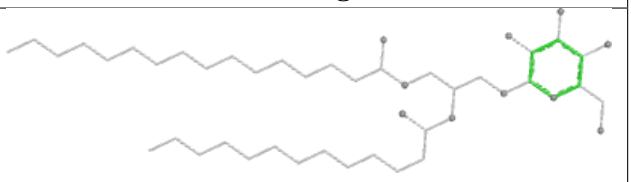
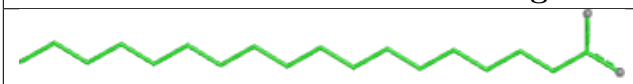

Rings

Ligand STE d 411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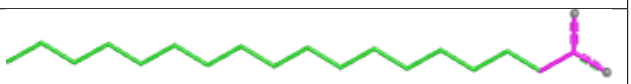
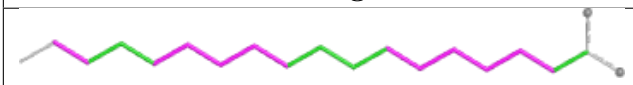
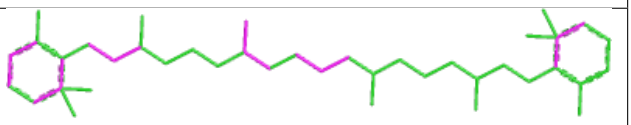

Bond angles

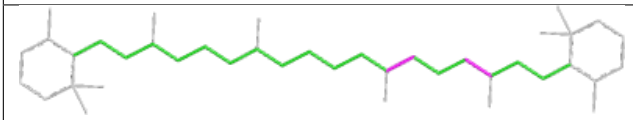

Torsions

Rings

Ligand BCR t 101

Bond lengths


Bond angles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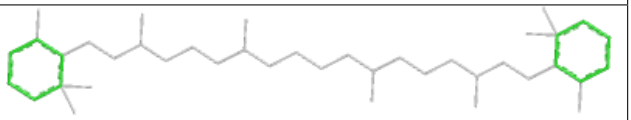
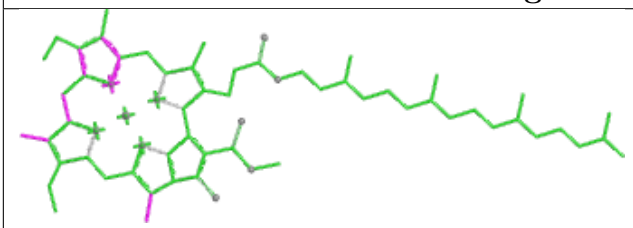

Rings

Ligand CLA B 606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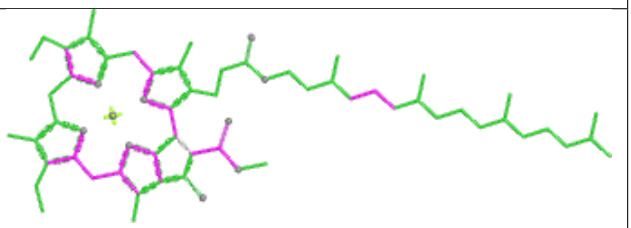
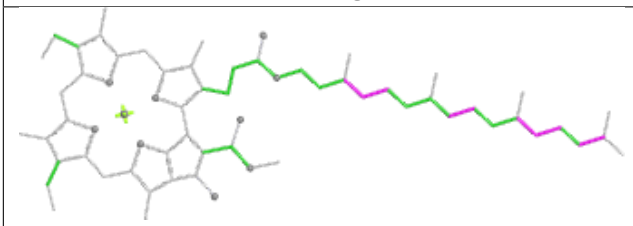
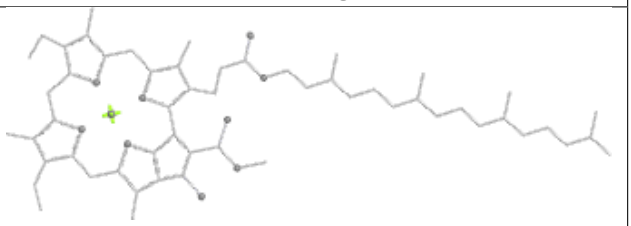
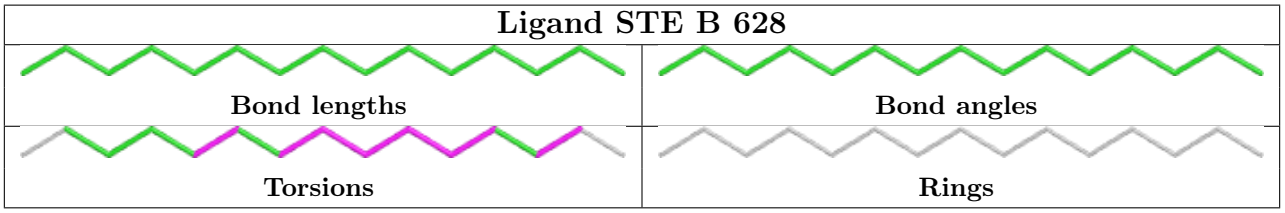

Bond angles


Torsions

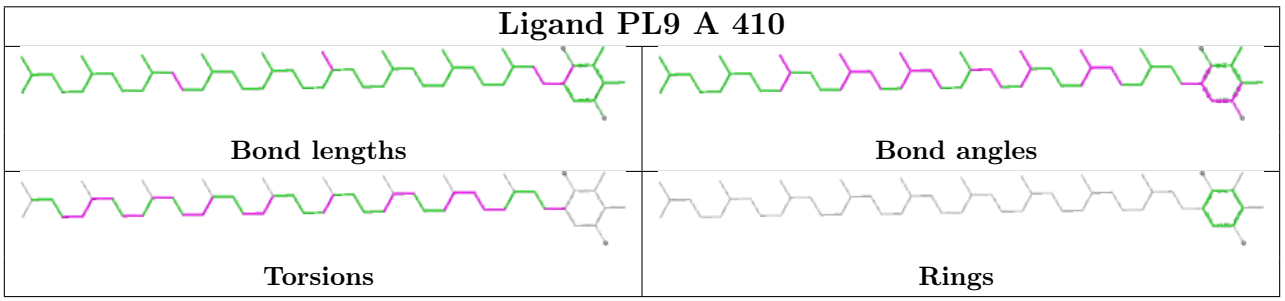

Rings

Ligand PL9 d 405

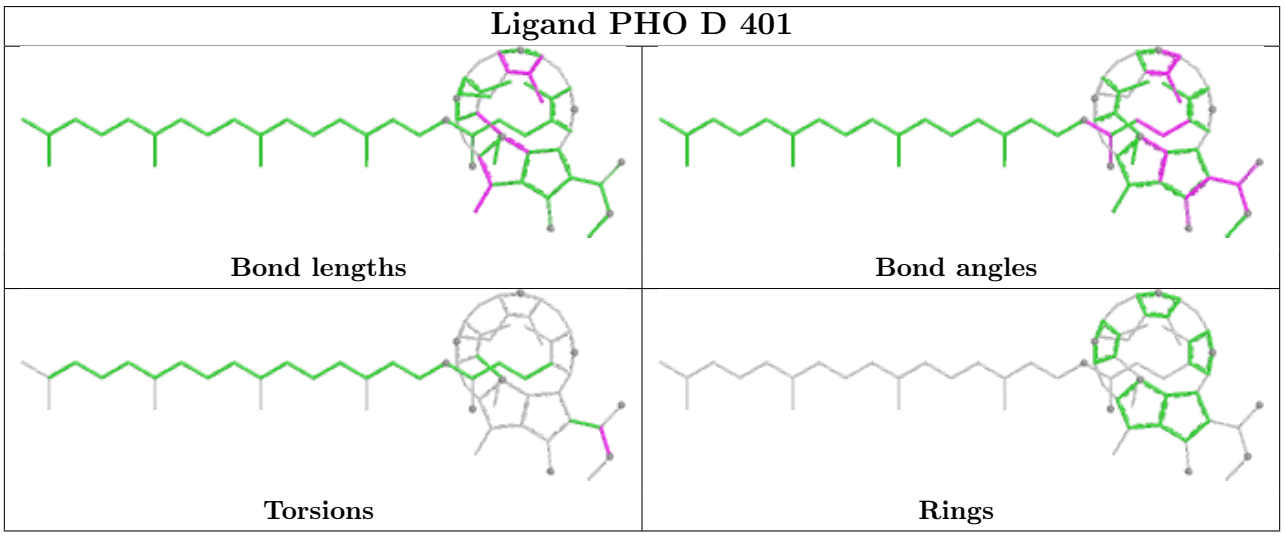
Ligand STE B 628



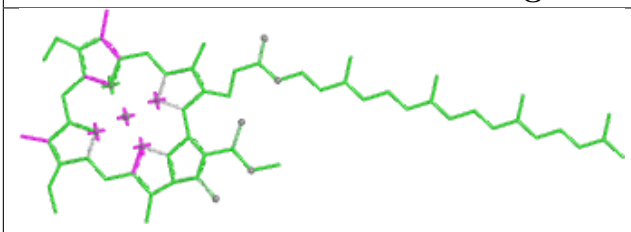
Ligand PL9 A 410



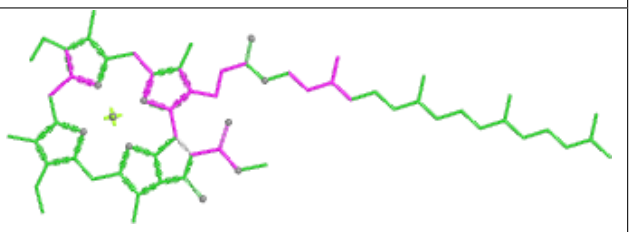
Ligand PHO D 401



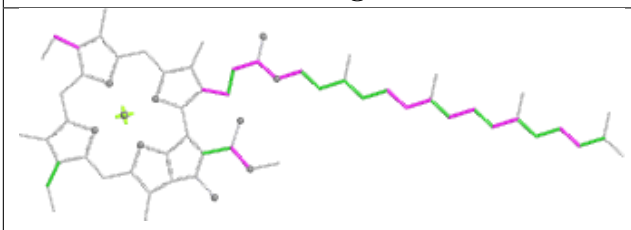
Ligand CLA B 602



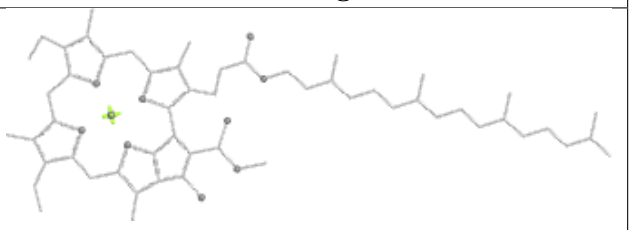
Bond lengths



Bond angles

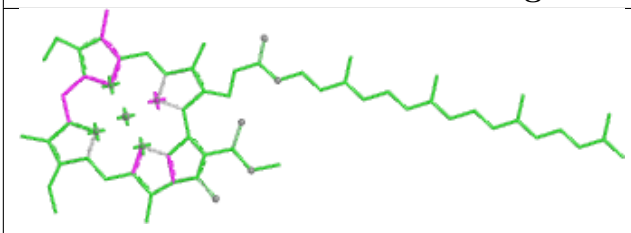


Torsions



Rings

Ligand CLA B 616



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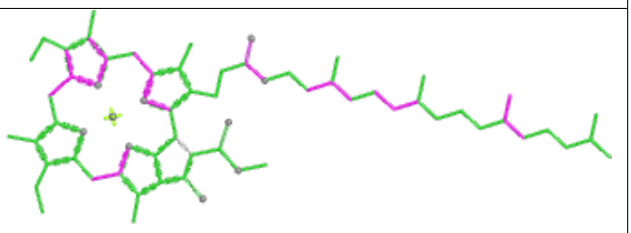
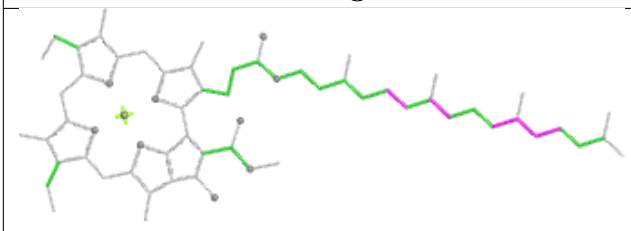
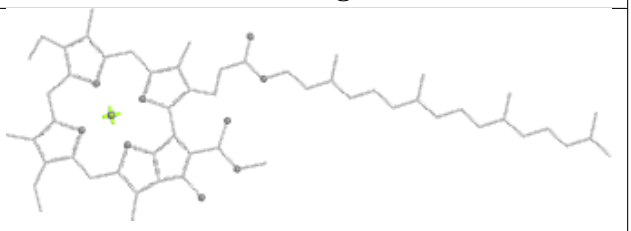


Bond angles

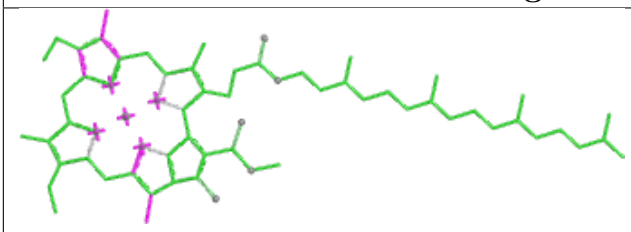


Torsions

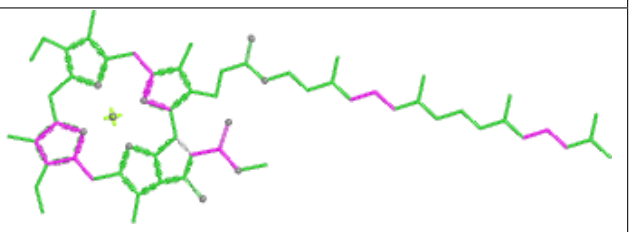


Rings

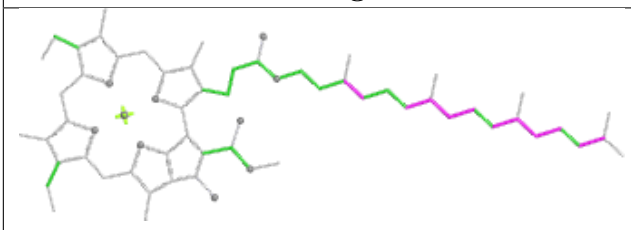
Ligand CLA B 612



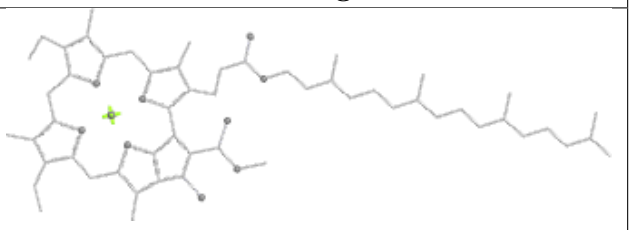
Bond lengths



Bond angles

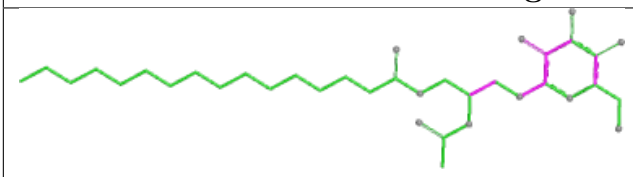


Torsions



Rings

Ligand LMG c 522



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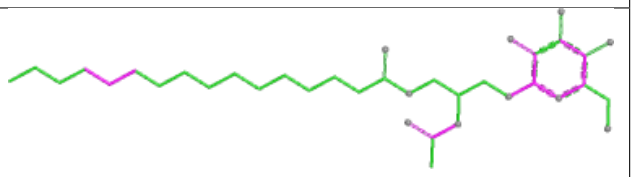
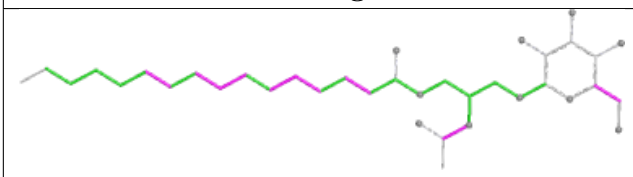
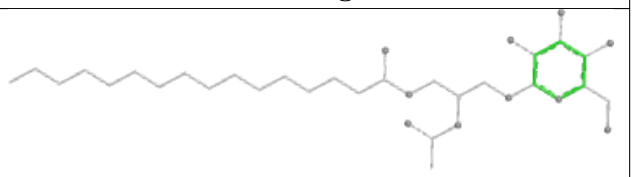


Bond angles

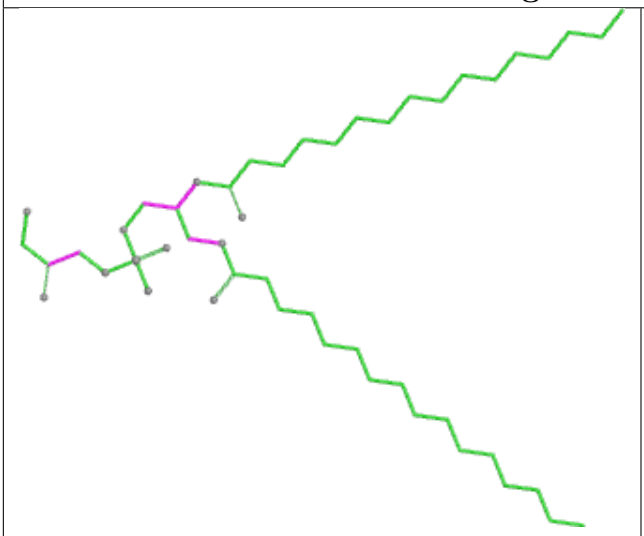


Torsions



Rings

Ligand LHG D 408



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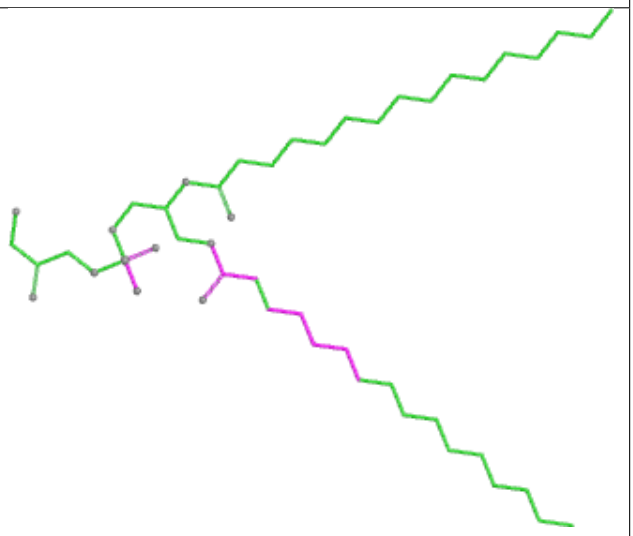
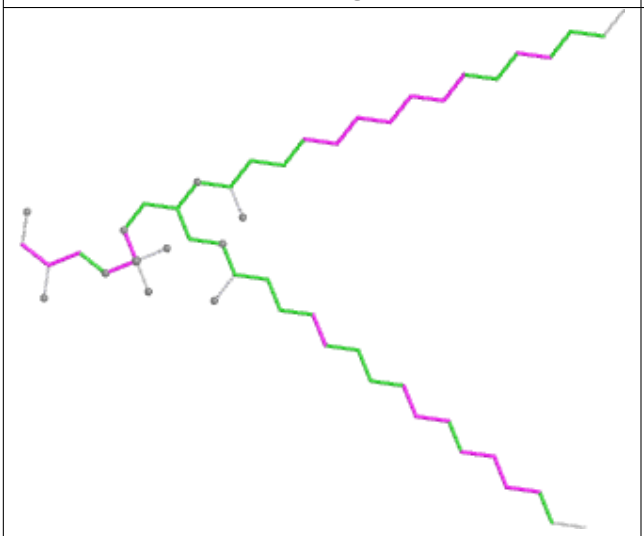


Bond angles



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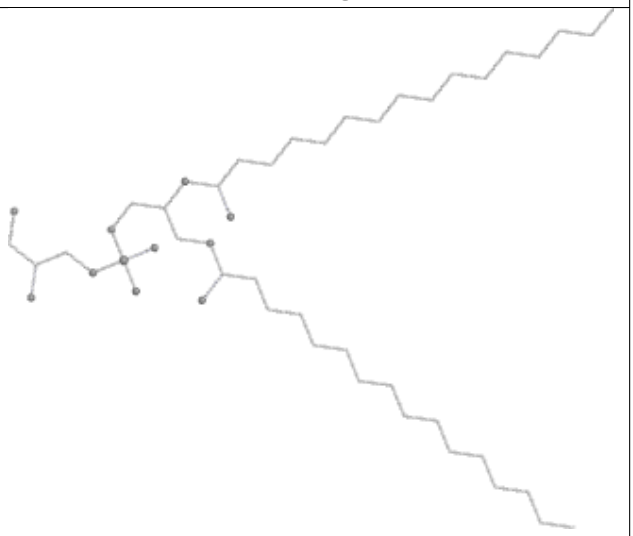
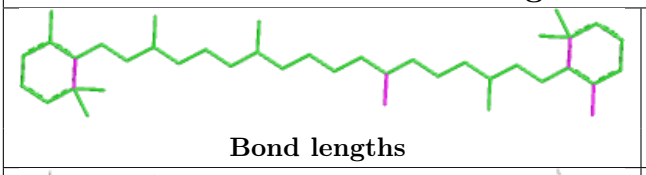


Rings

Ligand BCR b 617



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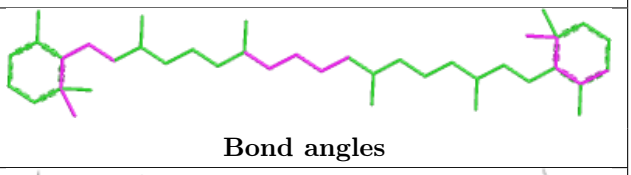

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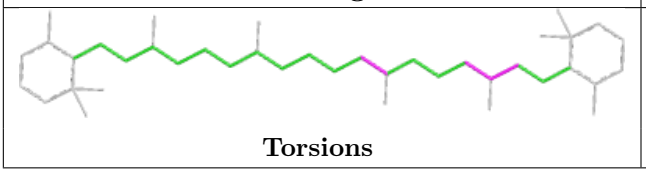

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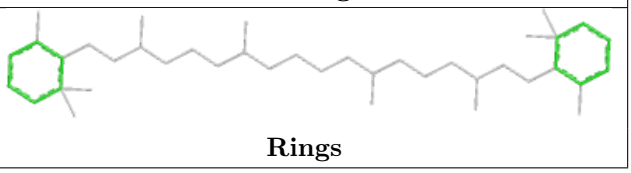
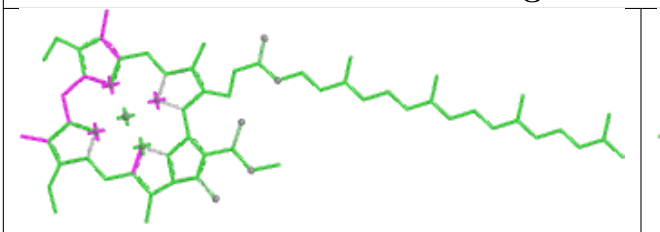
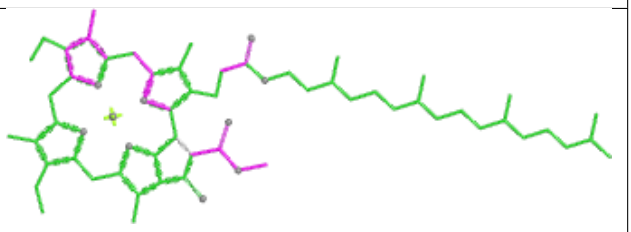


Rings

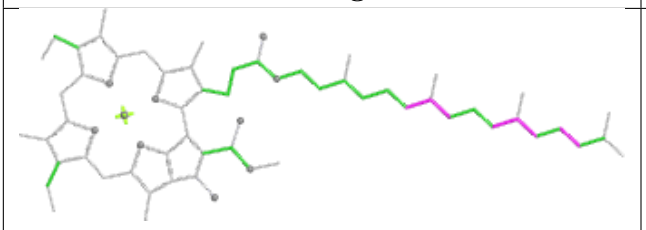
Ligand CLA A 403



Bond lengths



Bond angles



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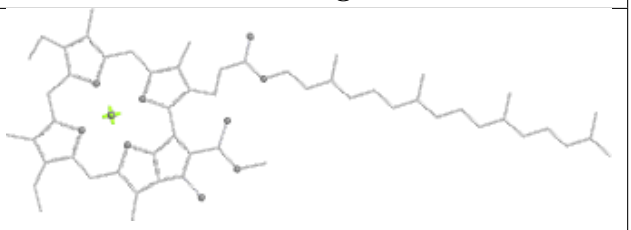
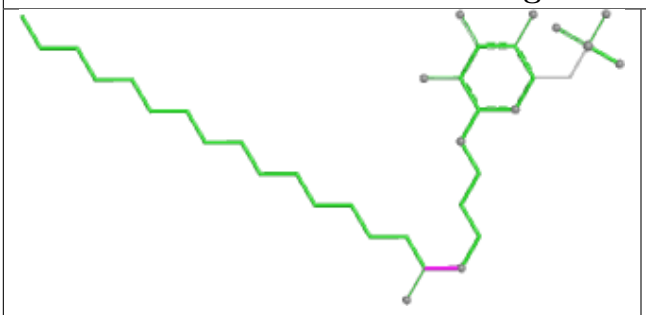


Rings

Ligand SQD D 407



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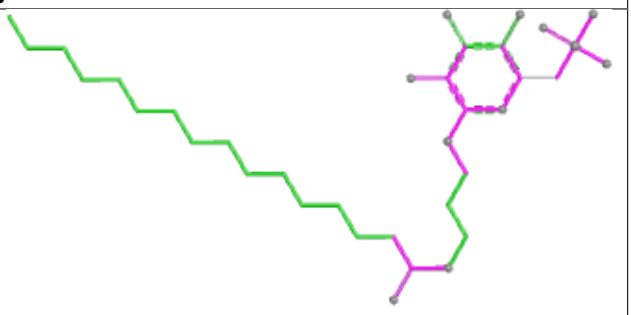
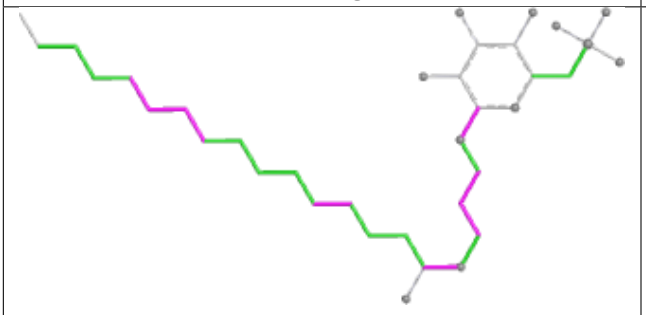
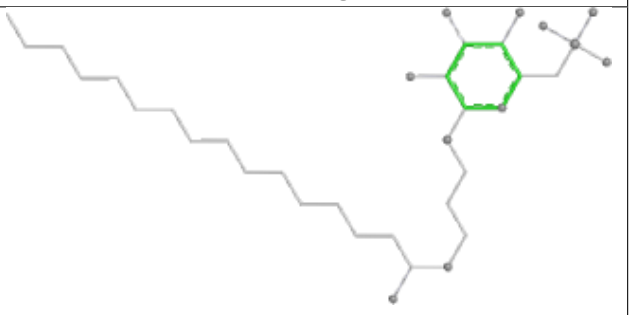


Bond angles

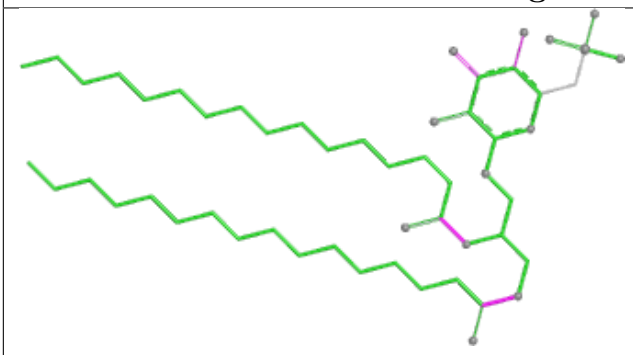


Torsions



Rings

Ligand SQD a 412



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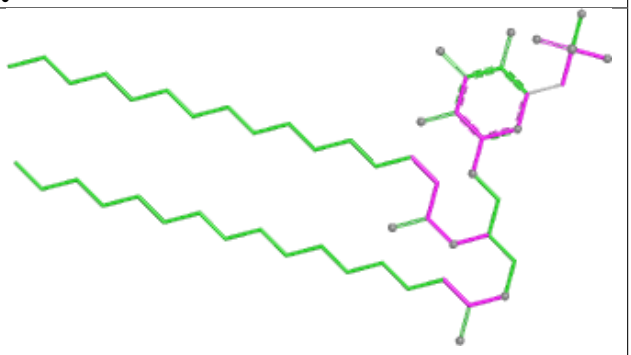
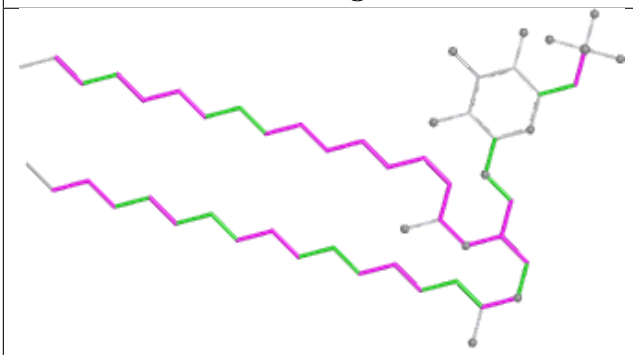


Bond angles



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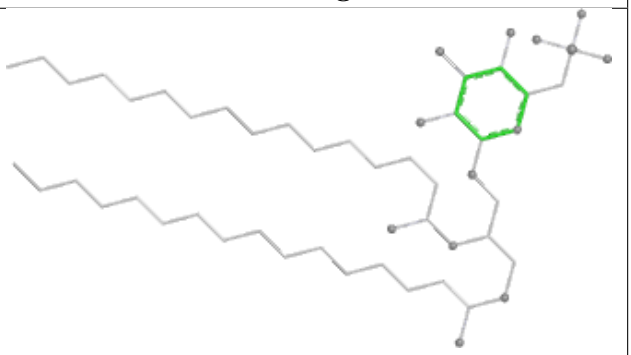
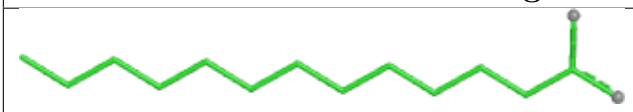


Rings

Ligand STE M 102



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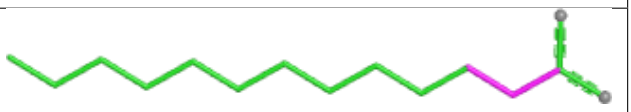
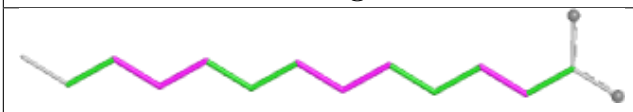


Bond angles



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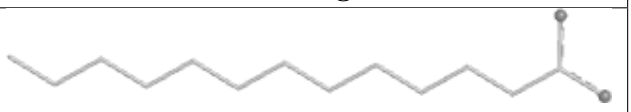
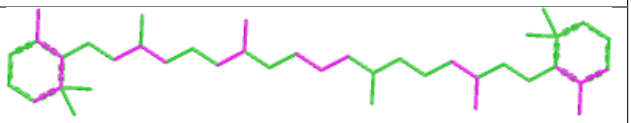


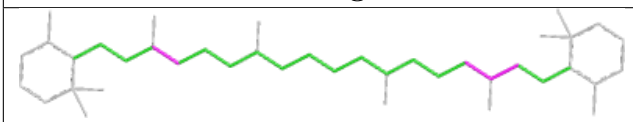
Rings

Ligand BCR x 101

Bond lengths



Bond angles



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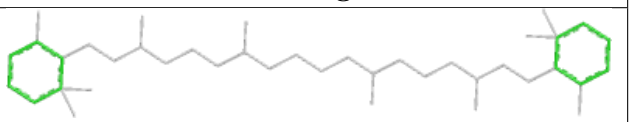
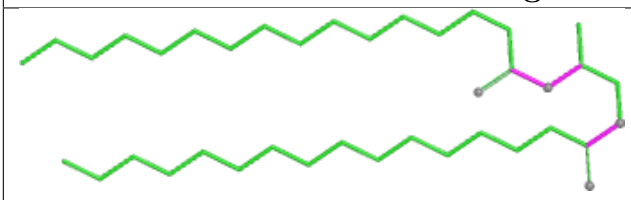


Rings

Ligand SQD A 414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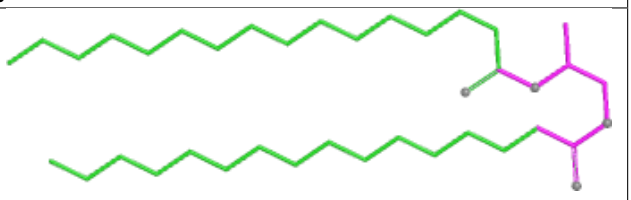
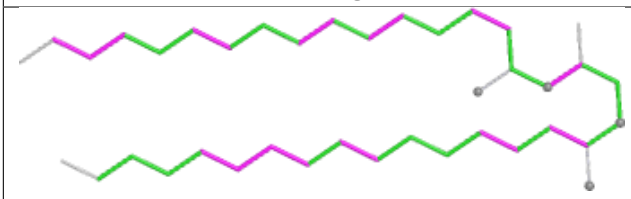

Bond angles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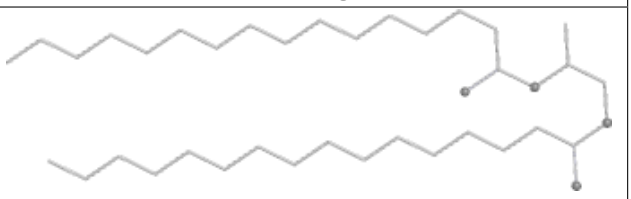
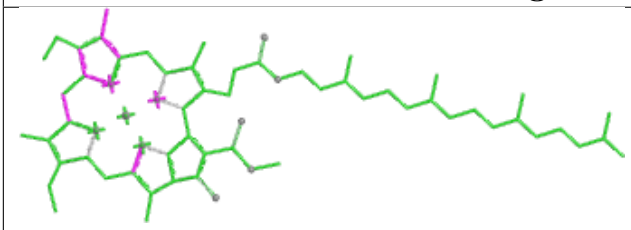
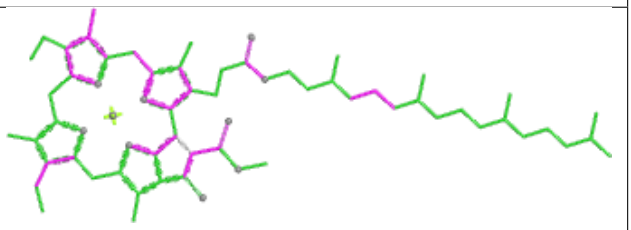
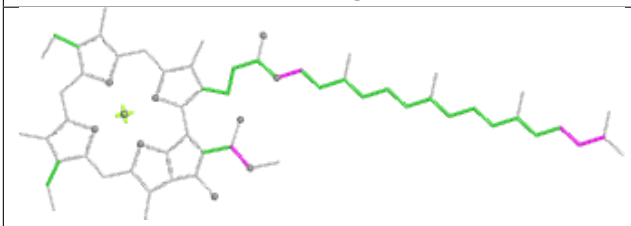
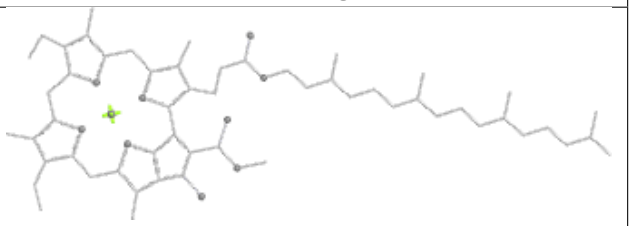

Rings

Ligand CLA a 402

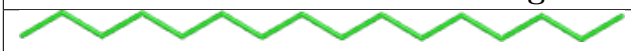

Bond lengths


Bond angles


Torsions


Rings

Ligand STE B 627


Bond lengths

Bond angles

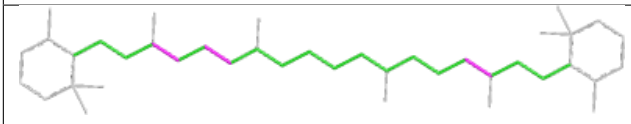
Torsions

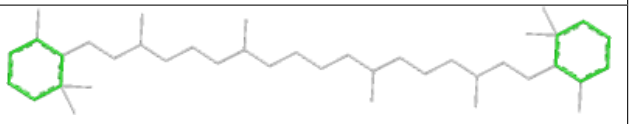
Rings

Ligand BCR B 620

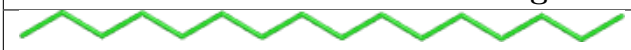
Bond lengths

Bond angles

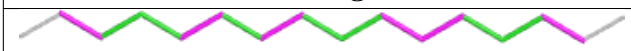

Torsions


Rings

Ligand STE b 620

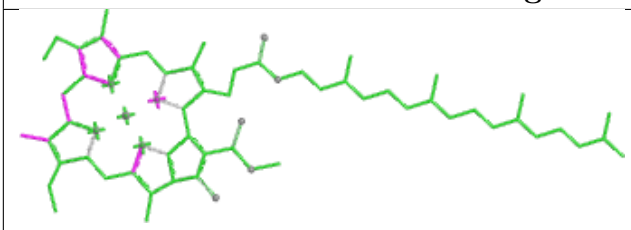

Bond lengths

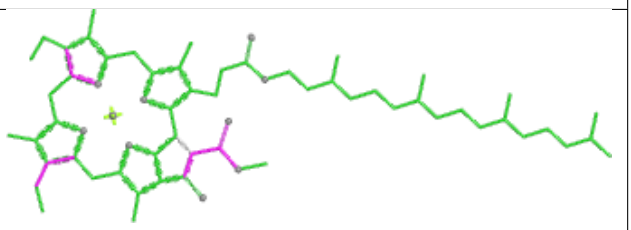
Bond angles

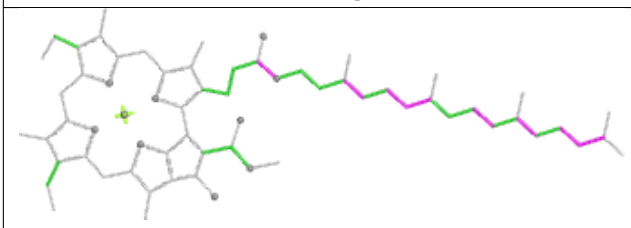

Torsions

Rings

Ligand CLA C 506


Bond lengths


Bond angles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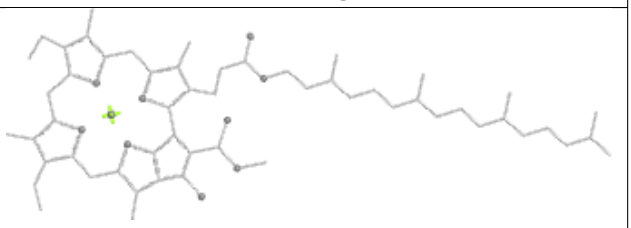
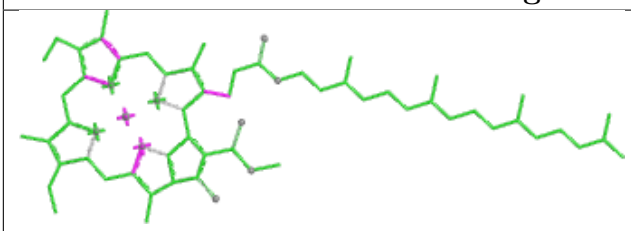
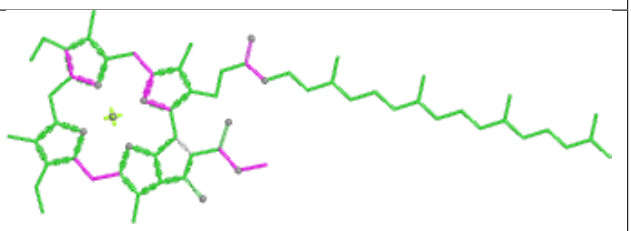
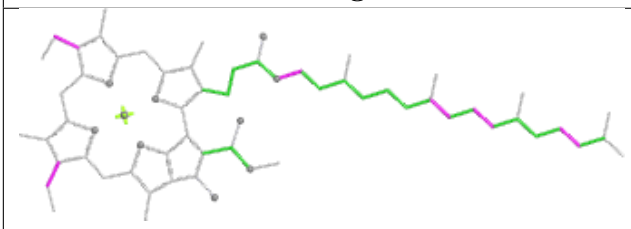
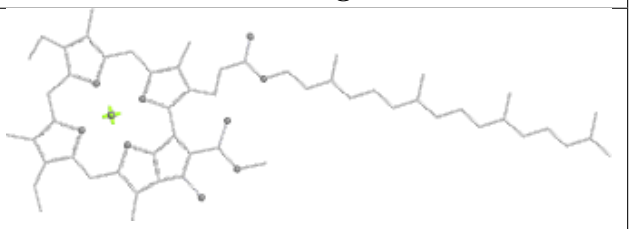

Rings

Ligand CLA D 402

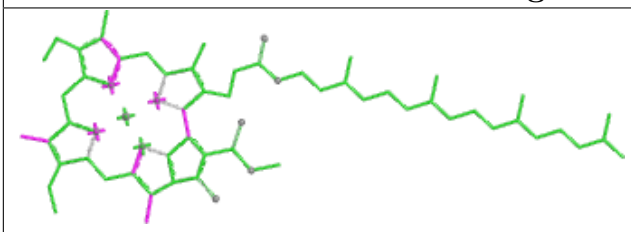

Bond lengths


Bond angles

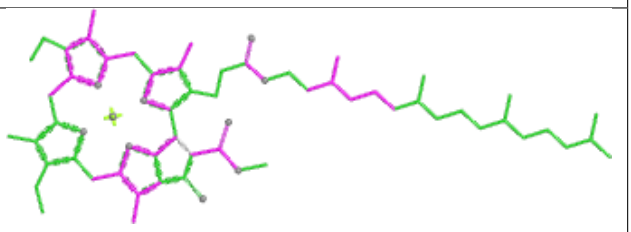

Torsions


Rings

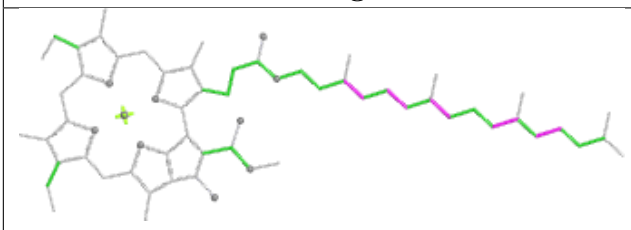
Ligand CLA b 602



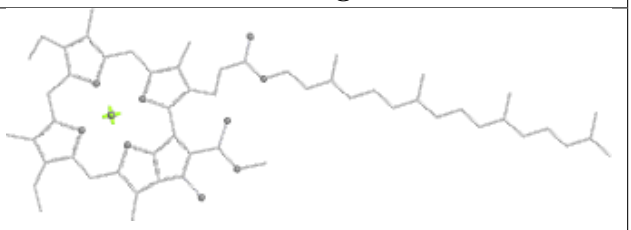
Bond lengths



Bond angles



Torsions

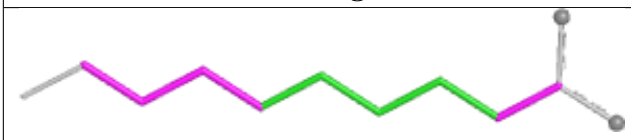


Rings

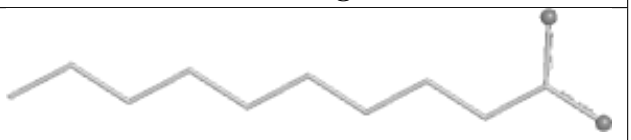
Ligand STE c 501

Bond lengths

Bond angles

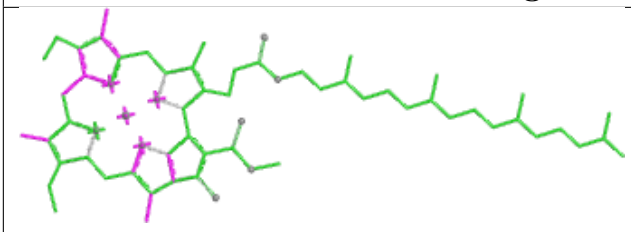


Torsions

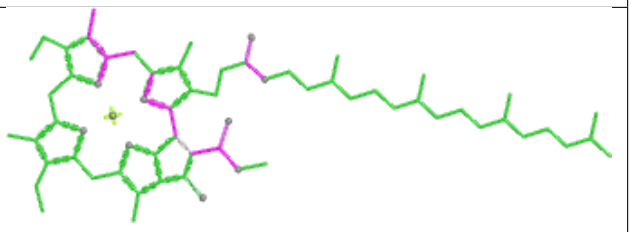


Rings

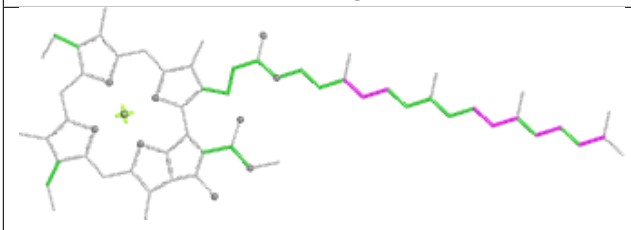
Ligand CLA D 403



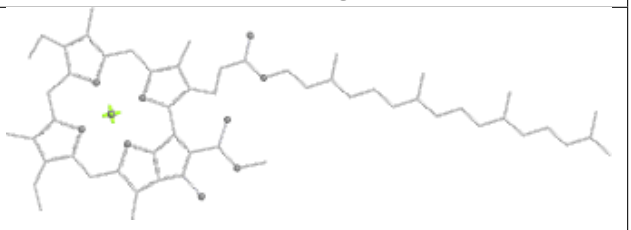
Bond lengths



Bond angles

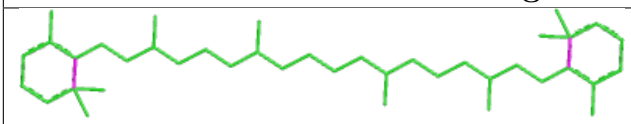


Torsions

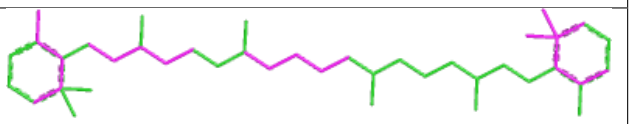


Rings

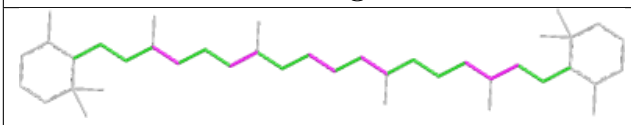
Ligand BCR B 619



Bond lengths



Bond angles



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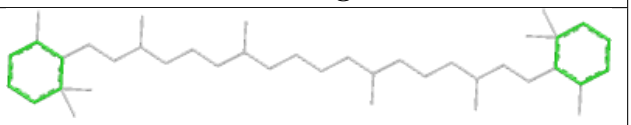
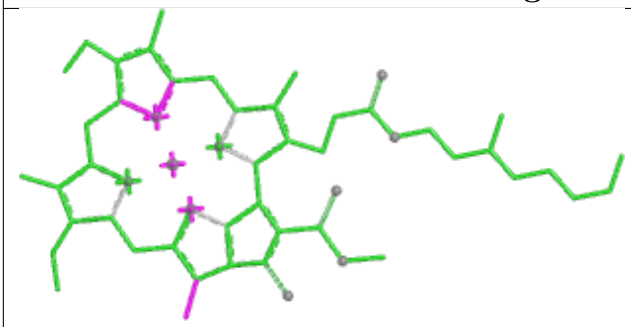


Rings

Ligand CLA A 405



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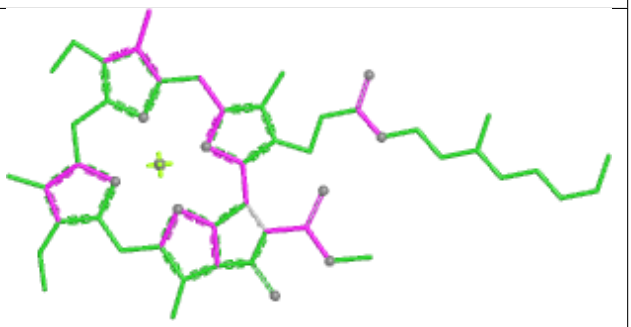
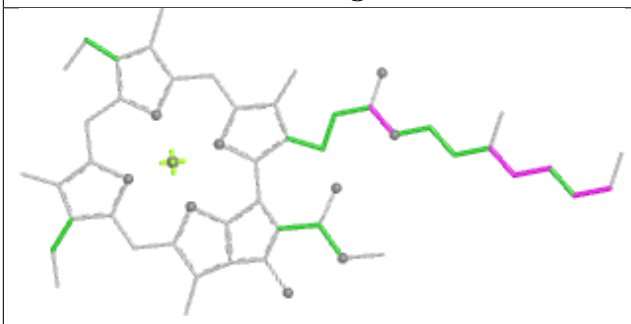


Bond angles



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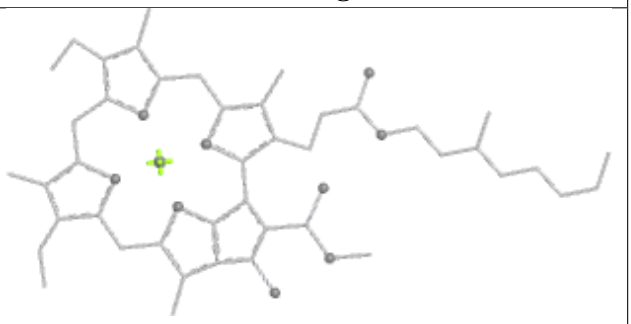
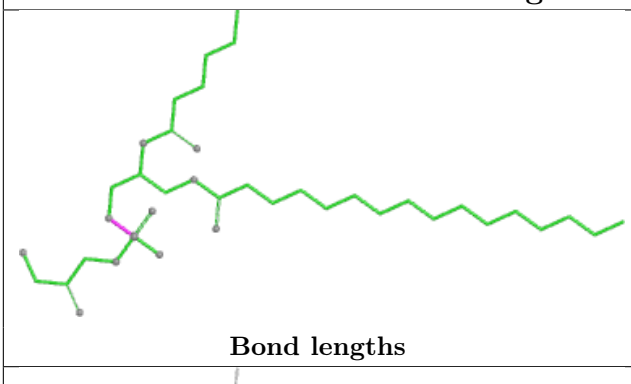
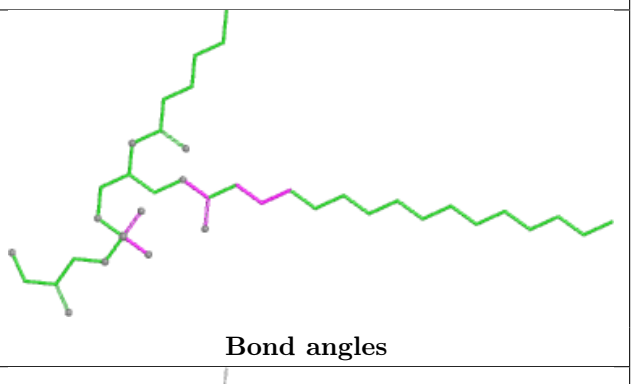


Rings

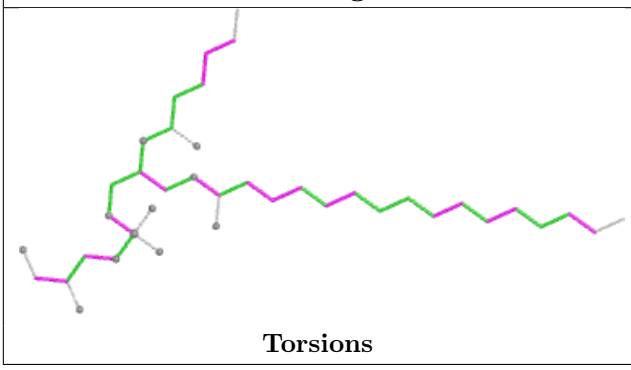
Ligand LHG d 408



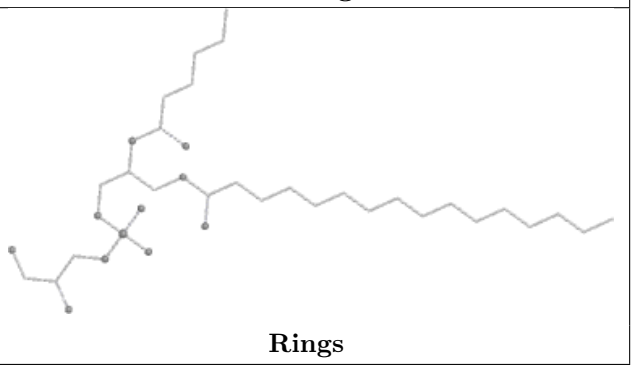
Bond lengths



Bond angles

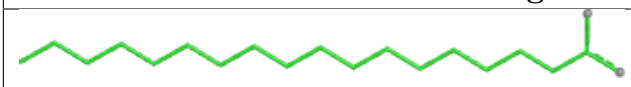


Torsions



Rings

Ligand STE X 101



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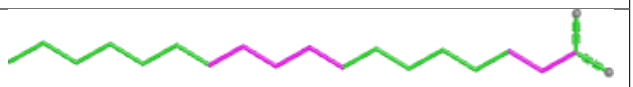
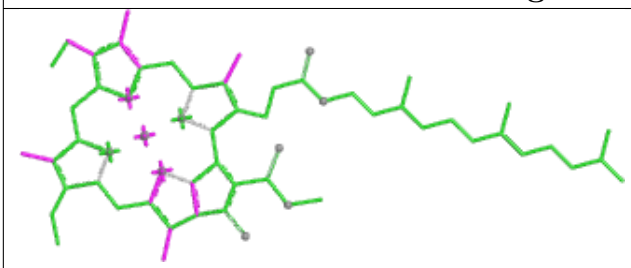


Bond angles

Torsions

Rings

Ligand CLA b 615



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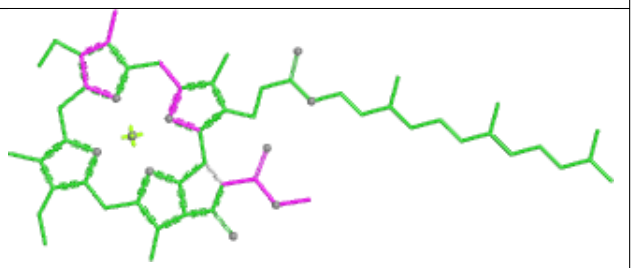
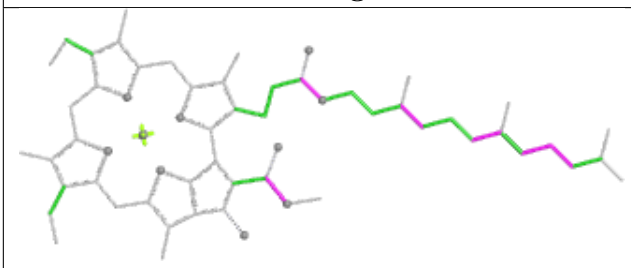


Bond angles



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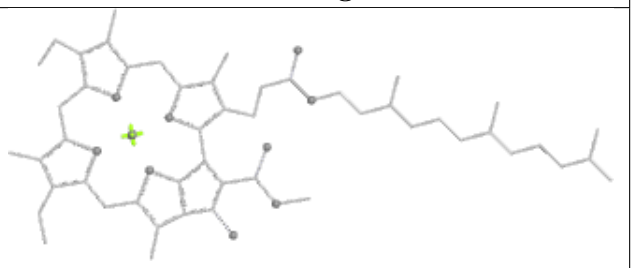
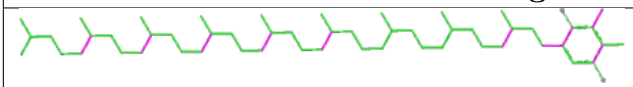
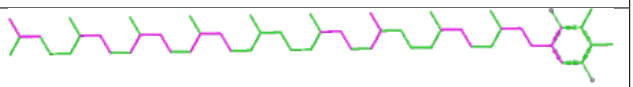


Rings

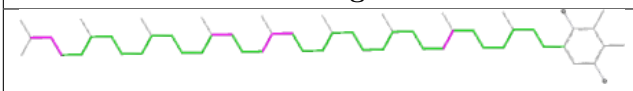
Ligand PL9 D 405



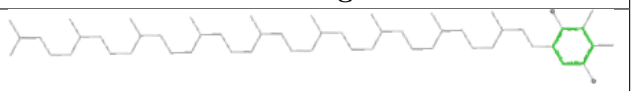
Bond lengths



Bond angles

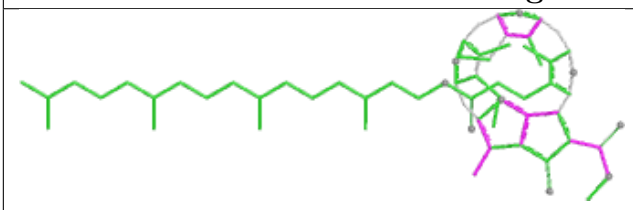


Torsions

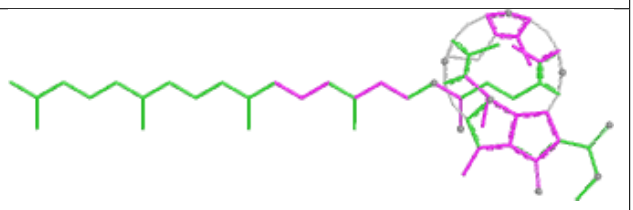


Rings

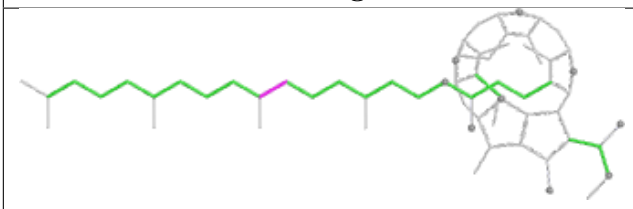
Ligand PHO a 404



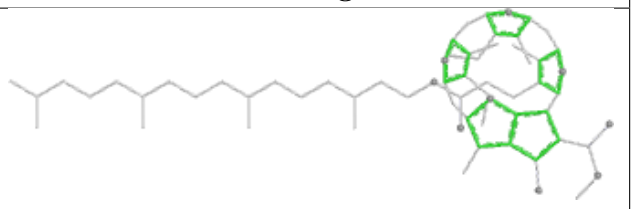
Bond lengths



Bond angles



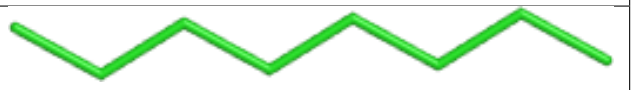
Torsions



Rings

Ligand STE Z 102

Bond lengths

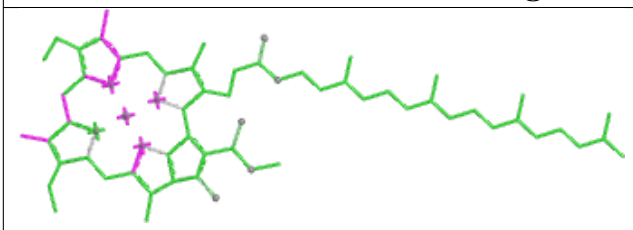


Bond angles

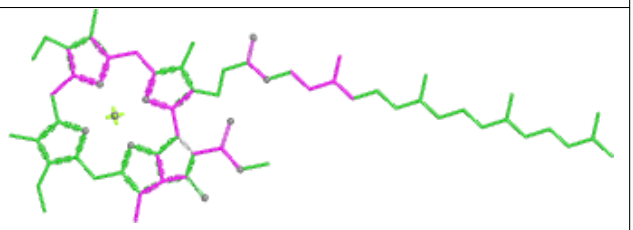
Torsions

Rings

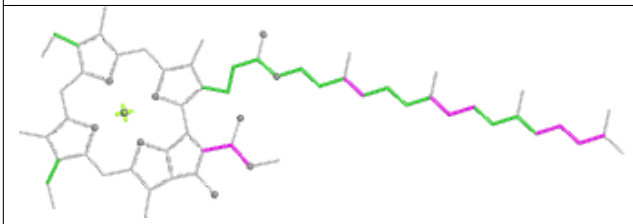
Ligand CLA B 615



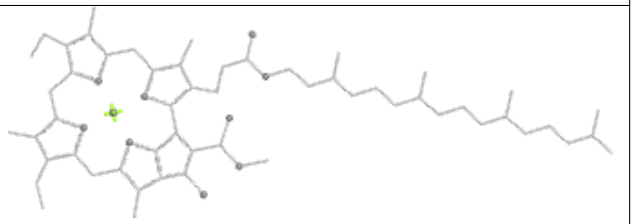
Bond lengths



Bond angles

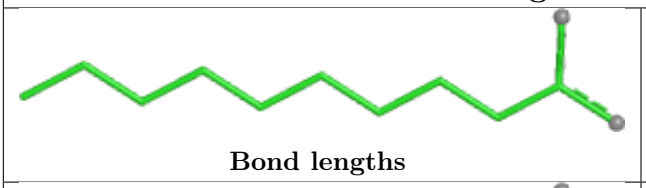


Torsions



Rings

Ligand STE L 101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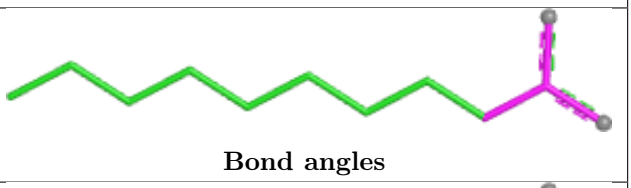
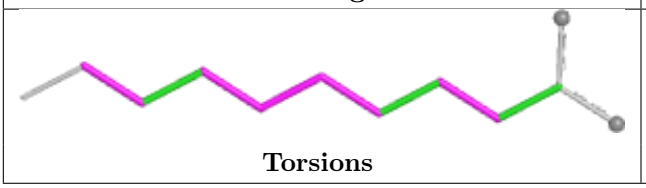
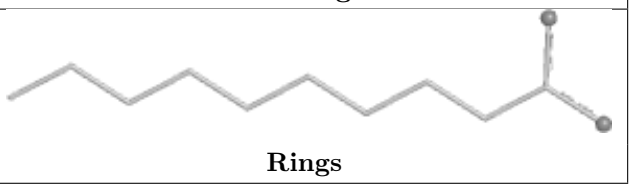
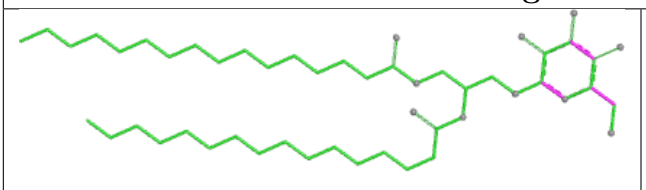

Bond angles


Torsions


Rings

Ligand LMG b 621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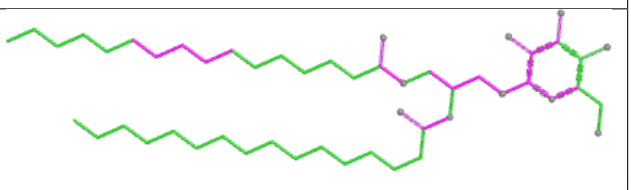
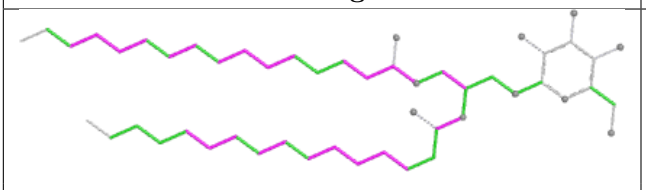
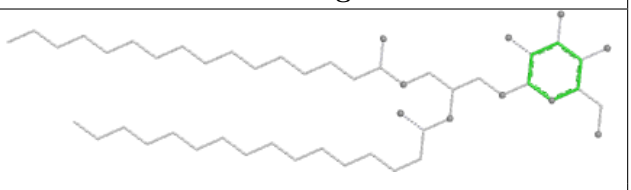
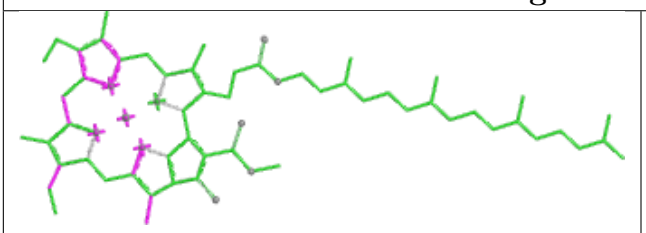

Bond angles


Torsions


Rings

Ligand CLA c 508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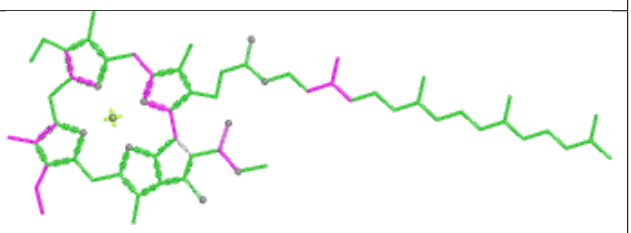
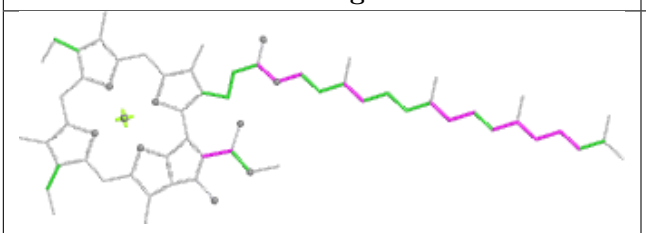

Bond angles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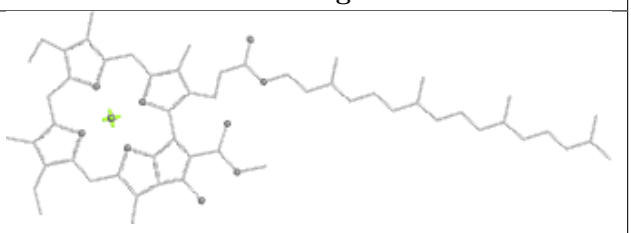
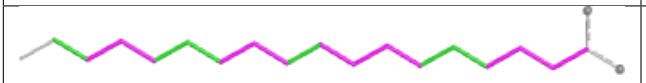

Rings

Ligand STE b 622

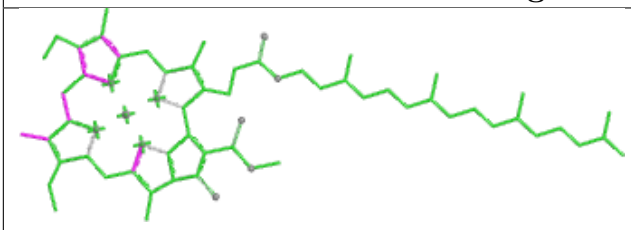
Bond lengths

Bond angles

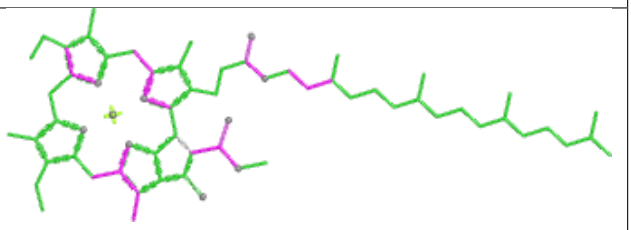

Torsions

Rings

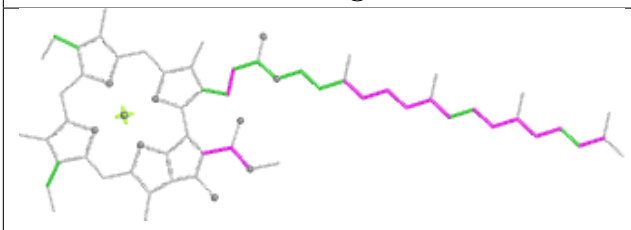
Ligand CLA b 613



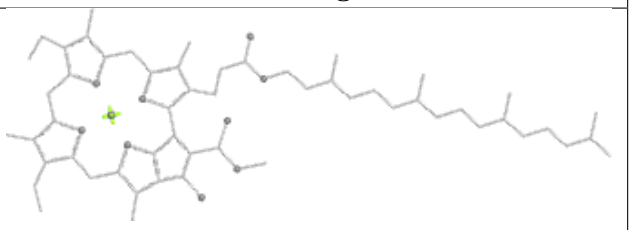
Bond lengths



Bond angles

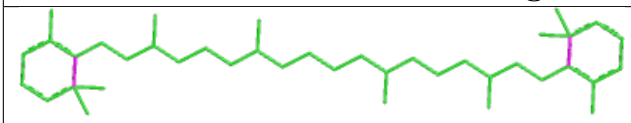


Torsions

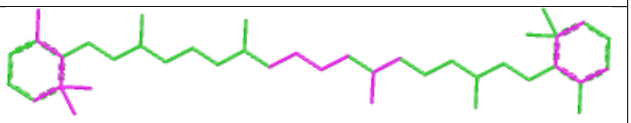


Rings

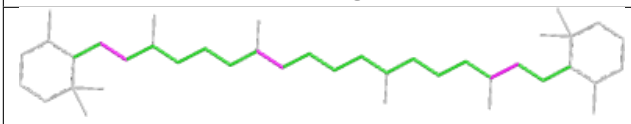
Ligand BCR b 618



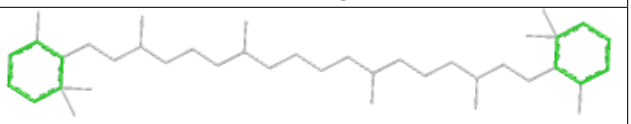
Bond lengths



Bond angles

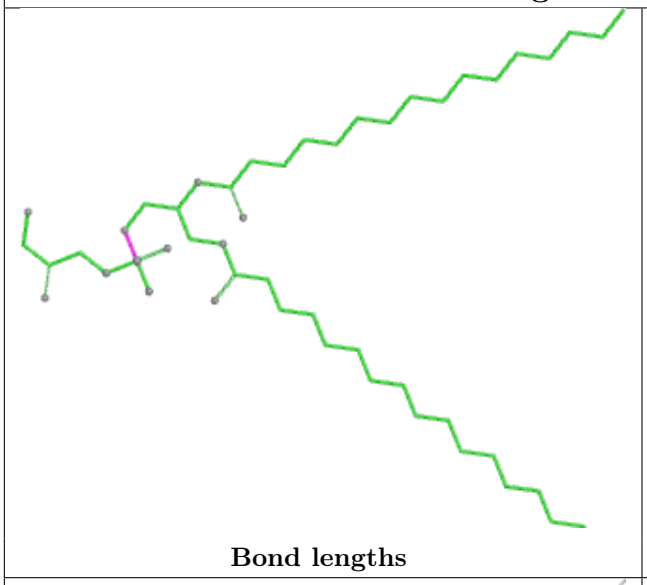


Torsions



Rings

Ligand LHG l 101



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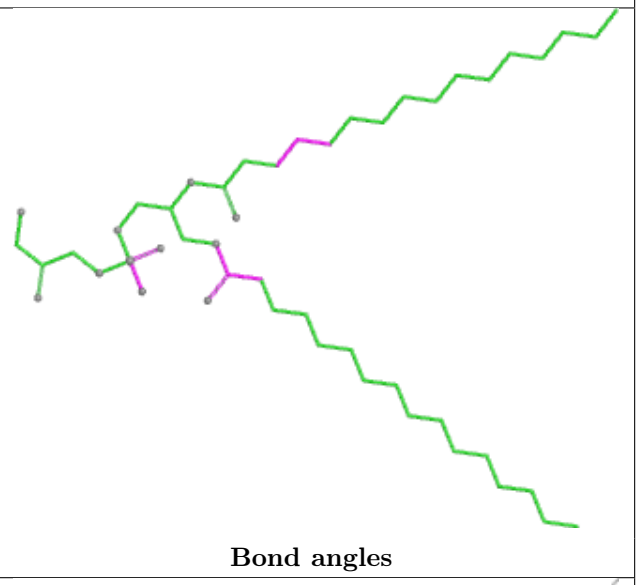
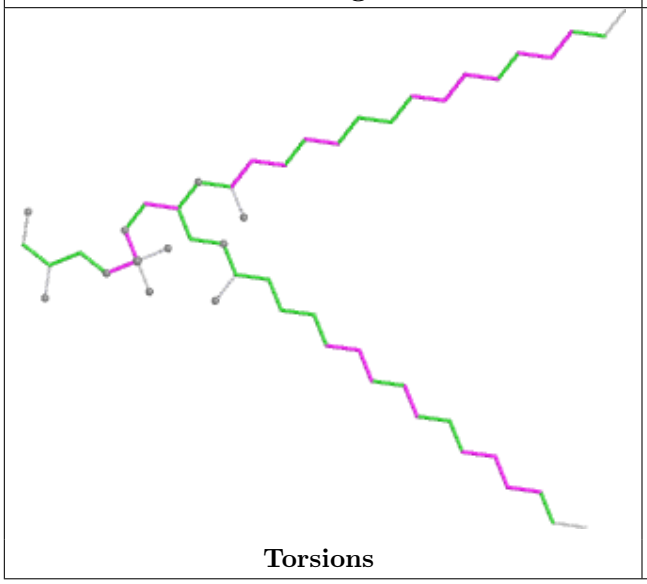


Bond angles



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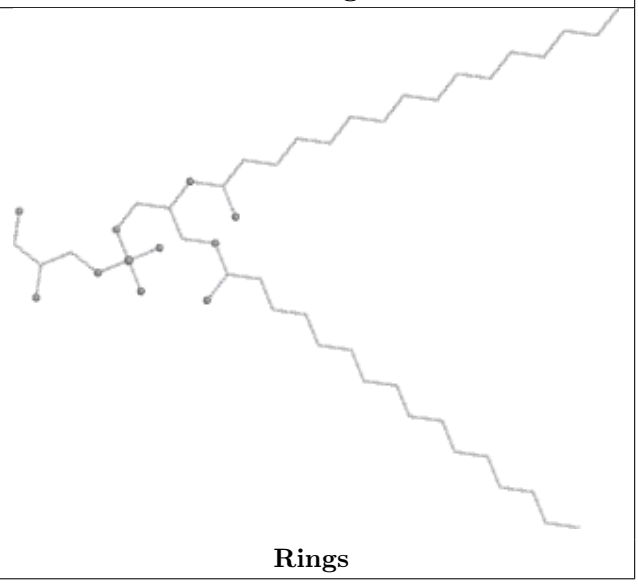
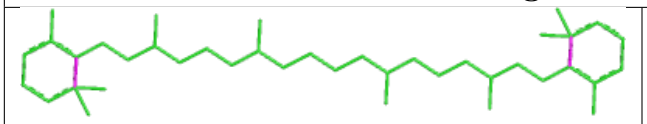


Rings

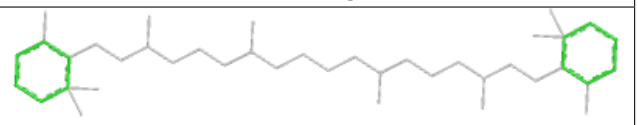
Ligand BCR D 404



Bond lengths

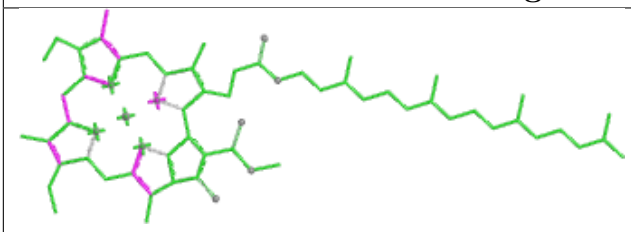
Bond angles

Torsions

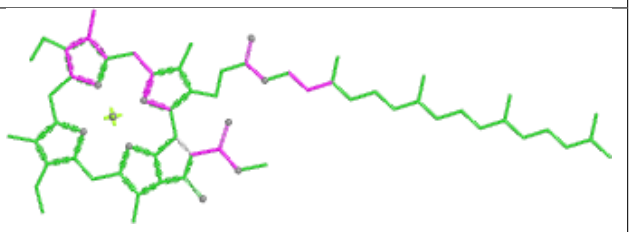


Rings

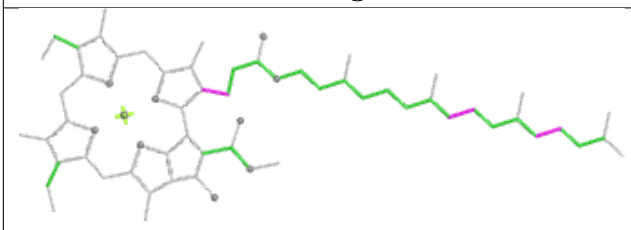
Ligand CLA B 603



Bond lengths



Bond angles



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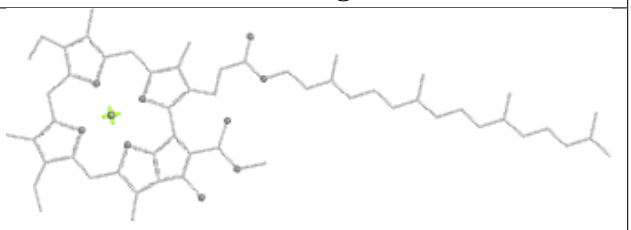
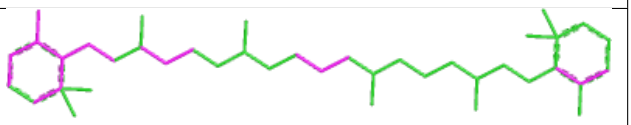


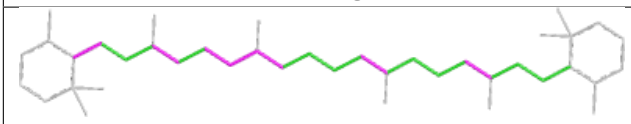
Rings

Ligand BCR B 618

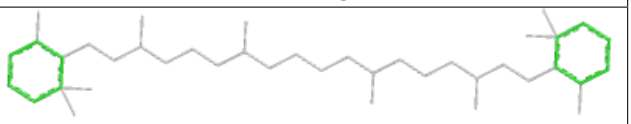
Bond lengths



Bond angles

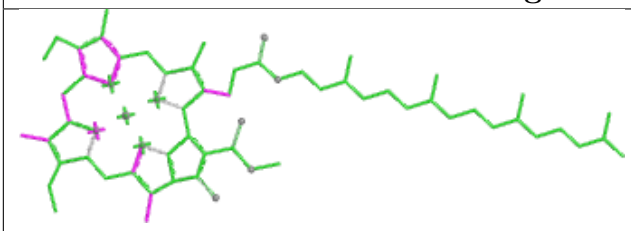


Torsions



Rings

Ligand CLA C 511



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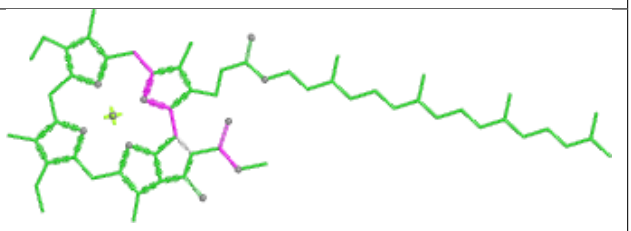
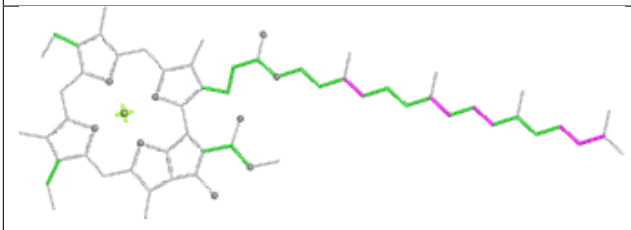
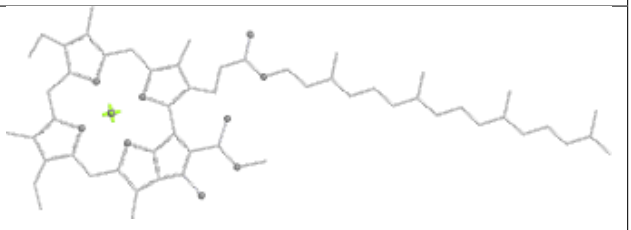


Bond angles

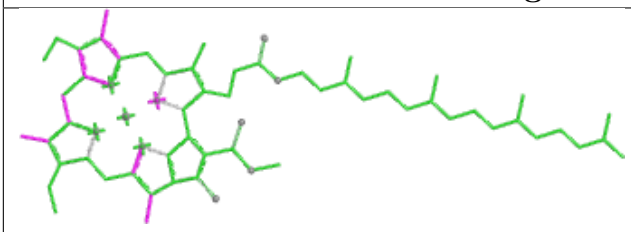


Torsions

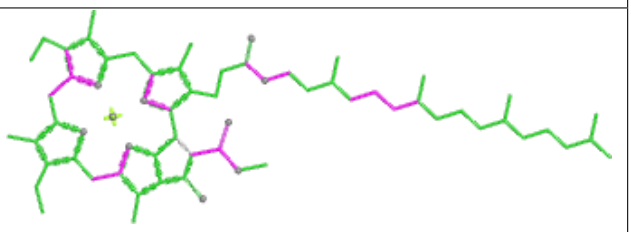


Rings

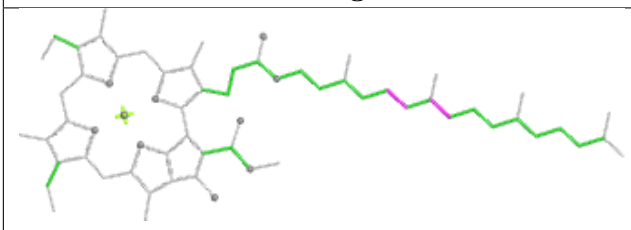
Ligand CLA C 504



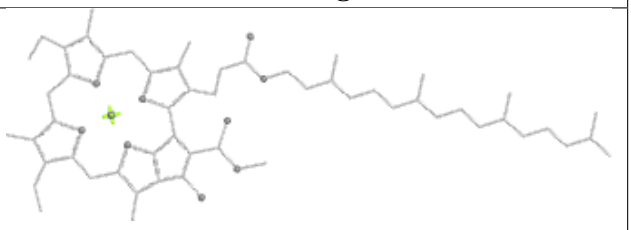
Bond lengths



Bond angles

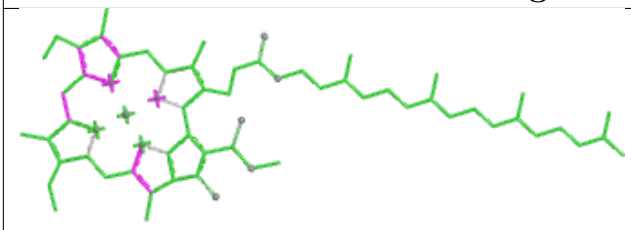


Torsions

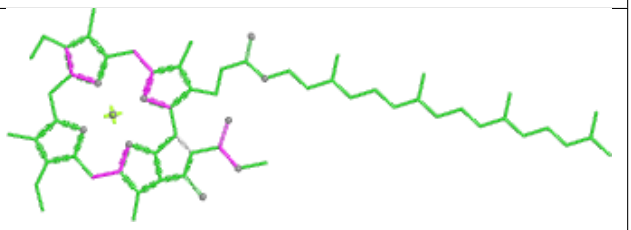


Rings

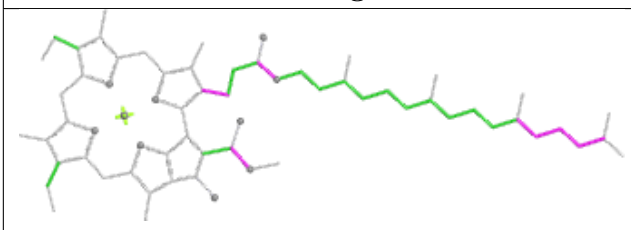
Ligand CLA c 513



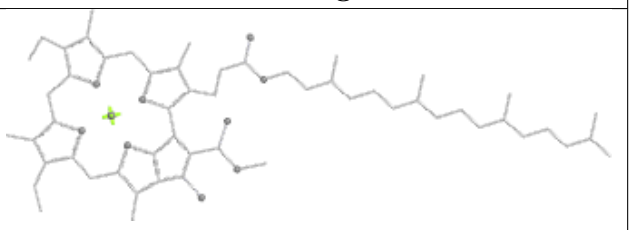
Bond lengths



Bond angles

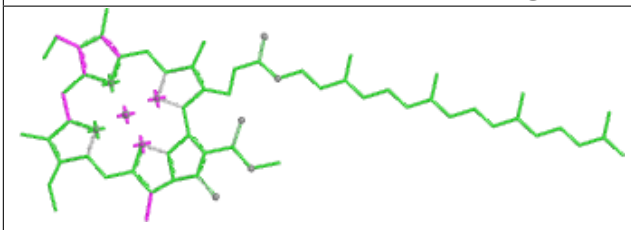


Torsions

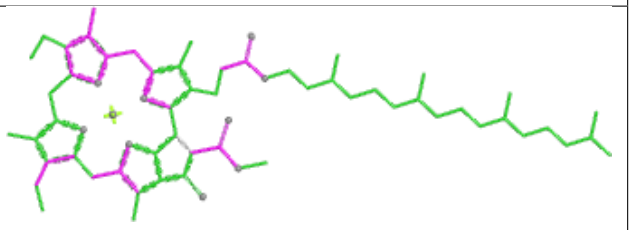


Rings

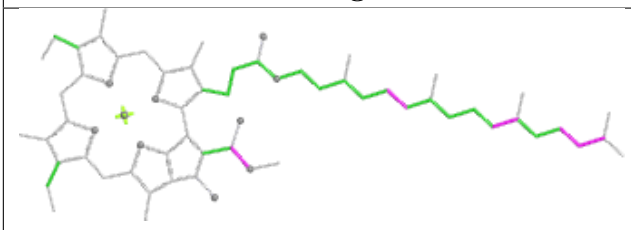
Ligand CLA B 604



Bond lengths



Bond angles



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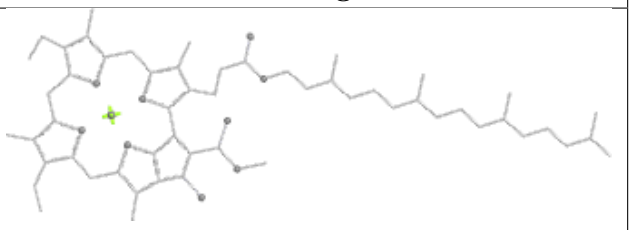
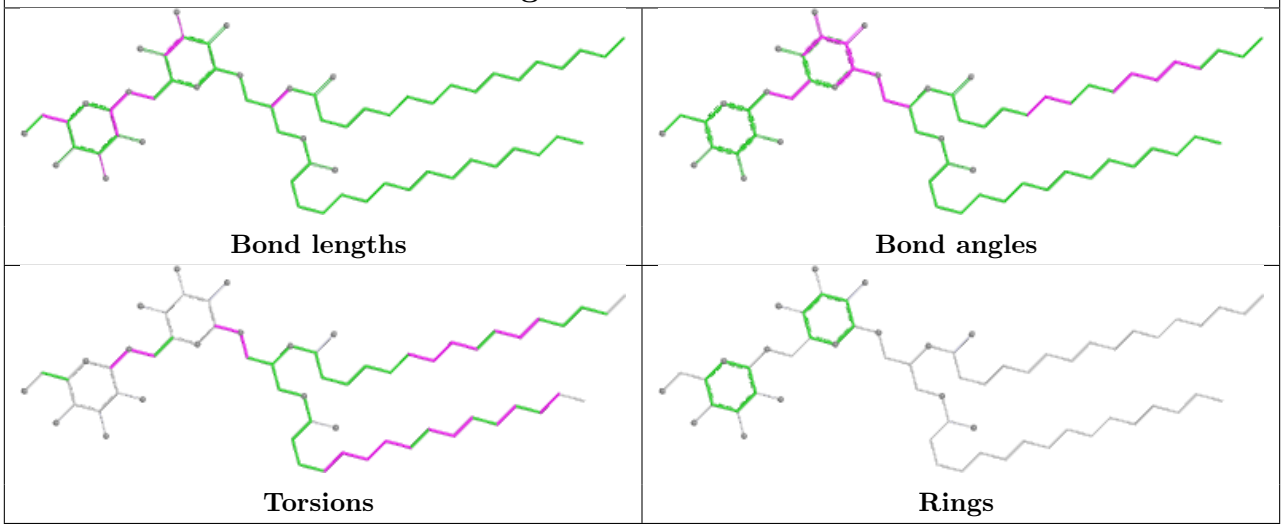
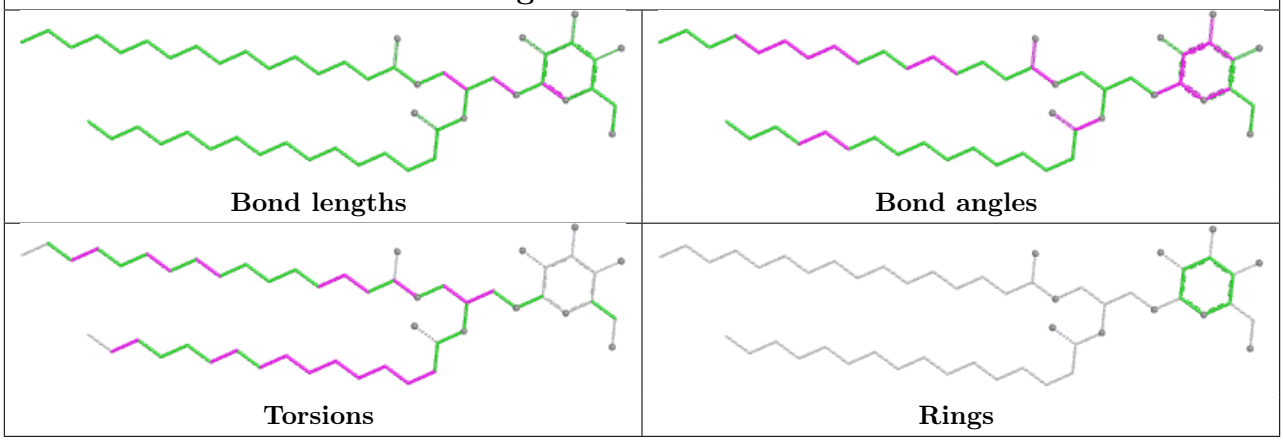


Rings

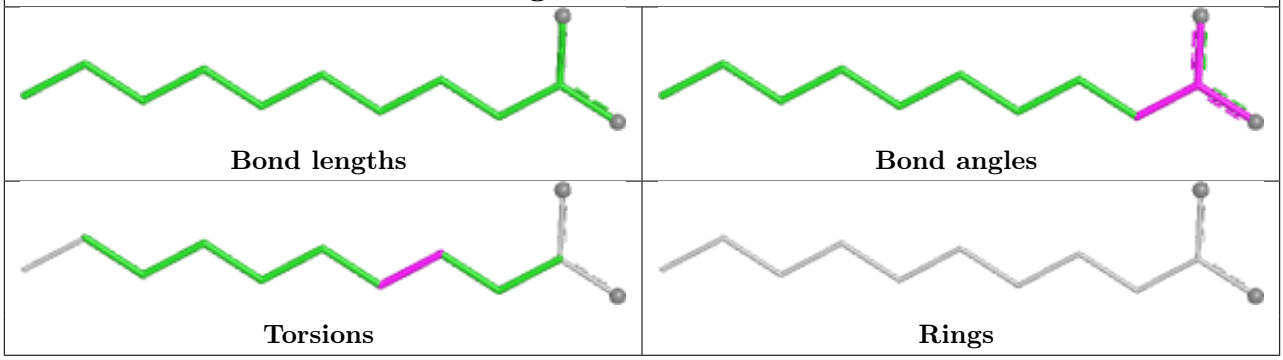
Ligand DGD C 517

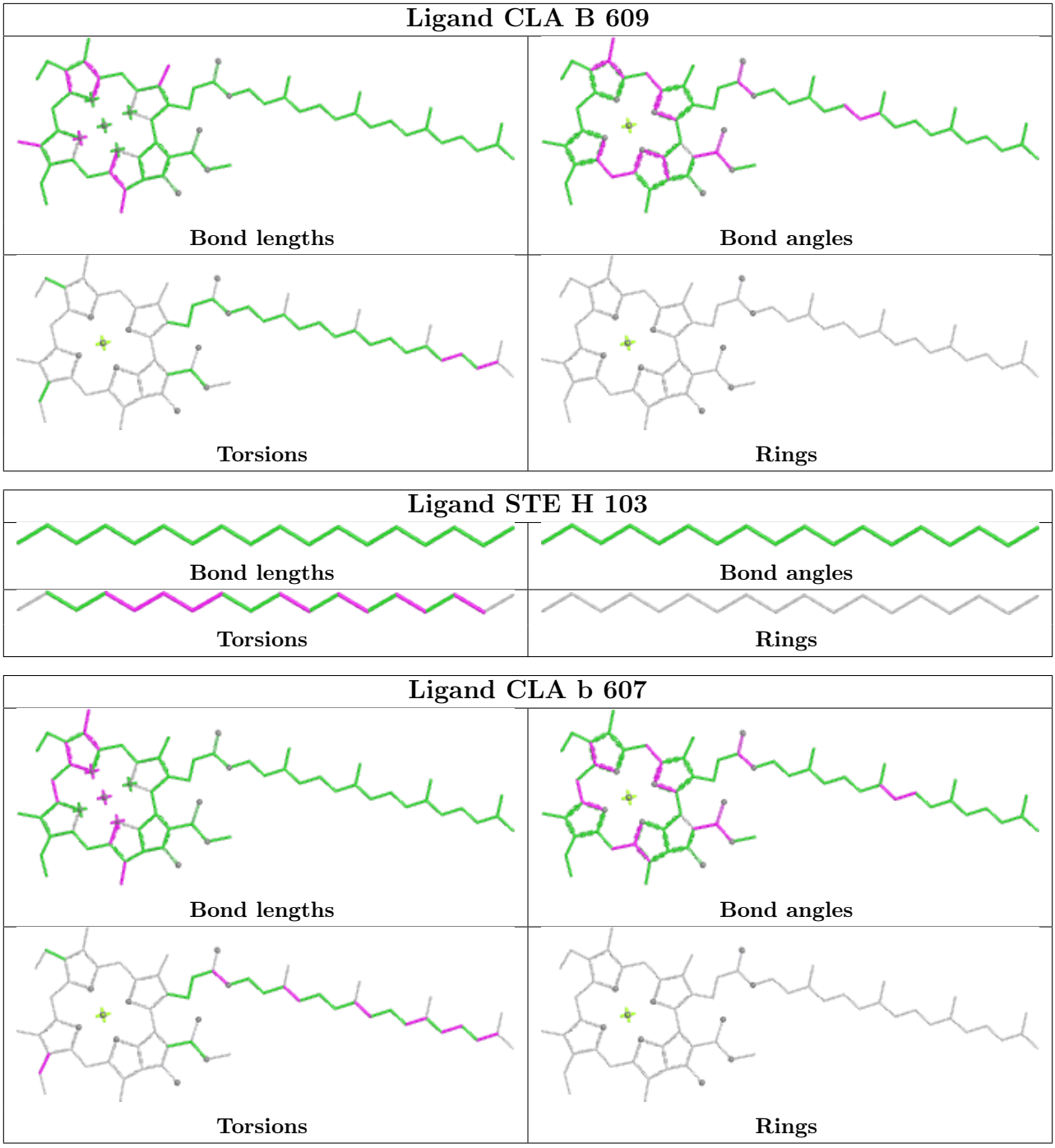


Ligand LMG M 101



Ligand STE B 601





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	30:GLN	C	31:VAL	N	3.77

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%)	-0.49	1 (0%) 90 91	13, 30, 48, 83	60 (17%)
1	a	334/344 (97%)	-0.39	3 (0%) 81 83	13, 32, 58, 87	60 (17%)
2	B	505/510 (99%)	-0.49	2 (0%) 88 90	19, 35, 65, 96	4 (0%)
2	b	505/510 (99%)	-0.35	2 (0%) 88 90	24, 39, 72, 105	0
3	C	442/461 (95%)	-0.42	1 (0%) 91 92	15, 38, 55, 78	7 (1%)
3	c	451/461 (97%)	-0.33	1 (0%) 91 92	15, 42, 64, 101	8 (1%)
4	D	341/352 (96%)	-0.65	0 100 100	16, 32, 48, 85	1 (0%)
4	d	341/352 (96%)	-0.46	0 100 100	17, 36, 57, 82	2 (0%)
5	E	82/84 (97%)	0.09	1 (1%) 76 78	30, 52, 69, 88	1 (1%)
5	e	82/84 (97%)	0.19	1 (1%) 76 78	40, 60, 79, 92	0
6	F	34/45 (75%)	-0.18	0 100 100	37, 43, 64, 84	0
6	f	34/45 (75%)	-0.03	0 100 100	40, 51, 77, 90	0
7	H	65/66 (98%)	-0.31	1 (1%) 72 74	31, 42, 63, 71	0
7	h	63/66 (95%)	0.01	2 (3%) 50 53	39, 50, 68, 78	0
8	I	35/38 (92%)	-0.36	0 100 100	34, 41, 73, 85	0
8	i	35/38 (92%)	-0.06	1 (2%) 53 56	32, 42, 80, 94	0
9	J	36/40 (90%)	-0.26	0 100 100	35, 51, 73, 95	0
9	j	36/40 (90%)	-0.01	0 100 100	36, 53, 91, 102	0
10	K	37/46 (80%)	-0.11	0 100 100	42, 53, 72, 74	0
10	k	37/46 (80%)	-0.01	0 100 100	44, 55, 73, 74	0
11	L	37/37 (100%)	-0.60	0 100 100	28, 33, 68, 75	0
11	l	36/37 (97%)	-0.58	0 100 100	26, 34, 80, 90	0
12	M	32/36 (88%)	-0.50	0 100 100	29, 38, 62, 73	0
12	m	31/36 (86%)	-0.50	0 100 100	28, 37, 56, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.23	3 (1%) 76 78	25, 44, 87, 140	1 (0%)
13	o	244/272 (89%)	-0.23	2 (0%) 82 84	28, 43, 83, 129	0
14	R	34/41 (82%)	0.57	1 (2%) 53 56	58, 71, 95, 110	0
14	r	31/41 (75%)	1.10	3 (9%) 13 14	67, 87, 105, 121	0
15	T	29/32 (90%)	-0.61	0 100 100	27, 33, 67, 86	0
15	t	29/32 (90%)	-0.38	1 (3%) 48 50	30, 35, 83, 94	0
16	U	97/134 (72%)	-0.28	0 100 100	32, 46, 69, 90	0
16	u	97/134 (72%)	-0.36	0 100 100	33, 43, 61, 83	0
17	V	137/163 (84%)	-0.41	0 100 100	31, 42, 59, 83	0
17	v	137/163 (84%)	-0.15	1 (0%) 84 86	33, 48, 72, 85	0
18	X	38/41 (92%)	-0.17	0 100 100	38, 51, 75, 83	0
18	x	39/41 (95%)	0.14	1 (2%) 57 60	47, 58, 88, 103	0
19	Y	27/46 (58%)	0.75	1 (3%) 45 47	54, 72, 90, 111	0
19	y	30/46 (65%)	0.49	0 100 100	63, 69, 90, 101	0
20	Z	62/62 (100%)	0.61	4 (6%) 25 26	53, 66, 112, 120	0
20	z	62/62 (100%)	0.53	2 (3%) 50 53	55, 71, 109, 124	0
All	All	5302/5700 (93%)	-0.31	35 (0%) 84 86	13, 40, 75, 140	144 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	32	GLN	5.1
13	o	58	ASN	4.0
15	t	30	THR	3.7
20	Z	33	TRP	3.3
19	Y	25	ILE	3.3
20	z	33	TRP	3.2
14	R	35	LEU	3.1
20	Z	62	VAL	3.1
14	r	31	VAL	3.1
7	H	41	PHE	3.0
18	x	40	SER	3.0
13	O	59	LYS	2.9
13	O	60	ARG	2.9
13	O	56	PRO	2.7
1	a	250	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
5	e	79	PHE	2.7
20	Z	3	ILE	2.6
20	Z	30	PRO	2.6
3	c	23	ALA	2.6
2	b	495	PHE	2.5
1	a	11	ALA	2.3
8	i	36	ASP	2.3
1	A	13	LEU	2.2
5	E	3	GLY	2.1
2	B	479[A]	PHE	2.1
17	v	21	LEU	2.1
20	z	40	ILE	2.1
7	h	64	ALA	2.1
14	r	27	ALA	2.1
13	o	57	LYS	2.1
7	h	41	PHE	2.1
2	b	84	THR	2.0
1	a	248	ILE	2.0
3	C	43	ILE	2.0
2	B	495	PHE	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
12	FME	M	1	10/11	0.95	0.08	42,52,69,73	0
15	FME	T	1	10/11	0.95	0.07	29,40,67,67	0
15	FME	t	1	10/11	0.95	0.07	27,43,73,73	0
8	FME	I	1	10/11	0.96	0.07	35,42,57,69	0
12	FME	m	1	10/11	0.96	0.07	32,49,65,76	0
8	FME	i	1	10/11	0.97	0.07	37,46,63,63	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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
33	STE	b	626	10/20	0.74	0.17	43,58,68,71	0
33	STE	L	101	12/20	0.78	0.18	45,61,76,80	0
33	STE	H	103	18/20	0.79	0.16	49,70,84,84	0
33	STE	b	625	20/20	0.80	0.15	47,64,79,85	0
33	STE	h	103	14/20	0.80	0.17	50,65,88,91	0
33	STE	E	102	12/20	0.81	0.15	42,72,79,86	0
33	STE	d	412	20/20	0.81	0.14	39,63,81,82	0
28	LMG	B	629	55/55	0.81	0.14	35,58,81,93	0
34	LHG	E	101	49/49	0.81	0.13	46,74,98,118	0
28	LMG	b	623	55/55	0.82	0.16	49,77,101,110	0
33	STE	I	101	15/20	0.82	0.15	38,55,74,78	0
33	STE	a	414	10/20	0.83	0.14	34,65,74,75	0
28	LMG	c	524	48/55	0.83	0.14	47,71,106,116	0
33	STE	B	627	16/20	0.83	0.13	42,64,79,80	0
33	STE	B	601	12/20	0.84	0.14	44,63,83,88	0
33	STE	a	415	12/20	0.84	0.12	39,68,76,84	0
33	STE	c	501	12/20	0.84	0.11	45,66,83,85	0
34	LHG	e	102	42/49	0.84	0.14	61,78,99,119	0
33	STE	j	101	12/20	0.85	0.11	38,54,72,78	0
33	STE	B	628	15/20	0.85	0.15	39,62,75,80	0
29	SQD	a	413	36/54	0.85	0.13	31,61,87,90	0
28	LMG	D	410	33/55	0.86	0.12	33,53,78,93	0
30	DGD	A	415	66/66	0.86	0.11	41,62,85,89	0
33	STE	C	520	12/20	0.86	0.12	45,56,65,65	0
29	SQD	A	414	39/54	0.86	0.13	38,63,93,102	0
33	STE	b	622	20/20	0.86	0.12	39,58,75,78	0
33	STE	b	624	16/20	0.86	0.12	45,61,80,82	0
33	STE	B	626	18/20	0.86	0.12	39,63,82,84	0
33	STE	c	523	20/20	0.87	0.12	40,59,79,87	0
33	STE	b	620	16/20	0.87	0.13	35,50,75,81	0
28	LMG	A	412	48/55	0.88	0.10	36,54,79,101	0
28	LMG	c	525	49/55	0.88	0.11	35,54,95,112	0
33	STE	C	521	16/20	0.88	0.12	38,51,63,70	0
33	STE	B	621	17/20	0.88	0.10	35,49,69,71	0
33	STE	B	625	12/20	0.88	0.12	42,55,66,66	0
27	PL9	a	410	55/55	0.88	0.13	36,67,87,103	0
28	LMG	c	522	37/55	0.88	0.11	42,64,82,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	STE	B	624	14/20	0.89	0.10	32,49,66,66	0
22	CLA	h	101	65/65	0.89	0.10	37,64,87,99	0
27	PL9	A	410	55/55	0.89	0.12	35,65,88,95	0
33	STE	T	102	15/20	0.89	0.12	41,57,79,85	0
33	STE	l	102	18/20	0.89	0.12	33,50,77,89	0
33	STE	C	522	12/20	0.89	0.10	35,48,54,55	0
29	SQD	b	619	49/54	0.89	0.10	42,60,97,99	0
33	STE	Z	102	8/20	0.90	0.14	43,56,67,67	0
24	BCR	Z	101	40/40	0.90	0.11	38,56,69,70	0
33	STE	d	411	20/20	0.90	0.11	33,57,73,77	0
29	SQD	B	623	54/54	0.90	0.09	38,58,94,100	0
33	STE	J	101	12/20	0.90	0.10	45,60,72,73	0
28	LMG	b	621	51/55	0.90	0.10	29,51,77,92	0
33	STE	M	103	10/20	0.90	0.11	33,49,60,63	0
28	LMG	C	519	48/55	0.90	0.11	34,67,87,93	0
33	STE	X	101	20/20	0.90	0.10	27,50,73,76	0
24	BCR	c	516	40/40	0.91	0.09	43,58,71,73	0
26	BCT	a	409	4/4	0.91	0.10	26,33,40,48	0
24	BCR	Y	101	40/40	0.91	0.09	34,49,67,72	0
22	CLA	C	514	65/65	0.91	0.10	39,62,91,98	0
28	LMG	D	411	28/55	0.91	0.11	25,49,62,67	0
33	STE	M	102	15/20	0.92	0.10	34,48,62,68	0
29	SQD	f	101	41/54	0.92	0.12	47,78,110,116	0
33	STE	d	410	17/20	0.92	0.09	38,52,60,66	0
22	CLA	B	602	65/65	0.92	0.10	30,57,92,101	0
30	DGD	h	102	62/66	0.92	0.09	24,49,65,74	0
29	SQD	a	412	54/54	0.93	0.10	38,64,93,96	0
24	BCR	D	404	40/40	0.93	0.08	24,42,81,90	0
24	BCR	c	518	40/40	0.93	0.10	39,51,61,68	0
24	BCR	d	404	40/40	0.93	0.09	28,48,86,102	0
28	LMG	M	101	51/55	0.93	0.08	26,48,73,85	0
30	DGD	C	517	62/66	0.93	0.09	27,50,99,120	0
30	DGD	H	102	62/66	0.93	0.08	26,43,58,61	0
24	BCR	x	101	40/40	0.93	0.08	29,48,66,73	0
24	BCR	y	101	40/40	0.93	0.09	38,59,75,79	0
24	BCR	H	101	40/40	0.93	0.09	22,44,58,70	0
22	CLA	c	514	65/65	0.93	0.09	36,55,95,110	0
22	CLA	c	513	65/65	0.93	0.09	38,53,68,75	0
24	BCR	b	617	40/40	0.93	0.07	25,40,55,61	0
24	BCR	b	618	40/40	0.93	0.08	26,44,66,67	0
29	SQD	D	407	36/54	0.93	0.10	43,66,86,99	0
24	BCR	c	517	40/40	0.94	0.08	25,43,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	513	65/65	0.94	0.09	33,54,85,98	0
24	BCR	K	101	40/40	0.94	0.09	30,48,58,62	0
28	LMG	d	409	44/55	0.94	0.09	28,50,79,91	0
29	SQD	A	413	52/54	0.94	0.09	28,56,88,98	0
30	DGD	c	520	62/66	0.94	0.08	32,50,88,94	0
23	PHO	d	401	64/64	0.94	0.07	26,37,46,48	0
24	BCR	B	619	40/40	0.94	0.07	23,38,49,57	0
24	BCR	B	620	40/40	0.94	0.07	26,41,58,69	0
24	BCR	C	515	40/40	0.94	0.08	25,41,53,65	0
34	LHG	d	406	49/49	0.94	0.10	32,48,82,87	0
22	CLA	c	515	65/65	0.94	0.10	39,66,105,110	0
22	CLA	c	508	65/65	0.95	0.09	27,46,95,106	0
27	PL9	d	405	55/55	0.95	0.06	19,34,45,46	0
22	CLA	c	510	64/65	0.95	0.08	30,45,86,105	0
30	DGD	C	516	62/66	0.95	0.08	21,39,75,91	0
22	CLA	c	511	65/65	0.95	0.07	30,45,62,67	0
30	DGD	C	518	62/66	0.95	0.08	26,46,75,85	0
24	BCR	T	101	40/40	0.95	0.06	21,38,55,67	0
28	LMG	D	406	51/55	0.95	0.10	28,54,88,96	0
30	DGD	c	521	62/66	0.95	0.09	28,52,93,108	0
22	CLA	c	512	65/65	0.95	0.07	30,46,62,71	0
22	CLA	C	506	65/65	0.95	0.09	23,40,69,82	0
24	BCR	b	616	40/40	0.95	0.07	21,41,52,59	0
22	CLA	C	511	65/65	0.95	0.07	26,43,58,66	0
22	CLA	C	512	65/65	0.95	0.08	27,48,66,70	0
22	CLA	d	403	65/65	0.95	0.09	26,46,89,103	0
22	CLA	B	607	65/65	0.95	0.08	21,35,74,78	0
22	CLA	C	504	65/65	0.95	0.07	24,40,54,56	0
24	BCR	A	406	40/40	0.95	0.07	22,34,47,51	0
24	BCR	t	101	40/40	0.95	0.06	23,38,51,53	0
24	BCR	B	618	40/40	0.95	0.07	27,39,57,69	0
22	CLA	b	605	65/65	0.95	0.08	25,39,73,80	0
22	CLA	b	608	65/65	0.95	0.08	29,43,57,64	0
22	CLA	c	504	65/65	0.95	0.07	27,42,62,69	0
34	LHG	d	408	39/49	0.95	0.08	28,45,68,75	0
27	PL9	D	405	55/55	0.95	0.06	20,33,48,49	0
34	LHG	l	101	49/49	0.95	0.08	31,43,60,69	0
26	BCT	A	409	4/4	0.96	0.09	31,33,36,43	0
22	CLA	c	507	65/65	0.96	0.07	25,39,67,76	0
22	CLA	C	503	65/65	0.96	0.07	24,39,61,66	0
22	CLA	c	509	65/65	0.96	0.07	27,43,57,64	0
22	CLA	B	605	65/65	0.96	0.07	19,34,72,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	505	59/65	0.96	0.08	27,40,78,90	0
22	CLA	A	402	65/65	0.96	0.06	15,27,42,61	0
22	CLA	C	507	65/65	0.96	0.09	22,40,87,99	0
22	CLA	C	508	65/65	0.96	0.07	21,38,53,59	0
22	CLA	C	509	65/65	0.96	0.07	25,43,98,114	0
22	CLA	d	402	65/65	0.96	0.06	18,35,52,67	0
22	CLA	C	510	65/65	0.96	0.08	24,43,64,68	0
22	CLA	B	610	65/65	0.96	0.07	23,37,58,69	0
23	PHO	D	401	64/64	0.96	0.05	23,34,44,48	0
22	CLA	B	611	65/65	0.96	0.07	19,33,46,47	0
22	CLA	B	613	65/65	0.96	0.07	17,33,49,53	0
22	CLA	B	615	65/65	0.96	0.08	22,35,80,90	0
22	CLA	a	403	65/65	0.96	0.09	24,41,95,107	0
22	CLA	a	405	65/65	0.96	0.07	18,38,79,87	0
22	CLA	a	411	65/65	0.96	0.06	19,29,45,50	0
22	CLA	b	601	65/65	0.96	0.07	25,42,62,70	0
22	CLA	b	602	65/65	0.96	0.07	22,36,67,77	0
22	CLA	b	604	65/65	0.96	0.06	18,35,50,58	0
22	CLA	B	616	65/65	0.96	0.07	22,36,61,64	0
22	CLA	b	607	65/65	0.96	0.06	23,39,59,62	0
22	CLA	B	617	60/65	0.96	0.08	21,38,87,94	0
24	BCR	a	406	40/40	0.96	0.06	19,33,47,52	0
22	CLA	b	609	65/65	0.96	0.07	23,39,51,57	0
22	CLA	b	610	65/65	0.96	0.06	21,34,53,59	0
22	CLA	b	611	65/65	0.96	0.07	21,35,52,56	0
22	CLA	b	613	65/65	0.96	0.07	22,40,81,91	0
22	CLA	b	614	65/65	0.96	0.07	23,39,56,60	0
30	DGD	c	519	62/66	0.96	0.08	22,41,74,96	0
34	LHG	D	408	49/49	0.96	0.07	18,41,53,59	0
34	LHG	D	409	47/49	0.96	0.09	27,48,87,104	0
34	LHG	D	412	49/49	0.96	0.08	27,43,71,77	0
22	CLA	b	615	60/65	0.96	0.08	26,42,84,93	0
22	CLA	c	503	65/65	0.96	0.06	22,40,53,61	0
22	CLA	C	502	65/65	0.96	0.07	20,34,53,55	0
22	CLA	c	505	65/65	0.96	0.07	30,43,53,59	0
22	CLA	c	506	60/65	0.96	0.07	29,42,79,84	0
22	CLA	a	402	65/65	0.97	0.05	18,29,47,59	0
22	CLA	B	603	65/65	0.97	0.06	22,37,54,60	0
22	CLA	B	612	65/65	0.97	0.06	21,32,51,52	0
23	PHO	A	404	64/64	0.97	0.05	18,28,37,39	0
22	CLA	B	604	65/65	0.97	0.06	17,34,61,63	0
23	PHO	a	404	64/64	0.97	0.05	17,31,42,45	0

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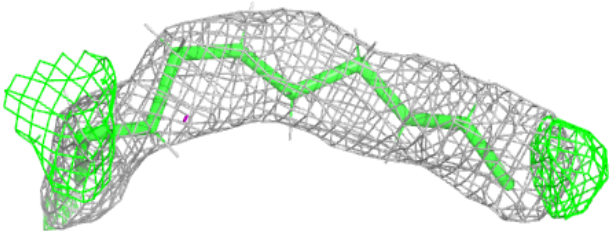
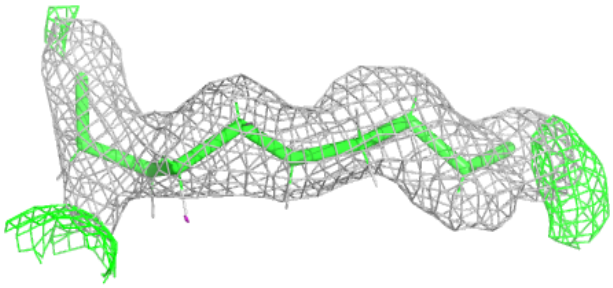
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	B	614	65/65	0.97	0.07	18,31,67,71	0
22	CLA	A	405	54/65	0.97	0.06	18,33,61,69	0
22	CLA	b	603	65/65	0.97	0.07	17,37,85,98	0
22	CLA	B	606	65/65	0.97	0.07	21,33,47,52	0
34	LHG	B	622	49/49	0.97	0.06	25,41,56,64	0
22	CLA	A	411	65/65	0.97	0.06	16,27,54,64	0
22	CLA	b	606	65/65	0.97	0.07	19,36,71,78	0
22	CLA	B	608	65/65	0.97	0.07	17,34,65,74	0
22	CLA	B	609	65/65	0.97	0.06	21,36,57,63	0
22	CLA	A	403	65/65	0.97	0.07	22,36,90,100	0
34	LHG	d	407	49/49	0.97	0.07	25,42,55,61	0
22	CLA	D	402	65/65	0.97	0.06	13,30,52,59	0
22	CLA	D	403	65/65	0.97	0.07	21,42,102,116	0
22	CLA	b	612	65/65	0.97	0.06	19,33,72,90	0
35	HEC	F	101	43/43	0.97	0.08	26,44,64,66	0
35	HEC	e	101	43/43	0.97	0.08	36,52,72,81	0
35	HEC	V	201	43/43	0.98	0.06	21,31,44,53	0
35	HEC	v	201	43/43	0.98	0.07	25,37,45,48	0
25	CL	A	407	1/1	0.99	0.02	27,27,27,27	0
25	CL	a	407	1/1	0.99	0.04	28,28,28,28	0
25	CL	a	408	1/1	0.99	0.08	28,28,28,28	0
31	OEX	A	416[A]	10/10	0.99	0.03	25,30,31,31	10
31	OEX	a	416[A]	10/10	0.99	0.03	27,28,30,30	10
32	OEY	A	417[B]	11/11	0.99	0.03	21,27,31,34	11
32	OEY	a	417[B]	11/11	0.99	0.03	22,26,28,31	11
21	FE2	A	401	1/1	1.00	0.01	26,26,26,26	0
25	CL	A	408	1/1	1.00	0.04	28,28,28,28	0
21	FE2	a	401	1/1	1.00	0.01	34,34,34,34	0

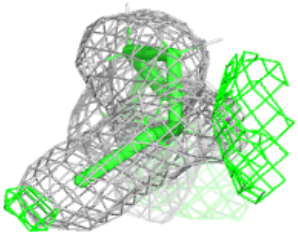
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE b 626:

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

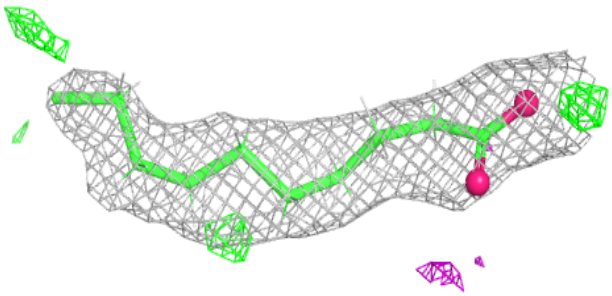


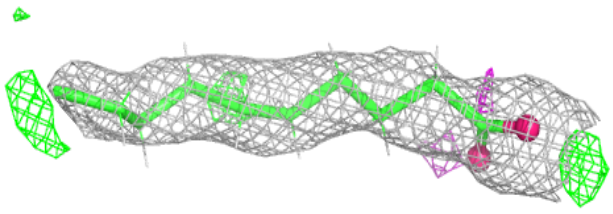


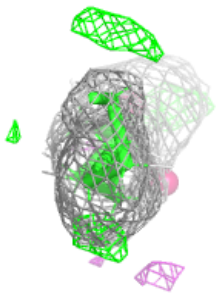


Electron density around STE L 101:

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

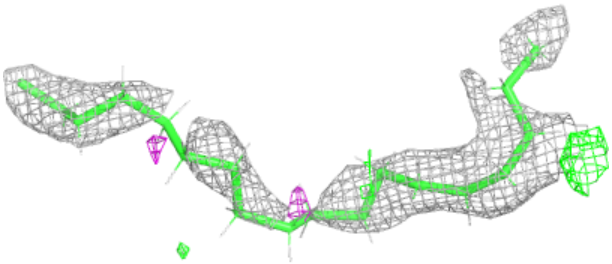


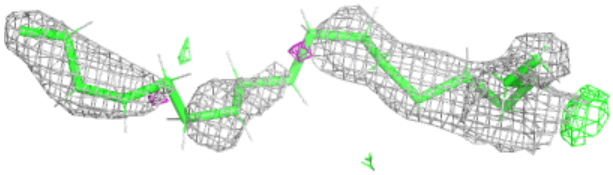


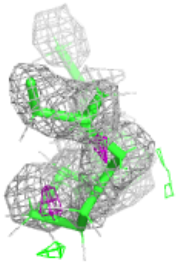


Electron density around STE H 103:

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

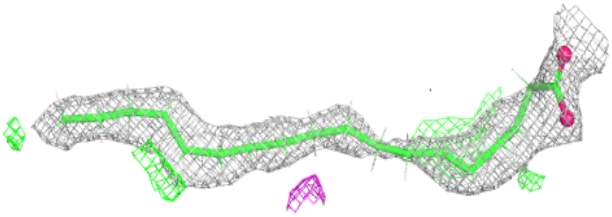


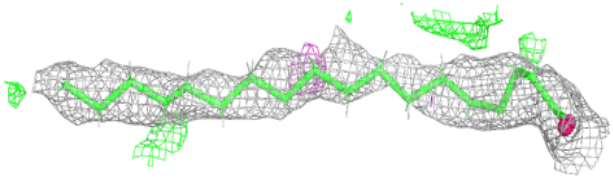


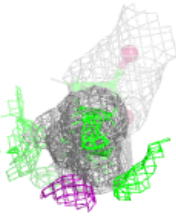


Electron density around STE b 625:

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

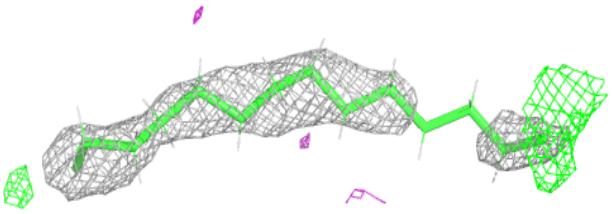


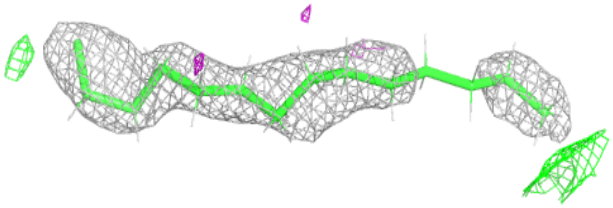


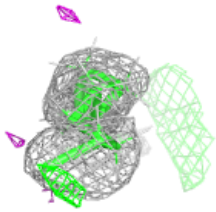


Electron density around STE h 103:

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

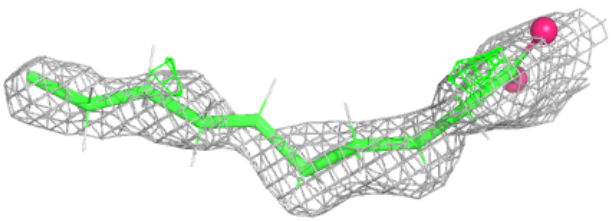


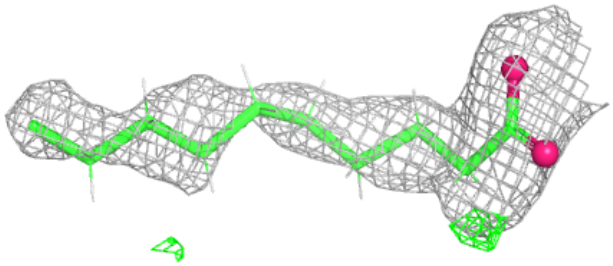


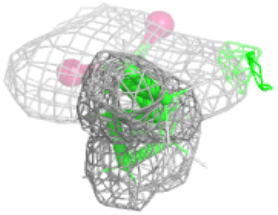


Electron density around STE E 102:

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

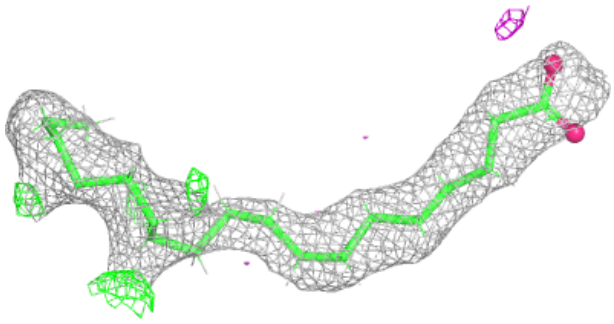


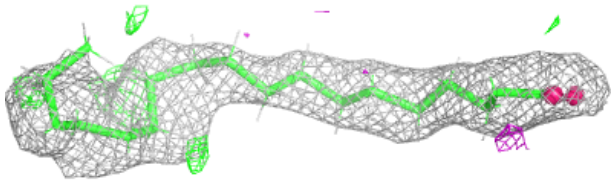


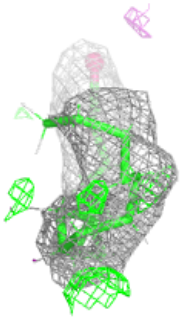


Electron density around STE d 412:

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

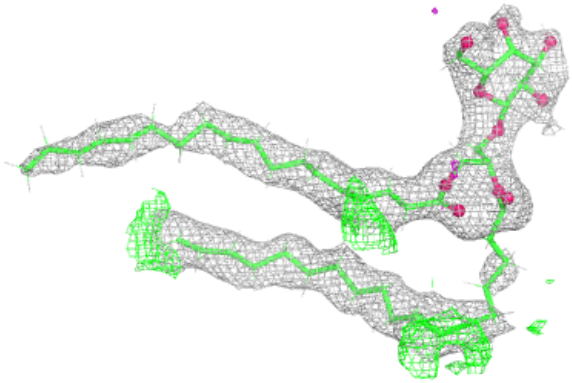


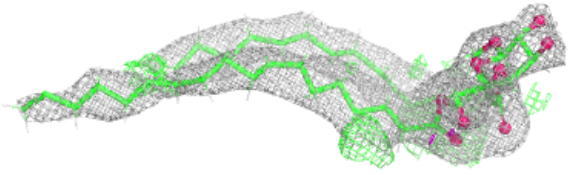




Electron density around LMG B 629:

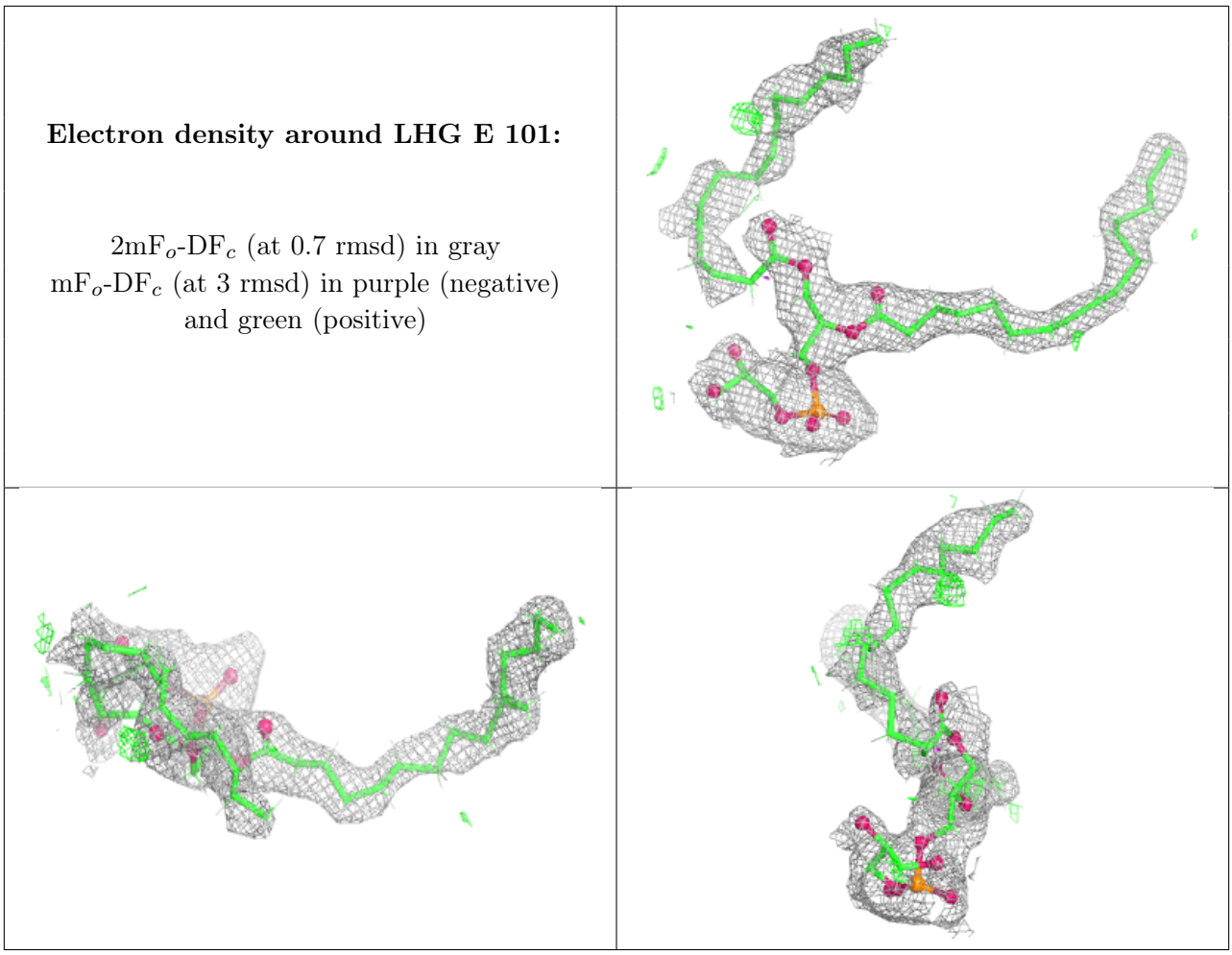
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





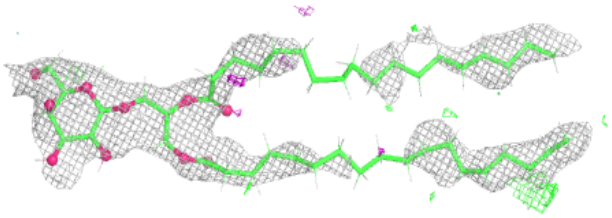
Electron density around LHG E 101:

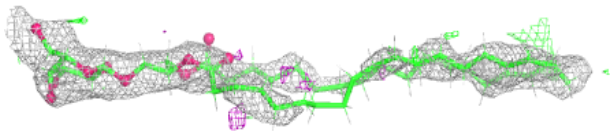
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

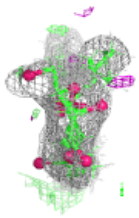


Electron density around LMG b 623:

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

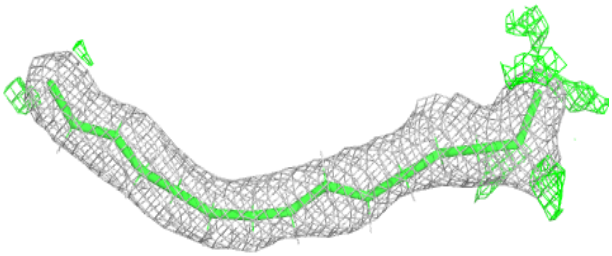


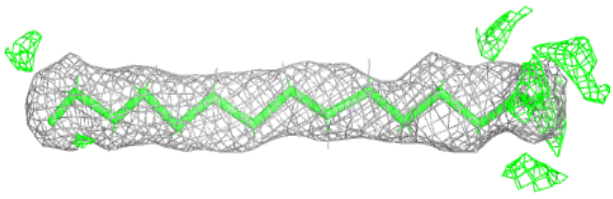


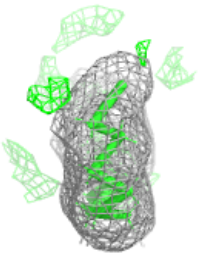


Electron density around STE I 101:

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

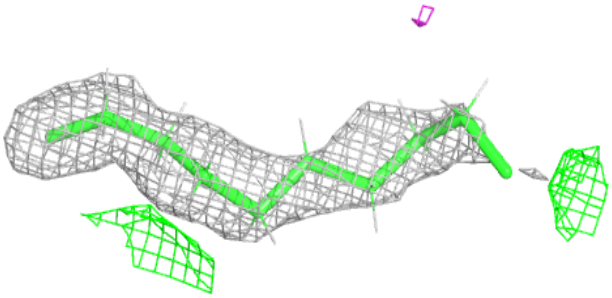


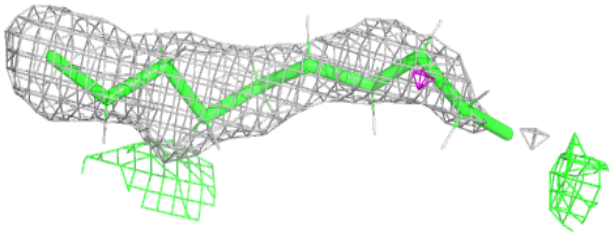


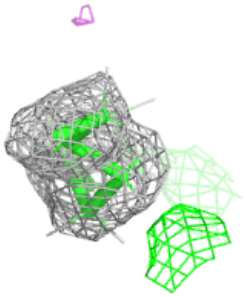


Electron density around STE a 414:

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

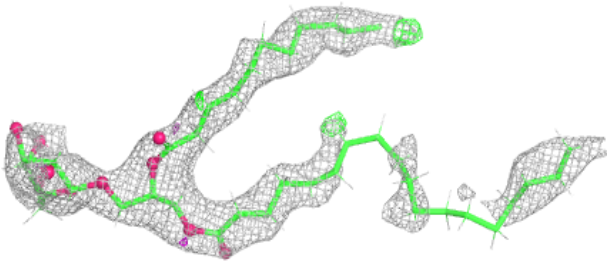


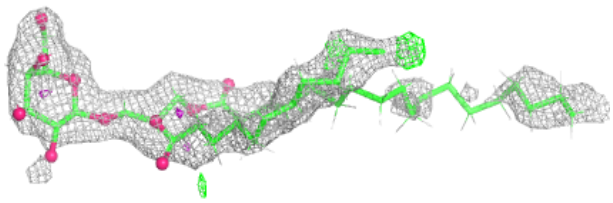


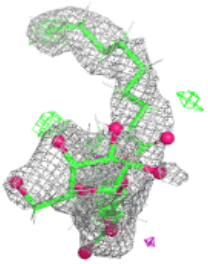


Electron density around LMG c 524:

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

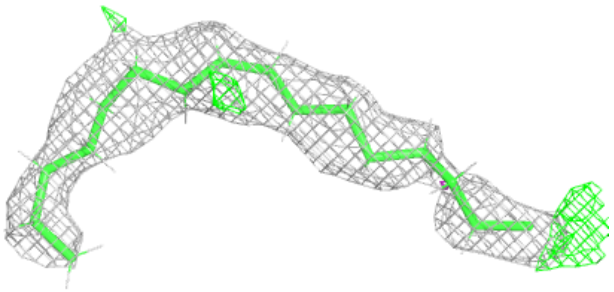


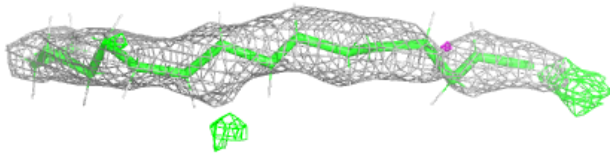


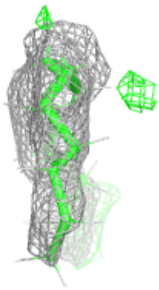


Electron density around STE B 627:

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

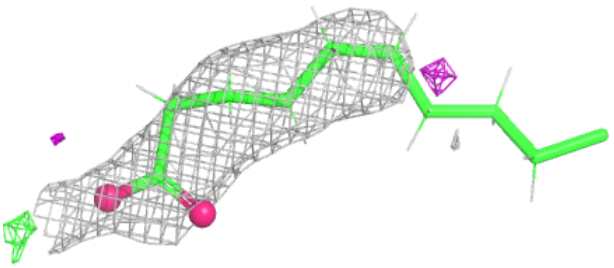


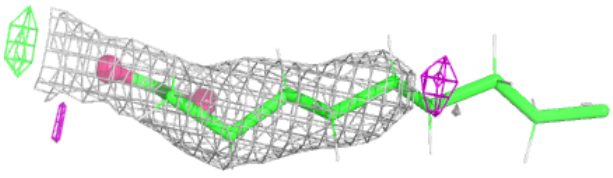


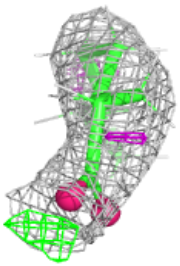


Electron density around STE B 601:

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

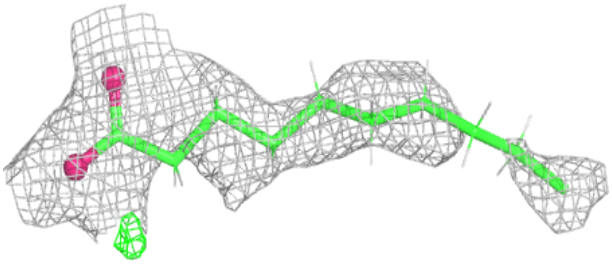


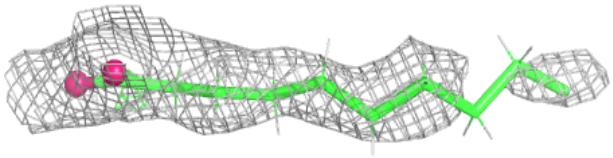


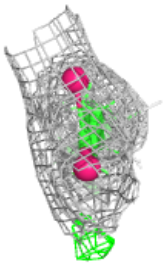


Electron density around STE a 415:

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

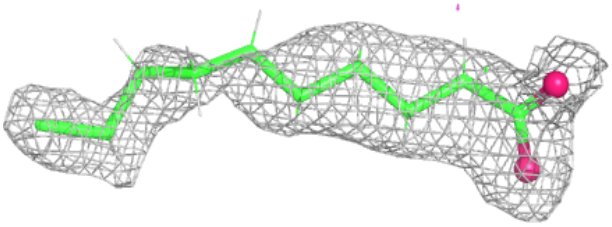


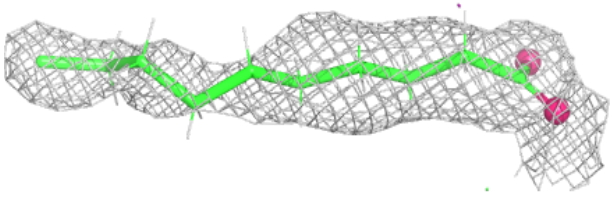


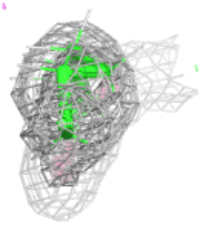


Electron density around STE c 501:

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

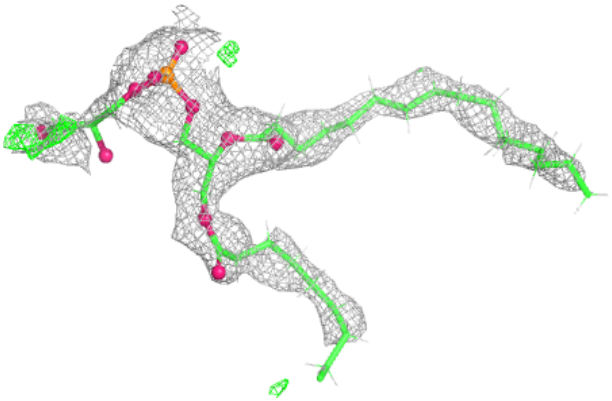


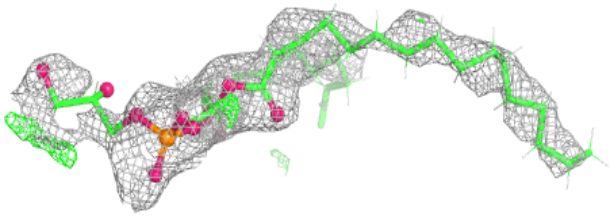


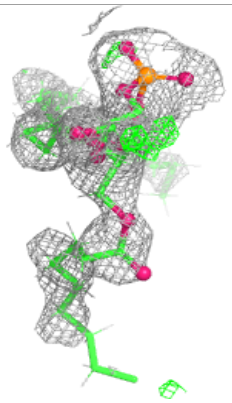


Electron density around LHG e 102:

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

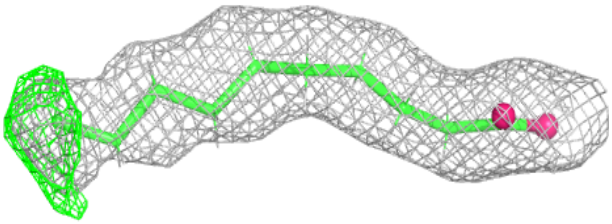


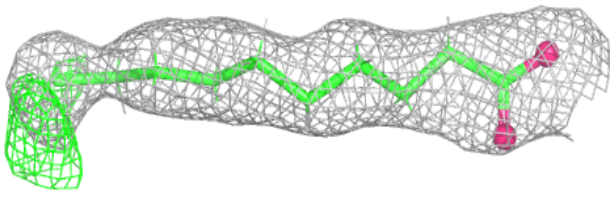


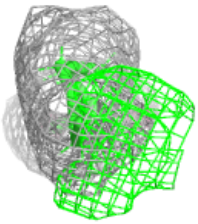


Electron density around STE j 101:

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

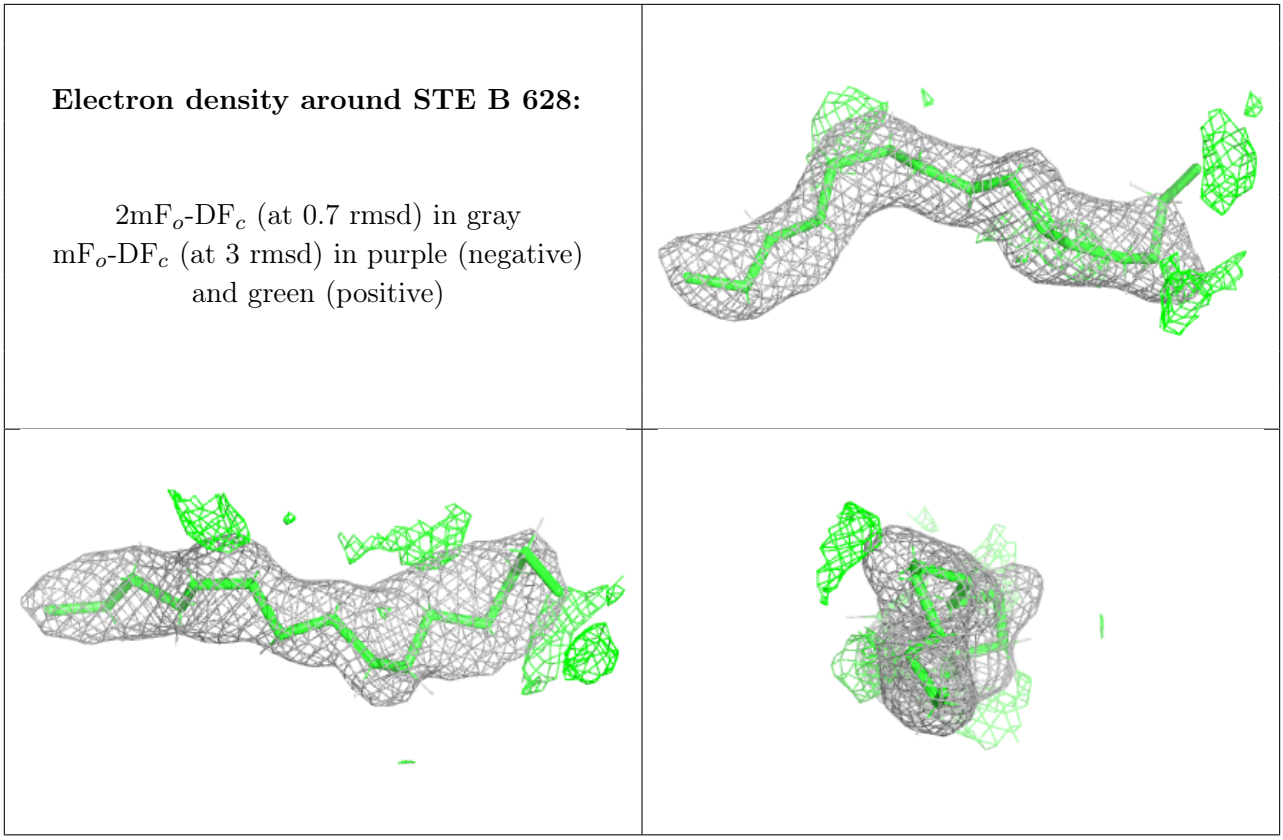






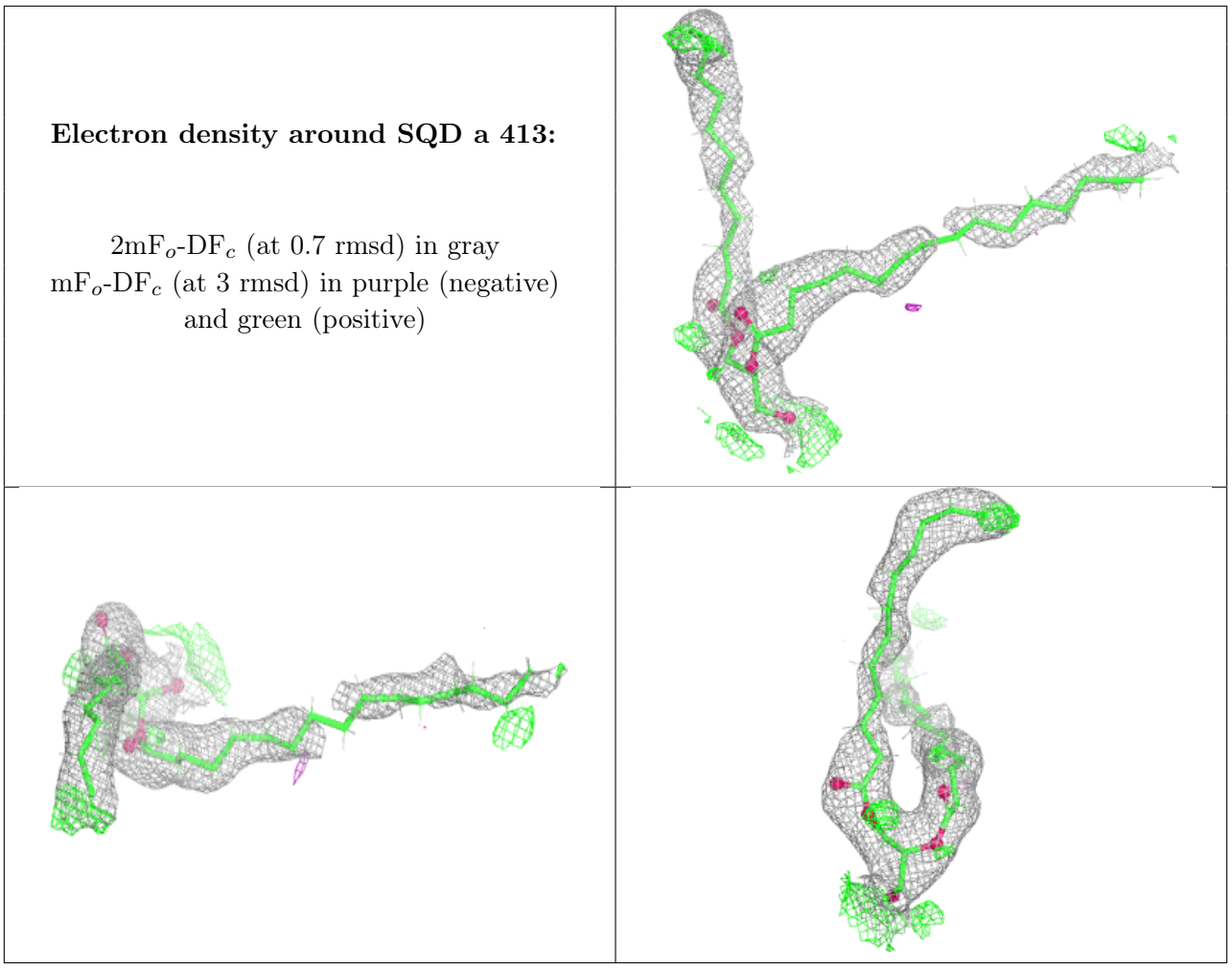
Electron density around STE B 628:

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



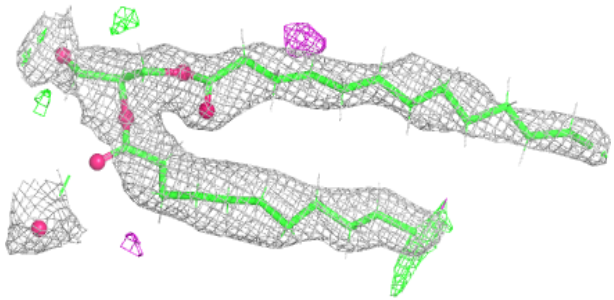
Electron density around SQD a 413:

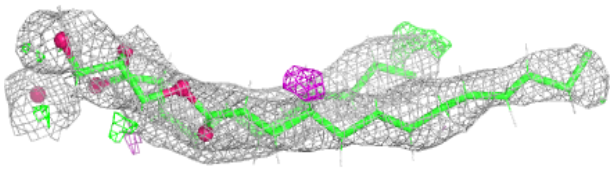
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

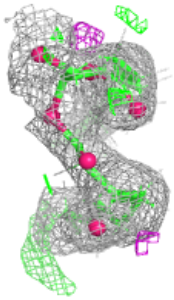


Electron density around LMG D 410:

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

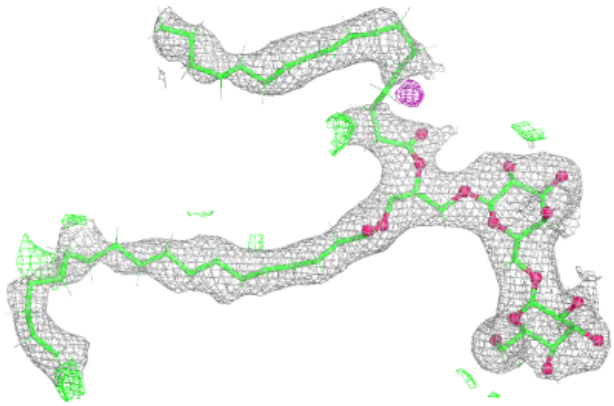


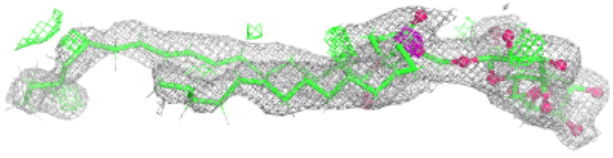




Electron density around DGD A 415:

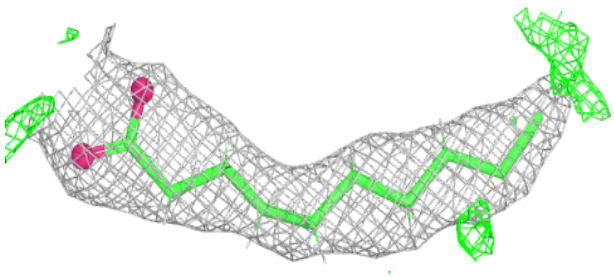
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

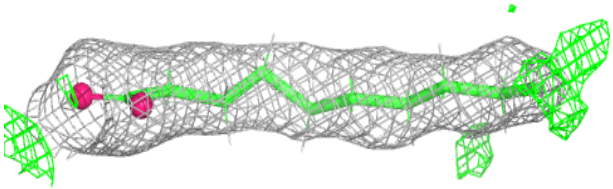


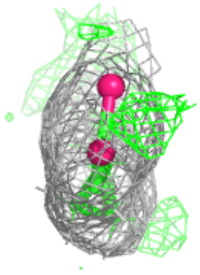


Electron density around STE C 520:

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

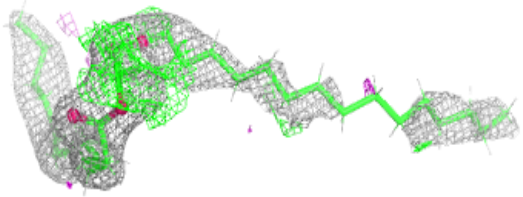


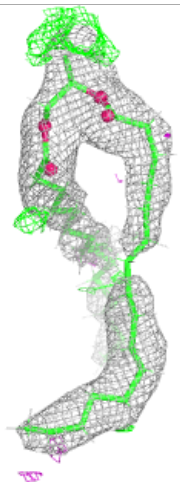




Electron density around SQD A 414:

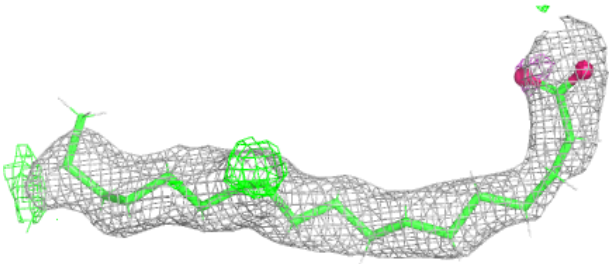
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

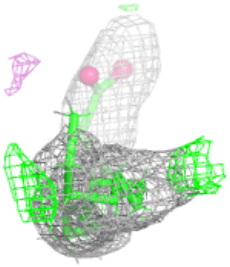




Electron density around STE b 622:

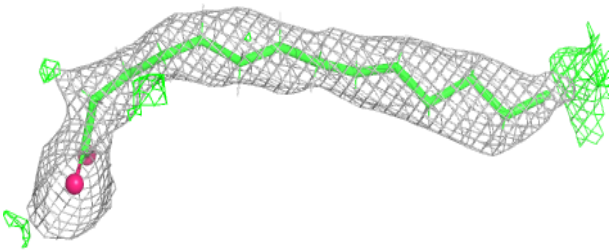
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

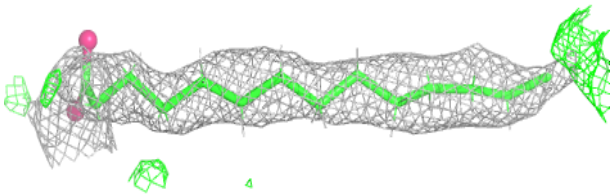


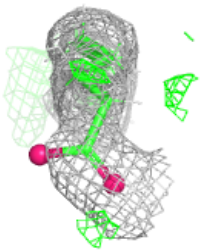


Electron density around STE b 624:

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

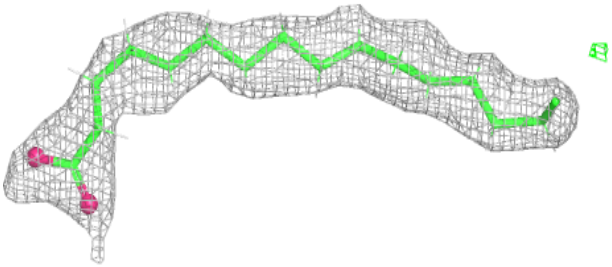


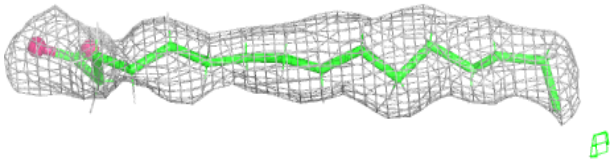


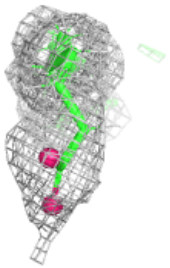


Electron density around STE B 626:

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

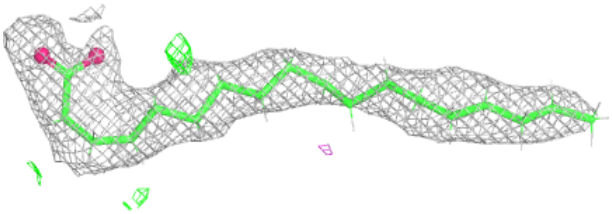


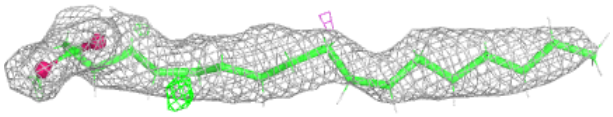


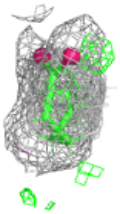


Electron density around STE c 523:

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

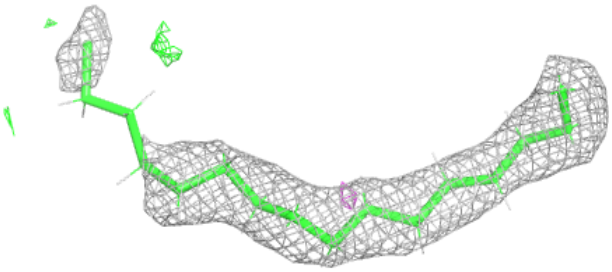


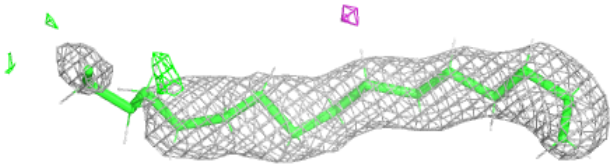


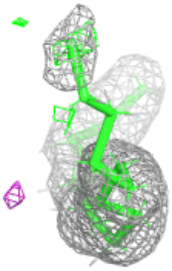


Electron density around STE b 620:

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

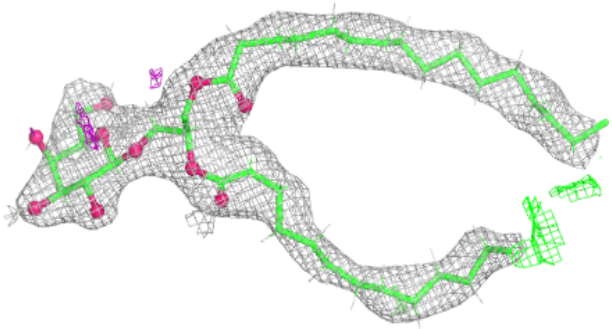


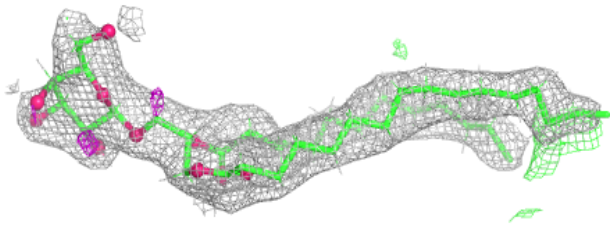


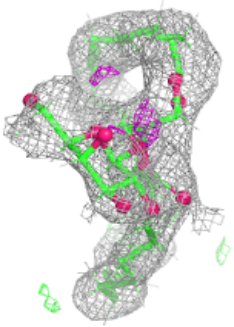


Electron density around LMG A 412:

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

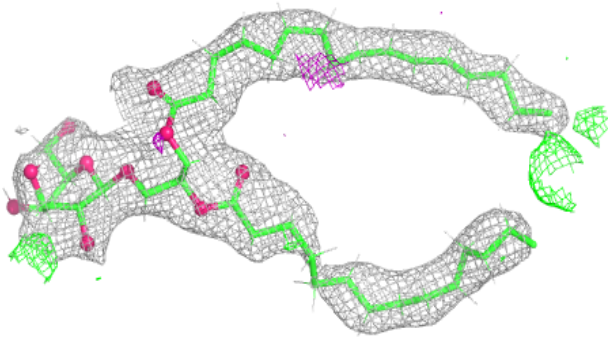


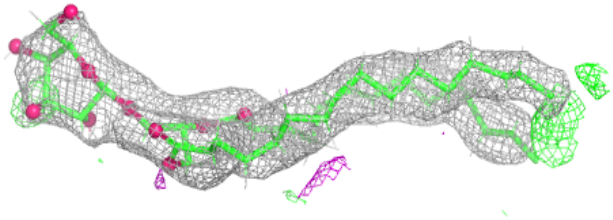


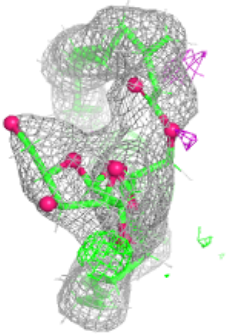


Electron density around LMG c 525:

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

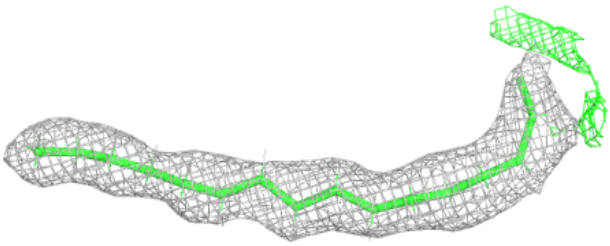


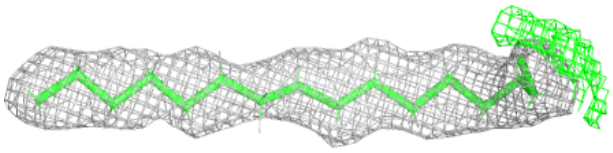


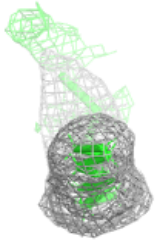


Electron density around STE C 521:

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

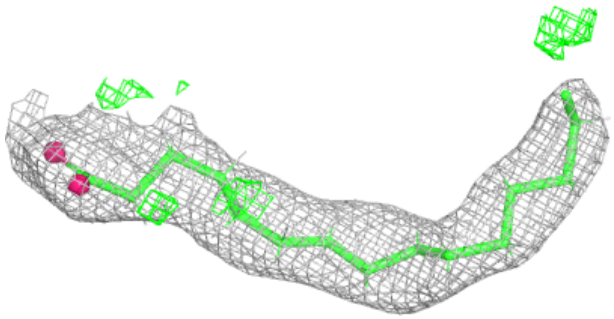


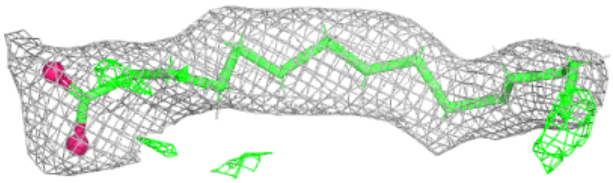


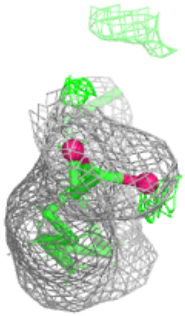


Electron density around STE B 621:

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

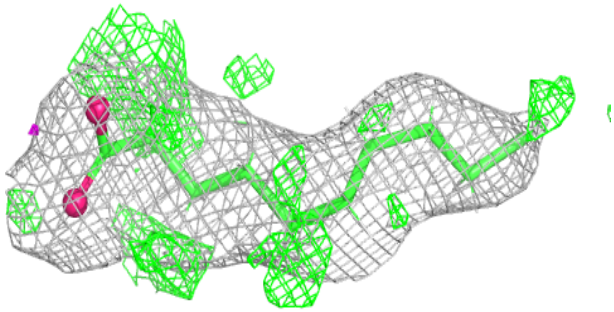


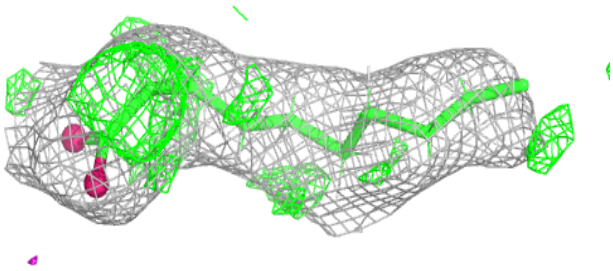


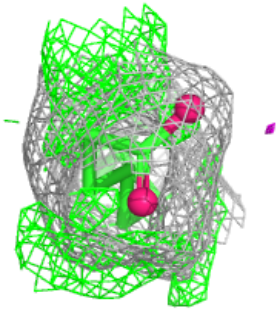


Electron density around STE B 625:

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

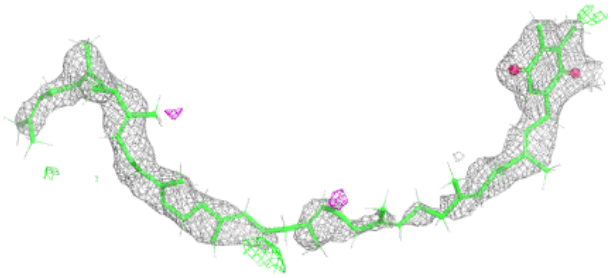


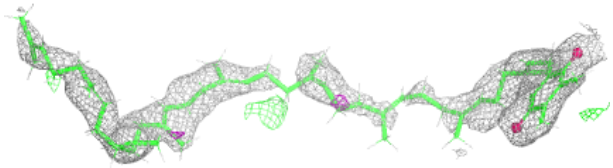


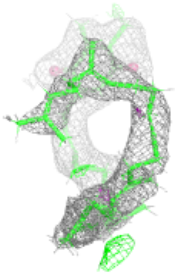


Electron density around PL9 a 410:

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

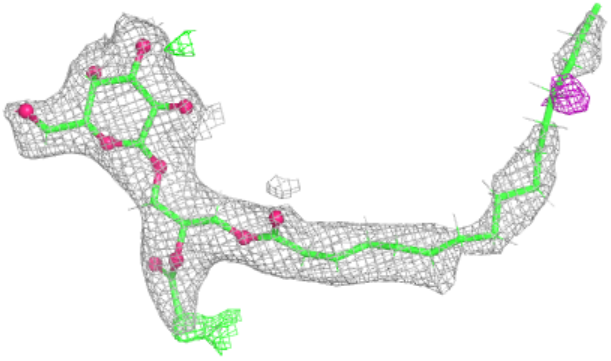


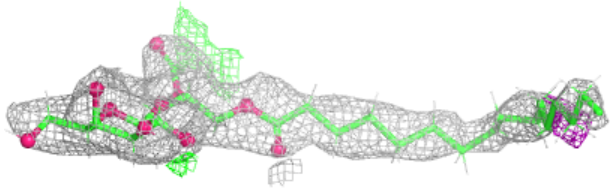


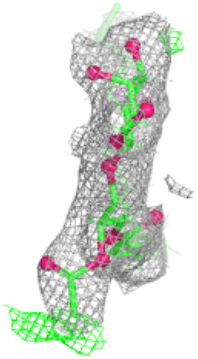


Electron density around LMG c 522:

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

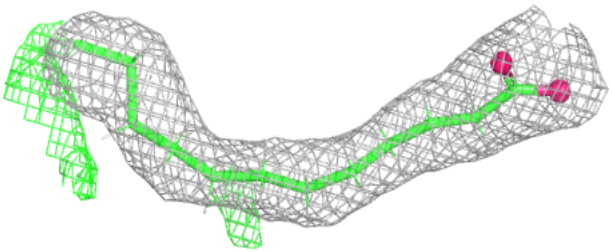


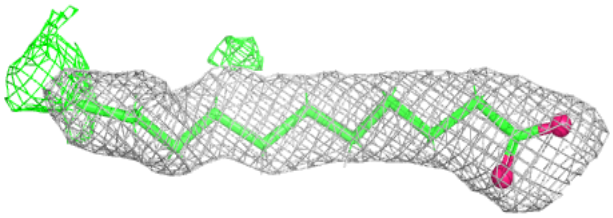


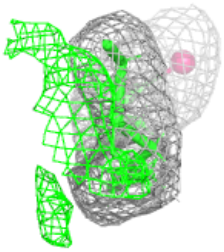


Electron density around STE B 624:

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

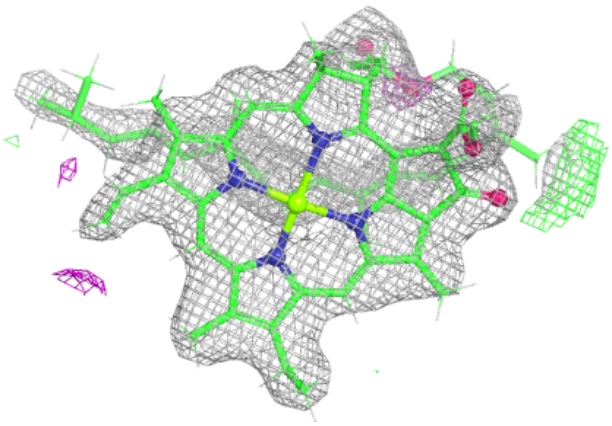


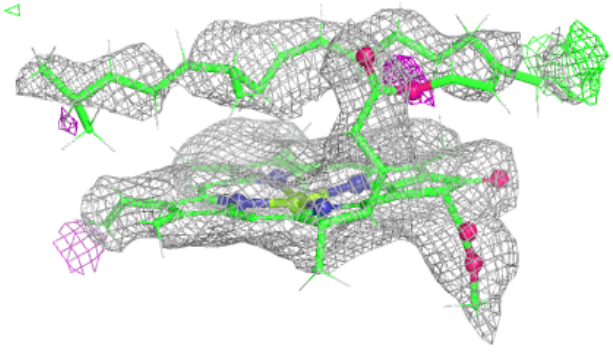


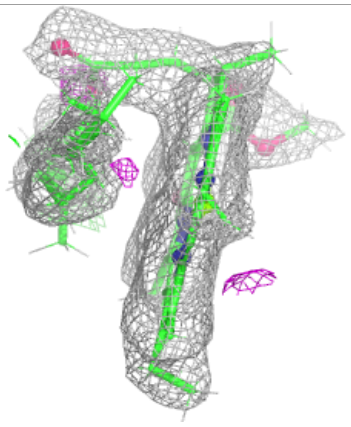


Electron density around CLA h 101:

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

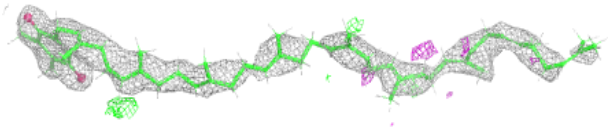


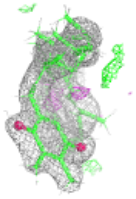




Electron density around PL9 A 410:

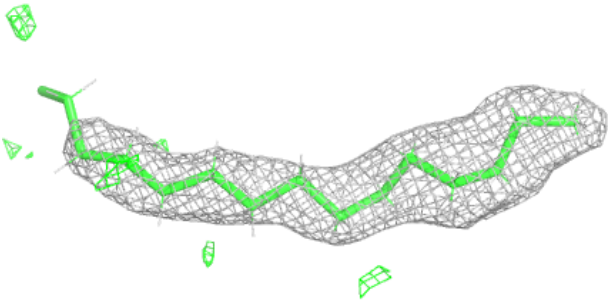
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

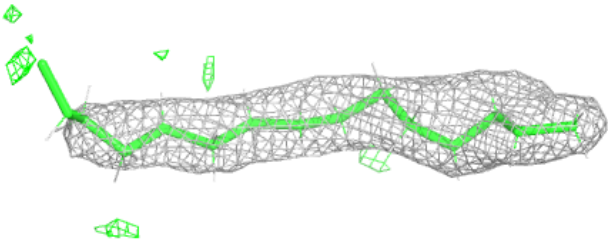


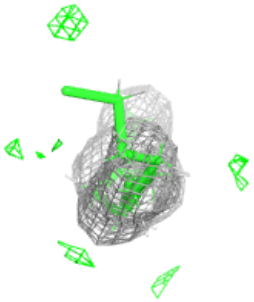


Electron density around STE T 102:

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

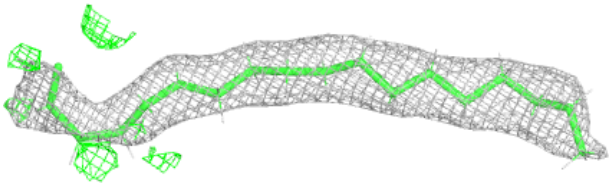


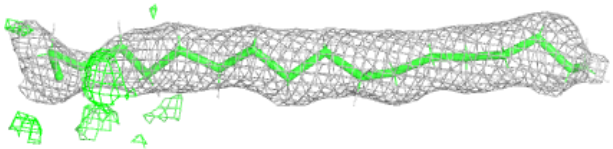


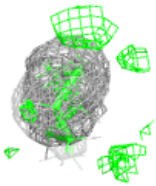


Electron density around STE l 102:

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

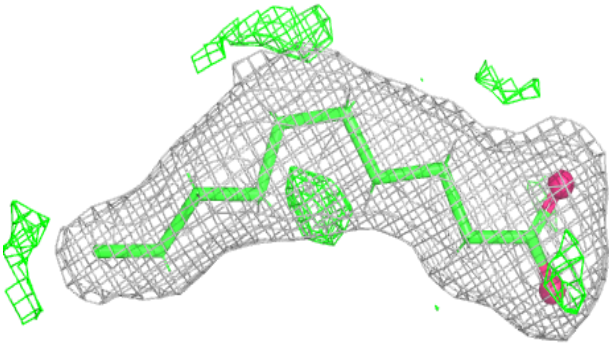


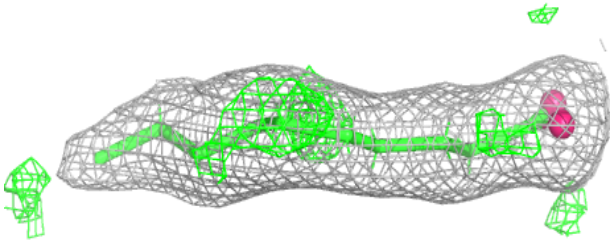


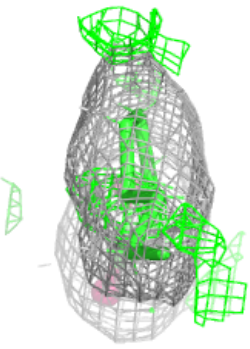


Electron density around STE C 522:

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

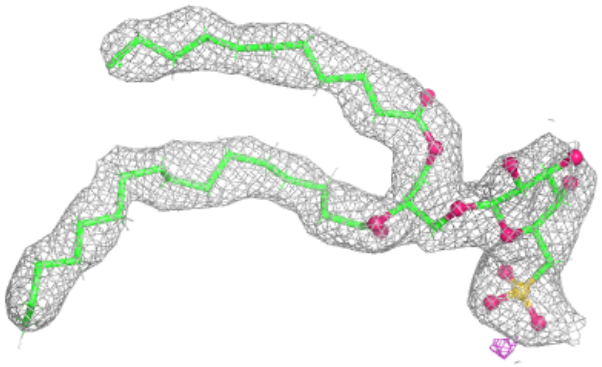


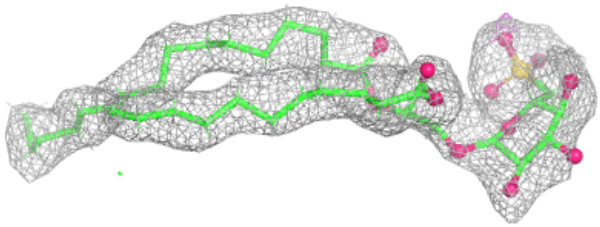


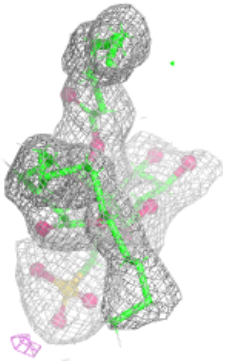


Electron density around SQD b 619:

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

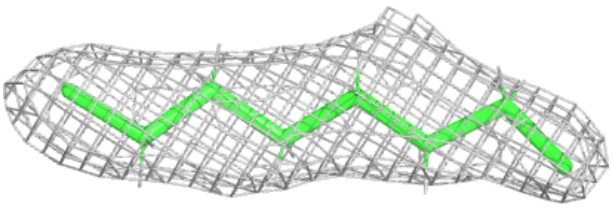


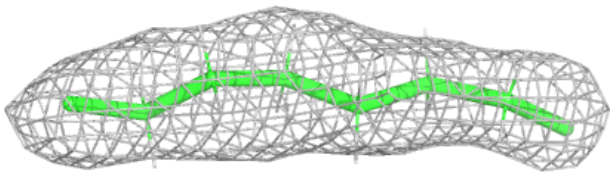


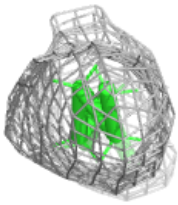


Electron density around STE Z 102:

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

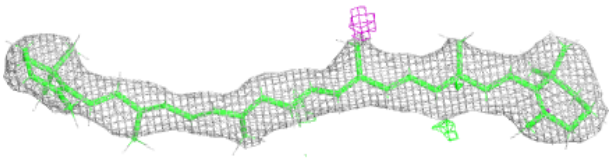


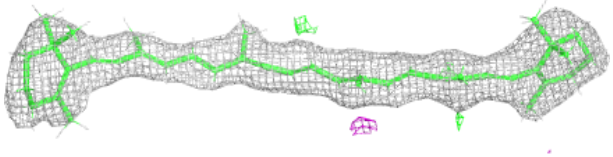


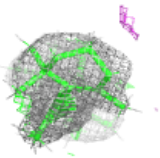


Electron density around BCR Z 101:

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

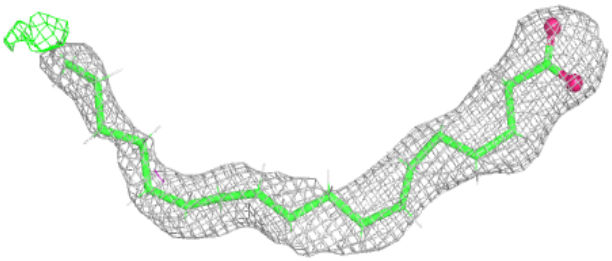


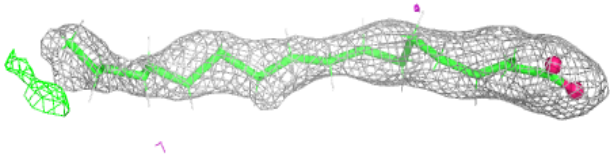


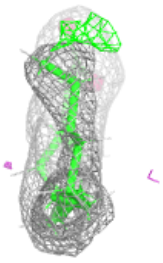


Electron density around STE d 411:

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

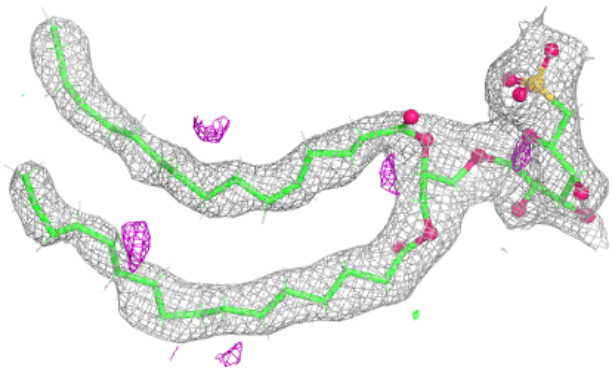


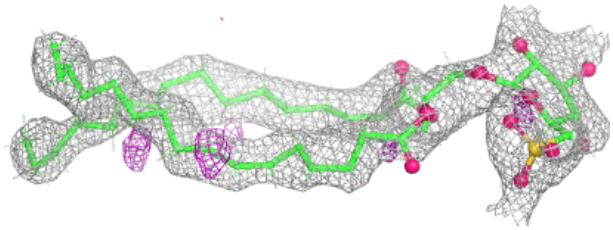


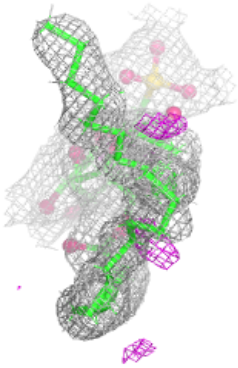


Electron density around SQD B 623:

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

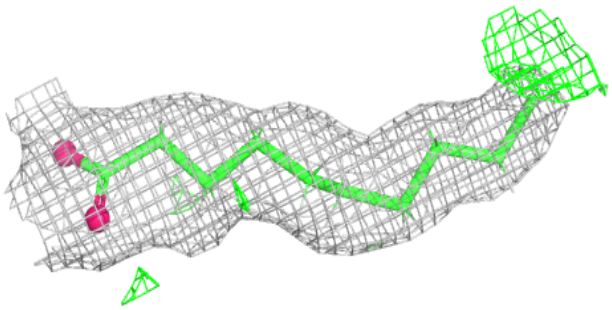


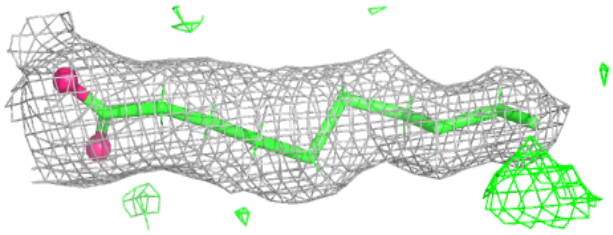


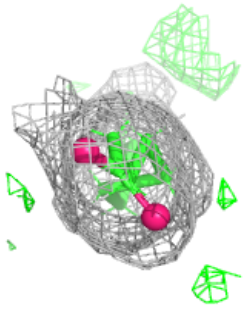


Electron density around STE J 101:

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

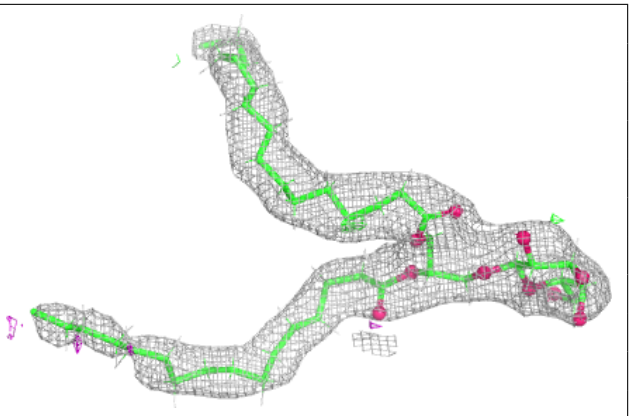


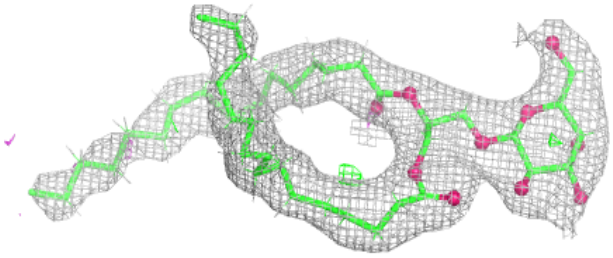




Electron density around LMG b 621:

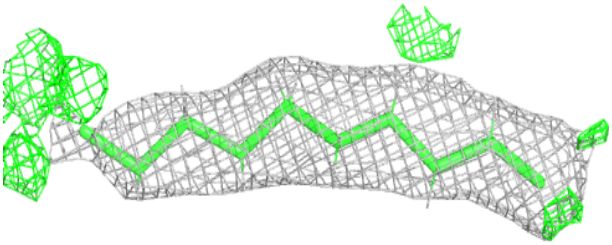
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

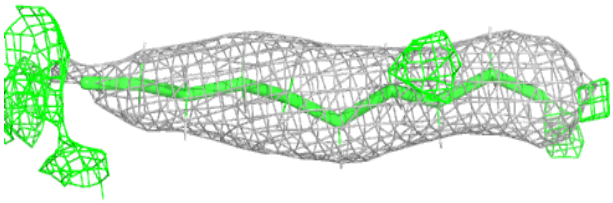


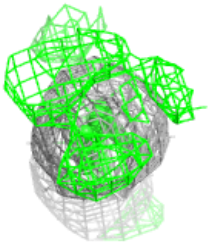


Electron density around STE M 103:

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

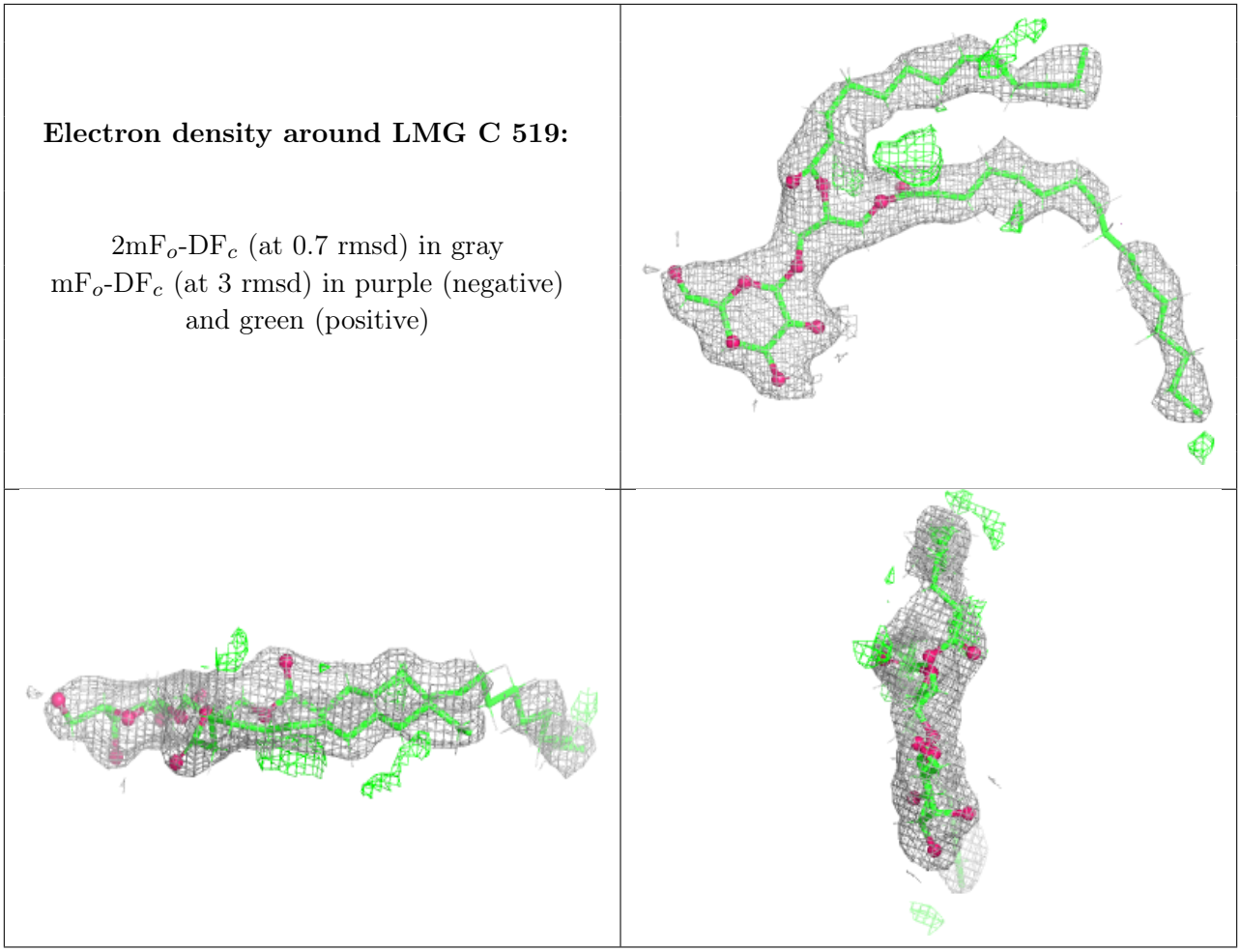






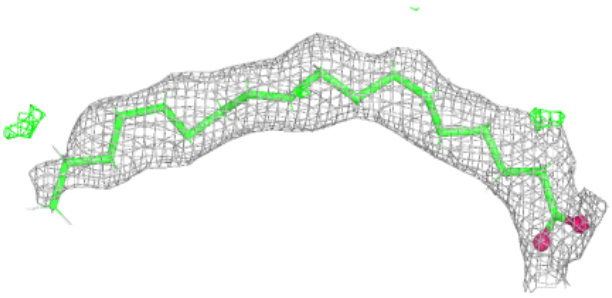
Electron density around LMG C 519:

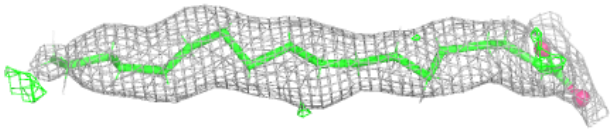
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

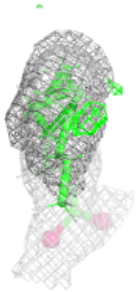


Electron density around STE X 101:

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

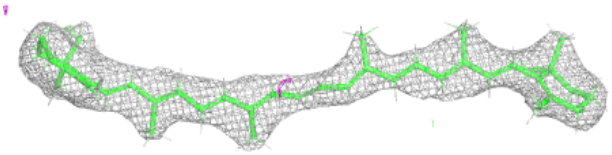


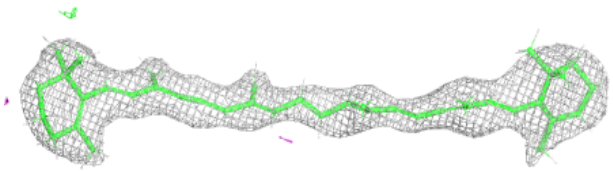


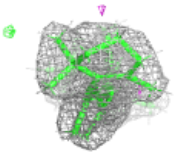


Electron density around BCR c 516:

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

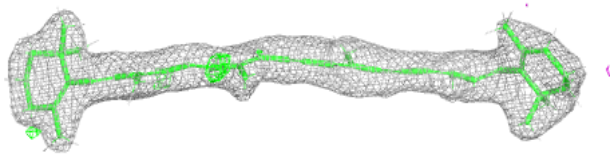






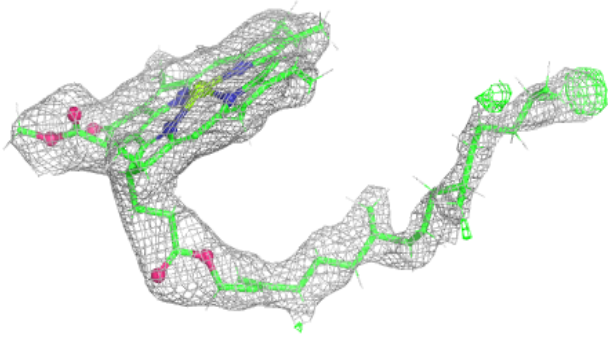
Electron density around BCR Y 101:

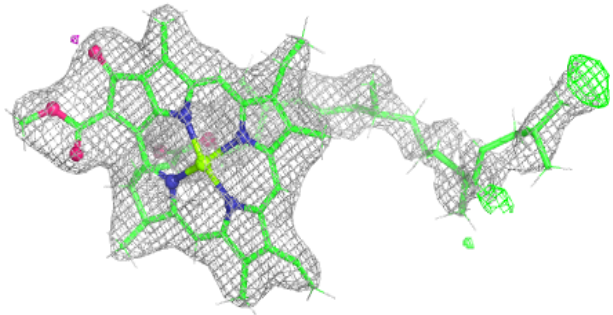
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

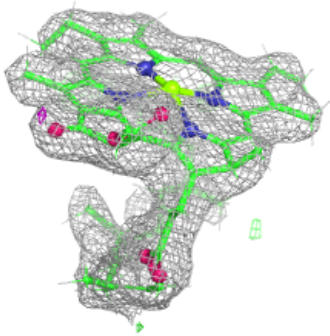


Electron density around CLA C 514:

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

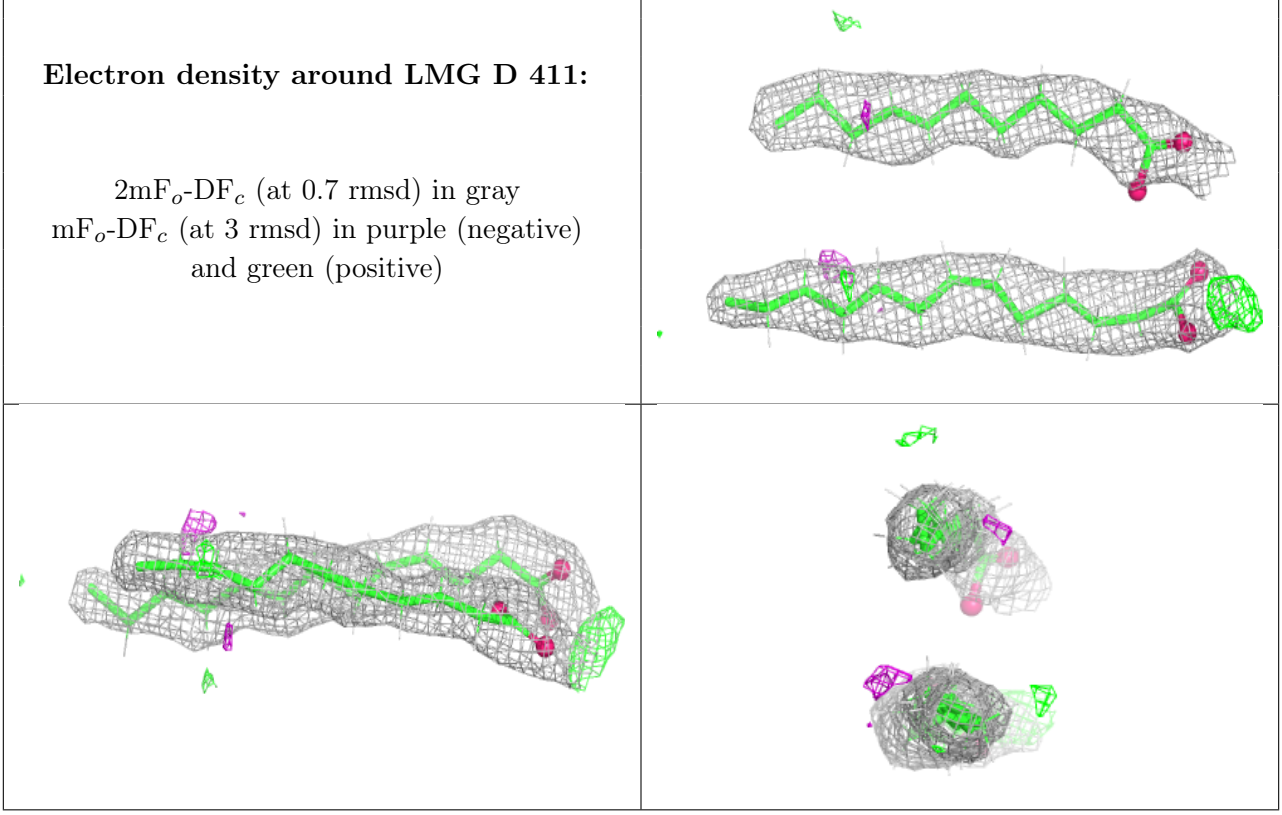






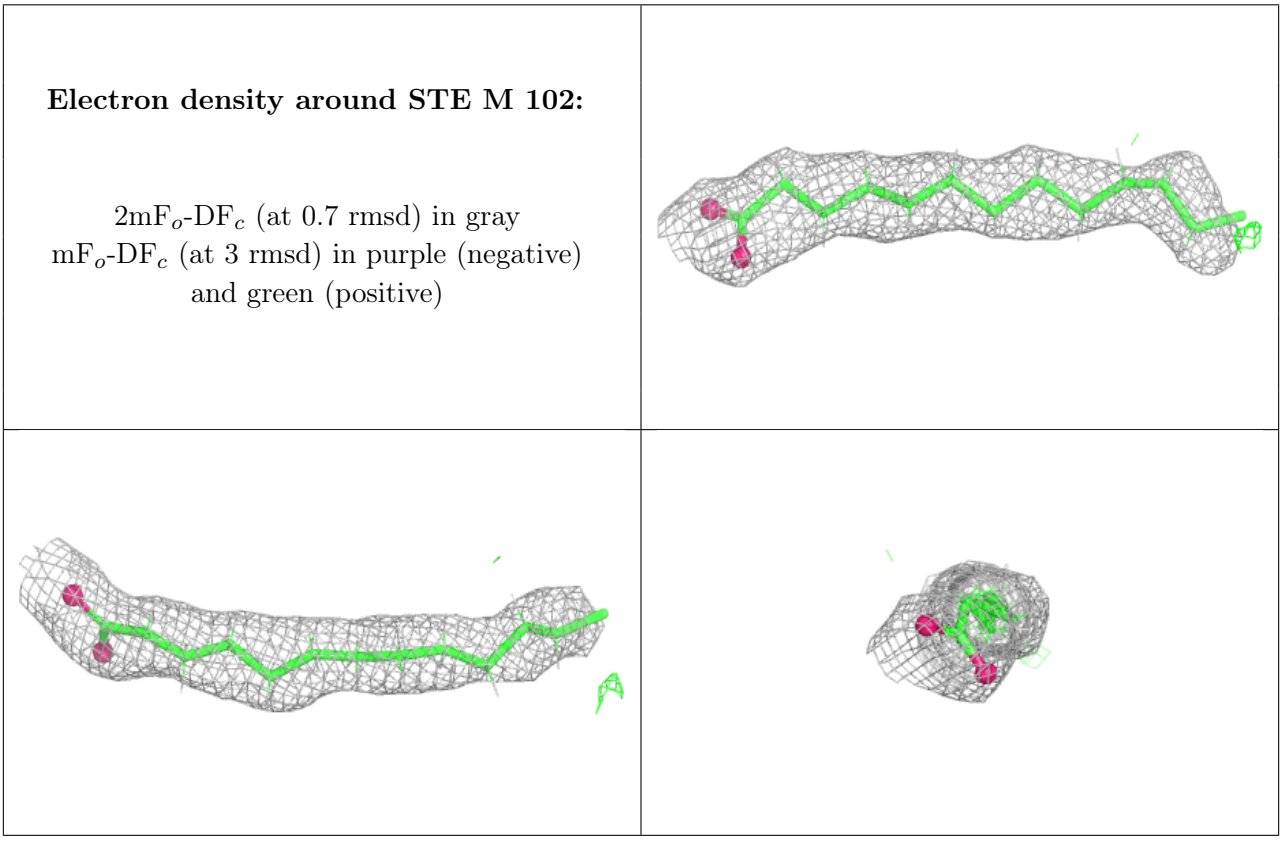
Electron density around LMG D 411:

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



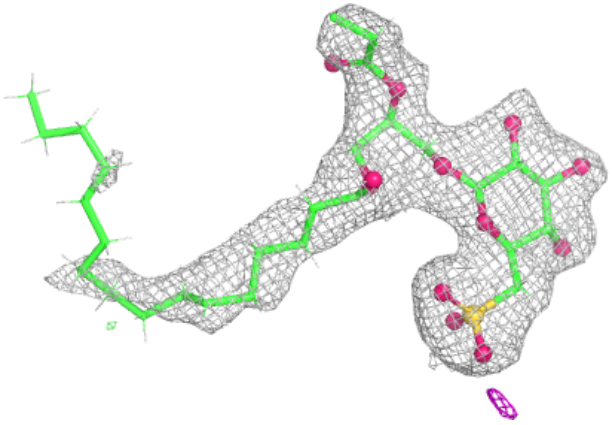
Electron density around STE M 102:

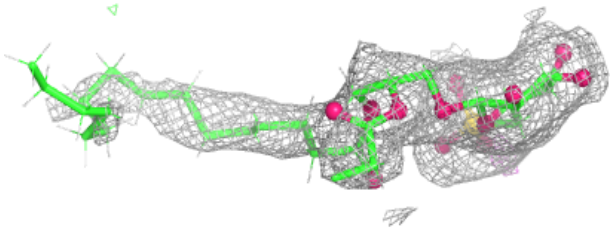
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

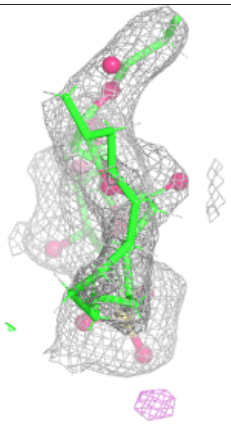


Electron density around SQD f 101:

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

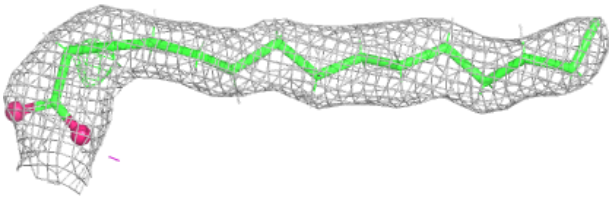


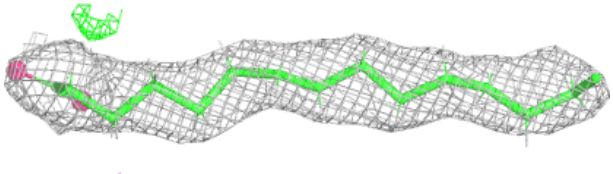


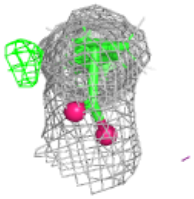


Electron density around STE d 410:

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

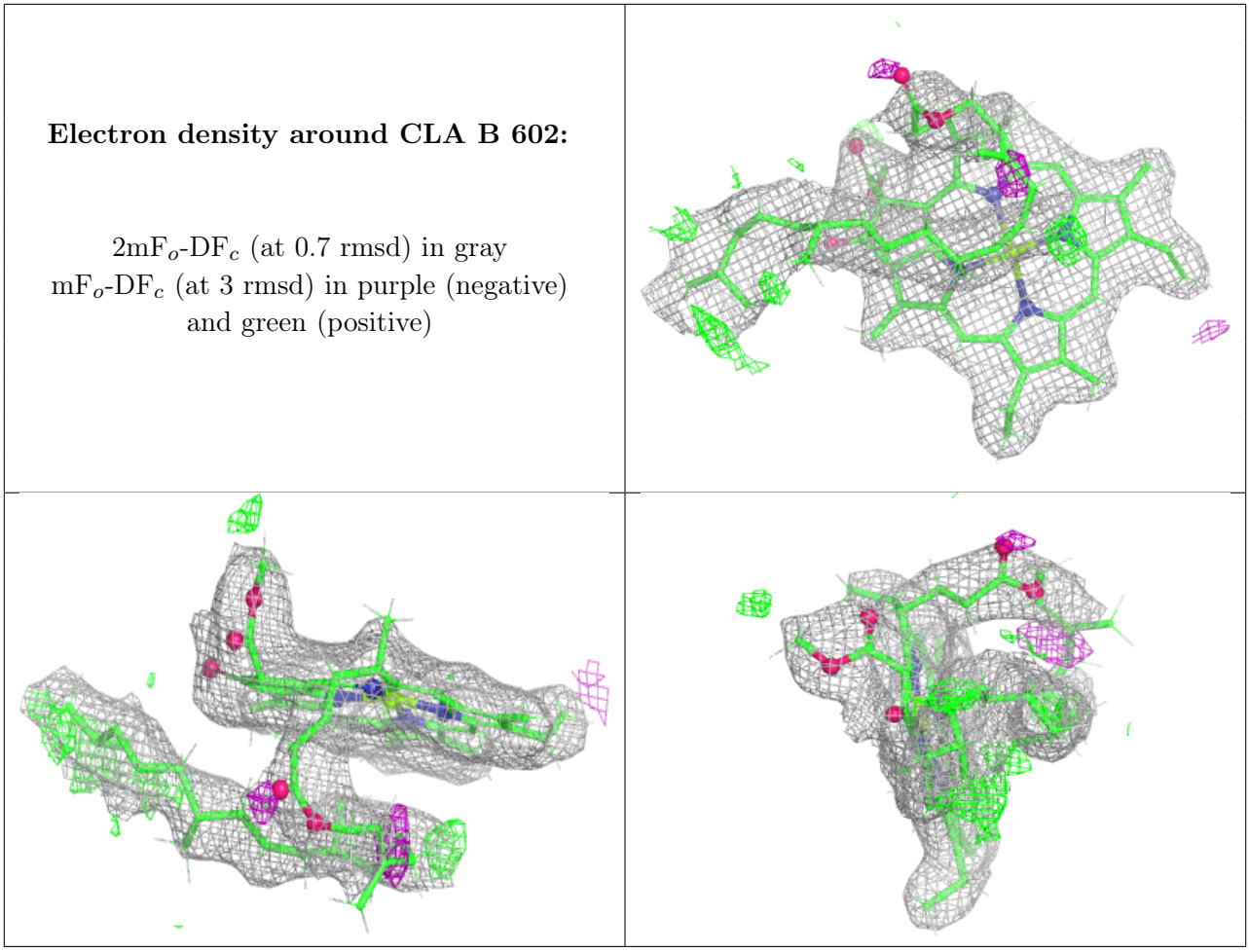






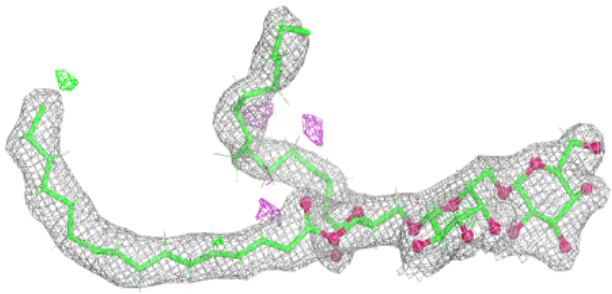
Electron density around CLA B 602:

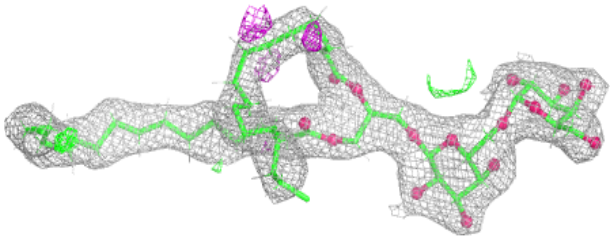
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

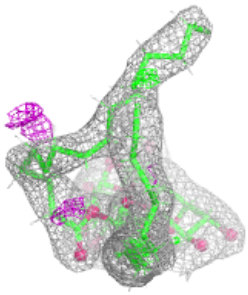


Electron density around DGD h 102:

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

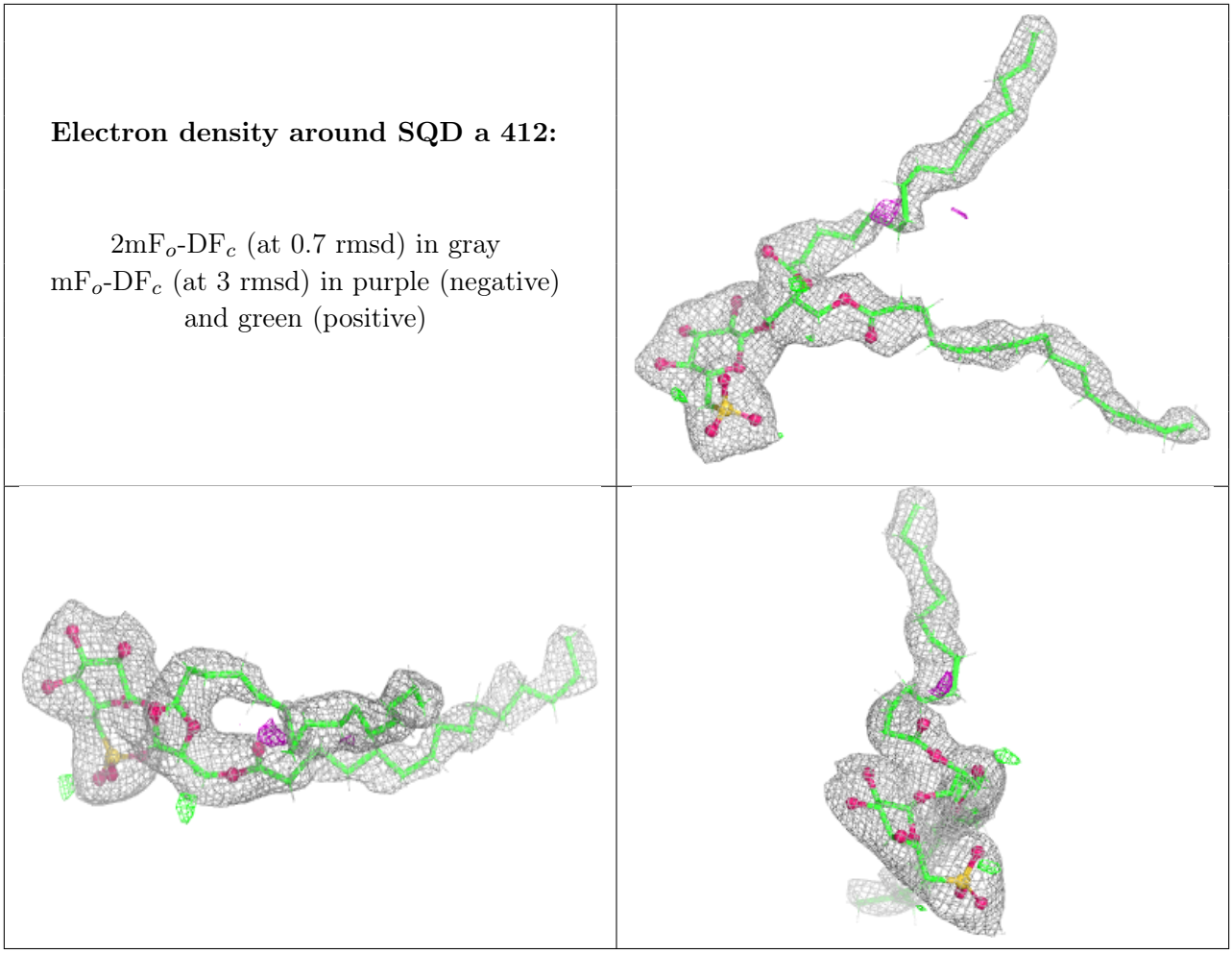






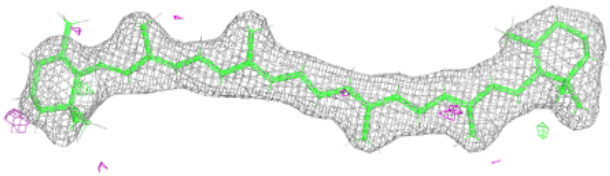
Electron density around SQD a 412:

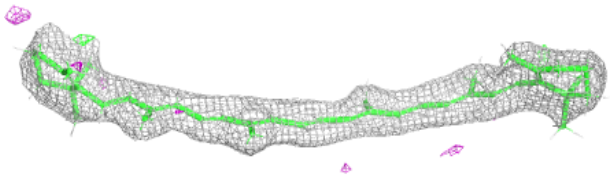
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

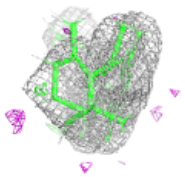


Electron density around BCR D 404:

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

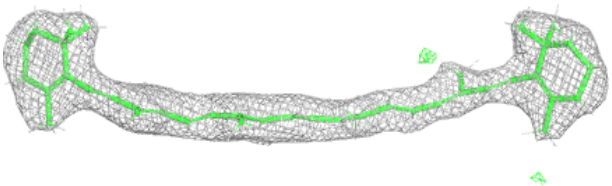


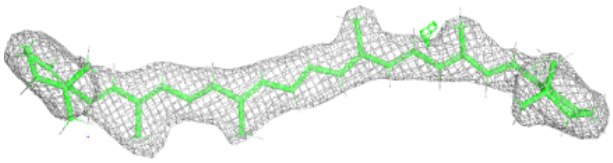


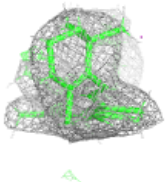


Electron density around BCR c 518:

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

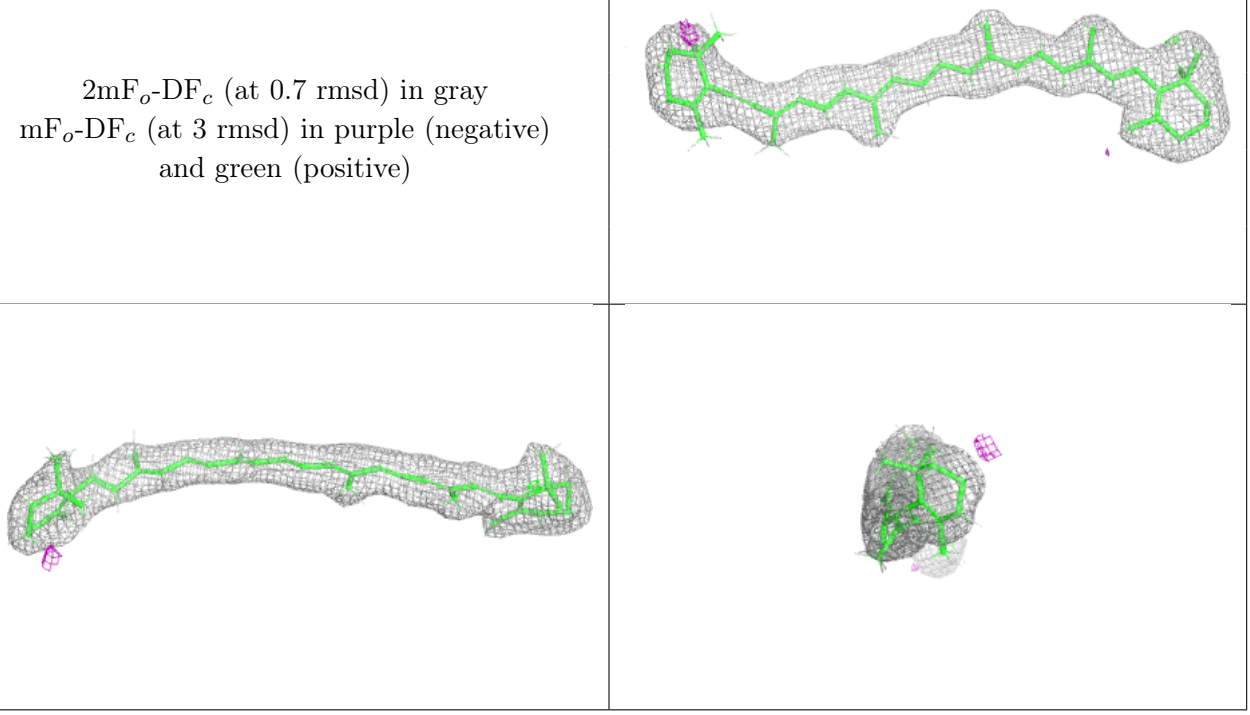






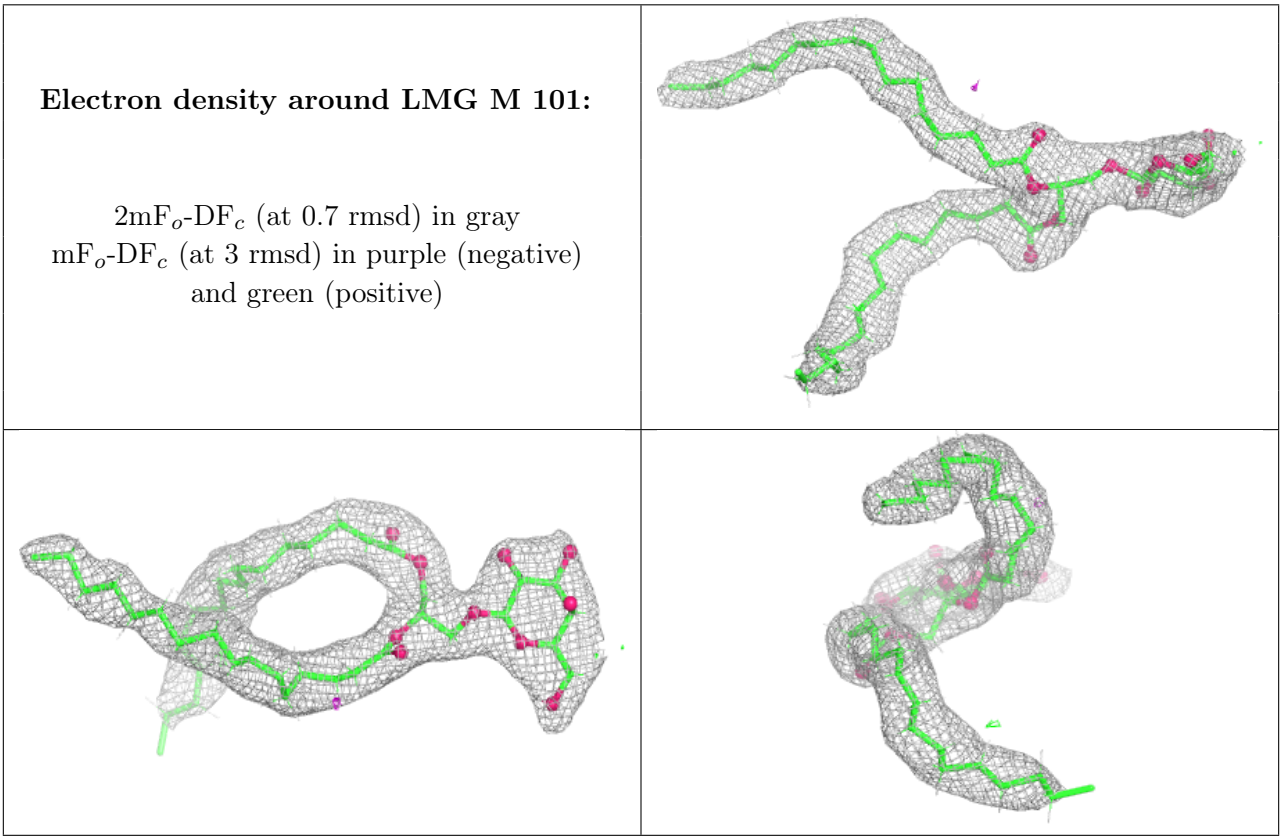
Electron density around BCR d 404:

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



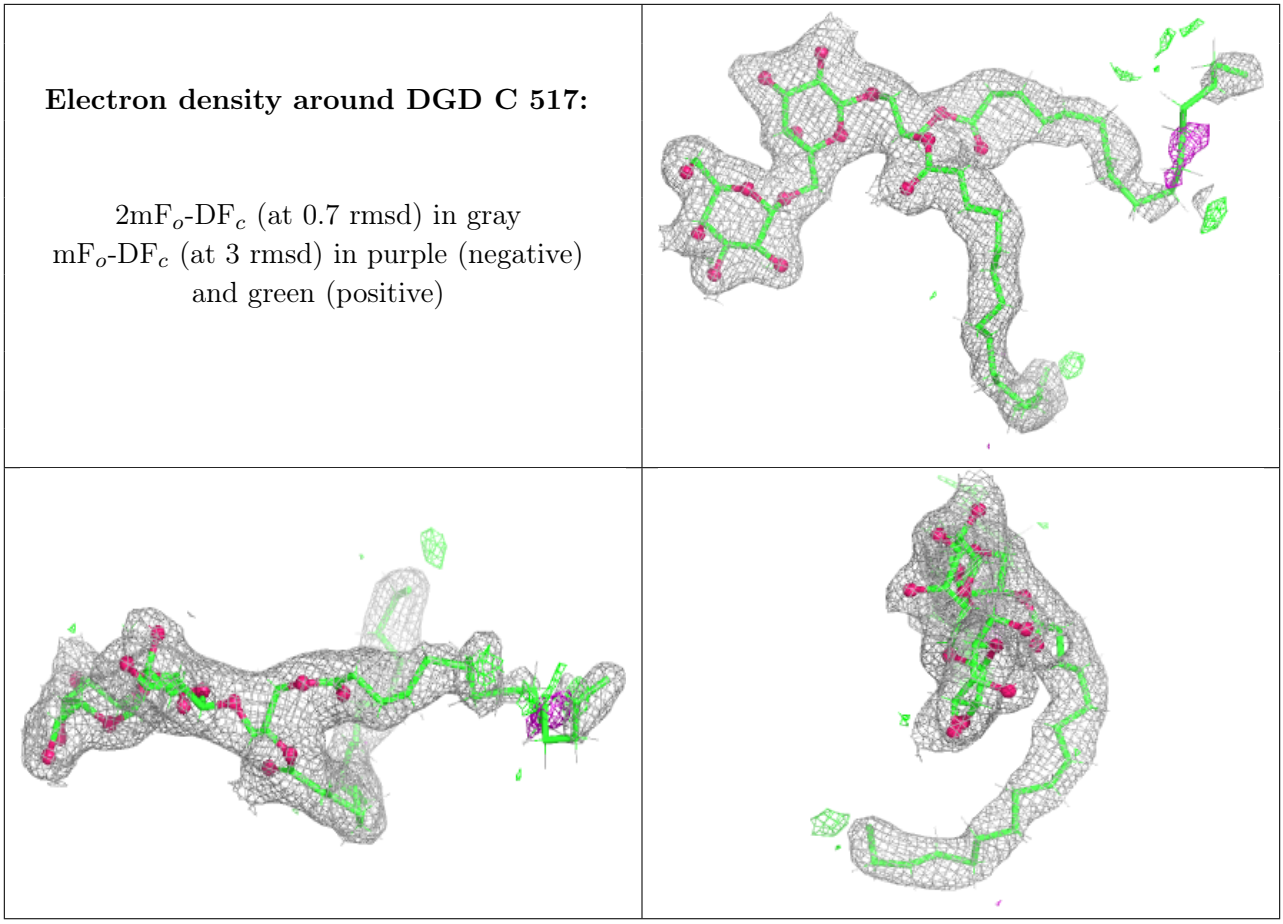
Electron density around LMG M 101:

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



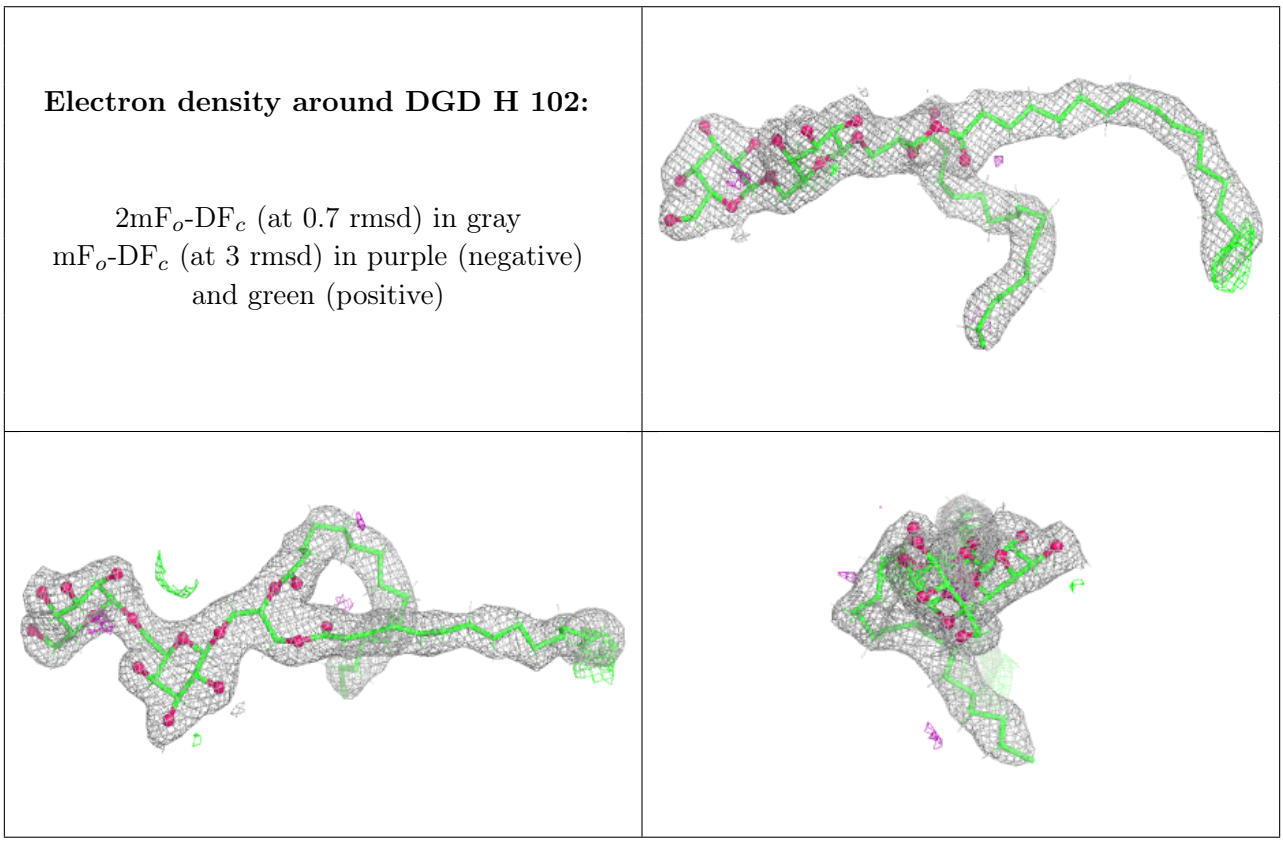
Electron density around DGD C 517:

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



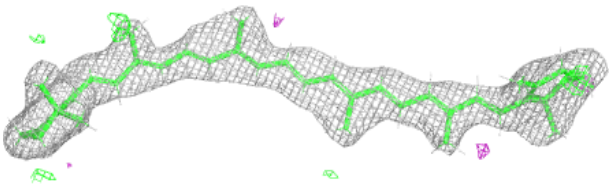
Electron density around DGD H 102:

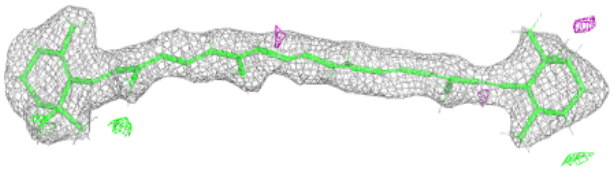
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

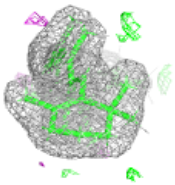


Electron density around BCR x 101:

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

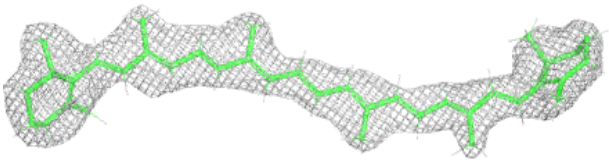


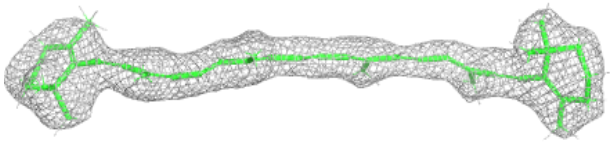


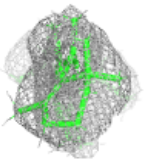


Electron density around BCR y 101:

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

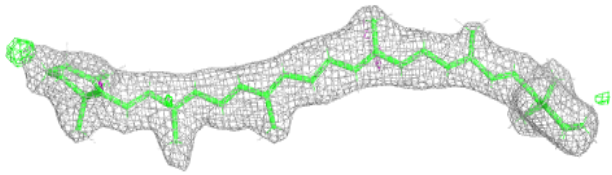


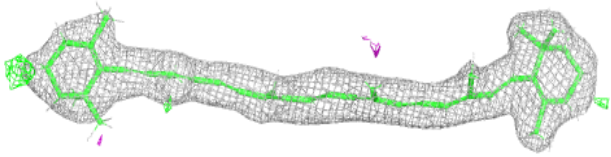


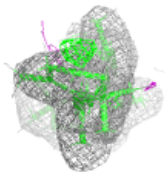


Electron density around BCR H 101:

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

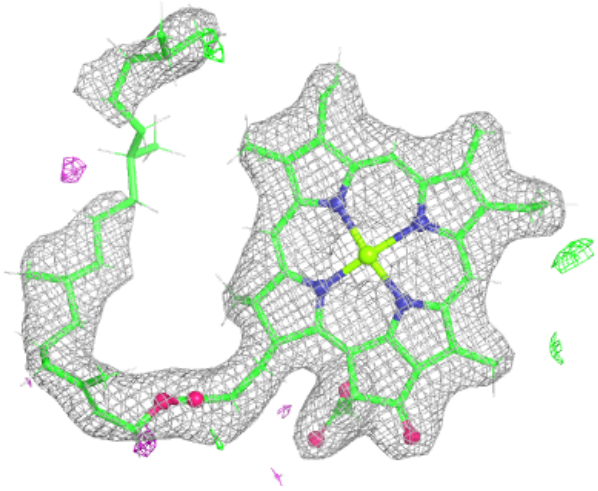


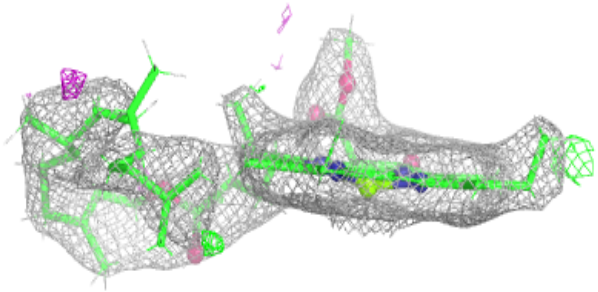


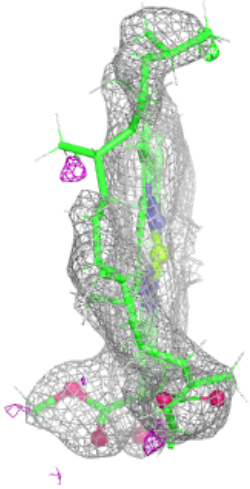


Electron density around CLA c 514:

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

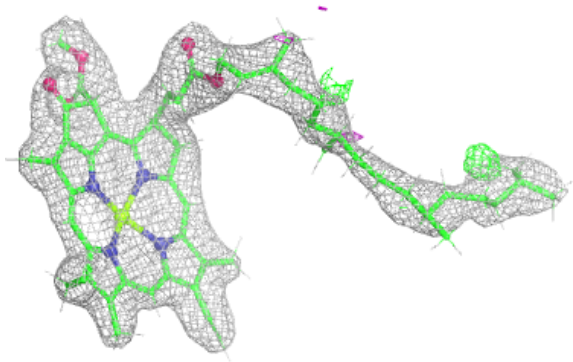


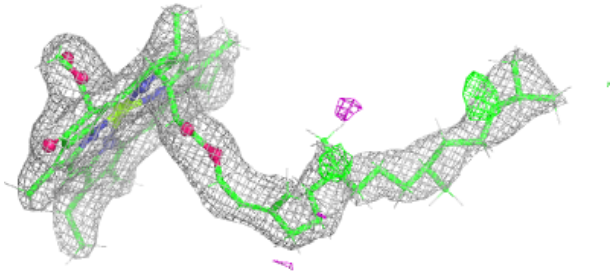


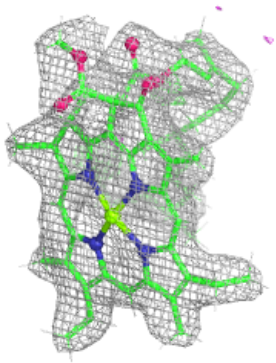


Electron density around CLA c 513:

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

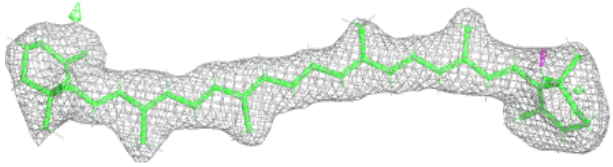


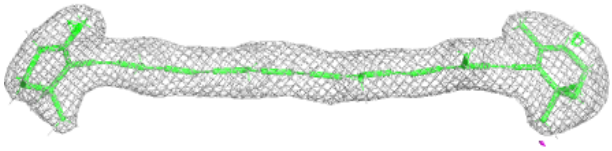


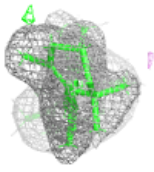


Electron density around BCR b 617:

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

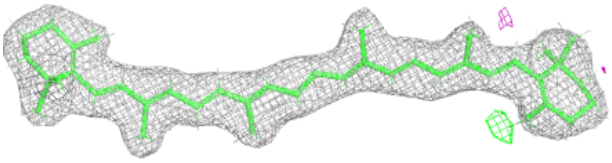


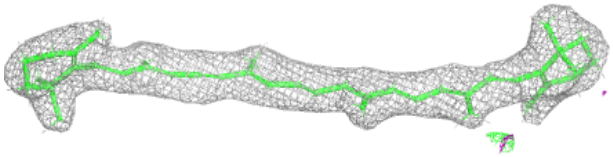


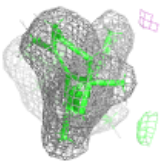


Electron density around BCR b 618:

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

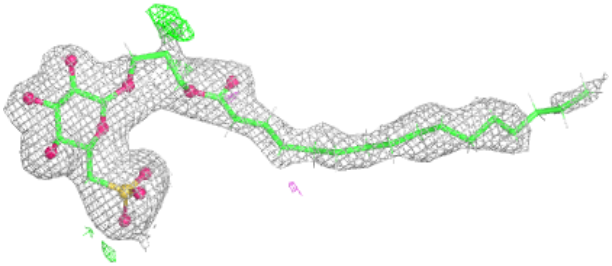


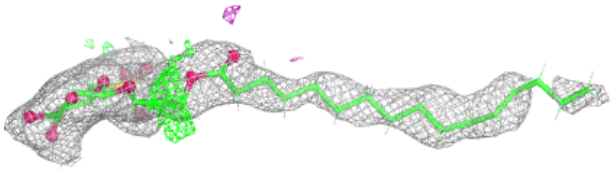


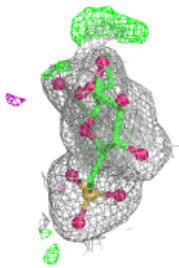


Electron density around SQD D 407:

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

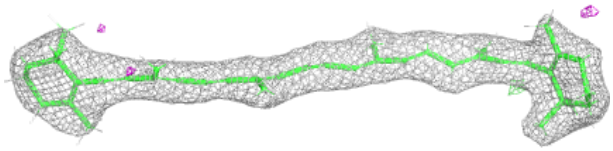


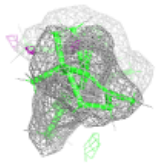




Electron density around BCR c 517:

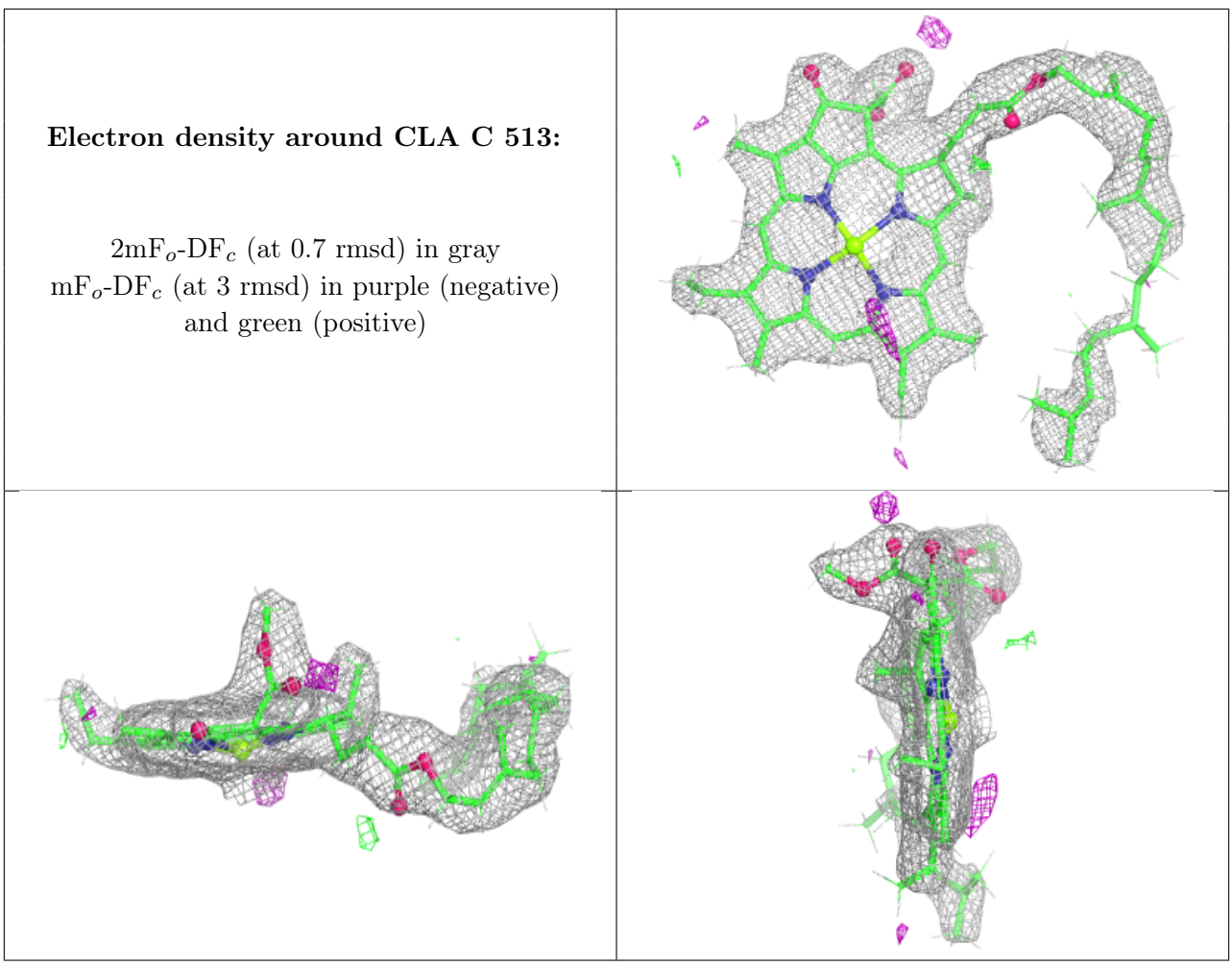
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





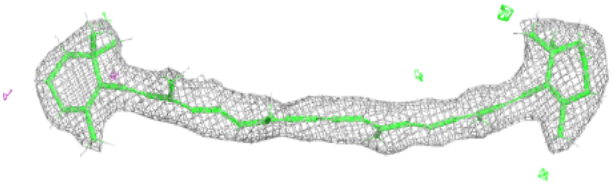
Electron density around CLA C 513:

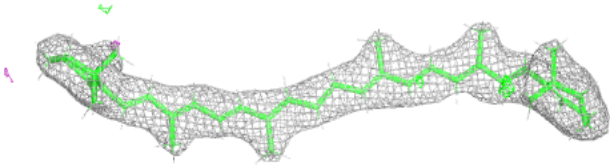
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

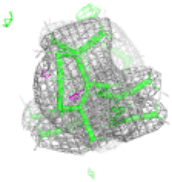


Electron density around BCR K 101:

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

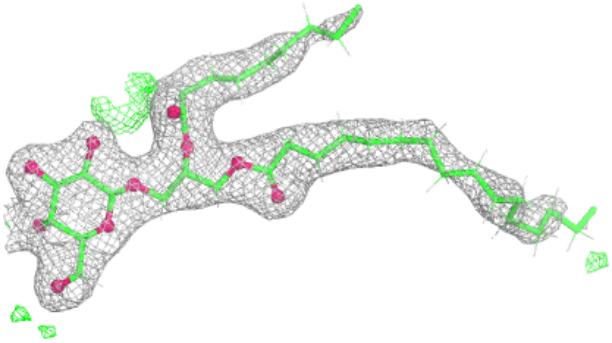


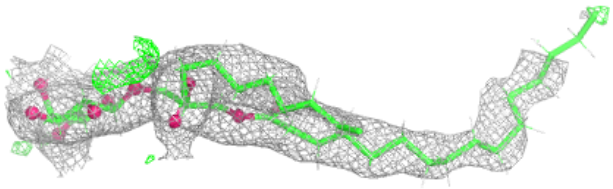


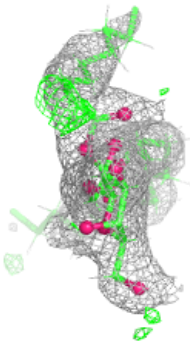


Electron density around LMG d 409:

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

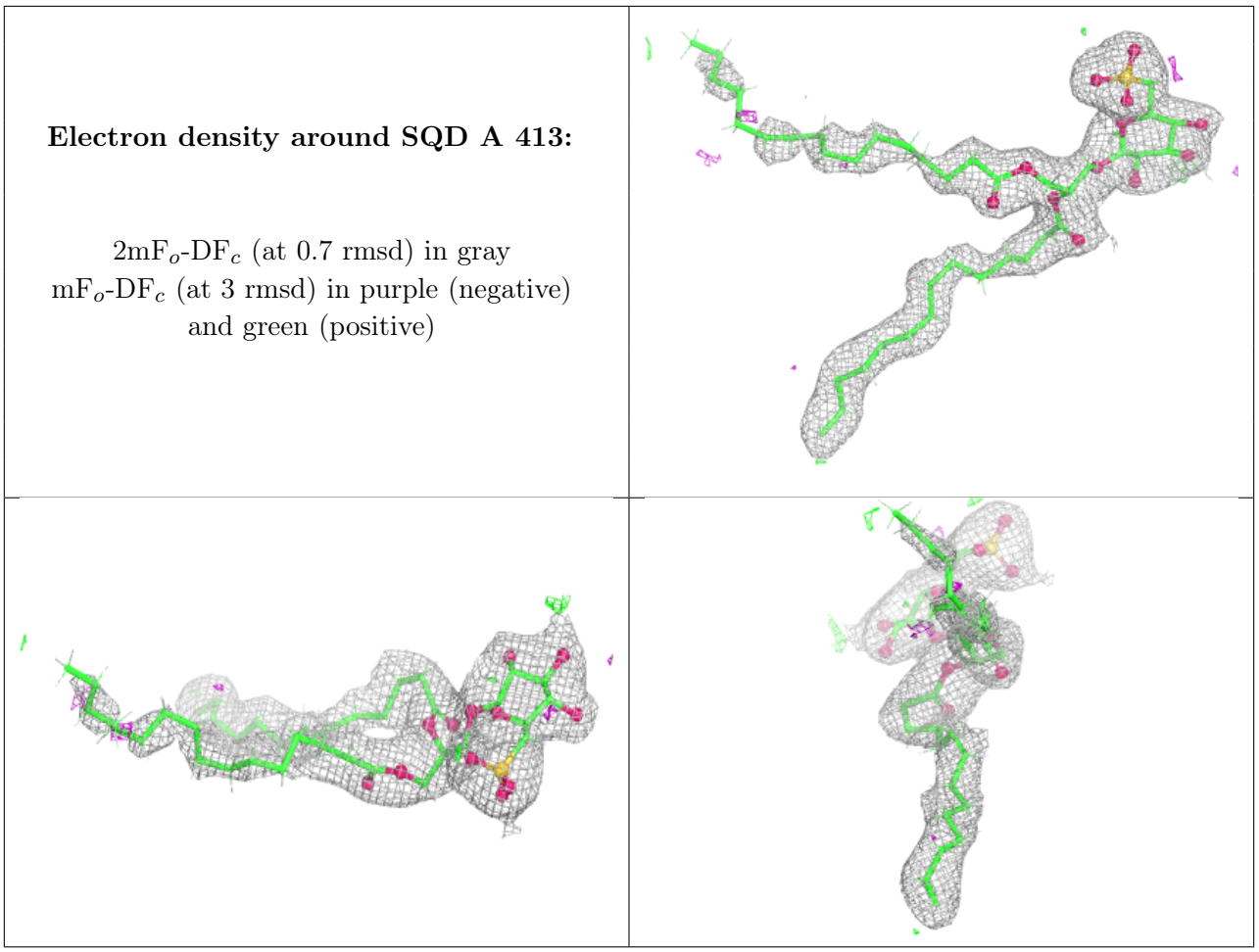






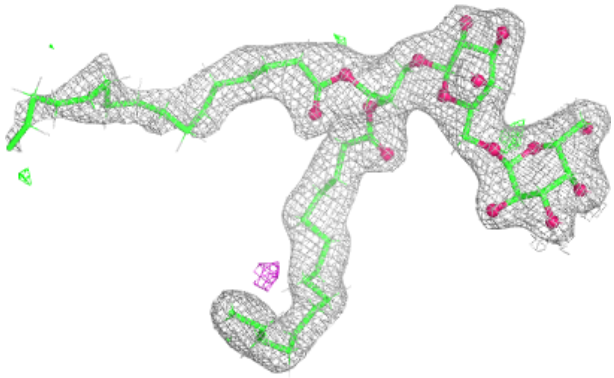
Electron density around SQD A 413:

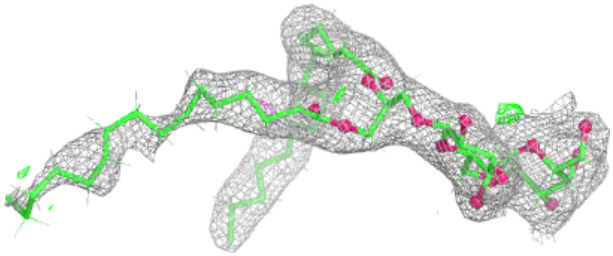
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

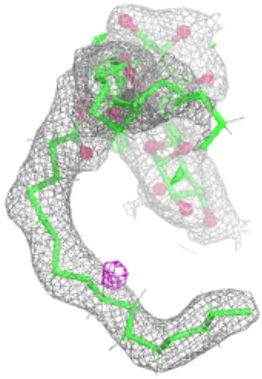


Electron density around DGD c 520:

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

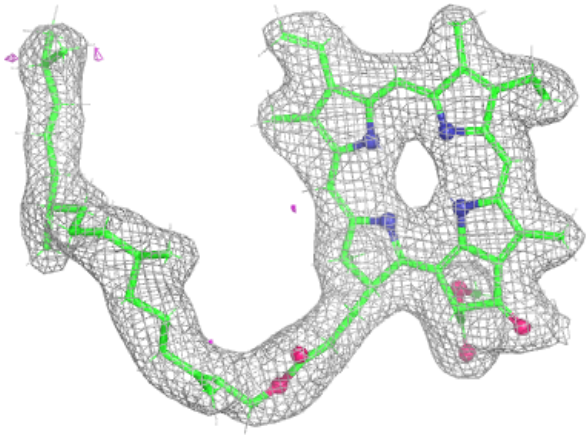


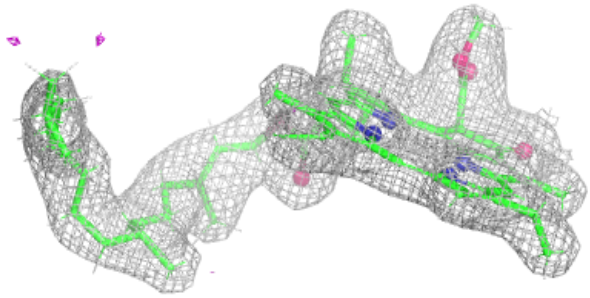




Electron density around PHO d 401:

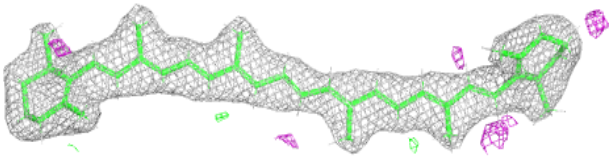
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

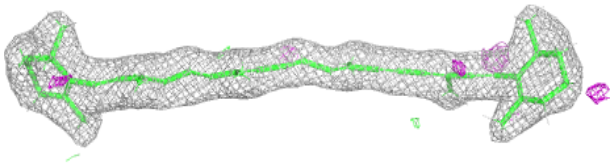


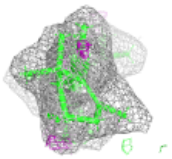


Electron density around BCR B 619:

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

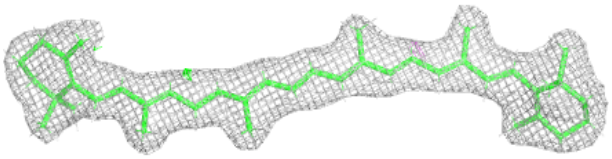


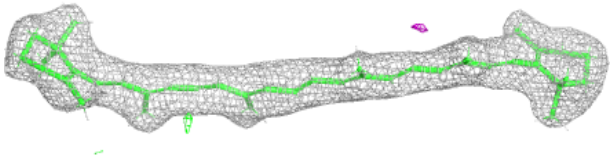


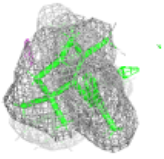


Electron density around BCR B 620:

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

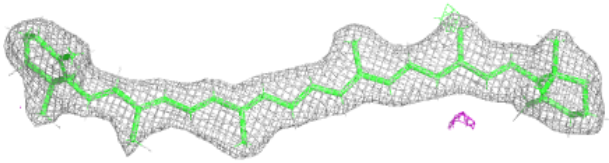


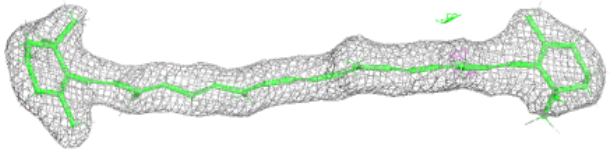


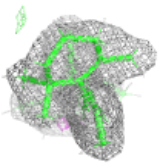


Electron density around BCR C 515:

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

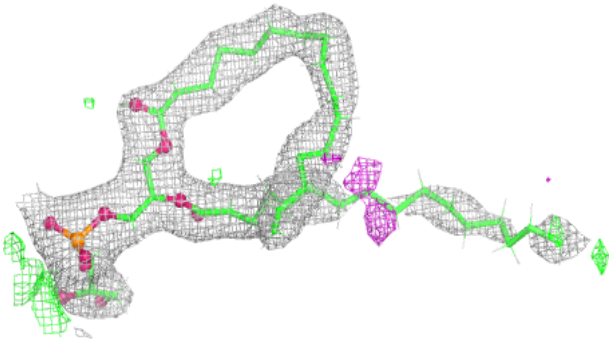


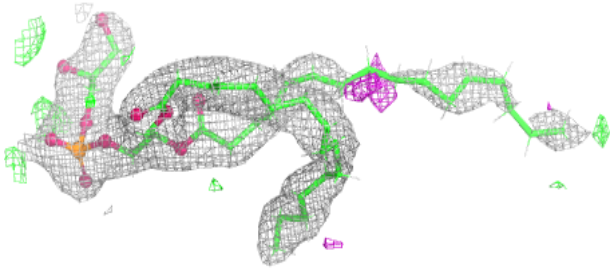




Electron density around LHG d 406:

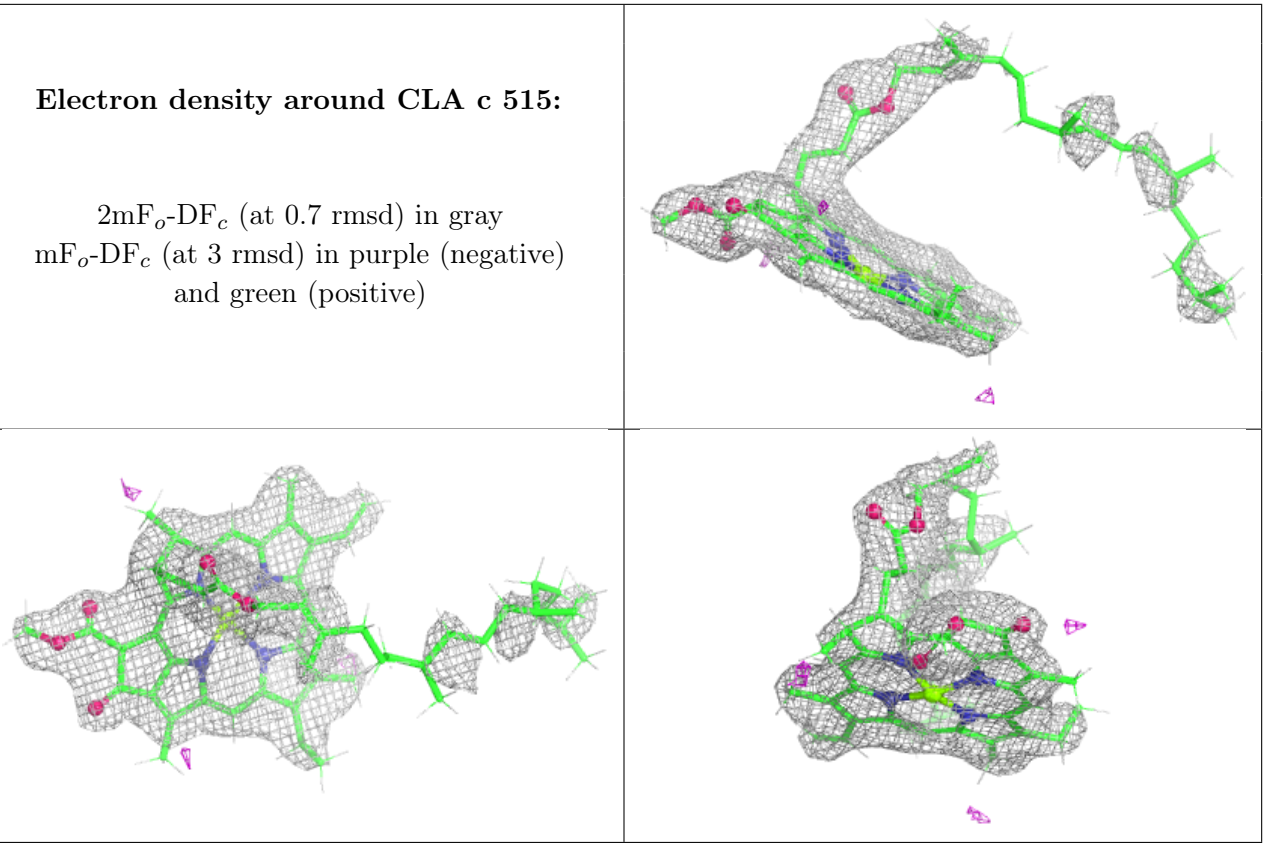
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





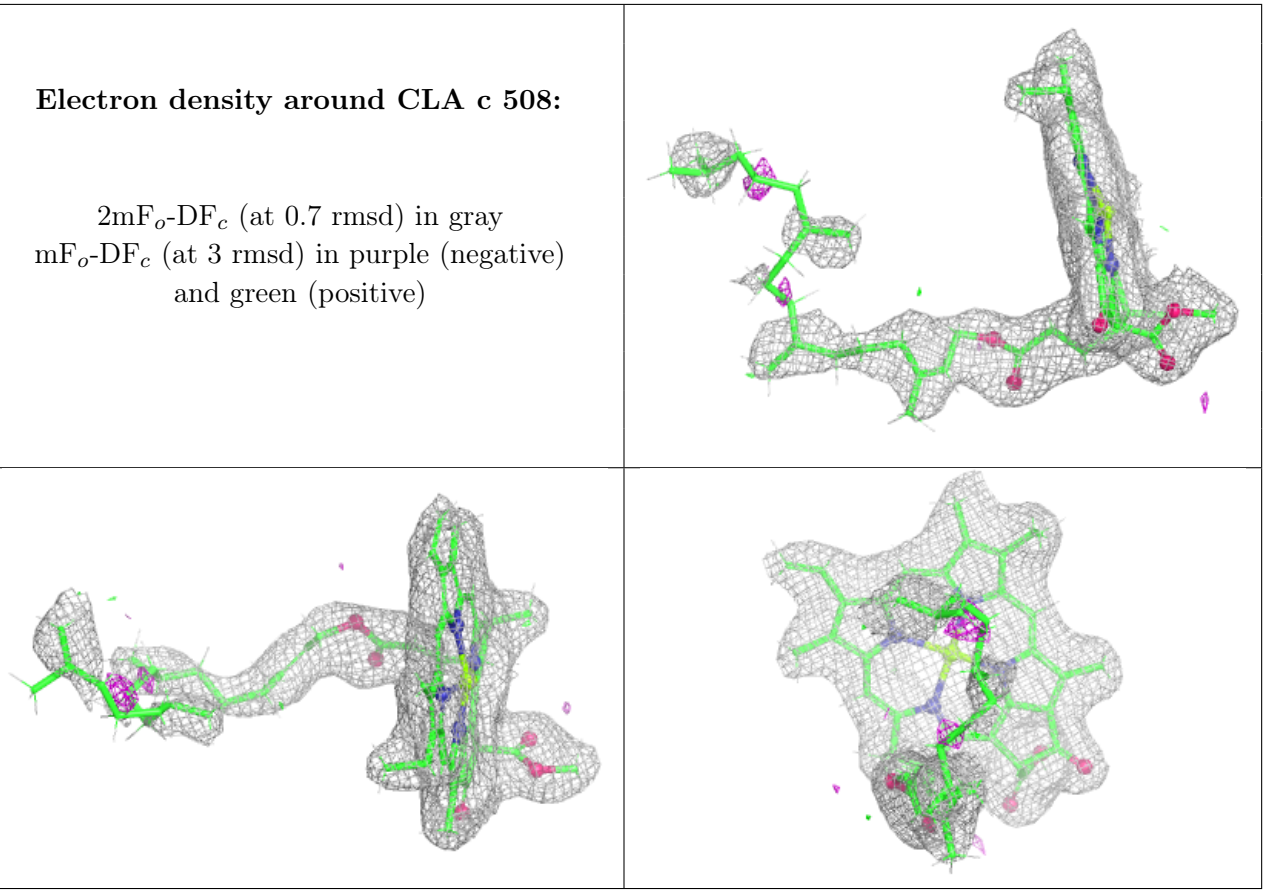
Electron density around CLA c 515:

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



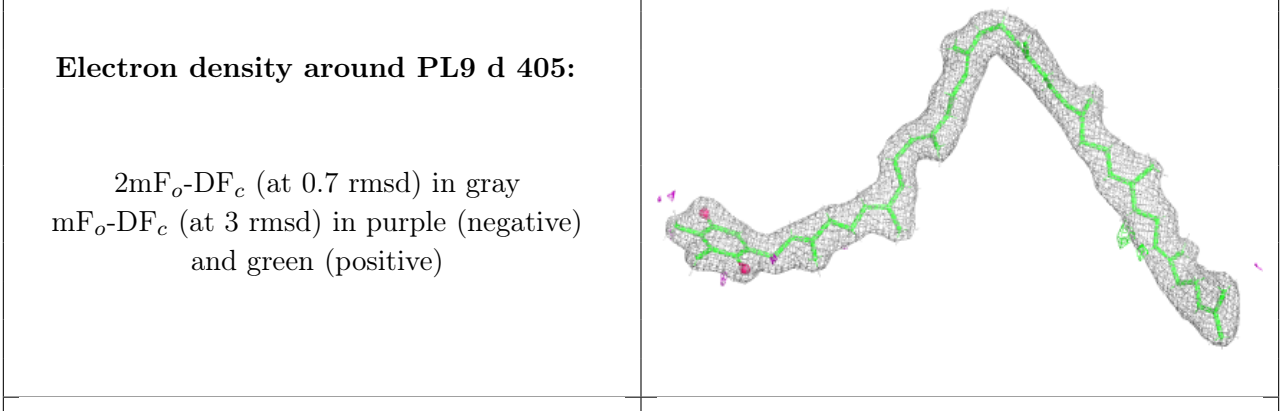
Electron density around CLA c 508:

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



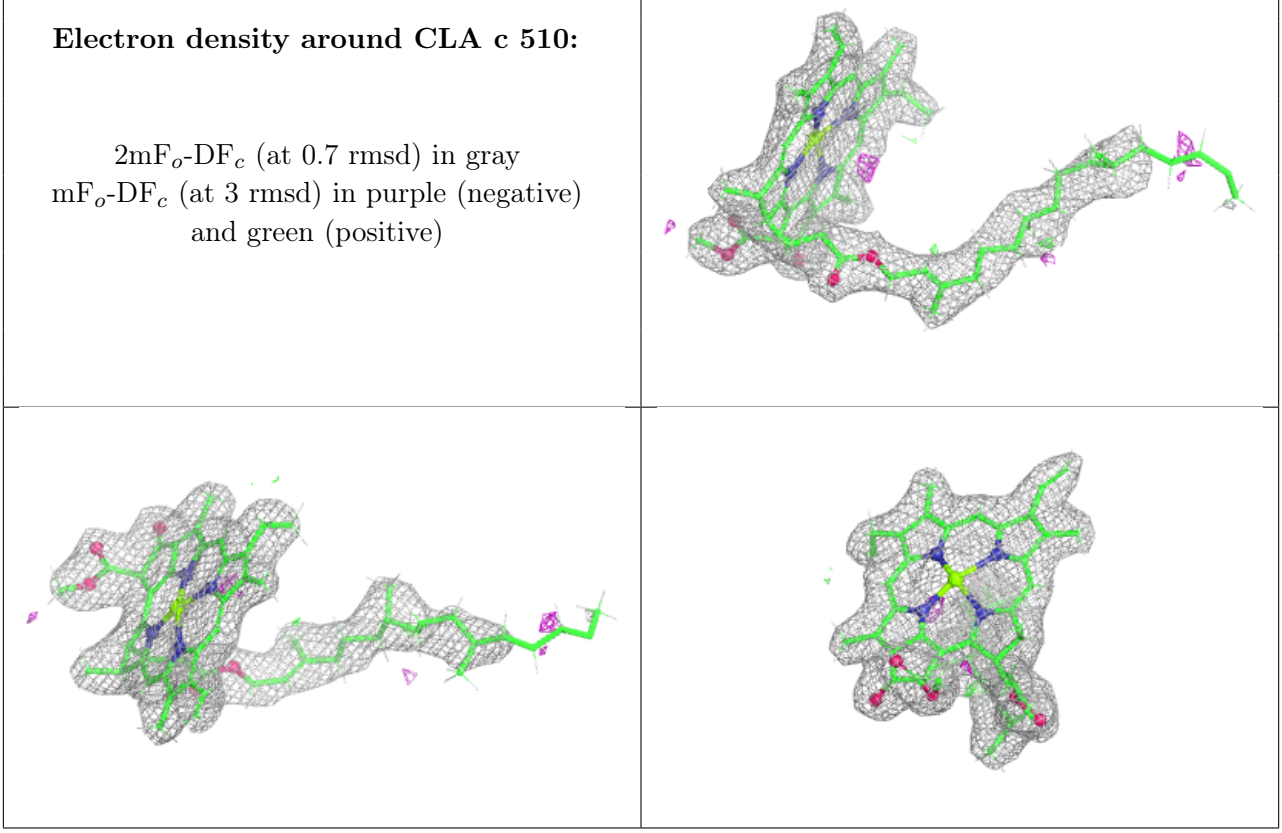
Electron density around PL9 d 405:

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



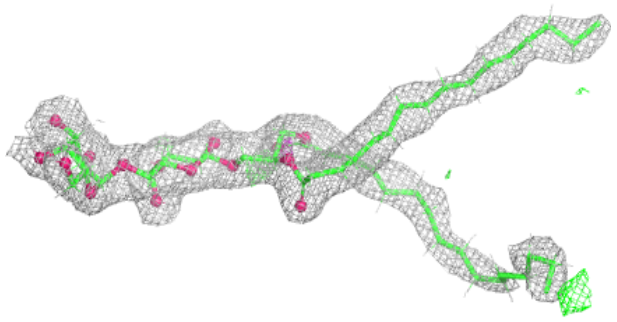
Electron density around CLA c 510:

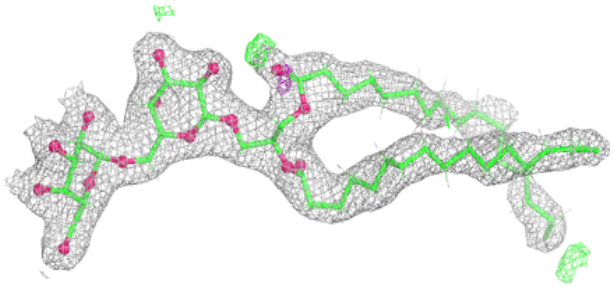
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

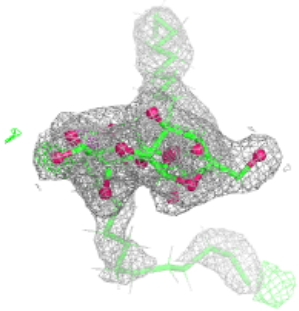


Electron density around DGD C 516:

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

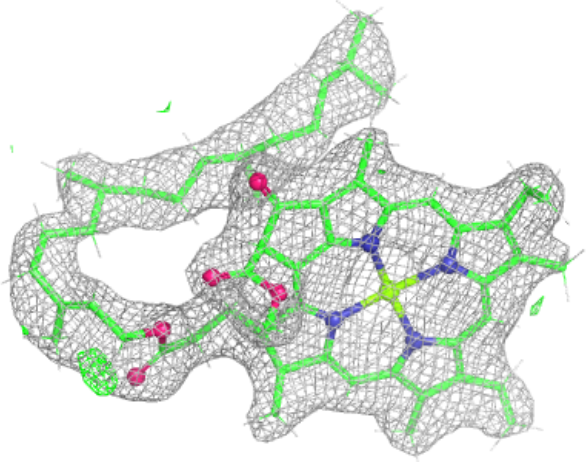


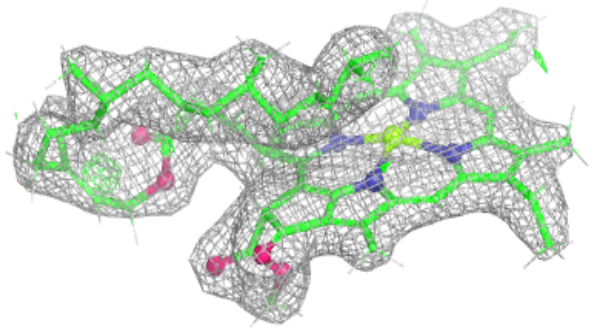


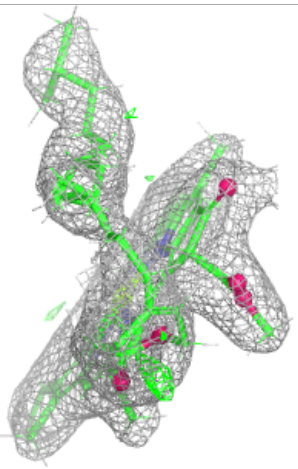


Electron density around CLA c 511:

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

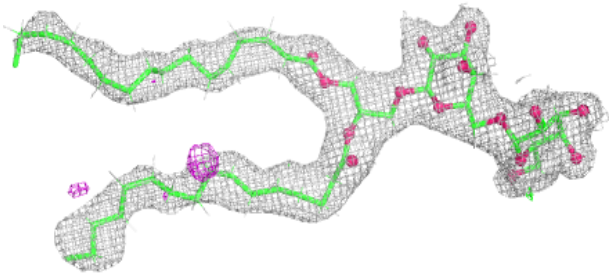


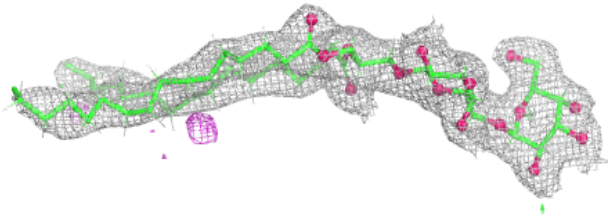


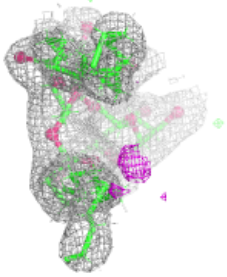


Electron density around DGD C 518:

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

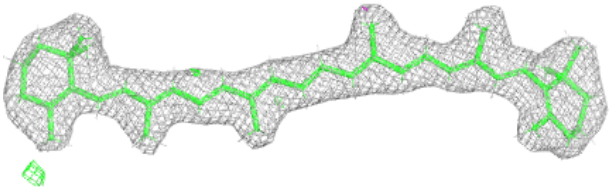


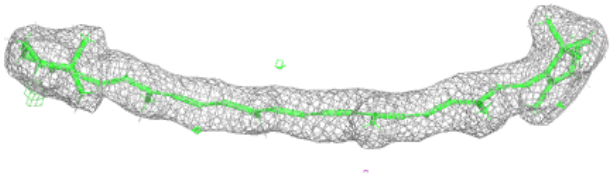


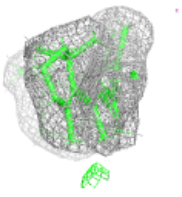


Electron density around BCR T 101:

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

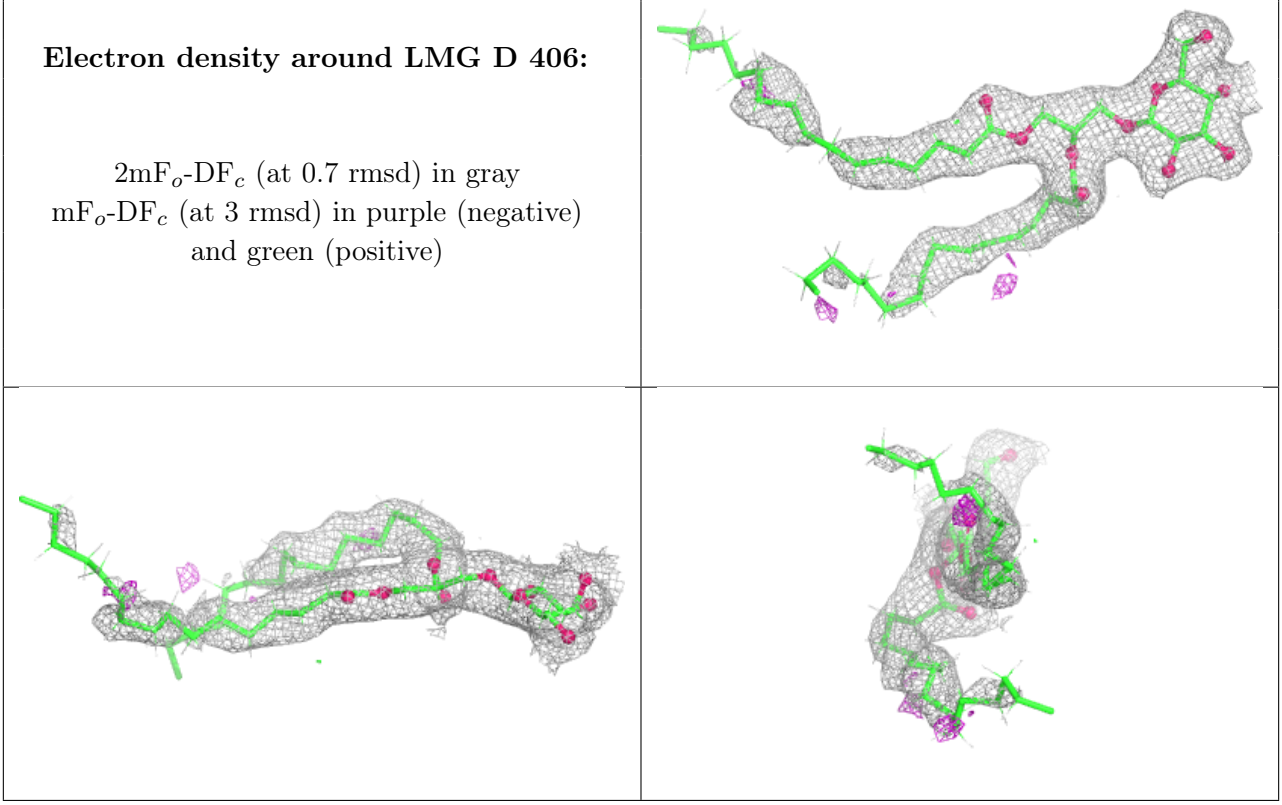






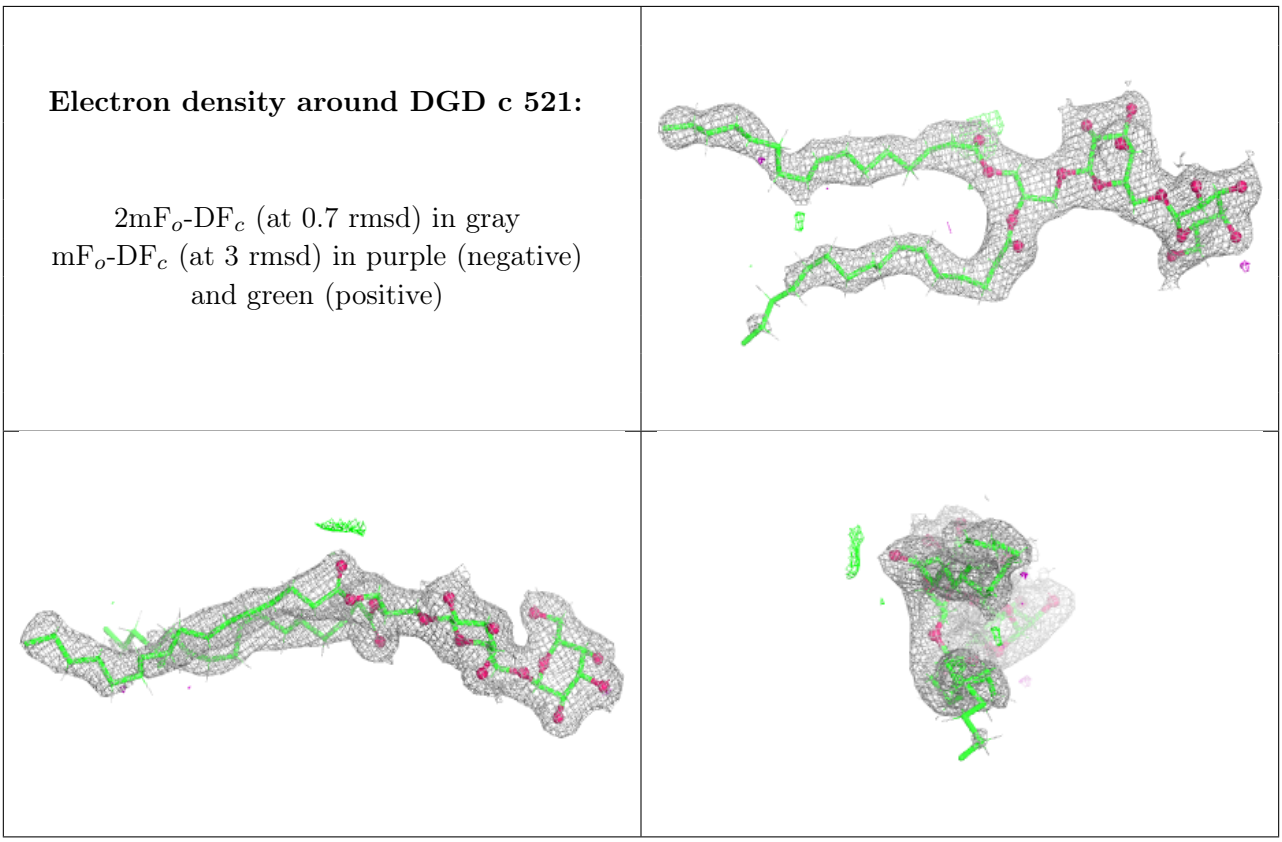
Electron density around LMG D 406:

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



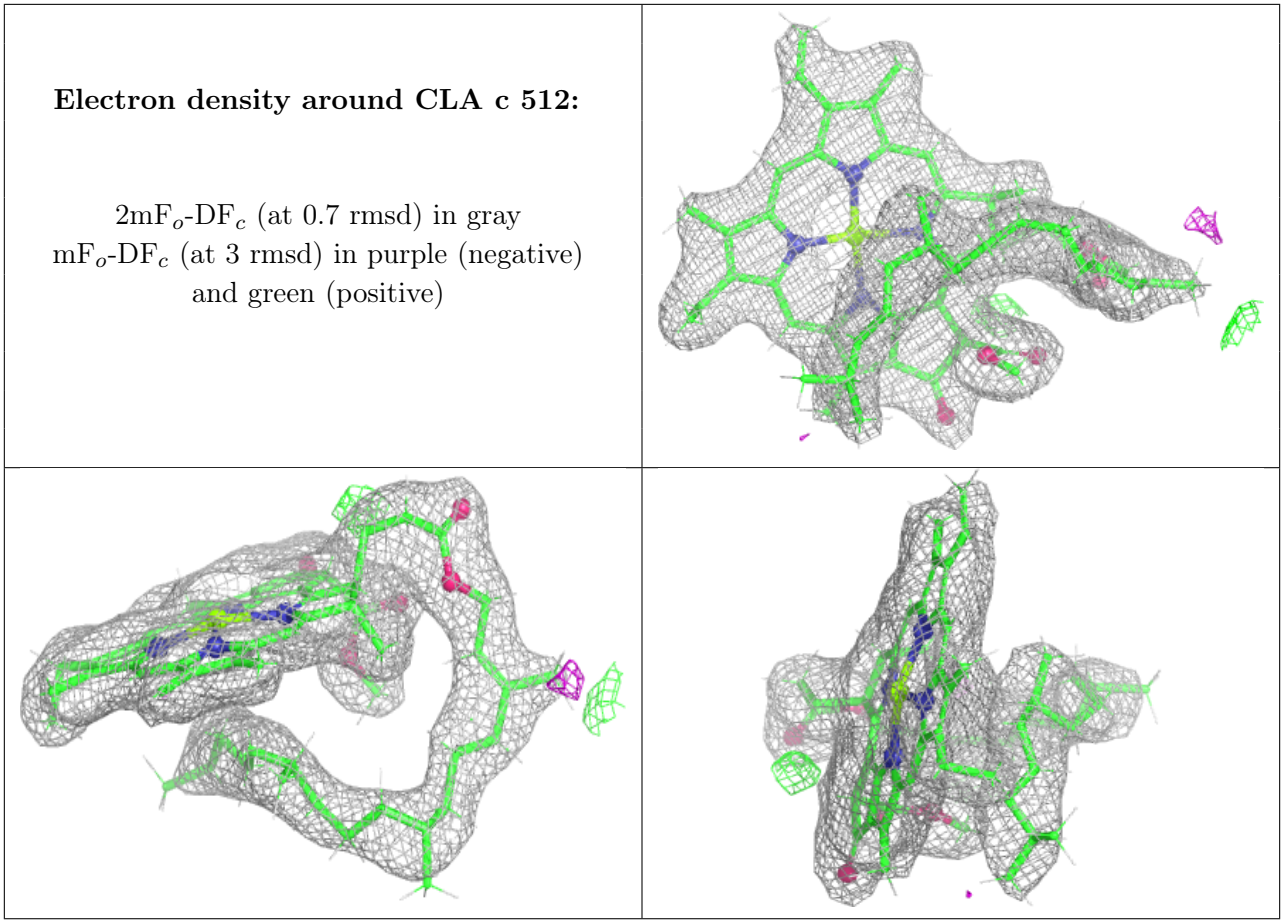
Electron density around DGD c 521:

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



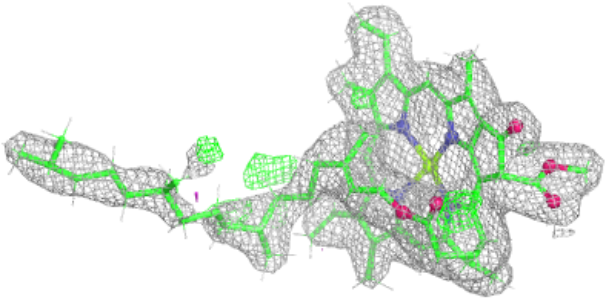
Electron density around CLA c 512:

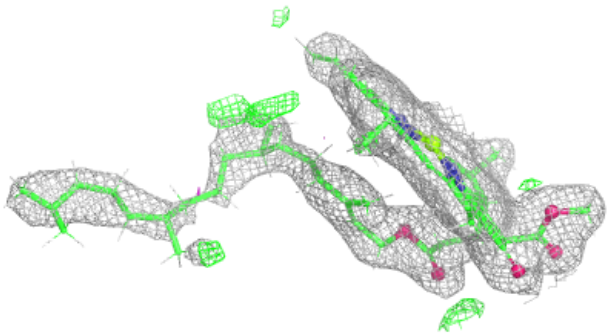
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

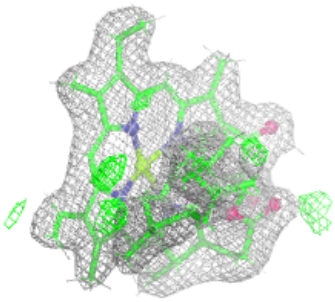


Electron density around CLA C 506:

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

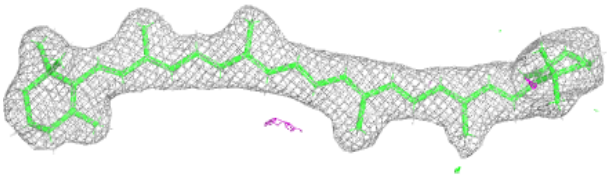


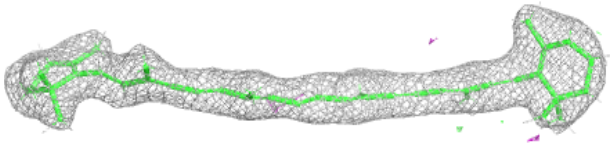


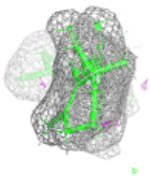


Electron density around BCR b 616:

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

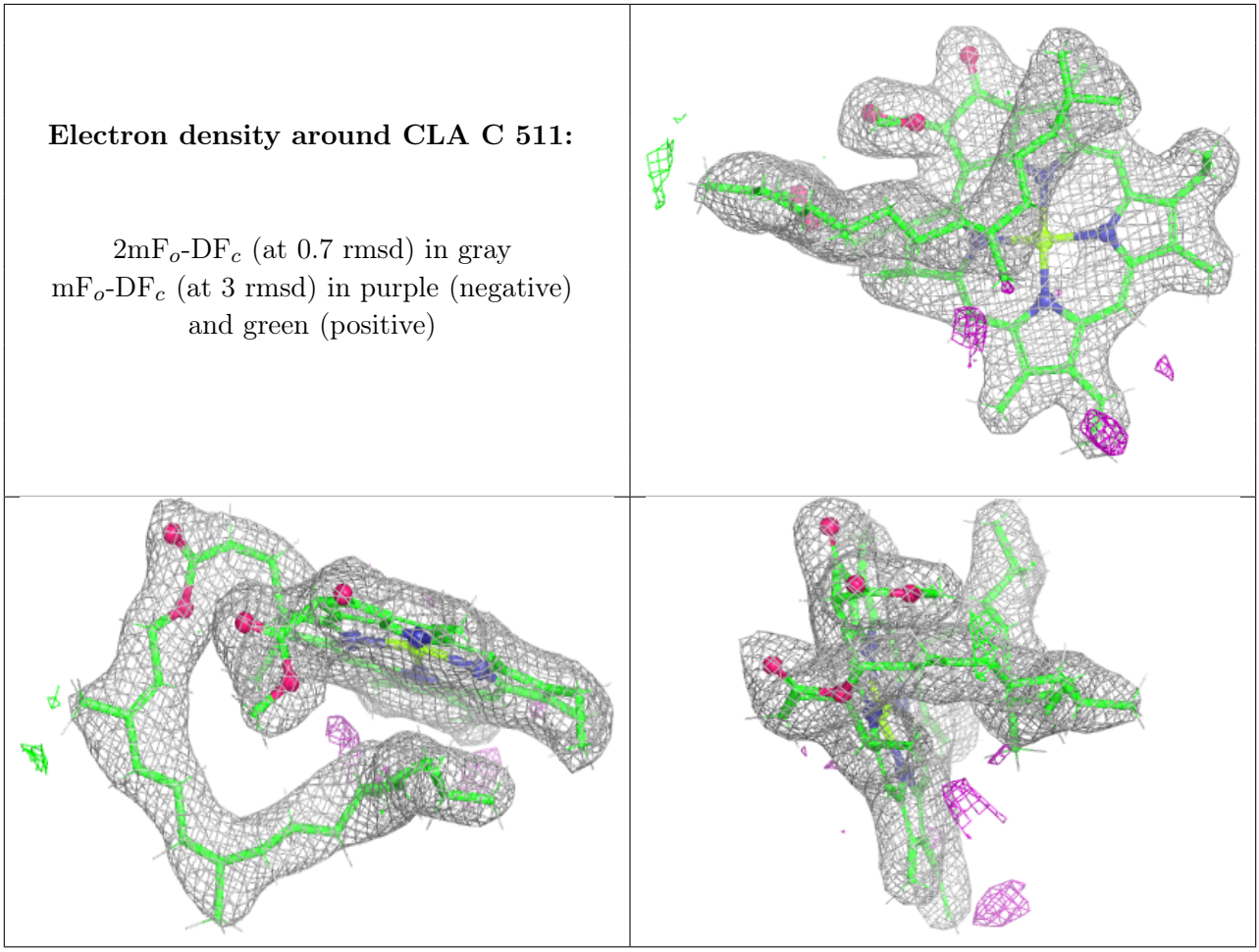






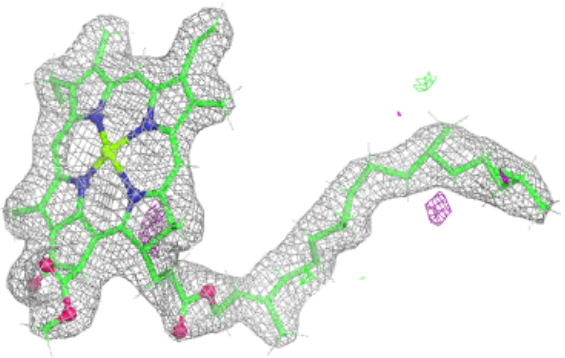
Electron density around CLA C 511:

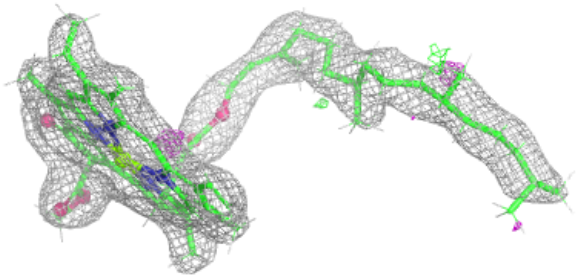
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

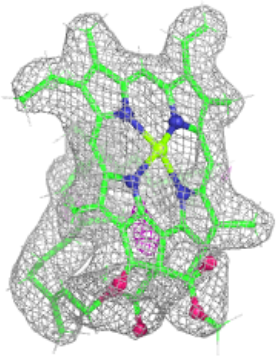


Electron density around CLA C 512:

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

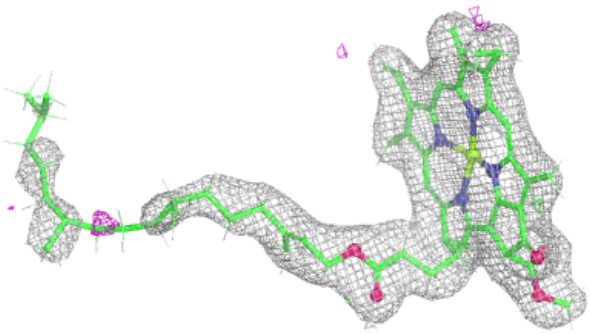


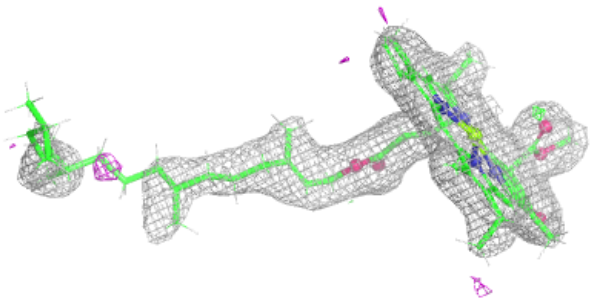


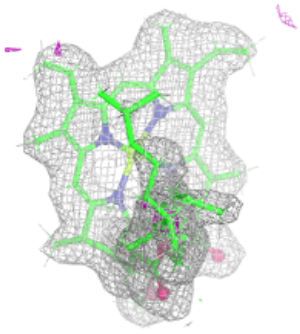


Electron density around CLA d 403:

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

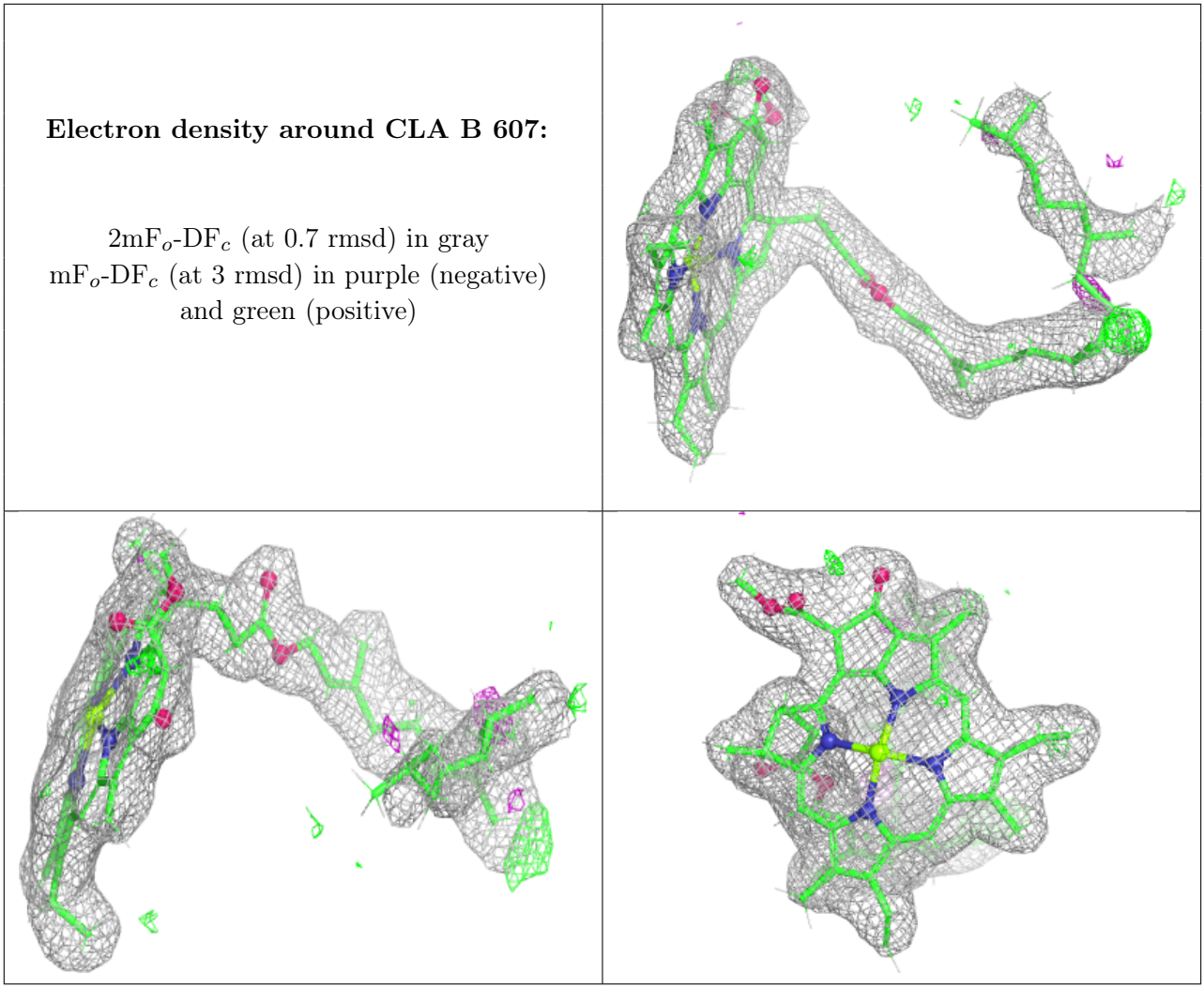






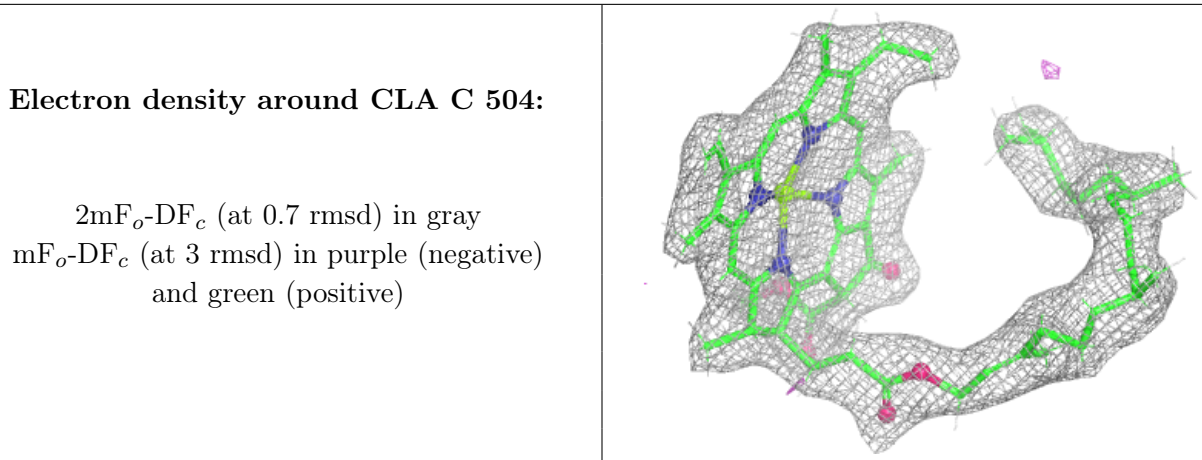
Electron density around CLA B 607:

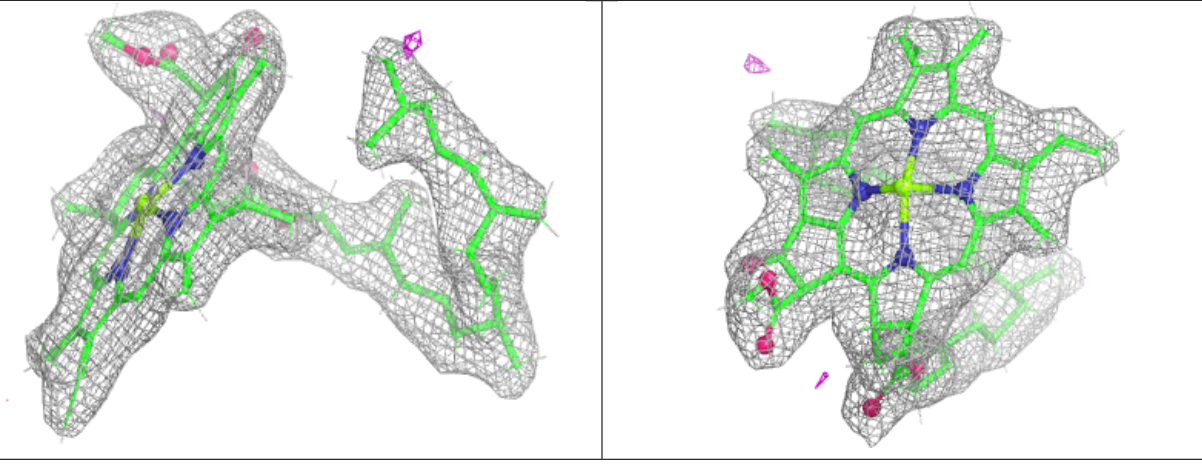
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA C 504:

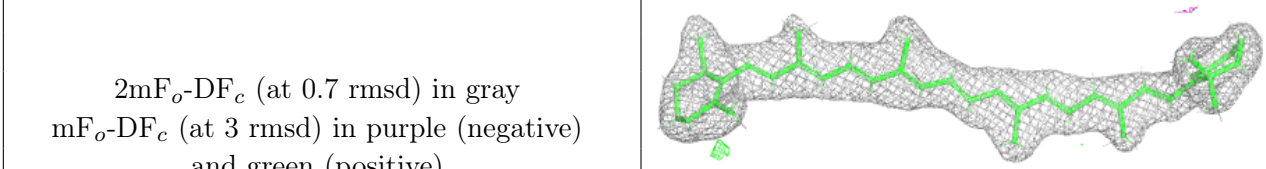
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

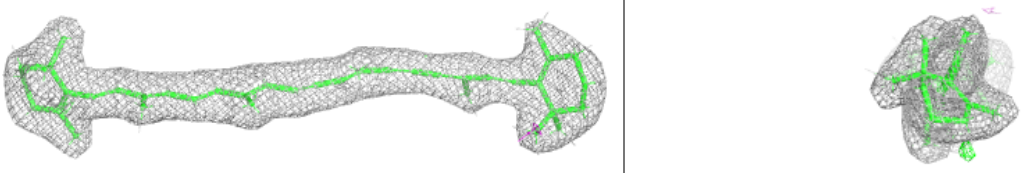




Electron density around BCR A 406:

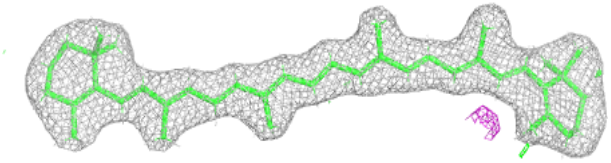
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

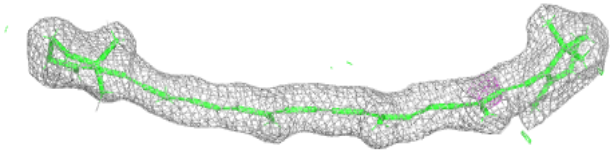


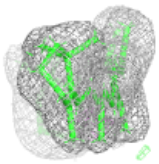


Electron density around BCR t 101:

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

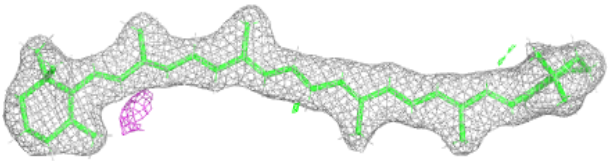


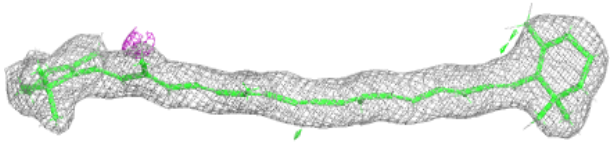


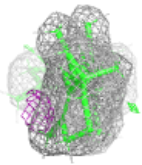


Electron density around BCR B 618:

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

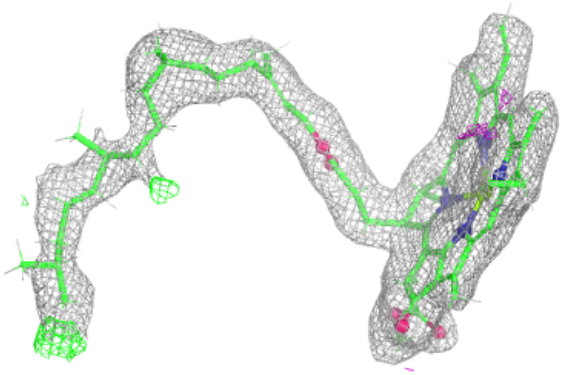


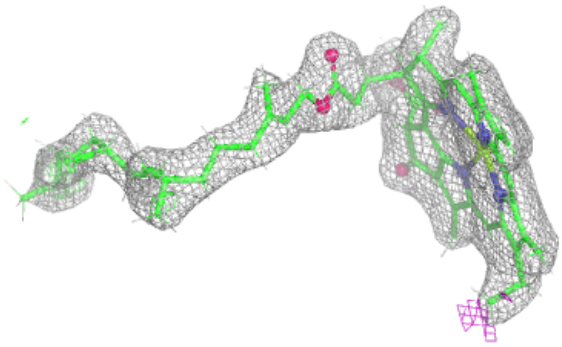


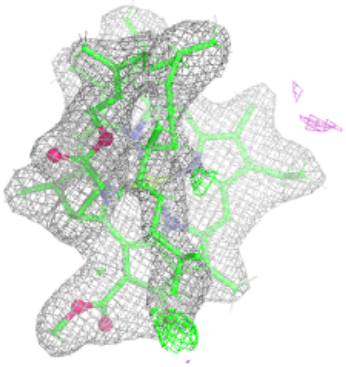


Electron density around CLA b 605:

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

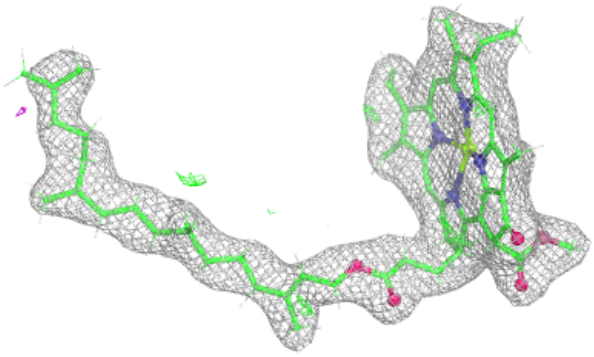


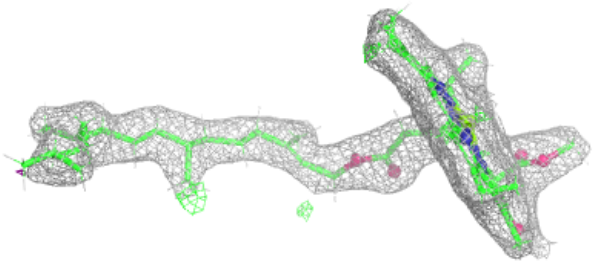


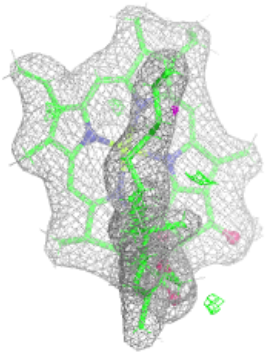


Electron density around CLA b 608:

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

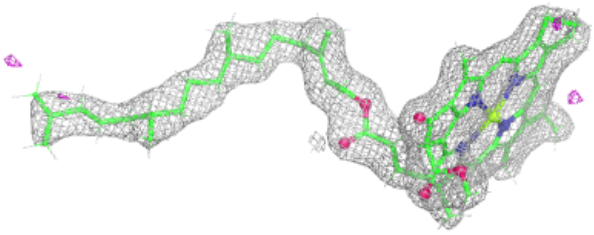


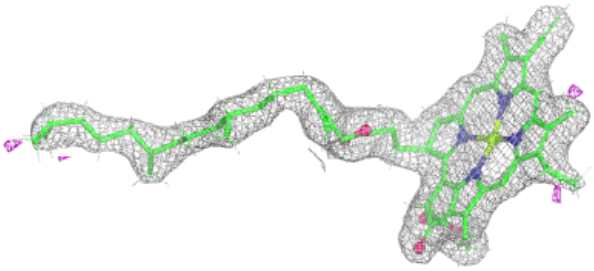


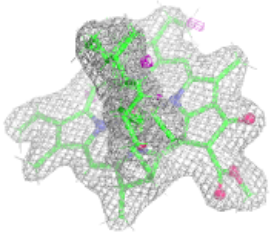


Electron density around CLA c 504:

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

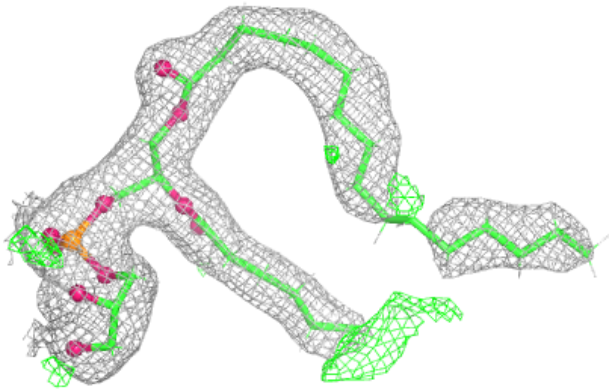


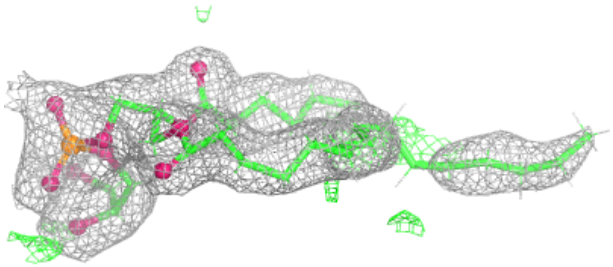




Electron density around LHG d 408:

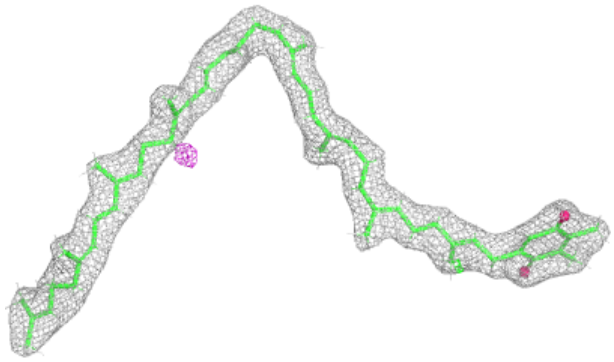
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

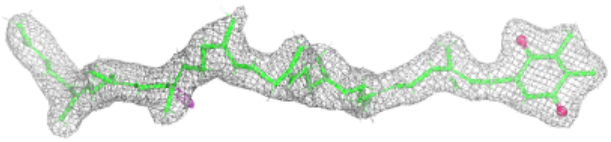


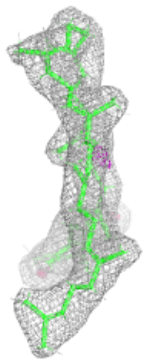


Electron density around PL9 D 405:

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

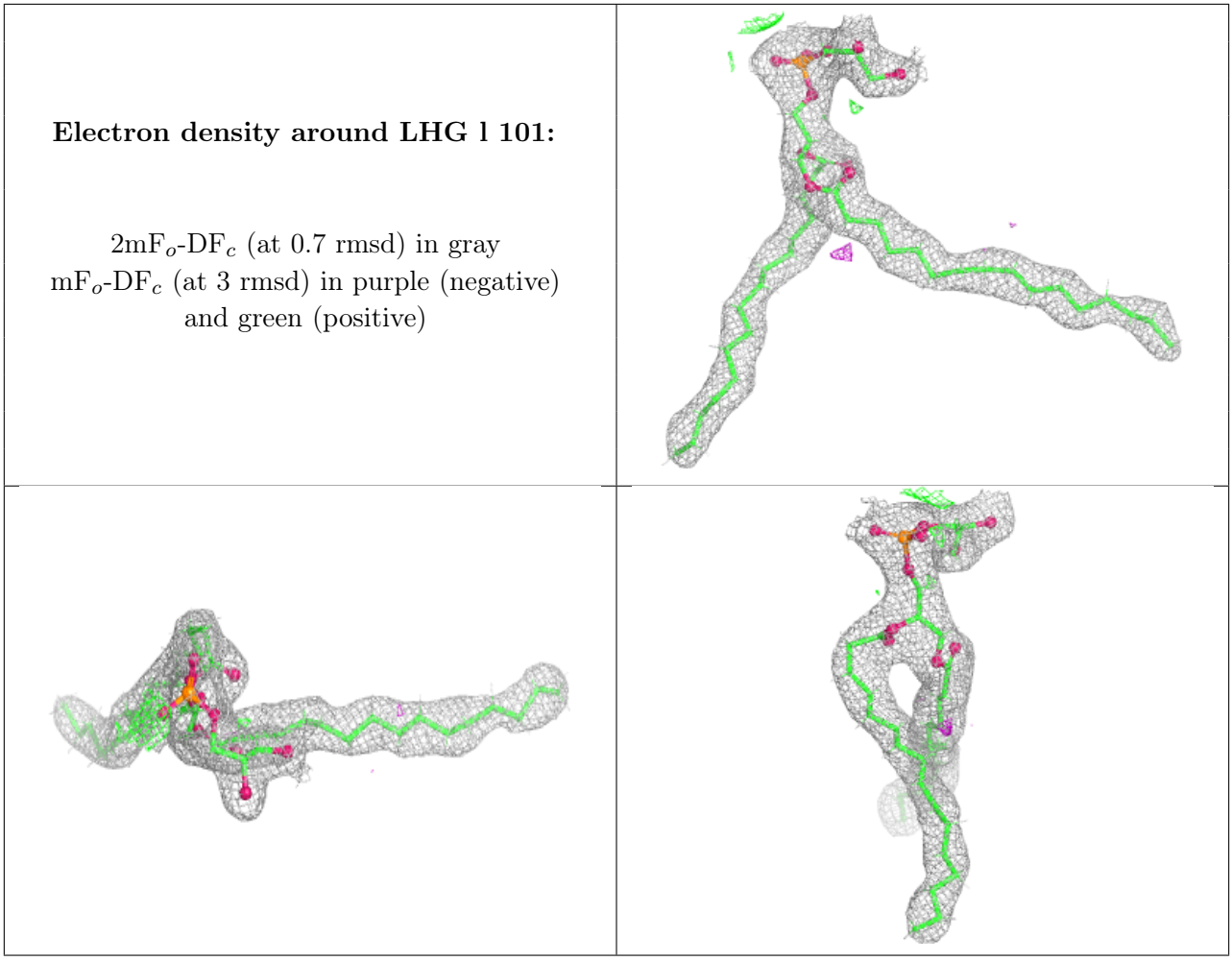






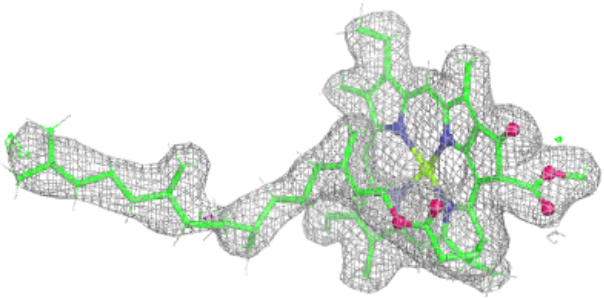
Electron density around LHG l 101:

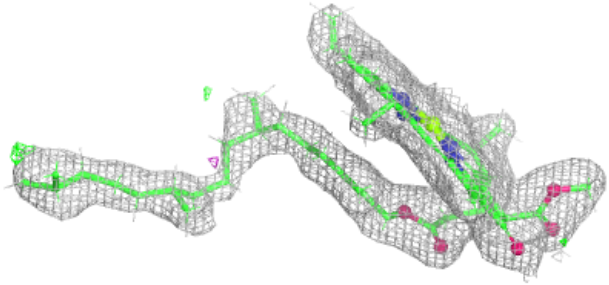
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

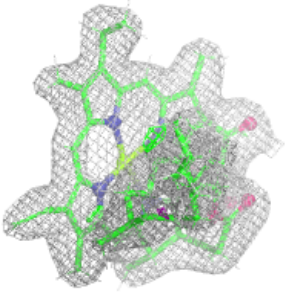


Electron density around CLA c 507:

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

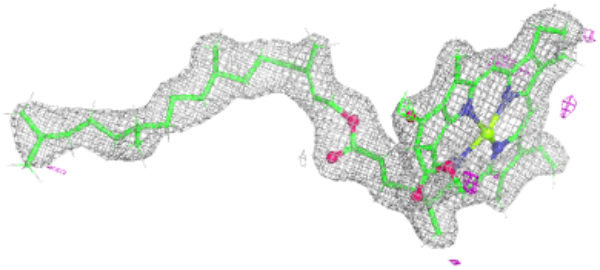


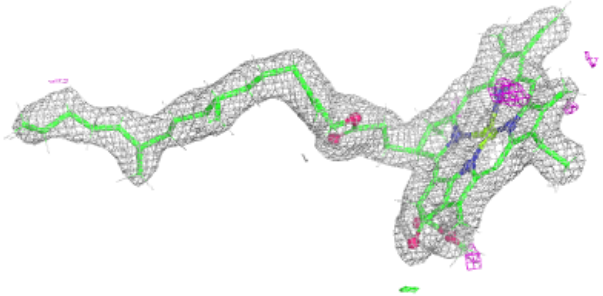


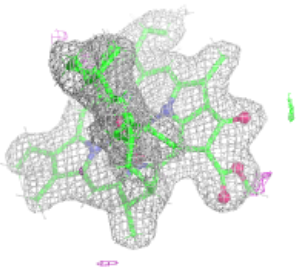


Electron density around CLA C 503:

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

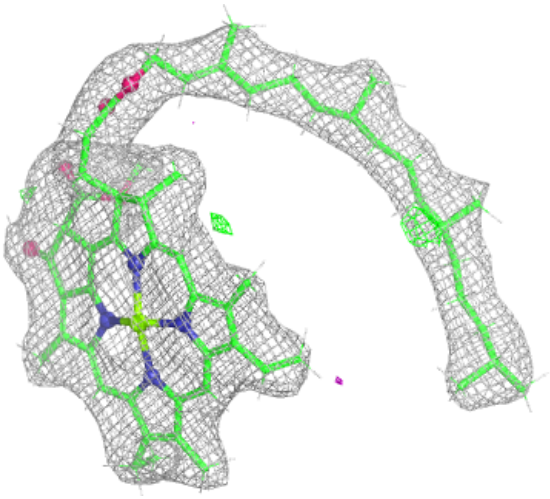


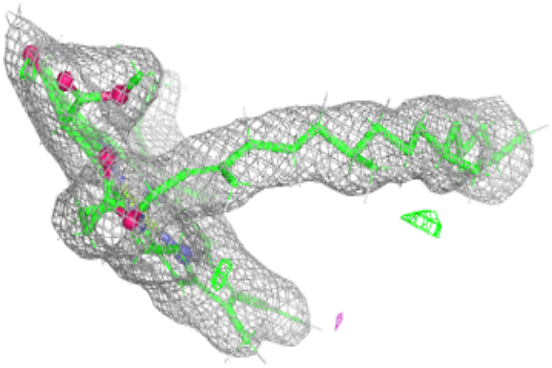


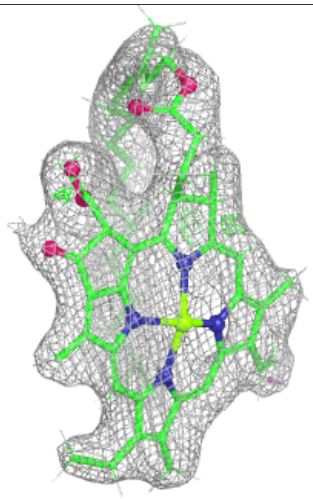


Electron density around CLA c 509:

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

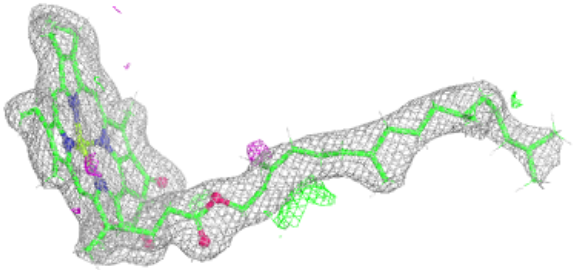


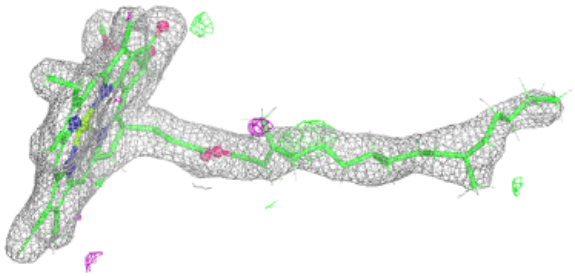


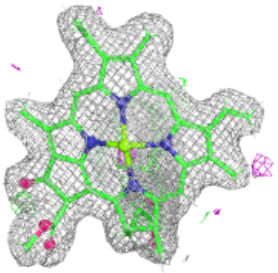


Electron density around CLA B 605:

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

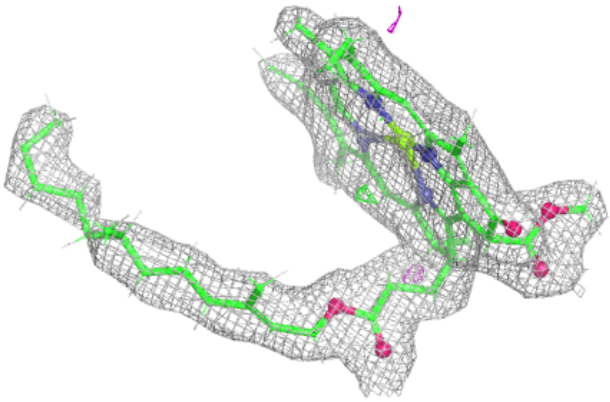


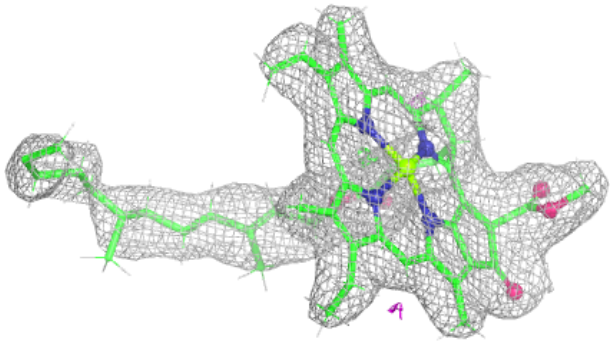


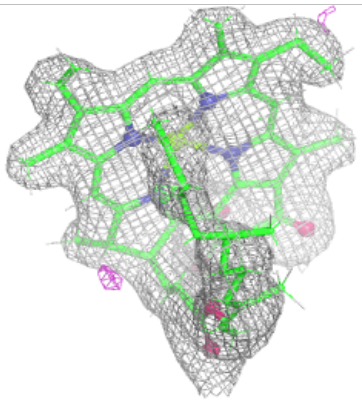


Electron density around CLA C 505:

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

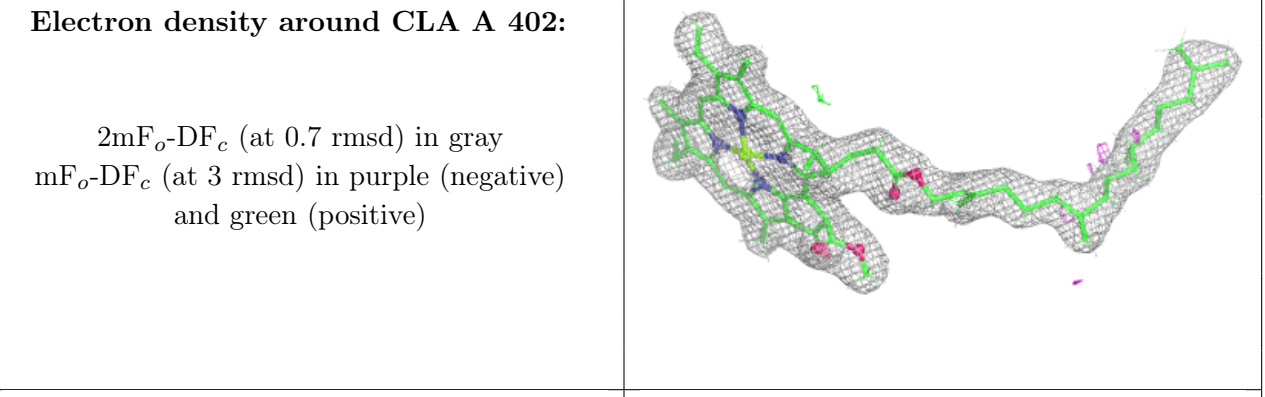






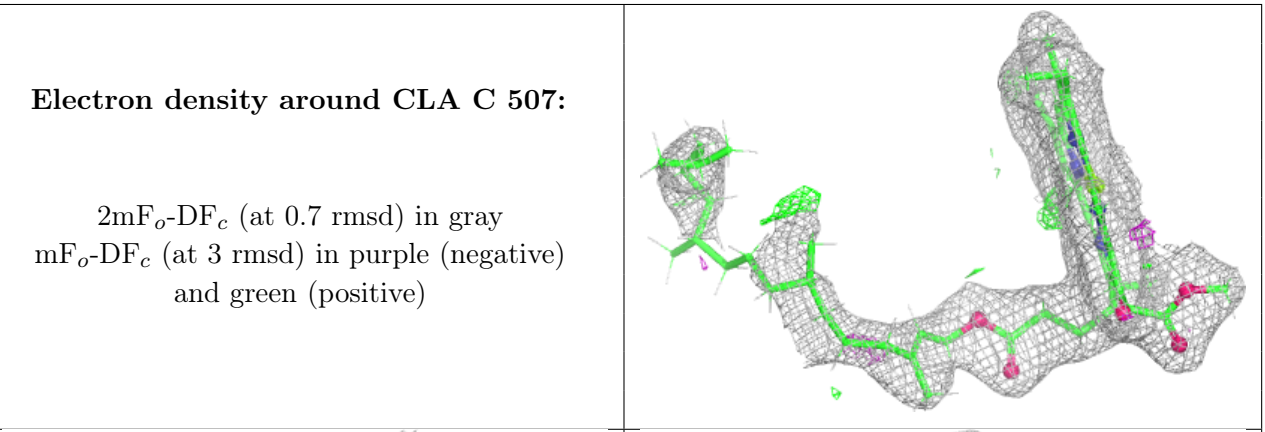
Electron density around CLA A 402:

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



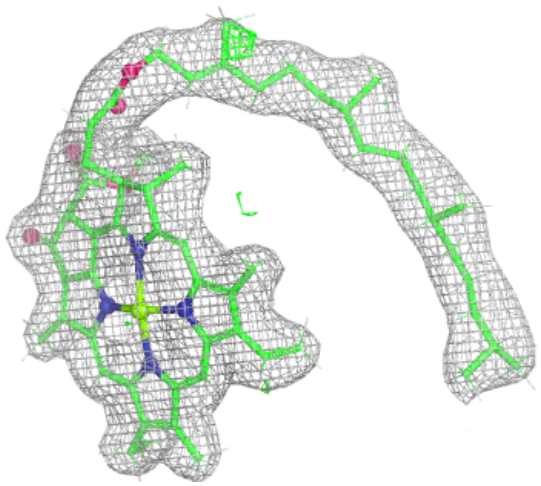
Electron density around CLA C 507:

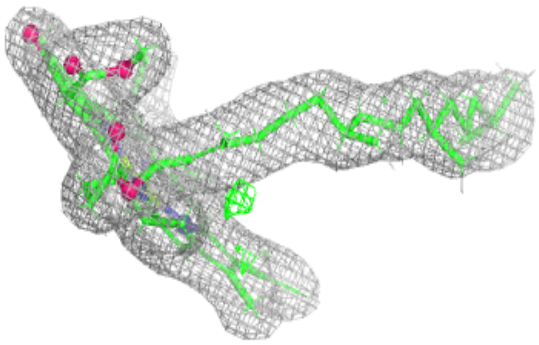
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

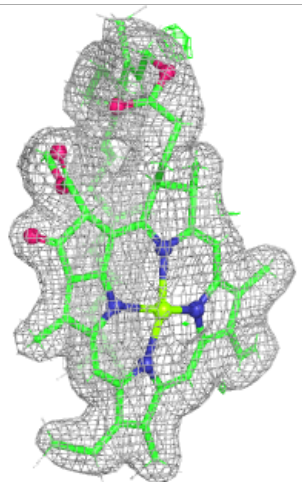


Electron density around CLA C 508:

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

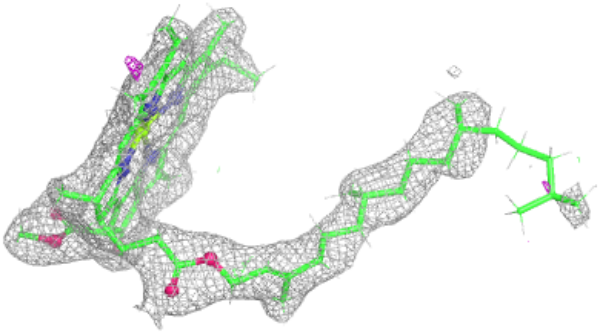


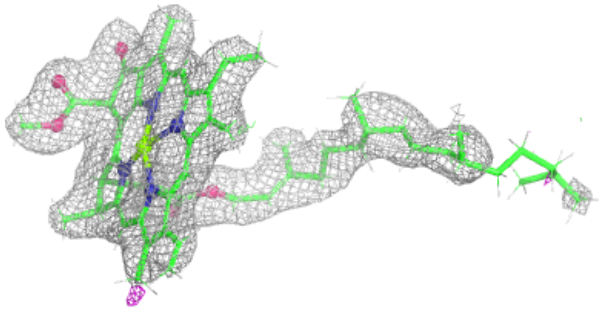


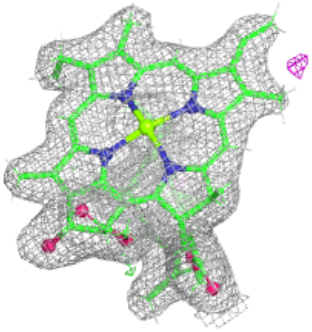


Electron density around CLA C 509:

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

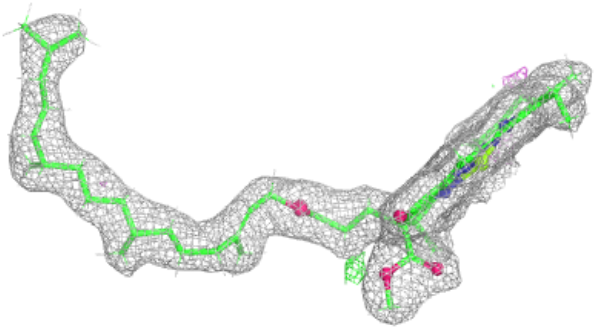


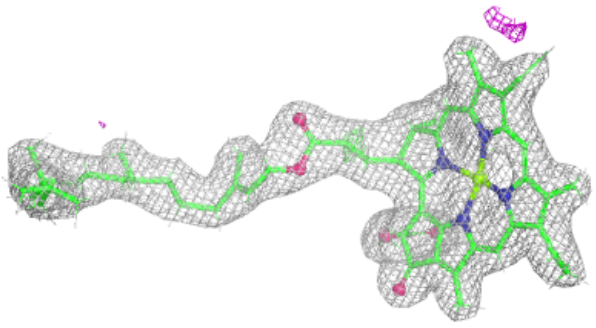


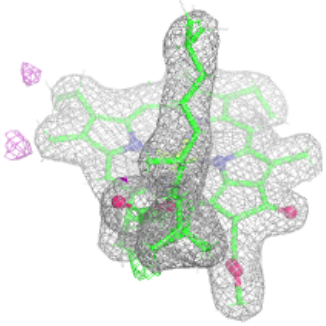


Electron density around CLA d 402:

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

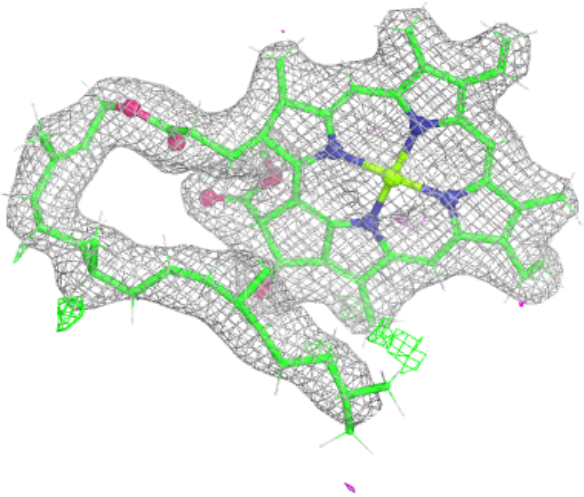


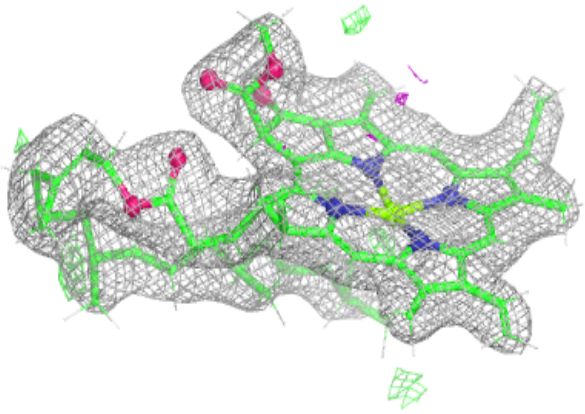


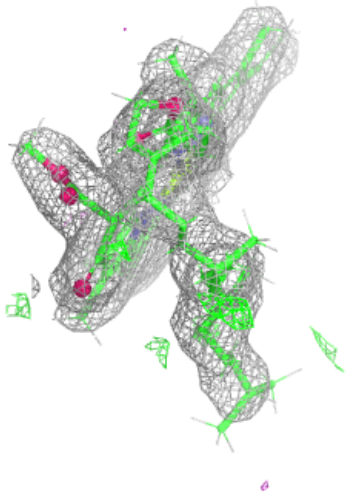


Electron density around CLA C 510:

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

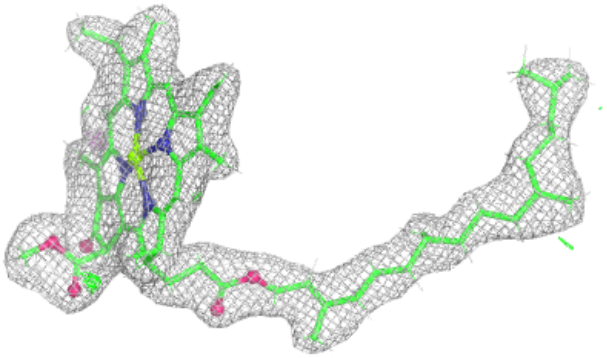


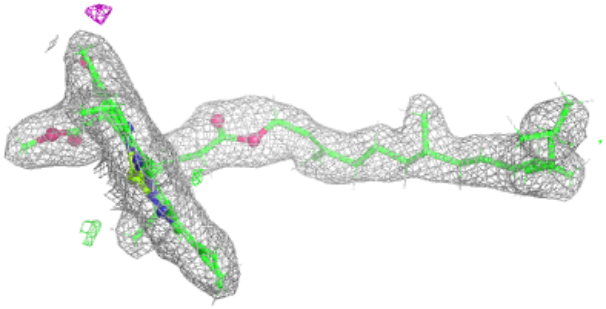


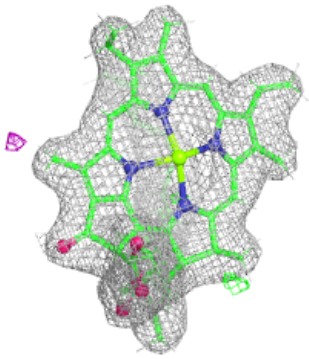


Electron density around CLA B 610:

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

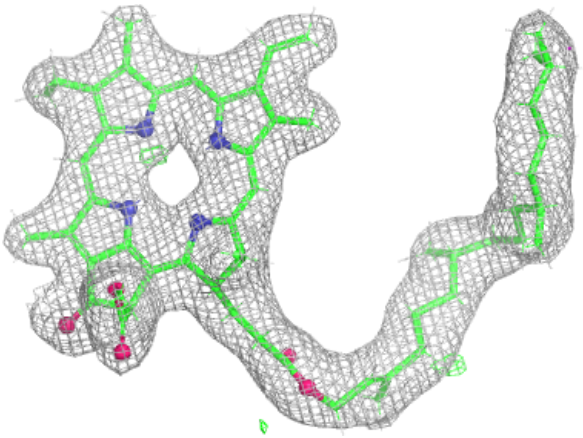


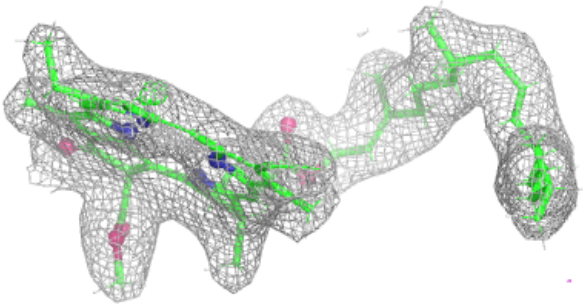


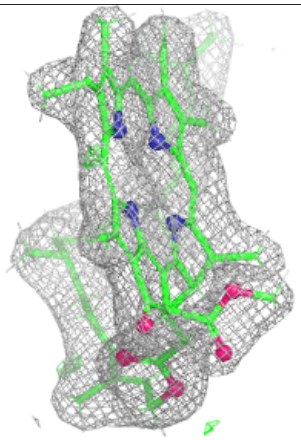


Electron density around PHO D 401:

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

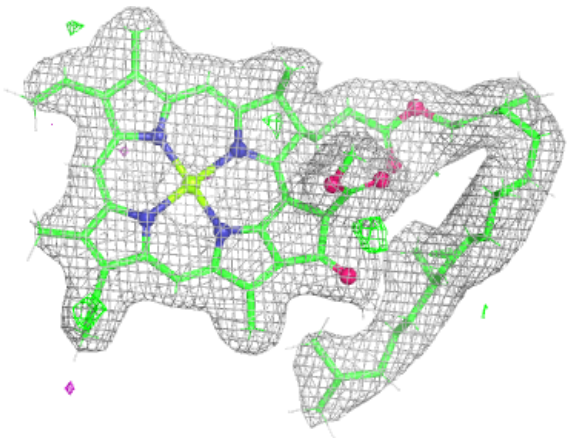


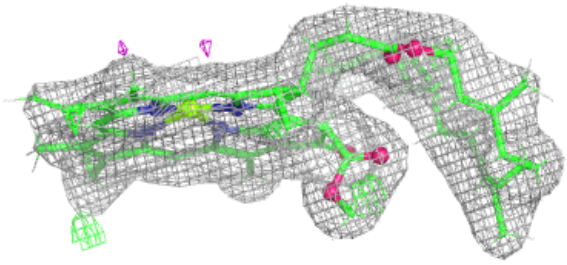


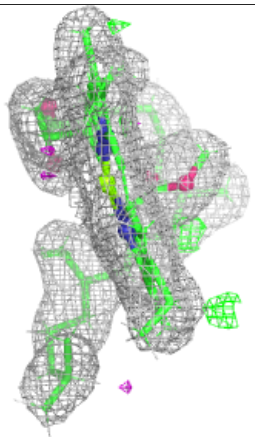


Electron density around CLA B 611:

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

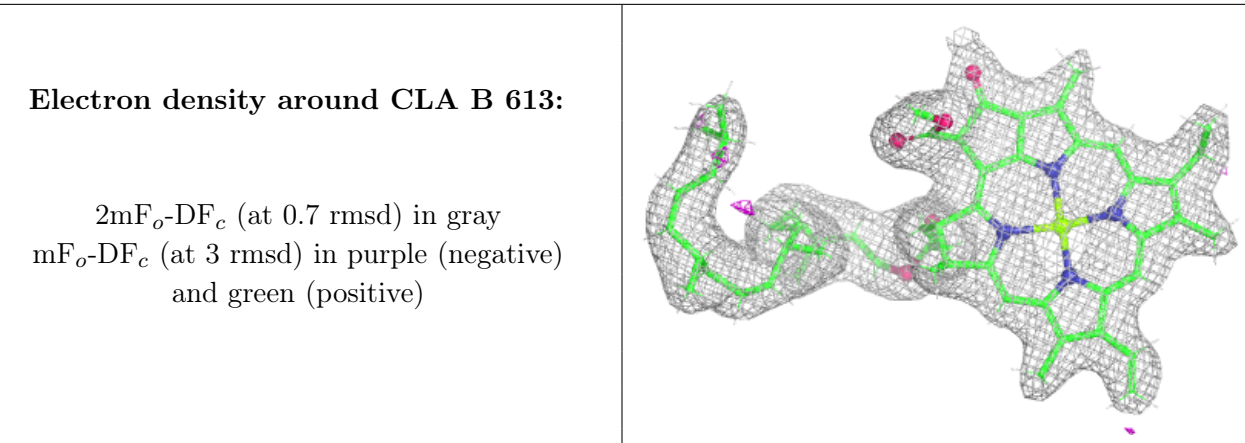


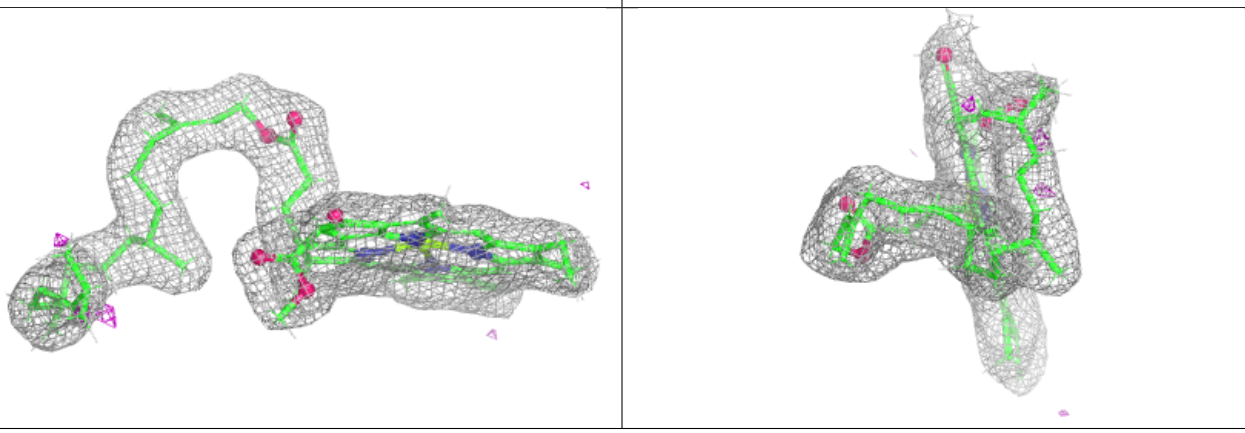




Electron density around CLA B 613:

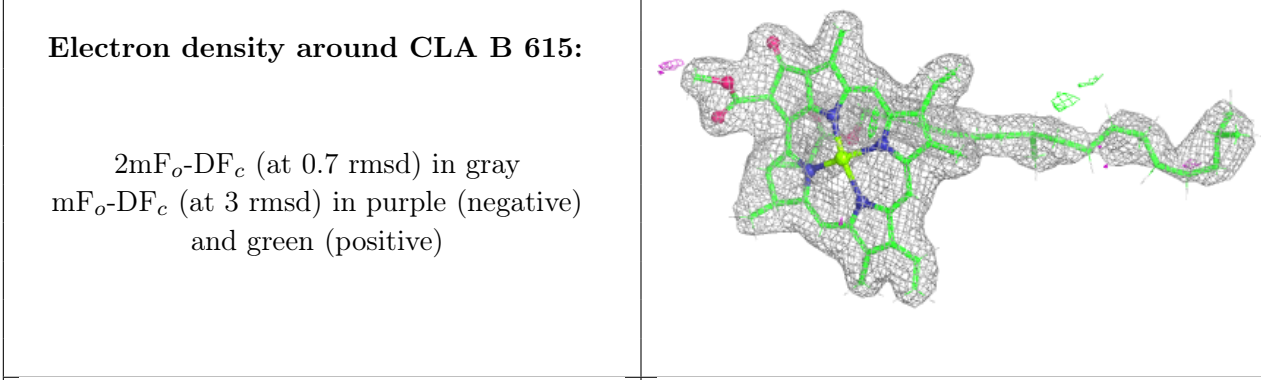
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

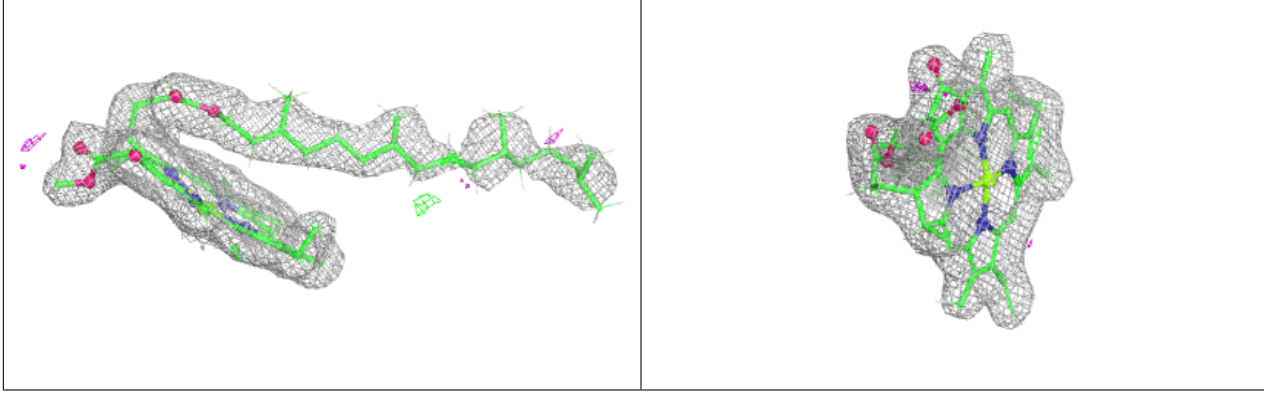




Electron density around CLA B 615:

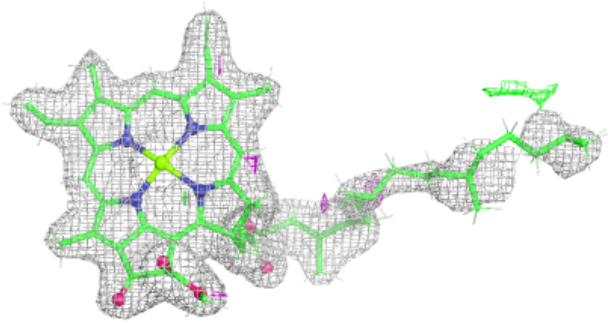
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

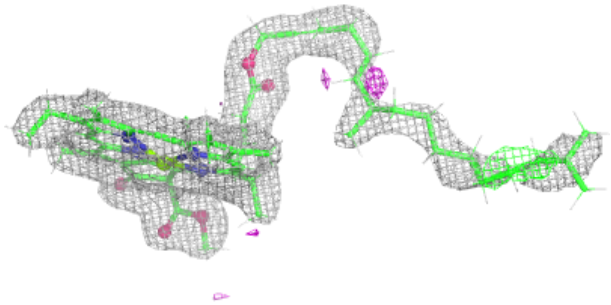


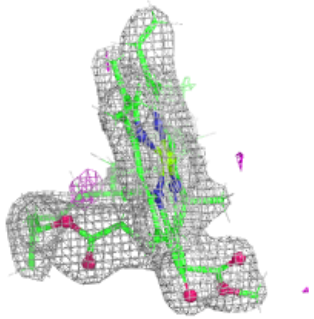


Electron density around CLA a 403:

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

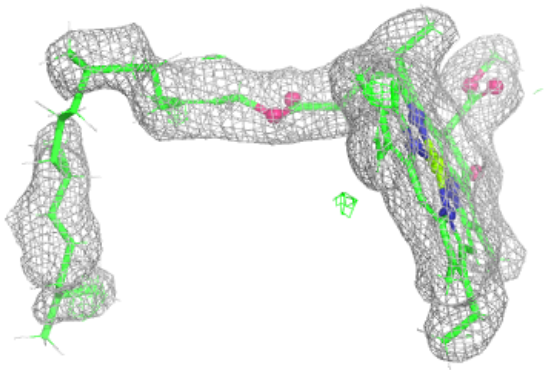


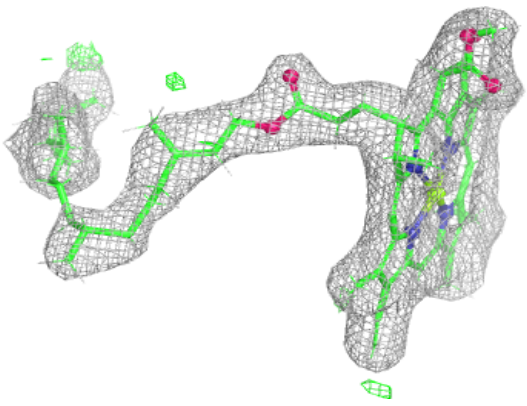


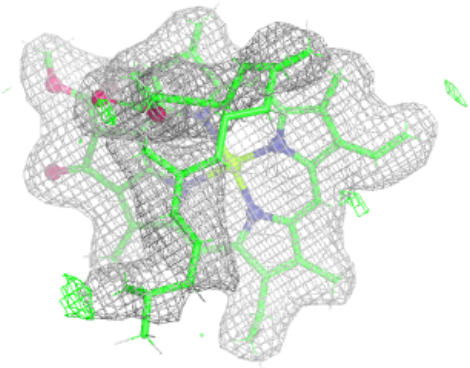


Electron density around CLA a 405:

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

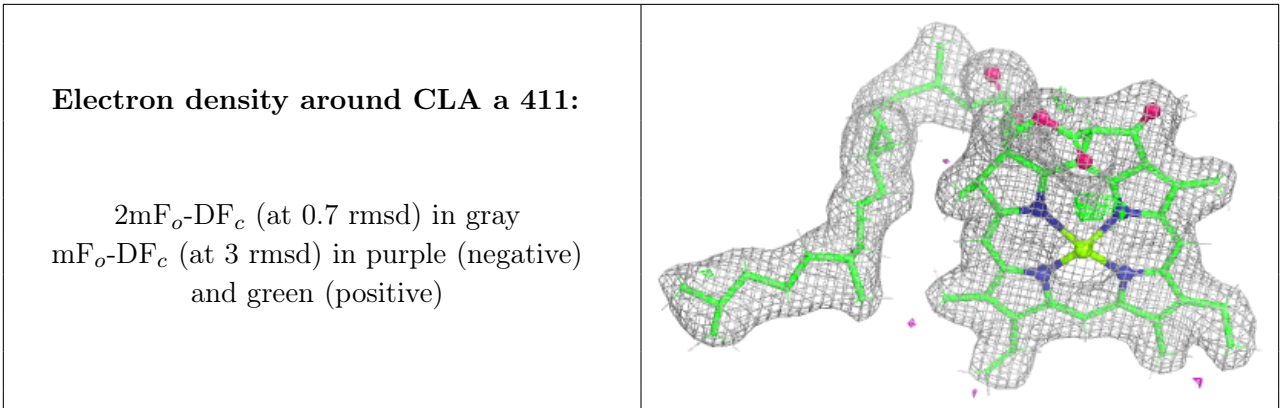


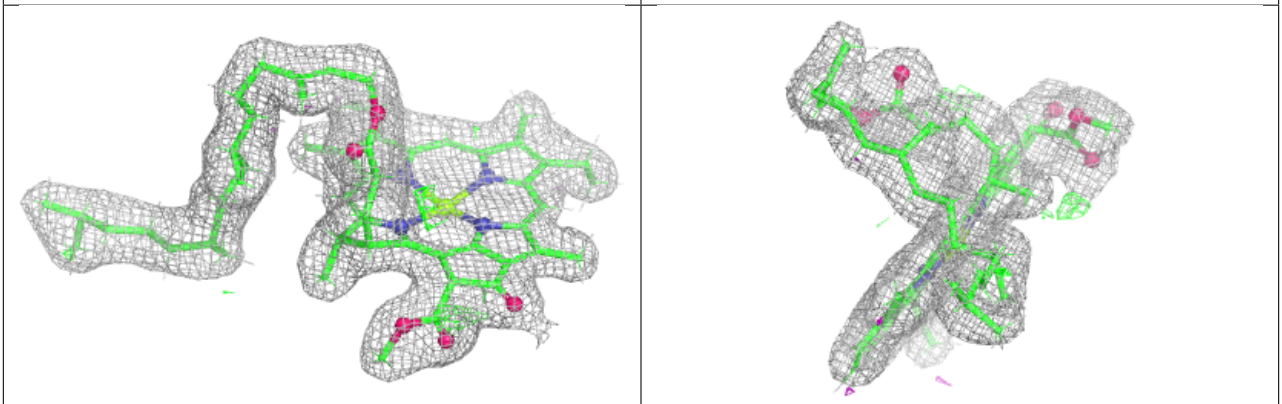




Electron density around CLA a 411:

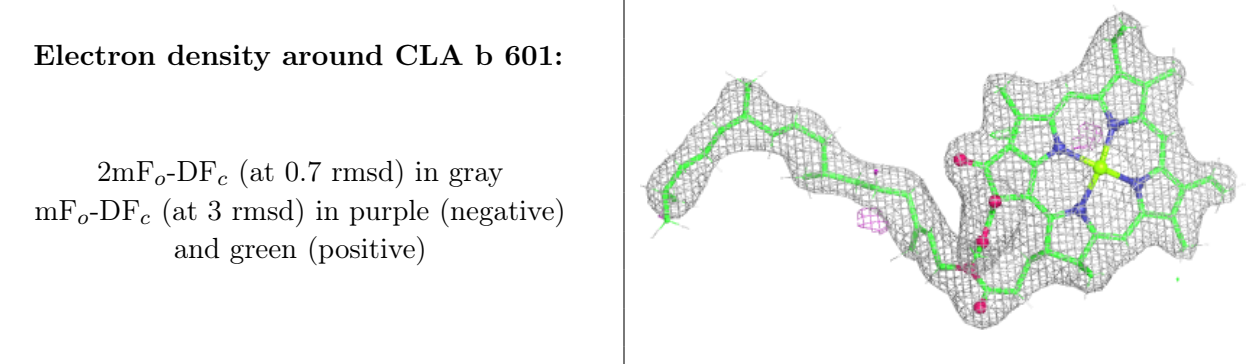
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

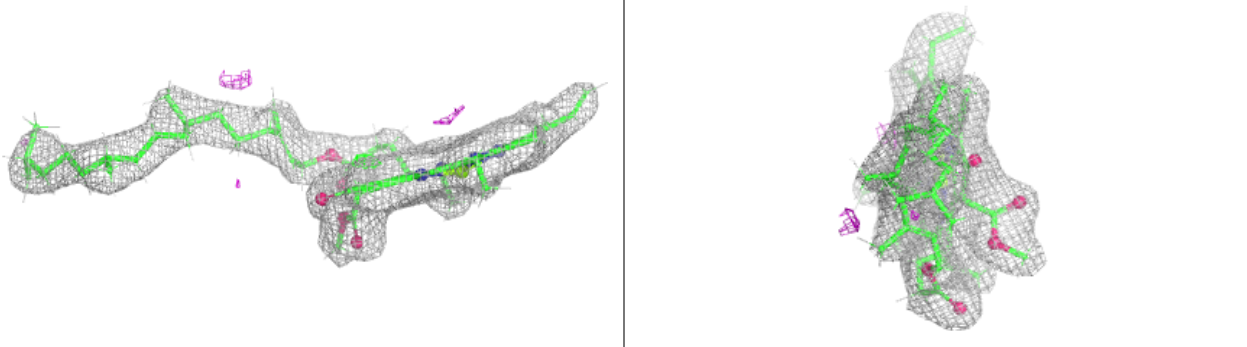




Electron density around CLA b 601:

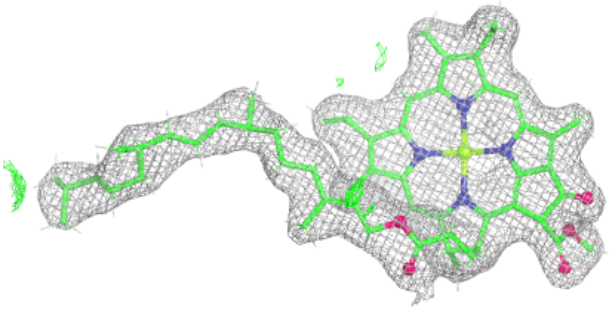
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

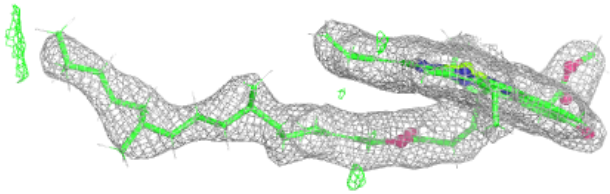


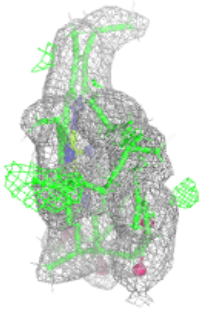


Electron density around CLA b 602:

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

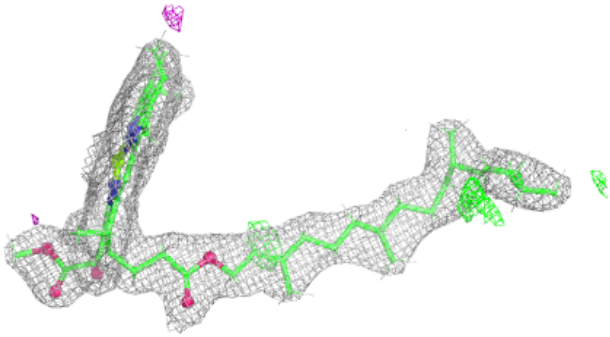


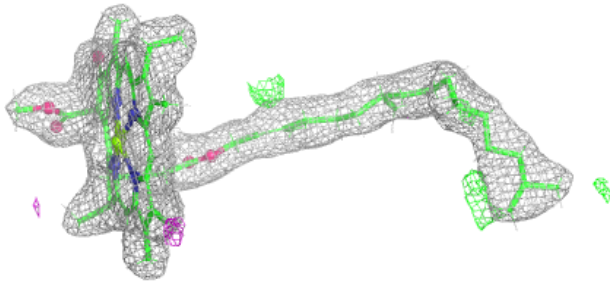


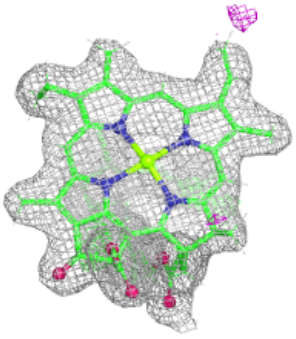


Electron density around CLA b 604:

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

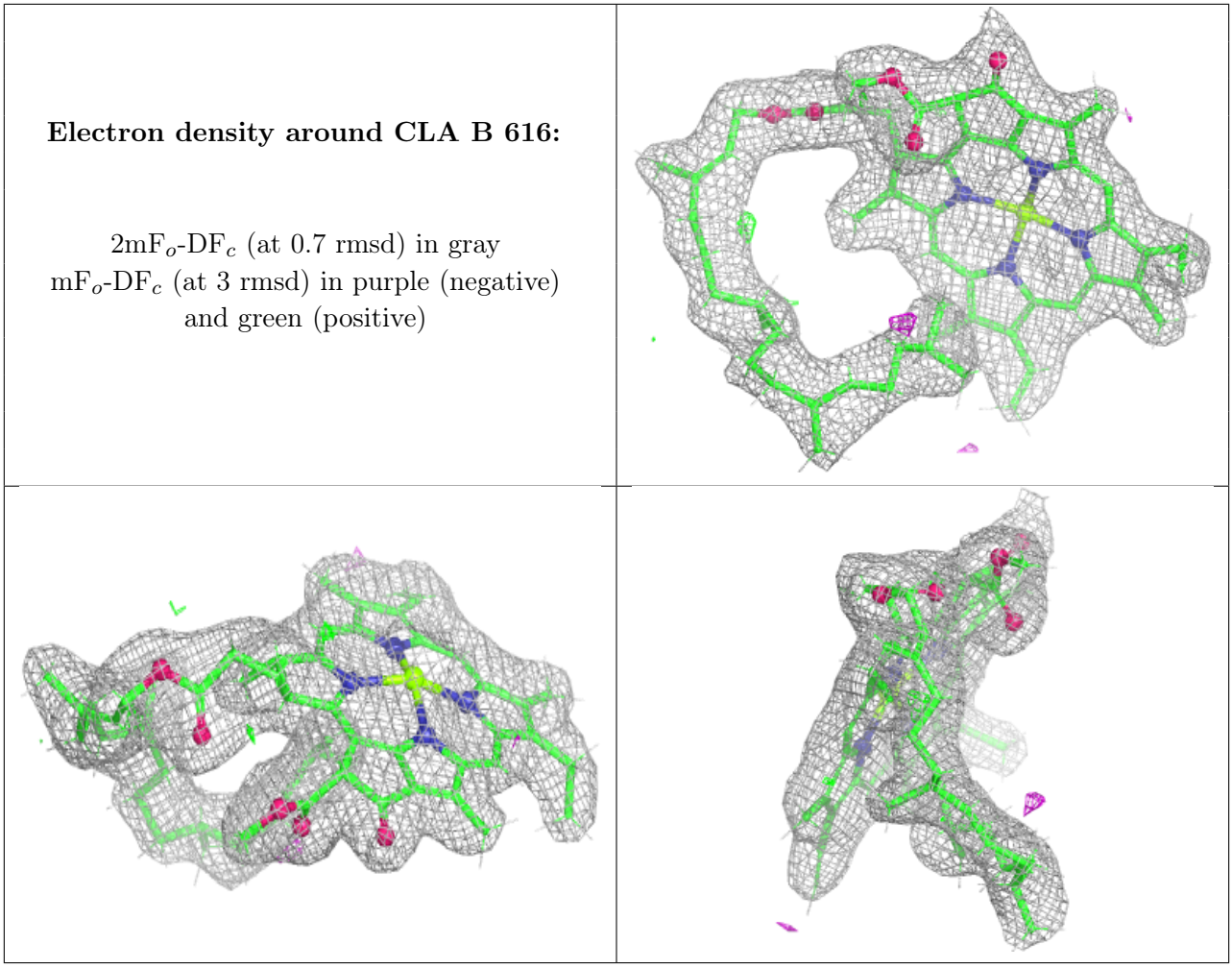






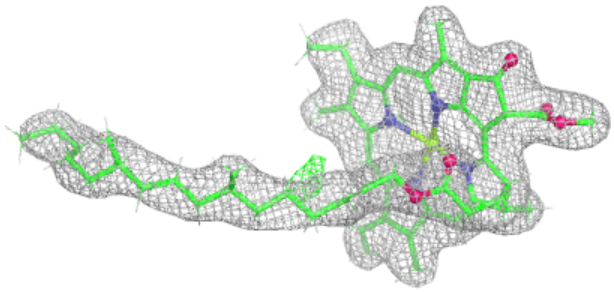
Electron density around CLA B 616:

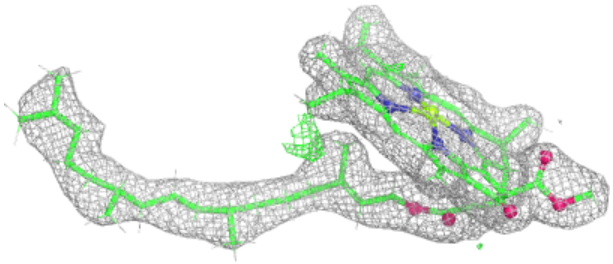
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

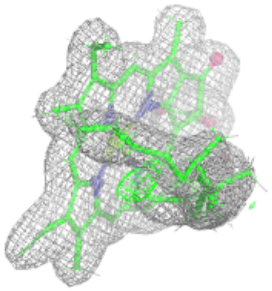


Electron density around CLA b 607:

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

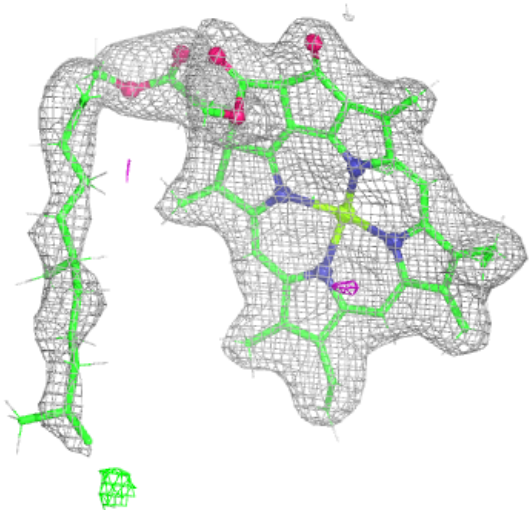


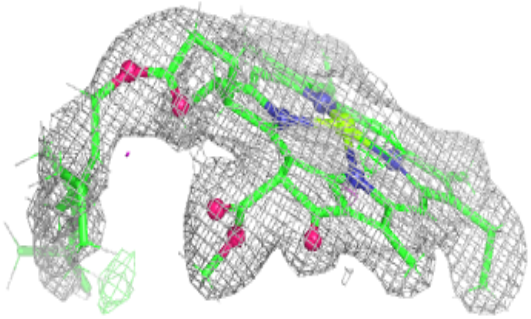


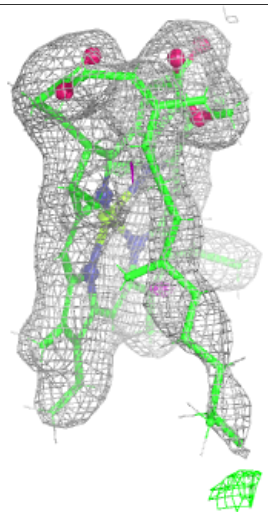


Electron density around CLA B 617:

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

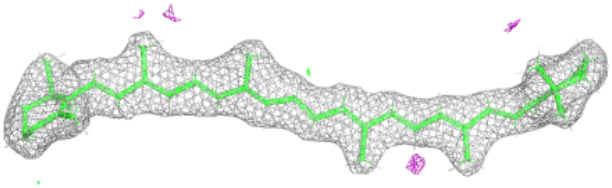


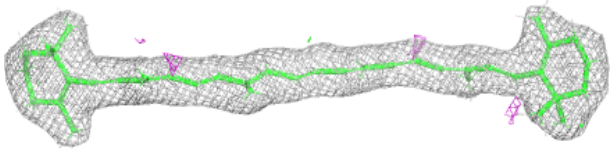


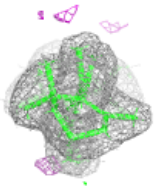


Electron density around BCR a 406:

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

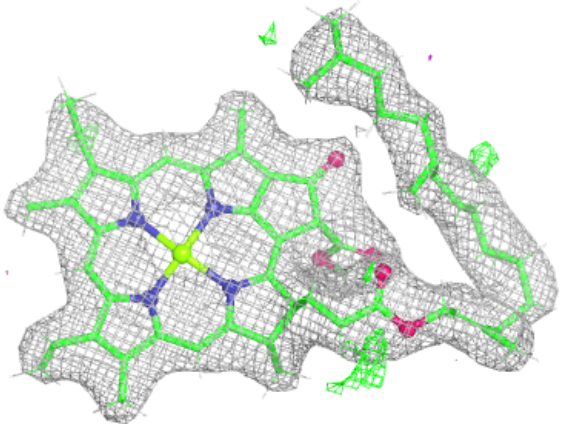


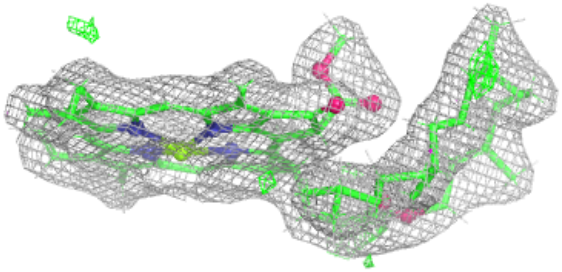


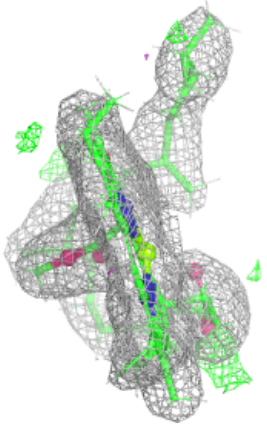


Electron density around CLA b 609:

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

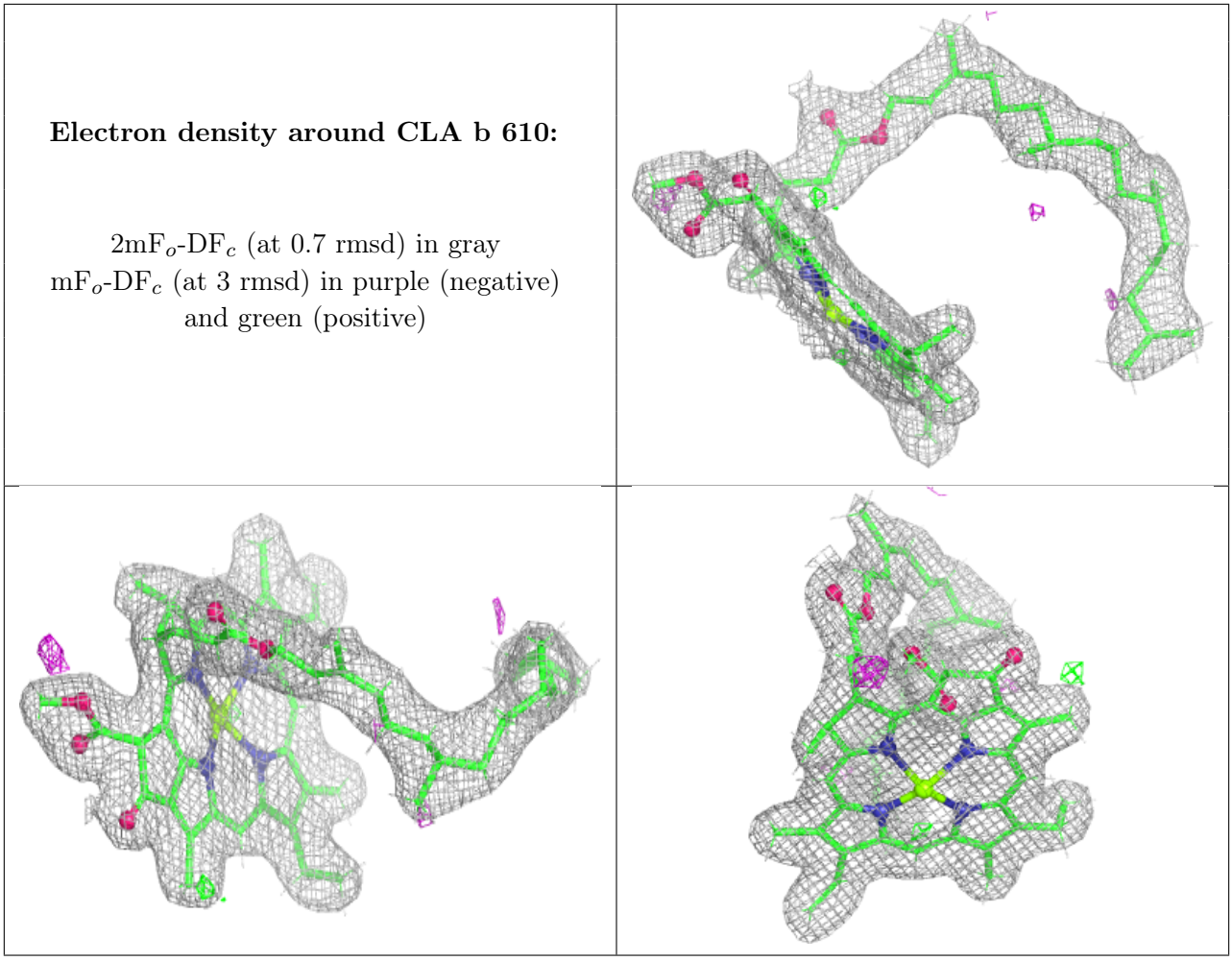






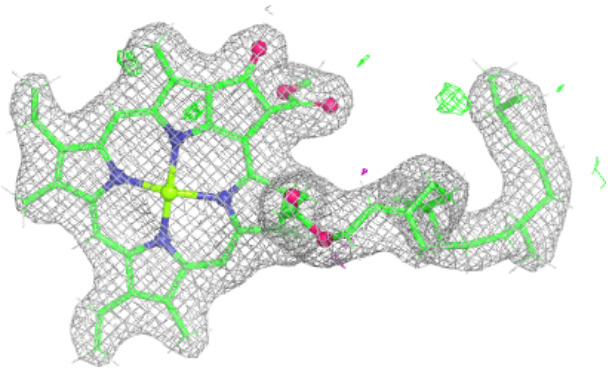
Electron density around CLA b 610:

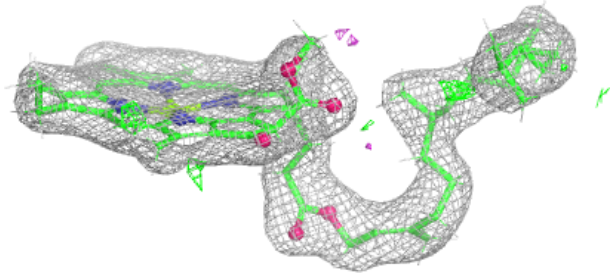
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

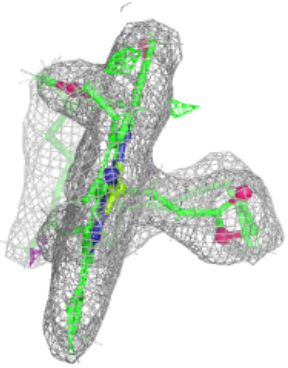


Electron density around CLA b 611:

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

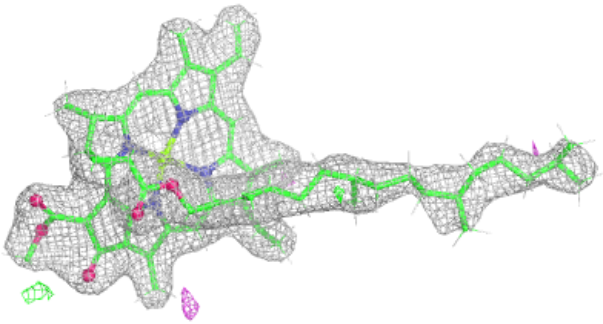


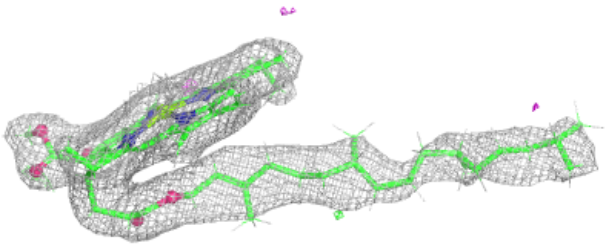


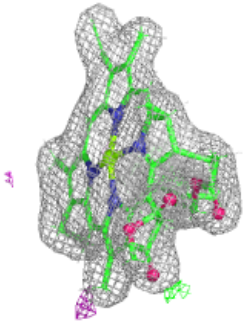


Electron density around CLA b 613:

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

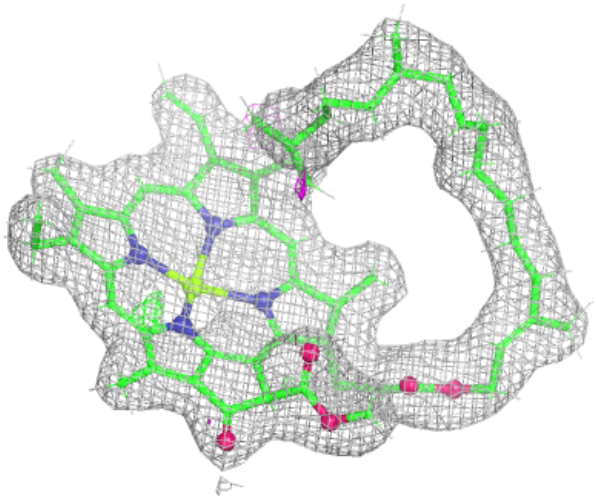


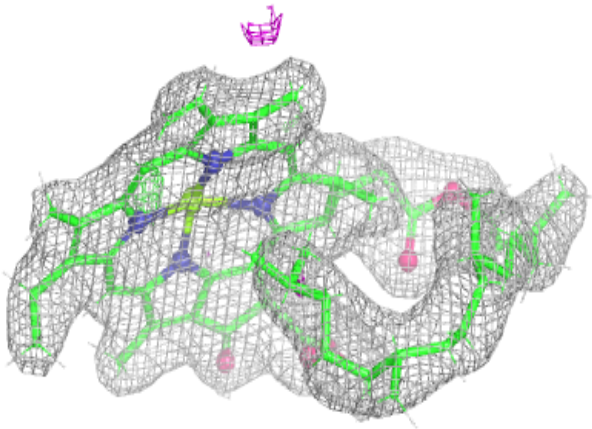


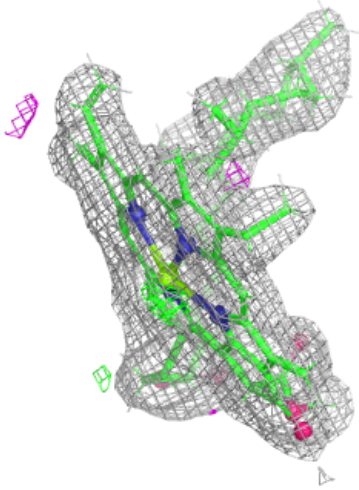


Electron density around CLA b 614:

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

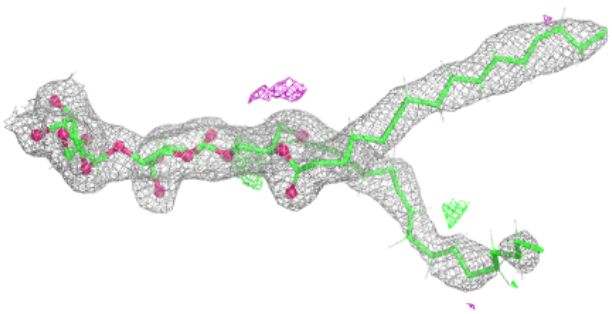


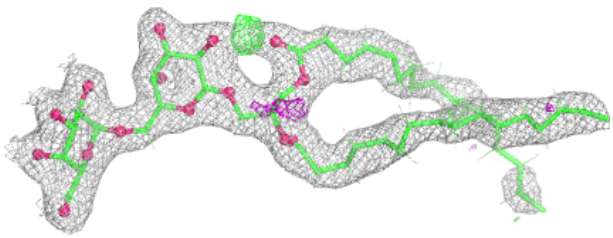




Electron density around DGD c 519:

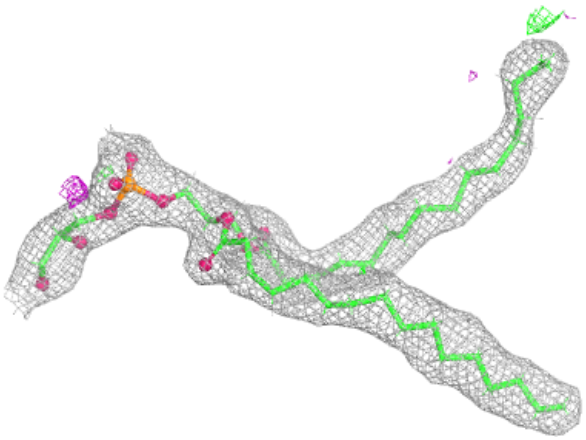
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

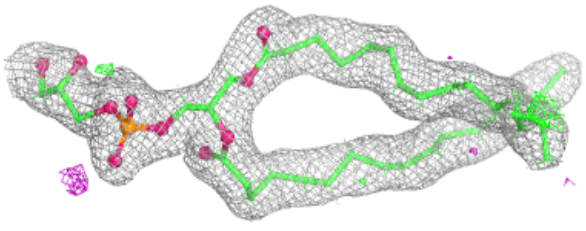


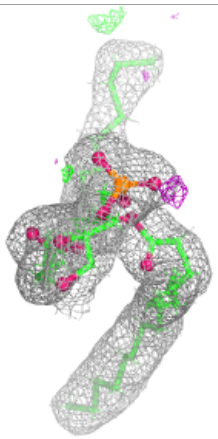


Electron density around LHG D 408:

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

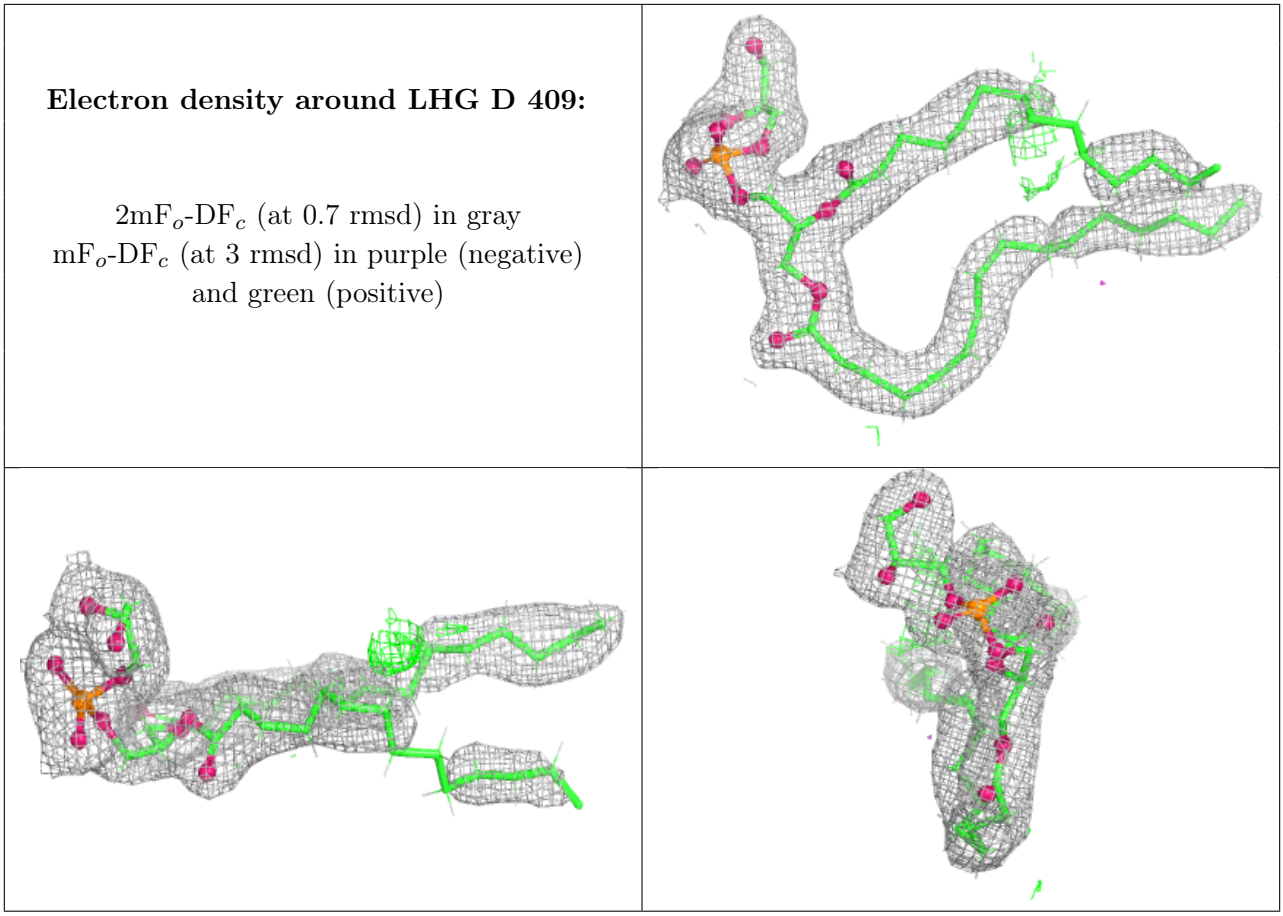






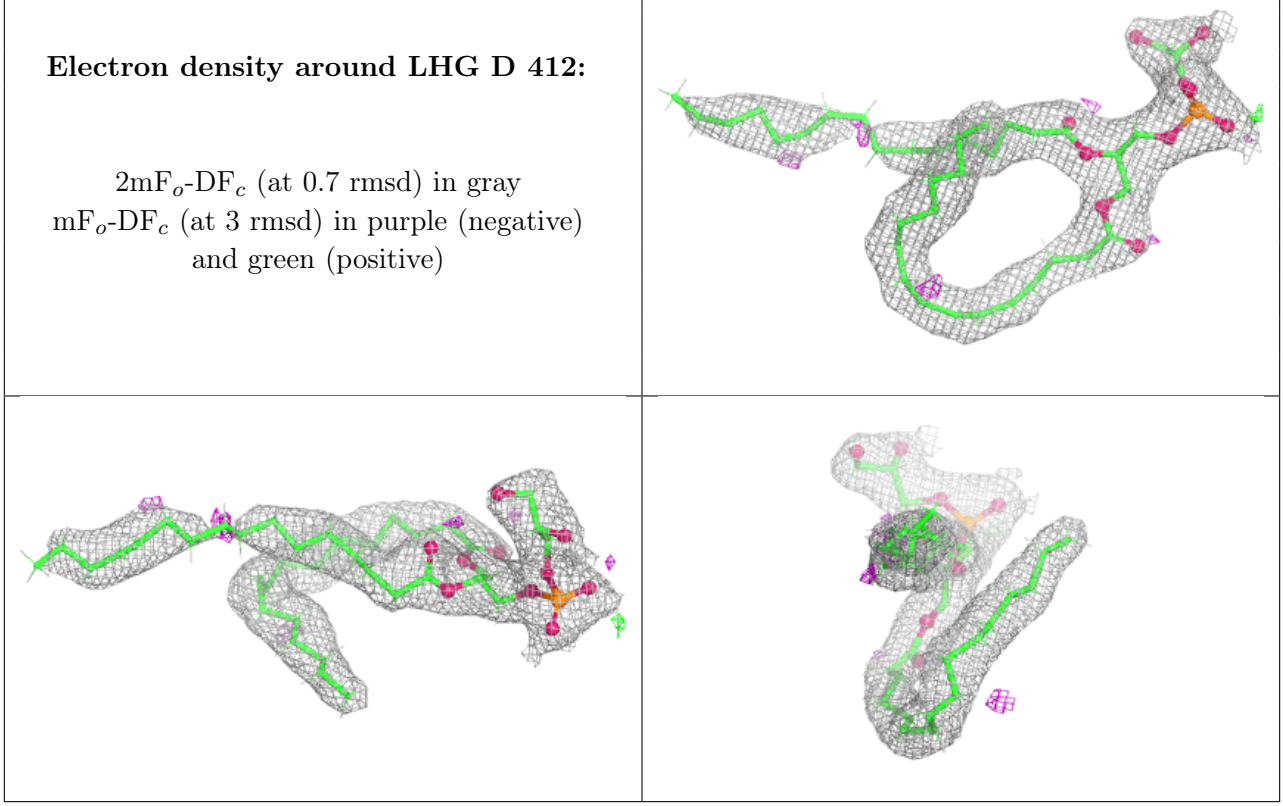
Electron density around LHG D 409:

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



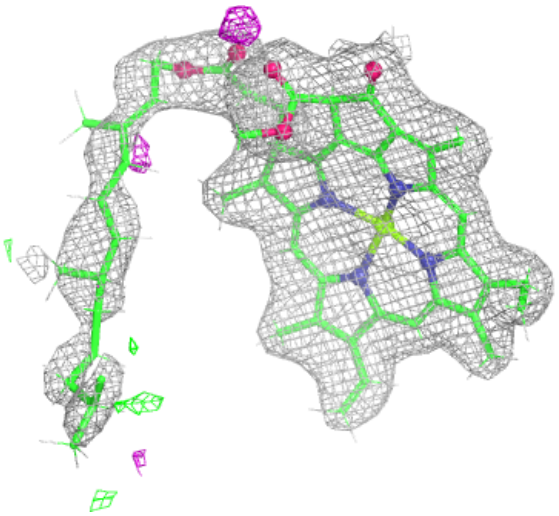
Electron density around LHG D 412:

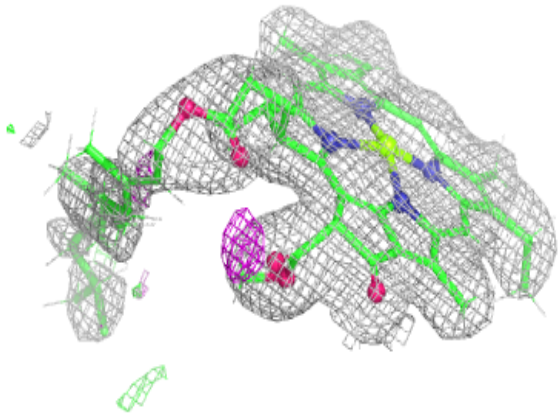
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

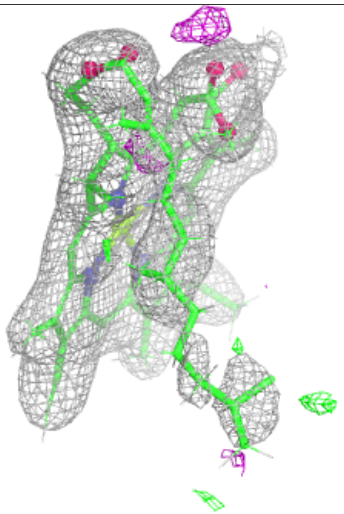


Electron density around CLA b 615:

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

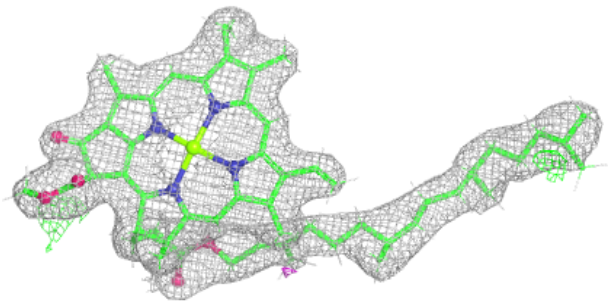


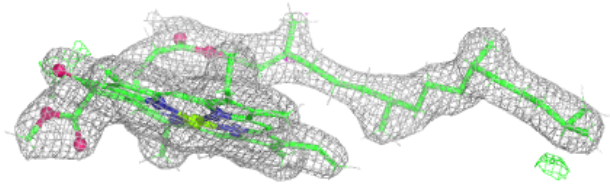


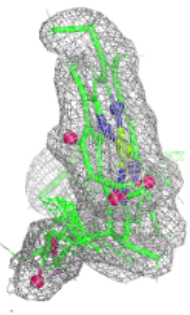


Electron density around CLA c 503:

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

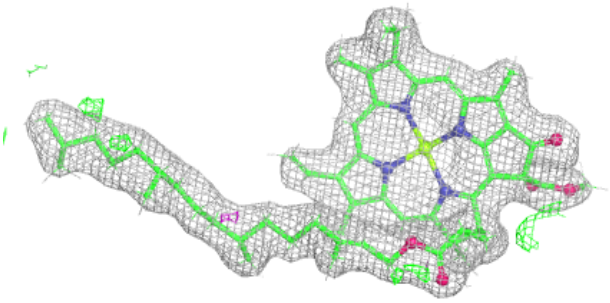


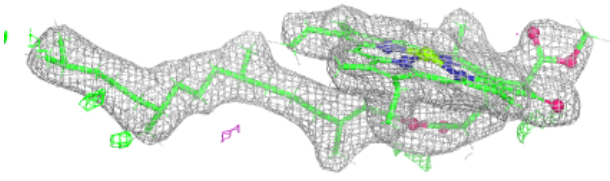


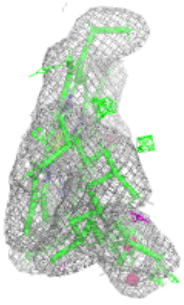


Electron density around CLA C 502:

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

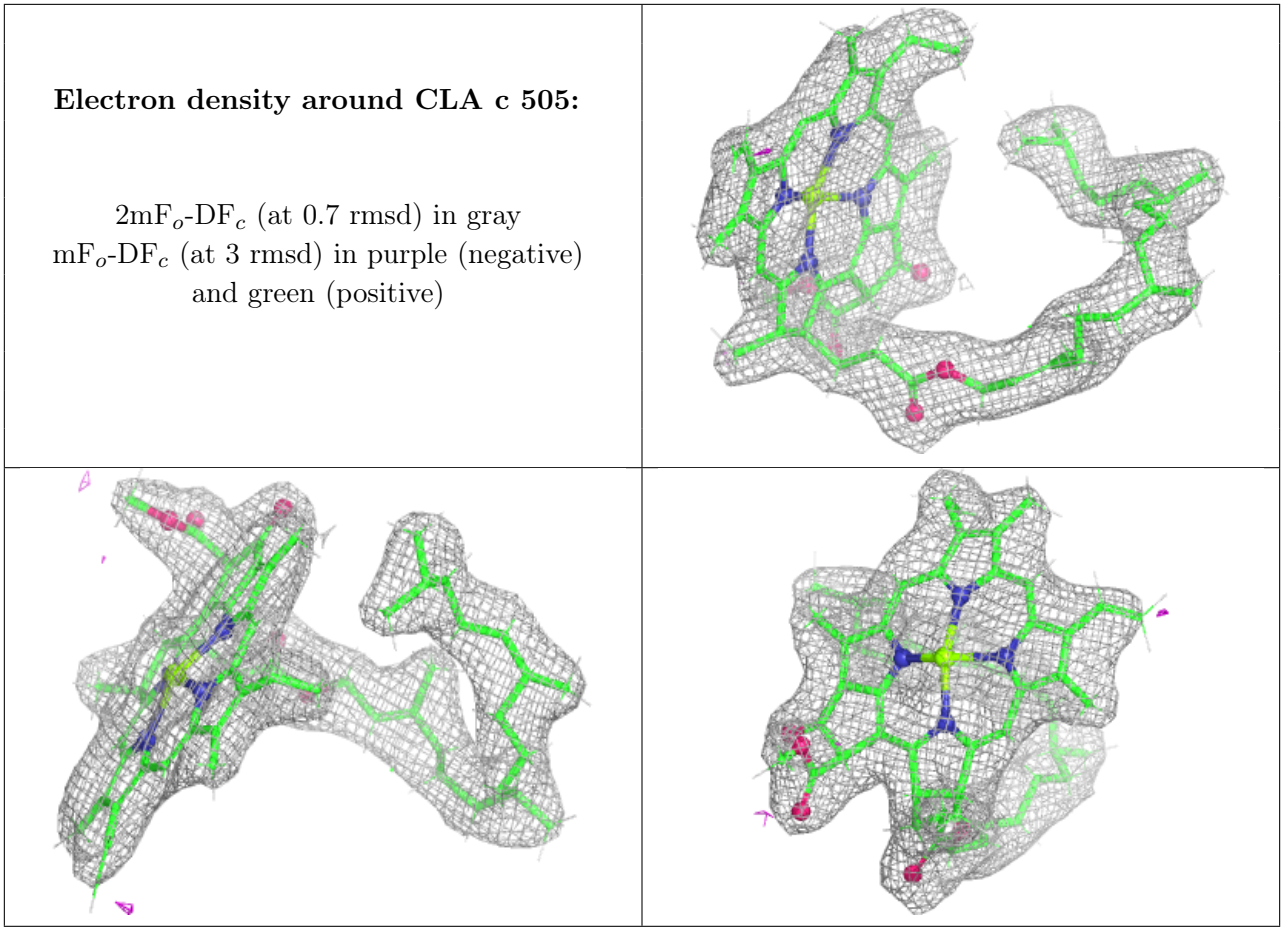






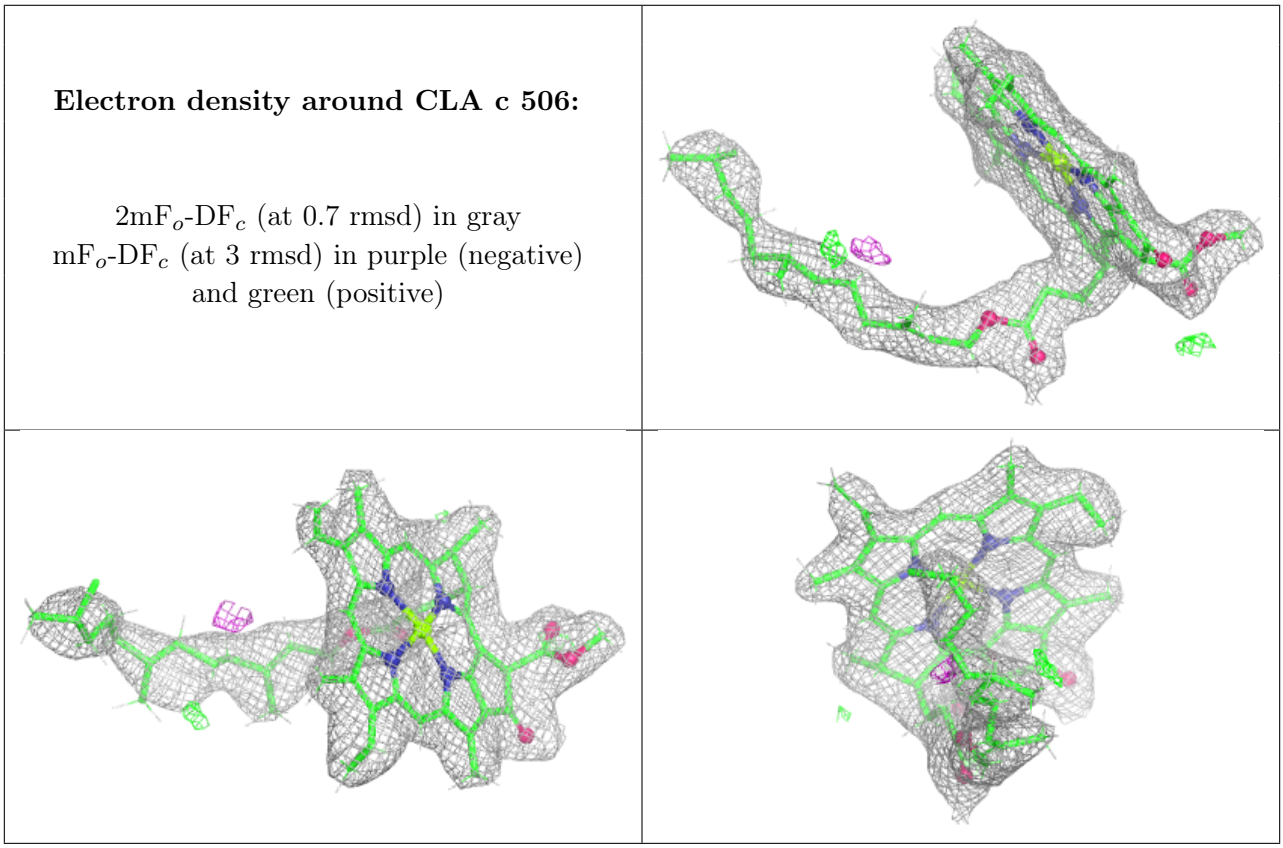
Electron density around CLA c 505:

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



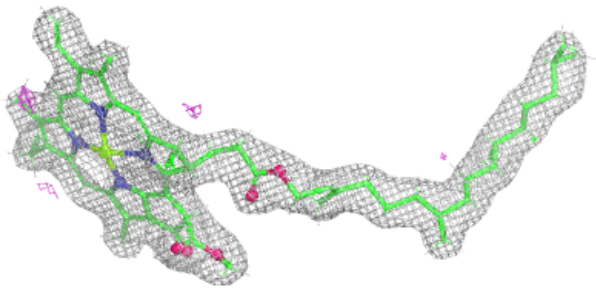
Electron density around CLA c 506:

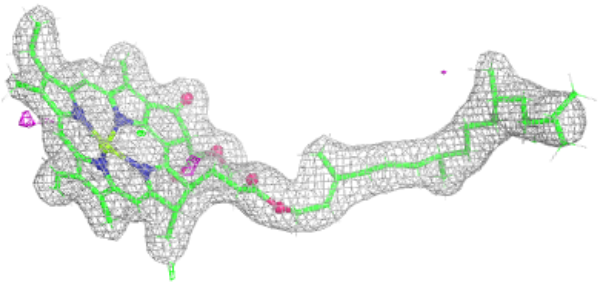
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

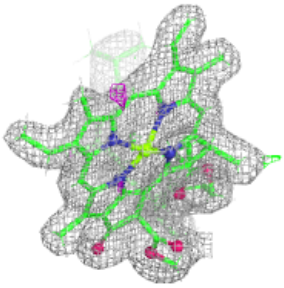


Electron density around CLA a 402:

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

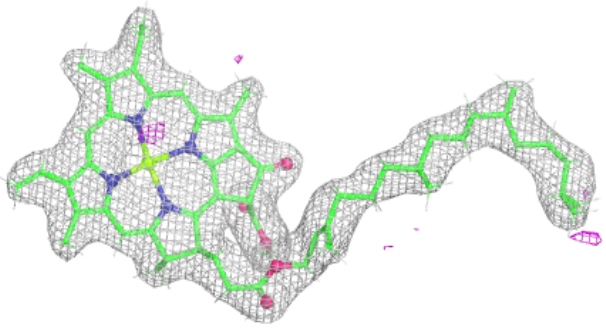


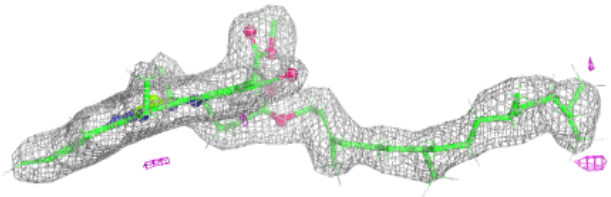


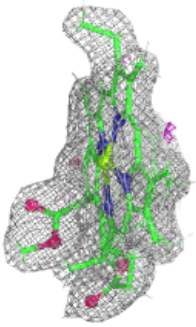


Electron density around CLA B 603:

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

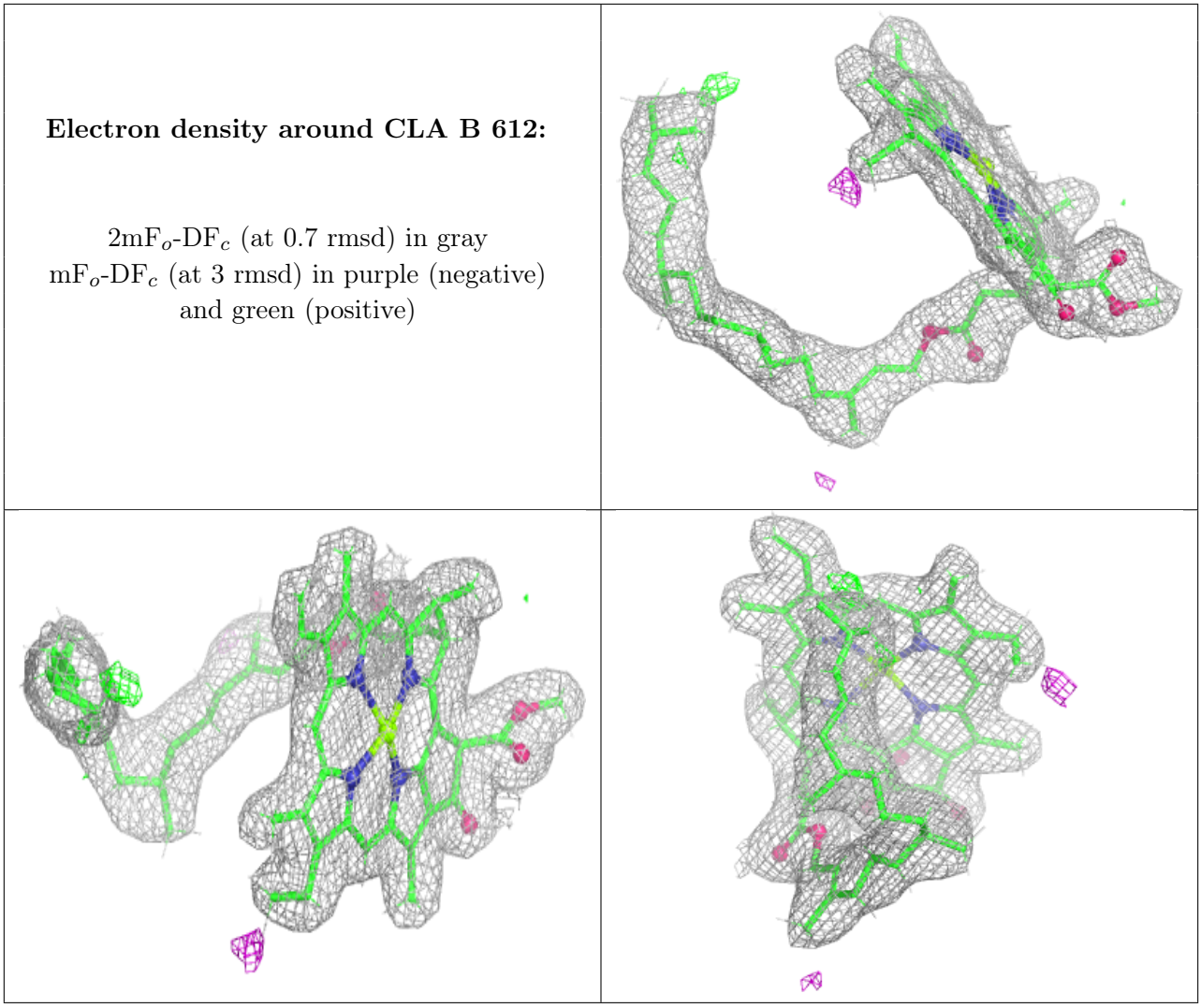






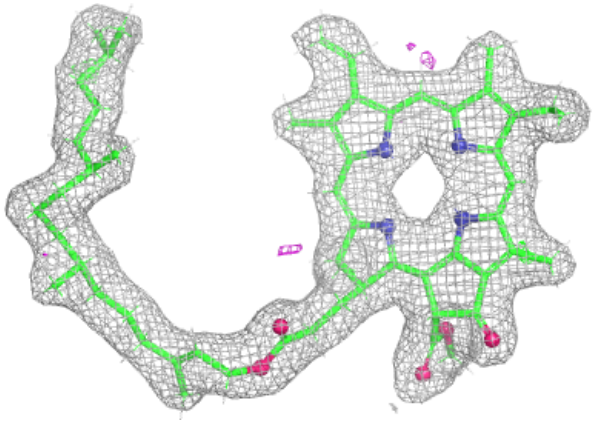
Electron density around CLA B 612:

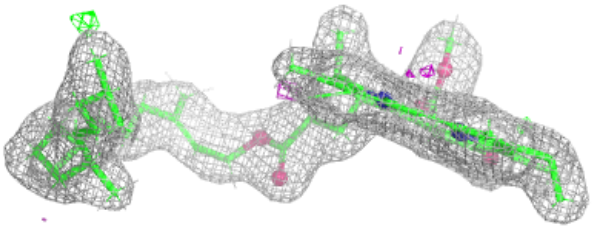
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO A 404:

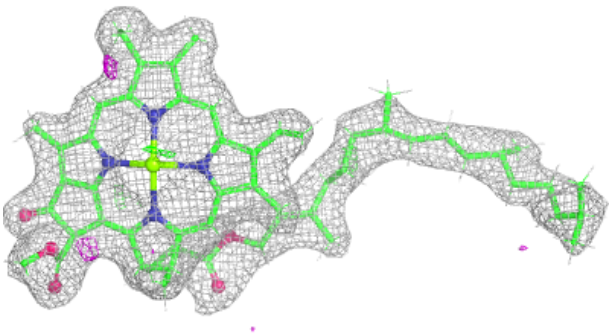
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

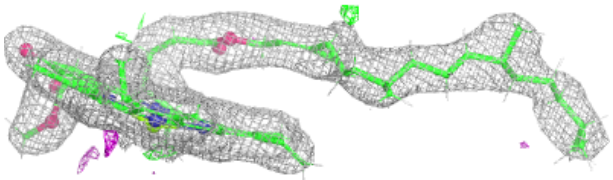


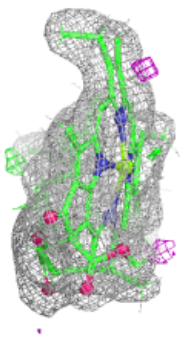


Electron density around CLA B 604:

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

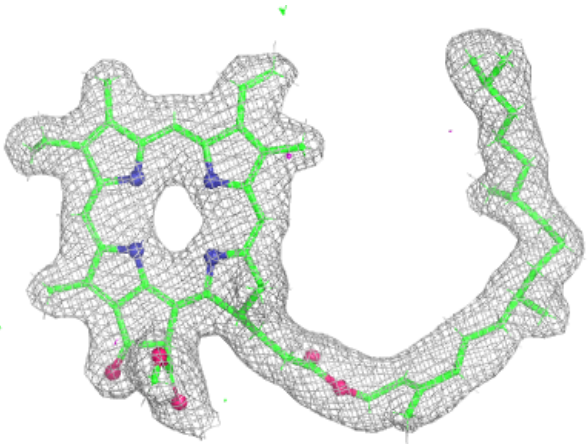


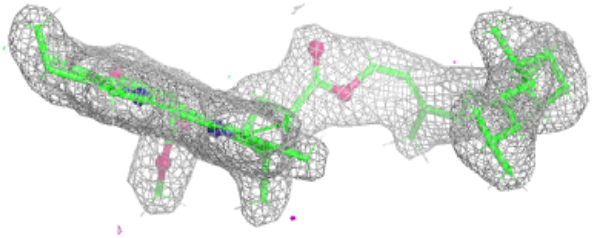


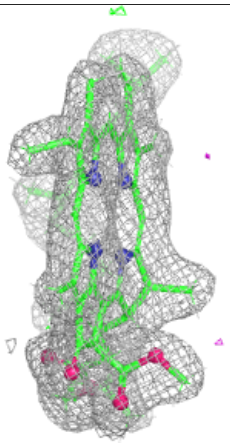


Electron density around PHO a 404:

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

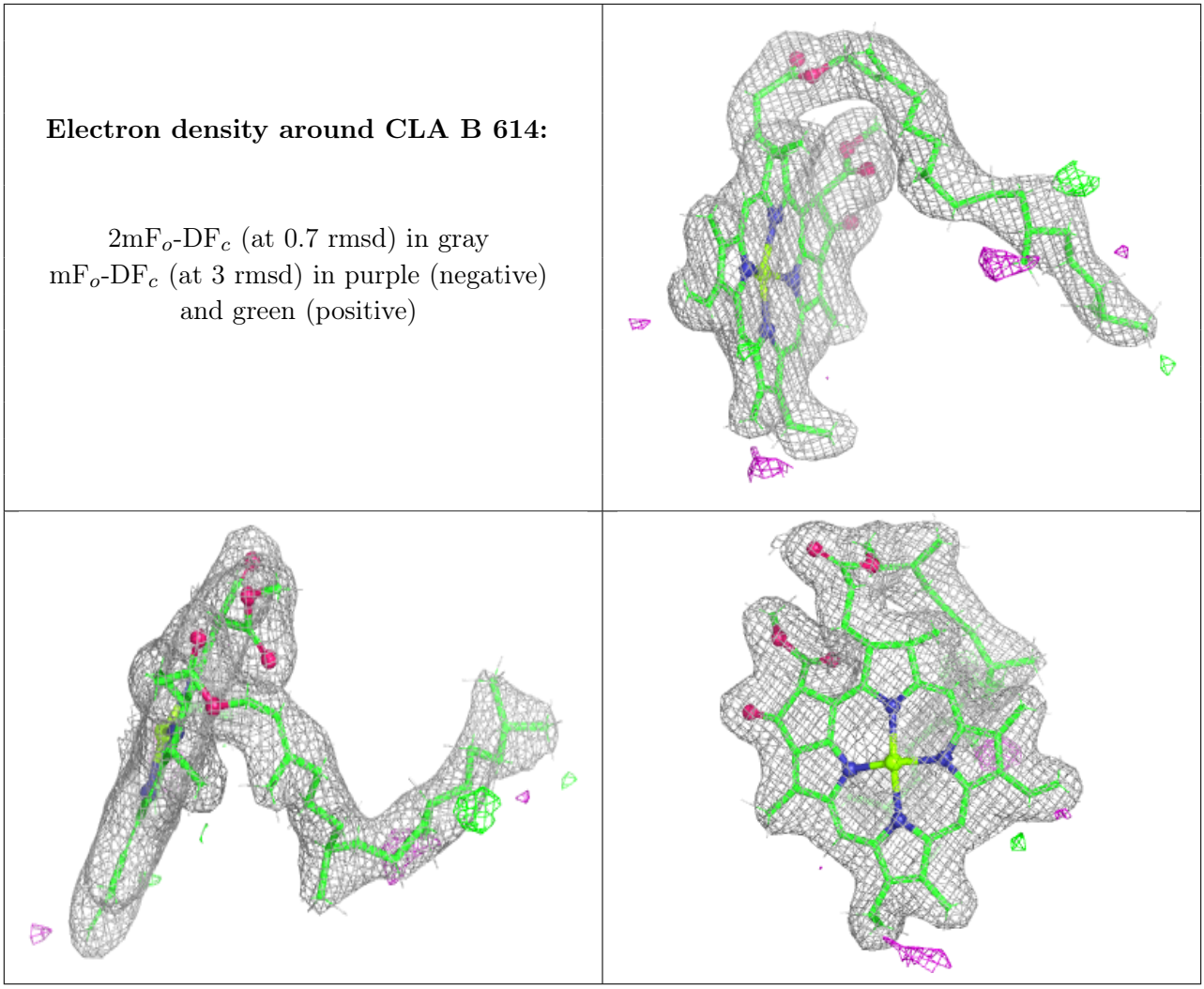






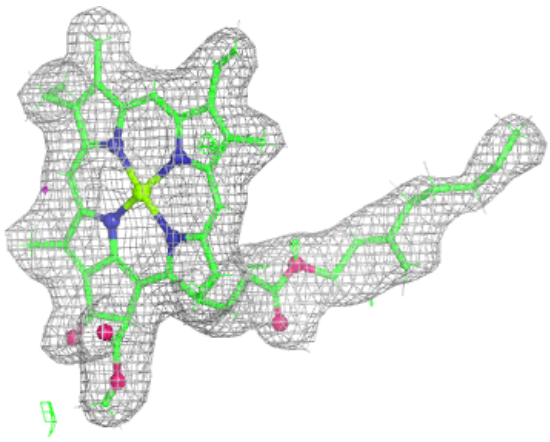
Electron density around CLA B 614:

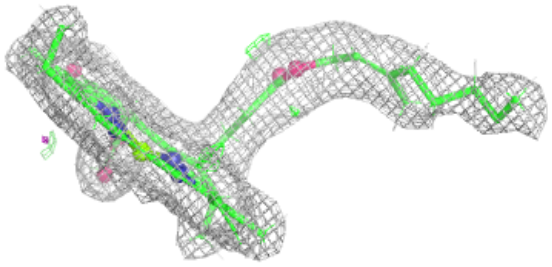
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

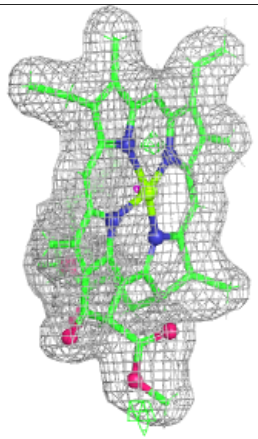


Electron density around CLA A 405:

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

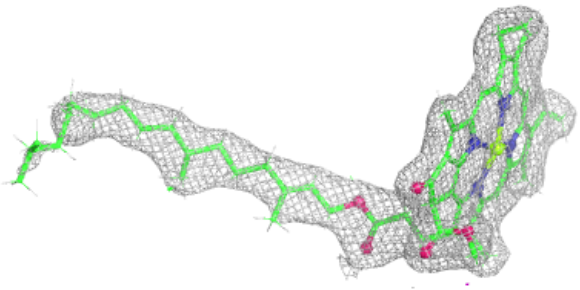


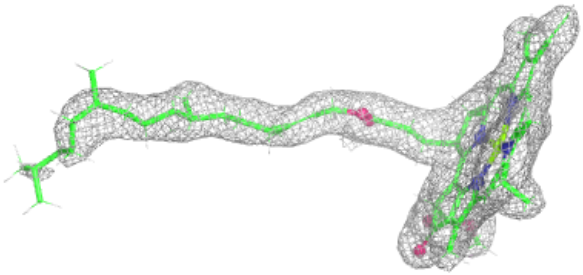


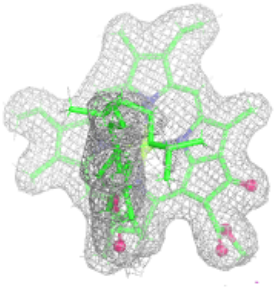


Electron density around CLA b 603:

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

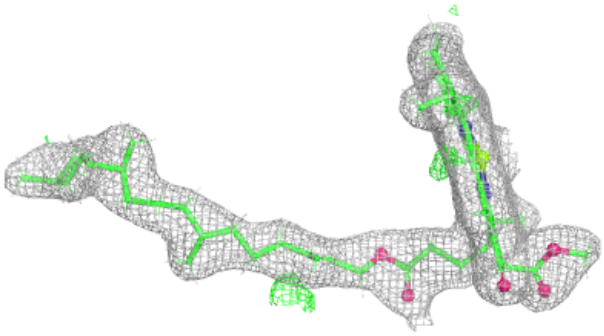


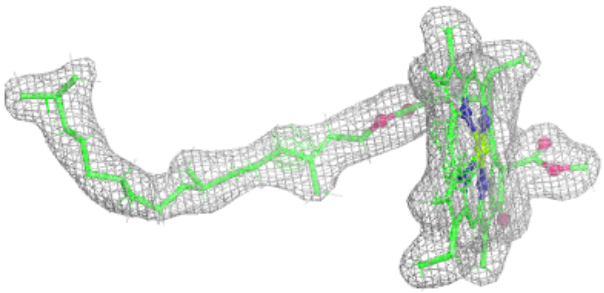


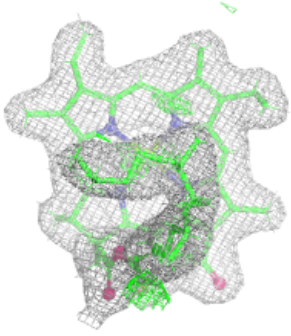


Electron density around CLA B 606:

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

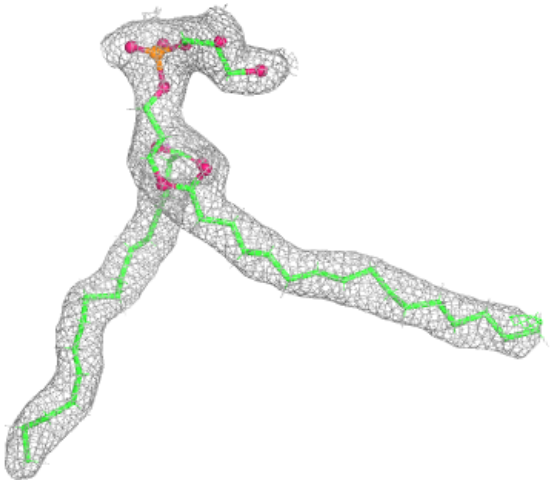


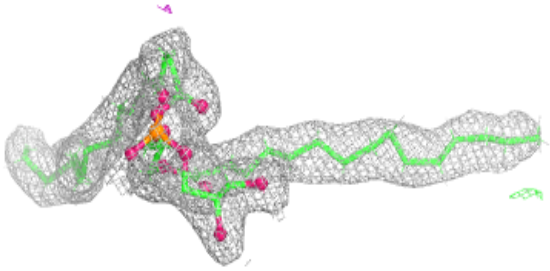


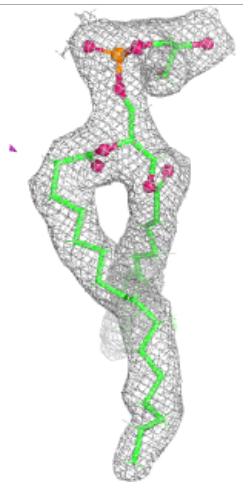


Electron density around LHG B 622:

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

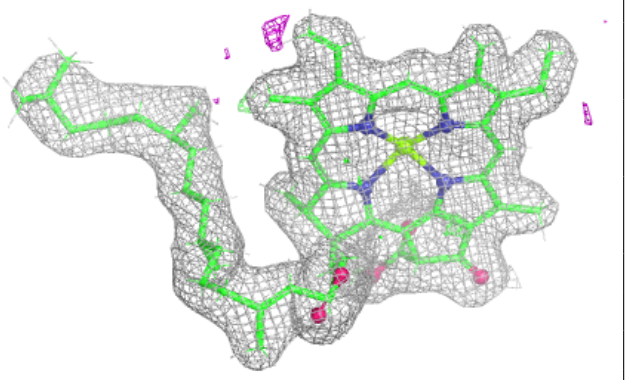


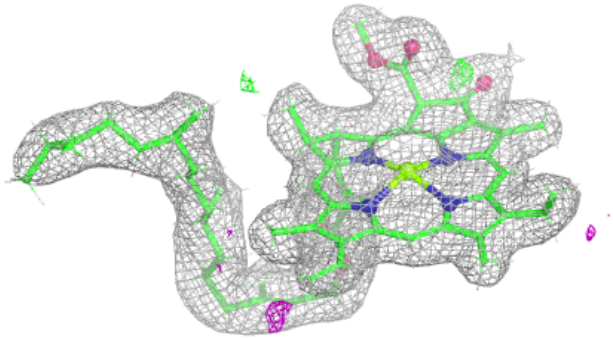


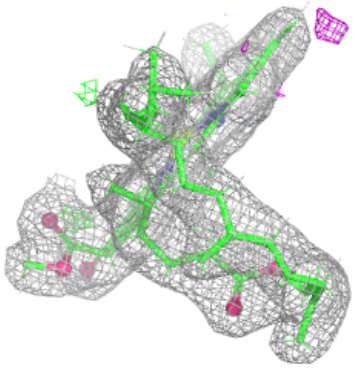


Electron density around CLA A 411:

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

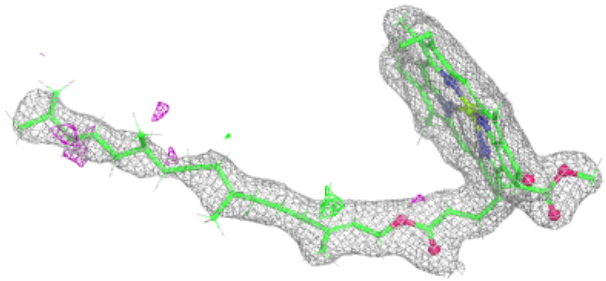


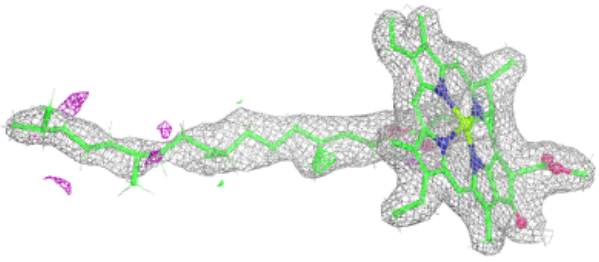


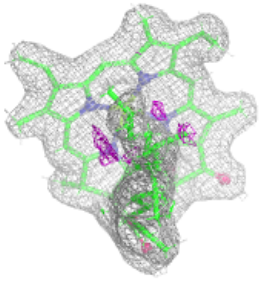


Electron density around CLA b 606:

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

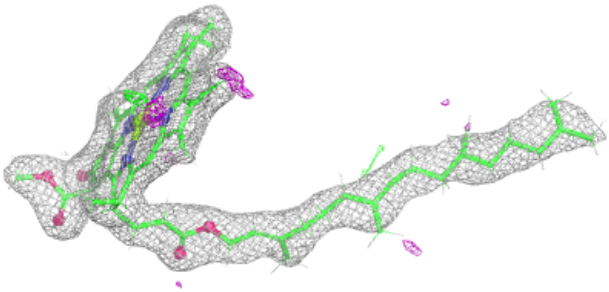


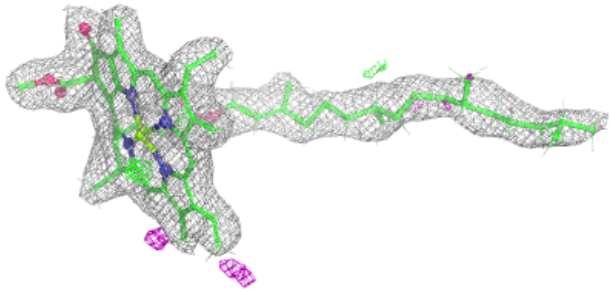


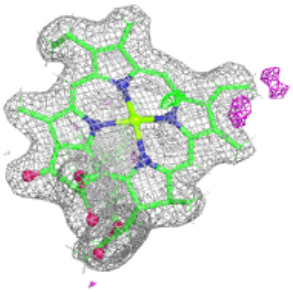


Electron density around CLA B 608:

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

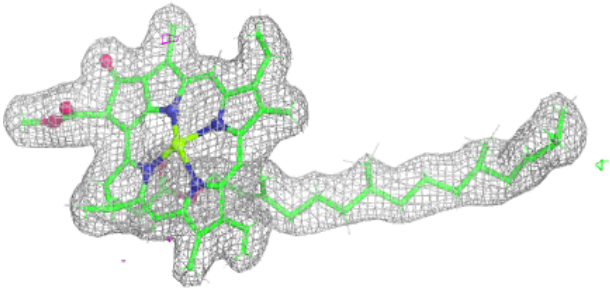


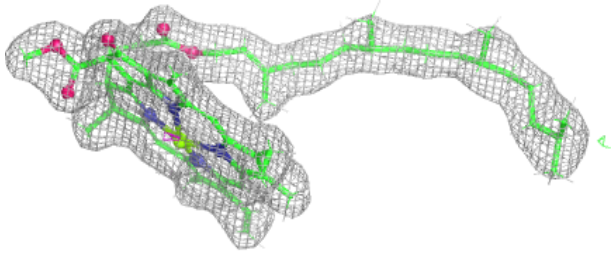


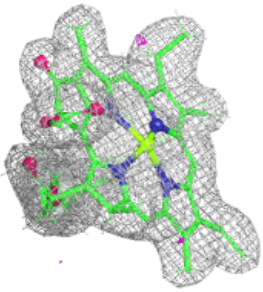


Electron density around CLA B 609:

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

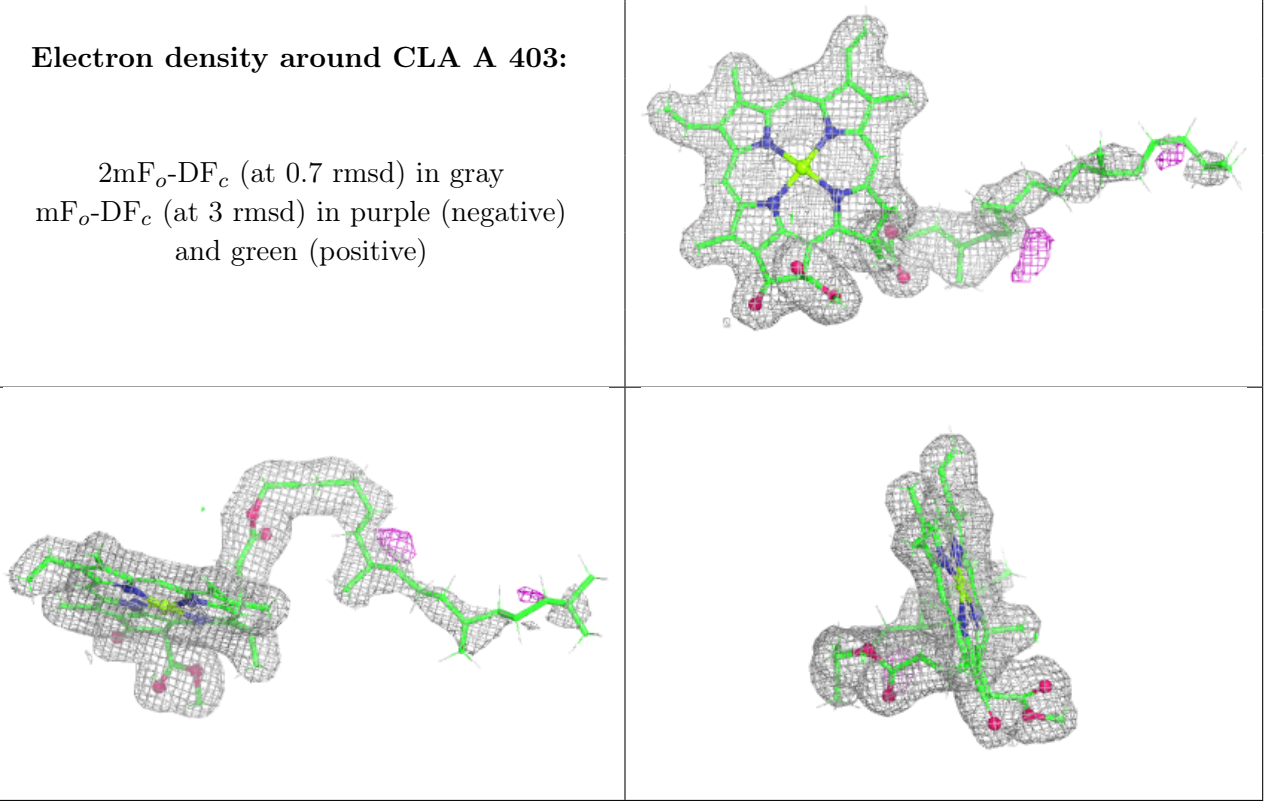






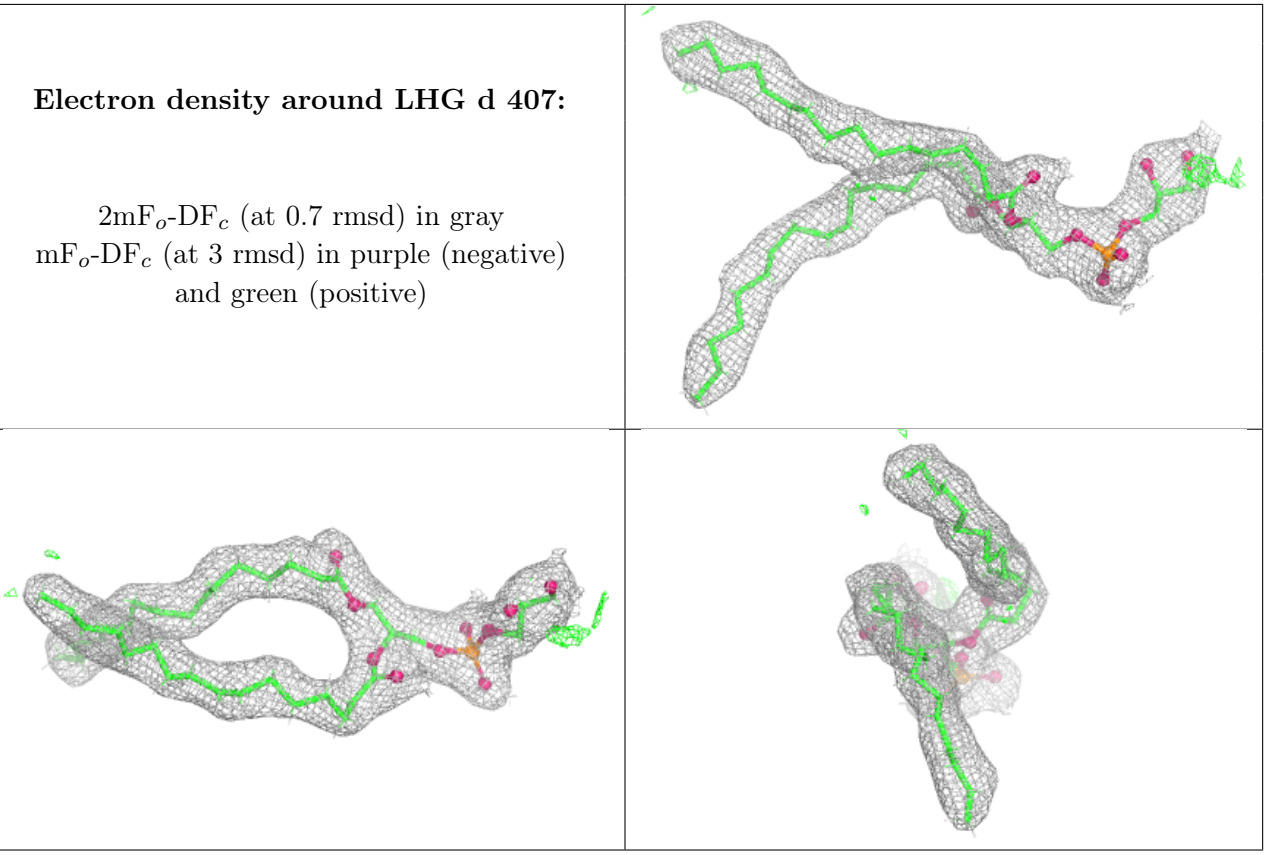
Electron density around CLA A 403:

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



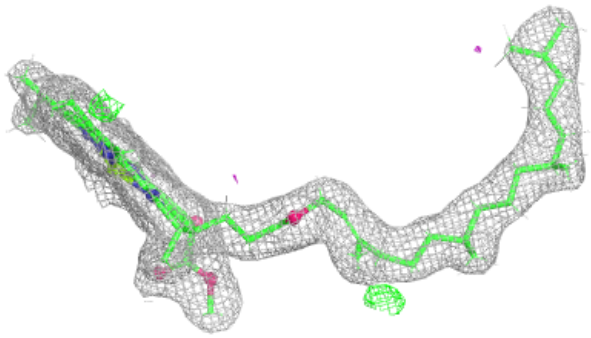
Electron density around LHG d 407:

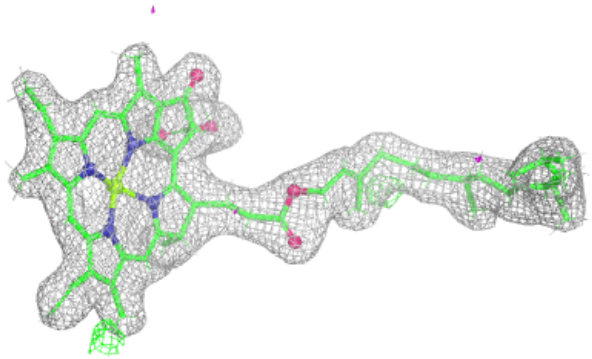
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

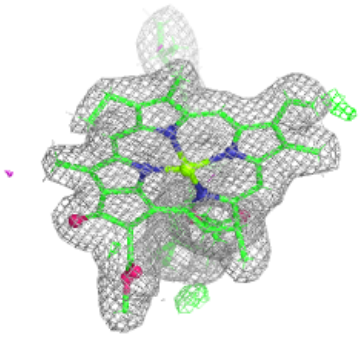


Electron density around CLA D 402:

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

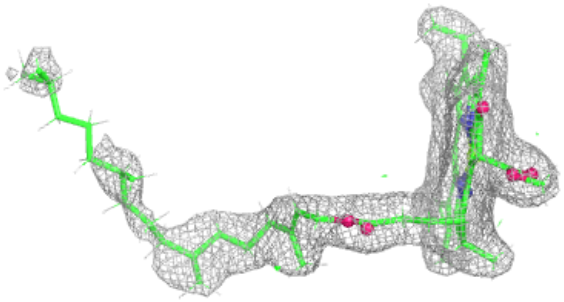


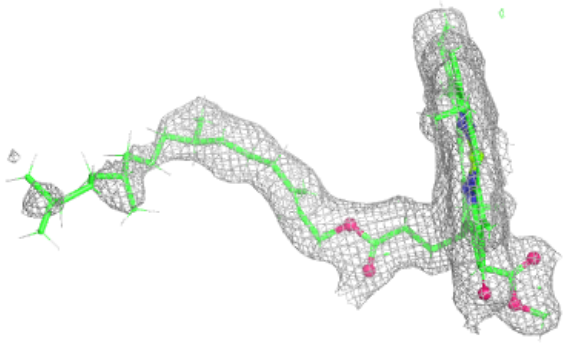


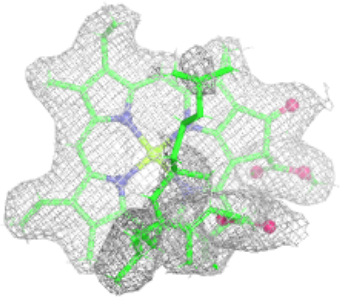


Electron density around CLA D 403:

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

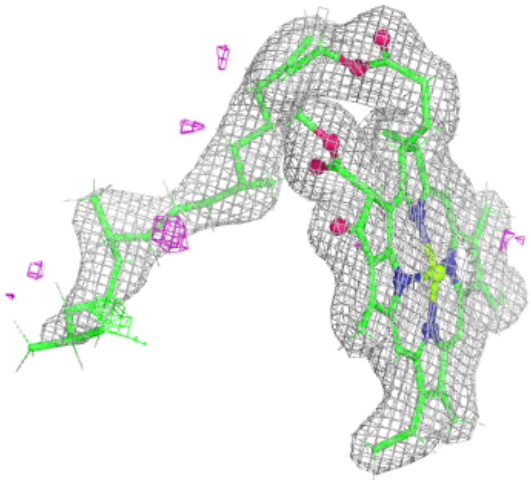


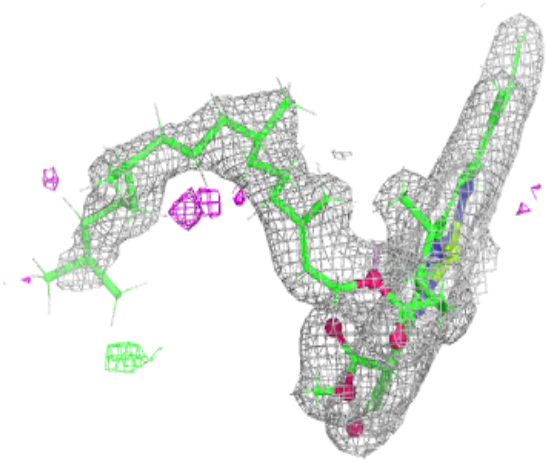


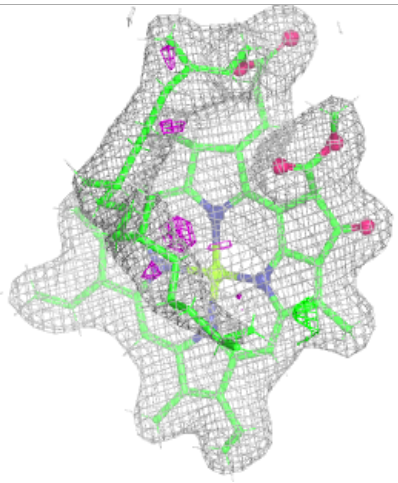


Electron density around CLA b 612:

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

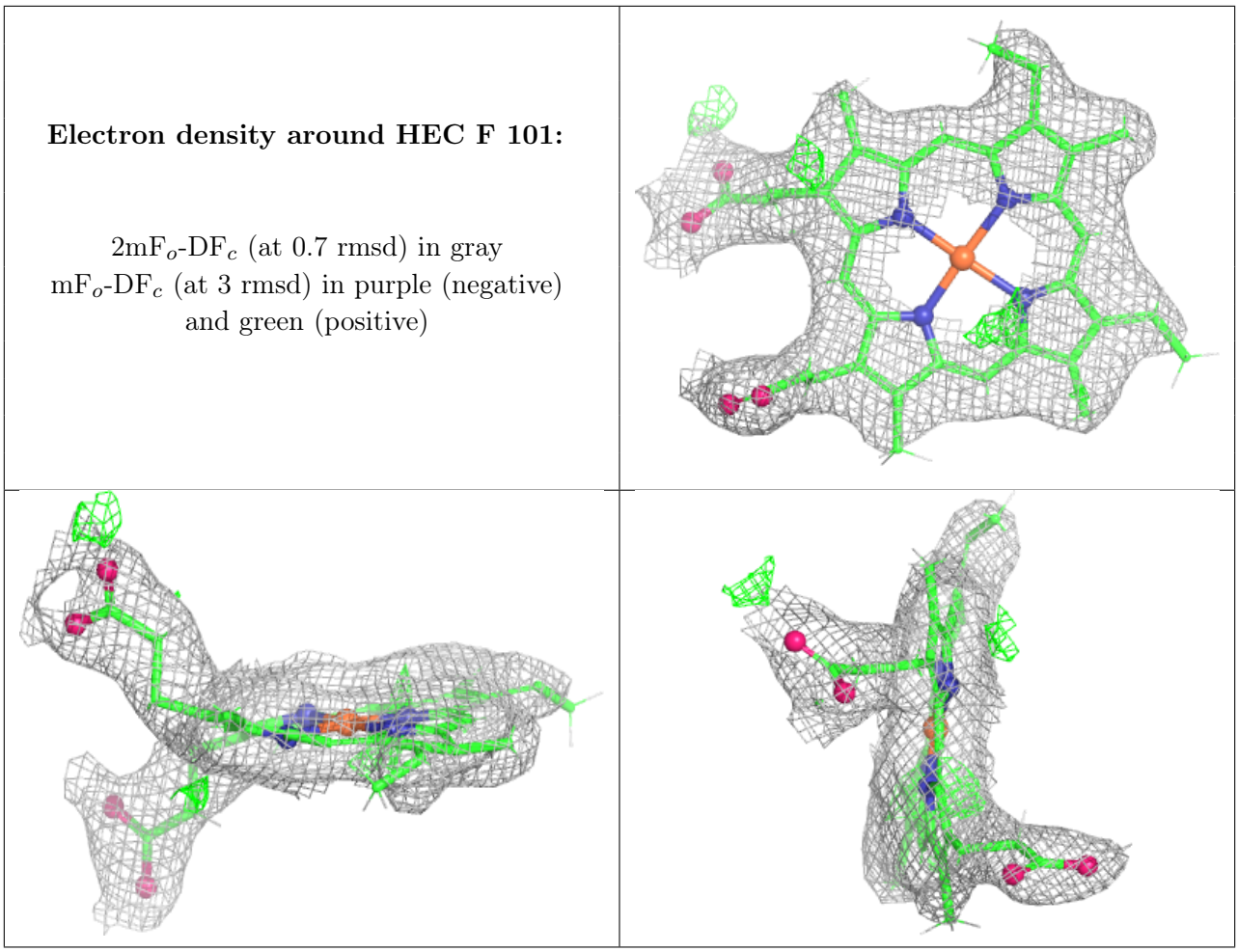






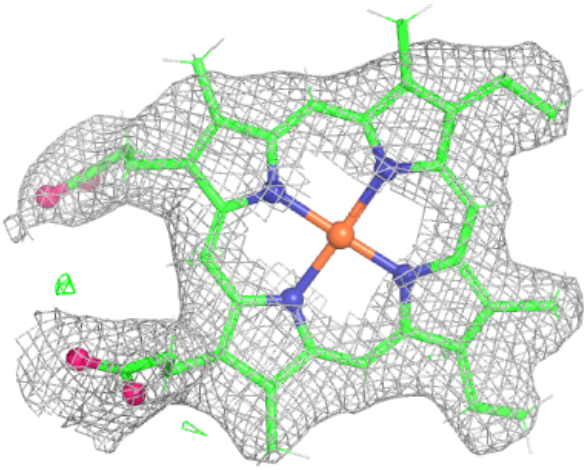
Electron density around HEC F 101:

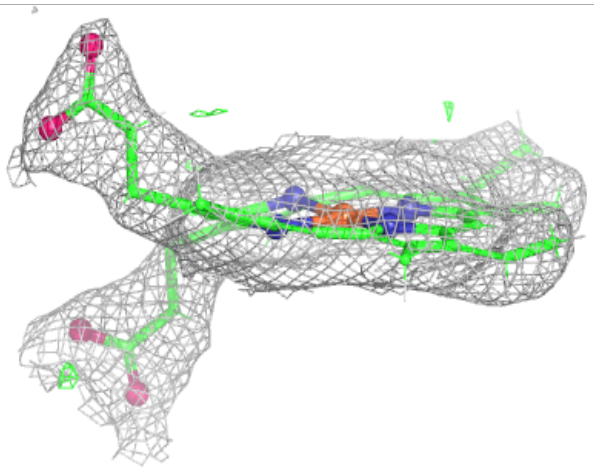
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

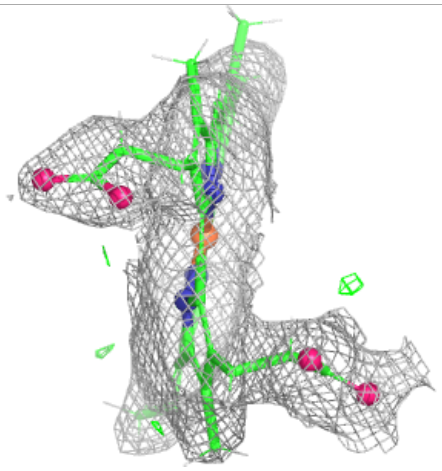


Electron density around HEC e 101:

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

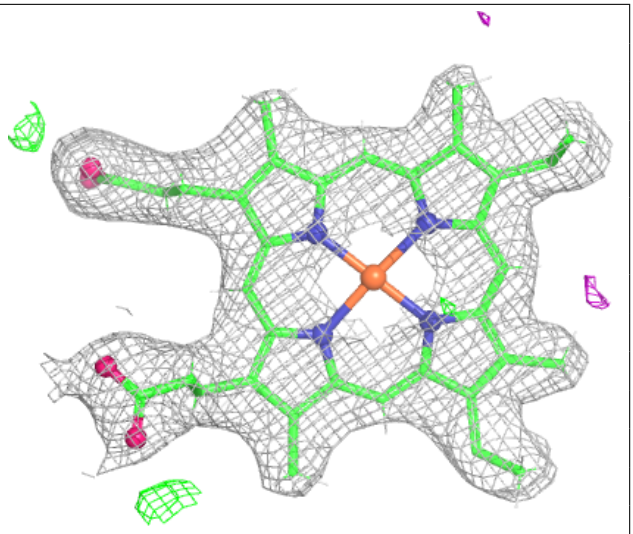


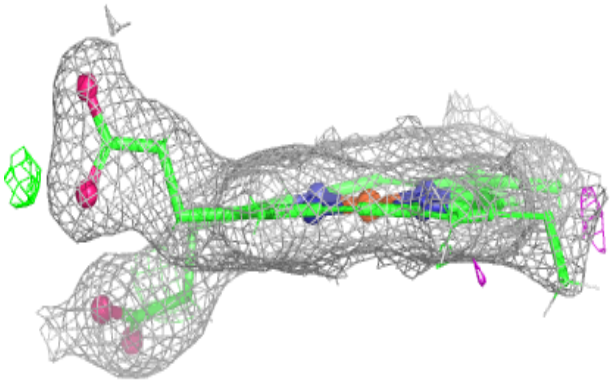




Electron density around HEC V 201:

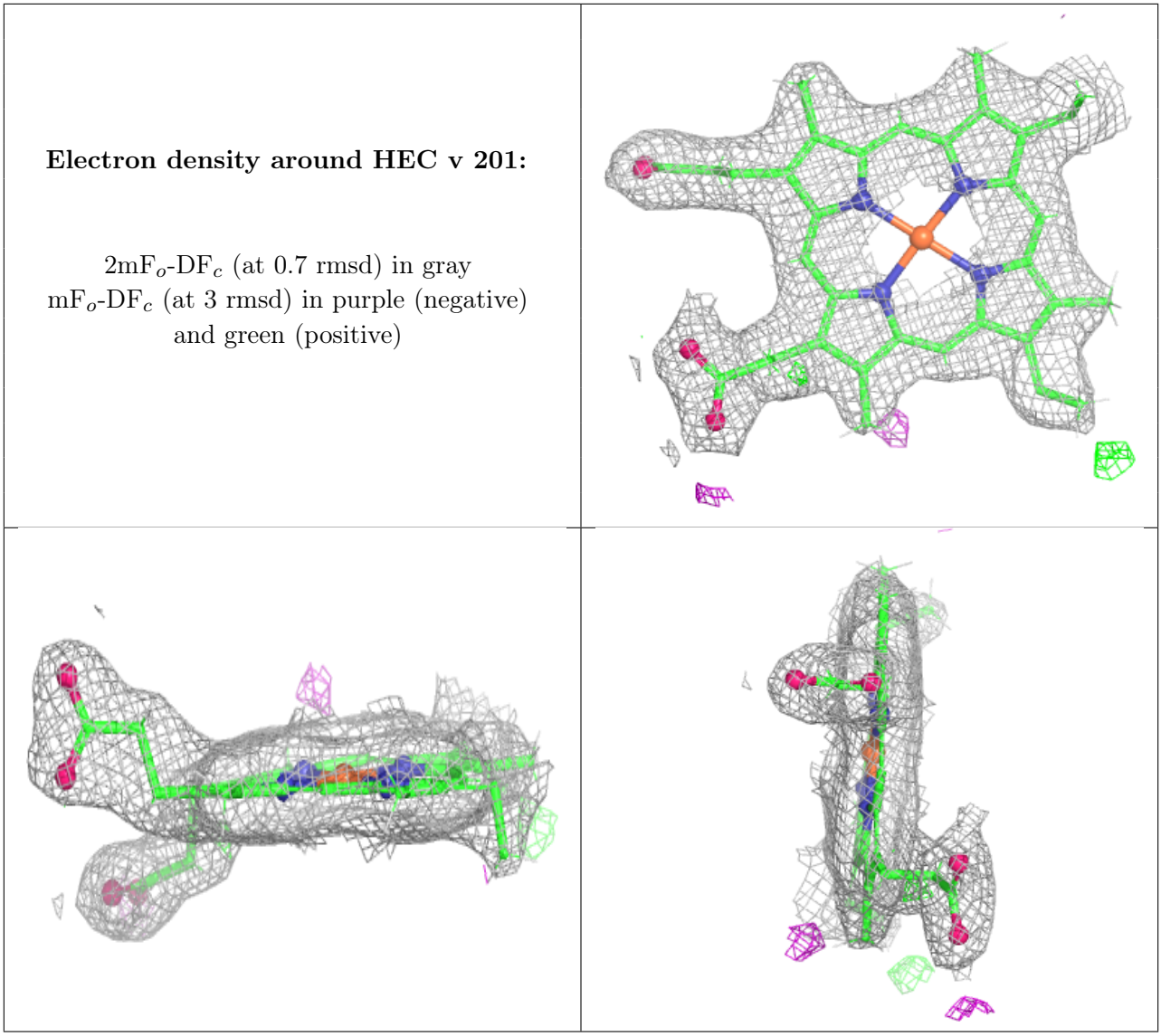
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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

There are no such residues in this entry.