Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2026 – 09:33 AM EDT

PDB ID	:	8F4J / pdb_00008f4j
Title	:	RT XFEL structure of Photosystem II 4000 microseconds after the third illumination at 2.00 Angstrom resolution
Authors	:	Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on	:	2022-11-10
Resolution	:	2.00 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 (1)) were used in the production of this report:

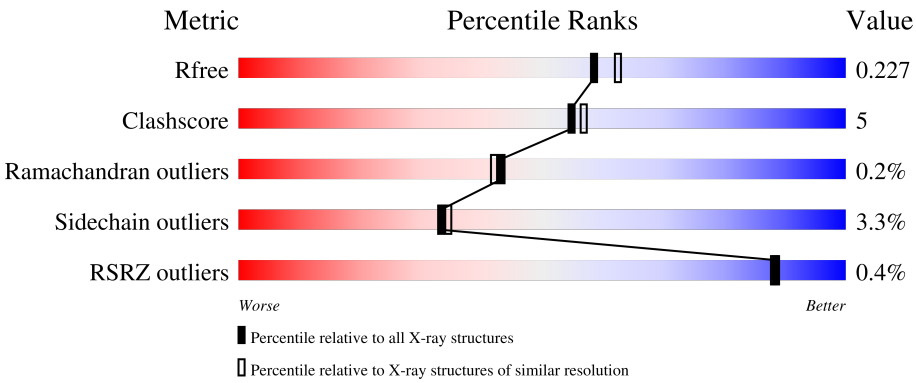
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0

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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	87% 10% •

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Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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Mol	Chain	Length	Quality of chain
1	a	344	86% 10% • •
2	B	510	88% 10% •
2	b	510	90% 8% • •
3	C	461	88% 8% • •
3	c	461	89% 8% • •
4	D	352	89% 7% • •
4	d	352	86% 11% •
5	E	84	83% 13% • •
5	e	84	70% 27% •
6	F	45	2% 69% 7% 24%
6	f	45	60% 11% • 24%
7	H	66	95% • •
7	h	66	88% 8% 5%
8	I	38	84% 11% 5%
8	i	38	79% 16% 5%
9	J	40	82% 8% 10%
9	j	40	2% 78% 12% 10%
10	K	46	65% 15% 20%
10	k	46	59% 22% 20%
11	L	37	3% 89% 11%
11	l	37	86% 8% • •
12	M	36	75% 14% • 8%
12	m	36	78% 8% • 11%
13	O	272	% 77% 12% • 10%
13	o	272	83% 6% • 10%

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Mol	Chain	Length	Quality of chain
14	T	32	84% 9% 6%
14	t	32	84% 9% 6%
15	U	134	64% 7% • 28%
15	u	134	% 64% 7% • 28%
16	V	163	77% 6% • 16%
16	v	163	67% 16% • 16%
17	Y	46	2% 41% 17% 41%
17	y	46	54% 9% • 35%
18	X	41	76% 15% • 7%
18	x	41	2% 83% 12% 5%
19	Z	62	3% 76% 21% •
19	z	62	2% 87% 13%
20	R	41	2% 68% 15% 17%
20	r	41	2% 51% 17% 7% 24%

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
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 54524 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	3604	2343	595	643	23	0	64	0
1	a	334	3601	2340	595	643	23	0	64	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	505	4005	2631	666	695	13	0	4	0
2	b	505	3978	2610	665	690	13	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	442	3592	2355	601	621	15	0	11	0
3	c	451	3666	2396	617	638	15	0	12	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	341	2745	1818	448	467	12	0	2	0
4	d	341	2751	1822	448	469	12	0	3	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	82	666	436	107	123	0	1	0
5	e	82	664	434	108	122	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	34	275	187	45	42	1	0	0	0
6	f	34	275	187	45	42	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	H	65	510	341	82	85	2	0	0	0
7	h	63	498	333	80	83	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	I	36	296	200	46	49	1	0	0	0
8	i	36	296	200	46	49	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	J	36	257	174	40	42	1	0	0	0
9	j	36	257	174	40	42	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	K	37	293	204	43	46	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	k	37	293	204	43	46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	L	37	304	202	48	53	1	0	0	0
			Total	C	N	O				
11	l	36	296	197	47	52		0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	M	33	256	171	37	47	1	0	0	0
			Total	C	N	O	S			
12	m	32	251	168	36	46	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	O	244	1870	1168	313	385	4	0	1	0
			Total	C	N	O	S			
13	o	244	1874	1170	317	383	4	0	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	T	30	258	181	36	39	2	0	0	0
			Total	C	N	O	S			
14	t	30	256	180	36	38	2	0	0	0

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	U	97	774	491	129	154	0	0	0
			Total	C	N	O			
15	u	97	774	491	129	154	0	0	0

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	V	137	1064	675	177	208	4	0	0	0
16	v	137	1064	675	177	208	4	0	0	0

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Y	27	196	128	35	30	3	0	0	0
17	y	30	218	144	35	36	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	X	38	281	188	45	48	0	0	0
18	x	39	286	191	46	49	0	0	0

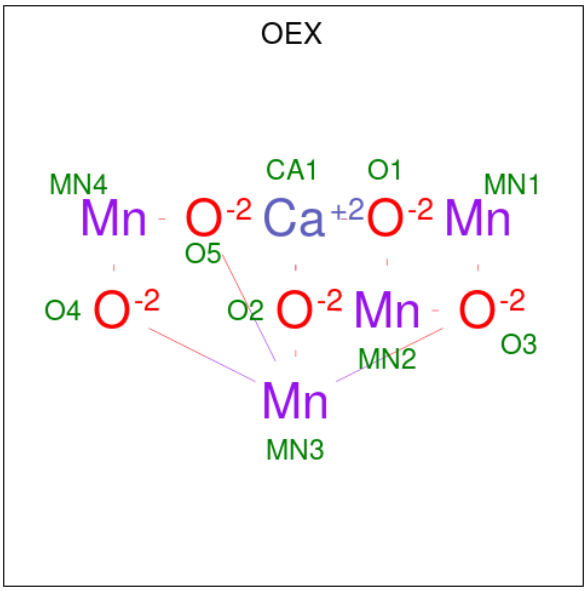
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Z	62	479	328	72	77	2	0	0	0
19	z	62	477	326	72	77	2	0	0	0

- Molecule 20 is a protein called Photosystem II protein Y.

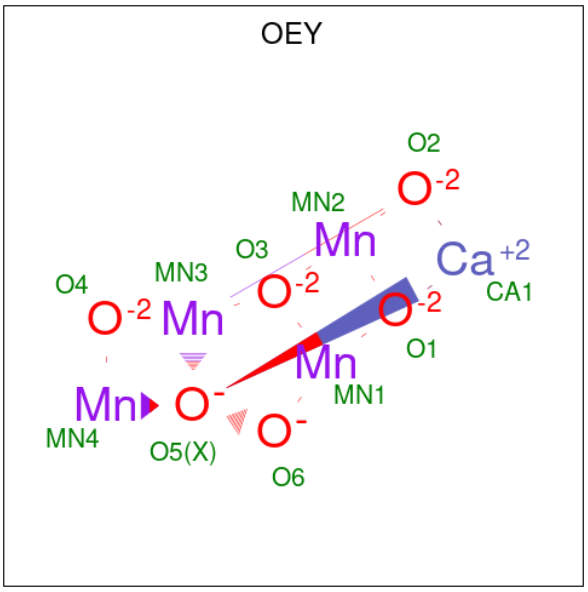
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	R	34	271	184	47	40	0	0	0
20	r	31	246	166	43	37	0	0	0

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Ca	Mn	O		
21	A	1	20	2	8	10	0	1
21	a	1	20	2	8	10	0	1

- Molecule 22 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: $CaMn_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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

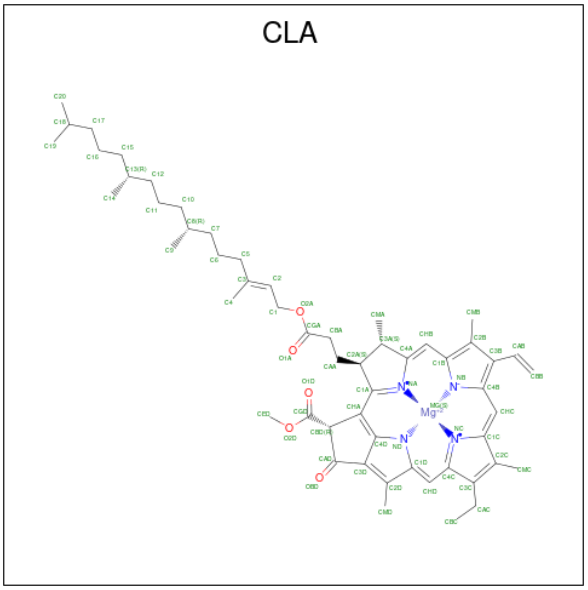
- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	A	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
25	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	C	1	59	49	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	D	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	a	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	b	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	64	54	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0

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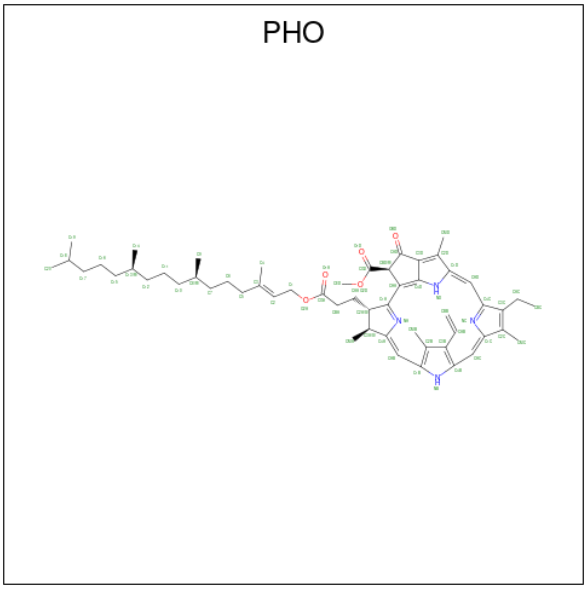
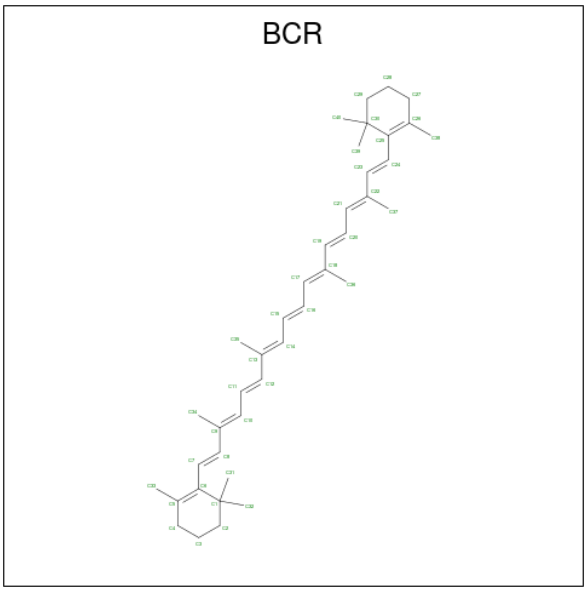
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	c	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	d	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
25	h	1	65	55	1	4	5	0	0

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
27	A	1	40	40	0	0
27	B	1	40	40	0	0
27	B	1	40	40	0	0
27	B	1	40	40	0	0
27	C	1	40	40	0	0
27	D	1	40	40	0	0
27	H	1	40	40	0	0
27	K	1	40	40	0	0
27	K	1	40	40	0	0
27	K	1	40	40	0	0
27	T	1	40	40	0	0
27	a	1	40	40	0	0
27	b	1	40	40	0	0
27	b	1	40	40	0	0

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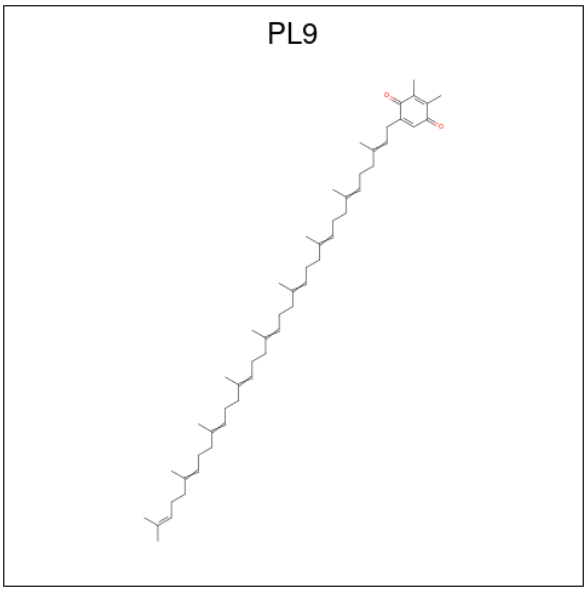
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
27	b	1	40	40	0	0
			Total	C		
27	c	1	40	40	0	0
			Total	C		
27	c	1	40	40	0	0
			Total	C		
27	d	1	40	40	0	0
			Total	C		
27	h	1	40	40	0	0
			Total	C		
27	k	1	40	40	0	0
			Total	C		
27	k	1	40	40	0	0
			Total	C		
27	t	1	40	40	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

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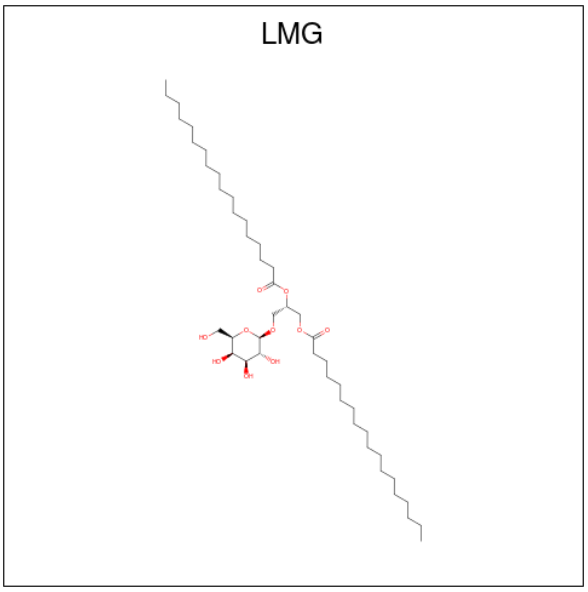
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
28	a	1	55	53	2	0	0
28	d	1	55	53	2	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	A	1	48	38	10	0	0
29	B	1	28	24	4	0	0
29	C	1	48	38	10	0	0
29	D	1	51	41	10	0	0
29	D	1	33	27	6	0	0
29	M	1	51	41	10	0	0
29	b	1	55	45	10	0	0
29	c	1	37	27	10	0	0
29	c	1	48	38	10	0	0

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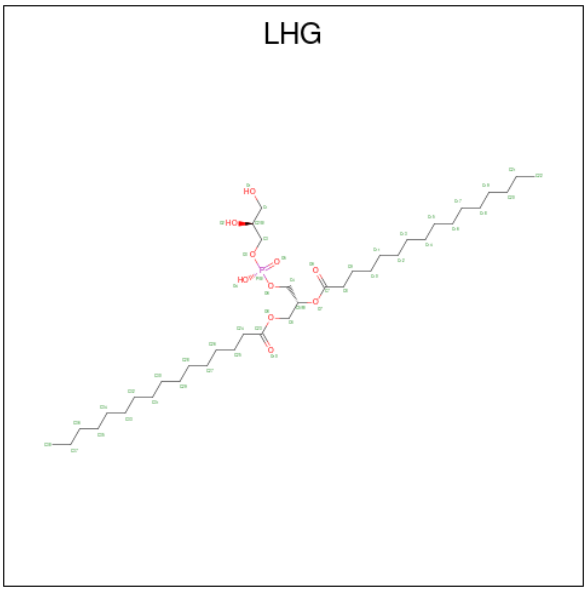
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
29	c	1	49	39	10		0	0
			Total	C	O			
29	d	1	23	21	2		0	0
			Total	C	O			
29	d	1	44	34	10		0	0
			Total	C	O			
29	m	1	51	41	10		0	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
30	A	1	47	36	10	1	0	0
			Total	C	O	P		
30	B	1	49	38	10	1	0	0
			Total	C	O	P		
30	D	1	49	38	10	1	0	0
			Total	C	O	P		
30	E	1	49	38	10	1	0	0
			Total	C	O	P		
30	L	1	49	38	10	1	0	0
			Total	C	O	P		
30	a	1	49	38	10	1	0	0
			Total	C	O	P		
30	d	1	49	38	10	1	0	0

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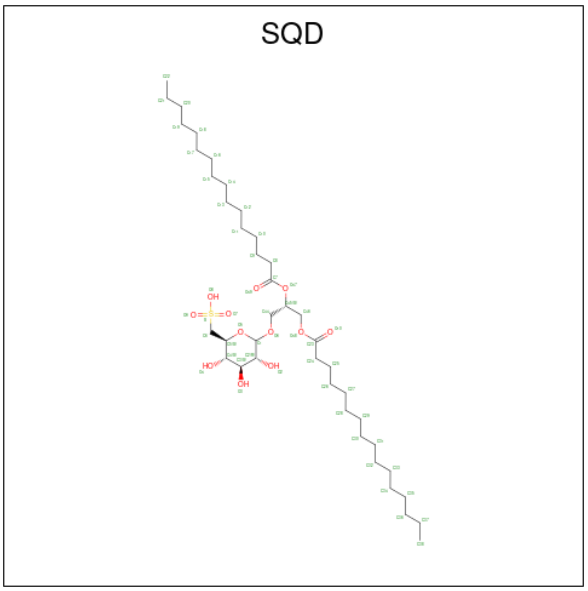
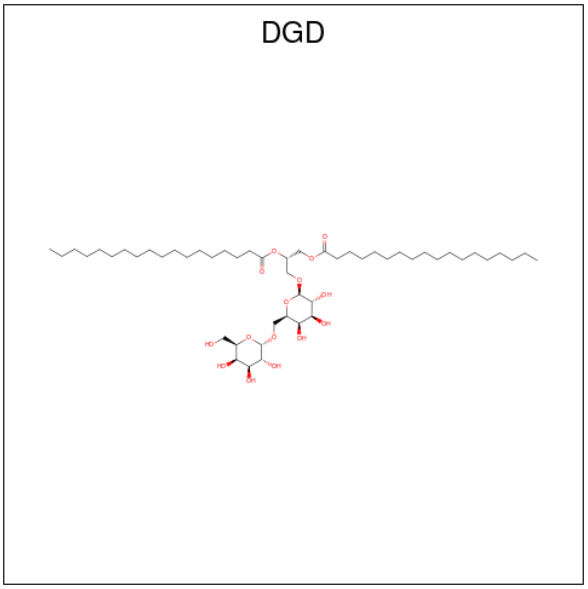
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
30	d	1	39	28	10	1	0	0
			Total	C	O	P		
30	e	1	42	31	10	1	0	0
			Total	C	O	P		
30	l	1	49	38	10	1	0	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



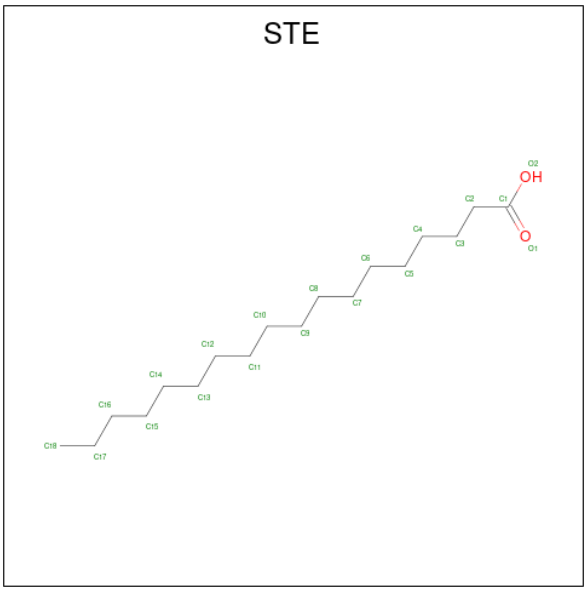
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
31	A	1	52	39	12	1	0	0
			Total	C	O			
31	A	1	39	35	4		0	0
			Total	C	O	S		
31	B	1	54	41	12	1	0	0
			Total	C	O	S		
31	F	1	36	25	10	1	0	0
			Total	C	O	S		
31	a	1	54	41	12	1	0	0
			Total	C	O			
31	a	1	36	31	5		0	0
			Total	C	O	S		
31	b	1	49	36	12	1	0	0
			Total	C	O	S		
31	f	1	41	28	12	1	0	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
32	A	1	66	51	15	0	0
32	C	1	62	47	15	0	0
32	C	1	62	47	15	0	0
32	C	1	62	47	15	0	0
32	H	1	62	47	15	0	0
32	a	1	44	39	5	0	0
32	c	1	62	47	15	0	0
32	c	1	62	47	15	0	0
32	c	1	62	47	15	0	0
32	h	1	62	47	15	0	0

- 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 O 17 15 2	0	0
33	B	1	Total C O 12 10 2	0	0
33	B	1	Total C O 12 10 2	0	0
33	B	1	Total C 16 16	0	0
33	C	1	Total C O 12 10 2	0	0
33	C	1	Total C O 12 10 2	0	0
33	C	1	Total C 16 16	0	0
33	E	1	Total C O 12 10 2	0	0
33	H	1	Total C 18 18	0	0
33	I	1	Total C 15 15	0	0
33	J	1	Total C O 12 10 2	0	0
33	M	1	Total C O 15 13 2	0	0
33	M	1	Total C 10 10	0	0
33	X	1	Total C O 20 18 2	0	0

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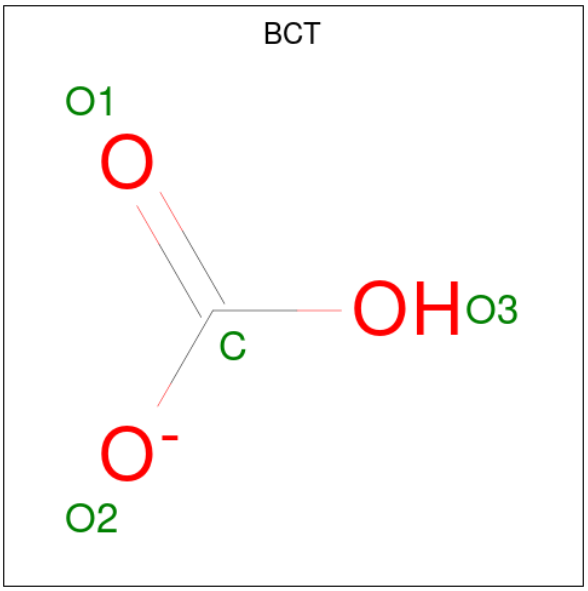
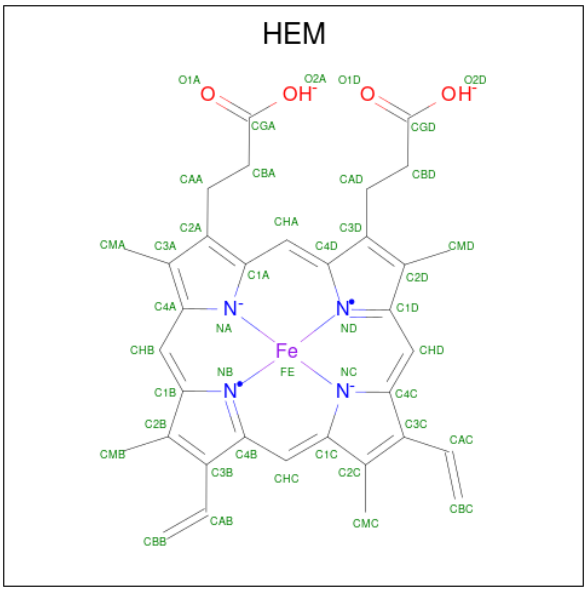
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C 16 16	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C O 16 14 2	0	0
33	b	1	Total C 15 15	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	d	1	Total C O 17 15 2	0	0
33	j	1	Total C O 12 10 2	0	0
33	k	1	Total C O 12 10 2	0	0
33	l	1	Total C 18 18	0	0
33	m	1	Total C O 12 10 2	0	0
33	t	1	Total C O 14 12 2	0	0
33	t	1	Total C 10 10	0	0
33	t	1	Total C O 18 16 2	0	0
33	x	1	Total C O 20 18 2	0	0

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	D	1	4	1	3	0	0
			Total	C	O		
34	a	1	4	1	3	0	0

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
35	F	1	43	34	1	4	4	0	0

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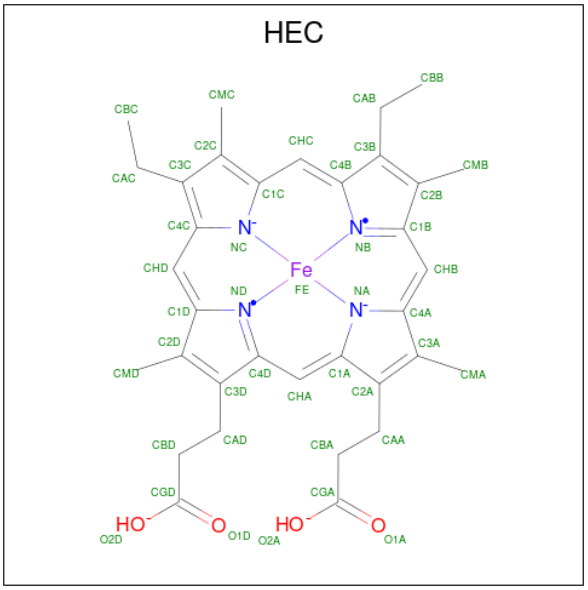
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
35	e	1	43	34	1	4	4	0	0

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
37	A	150	158	158	0	4
			Total	O		
37	B	214	214	214	0	0
			Total	O		
37	C	196	196	196	0	0
			Total	O		
37	D	115	115	115	0	0
			Total	O		
37	E	33	33	33	0	0
			Total	O		
37	F	6	6	6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	27	Total O 27 27	0	0
37	I	20	Total O 20 20	0	0
37	J	13	Total O 13 13	0	0
37	K	5	Total O 5 5	0	0
37	L	10	Total O 10 10	0	0
37	M	7	Total O 7 7	0	0
37	O	89	Total O 89 89	0	0
37	T	9	Total O 9 9	0	0
37	U	40	Total O 40 40	0	0
37	V	61	Total O 61 61	0	0
37	X	12	Total O 12 12	0	0
37	Z	6	Total O 6 6	0	0
37	a	123	Total O 131 131	0	4
37	b	199	Total O 199 199	0	0
37	c	150	Total O 150 150	0	0
37	d	109	Total O 109 109	0	0
37	e	17	Total O 17 17	0	0
37	f	3	Total O 3 3	0	0
37	h	17	Total O 17 17	0	0
37	i	17	Total O 17 17	0	0
37	j	14	Total O 14 14	0	0

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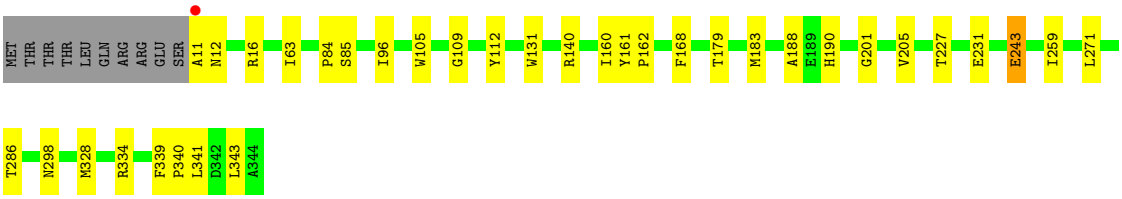
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	k	7	Total O 7 7	0	0
37	l	7	Total O 7 7	0	0
37	m	9	Total O 9 9	0	0
37	o	85	Total O 85 85	0	0
37	t	14	Total O 14 14	0	0
37	u	48	Total O 48 48	0	0
37	v	56	Total O 56 56	0	0
37	x	10	Total O 10 10	0	0
37	z	5	Total O 5 5	0	0
37	r	2	Total O 2 2	0	0

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.

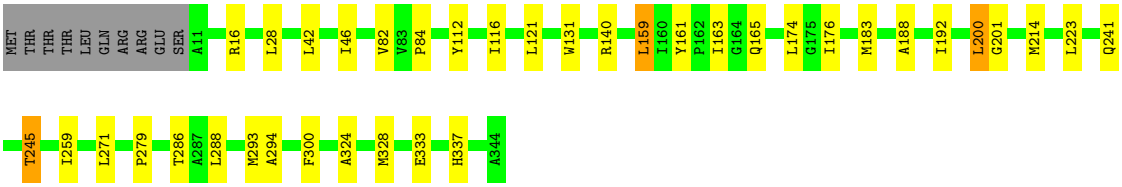
• Molecule 1: Photosystem II protein D1 1

Chain A:



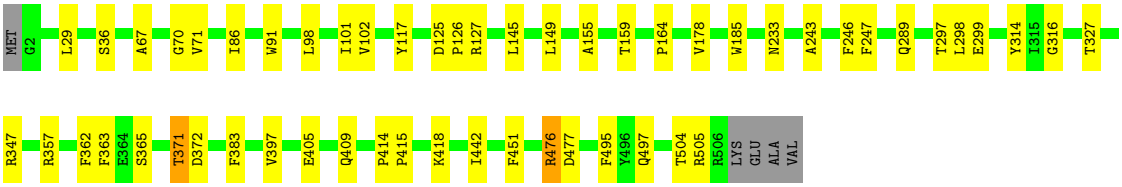
• Molecule 1: Photosystem II protein D1 1

Chain a:



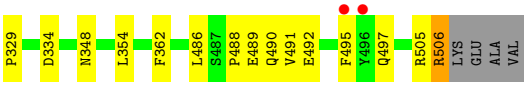
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



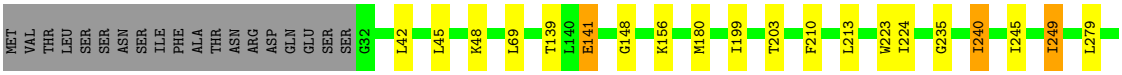
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



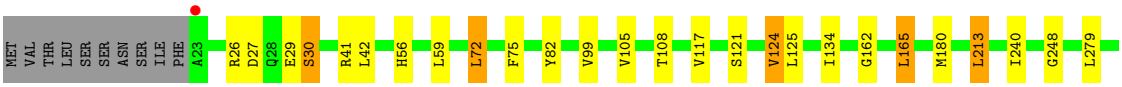
• Molecule 3: Photosystem II CP43 reaction center protein

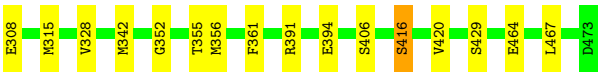
Chain C:



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



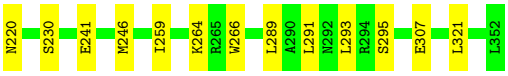


• Molecule 4: Photosystem II D2 protein

Chain D:

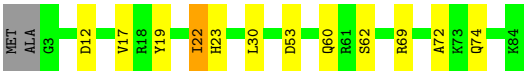
• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

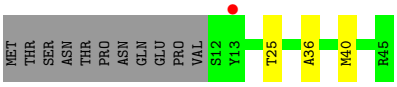


• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

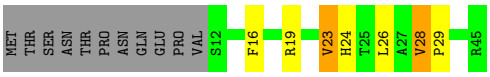
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



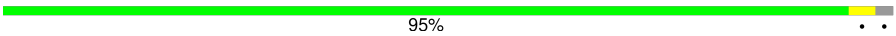
• Molecule 6: Cytochrome b559 subunit beta

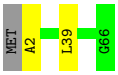
Chain f:



• Molecule 7: Photosystem II reaction center protein H

Chain H:



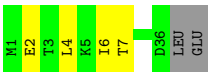


• Molecule 7: Photosystem II reaction center protein H

Chain h:

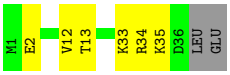
• Molecule 8: Photosystem II reaction center protein I

Chain I:



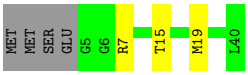
• Molecule 8: Photosystem II reaction center protein I

Chain i:



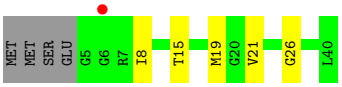
• Molecule 9: Photosystem II reaction center protein J

Chain J:



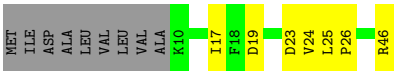
• Molecule 9: Photosystem II reaction center protein J

Chain j:



• Molecule 10: Photosystem II reaction center protein K

Chain K:

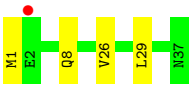


• Molecule 10: Photosystem II reaction center protein K

Chain k:

• Molecule 11: Photosystem II reaction center protein L

Chain L:



• Molecule 11: Photosystem II reaction center protein L

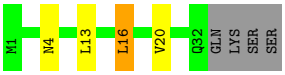
Chain l:

• Molecule 12: Photosystem II reaction center protein M

Chain M:

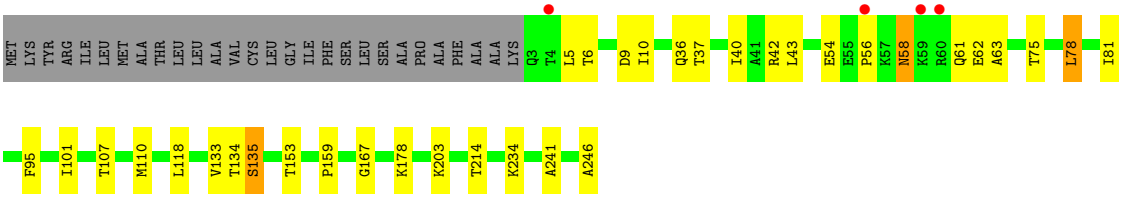
• Molecule 12: Photosystem II reaction center protein M

Chain m:



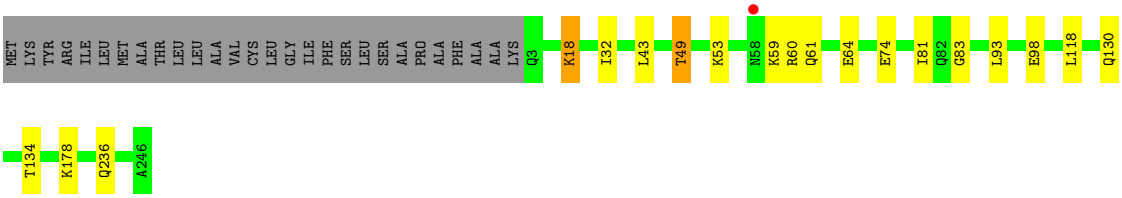
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



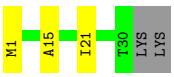
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



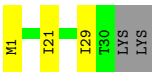
• Molecule 14: Photosystem II reaction center protein T

Chain T:



• Molecule 14: Photosystem II reaction center protein T

Chain t:

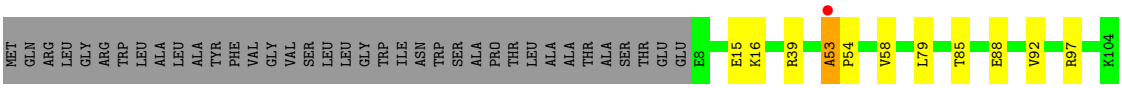


• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

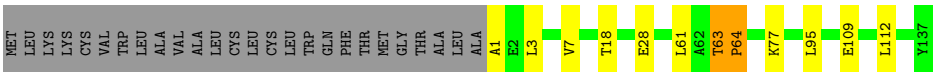
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



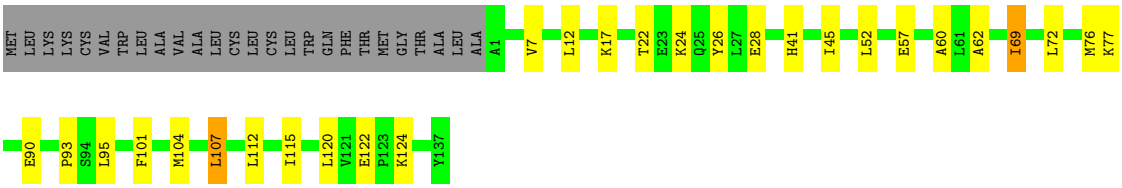
• Molecule 16: Cytochrome c-550

Chain V:



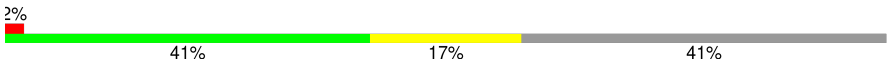
• Molecule 16: Cytochrome c-550

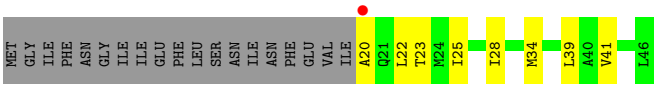
Chain v:



• Molecule 17: Photosystem II reaction center protein Ycf12

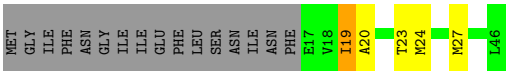
Chain Y:





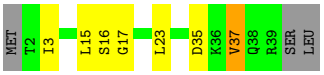
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 18: Photosystem II reaction center X protein

Chain X:

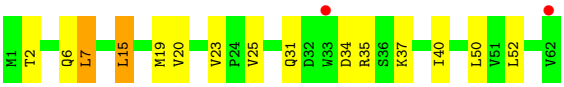


• Molecule 18: Photosystem II reaction center X protein

Chain x:

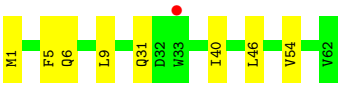
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



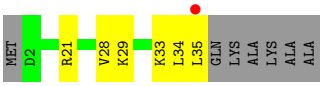
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



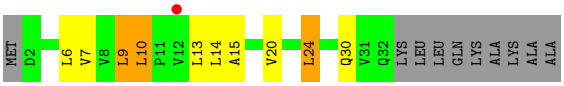
• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.34Å 222.83Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.74 – 2.00 19.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.74-2.00) 84.4 (19.74-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.33 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.226 0.182 , 0.227	Depositor DCC
R_{free} test set	4807 reflections (0.77%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	54524	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.28	0/3717	0.44	0/5060
1	a	0.26	0/3714	0.43	0/5056
2	B	0.32	0/4155	0.49	0/5661
2	b	0.32	0/4118	0.48	0/5611
3	C	0.31	0/3711	0.46	0/5051
3	c	0.29	0/3791	0.45	0/5158
4	D	0.34	0/2838	0.50	0/3862
4	d	0.33	0/2847	0.48	0/3874
5	E	0.26	0/688	0.45	0/940
5	e	0.24	0/683	0.45	0/932
6	F	0.30	0/284	0.47	0/387
6	f	0.25	0/284	0.52	0/387
7	H	0.32	0/523	0.50	0/713
7	h	0.28	0/511	0.45	0/697
8	I	0.30	0/293	0.46	0/396
8	i	0.32	0/293	0.43	0/396
9	J	0.26	0/263	0.41	0/356
9	j	0.23	0/263	0.43	0/356
10	K	0.27	0/303	0.42	0/416
10	k	0.27	0/303	0.43	0/416
11	L	0.34	0/311	0.45	0/422
11	l	0.33	0/303	0.46	0/412
12	M	0.31	0/249	0.49	0/341
12	m	0.31	0/244	0.51	0/334
13	O	0.32	0/1904	0.51	0/2585
13	o	0.31	0/1905	0.49	0/2583
14	T	0.32	0/257	0.54	0/349
14	t	0.33	0/255	0.45	0/346
15	U	0.27	0/785	0.47	0/1064
15	u	0.31	0/785	0.50	0/1064
16	V	0.29	0/1085	0.50	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.27	0/1085	0.43	0/1473
17	Y	0.24	0/197	0.38	0/264
17	y	0.20	0/219	0.37	0/294
18	X	0.24	0/284	0.39	0/384
18	x	0.22	0/289	0.31	0/391
19	Z	0.21	0/490	0.46	0/669
19	z	0.18	0/488	0.31	0/666
20	R	0.27	0/277	0.43	0/380
20	r	0.23	0/252	0.39	0/347
All	All	0.30	0/45246	0.46	0/61566

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	V	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	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	3604	0	3445	26	0
1	a	3601	0	3436	26	0
2	B	4005	0	3871	37	0
2	b	3978	0	3836	33	0
3	C	3592	0	3501	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3666	0	3574	25	0
4	D	2745	0	2653	19	0
4	d	2751	0	2659	29	0
5	E	666	0	651	9	0
5	e	664	0	648	17	0
6	F	275	0	282	2	0
6	f	275	0	282	6	0
7	H	510	0	532	2	0
7	h	498	0	518	3	0
8	I	296	0	311	2	0
8	i	296	0	311	3	0
9	J	257	0	268	2	0
9	j	257	0	268	4	0
10	K	293	0	305	3	0
10	k	293	0	305	7	0
11	L	304	0	316	4	0
11	l	296	0	304	1	0
12	M	256	0	269	5	0
12	m	251	0	267	4	0
13	O	1870	0	1830	22	0
13	o	1874	0	1846	9	0
14	T	258	0	261	2	0
14	t	256	0	256	1	0
15	U	774	0	773	5	0
15	u	774	0	773	7	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	20	0
17	Y	196	0	217	4	0
17	y	218	0	241	3	0
18	X	281	0	312	4	0
18	x	286	0	314	4	0
19	Z	479	0	516	7	0
19	z	477	0	509	4	0
20	R	271	0	298	0	0
20	r	246	0	263	6	0
21	A	20	0	0	0	0
21	a	20	0	0	0	0
22	A	11	0	0	1	0
22	a	11	0	0	1	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	2	0	0	0	0
25	A	249	0	264	6	0
25	B	1035	0	1139	29	0
25	C	839	0	922	15	0
25	D	130	0	144	2	0
25	a	260	0	288	11	0
25	b	970	0	1067	27	0
25	c	839	0	919	24	0
25	d	130	0	144	1	0
25	h	65	0	72	1	0
26	A	64	0	74	0	0
26	D	64	0	74	1	0
26	a	64	0	74	1	0
26	d	64	0	74	1	0
27	A	40	0	56	2	0
27	B	120	0	168	7	0
27	C	40	0	56	4	0
27	D	40	0	56	1	0
27	H	40	0	56	2	0
27	K	120	0	168	4	0
27	T	40	0	56	3	0
27	a	40	0	56	1	0
27	b	120	0	168	4	0
27	c	80	0	112	5	0
27	d	40	0	56	0	0
27	h	40	0	56	2	0
27	k	80	0	112	1	0
27	t	40	0	56	3	0
28	A	55	0	80	4	0
28	D	55	0	80	2	0
28	a	55	0	80	2	0
28	d	55	0	80	1	0
29	A	48	0	66	1	0
29	B	28	0	40	0	0
29	C	48	0	66	1	0
29	D	84	0	117	4	0
29	M	51	0	72	2	0
29	b	55	0	86	0	0
29	c	134	0	181	4	0
29	d	67	0	92	0	0
29	m	51	0	72	2	0
30	A	47	0	67	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	49	0	74	1	0
30	D	49	0	74	1	0
30	E	49	0	74	2	0
30	L	49	0	74	3	0
30	a	49	0	74	2	0
30	d	88	0	125	5	0
30	e	42	0	57	2	0
30	l	49	0	74	1	0
31	A	91	0	136	6	0
31	B	54	0	78	2	0
31	F	36	0	46	1	0
31	a	90	0	134	1	0
31	b	49	0	65	2	0
31	f	41	0	49	1	0
32	A	66	0	96	4	0
32	C	186	0	246	6	0
32	H	62	0	82	2	0
32	a	44	0	75	0	0
32	c	186	0	246	5	0
32	h	62	0	82	2	0
33	B	57	0	89	2	0
33	C	40	0	63	1	0
33	E	12	0	16	0	0
33	H	18	0	35	2	0
33	I	15	0	26	1	0
33	J	12	0	16	0	0
33	M	25	0	38	0	0
33	X	20	0	35	2	0
33	a	12	0	16	0	0
33	b	97	0	170	7	0
33	c	20	0	35	1	0
33	d	17	0	26	0	0
33	j	12	0	16	1	0
33	k	12	0	16	0	0
33	l	18	0	35	3	0
33	m	12	0	16	1	0
33	t	42	0	64	0	0
33	x	20	0	35	2	0
34	D	4	0	1	0	0
34	a	4	0	1	0	0
35	F	43	0	30	3	0
35	e	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	0	30	0	0
36	v	43	0	30	1	0
37	A	158	0	0	2	0
37	B	214	0	0	1	0
37	C	196	0	0	0	0
37	D	115	0	0	0	0
37	E	33	0	0	0	0
37	F	6	0	0	0	0
37	H	27	0	0	1	0
37	I	20	0	0	0	0
37	J	13	0	0	0	0
37	K	5	0	0	2	0
37	L	10	0	0	1	0
37	M	7	0	0	0	0
37	O	89	0	0	1	0
37	T	9	0	0	0	0
37	U	40	0	0	1	0
37	V	61	0	0	3	0
37	X	12	0	0	0	0
37	Z	6	0	0	0	0
37	a	131	0	0	1	0
37	b	199	0	0	3	0
37	c	150	0	0	1	0
37	d	109	0	0	0	0
37	e	17	0	0	0	0
37	f	3	0	0	0	0
37	h	17	0	0	0	0
37	i	17	0	0	0	0
37	j	14	0	0	0	0
37	k	7	0	0	0	0
37	l	7	0	0	0	0
37	m	9	0	0	1	0
37	o	85	0	0	0	0
37	r	2	0	0	0	0
37	t	14	0	0	0	0
37	u	48	0	0	0	0
37	v	56	0	0	1	0
37	x	10	0	0	0	0
37	z	5	0	0	0	0
All	All	54524	0	53863	507	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 5.

All (507) 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)
6:f:16:PHE:H	20:r:30:GLN:HE22	1.16	0.92
28:A:611:PL9:H361	6:F:25:THR:HG21	1.55	0.88
25:c:501:CLA:H192	25:c:507:CLA:HBB1	1.54	0.86
22:a:602[A]:OEY:O6	22:a:602[A]:OEY:O5	1.97	0.81
2:B:91:TRP:HE1	33:B:620:STE:H32	1.46	0.80
18:X:17:GLY:HA2	33:X:101:STE:H142	1.63	0.78
16:V:109:GLU:OE1	37:V:301:HOH:O	2.03	0.76
22:A:602[A]:OEY:O6	22:A:602[A]:OEY:O5	2.03	0.75
4:D:279:LEU:HD22	26:D:402:PHO:HBC3	1.67	0.75
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.70	0.74
25:b:614:CLA:H2	25:b:615:CLA:HBB2	1.70	0.73
9:J:15:THR:HG22	9:J:19:MET:HE2	1.70	0.72
2:b:497:GLN:HE21	4:d:24:ARG:HH12	1.38	0.72
6:f:16:PHE:H	20:r:30:GLN:NE2	1.87	0.72
32:A:617:DGD:HE4	2:b:76:SER:HB3	1.72	0.71
13:O:5:LEU:HD13	13:O:10:ILE:HD11	1.73	0.71
10:K:19:ASP:OD1	37:K:201:HOH:O	2.09	0.70
10:K:23:ASP:OD2	37:K:201:HOH:O	2.10	0.70
31:A:616:SQD:H383	25:b:605:CLA:H93	1.73	0.69
25:b:602:CLA:H202	25:b:608:CLA:H111	1.73	0.69
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.75	0.69
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.75	0.69
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.57	0.68
25:C:502:CLA:H61	25:C:512:CLA:H42	1.75	0.68
2:b:39:LEU:HD22	33:b:625:STE:H52	1.76	0.66
3:C:406:SER:HA	3:C:420:VAL:HG23	1.76	0.66
2:B:357:ARG:NE	37:B:701:HOH:O	2.22	0.65
27:t:101:BCR:H321	27:t:101:BCR:HC8	1.78	0.64
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.78	0.64
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.78	0.64
3:C:148:GLY:O	3:C:156:LYS:NZ	2.29	0.64
35:e:101:HEM:HBC2	35:e:101:HEM:HMC2	1.79	0.64
25:A:607:CLA:H91	29:D:407:LMG:H242	1.80	0.64
35:e:101:HEM:HHC	35:e:101:HEM:HBB2	1.79	0.64
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.80	0.63
2:B:371:THR:HG23	2:B:372:ASP:O	1.98	0.63
1:A:11:ALA:O	1:A:16:ARG:NH2	2.33	0.62
32:A:617:DGD:HBF2	8:I:7:THR:HG21	1.83	0.61
16:v:104:MET:HA	16:v:107:LEU:HD22	1.81	0.61
17:Y:20:ALA:N	17:Y:23:THR:HG1	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:21:LEU:HD13	17:y:24:MET:HE2	1.81	0.61
9:j:15:THR:HG22	9:j:19:MET:HE2	1.83	0.61
12:m:4:ASN:ND2	29:m:101:LMG:O10	2.34	0.61
29:A:613:LMG:H132	25:C:505:CLA:H203	1.82	0.61
28:D:406:PL9:H412	11:L:29:LEU:HD23	1.83	0.61
3:C:210:PHE:HA	3:C:213:LEU:HD13	1.84	0.60
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.82	0.60
30:D:408:LHG:H321	14:T:21:ILE:HD11	1.84	0.60
25:B:606:CLA:H72	27:B:619:BCR:H311	1.84	0.59
25:b:609:CLA:HBB1	27:h:102:BCR:HC21	1.84	0.59
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.85	0.59
2:B:327:THR:HG21	29:M:101:LMG:H291	1.83	0.58
25:a:613:CLA:H151	30:d:406:LHG:H222	1.85	0.58
28:A:611:PL9:H261	30:E:101:LHG:H202	1.85	0.58
13:O:56:PRO:O	13:O:58:ASN:ND2	2.37	0.58
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.85	0.57
25:B:609:CLA:H203	7:H:39:LEU:HD12	1.86	0.57
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.86	0.57
25:b:613:CLA:H43	31:b:619:SQD:H102	1.86	0.57
29:c:521:LMG:H292	29:c:521:LMG:H112	1.85	0.57
33:b:623:STE:O1	37:b:702:HOH:O	2.17	0.57
3:C:313:GLN:HB2	3:C:396:MET:HG3	1.86	0.57
12:M:6:LEU:HD12	29:M:101:LMG:HC92	1.87	0.57
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.19	0.57
26:d:401:PHO:HMB3	26:d:401:PHO:HBB1	1.87	0.57
25:B:601:CLA:HBA1	25:B:601:CLA:HBD	1.87	0.57
30:A:614:LHG:H192	30:A:614:LHG:H362	1.87	0.56
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.53	0.56
18:X:16:SER:HB3	33:X:101:STE:H91	1.85	0.56
5:e:26:THR:HA	20:r:15:ALA:HB1	1.87	0.56
1:A:227:THR:HB	1:A:231:GLU:HG3	1.86	0.56
1:a:46:ILE:HD12	27:a:611:BCR:H15C	1.87	0.56
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.88	0.56
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.88	0.56
25:a:610:CLA:H41	25:a:610:CLA:H142	1.86	0.56
14:T:15:ALA:HB2	27:T:101:BCR:H14C	1.88	0.55
15:U:58:VAL:O	15:U:61:VAL:HG22	2.06	0.55
16:v:12:LEU:HD23	16:v:17:LYS:HD3	1.86	0.55
3:c:406:SER:HA	3:c:420:VAL:HG23	1.88	0.55
4:d:126:MET:HE3	4:d:143:ALA:O	2.06	0.55
5:e:8:ARG:NH1	5:e:12:ASP:OD2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:504:CLA:H143	25:C:508:CLA:H141	1.88	0.55
13:O:56:PRO:O	13:O:58:ASN:N	2.32	0.55
2:b:226:TYR:OH	37:b:701:HOH:O	2.14	0.55
3:C:213:LEU:HD11	27:C:514:BCR:H373	1.89	0.55
2:b:488:PRO:O	2:b:492:GLU:HG2	2.06	0.55
10:k:17:ILE:HD11	19:z:6:GLN:HG2	1.87	0.55
2:b:12:LEU:HB2	25:b:611:CLA:HMC2	1.89	0.55
30:a:614:LHG:H212	25:b:612:CLA:H172	1.88	0.55
27:T:101:BCR:H321	27:T:101:BCR:HC8	1.87	0.54
18:x:12:ILE:HD13	33:x:101:STE:H152	1.89	0.54
16:V:18:THR:OG1	37:V:302:HOH:O	2.18	0.54
25:a:610:CLA:H2	8:i:12:VAL:HG11	1.89	0.54
1:A:188[C]:ALA:HB2	1:A:328[C]:MET:HB2	1.88	0.54
28:d:405:PL9:H201	30:l:101:LHG:H202	1.90	0.54
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.90	0.54
25:c:503:CLA:H203	25:c:510:CLA:HAB	1.88	0.54
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.90	0.54
2:B:247:PHE:CE1	25:B:602:CLA:H102	2.42	0.53
15:u:16:LYS:NZ	15:u:85:THR:OG1	2.41	0.53
3:c:464:GLU:HB3	3:c:467:LEU:HD12	1.90	0.53
3:c:342:MET:SD	3:c:356[B]:MET:HE2	2.49	0.53
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.91	0.53
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.44	0.53
1:A:271:LEU:HD11	28:A:611:PL9:HC71	1.91	0.53
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.89	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
25:c:501:CLA:C3D	25:c:503:CLA:H2	2.39	0.53
1:a:188[C]:ALA:HB2	1:a:328[C]:MET:HB2	1.91	0.53
5:e:56:TYR:HA	5:e:60:GLN:HE21	1.74	0.52
2:B:477:ASP:OD1	2:B:477:ASP:N	2.42	0.52
19:Z:34:ASP:O	19:Z:37:LYS:HG2	2.09	0.52
32:c:517:DGD:HAH1	32:c:518:DGD:HA81	1.91	0.52
1:a:183[B]:MET:HA	25:a:607:CLA:HMD1	1.89	0.52
33:m:102:STE:O2	37:m:201:HOH:O	2.19	0.52
31:f:101:SQD:H312	18:x:27:VAL:HG11	1.91	0.52
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.42	0.52
25:b:614:CLA:H2	25:b:615:CLA:CBB	2.40	0.51
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.91	0.51
25:B:614:CLA:H143	31:B:623:SQD:H382	1.93	0.51
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.93	0.51
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:ASN:HD21	2:B:476:ARG:NH1	2.09	0.51
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.93	0.51
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.93	0.51
6:f:24:HIS:O	6:f:28:VAL:HG13	2.11	0.51
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.92	0.50
5:E:30:LEU:HD11	35:F:101:HEM:HAB	1.92	0.50
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.93	0.50
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.94	0.50
11:L:26:VAL:HG11	30:L:101:LHG:H202	1.93	0.50
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.50
19:Z:6:GLN:HG3	19:Z:7:LEU:HD22	1.93	0.50
1:a:82:VAL:HB	1:a:174[C]:LEU:HB2	1.93	0.50
17:y:20:ALA:O	17:y:24:MET:HG2	2.10	0.50
1:A:341[C]:LEU:HD13	1:A:343[C]:LEU:HD21	1.93	0.50
2:b:124:ARG:HD2	7:h:2:ALA:HB2	1.94	0.50
4:d:21:TRP:HA	4:d:24:ARG:HD3	1.94	0.50
5:e:10:PHE:N	30:e:102:LHG:O4	2.40	0.50
2:B:495:PHE:HD2	2:B:505:ARG:NH1	2.09	0.49
3:C:349:ILE:HD12	13:O:101:ILE:HD13	1.95	0.49
2:B:149[B]:LEU:HD21	25:B:604:CLA:H171	1.93	0.49
11:l:7:ARG:HH12	33:l:102:STE:C1	2.26	0.49
25:A:612:CLA:HMB3	25:A:612:CLA:HBB1	1.95	0.49
2:b:224:ARG:HG3	7:h:25:TRP:CD2	2.48	0.49
3:c:26:ARG:HD3	10:k:46:ARG:NH2	2.27	0.49
20:r:20:VAL:O	20:r:24:LEU:HB2	2.12	0.49
1:a:279:PRO:HG2	4:d:212:ALA:HB2	1.95	0.49
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.94	0.49
25:B:607:CLA:H203	30:B:622:LHG:H142	1.94	0.49
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.94	0.49
2:B:247:PHE:HE1	25:B:602:CLA:H102	1.77	0.49
3:c:124:VAL:HG11	27:c:514:BCR:H16C	1.94	0.48
6:f:26:LEU:O	6:f:29:PRO:HD2	2.14	0.48
1:A:179[C]:THR:O	1:A:183[C]:MET:HG3	2.14	0.48
3:C:42:LEU:HD21	25:C:511:CLA:H2A	1.95	0.48
6:F:36:ALA:O	6:F:40:MET:HG3	2.12	0.48
13:O:133:VAL:C	13:O:135:SER:H	2.21	0.48
16:V:95:LEU:HD11	16:V:112:LEU:HD11	1.94	0.48
2:b:247:PHE:CE1	25:b:601:CLA:H102	2.48	0.48
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.78	0.48
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.95	0.48
31:A:616:SQD:H341	25:b:615:CLA:H93	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:513:CLA:H8	27:c:514:BCR:H23C	1.96	0.48
1:A:160[B]:ILE:HD11	32:C:515:DGD:HB92	1.94	0.48
3:c:213:LEU:HD21	27:c:515:BCR:C20	2.42	0.48
3:C:45:LEU:HA	3:C:139:THR:HG22	1.95	0.48
25:C:508:CLA:H203	32:C:516:DGD:HAE1	1.96	0.48
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.49	0.48
4:d:241:GLU:CD	4:d:241:GLU:H	2.21	0.48
1:A:334[B]:ARG:NH2	37:A:708:HOH:O	2.47	0.48
1:a:300:PHE:HZ	32:c:518:DGD:HB61	1.79	0.48
2:b:91:TRP:HE1	33:b:621:STE:H111	1.79	0.48
4:D:24:ARG:NH2	18:X:35:ASP:OD2	2.47	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.48
25:a:610:CLA:H111	25:a:610:CLA:H52	1.96	0.47
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.49	0.47
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.96	0.47
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.14	0.47
1:A:84:PRO:HA	1:A:112:TYR:CG	2.50	0.47
28:A:611:PL9:H422	28:A:611:PL9:H401	1.68	0.47
25:B:601:CLA:H51	33:H:103:STE:H151	1.96	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.47
4:d:266:TRP:CD1	30:d:406:LHG:HC31	2.50	0.47
32:A:617:DGD:HD5	2:b:75:TRP:HB3	1.96	0.47
1:a:165[C]:GLN:NE2	1:a:294:ALA:O	2.48	0.47
13:o:18:LYS:NZ	13:o:74:GLU:OE1	2.48	0.47
17:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.97	0.47
10:k:26:PRO:O	10:k:29:PRO:HD2	2.15	0.47
2:B:67:ALA:HA	2:B:71:VAL:O	2.15	0.47
29:D:409:LMG:H112	29:D:409:LMG:H141	1.83	0.47
1:A:85:SER:HA	1:A:109:GLY:HA3	1.97	0.47
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.77	0.47
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.50	0.47
25:c:507:CLA:H92	25:c:507:CLA:H61	1.73	0.47
2:B:155:ALA:O	2:B:159:THR:OG1	2.31	0.46
25:C:512:CLA:H141	25:C:512:CLA:H162	1.62	0.46
16:v:7:VAL:O	16:v:124:LYS:NZ	2.44	0.46
2:B:149[B]:LEU:HD11	25:B:604:CLA:H112	1.97	0.46
25:b:604:CLA:HMA1	25:b:605:CLA:H3A	1.98	0.46
16:v:90:GLU:HB2	37:v:315:HOH:O	2.15	0.46
2:B:149[B]:LEU:HD11	25:B:604:CLA:H162	1.98	0.46
25:B:606:CLA:H91	25:B:606:CLA:H112	1.57	0.46
25:B:611:CLA:H72	25:B:611:CLA:H112	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:334:PRO:HA	13:O:153:THR:OG1	2.15	0.46
25:C:508:CLA:H121	25:C:508:CLA:H161	1.78	0.46
2:b:36:SER:OG	27:b:617:BCR:H362	2.15	0.46
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.97	0.46
32:C:516:DGD:HAN2	32:C:516:DGD:HAW1	1.41	0.46
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.81	0.46
17:y:19:ILE:O	17:y:23:THR:HG22	2.16	0.46
2:B:36:SER:OG	27:B:618:BCR:H362	2.16	0.46
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.98	0.46
13:O:36:GLN:HE21	13:O:37:THR:H	1.64	0.46
13:O:203:LYS:NZ	37:O:306:HOH:O	2.46	0.46
1:a:201:GLY:HA3	1:a:286:THR:HB	1.96	0.46
28:a:612:PL9:H503	4:d:39:PRO:HG3	1.98	0.46
13:O:178:LYS:H	13:O:178:LYS:HG2	1.48	0.46
16:V:28:GLU:HG2	37:V:332:HOH:O	2.15	0.46
2:b:92:SER:O	2:b:96:VAL:HG23	2.15	0.46
27:t:101:BCR:HC7	27:t:101:BCR:H331	1.79	0.46
25:a:607:CLA:HBB1	25:a:607:CLA:HMB3	1.98	0.46
3:c:117:VAL:HG12	33:c:520:STE:H141	1.97	0.46
25:c:508:CLA:H141	25:c:510:CLA:H192	1.98	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.98	0.46
5:E:53:ASP:O	16:V:1:ALA:N	2.49	0.46
2:b:489:GLU:HA	2:b:495:PHE:CD2	2.51	0.46
3:c:429:SER:HB3	32:c:517:DGD:HBE1	1.98	0.46
4:d:12:ARG:HD3	4:d:12:ARG:HA	1.74	0.46
5:e:14:ILE:O	5:e:20:TRP:NE1	2.49	0.46
1:A:131:TRP:CH2	25:C:505:CLA:HAA2	2.50	0.45
2:B:102:VAL:HG11	25:B:606:CLA:H111	1.97	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.33	0.45
25:B:603:CLA:H141	25:B:603:CLA:H161	1.68	0.45
25:C:505:CLA:H2	25:C:505:CLA:H61	1.74	0.45
13:o:32:ILE:HG13	13:o:93:LEU:HD11	1.98	0.45
1:A:334[C]:ARG:HH21	13:O:159:PRO:HA	1.81	0.45
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.51	0.45
13:O:54:GLU:O	13:O:63:ALA:HB3	2.16	0.45
2:b:149:LEU:HD21	33:b:621:STE:H22	1.97	0.45
5:e:81:GLU:O	5:e:84:LYS:HE2	2.17	0.45
6:f:19:ARG:O	6:f:23:VAL:HG13	2.16	0.45
25:B:606:CLA:H71	27:B:619:BCR:H342	1.98	0.45
27:C:514:BCR:H361	27:C:514:BCR:H20C	1.80	0.45
1:a:271:LEU:HD21	28:a:612:PL9:HC71	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:333[C]:GLU:HB2	1:a:337[C]:HIS:HE1	1.81	0.45
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.46	0.45
2:b:283:GLU:O	2:b:287:ARG:HG3	2.16	0.45
2:b:293:ALA:C	2:b:295:GLY:H	2.25	0.45
25:b:601:CLA:H42	32:h:103:DGD:HB41	1.98	0.45
3:C:245:ILE:O	3:C:249:ILE:HD12	2.17	0.45
25:b:611:CLA:H162	25:b:611:CLA:H122	1.78	0.45
25:c:513:CLA:H172	25:c:513:CLA:H13	1.70	0.45
16:v:41:HIS:HA	16:v:45:ILE:O	2.17	0.45
2:B:451:PHE:CD1	2:B:451:PHE:C	2.94	0.45
15:U:16:LYS:NZ	37:U:204:HOH:O	2.49	0.45
5:e:64:PRO:HB2	5:e:79:PHE:CD2	2.52	0.45
16:v:77:LYS:HG2	16:v:95:LEU:HD12	1.98	0.45
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.98	0.45
1:a:131:TRP:CH2	25:c:505:CLA:HAA2	2.52	0.45
4:d:103:ARG:HG3	5:e:73:LYS:HZ3	1.82	0.45
25:B:615:CLA:H2	25:B:616:CLA:HBB2	1.99	0.45
29:D:407:LMG:H151	29:D:407:LMG:H122	1.77	0.45
4:D:194:ASN:HA	4:D:295:SER:OG	2.18	0.44
3:c:180:MET:HE1	29:c:521:LMG:HC72	1.98	0.44
25:B:616:CLA:H41	25:B:616:CLA:H61	1.71	0.44
3:C:180:MET:HG2	3:C:199:ILE:O	2.16	0.44
8:I:2:GLU:O	8:I:6:ILE:HG12	2.17	0.44
1:a:200:LEU:HD13	32:c:518:DGD:HAW2	1.99	0.44
31:a:615:SQD:H111	31:a:615:SQD:H142	1.64	0.44
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.73	0.44
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.98	0.44
31:F:102:SQD:H372	31:F:102:SQD:H341	1.85	0.44
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.99	0.44
2:b:491:VAL:HG12	4:d:136:VAL:HG13	2.00	0.44
30:d:406:LHG:H321	14:t:21:ILE:HD11	2.00	0.44
1:A:334[A]:ARG:NH2	37:A:708:HOH:O	2.50	0.44
25:B:607:CLA:H141	25:B:607:CLA:H161	1.82	0.44
25:C:504:CLA:H121	32:C:517:DGD:HBN1	2.00	0.44
25:C:507:CLA:H92	25:C:507:CLA:H61	1.86	0.44
13:O:6:THR:HG22	13:O:9:ASP:CG	2.42	0.44
19:Z:23:VAL:HG22	19:Z:40:ILE:HD12	2.00	0.44
2:b:65:PHE:HE1	25:b:603:CLA:HED2	1.82	0.44
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.51	0.44
30:d:407:LHG:H242	30:d:407:LHG:H272	1.47	0.44
2:B:409:GLN:HE21	2:B:409:GLN:HB3	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:ILE:HD12	4:D:299:ILE:HG12	1.99	0.44
3:C:69:LEU:HA	3:C:69:LEU:HD23	1.80	0.44
19:Z:7:LEU:HD13	19:Z:7:LEU:HA	1.86	0.44
1:a:161[C]:TYR:OH	37:a:701:HOH:O	2.18	0.44
3:c:121:SER:O	3:c:124:VAL:HG13	2.17	0.44
25:d:403:CLA:H92	18:x:18:ALA:HB2	1.99	0.44
15:u:39:ARG:NH2	16:v:60:ALA:O	2.45	0.44
2:b:314:TYR:OH	2:b:334:ASP:OD2	2.36	0.44
25:c:513:CLA:HBB1	25:c:513:CLA:HMB3	1.99	0.44
18:x:8:LYS:HA	18:x:8:LYS:HD2	1.64	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
32:C:516:DGD:HA71	32:C:516:DGD:HAT1	1.69	0.44
16:v:24:LYS:HZ2	16:v:28:GLU:HB2	1.83	0.44
2:B:299[B]:GLU:H	2:B:299[B]:GLU:CD	2.25	0.44
28:D:406:PL9:H201	30:L:101:LHG:H211	2.00	0.44
3:c:27:ASP:OD1	3:c:30:SER:OG	2.33	0.44
3:c:165:LEU:HD13	25:c:507:CLA:HED1	2.00	0.44
15:U:45:LEU:HD21	15:U:71:GLN:HB3	2.00	0.43
3:c:352:GLY:O	3:c:355[C]:THR:HG22	2.17	0.43
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.53	0.43
32:A:617:DGD:HB41	33:I:101:STE:H62	1.99	0.43
5:E:60:GLN:NE2	5:E:62:SER:O	2.51	0.43
27:K:103:BCR:H20C	27:K:103:BCR:H361	1.88	0.43
27:b:617:BCR:H24C	27:b:617:BCR:H371	1.76	0.43
25:c:504:CLA:H92	25:c:504:CLA:H62	1.76	0.43
4:d:103:ARG:NE	4:d:106:GLN:OE1	2.37	0.43
11:L:8:GLN:OE1	37:L:201:HOH:O	2.20	0.43
25:c:503:CLA:H62	25:c:503:CLA:H102	1.74	0.43
1:a:112:TYR:O	1:a:116:ILE:HG12	2.19	0.43
2:b:39:LEU:HD22	33:b:625:STE:C5	2.46	0.43
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.00	0.43
25:c:510:CLA:H193	25:c:510:CLA:H161	1.72	0.43
16:v:24:LYS:NZ	16:v:28:GLU:HB2	2.33	0.43
3:C:344:SER:O	13:O:75:THR:HG22	2.19	0.43
2:b:58:GLN:C	2:b:329:PRO:HB3	2.43	0.43
3:c:134:ILE:HD12	25:c:511:CLA:H43	2.00	0.43
25:c:512:CLA:H92	25:c:512:CLA:H61	1.68	0.43
25:c:513:CLA:H91	25:c:513:CLA:H111	1.78	0.43
1:A:190[B]:HIS:ND1	1:A:298:ASN:OD1	2.52	0.43
2:B:117:TYR:HA	11:L:1:MET:HE1	2.01	0.43
25:B:611:CLA:H71	30:L:101:LHG:H321	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:616:BCR:H11C	27:b:616:BCR:H341	1.93	0.43
3:c:42:LEU:HD21	25:c:511:CLA:H2A	2.00	0.43
32:c:517:DGD:HB22	29:c:519:LMG:H302	2.00	0.43
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.86	0.43
3:C:459:ILE:HG21	3:C:464:GLU:HG3	2.01	0.43
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.00	0.43
2:b:62:VAL:HB	25:b:604:CLA:HED3	2.01	0.43
25:b:612:CLA:H143	25:b:612:CLA:H111	1.81	0.43
31:b:619:SQD:H151	31:b:619:SQD:H122	1.78	0.43
4:d:194:ASN:HA	4:d:295:SER:OG	2.19	0.43
5:e:78:THR:O	5:e:82:GLN:HG3	2.19	0.43
2:B:414:PRO:O	2:B:418:LYS:HG3	2.18	0.43
2:b:486:LEU:HD11	2:b:490:GLN:NE2	2.34	0.43
15:u:16:LYS:HE3	15:u:88:GLU:HB2	2.01	0.43
1:A:201:GLY:HA3	1:A:286:THR:HB	2.01	0.43
29:c:521:LMG:H382	29:c:521:LMG:H351	1.90	0.43
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.70	0.43
33:C:519:STE:H71	33:C:519:STE:H41	1.87	0.42
1:a:82:VAL:HB	1:a:174[C]:LEU:HD12	2.01	0.42
4:d:85:MET:HE1	5:e:72:ALA:CB	2.49	0.42
30:A:614:LHG:H151	31:A:615:SQD:H272	2.02	0.42
2:B:145:LEU:HD22	25:B:604:CLA:H193	2.01	0.42
27:B:618:BCR:H371	27:B:618:BCR:H24C	1.84	0.42
27:D:405:BCR:H20C	27:D:405:BCR:H361	1.88	0.42
15:U:67:LEU:HB3	15:U:72:LYS:HG3	2.01	0.42
25:a:610:CLA:H102	8:i:13:THR:HG23	2.01	0.42
2:b:505:ARG:HG3	2:b:506:ARG:N	2.34	0.42
25:c:501:CLA:C4D	25:c:503:CLA:H2	2.49	0.42
8:i:33:LYS:O	8:i:35:LYS:NZ	2.53	0.42
25:A:612:CLA:H193	25:A:612:CLA:H162	1.70	0.42
27:B:617:BCR:H24C	27:B:617:BCR:H371	1.85	0.42
3:C:410:VAL:HG22	3:C:413[B]:GLU:HG2	2.00	0.42
3:c:56:HIS:HA	3:c:59:LEU:HD12	2.01	0.42
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.54	0.42
16:v:76:MET:HE1	16:v:115:ILE:HD12	2.00	0.42
2:B:497:GLN:HB2	2:B:504:THR:HB	2.00	0.42
33:B:625:STE:H81	33:B:625:STE:H52	1.65	0.42
13:O:78:LEU:HB3	13:O:81:ILE:HD11	2.01	0.42
25:b:607:CLA:HHD	25:b:607:CLA:HAC2	1.91	0.42
33:b:621:STE:H31	33:b:621:STE:H61	1.85	0.42
4:d:180:ARG:HD3	4:d:180:ARG:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:102:STE:H52	33:l:102:STE:H21	1.74	0.42
1:A:162[A]:PRO:HB3	1:A:168[A]:PHE:HA	2.02	0.42
25:B:612:CLA:H13	25:B:612:CLA:H171	1.61	0.42
27:B:619:BCR:H20C	27:B:619:BCR:H361	1.84	0.42
25:a:607:CLA:CBD	25:a:613:CLA:HAC2	2.50	0.42
25:c:510:CLA:H111	25:c:510:CLA:H152	1.72	0.42
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.55	0.42
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.82	0.42
27:H:101:BCR:H15C	27:H:101:BCR:H351	1.90	0.42
12:M:31:SER:HB3	33:l:102:STE:H22	2.01	0.42
1:a:183[A]:MET:HA	25:a:607:CLA:HMD1	2.00	0.42
1:a:214:MET:HE3	1:a:214:MET:HB3	1.85	0.42
25:c:505:CLA:H161	25:c:505:CLA:H141	1.66	0.42
30:E:101:LHG:H311	30:E:101:LHG:H342	1.58	0.42
25:b:602:CLA:C4D	25:b:604:CLA:H43	2.49	0.42
3:c:72:LEU:HD21	3:c:108:THR:HB	2.02	0.42
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.54	0.42
27:c:515:BCR:H15C	27:c:515:BCR:H351	1.91	0.42
15:u:39:ARG:NH1	16:v:62:ALA:O	2.52	0.42
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.55	0.42
29:D:409:LMG:O9	29:D:409:LMG:HC71	2.20	0.42
5:E:17:VAL:HG23	9:J:7:ARG:HB2	2.00	0.42
16:V:63:THR:HG22	16:V:64:PRO:CD	2.50	0.42
2:b:25:MET:HG2	27:b:616:BCR:H23C	2.02	0.42
2:b:224:ARG:HG2	7:h:24:GLY:O	2.20	0.42
25:b:613:CLA:H41	25:b:613:CLA:H62	1.41	0.42
12:m:16:LEU:HA	12:m:16:LEU:HD13	1.82	0.42
29:m:101:LMG:H371	29:m:101:LMG:H342	1.64	0.42
27:t:101:BCR:H20C	27:t:101:BCR:H361	1.92	0.42
1:A:339[A]:PHE:HB3	1:A:340[A]:PRO:HD2	2.02	0.42
30:A:614:LHG:H172	31:A:615:SQD:H131	2.02	0.42
30:e:102:LHG:HC61	30:e:102:LHG:H241	1.80	0.42
3:C:467:LEU:HD23	3:C:467:LEU:HA	1.78	0.42
27:H:101:BCR:H371	27:H:101:BCR:H24C	1.79	0.42
4:d:266:TRP:CG	30:d:406:LHG:HC31	2.55	0.42
13:o:178:LYS:HD3	13:o:178:LYS:HA	1.67	0.42
16:v:57:GLU:H	16:v:57:GLU:CD	2.28	0.42
25:C:505:CLA:H43	27:C:514:BCR:HC7	2.01	0.41
4:D:246:MET:HE3	4:D:264:LYS:HG3	2.00	0.41
31:A:616:SQD:H132	27:T:101:BCR:HC41	2.02	0.41
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:603:CLA:H91	25:b:603:CLA:H111	1.85	0.41
3:c:41:ARG:NH1	25:c:511:CLA:HMD1	2.35	0.41
25:h:101:CLA:H111	25:h:101:CLA:H91	1.81	0.41
3:C:279:LEU:HD23	3:C:282:MET:HE3	2.02	0.41
25:C:509:CLA:H62	25:C:509:CLA:H92	1.74	0.41
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.35	0.41
12:M:20:VAL:CG2	12:m:20:VAL:HG11	2.49	0.41
13:O:42:ARG:O	13:O:241:ALA:HA	2.20	0.41
1:a:159[C]:LEU:O	1:a:163[C]:ILE:HG13	2.21	0.41
20:r:10:LEU:HD22	20:r:10:LEU:HA	1.93	0.41
2:B:164:PRO:HG3	25:B:606:CLA:O1D	2.20	0.41
25:B:614:CLA:H141	25:B:614:CLA:H161	1.70	0.41
27:B:619:BCR:H11C	27:B:619:BCR:H341	1.91	0.41
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.03	0.41
30:a:614:LHG:O4	4:d:141:TYR:OH	2.24	0.41
3:c:26:ARG:HD3	10:k:46:ARG:HH22	1.85	0.41
3:c:82:TYR:OH	3:c:394:GLU:OE2	2.35	0.41
25:c:512:CLA:H142	25:c:513:CLA:H151	2.02	0.41
27:K:102:BCR:H20C	27:K:102:BCR:H361	1.86	0.41
19:Z:2:THR:O	19:Z:6:GLN:HG2	2.19	0.41
2:B:363:PHE:HB3	2:B:365:SER:O	2.20	0.41
32:H:102:DGD:HB21	32:H:102:DGD:HB51	1.76	0.41
26:a:609:PHO:H13	26:a:609:PHO:H102	1.87	0.41
25:b:601:CLA:H91	25:b:601:CLA:H111	1.78	0.41
25:B:614:CLA:H61	25:B:614:CLA:H41	1.64	0.41
25:C:504:CLA:H101	32:C:517:DGD:HBN1	2.03	0.41
25:b:603:CLA:H41	25:b:603:CLA:H62	1.58	0.41
2:B:29:LEU:HD23	31:B:623:SQD:H211	2.02	0.41
3:C:406:SER:O	3:C:418:ASN:HA	2.21	0.41
4:D:186:GLN:HB2	25:D:403:CLA:HBC1	2.02	0.41
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.03	0.41
10:k:15:TYR:CZ	19:z:5:PHE:HZ	2.37	0.41
20:r:9:LEU:O	20:r:13:LEU:HG	2.20	0.41
1:A:339[B]:PHE:HB3	1:A:340[B]:PRO:HD2	2.03	0.41
25:A:606:CLA:HMB1	25:A:606:CLA:HBB1	2.03	0.41
31:A:616:SQD:H191	31:A:616:SQD:H223	1.65	0.41
25:B:602:CLA:H162	25:B:602:CLA:H122	1.65	0.41
25:D:404:CLA:H142	25:D:404:CLA:H111	1.85	0.41
16:V:61:LEU:HD23	16:V:61:LEU:HA	1.92	0.41
16:V:77:LYS:HG2	16:V:95:LEU:HD12	2.02	0.41
19:Z:15:LEU:HD22	19:Z:19:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:184:GLU:HB2	37:b:781:HOH:O	2.21	0.41
3:c:328[B]:VAL:HG22	37:c:623:HOH:O	2.21	0.41
27:h:102:BCR:H24C	27:h:102:BCR:H371	1.83	0.41
10:k:18:PHE:CE1	19:z:9:LEU:HD23	2.56	0.41
1:A:341[C]:LEU:HB2	3:C:313:GLN:OE1	2.21	0.41
25:A:606:CLA:HBD	25:A:612:CLA:HAC2	2.02	0.41
27:A:610:BCR:H20C	27:A:610:BCR:H361	1.81	0.41
4:D:123:ILE:HD11	32:H:102:DGD:HAH1	2.03	0.41
5:E:74:GLN:N	5:E:74:GLN:CD	2.79	0.41
7:H:2:ALA:N	37:H:204:HOH:O	2.54	0.41
10:K:25:LEU:N	10:K:26:PRO:HD2	2.36	0.41
1:a:176[C]:ILE:HD13	25:a:613:CLA:HED3	2.03	0.41
25:a:613:CLA:HED2	4:d:198:MET:SD	2.61	0.41
2:b:91:TRP:HE1	33:b:621:STE:H141	1.86	0.41
25:b:609:CLA:H8	25:b:609:CLA:H51	1.91	0.41
25:b:613:CLA:H112	25:b:613:CLA:H152	1.94	0.41
16:v:69:ILE:CD1	16:v:120:LEU:HD12	2.51	0.41
1:A:161[A]:TYR:HB3	1:A:162[A]:PRO:HD3	2.02	0.40
1:A:243:GLU:CD	1:A:243:GLU:H	2.29	0.40
25:C:506:CLA:H62	25:C:506:CLA:H2	1.79	0.40
25:c:505:CLA:H43	27:c:515:BCR:HC7	2.02	0.40
4:d:99:GLY:HA3	33:x:101:STE:H142	2.03	0.40
27:k:102:BCR:H20C	27:k:102:BCR:H361	1.88	0.40
13:o:32:ILE:HD13	13:o:32:ILE:HA	1.91	0.40
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.40
2:B:185:TRP:HB3	25:B:601:CLA:HMA3	2.03	0.40
27:C:514:BCR:H371	27:C:514:BCR:H24C	1.83	0.40
27:K:102:BCR:H10C	17:Y:28:ILE:HG23	2.02	0.40
15:U:17:LEU:HD23	15:U:17:LEU:HA	1.89	0.40
4:d:139:ARG:H	4:d:139:ARG:HG3	1.74	0.40
25:A:606:CLA:CBD	25:A:612:CLA:HAC2	2.52	0.40
2:B:414:PRO:N	2:B:415:PRO:HD2	2.36	0.40
3:C:139:THR:HB	3:C:141:GLU:OE2	2.21	0.40
29:C:518:LMG:H142	29:C:518:LMG:H111	1.86	0.40
4:D:241:GLU:H	4:D:241:GLU:CD	2.29	0.40
13:O:37:THR:OG1	13:O:246:ALA:HB3	2.20	0.40
25:b:601:CLA:H161	25:b:601:CLA:H203	1.88	0.40
25:b:607:CLA:H18	25:b:608:CLA:H192	2.03	0.40
16:v:26:TYR:OH	16:v:122:GLU:OE1	2.26	0.40
16:v:41:HIS:CD2	36:v:201:HEC:NB	2.89	0.40
27:A:610:BCR:H371	27:A:610:BCR:H24C	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.56	0.40
2:B:347:ARG:O	2:B:397:VAL:HA	2.22	0.40
25:B:613:CLA:H71	25:B:613:CLA:H112	1.88	0.40
4:D:246:MET:HE3	4:D:264:LYS:HE2	2.04	0.40
27:K:101:BCR:H20C	27:K:101:BCR:H361	1.91	0.40
25:b:607:CLA:H203	32:h:103:DGD:HA82	2.03	0.40
4:d:293:LEU:HD23	4:d:293:LEU:HA	1.98	0.40
16:v:69:ILE:HD12	16:v:120:LEU:HD12	2.02	0.40
25:B:601:CLA:H61	33:H:103:STE:H142	2.02	0.40
4:D:61:HIS:HE1	4:D:80:THR:O	2.05	0.40
12:M:16:LEU:HD12	12:M:16:LEU:HA	1.80	0.40
13:O:110:MET:HE2	13:O:110:MET:HB3	1.96	0.40
1:a:324:ALA:O	1:a:328[C]:MET:HG3	2.22	0.40
25:c:508:CLA:H92	25:c:508:CLA:H62	1.90	0.40
4:d:20:ASP:O	4:d:24:ARG:HG3	2.21	0.40
9:j:26:GLY:HA2	33:j:101:STE:H82	2.03	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	458/344 (133%)	445 (97%)	12 (3%)	1 (0%)	43	42
1	a	458/344 (133%)	440 (96%)	17 (4%)	1 (0%)	43	42
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	461/461 (100%)	449 (97%)	11 (2%)	1 (0%)	43	42
3	c	471/461 (102%)	457 (97%)	13 (3%)	1 (0%)	43	42
4	D	341/352 (97%)	332 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	342/352 (97%)	332 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
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%)	231 (95%)	9 (4%)	3 (1%)	10	6
13	o	242/272 (89%)	235 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	7
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	18	14
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	25 (100%)	0	0	100	100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	R	32/41 (78%)	31 (97%)	0	1 (3%)	3 1
20	r	29/41 (71%)	28 (97%)	1 (3%)	0	100 100
All	All	5534/5700 (97%)	5383 (97%)	141 (2%)	10 (0%)	43 42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
13	O	62	GLU
3	c	416	SER
15	u	53	ALA
13	O	58	ASN
13	O	134	THR
20	R	34	LEU
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	374/280 (134%)	371 (99%)	3 (1%)	73 80
1	a	373/280 (133%)	362 (97%)	11 (3%)	37 40
2	B	407/407 (100%)	397 (98%)	10 (2%)	42 45
2	b	402/407 (99%)	396 (98%)	6 (2%)	57 64
3	C	361/362 (100%)	355 (98%)	6 (2%)	53 60
3	c	370/362 (102%)	356 (96%)	14 (4%)	29 29
4	D	278/283 (98%)	273 (98%)	5 (2%)	51 58
4	d	279/283 (99%)	273 (98%)	6 (2%)	45 50
5	E	72/73 (99%)	69 (96%)	3 (4%)	26 25
5	e	71/73 (97%)	69 (97%)	2 (3%)	38 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	10
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	29
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	30 (94%)	2 (6%)	16	13
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	26	25
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	10
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	200 (97%)	6 (3%)	37	40
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	28
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	25/28 (89%)	24 (96%)	1 (4%)	28	27
15	U	84/112 (75%)	79 (94%)	5 (6%)	17	14
15	u	84/112 (75%)	83 (99%)	1 (1%)	63	70
16	V	117/138 (85%)	115 (98%)	2 (2%)	53	60
16	v	117/138 (85%)	113 (97%)	4 (3%)	32	33
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
17	y	22/37 (60%)	20 (91%)	2 (9%)	9	6
18	X	31/34 (91%)	27 (87%)	4 (13%)	4	2
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	35
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4	2
19	z	51/52 (98%)	47 (92%)	4 (8%)	11	8
20	R	28/33 (85%)	23 (82%)	5 (18%)	2	1
20	r	25/33 (76%)	19 (76%)	6 (24%)	1	0
All	All	4572/4654 (98%)	4426 (97%)	146 (3%)	33	35

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL
1	A	243	GLU
2	B	86	ILE
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	289	GLN
2	B	297	THR
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	476	ARG
3	C	48	LYS
3	C	141	GLU
3	C	240	ILE
3	C	249	ILE
3	C	289	PHE
3	C	315	MET
4	D	43	LEU
4	D	136	VAL
4	D	241	GLU
4	D	259	ILE
4	D	264	LYS
5	E	12	ASP
5	E	22[A]	ILE
5	E	22[B]	ILE
8	I	4	LEU
10	K	17	ILE
10	K	24	VAL
10	K	46	ARG
12	M	20	VAL
12	M	25	LEU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	214	THR
13	O	234	LYS
15	U	10	VAL
15	U	39	ARG
15	U	51	LYS

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Mol	Chain	Res	Type
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
17	Y	34	MET
17	Y	41	VAL
18	X	3	ILE
18	X	15	LEU
18	X	23	LEU
18	X	37	VAL
19	Z	7	LEU
19	Z	15	LEU
19	Z	20	VAL
19	Z	31	GLN
19	Z	35	ARG
19	Z	50	LEU
19	Z	52	LEU
20	R	21	ARG
20	R	28	VAL
20	R	29	LYS
20	R	33	LYS
20	R	35	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	159[C]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	245	THR
1	a	288	LEU
2	b	98	LEU
2	b	149	LEU
2	b	179	GLN
2	b	227	LYS
2	b	362	PHE
2	b	506	ARG
3	c	29	GLU
3	c	30	SER
3	c	72	LEU

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Mol	Chain	Res	Type
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	213	LEU
3	c	240	ILE
3	c	279	LEU
3	c	315	MET
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	416	SER
4	d	182	LEU
4	d	230	SER
4	d	259	ILE
4	d	291	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	83	LEU
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	56	ASP
8	i	2	GLU
8	i	34	ARG
9	j	21	VAL
10	k	10	LYS
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS
13	o	49	THR
13	o	53	LYS
13	o	60	ARG
13	o	64	GLU
13	o	118	LEU
13	o	130	GLN

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Mol	Chain	Res	Type
13	o	134	THR
14	t	29	ILE
15	u	15	GLU
16	v	22	THR
16	v	52	LEU
16	v	69	ILE
16	v	107	LEU
17	y	19	ILE
17	y	27	MET
18	x	15	LEU
19	z	1	MET
19	z	31	GLN
19	z	40	ILE
19	z	46	LEU
20	r	6	LEU
20	r	7	VAL
20	r	9	LEU
20	r	10	LEU
20	r	14	LEU
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	289	GLN
2	B	394	GLN
2	B	409	GLN
3	C	155	ASN
3	C	311	GLN
4	D	61	HIS
4	D	186	GLN
4	D	334	GLN
13	O	3	GLN
13	O	36	GLN
13	O	155	ASN
13	O	219	GLN
13	O	231	HIS
15	U	78	ASN
16	V	86	GLN
18	X	38	GLN
19	Z	38	GLN
20	R	32	GLN

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Mol	Chain	Res	Type
1	a	19	ASN
1	a	234	ASN
2	b	14	ASN
2	b	338	GLN
2	b	409	GLN
2	b	490	GLN
2	b	497	GLN
3	c	201	ASN
3	c	311	GLN
3	c	322	GLN
5	e	60	GLN
12	m	5	GLN
13	o	155	ASN
15	u	37	GLN
18	x	33	GLN
19	z	31	GLN
20	r	30	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	1.07	0	8,9,11	0.99	1 (12%)
14	FME	t	1	14	8,9,10	1.13	1 (12%)	8,9,11	1.10	0
12	FME	m	1	12	8,9,10	0.95	0	8,9,11	0.84	0
8	FME	i	1	8	8,9,10	1.04	0	8,9,11	0.90	0
12	FME	M	1	12	8,9,10	1.05	1 (12%)	8,9,11	0.88	0
8	FME	I	1	8	8,9,10	0.95	0	8,9,11	0.96	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
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-2.20	1.43	1.46
14	t	1	FME	CA-N	-2.17	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	C-CA-N	2.14	113.63	109.50

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 190 ligands modelled in this entry, 6 are monoatomic - leaving 184 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	$\#\|Z\| > 2$
33	STE	X	101	-	19,19,19	0.56	0	19,19,19	1.18	1 (5%)
25	CLA	c	511	3	69,73,73	1.58	8 (11%)	82,113,113	1.46	6 (7%)
29	LMG	c	521	-	48,48,55	0.95	3 (6%)	56,56,63	1.29	7 (12%)
25	CLA	B	605	2	69,73,73	1.29	8 (11%)	82,113,113	1.37	8 (9%)
25	CLA	a	610	1	69,73,73	1.31	6 (8%)	82,113,113	1.31	7 (8%)
25	CLA	c	506	3	69,73,73	1.32	10 (14%)	82,113,113	1.21	6 (7%)
25	CLA	B	615	2	69,73,73	1.29	9 (13%)	82,113,113	1.26	6 (7%)
21	OEX	A	601[C]	37,3,1	0,14,14	-	-	-		
25	CLA	C	502	3	69,73,73	1.23	9 (13%)	82,113,113	1.19	6 (7%)
29	LMG	D	407	-	51,51,55	0.75	1 (1%)	59,59,63	1.34	7 (11%)
33	STE	M	102	-	14,14,19	0.63	0	14,14,19	1.43	2 (14%)
27	BCR	B	617	-	41,41,41	1.04	3 (7%)	56,56,56	1.21	6 (10%)
33	STE	b	625	-	19,19,19	0.59	0	19,19,19	1.07	1 (5%)
31	SQD	B	623	-	52,54,54	1.56	8 (15%)	62,65,65	1.73	11 (17%)
25	CLA	B	612	2	69,73,73	1.16	6 (8%)	82,113,113	1.33	11 (13%)
33	STE	b	620	-	15,15,19	0.39	0	14,14,19	0.83	0
25	CLA	b	603	2	69,73,73	1.36	8 (11%)	82,113,113	1.44	10 (12%)
25	CLA	b	604	2	69,73,73	1.18	8 (11%)	82,113,113	1.59	11 (13%)
33	STE	H	103	-	17,17,19	0.42	0	16,16,19	0.68	0
32	DGD	C	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.35	8 (10%)
31	SQD	A	615	-	50,52,54	1.56	6 (12%)	60,63,65	1.86	10 (16%)
27	BCR	B	619	-	41,41,41	1.02	2 (4%)	56,56,56	1.28	5 (8%)
32	DGD	c	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.37	8 (10%)
36	HEC	v	201	16	50,50,50	1.68	6 (12%)	68,82,82	1.32	8 (11%)
27	BCR	C	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	6 (10%)
34	BCT	a	606	23	3,3,3	1.07	0	2,3,3	3.15	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	HEC	V	201	16	50,50,50	1.67	7 (14%)	68,82,82	1.30	6 (8%)
25	CLA	b	613	2	69,73,73	1.38	9 (13%)	82,113,113	1.22	6 (7%)
35	HEM	e	101	6,5	50,50,50	1.58	7 (14%)	67,82,82	1.22	4 (5%)
30	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.37	7 (13%)
25	CLA	C	508	3	69,73,73	1.30	9 (13%)	82,113,113	1.51	11 (13%)
25	CLA	B	602	2	69,73,73	1.29	7 (10%)	82,113,113	1.34	12 (14%)
27	BCR	K	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	6 (10%)
27	BCR	h	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.27	5 (8%)
27	BCR	k	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.07	3 (5%)
25	CLA	b	609	37	69,73,73	1.25	6 (8%)	82,113,113	1.28	6 (7%)
29	LMG	B	621	-	26,26,55	0.60	1 (3%)	26,26,63	1.35	2 (7%)
27	BCR	b	616	-	41,41,41	0.96	3 (7%)	56,56,56	1.23	4 (7%)
29	LMG	d	408	-	21,21,55	0.57	0	20,20,63	1.20	3 (15%)
33	STE	b	626	-	9,9,19	0.39	0	8,8,19	0.60	0
29	LMG	M	101	-	51,51,55	0.87	3 (5%)	59,59,63	1.44	10 (16%)
25	CLA	B	616	2	64,68,73	1.48	9 (14%)	76,107,113	1.36	8 (10%)
29	LMG	c	522	-	49,49,55	0.96	4 (8%)	57,57,63	1.29	4 (7%)
25	CLA	b	601	2	69,73,73	1.15	8 (11%)	82,113,113	1.41	8 (9%)
33	STE	B	620	-	16,16,19	0.70	0	16,16,19	1.06	0
25	CLA	B	606	2	69,73,73	1.38	8 (11%)	82,113,113	1.48	6 (7%)
33	STE	J	101	-	11,11,19	0.79	0	11,11,19	1.19	1 (9%)
25	CLA	C	512	3	69,73,73	1.52	10 (14%)	82,113,113	1.37	9 (10%)
25	CLA	A	612	37	69,73,73	1.21	8 (11%)	82,113,113	1.31	6 (7%)
33	STE	E	102	-	11,11,19	0.74	0	11,11,19	1.14	1 (9%)
27	BCR	b	618	-	41,41,41	0.95	2 (4%)	56,56,56	1.12	4 (7%)
21	OEX	A	601[B]	37,3,1	0,14,14	-	-	-		
25	CLA	C	501	3	69,73,73	1.56	10 (14%)	82,113,113	1.43	8 (9%)
25	CLA	B	609	2	69,73,73	1.24	6 (8%)	82,113,113	1.33	9 (10%)
25	CLA	A	607	37	69,73,73	1.14	6 (8%)	82,113,113	1.35	10 (12%)
30	LHG	d	406	-	48,48,48	0.71	2 (4%)	51,54,54	1.21	5 (9%)
33	STE	C	519	-	11,11,19	0.65	0	11,11,19	1.53	1 (9%)
21	OEX	a	601[C]	37,3,1	0,14,14	-	-	-		
27	BCR	d	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.18	4 (7%)
35	HEM	F	101	6,5	50,50,50	1.48	10 (20%)	67,82,82	1.22	4 (5%)
25	CLA	c	508	3	68,72,73	1.33	8 (11%)	80,111,113	1.36	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	C	504	37	63,67,73	1.30	8 (12%)	74,105,113	1.27	8 (10%)
32	DGD	A	617	-	67,67,67	1.11	6 (8%)	81,81,81	1.31	8 (9%)
25	CLA	b	615	2	64,68,73	1.18	5 (7%)	76,107,113	1.37	10 (13%)
25	CLA	c	503	3	69,73,73	1.37	9 (13%)	82,113,113	1.43	6 (7%)
25	CLA	b	614	2	69,73,73	1.27	9 (13%)	82,113,113	1.31	4 (4%)
30	LHG	a	614	-	48,48,48	0.76	3 (6%)	51,54,54	1.31	7 (13%)
33	STE	b	623	-	15,15,19	0.68	0	15,15,19	1.04	0
26	PHO	a	609	-	58,69,69	2.15	9 (15%)	55,99,99	1.44	7 (12%)
25	CLA	b	602	2	69,73,73	1.20	8 (11%)	82,113,113	1.29	9 (10%)
25	CLA	A	609	1	58,62,73	1.22	7 (12%)	68,99,113	1.42	8 (11%)
25	CLA	C	505	3	69,73,73	1.24	7 (10%)	82,113,113	1.30	7 (8%)
33	STE	k	103	-	11,11,19	0.75	0	11,11,19	1.09	0
33	STE	x	101	-	19,19,19	0.71	0	19,19,19	0.97	1 (5%)
33	STE	c	520	-	19,19,19	0.60	0	19,19,19	1.03	0
25	CLA	a	608	37	69,73,73	1.21	6 (8%)	82,113,113	1.35	8 (9%)
33	STE	B	625	-	11,11,19	0.68	0	11,11,19	1.31	2 (18%)
25	CLA	b	611	2	69,73,73	1.28	9 (13%)	82,113,113	1.34	9 (10%)
25	CLA	B	604	2	69,73,73	1.35	7 (10%)	82,113,113	1.53	7 (8%)
27	BCR	B	618	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
29	LMG	d	409	-	44,44,55	0.94	3 (6%)	52,52,63	1.30	6 (11%)
25	CLA	c	513	3	69,73,73	1.29	7 (10%)	82,113,113	1.28	10 (12%)
26	PHO	d	401	-	58,69,69	2.14	8 (13%)	55,99,99	1.57	10 (18%)
31	SQD	F	102	-	34,36,54	1.51	6 (17%)	42,45,65	1.95	10 (23%)
33	STE	t	103	-	9,9,19	0.35	0	8,8,19	0.80	0
25	CLA	C	511	3	69,73,73	1.37	8 (11%)	82,113,113	1.46	5 (6%)
25	CLA	h	101	37	69,73,73	1.37	9 (13%)	82,113,113	1.41	7 (8%)
25	CLA	b	608	2	69,73,73	1.29	8 (11%)	82,113,113	1.27	7 (8%)
25	CLA	B	607	37	69,73,73	1.26	6 (8%)	82,113,113	1.32	6 (7%)
25	CLA	c	501	3	69,73,73	1.22	9 (13%)	82,113,113	1.39	7 (8%)
22	OEY	A	602[A]	37,3,1	0,16,16	-	-	-		
30	LHG	d	407	-	38,38,48	0.76	1 (2%)	41,44,54	1.11	2 (4%)
33	STE	a	618	-	11,11,19	0.79	0	11,11,19	1.20	2 (18%)
32	DGD	c	517	-	63,63,67	0.95	2 (3%)	77,77,81	1.41	9 (11%)
25	CLA	c	512	3	69,73,73	1.27	10 (14%)	82,113,113	1.34	7 (8%)
25	CLA	C	506	3	69,73,73	1.19	6 (8%)	82,113,113	1.22	9 (10%)
30	LHG	A	614	-	46,46,48	0.84	3 (6%)	49,52,54	1.20	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	SQD	b	619	-	47,49,54	1.63	9 (19%)	57,60,65	1.73	10 (17%)
33	STE	d	410	-	16,16,19	0.61	0	16,16,19	1.30	1 (6%)
30	LHG	L	101	-	48,48,48	0.75	1 (2%)	51,54,54	1.16	2 (3%)
27	BCR	k	102	-	41,41,41	1.02	3 (7%)	56,56,56	1.15	4 (7%)
25	CLA	a	613	37	69,73,73	1.37	6 (8%)	82,113,113	1.44	7 (8%)
27	BCR	t	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.39	10 (17%)
27	BCR	c	514	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	5 (8%)
27	BCR	A	610	-	41,41,41	0.97	1 (2%)	56,56,56	1.13	4 (7%)
29	LMG	A	613	-	48,48,55	0.88	2 (4%)	56,56,63	1.29	4 (7%)
29	LMG	c	519	-	37,37,55	1.01	2 (5%)	45,45,63	1.36	6 (13%)
32	DGD	c	516	-	63,63,67	0.90	4 (6%)	77,77,81	1.38	11 (14%)
33	STE	B	624	-	11,11,19	0.75	0	11,11,19	1.24	0
26	PHO	A	608	-	58,69,69	1.95	10 (17%)	55,99,99	1.44	6 (10%)
25	CLA	B	611	2	69,73,73	1.23	6 (8%)	82,113,113	1.36	6 (7%)
25	CLA	c	510	3	69,73,73	1.34	8 (11%)	82,113,113	1.35	8 (9%)
25	CLA	c	505	3	69,73,73	1.12	7 (10%)	82,113,113	1.30	6 (7%)
25	CLA	b	606	37	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
33	STE	b	621	-	19,19,19	0.65	0	19,19,19	0.95	0
33	STE	t	102	-	13,13,19	0.65	0	13,13,19	1.33	2 (15%)
27	BCR	a	611	-	41,41,41	0.96	2 (4%)	56,56,56	1.24	5 (8%)
30	LHG	D	408	-	48,48,48	0.74	2 (4%)	51,54,54	1.30	6 (11%)
25	CLA	B	601	37	69,73,73	1.40	11 (15%)	82,113,113	1.35	11 (13%)
30	LHG	E	101	-	48,48,48	0.79	2 (4%)	51,54,54	1.25	6 (11%)
31	SQD	f	101	-	39,41,54	1.68	8 (20%)	49,52,65	1.64	10 (20%)
30	LHG	e	102	-	41,41,48	0.80	1 (2%)	44,47,54	1.30	5 (11%)
28	PL9	d	405	-	55,55,55	1.05	3 (5%)	68,69,69	1.62	14 (20%)
33	STE	B	626	-	15,15,19	0.36	0	14,14,19	0.90	0
25	CLA	B	608	2	69,73,73	1.17	8 (11%)	82,113,113	1.37	10 (12%)
32	DGD	a	617	-	43,43,67	0.79	3 (6%)	45,45,81	1.41	7 (15%)
25	CLA	B	610	37	69,73,73	1.24	10 (14%)	82,113,113	1.25	9 (10%)
33	STE	I	101	-	14,14,19	0.32	0	13,13,19	0.82	0
33	STE	j	101	-	11,11,19	0.78	0	11,11,19	1.29	2 (18%)
27	BCR	c	515	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	5 (8%)
25	CLA	d	402	4	69,73,73	1.18	7 (10%)	82,113,113	1.26	7 (8%)
27	BCR	K	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.12	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	b	612	2	69,73,73	1.22	8 (11%)	82,113,113	1.41	9 (10%)
33	STE	C	521	-	15,15,19	0.38	0	14,14,19	0.79	0
32	DGD	h	103	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	12 (15%)
25	CLA	D	403	4	69,73,73	1.29	9 (13%)	82,113,113	1.32	7 (8%)
33	STE	C	520	-	11,11,19	0.71	0	11,11,19	1.19	1 (9%)
22	OEY	a	602[A]	37,3,1	0,16,16	-	-	-		
25	CLA	b	607	2	69,73,73	1.24	7 (10%)	82,113,113	1.41	10 (12%)
25	CLA	c	507	37	69,73,73	1.34	10 (14%)	82,113,113	1.42	8 (9%)
31	SQD	a	615	-	52,54,54	1.59	7 (13%)	62,65,65	1.88	10 (16%)
31	SQD	A	616	-	38,38,54	1.78	5 (13%)	40,40,65	1.19	2 (5%)
32	DGD	C	516	-	63,63,67	1.06	5 (7%)	77,77,81	1.33	7 (9%)
25	CLA	c	504	37	64,68,73	1.16	4 (6%)	76,107,113	1.36	10 (13%)
25	CLA	C	510	3	69,73,73	1.21	7 (10%)	82,113,113	1.34	8 (9%)
25	CLA	d	403	4	69,73,73	1.24	7 (10%)	82,113,113	1.27	9 (10%)
27	BCR	T	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.31	6 (10%)
29	LMG	b	622	-	55,55,55	0.80	1 (1%)	63,63,63	1.37	12 (19%)
30	LHG	l	101	-	48,48,48	0.58	0	51,54,54	1.23	5 (9%)
34	BCT	D	401	23	3,3,3	1.07	0	2,3,3	3.28	1 (50%)
25	CLA	a	607	1	69,73,73	1.43	10 (14%)	82,113,113	1.34	6 (7%)
27	BCR	K	103	-	41,41,41	1.11	2 (4%)	56,56,56	1.13	2 (3%)
26	PHO	D	402	-	58,69,69	2.11	10 (17%)	55,99,99	1.53	7 (12%)
33	STE	m	102	-	11,11,19	0.70	0	11,11,19	1.44	2 (18%)
25	CLA	c	509	3	69,73,73	1.26	9 (13%)	82,113,113	1.42	5 (6%)
33	STE	t	104	-	17,17,19	0.65	0	17,17,19	1.10	1 (5%)
25	CLA	B	613	2	69,73,73	1.29	7 (10%)	82,113,113	1.46	11 (13%)
25	CLA	b	605	2	69,73,73	1.35	5 (7%)	82,113,113	1.48	9 (10%)
25	CLA	D	404	4	69,73,73	1.54	10 (14%)	82,113,113	1.19	8 (9%)
32	DGD	C	515	-	63,63,67	1.05	5 (7%)	77,77,81	1.36	11 (14%)
27	BCR	H	101	-	41,41,41	0.98	2 (4%)	56,56,56	1.20	6 (10%)
25	CLA	A	606	1	69,73,73	1.32	9 (13%)	82,113,113	1.21	7 (8%)
21	OEX	a	601[B]	37,3,1	0,14,14	-	-	-		
27	BCR	D	405	-	41,41,41	1.10	3 (7%)	56,56,56	1.18	5 (8%)
29	LMG	m	101	-	51,51,55	0.91	3 (5%)	59,59,63	1.48	7 (11%)
33	STE	b	624	-	14,14,19	0.32	0	13,13,19	0.89	0
25	CLA	C	503	3	69,73,73	1.44	9 (13%)	82,113,113	1.56	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	C	507	37	69,73,73	1.31	8 (11%)	82,113,113	1.39	11 (13%)
28	PL9	A	611	-	55,55,55	0.78	1 (1%)	68,69,69	1.47	13 (19%)
25	CLA	B	603	2	69,73,73	1.23	8 (11%)	82,113,113	1.22	6 (7%)
25	CLA	C	513	3	69,73,73	1.24	8 (11%)	82,113,113	1.40	7 (8%)
33	STE	l	102	-	17,17,19	0.34	0	16,16,19	0.89	0
25	CLA	C	509	3	69,73,73	1.27	11 (15%)	82,113,113	1.30	8 (9%)
27	BCR	b	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.09	4 (7%)
32	DGD	H	102	-	63,63,67	1.21	8 (12%)	77,77,81	1.33	8 (10%)
28	PL9	D	406	-	55,55,55	0.96	2 (3%)	68,69,69	1.72	12 (17%)
25	CLA	c	502	3	69,73,73	1.25	9 (13%)	82,113,113	1.27	7 (8%)
25	CLA	b	610	2	69,73,73	1.33	7 (10%)	82,113,113	1.33	10 (12%)
29	LMG	C	518	-	48,48,55	0.74	0	56,56,63	1.31	7 (12%)
29	LMG	D	409	-	31,31,55	0.84	2 (6%)	33,33,63	1.28	3 (9%)
28	PL9	a	612	-	55,55,55	0.78	2 (3%)	68,69,69	1.58	11 (16%)
33	STE	M	103	-	9,9,19	0.35	0	8,8,19	0.79	0
31	SQD	a	616	-	35,35,54	1.68	5 (14%)	37,37,65	1.43	6 (16%)
25	CLA	B	614	2	69,73,73	1.38	8 (11%)	82,113,113	1.50	9 (10%)

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
33	STE	X	101	-	-	8/17/17/17	-
25	CLA	c	511	3	-	9/39/115/115	-
29	LMG	c	521	-	-	23/43/63/70	0/1/1/1
25	CLA	B	605	2	-	12/39/115/115	-
25	CLA	a	610	1	-	8/39/115/115	-
25	CLA	c	506	3	-	13/39/115/115	-
25	CLA	B	615	2	-	16/39/115/115	-
25	CLA	C	502	3	-	9/39/115/115	-
29	LMG	D	407	-	-	19/46/66/70	0/1/1/1
33	STE	M	102	-	-	6/12/12/17	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
33	STE	b	625	-	-	7/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	B	623	-	-	20/49/69/69	0/1/1/1
25	CLA	B	612	2	-	7/39/115/115	-
33	STE	b	620	-	-	8/13/13/17	-
25	CLA	b	603	2	-	7/39/115/115	-
25	CLA	b	604	2	-	7/39/115/115	-
33	STE	H	103	-	-	11/15/15/17	-
32	DGD	C	517	-	-	17/51/91/95	0/2/2/2
31	SQD	A	615	-	-	14/47/67/69	0/1/1/1
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
36	HEC	v	201	16	1/1/3/7	4/14/54/54	-
32	DGD	c	518	-	-	19/51/91/95	0/2/2/2
27	BCR	C	514	-	-	1/29/63/63	0/2/2/2
36	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	CLA	b	613	2	-	18/39/115/115	-
35	HEM	e	101	6,5	-	3/14/54/54	-
30	LHG	B	622	-	-	16/53/53/53	-
25	CLA	C	508	3	-	7/39/115/115	-
25	CLA	B	602	2	-	7/39/115/115	-
27	BCR	K	101	-	-	11/29/63/63	0/2/2/2
27	BCR	h	102	-	-	3/29/63/63	0/2/2/2
27	BCR	k	101	-	-	8/29/63/63	0/2/2/2
25	CLA	b	609	37	-	3/39/115/115	-
29	LMG	B	621	-	-	6/22/22/70	-
27	BCR	b	616	-	-	5/29/63/63	0/2/2/2
29	LMG	d	408	-	-	11/17/17/70	-
33	STE	b	626	-	-	5/7/7/17	-
29	LMG	M	101	-	-	22/46/66/70	0/1/1/1
25	CLA	B	616	2	-	12/33/109/115	-
29	LMG	c	522	-	-	24/44/64/70	0/1/1/1
25	CLA	b	601	2	-	8/39/115/115	-
33	STE	B	620	-	-	5/14/14/17	-
25	CLA	B	606	2	-	11/39/115/115	-
33	STE	J	101	-	-	3/9/9/17	-
25	CLA	C	512	3	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	612	37	-	4/39/115/115	-
33	STE	E	102	-	-	6/9/9/17	-
27	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	C	501	3	-	4/39/115/115	-
25	CLA	B	609	2	-	1/39/115/115	-
25	CLA	A	607	37	-	10/39/115/115	-
30	LHG	d	406	-	-	21/53/53/53	-
33	STE	C	519	-	-	5/9/9/17	-
27	BCR	d	404	-	-	4/29/63/63	0/2/2/2
35	HEM	F	101	6,5	-	3/14/54/54	-
25	CLA	c	508	3	-	10/38/114/115	-
25	CLA	C	504	37	-	6/32/108/115	-
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2
25	CLA	b	615	2	-	7/33/109/115	-
25	CLA	c	503	3	-	7/39/115/115	-
25	CLA	b	614	2	-	10/39/115/115	-
30	LHG	a	614	-	-	21/53/53/53	-
33	STE	b	623	-	-	6/13/13/17	-
26	PHO	a	609	-	-	6/37/103/103	0/5/6/6
25	CLA	b	602	2	-	9/39/115/115	-
25	CLA	A	609	1	-	2/26/102/115	-
25	CLA	C	505	3	-	8/39/115/115	-
33	STE	k	103	-	-	6/9/9/17	-
33	STE	x	101	-	-	11/17/17/17	-
33	STE	c	520	-	-	13/17/17/17	-
25	CLA	a	608	37	-	12/39/115/115	-
33	STE	B	625	-	-	5/9/9/17	-
25	CLA	b	611	2	-	5/39/115/115	-
25	CLA	B	604	2	-	10/39/115/115	-
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2
29	LMG	d	409	-	-	11/39/59/70	0/1/1/1
25	CLA	c	513	3	-	11/39/115/115	-
26	PHO	d	401	-	-	7/37/103/103	0/5/6/6
31	SQD	F	102	-	-	7/28/48/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	t	103	-	-	4/7/7/17	-
25	CLA	C	511	3	-	3/39/115/115	-
25	CLA	h	101	37	-	14/39/115/115	-
25	CLA	b	608	2	-	9/39/115/115	-
25	CLA	B	607	37	-	6/39/115/115	-
25	CLA	c	501	3	-	5/39/115/115	-
30	LHG	d	407	-	-	11/43/43/53	-
33	STE	a	618	-	-	5/9/9/17	-
32	DGD	c	517	-	-	19/51/91/95	0/2/2/2
25	CLA	c	512	3	-	20/39/115/115	-
25	CLA	C	506	3	-	9/39/115/115	-
30	LHG	A	614	-	-	17/51/51/53	-
31	SQD	b	619	-	-	23/44/64/69	0/1/1/1
33	STE	d	410	-	-	10/14/14/17	-
30	LHG	L	101	-	-	21/53/53/53	-
27	BCR	k	102	-	-	3/29/63/63	0/2/2/2
25	CLA	a	613	37	-	3/39/115/115	-
27	BCR	t	101	-	-	1/29/63/63	0/2/2/2
27	BCR	c	514	-	-	8/29/63/63	0/2/2/2
27	BCR	A	610	-	-	0/29/63/63	0/2/2/2
29	LMG	A	613	-	-	22/43/63/70	0/1/1/1
29	LMG	c	519	-	-	13/31/51/70	0/1/1/1
32	DGD	c	516	-	-	19/51/91/95	0/2/2/2
33	STE	B	624	-	-	8/9/9/17	-
26	PHO	A	608	-	-	2/37/103/103	0/5/6/6
25	CLA	B	611	2	-	5/39/115/115	-
25	CLA	c	510	3	-	14/39/115/115	-
25	CLA	c	505	3	-	14/39/115/115	-
25	CLA	b	606	37	-	12/39/115/115	-
33	STE	b	621	-	-	10/17/17/17	-
33	STE	t	102	-	-	4/11/11/17	-
27	BCR	a	611	-	-	1/29/63/63	0/2/2/2
30	LHG	D	408	-	-	17/53/53/53	-
25	CLA	B	601	37	-	15/39/115/115	-
30	LHG	E	101	-	-	27/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	f	101	-	-	14/36/56/69	0/1/1/1
30	LHG	e	102	-	-	24/46/46/53	-
28	PL9	d	405	-	-	6/53/73/73	0/1/1/1
33	STE	B	626	-	-	2/13/13/17	-
25	CLA	B	608	2	-	4/39/115/115	-
32	DGD	a	617	-	-	21/45/45/95	-
25	CLA	B	610	37	-	6/39/115/115	-
33	STE	I	101	-	-	5/12/12/17	-
33	STE	j	101	-	-	4/9/9/17	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2
25	CLA	d	402	4	-	6/39/115/115	-
27	BCR	K	102	-	-	6/29/63/63	0/2/2/2
25	CLA	b	612	2	-	4/39/115/115	-
33	STE	C	521	-	-	8/13/13/17	-
32	DGD	h	103	-	-	19/51/91/95	0/2/2/2
25	CLA	D	403	4	-	4/39/115/115	-
33	STE	C	520	-	-	3/9/9/17	-
25	CLA	b	607	2	-	5/39/115/115	-
25	CLA	c	507	37	-	9/39/115/115	-
31	SQD	a	615	-	-	22/49/69/69	0/1/1/1
31	SQD	A	616	-	-	20/39/39/69	-
32	DGD	C	516	-	-	17/51/91/95	0/2/2/2
25	CLA	c	504	37	-	8/33/109/115	-
25	CLA	C	510	3	-	14/39/115/115	-
25	CLA	d	403	4	-	9/39/115/115	-
27	BCR	T	101	-	-	4/29/63/63	0/2/2/2
29	LMG	b	622	-	-	33/50/70/70	0/1/1/1
30	LHG	l	101	-	-	21/53/53/53	-
25	CLA	a	607	1	-	2/39/115/115	-
27	BCR	K	103	-	-	5/29/63/63	0/2/2/2
26	PHO	D	402	-	-	0/37/103/103	0/5/6/6
33	STE	m	102	-	-	5/9/9/17	-
25	CLA	c	509	3	-	11/39/115/115	-
33	STE	t	104	-	-	7/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	613	2	-	9/39/115/115	-
25	CLA	b	605	2	-	6/39/115/115	-
25	CLA	D	404	4	-	9/39/115/115	-
32	DGD	C	515	-	-	19/51/91/95	0/2/2/2
27	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	A	606	1	-	2/39/115/115	-
27	BCR	D	405	-	-	3/29/63/63	0/2/2/2
29	LMG	m	101	-	-	20/46/66/70	0/1/1/1
33	STE	b	624	-	-	9/12/12/17	-
25	CLA	C	503	3	-	4/39/115/115	-
25	CLA	C	507	37	-	5/39/115/115	-
28	PL9	A	611	-	-	24/53/73/73	0/1/1/1
25	CLA	B	603	2	-	9/39/115/115	-
25	CLA	C	513	3	-	6/39/115/115	-
33	STE	l	102	-	-	8/15/15/17	-
25	CLA	C	509	3	-	14/39/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
32	DGD	H	102	-	-	16/51/91/95	0/2/2/2
28	PL9	D	406	-	-	13/53/73/73	0/1/1/1
25	CLA	c	502	3	-	3/39/115/115	-
25	CLA	b	610	2	-	6/39/115/115	-
29	LMG	C	518	-	-	17/43/63/70	0/1/1/1
29	LMG	D	409	-	-	20/33/33/70	-
28	PL9	a	612	-	-	15/53/73/73	0/1/1/1
33	STE	M	103	-	-	3/7/7/17	-
31	SQD	a	616	-	-	17/37/37/69	-
25	CLA	B	614	2	-	8/39/115/115	-

All (810) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	609	PHO	C1B-C2B	9.67	1.50	1.39
26	d	401	PHO	C1B-C2B	9.37	1.49	1.39
26	d	401	PHO	C3B-C4B	9.05	1.50	1.41
26	D	402	PHO	C3B-C4B	8.87	1.50	1.41
26	a	609	PHO	C3B-C4B	8.63	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	402	PHO	C1B-C2B	8.50	1.48	1.39
25	c	511	CLA	MG-NA	8.45	2.26	2.06
26	A	608	PHO	C3B-C4B	8.02	1.49	1.41
26	A	608	PHO	C1B-C2B	7.41	1.47	1.39
36	v	201	HEC	C3D-C2D	7.29	1.52	1.36
36	V	201	HEC	C3D-C2D	7.26	1.52	1.36
25	D	404	CLA	MG-NB	-6.78	1.92	2.05
25	b	605	CLA	MG-NA	6.73	2.22	2.06
25	c	510	CLA	MG-NA	6.55	2.21	2.06
25	B	606	CLA	MG-NA	6.44	2.21	2.06
25	b	603	CLA	MG-NA	6.40	2.21	2.06
25	B	616	CLA	MG-NA	6.27	2.21	2.06
25	C	512	CLA	MG-NB	6.06	2.17	2.05
25	B	614	CLA	MG-NA	5.90	2.20	2.06
25	c	503	CLA	MG-NA	5.88	2.20	2.06
25	C	511	CLA	MG-NA	5.74	2.19	2.06
35	e	101	HEM	FE-NA	5.65	2.13	1.95
25	C	501	CLA	MG-NA	5.59	2.19	2.06
31	A	616	SQD	O47-C45	-5.56	1.37	1.47
25	C	512	CLA	MG-NC	5.53	2.19	2.06
25	a	613	CLA	MG-NA	5.41	2.19	2.06
36	V	201	HEC	FE-ND	5.34	2.11	1.94
25	B	601	CLA	MG-NA	5.12	2.18	2.06
25	b	609	CLA	MG-NB	-5.11	1.95	2.05
25	b	610	CLA	MG-NA	5.11	2.18	2.06
31	a	615	SQD	O48-C23	5.09	1.48	1.33
25	C	503	CLA	MG-NC	5.08	2.18	2.06
25	B	604	CLA	MG-NC	5.07	2.18	2.06
35	e	101	HEM	FE-NB	5.02	2.10	1.94
31	b	619	SQD	O48-C23	5.00	1.47	1.33
25	h	101	CLA	MG-NA	5.00	2.18	2.06
25	c	507	CLA	MG-NA	4.99	2.18	2.06
31	B	623	SQD	O48-C23	4.93	1.47	1.33
25	C	505	CLA	MG-NA	4.92	2.18	2.06
25	A	606	CLA	MG-NA	4.87	2.17	2.06
25	b	608	CLA	MG-NA	4.82	2.17	2.06
31	A	616	SQD	O48-C23	4.81	1.47	1.33
25	C	501	CLA	MG-ND	-4.76	1.96	2.05
26	D	402	PHO	C1D-C2D	4.75	1.44	1.39
25	B	602	CLA	MG-NA	4.71	2.17	2.06
25	b	611	CLA	MG-ND	-4.70	1.96	2.05
25	b	607	CLA	MG-NA	4.70	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	513	CLA	MG-NA	4.68	2.17	2.06
31	F	102	SQD	O48-C23	4.66	1.46	1.33
25	a	607	CLA	MG-NA	4.65	2.17	2.06
26	d	401	PHO	C1D-C2D	4.64	1.44	1.39
25	D	403	CLA	MG-NA	4.64	2.17	2.06
31	f	101	SQD	O48-C23	4.61	1.46	1.33
25	D	404	CLA	MG-NC	4.58	2.17	2.06
35	F	101	HEM	FE-NC	4.58	2.10	1.95
25	B	603	CLA	MG-NA	4.57	2.17	2.06
31	A	615	SQD	O48-C23	4.53	1.46	1.33
31	a	616	SQD	O48-C23	4.49	1.46	1.33
26	a	609	PHO	C1D-C2D	4.38	1.44	1.39
25	a	610	CLA	C1D-ND	4.28	1.43	1.37
25	b	612	CLA	MG-NA	4.27	2.16	2.06
25	C	501	CLA	MG-NB	4.25	2.14	2.05
25	C	503	CLA	MG-ND	4.23	2.14	2.05
25	C	507	CLA	MG-NA	4.20	2.16	2.06
25	B	604	CLA	MG-NA	4.18	2.16	2.06
25	B	612	CLA	MG-ND	-4.13	1.97	2.05
28	d	405	PL9	C6-C1	-4.13	1.41	1.48
26	A	608	PHO	C1D-C2D	4.12	1.44	1.39
25	B	613	CLA	MG-ND	-4.12	1.97	2.05
25	B	605	CLA	MG-NA	4.12	2.16	2.06
27	c	515	BCR	C1-C6	-4.10	1.48	1.53
25	a	610	CLA	MG-ND	-4.07	1.97	2.05
25	B	607	CLA	C1D-ND	4.02	1.43	1.37
36	v	201	HEC	FE-ND	4.01	2.07	1.94
25	B	611	CLA	C1D-ND	4.01	1.43	1.37
25	b	611	CLA	C1D-ND	4.00	1.43	1.37
25	b	602	CLA	MG-NA	4.00	2.15	2.06
25	b	609	CLA	C1D-ND	3.99	1.43	1.37
25	b	614	CLA	MG-NB	3.99	2.13	2.05
25	C	509	CLA	C1D-ND	3.99	1.43	1.37
25	D	404	CLA	C1D-ND	3.97	1.43	1.37
25	B	601	CLA	C1D-ND	3.95	1.43	1.37
25	c	508	CLA	MG-NA	3.91	2.15	2.06
25	B	615	CLA	MG-NA	3.89	2.15	2.06
25	B	605	CLA	C1D-ND	3.89	1.43	1.37
25	B	613	CLA	MG-NB	3.88	2.13	2.05
25	C	501	CLA	C1D-ND	3.87	1.42	1.37
25	b	610	CLA	C1D-ND	3.86	1.42	1.37
31	A	615	SQD	O47-C45	-3.84	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	C1B-C2B	3.83	1.52	1.43
25	C	504	CLA	MG-NB	3.83	2.13	2.05
25	C	510	CLA	MG-NA	3.82	2.15	2.06
25	c	503	CLA	C1D-ND	3.81	1.42	1.37
25	B	604	CLA	C1D-ND	3.80	1.42	1.37
25	A	609	CLA	C1D-ND	3.79	1.42	1.37
25	b	613	CLA	C1D-ND	3.75	1.42	1.37
25	c	509	CLA	C1D-ND	3.74	1.42	1.37
25	B	607	CLA	MG-NA	3.74	2.15	2.06
25	c	513	CLA	C1D-ND	3.73	1.42	1.37
27	d	404	BCR	C30-C25	-3.72	1.49	1.53
25	B	602	CLA	C1D-ND	3.71	1.42	1.37
32	A	617	DGD	C4D-C3D	3.71	1.62	1.52
25	c	512	CLA	C1D-ND	3.70	1.42	1.37
31	f	101	SQD	O47-C7	3.69	1.44	1.34
25	h	101	CLA	C1D-ND	3.69	1.42	1.37
31	a	616	SQD	O47-C7	3.68	1.44	1.34
27	d	404	BCR	C1-C6	-3.66	1.49	1.53
25	B	615	CLA	MG-NB	3.65	2.13	2.05
25	B	609	CLA	C1D-ND	3.65	1.42	1.37
36	v	201	HEC	FE-NA	3.65	2.07	1.95
31	B	623	SQD	O47-C7	3.64	1.44	1.34
27	B	618	BCR	C30-C25	-3.63	1.49	1.53
25	a	607	CLA	C1B-C2B	3.63	1.51	1.43
32	H	102	DGD	O5D-C1E	3.62	1.46	1.40
25	B	606	CLA	C1D-ND	3.61	1.42	1.37
25	C	513	CLA	MG-NA	3.61	2.14	2.06
25	C	513	CLA	C1D-ND	3.60	1.42	1.37
25	C	507	CLA	MG-NB	-3.60	1.98	2.05
31	b	619	SQD	O47-C7	3.60	1.44	1.34
25	B	616	CLA	C1D-ND	3.60	1.42	1.37
25	a	610	CLA	C4B-NB	3.59	1.42	1.37
25	c	502	CLA	MG-NA	3.58	2.14	2.06
25	c	509	CLA	C1B-C2B	3.58	1.51	1.43
25	C	503	CLA	C1D-ND	3.58	1.42	1.37
25	C	507	CLA	C4B-NB	3.57	1.42	1.37
25	C	509	CLA	MG-NA	3.56	2.14	2.06
25	A	606	CLA	MG-NB	3.56	2.12	2.05
25	b	614	CLA	MG-NA	3.55	2.14	2.06
27	K	102	BCR	C1-C6	-3.55	1.49	1.53
31	A	616	SQD	O47-C7	3.55	1.44	1.34
27	k	101	BCR	C30-C25	-3.54	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	C1D-ND	3.54	1.42	1.37
25	A	612	CLA	C1D-ND	3.54	1.42	1.37
25	a	607	CLA	MG-NC	3.54	2.14	2.06
25	a	613	CLA	C1D-ND	3.53	1.42	1.37
25	C	503	CLA	MG-NA	3.53	2.14	2.06
25	b	604	CLA	C1D-ND	3.53	1.42	1.37
25	d	402	CLA	C1D-ND	3.52	1.42	1.37
27	C	514	BCR	C1-C6	-3.52	1.49	1.53
25	b	613	CLA	MG-NA	3.51	2.14	2.06
25	C	511	CLA	C1D-ND	3.51	1.42	1.37
25	c	502	CLA	C1D-ND	3.51	1.42	1.37
25	b	606	CLA	C1D-ND	3.51	1.42	1.37
25	A	606	CLA	C1D-ND	3.50	1.42	1.37
31	a	615	SQD	O47-C45	-3.49	1.38	1.46
25	C	508	CLA	MG-NA	3.49	2.14	2.06
27	B	617	BCR	C1-C6	-3.49	1.49	1.53
27	K	103	BCR	C30-C25	-3.49	1.49	1.53
25	b	603	CLA	C1D-ND	3.48	1.42	1.37
26	a	609	PHO	C4D-CHA	3.48	1.44	1.39
25	h	101	CLA	C4B-NB	3.47	1.42	1.37
25	B	614	CLA	C4B-NB	3.47	1.42	1.37
25	A	606	CLA	MG-ND	-3.47	1.98	2.05
25	c	508	CLA	C1D-ND	3.47	1.42	1.37
25	c	501	CLA	MG-ND	-3.46	1.98	2.05
25	B	609	CLA	MG-NC	3.45	2.14	2.06
25	d	403	CLA	C4B-NB	3.45	1.42	1.37
27	k	101	BCR	C1-C6	-3.43	1.49	1.53
25	C	512	CLA	C1D-ND	3.42	1.42	1.37
25	D	403	CLA	C1D-ND	3.42	1.42	1.37
25	a	607	CLA	MG-NB	3.42	2.12	2.05
25	b	613	CLA	MG-ND	-3.41	1.99	2.05
25	B	615	CLA	C1D-ND	3.41	1.42	1.37
27	K	101	BCR	C30-C25	-3.41	1.49	1.53
25	B	611	CLA	MG-NA	3.41	2.14	2.06
25	a	607	CLA	C1D-ND	3.41	1.42	1.37
25	A	607	CLA	C4B-NB	3.41	1.42	1.37
27	K	103	BCR	C1-C6	-3.41	1.49	1.53
25	c	509	CLA	MG-NA	3.41	2.14	2.06
27	D	405	BCR	C30-C25	-3.40	1.49	1.53
25	a	608	CLA	C1D-ND	3.40	1.42	1.37
25	b	603	CLA	C4B-NB	3.39	1.42	1.37
25	c	511	CLA	C1D-ND	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C1D-ND	3.38	1.42	1.37
25	B	603	CLA	C1D-ND	3.38	1.42	1.37
25	c	506	CLA	MG-NA	3.38	2.14	2.06
25	b	608	CLA	C1D-ND	3.37	1.42	1.37
25	b	612	CLA	C1D-ND	3.36	1.42	1.37
25	c	506	CLA	C1D-ND	3.36	1.42	1.37
31	A	615	SQD	C24-C23	3.35	1.60	1.50
25	b	601	CLA	C1D-ND	3.35	1.42	1.37
25	b	615	CLA	C1D-ND	3.34	1.42	1.37
31	b	619	SQD	O5-C1	3.33	1.50	1.41
25	b	613	CLA	C4B-NB	3.33	1.42	1.37
25	B	601	CLA	C4B-NB	3.32	1.42	1.37
25	c	506	CLA	MG-ND	-3.32	1.99	2.05
25	C	506	CLA	C1D-ND	3.30	1.42	1.37
25	C	501	CLA	C4B-NB	3.30	1.42	1.37
35	F	101	HEM	FE-NB	3.29	2.05	1.94
31	B	623	SQD	O47-C45	-3.28	1.38	1.46
28	D	406	PL9	C6-C1	-3.28	1.43	1.48
26	d	401	PHO	C4D-CHA	3.28	1.44	1.39
27	c	514	BCR	C1-C6	-3.26	1.49	1.53
25	C	509	CLA	C4B-NB	3.25	1.42	1.37
25	D	403	CLA	MG-NC	3.25	2.14	2.06
25	b	602	CLA	C4B-NB	3.24	1.42	1.37
25	C	510	CLA	C4B-NB	3.24	1.42	1.37
25	b	614	CLA	C1D-ND	3.23	1.42	1.37
31	a	615	SQD	O47-C7	3.23	1.43	1.34
25	A	612	CLA	MG-NB	3.22	2.12	2.05
25	a	608	CLA	MG-NC	3.22	2.13	2.06
25	c	512	CLA	MG-NB	3.22	2.12	2.05
25	b	604	CLA	C4B-NB	3.21	1.42	1.37
25	a	608	CLA	C4B-NB	3.20	1.42	1.37
25	b	610	CLA	C1B-C2B	3.20	1.50	1.43
31	F	102	SQD	C24-C23	3.20	1.60	1.50
25	c	511	CLA	C4B-NB	3.19	1.42	1.37
25	B	611	CLA	C1B-C2B	3.19	1.50	1.43
27	b	617	BCR	C30-C25	-3.19	1.49	1.53
31	a	616	SQD	O47-C45	-3.18	1.39	1.46
25	c	501	CLA	C1D-ND	3.18	1.42	1.37
25	B	607	CLA	MG-NC	3.17	2.13	2.06
25	C	506	CLA	MG-ND	-3.17	1.99	2.05
25	A	609	CLA	C4B-NB	3.17	1.42	1.37
25	c	507	CLA	MG-NB	-3.17	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	613	CLA	C4B-NB	3.16	1.42	1.37
25	a	610	CLA	C1B-C2B	3.16	1.50	1.43
26	A	608	PHO	C4D-CHA	3.16	1.44	1.39
25	B	616	CLA	C1B-C2B	3.16	1.50	1.43
25	B	602	CLA	C4B-NB	3.15	1.42	1.37
31	f	101	SQD	C24-C23	3.15	1.59	1.50
32	H	102	DGD	C6D-C5D	3.14	1.61	1.51
25	b	613	CLA	MG-NB	3.14	2.12	2.05
35	F	101	HEM	CAC-C3C	3.13	1.55	1.47
25	C	511	CLA	C4B-NB	3.13	1.42	1.37
25	C	510	CLA	C1D-ND	3.13	1.42	1.37
25	B	612	CLA	C1D-ND	3.12	1.42	1.37
32	A	617	DGD	C4D-C5D	3.12	1.59	1.53
25	c	513	CLA	MG-ND	-3.12	1.99	2.05
31	f	101	SQD	O47-C45	-3.12	1.39	1.46
25	d	402	CLA	MG-NC	3.12	2.13	2.06
32	C	515	DGD	O2G-C2G	-3.12	1.39	1.46
27	T	101	BCR	C30-C25	-3.12	1.49	1.53
27	A	610	BCR	C1-C6	-3.10	1.49	1.53
31	A	616	SQD	C24-C23	3.10	1.59	1.50
25	a	613	CLA	C1B-C2B	3.10	1.50	1.43
25	B	610	CLA	C1D-ND	3.09	1.41	1.37
25	B	614	CLA	MG-ND	-3.09	1.99	2.05
31	a	616	SQD	C24-C23	3.08	1.59	1.50
27	B	619	BCR	C1-C6	-3.08	1.49	1.53
30	L	101	LHG	O7-C5	-3.07	1.39	1.46
27	b	617	BCR	C1-C6	-3.07	1.49	1.53
32	C	516	DGD	C4D-C3D	3.06	1.60	1.52
31	B	623	SQD	O5-C1	3.06	1.49	1.41
27	k	102	BCR	C1-C6	-3.05	1.49	1.53
35	F	101	HEM	CAB-C3B	3.05	1.55	1.47
27	h	102	BCR	C30-C25	-3.05	1.49	1.53
25	b	607	CLA	CHC-C1C	3.05	1.44	1.38
25	b	601	CLA	C1B-C2B	3.04	1.50	1.43
25	b	605	CLA	C1D-ND	3.04	1.41	1.37
25	b	608	CLA	C4B-NB	3.04	1.41	1.37
31	a	615	SQD	C24-C23	3.04	1.59	1.50
25	B	610	CLA	MG-NA	3.04	2.13	2.06
29	m	101	LMG	O7-C8	-3.04	1.39	1.46
25	C	507	CLA	C1D-ND	3.04	1.41	1.37
25	B	616	CLA	MG-NB	-3.04	1.99	2.05
27	H	101	BCR	C30-C25	-3.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	C4B-NB	3.03	1.41	1.37
29	d	409	LMG	C4-C5	3.03	1.59	1.53
25	c	512	CLA	C4B-NB	3.03	1.41	1.37
25	B	607	CLA	MG-ND	-3.03	1.99	2.05
25	C	504	CLA	C1D-ND	3.03	1.41	1.37
25	c	502	CLA	C4B-NB	3.02	1.41	1.37
25	A	607	CLA	C1D-ND	3.02	1.41	1.37
25	C	513	CLA	C1B-C2B	3.02	1.50	1.43
31	a	615	SQD	O5-C1	3.02	1.49	1.41
25	C	502	CLA	C4B-NB	3.02	1.41	1.37
32	a	617	DGD	O1G-C1A	3.02	1.42	1.33
25	C	505	CLA	C4B-NB	3.01	1.41	1.37
25	B	611	CLA	C4B-NB	3.01	1.41	1.37
25	b	613	CLA	CHC-C1C	3.01	1.44	1.38
25	c	507	CLA	C1B-C2B	3.00	1.50	1.43
25	C	508	CLA	C1D-ND	3.00	1.41	1.37
27	a	611	BCR	C1-C6	-3.00	1.49	1.53
25	b	607	CLA	C1D-ND	3.00	1.41	1.37
25	B	602	CLA	C1B-C2B	3.00	1.50	1.43
25	B	610	CLA	C4B-NB	2.99	1.41	1.37
25	c	506	CLA	C1B-C2B	2.99	1.50	1.43
36	v	201	HEC	FE-NC	2.99	2.05	1.95
25	c	508	CLA	MG-ND	2.98	2.11	2.05
25	b	602	CLA	C1D-ND	2.98	1.41	1.37
25	c	509	CLA	C4B-NB	2.98	1.41	1.37
25	c	508	CLA	C4B-NB	2.97	1.41	1.37
30	B	622	LHG	O7-C5	-2.97	1.39	1.46
25	d	402	CLA	C1B-C2B	2.96	1.50	1.43
25	C	505	CLA	MG-ND	-2.96	1.99	2.05
27	B	619	BCR	C30-C25	-2.95	1.50	1.53
25	b	610	CLA	C4B-NB	2.95	1.41	1.37
25	b	605	CLA	C1B-C2B	2.95	1.50	1.43
25	c	508	CLA	C1B-C2B	2.95	1.50	1.43
25	c	501	CLA	C1B-C2B	2.95	1.50	1.43
27	D	405	BCR	C1-C6	-2.95	1.50	1.53
30	A	614	LHG	P-O6	2.94	1.70	1.59
25	C	511	CLA	C1B-C2B	2.94	1.50	1.43
25	D	404	CLA	C4B-NB	2.94	1.41	1.37
25	b	613	CLA	C3B-C4B	2.94	1.51	1.42
32	H	102	DGD	C4E-C5E	2.94	1.59	1.53
26	D	402	PHO	C4D-CHA	2.94	1.43	1.39
27	K	102	BCR	C30-C25	-2.94	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	515	BCR	C30-C25	-2.94	1.50	1.53
25	B	608	CLA	MG-NA	2.93	2.13	2.06
25	B	609	CLA	C4B-NB	2.93	1.41	1.37
27	C	514	BCR	C30-C25	-2.93	1.50	1.53
36	V	201	HEC	FE-NC	2.92	2.04	1.95
25	c	511	CLA	C1B-C2B	2.92	1.50	1.43
25	C	513	CLA	C4B-NB	2.92	1.41	1.37
27	b	618	BCR	C1-C6	-2.92	1.50	1.53
25	h	101	CLA	CHC-C1C	2.92	1.44	1.38
25	C	508	CLA	C1B-C2B	2.91	1.50	1.43
25	b	611	CLA	C4B-NB	2.91	1.41	1.37
35	F	101	HEM	FE-NA	2.91	2.04	1.95
25	A	612	CLA	MG-NA	2.90	2.13	2.06
25	c	506	CLA	C4B-NB	2.90	1.41	1.37
26	A	608	PHO	C3D-C4D	2.90	1.45	1.41
25	b	607	CLA	C4B-NB	2.90	1.41	1.37
25	B	613	CLA	C1D-ND	2.89	1.41	1.37
25	C	501	CLA	C1B-C2B	2.89	1.49	1.43
25	C	508	CLA	C4B-NB	2.89	1.41	1.37
30	E	101	LHG	P-O6	2.89	1.70	1.59
26	A	608	PHO	CMC-C2C	-2.88	1.46	1.50
25	B	601	CLA	C1B-C2B	2.88	1.49	1.43
25	C	502	CLA	C1B-C2B	2.87	1.49	1.43
31	b	619	SQD	O47-C45	-2.87	1.39	1.46
29	c	522	LMG	C4-C5	2.87	1.59	1.53
25	B	609	CLA	C1B-C2B	2.87	1.49	1.43
25	b	615	CLA	C4B-NB	2.86	1.41	1.37
32	h	103	DGD	C4D-C3D	2.86	1.59	1.52
25	h	101	CLA	C1B-C2B	2.86	1.49	1.43
31	f	101	SQD	O5-C1	2.86	1.49	1.41
25	B	614	CLA	C1D-ND	2.86	1.41	1.37
25	B	608	CLA	C1D-ND	2.85	1.41	1.37
25	b	612	CLA	C4B-NB	2.85	1.41	1.37
25	D	404	CLA	C1B-C2B	2.85	1.49	1.43
25	c	508	CLA	CHC-C1C	2.85	1.44	1.38
25	a	607	CLA	C4B-NB	2.85	1.41	1.37
27	c	514	BCR	C30-C25	-2.85	1.50	1.53
25	a	608	CLA	CHC-C1C	2.85	1.44	1.38
25	B	615	CLA	C1B-C2B	2.85	1.49	1.43
25	c	504	CLA	C4B-NB	2.85	1.41	1.37
25	d	403	CLA	C1D-ND	2.85	1.41	1.37
25	B	613	CLA	C4B-NB	2.84	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	505	CLA	C1D-ND	2.84	1.41	1.37
31	b	619	SQD	C24-C23	2.84	1.58	1.50
25	a	613	CLA	MG-NC	2.84	2.13	2.06
25	C	510	CLA	C1B-C2B	2.84	1.49	1.43
25	B	606	CLA	C1B-C2B	2.84	1.49	1.43
25	b	601	CLA	MG-ND	2.83	2.11	2.05
25	d	403	CLA	MG-NB	-2.83	2.00	2.05
25	B	613	CLA	C1B-C2B	2.83	1.49	1.43
31	A	615	SQD	O47-C7	2.83	1.42	1.34
25	c	510	CLA	C1D-ND	2.83	1.41	1.37
29	c	521	LMG	C4-C3	2.82	1.59	1.52
25	c	511	CLA	CHC-C1C	2.82	1.44	1.38
25	b	604	CLA	C1B-C2B	2.81	1.49	1.43
35	e	101	HEM	CAC-C3C	2.80	1.54	1.47
25	b	606	CLA	C4B-NB	2.80	1.41	1.37
31	A	615	SQD	O5-C1	2.79	1.49	1.41
29	c	521	LMG	C3-C2	2.79	1.59	1.52
25	b	612	CLA	C1B-C2B	2.79	1.49	1.43
29	c	519	LMG	C4-C5	2.79	1.59	1.53
25	B	603	CLA	C1B-C2B	2.78	1.49	1.43
31	F	102	SQD	O5-C1	2.78	1.49	1.41
25	B	614	CLA	C1B-C2B	2.78	1.49	1.43
25	b	609	CLA	C1B-C2B	2.78	1.49	1.43
27	K	101	BCR	C1-C6	-2.77	1.50	1.53
25	b	614	CLA	C1B-C2B	2.77	1.49	1.43
25	d	403	CLA	MG-NA	2.77	2.12	2.06
25	C	508	CLA	C3B-C4B	2.77	1.50	1.42
25	C	507	CLA	C1B-C2B	2.76	1.49	1.43
25	C	505	CLA	CHC-C1C	2.76	1.44	1.38
25	C	503	CLA	C3B-C4B	2.76	1.50	1.42
25	b	611	CLA	C1B-C2B	2.75	1.49	1.43
25	C	504	CLA	C3B-C4B	2.75	1.50	1.42
25	C	511	CLA	C3B-C4B	2.74	1.50	1.42
25	c	502	CLA	C1B-C2B	2.74	1.49	1.43
25	B	612	CLA	C4B-NB	2.74	1.41	1.37
32	C	515	DGD	C4E-C3E	2.73	1.59	1.52
25	A	612	CLA	C1B-C2B	2.73	1.49	1.43
25	B	609	CLA	MG-NA	2.72	2.12	2.06
25	B	610	CLA	C1B-C2B	2.72	1.49	1.43
25	B	604	CLA	C4B-NB	2.72	1.41	1.37
25	B	608	CLA	C1B-C2B	2.72	1.49	1.43
25	b	606	CLA	C1B-C2B	2.71	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	505	CLA	C1D-ND	2.71	1.41	1.37
25	c	506	CLA	CHC-C1C	2.71	1.43	1.38
25	c	512	CLA	CHC-C1C	2.71	1.43	1.38
26	D	402	PHO	C3D-C4D	2.70	1.44	1.41
30	D	408	LHG	O7-C5	-2.70	1.40	1.46
32	c	518	DGD	C4D-C5D	2.70	1.58	1.53
25	b	610	CLA	CHC-C1C	2.70	1.43	1.38
25	c	513	CLA	C4B-NB	2.69	1.41	1.37
25	c	505	CLA	C1B-C2B	2.69	1.49	1.43
28	d	405	PL9	C3-C4	-2.69	1.45	1.49
25	c	510	CLA	C1B-C2B	2.69	1.49	1.43
25	c	501	CLA	MG-NA	2.69	2.12	2.06
32	c	516	DGD	C4E-C3E	2.68	1.59	1.52
25	c	505	CLA	C4B-NB	2.68	1.41	1.37
35	e	101	HEM	CAB-C3B	2.68	1.54	1.47
25	b	613	CLA	C1B-C2B	2.68	1.49	1.43
25	B	608	CLA	C4B-NB	2.68	1.41	1.37
25	c	512	CLA	C1B-C2B	2.67	1.49	1.43
25	d	403	CLA	C1B-C2B	2.67	1.49	1.43
26	d	401	PHO	CMD-C2D	-2.66	1.46	1.51
25	C	509	CLA	C1B-C2B	2.66	1.49	1.43
25	B	616	CLA	C4B-NB	2.66	1.41	1.37
25	c	513	CLA	C3B-C4B	2.66	1.50	1.42
29	b	622	LMG	C4-C3	2.66	1.59	1.52
25	b	601	CLA	C4B-NB	2.66	1.41	1.37
25	B	604	CLA	C1B-C2B	2.66	1.49	1.43
25	C	508	CLA	MG-NB	2.66	2.11	2.05
25	D	403	CLA	C1B-C2B	2.65	1.49	1.43
32	c	518	DGD	O2G-C2G	-2.64	1.40	1.46
31	A	616	SQD	C46-C45	2.64	1.56	1.50
25	C	503	CLA	C4B-NB	2.64	1.41	1.37
25	C	501	CLA	CHC-C1C	2.64	1.43	1.38
25	b	615	CLA	MG-NA	2.63	2.12	2.06
25	A	606	CLA	C1B-C2B	2.63	1.49	1.43
31	B	623	SQD	C24-C23	2.63	1.58	1.50
30	e	102	LHG	P-O6	2.62	1.69	1.59
25	B	616	CLA	MG-ND	2.62	2.11	2.05
25	C	505	CLA	C1B-C2B	2.62	1.49	1.43
27	b	616	BCR	C1-C6	-2.62	1.50	1.53
25	c	505	CLA	MG-NA	2.61	2.12	2.06
25	C	512	CLA	MG-ND	-2.61	2.00	2.05
25	b	615	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	510	CLA	CHC-C1C	2.61	1.43	1.38
29	A	613	LMG	C1-C2	2.60	1.60	1.52
25	c	503	CLA	C4B-NB	2.60	1.41	1.37
25	b	604	CLA	CHC-C1C	2.59	1.43	1.38
25	c	508	CLA	C3B-C4B	2.59	1.50	1.42
25	C	503	CLA	C1B-C2B	2.59	1.49	1.43
27	B	617	BCR	C30-C25	-2.59	1.50	1.53
25	a	613	CLA	CHC-C1C	2.58	1.43	1.38
25	B	612	CLA	C1B-C2B	2.58	1.49	1.43
25	C	512	CLA	C1B-C2B	2.58	1.49	1.43
25	C	503	CLA	CHC-C1C	2.58	1.43	1.38
25	b	608	CLA	MG-ND	-2.57	2.00	2.05
25	B	606	CLA	CHC-C1C	2.57	1.43	1.38
25	c	513	CLA	C1B-C2B	2.56	1.49	1.43
25	c	501	CLA	C4B-NB	2.56	1.41	1.37
30	d	406	LHG	O8-C6	-2.56	1.39	1.45
25	c	511	CLA	C3B-C4B	2.56	1.50	1.42
29	D	409	LMG	C7-C8	2.56	1.57	1.51
29	c	522	LMG	C3-C2	2.55	1.59	1.52
32	C	516	DGD	O2G-C2G	-2.55	1.40	1.46
25	D	404	CLA	C3B-C4B	2.55	1.50	1.42
25	c	504	CLA	C1B-C2B	2.54	1.49	1.43
25	c	503	CLA	C1B-C2B	2.54	1.49	1.43
29	D	409	LMG	C9-C8	2.54	1.58	1.50
25	A	607	CLA	C1B-C2B	2.54	1.49	1.43
25	b	607	CLA	C3B-C4B	2.54	1.50	1.42
25	b	603	CLA	C1B-C2B	2.53	1.49	1.43
25	C	502	CLA	CMC-C2C	-2.53	1.45	1.50
25	b	611	CLA	CHC-C1C	2.53	1.43	1.38
28	d	405	PL9	C31-C29	-2.53	1.46	1.51
29	M	101	LMG	O7-C8	-2.53	1.40	1.46
32	C	516	DGD	C4E-C3E	2.52	1.58	1.52
25	C	501	CLA	C3B-C4B	2.52	1.50	1.42
27	t	101	BCR	C30-C25	-2.52	1.50	1.53
25	h	101	CLA	C3B-C4B	2.51	1.50	1.42
25	b	614	CLA	C4B-NB	2.51	1.41	1.37
32	C	516	DGD	C1G-C2G	2.51	1.58	1.50
25	B	615	CLA	C4B-NB	2.51	1.41	1.37
27	T	101	BCR	C1-C6	-2.50	1.50	1.53
25	b	605	CLA	C4B-NB	2.50	1.41	1.37
25	C	508	CLA	MG-ND	2.50	2.10	2.05
25	C	508	CLA	MG-NC	2.50	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C3B-C4B	2.50	1.50	1.42
25	c	512	CLA	C3B-C4B	2.50	1.50	1.42
25	D	403	CLA	C4B-NB	2.50	1.41	1.37
25	C	510	CLA	C3B-C4B	2.50	1.50	1.42
36	V	201	HEC	CMB-C2B	2.49	1.55	1.50
25	b	611	CLA	C3B-C4B	2.49	1.50	1.42
26	a	609	PHO	C4D-ND	-2.49	1.34	1.38
26	D	402	PHO	CMB-C2B	-2.49	1.46	1.51
25	c	502	CLA	MG-NB	-2.49	2.00	2.05
27	H	101	BCR	C1-C6	-2.49	1.50	1.53
25	C	511	CLA	CHC-C1C	2.49	1.43	1.38
25	b	606	CLA	MG-NC	2.48	2.12	2.06
25	A	606	CLA	CHC-C1C	2.48	1.43	1.38
32	H	102	DGD	C1E-C2E	2.48	1.59	1.52
25	B	610	CLA	C3B-C4B	2.48	1.49	1.42
25	c	501	CLA	CHC-C1C	2.48	1.43	1.38
25	C	502	CLA	C3B-C4B	2.48	1.49	1.42
25	c	509	CLA	MG-NB	-2.47	2.00	2.05
25	A	607	CLA	CHC-C1C	2.47	1.43	1.38
25	C	512	CLA	CMD-C2D	-2.47	1.45	1.50
25	c	504	CLA	CHC-C1C	2.47	1.43	1.38
25	B	614	CLA	MG-NB	2.47	2.10	2.05
25	B	610	CLA	MG-ND	-2.46	2.00	2.05
25	B	610	CLA	CMB-C2B	-2.46	1.45	1.50
30	d	406	LHG	O7-C5	-2.46	1.40	1.46
25	C	508	CLA	CHC-C1C	2.46	1.43	1.38
32	h	103	DGD	C1E-C2E	2.46	1.59	1.52
25	b	604	CLA	C3B-C4B	2.46	1.49	1.42
25	C	513	CLA	MG-NC	2.46	2.12	2.06
25	c	504	CLA	C1D-ND	2.45	1.41	1.37
30	d	407	LHG	P-O6	2.45	1.69	1.59
26	a	609	PHO	C3D-C4D	2.45	1.44	1.41
26	A	608	PHO	CMD-C2D	-2.45	1.46	1.51
25	A	612	CLA	C3B-C4B	2.45	1.49	1.42
27	k	102	BCR	C30-C25	-2.45	1.50	1.53
29	m	101	LMG	O1-C7	-2.45	1.39	1.43
32	c	517	DGD	C3E-C2E	2.45	1.58	1.52
25	C	512	CLA	C3B-C4B	2.45	1.49	1.42
25	a	608	CLA	C1B-C2B	2.44	1.48	1.43
26	a	609	PHO	CMC-C2C	-2.44	1.46	1.50
25	D	404	CLA	MG-NA	2.44	2.12	2.06
25	C	506	CLA	C4B-NB	2.43	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	505	CLA	C3B-C4B	2.43	1.49	1.42
25	c	507	CLA	C4B-NB	2.42	1.41	1.37
25	d	402	CLA	C4B-NB	2.42	1.41	1.37
30	a	614	LHG	P-O6	2.42	1.68	1.59
25	B	601	CLA	MG-ND	-2.42	2.01	2.05
32	C	515	DGD	C3E-C2E	2.42	1.58	1.52
30	a	614	LHG	O7-C5	-2.42	1.40	1.46
25	B	611	CLA	CHC-C1C	2.42	1.43	1.38
25	b	613	CLA	CMC-C2C	-2.42	1.45	1.50
30	A	614	LHG	O3-C3	-2.42	1.35	1.44
25	B	601	CLA	C3B-C4B	2.41	1.49	1.42
28	A	611	PL9	C53-C6	-2.41	1.45	1.50
25	b	608	CLA	C1B-C2B	2.40	1.48	1.43
25	B	611	CLA	C3B-C4B	2.40	1.49	1.42
30	E	101	LHG	O7-C5	-2.40	1.41	1.46
25	B	603	CLA	C4B-NB	2.40	1.41	1.37
29	m	101	LMG	C4-C3	2.39	1.58	1.52
30	D	408	LHG	P-O6	2.39	1.68	1.59
25	B	612	CLA	C3B-C4B	2.39	1.49	1.42
25	c	507	CLA	MG-ND	2.39	2.10	2.05
25	B	610	CLA	MG-NB	-2.39	2.01	2.05
25	D	403	CLA	CHC-C1C	2.39	1.43	1.38
25	c	506	CLA	MG-NC	2.39	2.11	2.06
25	A	609	CLA	C1B-C2B	2.39	1.48	1.43
28	a	612	PL9	C7-C3	-2.39	1.48	1.51
25	B	604	CLA	C3B-C4B	2.38	1.49	1.42
29	c	522	LMG	C4-C3	2.38	1.58	1.52
29	M	101	LMG	O1-C7	-2.37	1.39	1.43
25	C	504	CLA	C1B-C2B	2.37	1.48	1.43
25	C	507	CLA	CHC-C1C	2.37	1.43	1.38
27	B	618	BCR	C1-C6	-2.37	1.50	1.53
32	C	515	DGD	C3G-C2G	2.37	1.58	1.50
25	c	507	CLA	CHC-C1C	2.37	1.43	1.38
26	A	608	PHO	C4D-ND	-2.37	1.35	1.38
25	B	603	CLA	C3B-C4B	2.36	1.49	1.42
25	d	403	CLA	CHC-C1C	2.36	1.43	1.38
25	B	607	CLA	C1B-C2B	2.36	1.48	1.43
25	a	610	CLA	C3B-C4B	2.36	1.49	1.42
27	b	616	BCR	C30-C25	-2.36	1.50	1.53
25	b	614	CLA	C3B-C4B	2.35	1.49	1.42
25	C	506	CLA	C3B-C4B	2.35	1.49	1.42
31	f	101	SQD	O9-S	2.35	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	501	CLA	MG-NC	2.35	2.11	2.06
26	a	609	PHO	CMB-C2B	-2.35	1.46	1.51
31	b	619	SQD	O9-S	2.35	1.51	1.45
25	C	512	CLA	C4B-NB	2.35	1.40	1.37
25	b	601	CLA	CHC-C1C	2.34	1.43	1.38
25	C	509	CLA	C3B-C4B	2.34	1.49	1.42
25	a	607	CLA	C3B-C4B	2.34	1.49	1.42
32	c	516	DGD	C3G-C2G	2.34	1.58	1.50
25	B	605	CLA	MG-NB	2.34	2.10	2.05
25	c	503	CLA	MG-NC	2.34	2.11	2.06
25	A	612	CLA	CHC-C1C	2.33	1.43	1.38
25	b	602	CLA	CMD-C2D	-2.33	1.46	1.50
25	b	614	CLA	CMD-C2D	-2.33	1.46	1.50
27	a	611	BCR	C30-C25	-2.33	1.50	1.53
32	h	103	DGD	C6D-C5D	2.33	1.58	1.51
25	B	615	CLA	CHC-C1C	2.32	1.43	1.38
25	A	607	CLA	C3B-C4B	2.32	1.49	1.42
25	b	610	CLA	C3B-C4B	2.32	1.49	1.42
25	b	602	CLA	C3B-C4B	2.31	1.49	1.42
27	B	617	BCR	C33-C5	-2.31	1.47	1.50
25	b	609	CLA	C4B-NB	2.31	1.40	1.37
25	b	602	CLA	C1B-C2B	2.31	1.48	1.43
29	c	522	LMG	O8-C9	-2.30	1.40	1.45
25	a	610	CLA	CMC-C2C	-2.30	1.46	1.50
26	D	402	PHO	CMD-C2D	-2.30	1.47	1.51
32	C	516	DGD	C1E-C2E	2.30	1.59	1.52
25	c	506	CLA	C3B-C4B	2.30	1.49	1.42
25	b	601	CLA	C3B-C4B	2.30	1.49	1.42
25	B	613	CLA	C3B-C4B	2.29	1.49	1.42
28	D	406	PL9	C26-C24	-2.29	1.46	1.51
25	B	606	CLA	C4B-NB	2.29	1.40	1.37
30	a	614	LHG	C24-C23	2.28	1.57	1.50
35	e	101	HEM	CMC-C2C	2.28	1.55	1.50
25	c	512	CLA	MG-ND	-2.28	2.01	2.05
31	f	101	SQD	O7-S	2.28	1.51	1.45
25	a	608	CLA	C3B-C4B	2.28	1.49	1.42
27	b	618	BCR	C30-C25	-2.27	1.50	1.53
25	c	510	CLA	CMB-C2B	-2.27	1.46	1.50
29	M	101	LMG	O8-C9	-2.27	1.40	1.45
25	b	606	CLA	MG-NA	2.27	2.11	2.06
29	d	409	LMG	C7-C8	2.27	1.57	1.50
25	B	612	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	615	SQD	O7-S	2.26	1.51	1.45
29	c	519	LMG	C1-C2	2.26	1.59	1.52
36	V	201	HEC	CMC-C2C	2.26	1.55	1.50
25	B	605	CLA	C4B-NB	2.25	1.40	1.37
25	C	504	CLA	CHC-C1C	2.25	1.43	1.38
25	C	504	CLA	CMD-C2D	-2.25	1.46	1.50
32	A	617	DGD	C6E-C5E	2.24	1.59	1.51
26	D	402	PHO	CMC-C2C	-2.24	1.47	1.50
31	B	623	SQD	O9-S	2.24	1.51	1.45
25	b	612	CLA	CMB-C2B	-2.24	1.46	1.50
32	A	617	DGD	O1G-C1G	-2.24	1.40	1.45
26	d	401	PHO	C3D-C4D	2.24	1.44	1.41
32	H	102	DGD	O2G-C2G	-2.24	1.41	1.46
26	d	401	PHO	CMC-C2C	-2.24	1.47	1.50
25	c	503	CLA	CHC-C1C	2.24	1.43	1.38
31	a	616	SQD	C44-C45	2.24	1.56	1.51
36	V	201	HEC	CAC-C3C	2.23	1.56	1.51
25	c	512	CLA	CMB-C2B	-2.23	1.46	1.50
25	C	513	CLA	C3B-C4B	2.23	1.49	1.42
25	d	402	CLA	C3B-C4B	2.23	1.49	1.42
25	C	506	CLA	CHC-C1C	2.23	1.43	1.38
25	C	509	CLA	CMC-C2C	-2.23	1.46	1.50
32	A	617	DGD	O2G-C2G	-2.23	1.41	1.46
25	a	607	CLA	CHC-C1C	2.22	1.42	1.38
25	c	505	CLA	CHC-C1C	2.22	1.42	1.38
25	C	512	CLA	CHC-C1C	2.22	1.42	1.38
25	C	512	CLA	CMB-C2B	-2.22	1.46	1.50
25	h	101	CLA	CMC-C2C	-2.22	1.46	1.50
25	b	611	CLA	CMC-C2C	-2.22	1.46	1.50
25	A	612	CLA	C1D-C2D	2.22	1.49	1.45
25	B	608	CLA	CMD-C2D	-2.22	1.46	1.50
25	c	512	CLA	C1D-C2D	2.22	1.49	1.45
32	H	102	DGD	C4E-C3E	2.22	1.58	1.52
36	v	201	HEC	CMA-C3A	2.22	1.55	1.50
25	B	605	CLA	C3B-C4B	2.22	1.49	1.42
25	b	607	CLA	C1B-C2B	2.22	1.48	1.43
25	b	603	CLA	C3B-C4B	2.22	1.49	1.42
29	d	409	LMG	O7-C8	-2.21	1.41	1.46
29	D	407	LMG	C4-C5	2.21	1.57	1.53
32	A	617	DGD	C3G-C2G	2.21	1.57	1.50
31	F	102	SQD	O9-S	2.21	1.51	1.45
25	b	604	CLA	C3D-C4D	2.20	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	501	CLA	C1D-C2D	2.20	1.49	1.45
25	B	608	CLA	CMC-C2C	-2.20	1.46	1.50
25	B	606	CLA	C3B-C4B	2.20	1.49	1.42
25	B	603	CLA	CMC-C2C	-2.20	1.46	1.50
25	b	608	CLA	C3B-C4B	2.20	1.49	1.42
25	B	610	CLA	CHC-C1C	2.20	1.42	1.38
25	b	606	CLA	C3B-C4B	2.19	1.49	1.42
32	c	516	DGD	O2G-C2G	-2.19	1.41	1.46
25	B	615	CLA	C3B-C4B	2.19	1.49	1.42
32	C	515	DGD	C4E-C5E	2.19	1.57	1.53
25	d	402	CLA	CMD-C2D	-2.19	1.46	1.50
25	B	614	CLA	MG-NC	2.19	2.11	2.06
25	D	403	CLA	C3B-C4B	2.19	1.49	1.42
32	C	517	DGD	O2G-C2G	-2.18	1.41	1.46
25	D	404	CLA	CMD-C2D	-2.18	1.46	1.50
25	C	506	CLA	C1B-C2B	2.18	1.48	1.43
25	b	612	CLA	MG-NB	-2.18	2.01	2.05
25	C	507	CLA	C3B-C4B	2.18	1.49	1.42
25	B	601	CLA	MG-NB	-2.18	2.01	2.05
25	B	602	CLA	C3B-C4B	2.18	1.49	1.42
25	B	614	CLA	CHC-C1C	2.18	1.42	1.38
30	A	614	LHG	O7-C7	2.18	1.40	1.34
31	B	623	SQD	O7-S	2.18	1.51	1.45
25	B	608	CLA	CHC-C1C	2.17	1.42	1.38
25	B	604	CLA	CHC-C1C	2.17	1.42	1.38
25	b	605	CLA	C3B-C4B	2.17	1.49	1.42
25	c	509	CLA	C3B-C4B	2.17	1.49	1.42
35	e	101	HEM	CMA-C3A	2.17	1.55	1.50
25	a	607	CLA	MG-ND	-2.17	2.01	2.05
25	B	605	CLA	CHC-C1C	2.17	1.42	1.38
25	B	608	CLA	C3B-C4B	2.17	1.49	1.42
25	b	602	CLA	CMB-C2B	-2.17	1.46	1.50
32	a	617	DGD	O2G-C1B	2.17	1.40	1.34
26	D	402	PHO	CAC-C3C	-2.16	1.47	1.51
32	c	516	DGD	C4D-C3D	2.16	1.58	1.52
25	B	606	CLA	MG-NB	2.16	2.10	2.05
25	c	511	CLA	CMD-C2D	-2.16	1.46	1.50
25	A	606	CLA	C3B-C4B	2.16	1.49	1.42
25	A	607	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	611	CLA	MG-NC	2.16	2.11	2.06
25	c	507	CLA	C3D-C4D	2.16	1.49	1.44
26	d	401	PHO	CAC-C3C	-2.15	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	101	HEM	CMD-C2D	2.15	1.55	1.50
25	c	511	CLA	MG-NB	2.15	2.10	2.05
25	c	501	CLA	C3B-C4B	2.15	1.49	1.42
25	B	607	CLA	C3B-C4B	2.15	1.49	1.42
25	B	605	CLA	C1B-NB	-2.14	1.35	1.37
31	b	619	SQD	C46-C45	2.14	1.57	1.50
25	A	606	CLA	CMC-C2C	-2.14	1.46	1.50
25	c	503	CLA	C3B-C4B	2.14	1.49	1.42
25	B	602	CLA	MG-NB	-2.14	2.01	2.05
25	C	502	CLA	CHC-C1C	2.13	1.42	1.38
25	D	403	CLA	CMC-C2C	-2.13	1.46	1.50
25	A	609	CLA	CHC-C1C	2.13	1.42	1.38
25	b	609	CLA	CMD-C2D	-2.13	1.46	1.50
25	B	616	CLA	CMC-C2C	-2.13	1.46	1.50
25	B	616	CLA	CHC-C1C	2.13	1.42	1.38
25	C	501	CLA	CMD-C2D	-2.13	1.46	1.50
25	b	610	CLA	MG-NC	2.13	2.11	2.06
25	B	603	CLA	CHC-C1C	2.13	1.42	1.38
25	b	604	CLA	MG-NB	2.13	2.10	2.05
25	C	509	CLA	MG-ND	-2.13	2.01	2.05
36	v	201	HEC	CMD-C2D	2.13	1.55	1.50
25	b	606	CLA	CMD-C2D	-2.13	1.46	1.50
32	a	617	DGD	C1G-C2G	2.12	1.57	1.50
25	c	510	CLA	CHC-C1C	2.12	1.42	1.38
25	c	501	CLA	CMC-C2C	-2.12	1.46	1.50
25	B	601	CLA	CMB-C2B	-2.12	1.46	1.50
25	c	505	CLA	CMB-C2B	-2.12	1.46	1.50
31	F	102	SQD	O5-C5	2.12	1.49	1.44
25	A	612	CLA	C4B-NB	2.12	1.40	1.37
25	d	403	CLA	C3B-C4B	2.11	1.48	1.42
25	C	513	CLA	CHC-C1C	2.11	1.42	1.38
25	c	502	CLA	C3B-C4B	2.11	1.48	1.42
25	c	503	CLA	CMC-C2C	-2.11	1.46	1.50
25	b	614	CLA	CHC-C1C	2.11	1.42	1.38
25	c	513	CLA	CHC-C1C	2.11	1.42	1.38
25	C	509	CLA	CMB-C2B	-2.11	1.46	1.50
29	A	613	LMG	O1-C1	2.11	1.43	1.40
25	b	602	CLA	CMC-C2C	-2.11	1.46	1.50
32	c	517	DGD	C1E-C2E	2.11	1.58	1.52
27	D	405	BCR	C38-C26	-2.10	1.47	1.50
35	F	101	HEM	C2A-C3A	-2.10	1.33	1.38
25	B	615	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	502	CLA	MG-ND	-2.10	2.01	2.05
25	c	507	CLA	CMC-C2C	-2.10	1.46	1.50
26	a	609	PHO	CMD-C2D	-2.10	1.47	1.51
36	V	201	HEC	FE-NB	2.10	2.01	1.94
25	b	603	CLA	MG-NB	-2.10	2.01	2.05
26	D	402	PHO	O2D-CGD	2.10	1.38	1.33
32	H	102	DGD	C4D-C5D	2.10	1.57	1.53
25	B	606	CLA	CMD-C2D	-2.10	1.46	1.50
25	b	603	CLA	CHC-C1C	2.09	1.42	1.38
25	c	502	CLA	CMC-C2C	-2.09	1.46	1.50
31	F	102	SQD	O7-S	2.09	1.51	1.45
25	b	607	CLA	CMB-C2B	-2.09	1.46	1.50
29	c	521	LMG	C1-C2	2.09	1.58	1.52
31	A	615	SQD	C8-C7	2.08	1.56	1.50
25	D	404	CLA	CMB-C2B	-2.08	1.46	1.50
32	C	517	DGD	C6D-C5D	2.08	1.57	1.51
35	F	101	HEM	CMC-C2C	2.08	1.55	1.50
25	C	507	CLA	CMD-C2D	-2.08	1.46	1.50
25	C	509	CLA	CHC-C1C	2.08	1.42	1.38
25	c	508	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	601	CLA	C1D-C2D	2.08	1.49	1.45
25	c	506	CLA	MG-NB	2.08	2.09	2.05
25	C	510	CLA	CMD-C2D	-2.08	1.46	1.50
25	D	403	CLA	CMD-C2D	-2.08	1.46	1.50
28	a	612	PL9	C53-C6	-2.07	1.46	1.50
25	C	509	CLA	C3D-C4D	2.07	1.48	1.44
25	B	615	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	510	CLA	C4B-NB	2.07	1.40	1.37
25	B	613	CLA	CHC-C1C	2.07	1.42	1.38
25	d	402	CLA	CHC-C1C	2.07	1.42	1.38
27	b	616	BCR	C33-C5	-2.07	1.47	1.50
25	c	509	CLA	CMD-C2D	-2.07	1.46	1.50
25	C	503	CLA	CMD-C2D	-2.06	1.46	1.50
25	C	511	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	608	CLA	CMC-C2C	-2.06	1.46	1.50
25	c	507	CLA	C3B-C4B	2.06	1.48	1.42
27	h	102	BCR	C1-C6	-2.06	1.51	1.53
31	f	101	SQD	O5-C5	2.06	1.49	1.44
25	B	602	CLA	CHC-C1C	2.06	1.42	1.38
25	b	612	CLA	CMD-C2D	-2.06	1.46	1.50
25	b	601	CLA	CMD-C2D	-2.06	1.46	1.50
31	b	619	SQD	O5-C5	2.06	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	CLA	C3D-C4D	2.06	1.48	1.44
25	c	509	CLA	MG-ND	-2.05	2.01	2.05
25	C	502	CLA	MG-NB	-2.05	2.01	2.05
31	b	619	SQD	O7-S	2.05	1.50	1.45
35	F	101	HEM	CMB-C2B	2.05	1.55	1.50
27	k	102	BCR	C38-C26	-2.05	1.47	1.50
25	b	612	CLA	C3B-C4B	2.05	1.48	1.42
25	b	603	CLA	C3D-C4D	2.05	1.48	1.44
25	B	601	CLA	C3D-C4D	2.05	1.48	1.44
25	c	512	CLA	C3D-C4D	2.05	1.48	1.44
25	b	601	CLA	C1D-C2D	2.05	1.49	1.45
25	C	511	CLA	CMB-C2B	-2.05	1.46	1.50
25	A	609	CLA	CMD-C2D	-2.04	1.46	1.50
25	B	610	CLA	C1D-C2D	2.04	1.49	1.45
26	A	608	PHO	CMB-C2B	-2.04	1.47	1.51
25	C	509	CLA	O2D-CGD	2.04	1.38	1.33
25	C	502	CLA	CMB-C2B	-2.04	1.46	1.50
25	C	502	CLA	MG-NC	2.04	2.11	2.06
29	B	621	LMG	O8-C28	2.04	1.37	1.30
25	D	404	CLA	C3D-C4D	2.04	1.48	1.44
25	C	513	CLA	CMC-C2C	-2.04	1.46	1.50
35	e	101	HEM	C2A-C3A	-2.04	1.33	1.38
25	c	503	CLA	CMD-C2D	-2.04	1.46	1.50
25	C	505	CLA	C3B-C4B	2.03	1.48	1.42
31	a	615	SQD	O9-S	2.03	1.50	1.45
25	c	509	CLA	CMB-C2B	-2.03	1.46	1.50
25	c	502	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	609	CLA	C3B-C4B	2.03	1.48	1.42
25	B	601	CLA	CHC-C1C	2.03	1.42	1.38
25	h	101	CLA	O2A-CGA	2.03	1.39	1.33
25	A	609	CLA	MG-ND	-2.02	2.01	2.05
25	c	510	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	604	CLA	MG-NC	2.02	2.11	2.06
31	B	623	SQD	C46-C45	2.02	1.57	1.50
25	b	615	CLA	CMD-C2D	-2.02	1.46	1.50
25	A	606	CLA	CMD-C2D	-2.02	1.46	1.50
25	a	607	CLA	CMB-C2B	-2.02	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	609	CLA	C3B-C4B	2.02	1.48	1.42
35	F	101	HEM	CMA-C3A	2.02	1.54	1.50
25	b	614	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	603	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	C4C-NC	2.01	1.43	1.37
25	b	608	CLA	O2D-CGD	2.01	1.38	1.33
25	C	504	CLA	CMB-C2B	-2.00	1.46	1.50
25	b	611	CLA	CMB-C2B	-2.00	1.46	1.50
25	B	616	CLA	C3B-C4B	2.00	1.48	1.42
25	h	101	CLA	C1D-C2D	2.00	1.49	1.45
32	H	102	DGD	C1G-C2G	2.00	1.57	1.50

All (1080) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	604	CLA	C4A-NA-C1A	9.04	110.80	106.68
25	C	511	CLA	C4A-NA-C1A	8.55	110.58	106.68
25	c	511	CLA	C4A-NA-C1A	8.52	110.57	106.68
25	b	605	CLA	C4A-NA-C1A	8.36	110.49	106.68
25	C	508	CLA	C4A-NA-C1A	8.18	110.41	106.68
25	C	503	CLA	C4A-NA-C1A	7.95	110.31	106.68
25	B	606	CLA	C4A-NA-C1A	7.90	110.28	106.68
25	c	507	CLA	C4A-NA-C1A	7.89	110.28	106.68
25	C	513	CLA	C4A-NA-C1A	7.78	110.23	106.68
25	b	604	CLA	C4A-NA-C1A	7.77	110.22	106.68
25	c	509	CLA	C4A-NA-C1A	7.66	110.17	106.68
25	B	614	CLA	C4A-NA-C1A	7.54	110.12	106.68
25	b	603	CLA	C4A-NA-C1A	7.40	110.06	106.68
25	h	101	CLA	C4A-NA-C1A	7.28	110.00	106.68
25	C	507	CLA	C4A-NA-C1A	7.26	109.99	106.68
25	a	613	CLA	C4A-NA-C1A	7.23	109.98	106.68
25	b	601	CLA	C4A-NA-C1A	7.22	109.97	106.68
25	B	616	CLA	C4A-NA-C1A	7.19	109.96	106.68
25	c	503	CLA	C4A-NA-C1A	7.17	109.95	106.68
25	B	607	CLA	C4A-NA-C1A	7.11	109.92	106.68
25	b	614	CLA	C4A-NA-C1A	7.09	109.91	106.68
25	c	501	CLA	C4A-NA-C1A	7.06	109.90	106.68
25	B	605	CLA	C4A-NA-C1A	6.93	109.84	106.68
25	a	607	CLA	C4A-NA-C1A	6.81	109.79	106.68
26	a	609	PHO	C4D-CHA-CBD	-6.76	105.21	108.45
25	C	510	CLA	C4A-NA-C1A	6.76	109.76	106.68
25	B	608	CLA	C4A-NA-C1A	6.72	109.74	106.68
25	c	510	CLA	C4A-NA-C1A	6.69	109.73	106.68
31	A	615	SQD	O6-C1-C2	6.68	118.41	108.27
31	a	615	SQD	C1-O5-C5	-6.66	100.72	113.72
31	a	615	SQD	O6-C1-C2	6.65	118.38	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	501	CLA	C4A-NA-C1A	6.60	109.69	106.68
25	c	505	CLA	C4A-NA-C1A	6.47	109.63	106.68
28	D	406	PL9	C7-C3-C4	6.45	122.22	116.91
25	c	504	CLA	C4A-NA-C1A	6.45	109.62	106.68
25	b	610	CLA	C4A-NA-C1A	6.34	109.57	106.68
25	B	615	CLA	C4A-NA-C1A	6.25	109.53	106.68
25	c	508	CLA	C4A-NA-C1A	6.25	109.53	106.68
25	B	611	CLA	C4A-NA-C1A	6.21	109.51	106.68
25	B	601	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	d	403	CLA	C4A-NA-C1A	5.97	109.40	106.68
25	C	512	CLA	C4A-NA-C1A	5.86	109.35	106.68
25	B	609	CLA	C4A-NA-C1A	5.86	109.35	106.68
28	a	612	PL9	C7-C3-C4	5.85	121.73	116.91
25	C	509	CLA	C4A-NA-C1A	5.79	109.32	106.68
25	D	403	CLA	C4A-NA-C1A	5.78	109.32	106.68
25	b	607	CLA	C4A-NA-C1A	5.76	109.31	106.68
28	d	405	PL9	C7-C3-C4	5.70	121.60	116.91
25	b	612	CLA	C4A-NA-C1A	5.68	109.27	106.68
25	d	402	CLA	C4A-NA-C1A	5.62	109.24	106.68
31	b	619	SQD	O6-C1-C2	5.59	116.77	108.27
26	A	608	PHO	C4D-CHA-CBD	-5.53	105.80	108.45
25	c	506	CLA	C4A-NA-C1A	5.40	109.14	106.68
25	b	606	CLA	C4A-NA-C1A	5.38	109.13	106.68
25	c	502	CLA	C4A-NA-C1A	5.28	109.09	106.68
25	c	512	CLA	C4A-NA-C1A	5.28	109.09	106.68
25	b	608	CLA	C4A-NA-C1A	5.21	109.06	106.68
25	C	502	CLA	C4A-NA-C1A	5.18	109.04	106.68
25	a	608	CLA	C4A-NA-C1A	5.14	109.02	106.68
25	A	612	CLA	C4A-NA-C1A	5.11	109.01	106.68
25	b	615	CLA	C4A-NA-C1A	5.10	109.01	106.68
25	B	613	CLA	C1-C2-C3	-5.08	117.88	126.20
31	F	102	SQD	C1-O5-C5	-5.08	103.81	113.72
25	B	613	CLA	C4A-NA-C1A	4.99	108.96	106.68
25	C	505	CLA	C4A-NA-C1A	4.99	108.96	106.68
25	B	602	CLA	C4A-NA-C1A	4.99	108.96	106.68
25	D	404	CLA	C4A-NA-C1A	4.98	108.95	106.68
25	A	607	CLA	C4A-NA-C1A	4.96	108.94	106.68
25	c	513	CLA	C4A-NA-C1A	4.94	108.93	106.68
31	F	102	SQD	O6-C1-C2	4.90	115.71	108.27
31	A	615	SQD	C1-O5-C5	-4.88	104.20	113.72
36	V	201	HEC	C1D-ND-C4D	4.81	110.90	105.21
25	c	512	CLA	C1-C2-C3	-4.76	118.40	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	616	SQD	O47-C7-C8	4.72	121.68	111.48
28	a	612	PL9	C7-C3-C2	-4.71	117.83	123.39
36	v	201	HEC	C1D-ND-C4D	4.70	110.77	105.21
25	a	610	CLA	C4A-NA-C1A	4.67	108.81	106.68
31	B	623	SQD	O6-C1-C2	4.64	115.32	108.27
25	b	613	CLA	C4A-NA-C1A	4.59	108.77	106.68
31	B	623	SQD	O47-C7-C8	4.58	121.38	111.48
25	A	609	CLA	C4A-NA-C1A	4.58	108.77	106.68
25	C	506	CLA	C4A-NA-C1A	4.55	108.76	106.68
25	A	606	CLA	C4A-NA-C1A	4.51	108.74	106.68
25	B	614	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
25	A	609	CLA	O2D-CGD-O1D	-4.43	115.23	123.85
27	b	616	BCR	C2-C1-C6	4.41	116.84	110.44
31	B	623	SQD	O7-S-C6	4.38	113.30	106.76
31	A	615	SQD	C1-C2-C3	-4.38	100.79	110.01
25	C	504	CLA	C4A-NA-C1A	4.38	108.68	106.68
30	e	102	LHG	O4-P-O5	4.34	132.64	112.44
25	a	610	CLA	O2D-CGD-O1D	-4.31	115.45	123.85
25	a	610	CLA	O2D-CGD-CBD	4.31	118.77	111.23
30	B	622	LHG	O4-P-O5	4.30	132.43	112.44
30	d	406	LHG	O4-P-O5	4.29	132.39	112.44
28	A	611	PL9	C7-C3-C4	4.26	120.42	116.91
25	B	610	CLA	O2D-CGD-O1D	-4.26	115.56	123.85
31	a	615	SQD	O9-S-O7	-4.25	100.00	113.82
25	b	604	CLA	C1-C2-C3	-4.25	119.23	126.20
34	D	401	BCT	O2-C-O1	4.25	130.53	119.68
30	L	101	LHG	O4-P-O5	4.23	132.12	112.44
30	l	101	LHG	O4-P-O5	4.22	132.09	112.44
30	E	101	LHG	O4-P-O5	4.22	132.08	112.44
30	D	408	LHG	O4-P-O5	4.20	132.00	112.44
32	a	617	DGD	O3G-C3G-C2G	-4.20	100.97	111.77
25	b	612	CLA	C1-C2-C3	-4.19	119.33	126.20
34	a	606	BCT	O2-C-O1	4.19	130.38	119.68
25	c	501	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
25	c	509	CLA	O2A-CGA-O1A	-4.09	113.39	123.63
30	a	614	LHG	O4-P-O5	4.09	131.46	112.44
30	d	407	LHG	O4-P-O5	4.08	131.43	112.44
30	A	614	LHG	O4-P-O5	4.06	131.33	112.44
25	b	607	CLA	C3B-C4B-NB	-4.05	106.92	110.53
26	D	402	PHO	C4D-CHA-CBD	-4.04	106.52	108.45
25	B	612	CLA	C4A-NA-C1A	4.03	108.52	106.68
26	d	401	PHO	C1-C2-C3	-4.02	119.60	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	403	CLA	C3B-C4B-NB	-3.99	106.96	110.53
25	b	604	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
25	b	602	CLA	C4A-NA-C1A	3.98	108.49	106.68
31	f	101	SQD	O5-C5-C4	3.97	116.84	109.70
25	b	605	CLA	O2D-CGD-O1D	-3.96	116.14	123.85
28	D	406	PL9	C7-C3-C2	-3.96	118.73	123.39
25	C	503	CLA	C3B-C4B-NB	-3.95	107.00	110.53
35	e	101	HEM	CBD-CAD-C3D	-3.94	101.63	112.53
35	F	101	HEM	CBD-CAD-C3D	-3.94	101.64	112.53
25	b	602	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
25	C	501	CLA	O2D-CGD-O1D	-3.93	116.21	123.85
25	b	615	CLA	O2D-CGD-O1D	-3.92	116.21	123.85
26	D	402	PHO	C2B-C1B-NB	-3.91	106.60	109.43
25	a	608	CLA	C3B-C4B-NB	-3.91	107.04	110.53
31	F	102	SQD	C1-C2-C3	-3.90	101.80	110.01
32	C	516	DGD	O3G-C3G-C2G	-3.89	101.35	110.82
32	C	517	DGD	O3G-C3G-C2G	-3.88	101.37	110.82
25	d	402	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
25	b	604	CLA	C3B-C4B-NB	-3.88	107.06	110.53
25	C	513	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
25	B	614	CLA	C3B-C4B-NB	-3.86	107.08	110.53
26	D	402	PHO	C1-C2-C3	-3.85	119.88	126.20
25	b	611	CLA	C4A-NA-C1A	3.85	108.44	106.68
25	c	511	CLA	C3B-C4B-NB	-3.85	107.10	110.53
32	H	102	DGD	O3G-C3G-C2G	-3.85	101.46	110.82
25	C	512	CLA	C1-C2-C3	-3.84	119.91	126.20
25	B	611	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
25	C	505	CLA	C3B-C4B-NB	-3.80	107.14	110.53
25	B	606	CLA	C3B-C4B-NB	-3.80	107.14	110.53
28	d	405	PL9	C7-C3-C2	-3.79	118.92	123.39
31	f	101	SQD	O9-S-O7	-3.79	101.51	113.82
31	A	615	SQD	O9-S-O7	-3.78	101.53	113.82
31	b	619	SQD	O7-S-C6	3.77	112.39	106.76
25	B	602	CLA	O2D-CGD-CBD	3.76	117.81	111.23
27	c	514	BCR	C15-C14-C13	-3.76	122.00	127.28
31	B	623	SQD	O9-S-O7	-3.76	101.59	113.82
31	B	623	SQD	C1-O5-C5	-3.75	106.41	113.72
32	c	517	DGD	O3G-C3G-C2G	-3.74	101.73	110.82
25	B	601	CLA	O2D-CGD-O1D	-3.73	116.58	123.85
25	b	611	CLA	C1-C2-C3	-3.72	120.11	126.20
25	C	510	CLA	C3B-C4B-NB	-3.70	107.22	110.53
26	A	608	PHO	CMB-C2B-C3B	3.69	132.06	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	603	CLA	C4A-NA-C1A	3.69	108.36	106.68
31	F	102	SQD	O9-S-C6	3.68	112.24	106.76
25	b	614	CLA	C3B-C4B-NB	-3.66	107.26	110.53
28	D	406	PL9	C27-C28-C29	-3.66	119.24	127.62
31	a	615	SQD	O47-C7-C8	3.66	119.39	111.48
26	D	402	PHO	CMB-C2B-C3B	3.65	131.98	124.68
25	A	607	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
25	h	101	CLA	O2D-CGD-O1D	-3.65	116.75	123.85
25	A	609	CLA	O2D-CGD-CBD	3.61	117.54	111.23
29	b	622	LMG	C1-O6-C5	-3.60	106.69	113.72
25	C	501	CLA	O2D-CGD-CBD	3.59	117.51	111.23
25	B	615	CLA	CHB-C4A-NA	3.59	129.58	124.40
25	B	606	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
27	B	617	BCR	C2-C1-C6	3.57	115.63	110.44
31	a	615	SQD	C1-C2-C3	-3.57	102.50	110.01
25	c	505	CLA	C3B-C4B-NB	-3.57	107.34	110.53
32	h	103	DGD	O3G-C3G-C2G	-3.57	102.15	110.82
25	c	508	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
31	f	101	SQD	O6-C1-C2	3.55	113.67	108.27
25	h	101	CLA	C3B-C4B-NB	-3.55	107.36	110.53
27	h	102	BCR	C2-C1-C6	3.55	115.60	110.44
28	d	405	PL9	C37-C38-C39	-3.54	119.51	127.62
31	b	619	SQD	O47-C7-C8	3.53	119.12	111.48
25	A	607	CLA	C3B-C4B-NB	-3.53	107.38	110.53
25	C	508	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
25	B	604	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
25	a	613	CLA	C1-C2-C3	-3.52	120.43	126.20
31	A	615	SQD	O5-C1-C2	-3.52	103.15	110.37
25	B	603	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
25	B	604	CLA	C3B-C4B-NB	-3.51	107.40	110.53
31	f	101	SQD	O7-S-C6	3.51	111.99	106.76
25	b	608	CLA	C3B-C4B-NB	-3.50	107.41	110.53
25	b	610	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
32	C	517	DGD	O6D-C1D-O3G	-3.49	101.79	110.04
26	d	401	PHO	CMB-C2B-C3B	3.49	131.66	124.68
30	D	408	LHG	O8-C23-C24	3.48	122.44	111.83
25	d	403	CLA	C3B-C4B-NB	-3.48	107.43	110.53
30	a	614	LHG	O8-C23-C24	3.47	122.43	111.83
25	b	601	CLA	CHB-C4A-NA	3.47	129.40	124.40
25	C	501	CLA	C3B-C4B-NB	-3.46	107.44	110.53
31	a	616	SQD	O48-C23-C24	3.46	122.37	111.83
31	a	615	SQD	O48-C23-C24	3.45	122.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	611	PL9	C40-C39-C41	3.44	121.20	115.23
25	b	609	CLA	C4A-NA-C1A	3.44	108.25	106.68
25	B	608	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
25	D	403	CLA	C1-C2-C3	-3.41	120.60	126.20
25	c	509	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
25	b	609	CLA	C1-C2-C3	-3.39	120.64	126.20
25	c	502	CLA	C1-C2-C3	-3.39	120.65	126.20
31	A	615	SQD	O47-C7-C8	3.39	118.81	111.48
25	b	605	CLA	O2D-CGD-CBD	3.39	117.15	111.23
31	A	616	SQD	O47-C7-C8	3.38	118.79	111.48
31	b	619	SQD	O5-C5-C4	3.38	115.79	109.70
26	a	609	PHO	C2B-C1B-NB	-3.37	107.00	109.43
25	B	612	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
25	C	512	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
25	B	611	CLA	O2D-CGD-CBD	3.34	117.06	111.23
25	B	611	CLA	C1-C2-C3	-3.33	120.74	126.20
25	c	512	CLA	C3B-C4B-NB	-3.32	107.56	110.53
28	D	406	PL9	C22-C23-C24	-3.32	120.03	127.62
25	A	607	CLA	O2D-CGD-CBD	3.31	117.02	111.23
27	B	619	BCR	C2-C1-C6	3.31	115.25	110.44
25	B	603	CLA	C3B-C4B-NB	-3.31	107.58	110.53
25	B	610	CLA	O2A-CGA-O1A	-3.31	115.35	123.63
28	d	405	PL9	C7-C8-C9	-3.30	121.14	126.83
32	c	516	DGD	O3G-C3G-C2G	-3.30	102.78	110.82
26	D	402	PHO	C3B-C4B-NB	-3.30	105.31	107.46
25	b	612	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
25	C	512	CLA	CHB-C4A-NA	3.29	129.15	124.40
26	d	401	PHO	O1D-CGD-CBD	3.29	129.71	124.72
25	b	601	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
25	b	606	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
25	c	503	CLA	C3B-C4B-NB	-3.28	107.60	110.53
25	A	612	CLA	O2D-CGD-CBD	3.28	116.96	111.23
28	D	406	PL9	C37-C38-C39	-3.28	120.13	127.62
28	d	405	PL9	C22-C23-C24	-3.27	120.15	127.62
25	A	609	CLA	CHB-C4A-NA	3.26	129.10	124.40
25	c	508	CLA	C3B-C4B-NB	-3.26	107.62	110.53
27	C	514	BCR	C15-C16-C17	-3.25	116.86	123.52
29	c	519	LMG	O6-C1-O1	-3.25	102.37	110.04
31	B	623	SQD	O48-C23-C24	3.24	121.73	111.83
26	d	401	PHO	C2B-C1B-NB	-3.24	107.09	109.43
32	h	103	DGD	O6E-C5E-C4E	3.24	115.54	109.70
25	B	608	CLA	CMB-C2B-C1B	-3.24	120.49	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	401	PHO	O2D-CGD-O1D	-3.24	117.55	123.85
25	b	613	CLA	C3B-C4B-NB	-3.23	107.64	110.53
31	A	615	SQD	O7-S-C6	3.23	111.58	106.76
25	B	609	CLA	O2A-CGA-O1A	-3.23	115.54	123.63
25	B	614	CLA	CHC-C4B-NB	3.23	128.89	124.05
25	D	404	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
32	C	516	DGD	O6D-C1D-O3G	-3.23	102.42	110.04
25	B	605	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
26	d	401	PHO	C4D-CHA-CBD	-3.22	106.91	108.45
31	F	102	SQD	O9-S-O7	-3.22	103.35	113.82
30	B	622	LHG	O8-C23-C24	3.22	121.64	111.83
27	c	515	BCR	C11-C10-C9	-3.22	122.77	127.28
31	b	619	SQD	O48-C23-C24	3.21	121.63	111.83
25	c	512	CLA	CHB-C4A-NA	3.21	129.03	124.40
25	a	608	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
27	c	515	BCR	C7-C8-C9	-3.19	121.51	126.23
25	A	612	CLA	C3B-C4B-NB	-3.18	107.69	110.53
25	b	611	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
27	D	405	BCR	C27-C26-C25	3.17	126.99	122.70
28	D	406	PL9	C7-C8-C9	-3.17	121.37	126.83
32	C	515	DGD	O5D-C6D-C5D	-3.17	102.27	109.42
31	b	619	SQD	O9-S-O7	-3.17	103.51	113.82
31	F	102	SQD	O8-S-C6	3.17	112.09	105.97
25	B	612	CLA	CHB-C4A-NA	3.16	128.96	124.40
32	c	518	DGD	O3G-C3G-C2G	-3.16	103.13	110.82
25	B	612	CLA	C1-C2-C3	-3.15	121.03	126.20
25	b	613	CLA	C1-C2-C3	-3.15	121.04	126.20
27	K	101	BCR	C24-C23-C22	-3.15	121.58	126.23
25	c	510	CLA	CMB-C2B-C1B	-3.15	120.63	125.42
29	m	101	LMG	O1-C7-C8	-3.14	103.17	110.82
25	B	613	CLA	C3B-C4B-NB	-3.14	107.73	110.53
32	c	516	DGD	CDB-CCB-CBB	-3.14	98.52	114.37
25	C	508	CLA	CHD-C1D-ND	-3.13	120.40	124.80
33	M	102	STE	C3-C2-C1	-3.13	106.35	114.51
32	c	517	DGD	O6D-C1D-O3G	-3.12	102.68	110.04
25	d	402	CLA	C3B-C4B-NB	-3.12	107.75	110.53
25	a	613	CLA	O2D-CGD-CBD	3.11	116.67	111.23
25	B	604	CLA	O2A-CGA-O1A	-3.11	115.86	123.63
29	d	409	LMG	O6-C1-O1	-3.10	102.71	110.04
27	h	102	BCR	C27-C26-C25	3.10	126.89	122.70
25	b	611	CLA	C3B-C4B-NB	-3.09	107.77	110.53
25	C	505	CLA	O2D-CGD-O1D	-3.09	117.83	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	v	201	HEC	CHB-C1B-NB	3.09	127.75	124.42
28	A	611	PL9	C7-C3-C2	-3.09	119.75	123.39
25	b	611	CLA	C11-C12-C13	-3.09	105.71	115.97
25	b	601	CLA	C1-C2-C3	-3.08	121.14	126.20
28	a	612	PL9	C22-C23-C24	-3.08	120.57	127.62
36	v	201	HEC	CHA-C4D-ND	3.07	127.72	124.42
25	c	512	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
25	C	502	CLA	C1-C2-C3	-3.06	121.18	126.20
27	t	101	BCR	C15-C14-C13	-3.06	122.98	127.28
29	m	101	LMG	O6-C1-O1	-3.06	102.81	110.04
25	A	606	CLA	C3B-C4B-NB	-3.05	107.80	110.53
25	c	504	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
25	b	604	CLA	O2A-CGA-O1A	-3.05	116.01	123.63
25	c	503	CLA	C7-C6-C5	-3.04	105.16	113.26
33	C	519	STE	C3-C2-C1	-3.04	106.58	114.51
25	a	607	CLA	O2A-CGA-O1A	-3.04	116.03	123.63
27	B	619	BCR	C29-C30-C25	3.04	114.85	110.44
29	c	522	LMG	C1-O6-C5	-3.02	107.82	113.72
25	b	602	CLA	O2D-CGD-CBD	3.02	116.50	111.23
25	c	513	CLA	CMB-C2B-C1B	-3.01	120.84	125.42
25	b	615	CLA	CHB-C4A-NA	3.00	128.74	124.40
31	b	619	SQD	C1-C2-C3	-3.00	103.69	110.01
32	h	103	DGD	C1D-C2D-C3D	-3.00	103.71	110.01
31	f	101	SQD	O48-C23-C24	2.99	120.96	111.83
32	A	617	DGD	O3G-C3G-C2G	-2.99	103.55	110.82
32	C	515	DGD	O3G-C3G-C2G	-2.98	103.56	110.82
25	c	507	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
25	C	509	CLA	CED-O2D-CGD	2.98	122.68	115.92
25	C	512	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	a	615	SQD	O7-S-C6	2.97	111.19	106.76
25	b	602	CLA	C3B-C4B-NB	-2.97	107.88	110.53
27	d	404	BCR	C27-C26-C25	2.97	126.72	122.70
25	b	607	CLA	CMB-C2B-C1B	-2.97	120.90	125.42
27	T	101	BCR	C15-C14-C13	-2.96	123.12	127.28
28	D	406	PL9	C40-C39-C41	2.96	120.37	115.23
29	m	101	LMG	O1-C1-C2	-2.96	103.78	108.27
25	b	615	CLA	CMB-C2B-C1B	-2.95	120.93	125.42
25	B	603	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
36	V	201	HEC	CBD-CAD-C3D	-2.95	104.38	112.53
25	b	611	CLA	O2A-CGA-O1A	-2.95	116.26	123.63
25	b	603	CLA	C1-C2-C3	-2.94	121.37	126.20
25	C	503	CLA	CHB-C4A-NA	2.94	128.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	101	BCR	C27-C26-C25	2.94	126.68	122.70
25	C	511	CLA	C3B-C4B-NB	-2.94	107.90	110.53
30	l	101	LHG	O8-C23-C24	2.94	120.80	111.83
25	b	609	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
25	c	502	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
31	f	101	SQD	O5-C1-C2	-2.93	104.34	110.37
25	B	610	CLA	C4A-NA-C1A	2.93	108.02	106.68
25	c	510	CLA	C3B-C4B-NB	-2.93	107.92	110.53
31	F	102	SQD	O48-C23-C24	2.93	120.75	111.83
29	m	101	LMG	O3-C3-C2	-2.92	103.48	110.38
25	c	507	CLA	C3B-C4B-NB	-2.92	107.92	110.53
27	H	101	BCR	C2-C1-C6	2.92	114.68	110.44
25	b	609	CLA	CHB-C4A-NA	2.92	128.61	124.40
25	A	606	CLA	CHB-C4A-NA	2.92	128.61	124.40
25	d	402	CLA	O2D-CGD-CBD	2.91	116.32	111.23
25	b	615	CLA	C3B-C4B-NB	-2.91	107.93	110.53
25	B	602	CLA	CMB-C2B-C1B	-2.91	120.99	125.42
27	c	515	BCR	C27-C26-C25	2.91	126.63	122.70
32	c	518	DGD	O6D-C1D-O3G	-2.90	103.18	110.04
30	a	614	LHG	O8-C23-O10	-2.90	116.36	123.63
25	B	609	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
32	A	617	DGD	C3G-C2G-C1G	-2.90	105.03	111.78
27	c	514	BCR	C15-C16-C17	-2.90	117.59	123.52
27	k	101	BCR	C33-C5-C6	-2.89	121.33	124.48
25	A	612	CLA	CHB-C4A-NA	2.89	128.56	124.40
25	b	606	CLA	C3B-C4B-NB	-2.89	107.95	110.53
27	t	101	BCR	C15-C16-C17	-2.88	117.63	123.52
27	K	102	BCR	C27-C26-C25	2.88	126.59	122.70
25	C	511	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
25	B	602	CLA	CGD-CBD-CAD	-2.87	101.55	110.85
27	C	514	BCR	C2-C1-C6	2.87	114.61	110.44
25	a	613	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	C	503	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
25	b	607	CLA	CHB-C1B-NB	2.86	128.34	124.05
25	C	502	CLA	C3B-C4B-NB	-2.86	107.98	110.53
27	a	611	BCR	C27-C26-C25	2.86	126.57	122.70
25	b	603	CLA	C3B-C4B-NB	-2.86	107.98	110.53
25	A	606	CLA	O2A-CGA-O1A	-2.86	116.48	123.63
28	A	611	PL9	C7-C8-C9	-2.85	121.91	126.83
32	C	515	DGD	CDB-CCB-CBB	-2.84	100.00	114.37
27	T	101	BCR	C7-C8-C9	-2.84	122.03	126.23
32	C	515	DGD	C3D-C4D-C5D	-2.84	105.08	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	602	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
26	D	402	PHO	O2D-CGD-O1D	-2.84	118.33	123.85
25	B	613	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
28	a	612	PL9	O2-C1-C6	2.83	124.99	120.48
27	c	514	BCR	C27-C26-C25	2.83	126.53	122.70
25	C	510	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
27	b	616	BCR	C27-C26-C25	2.83	126.52	122.70
31	b	619	SQD	O8-S-C6	2.83	111.43	105.97
30	E	101	LHG	O8-C23-C24	2.82	120.45	111.83
31	A	615	SQD	O48-C23-C24	2.82	120.44	111.83
25	C	509	CLA	CMB-C2B-C1B	-2.82	121.13	125.42
30	e	102	LHG	O8-C23-C24	2.82	120.42	111.83
25	A	612	CLA	C1-C2-C3	-2.81	121.59	126.20
25	a	607	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
32	c	516	DGD	O6D-C1D-O3G	-2.81	103.41	110.04
32	H	102	DGD	O6D-C1D-O3G	-2.80	103.42	110.04
27	K	101	BCR	C27-C26-C25	2.80	126.49	122.70
25	c	505	CLA	O2D-CGD-CBD	2.80	116.12	111.23
27	B	618	BCR	C27-C26-C25	2.79	126.48	122.70
25	A	607	CLA	CHB-C4A-NA	2.79	128.43	124.40
26	A	608	PHO	O2D-CGD-CBD	2.79	114.01	110.95
25	C	504	CLA	CHB-C4A-NA	2.79	128.43	124.40
28	d	405	PL9	C40-C39-C41	2.79	120.06	115.23
27	A	610	BCR	C27-C26-C25	2.78	126.47	122.70
25	B	611	CLA	C3B-C4B-NB	-2.78	108.05	110.53
27	B	618	BCR	C15-C14-C13	-2.78	123.38	127.28
32	c	517	DGD	CDB-CCB-CBB	-2.78	100.31	114.37
25	c	504	CLA	C3B-C4B-NB	-2.78	108.05	110.53
28	D	406	PL9	C36-C34-C33	-2.78	114.94	121.17
35	F	101	HEM	CHC-C4B-NB	2.77	127.41	124.42
25	C	508	CLA	C3B-C4B-NB	-2.76	108.06	110.53
36	v	201	HEC	CBD-CAD-C3D	-2.76	104.89	112.53
25	h	101	CLA	CHB-C4A-NA	2.76	128.38	124.40
32	C	516	DGD	C1D-C2D-C3D	-2.76	104.20	110.01
25	C	503	CLA	C7-C6-C5	-2.76	105.91	113.26
25	B	615	CLA	C3B-C4B-NB	-2.76	108.07	110.53
25	B	613	CLA	CHB-C4A-NA	2.76	128.38	124.40
27	K	101	BCR	C11-C10-C9	-2.76	123.41	127.28
27	T	101	BCR	C33-C5-C6	-2.75	121.48	124.48
30	B	622	LHG	C11-C10-C9	-2.75	100.45	114.37
32	C	517	DGD	CDB-CCB-CBB	-2.75	100.46	114.37
25	A	607	CLA	C1-C2-C3	-2.75	121.69	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	619	SQD	C3-C4-C5	2.75	115.21	110.23
27	A	610	BCR	C2-C1-C6	2.74	114.42	110.44
28	a	612	PL9	C27-C28-C29	-2.74	121.34	127.62
25	B	601	CLA	C3B-C4B-NB	-2.74	108.08	110.53
31	B	623	SQD	C3-C4-C5	2.74	115.20	110.23
25	B	614	CLA	O1D-CGD-CBD	2.74	129.92	124.52
25	c	508	CLA	O2D-CGD-CBD	2.74	116.02	111.23
25	B	601	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
25	B	610	CLA	C3B-C4B-NB	-2.74	108.09	110.53
32	A	617	DGD	O6D-C1D-O3G	-2.74	103.58	110.04
25	A	612	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
25	b	601	CLA	C3B-C4B-NB	-2.73	108.09	110.53
25	a	608	CLA	CHB-C4A-NA	2.73	128.33	124.40
25	b	601	CLA	O2D-CGD-CBD	2.73	115.99	111.23
25	C	506	CLA	O2A-CGA-O1A	-2.72	116.81	123.63
32	h	103	DGD	O6D-C1D-O3G	-2.72	103.61	110.04
25	c	507	CLA	CHB-C4A-NA	2.72	128.33	124.40
32	c	516	DGD	O3E-C3E-C2E	-2.72	103.96	110.38
28	a	612	PL9	O2-C1-C2	-2.72	115.64	121.83
25	a	607	CLA	O1D-CGD-CBD	2.72	129.88	124.52
25	A	607	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
25	C	512	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
29	D	409	LMG	O1-C7-C8	-2.71	104.81	111.77
25	B	608	CLA	O2D-CGD-CBD	2.71	115.96	111.23
25	a	608	CLA	O2D-CGD-CBD	2.71	115.96	111.23
30	d	406	LHG	O8-C23-C24	2.71	120.09	111.83
25	b	611	CLA	CAC-C3C-C4C	2.71	128.31	124.79
25	C	513	CLA	C3B-C4B-NB	-2.70	108.12	110.53
25	B	606	CLA	O2D-CGD-CBD	2.70	115.95	111.23
31	F	102	SQD	O5-C5-C4	2.70	114.56	109.70
25	b	608	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
32	C	515	DGD	O6D-C1D-O3G	-2.70	103.67	110.04
25	c	510	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
33	m	102	STE	O2-C1-C2	2.69	122.52	114.00
32	A	617	DGD	CDB-CCB-CBB	-2.69	100.75	114.37
25	a	610	CLA	CHB-C4A-NA	2.69	128.28	124.40
25	d	403	CLA	CHD-C1D-ND	-2.69	121.02	124.80
25	c	506	CLA	C3B-C4B-NB	-2.69	108.13	110.53
25	a	608	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
25	c	505	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
25	c	511	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
25	C	504	CLA	CHC-C1C-NC	2.68	128.34	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	M	101	LMG	C38-C37-C36	-2.67	100.85	114.37
25	B	612	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
27	T	101	BCR	C27-C26-C25	2.66	126.29	122.70
25	b	613	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
28	d	405	PL9	C20-C19-C21	2.65	119.83	115.23
29	b	622	LMG	O1-C1-C2	-2.65	104.25	108.27
25	C	507	CLA	CHB-C4A-NA	2.65	128.22	124.40
26	D	402	PHO	O1D-CGD-CBD	2.65	128.74	124.72
26	d	401	PHO	CMA-C3A-C4A	-2.65	108.91	114.61
25	C	502	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
25	B	614	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
25	c	507	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
30	d	407	LHG	O8-C23-C24	2.63	119.86	111.83
25	c	513	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
25	b	611	CLA	CHB-C4A-NA	2.63	128.19	124.40
29	M	101	LMG	C1-C2-C3	-2.62	104.50	110.01
25	b	603	CLA	O2D-CGD-CBD	2.62	115.80	111.23
27	k	102	BCR	C11-C10-C9	-2.62	123.61	127.28
27	d	404	BCR	C30-C25-C26	-2.62	119.06	122.64
31	A	615	SQD	O8-S-C6	2.61	111.02	105.97
25	B	605	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
25	a	610	CLA	C1-C2-C3	-2.61	121.92	126.20
29	b	622	LMG	C8-O7-C10	2.61	124.04	117.80
25	b	607	CLA	CHB-C4A-NA	2.60	128.16	124.40
27	d	404	BCR	C38-C26-C25	-2.60	121.64	124.48
32	c	518	DGD	CDB-CCB-CBB	-2.60	101.20	114.37
25	C	506	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
25	a	607	CLA	CHB-C4A-NA	2.60	128.15	124.40
32	c	516	DGD	C3D-C4D-C5D	-2.59	105.53	110.23
25	c	513	CLA	C1-C2-C3	-2.59	121.95	126.20
25	b	610	CLA	O2D-CGD-CBD	2.59	115.76	111.23
28	a	612	PL9	C7-C8-C9	-2.59	122.37	126.83
25	C	506	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	C	507	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
25	B	602	CLA	C3B-C4B-NB	-2.59	108.22	110.53
25	D	404	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
25	a	613	CLA	CHC-C4B-NB	2.59	127.93	124.05
25	B	612	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
31	f	101	SQD	O9-S-C6	2.58	110.61	106.76
27	K	103	BCR	C27-C26-C25	2.58	126.19	122.70
25	c	501	CLA	C1-C2-C3	-2.58	121.97	126.20
29	M	101	LMG	C40-C39-C38	-2.58	101.31	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	610	CLA	O2D-CGD-CBD	2.58	115.74	111.23
28	d	405	PL9	C42-C43-C44	-2.58	121.72	127.62
26	d	401	PHO	C3B-C4B-NB	-2.58	105.78	107.46
27	B	618	BCR	C2-C1-C6	2.58	114.18	110.44
25	B	616	CLA	C3B-C4B-NB	-2.58	108.23	110.53
27	D	405	BCR	C7-C8-C9	-2.57	122.43	126.23
27	c	515	BCR	C15-C16-C17	-2.57	118.26	123.52
25	C	507	CLA	C3B-C4B-NB	-2.57	108.24	110.53
25	b	603	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
27	D	405	BCR	C24-C23-C22	-2.57	122.44	126.23
25	c	504	CLA	O2A-CGA-O1A	-2.56	117.21	123.63
25	B	608	CLA	CHB-C4A-NA	2.56	128.10	124.40
29	C	518	LMG	O1-C7-C8	-2.56	104.59	110.82
25	C	513	CLA	O2D-CGD-CBD	2.56	115.71	111.23
25	b	605	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
25	b	603	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
27	k	102	BCR	C33-C5-C6	-2.56	121.69	124.48
25	b	612	CLA	O2A-CGA-O1A	-2.56	117.24	123.63
25	B	610	CLA	CHB-C4A-NA	2.55	128.09	124.40
28	a	612	PL9	C37-C38-C39	-2.55	121.78	127.62
33	d	410	STE	O2-C1-C2	2.55	122.07	114.00
30	D	408	LHG	O8-C23-O10	-2.55	117.24	123.63
25	C	506	CLA	CMB-C2B-C1B	-2.55	121.53	125.42
25	B	604	CLA	CHB-C4A-NA	2.55	128.08	124.40
32	c	518	DGD	CAB-C9B-C8B	-2.55	101.48	114.37
28	a	612	PL9	C40-C39-C41	2.55	119.65	115.23
32	h	103	DGD	C1E-O6E-C5E	2.55	118.70	113.72
29	m	101	LMG	C38-C37-C36	-2.55	101.49	114.37
26	a	609	PHO	CMB-C2B-C3B	2.55	129.77	124.68
31	a	615	SQD	O8-S-C6	2.55	110.89	105.97
30	d	406	LHG	O8-C23-O10	-2.54	117.26	123.63
25	b	609	CLA	O2A-CGA-O1A	-2.54	117.27	123.63
25	C	509	CLA	C1-C2-C3	-2.54	122.03	126.20
29	c	521	LMG	O8-C28-O10	-2.54	117.28	123.63
30	D	408	LHG	C27-C26-C25	-2.54	101.53	114.37
26	A	608	PHO	O2D-CGD-O1D	-2.54	118.91	123.85
30	a	614	LHG	C11-C10-C9	-2.54	101.55	114.37
27	k	102	BCR	C27-C26-C25	2.53	126.13	122.70
25	B	602	CLA	CMB-C2B-C3B	2.53	132.51	126.55
25	b	604	CLA	O1D-CGD-CBD	2.53	129.51	124.52
25	B	612	CLA	CMB-C2B-C3B	2.53	132.50	126.55
25	c	502	CLA	C3B-C4B-NB	-2.53	108.27	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	513	CLA	C3B-C4B-NB	-2.53	108.27	110.53
33	x	101	STE	C3-C2-C1	-2.53	107.91	114.51
29	C	518	LMG	C1-O6-C5	-2.53	108.78	113.72
31	f	101	SQD	O47-C7-C8	2.53	120.21	110.93
27	c	514	BCR	C7-C8-C9	-2.53	122.50	126.23
25	b	610	CLA	C3B-C4B-NB	-2.52	108.28	110.53
25	c	512	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
28	A	611	PL9	C22-C23-C24	-2.52	121.86	127.62
30	D	408	LHG	C11-C10-C9	-2.52	101.65	114.37
30	E	101	LHG	C20-C19-C18	-2.52	101.65	114.37
27	b	617	BCR	C27-C26-C25	2.51	126.10	122.70
29	D	407	LMG	O6-C1-O1	-2.51	104.11	110.04
25	c	513	CLA	CMB-C2B-C3B	2.51	132.46	126.55
25	B	602	CLA	CHB-C4A-NA	2.51	128.02	124.40
27	b	616	BCR	C33-C5-C6	-2.51	121.75	124.48
28	D	406	PL9	C42-C43-C44	-2.51	121.88	127.62
25	C	512	CLA	O2D-CGD-CBD	2.51	115.61	111.23
27	K	102	BCR	C33-C5-C6	-2.50	121.76	124.48
25	B	606	CLA	CGD-CBD-CAD	-2.50	102.76	110.85
25	C	501	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
25	B	613	CLA	CAC-C3C-C4C	2.49	128.04	124.79
25	C	504	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
27	K	101	BCR	C33-C5-C6	-2.49	121.77	124.48
31	A	616	SQD	O48-C23-C24	2.49	119.42	111.83
27	B	617	BCR	C27-C26-C25	2.49	126.06	122.70
36	v	201	HEC	CBA-CAA-C2A	-2.49	105.66	112.53
31	a	615	SQD	C44-O6-C1	-2.49	108.47	113.80
27	B	617	BCR	C33-C5-C6	-2.49	121.77	124.48
29	c	519	LMG	C38-C37-C36	-2.48	101.83	114.37
27	a	611	BCR	C2-C1-C6	2.48	114.04	110.44
32	c	517	DGD	O3G-C1D-C2D	-2.48	104.51	108.27
25	B	601	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
25	C	509	CLA	C3B-C4B-NB	-2.47	108.32	110.53
32	h	103	DGD	CDB-CCB-CBB	-2.47	101.86	114.37
31	f	101	SQD	C3-C4-C5	2.47	114.72	110.23
25	B	612	CLA	C16-C15-C13	-2.47	107.75	115.97
25	b	615	CLA	CMB-C2B-C3B	2.47	132.36	126.55
25	h	101	CLA	O2D-CGD-CBD	2.47	115.55	111.23
35	e	101	HEM	CHD-C4C-NC	2.47	127.14	124.45
25	B	603	CLA	CHB-C1B-NB	2.47	127.75	124.05
33	t	102	STE	C3-C2-C1	-2.46	108.08	114.51
25	B	601	CLA	O2D-CGD-CBD	2.46	115.53	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	614	CLA	CHB-C4A-NA	2.46	127.95	124.40
27	k	101	BCR	C27-C26-C25	2.46	126.03	122.70
30	e	102	LHG	C11-C10-C9	-2.46	101.94	114.37
32	C	517	DGD	O3E-C3E-C2E	-2.46	104.58	110.38
29	D	407	LMG	O8-C28-O10	-2.46	117.49	123.63
25	B	608	CLA	CMB-C2B-C3B	2.46	132.32	126.55
25	b	614	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
25	C	503	CLA	O1D-CGD-CBD	2.45	129.35	124.52
27	B	617	BCR	C24-C23-C22	-2.45	122.61	126.23
25	b	604	CLA	CHB-C4A-NA	2.45	127.94	124.40
27	b	618	BCR	C2-C1-C6	2.45	114.00	110.44
25	b	607	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
25	b	606	CLA	CHB-C4A-NA	2.45	127.93	124.40
28	A	611	PL9	C36-C34-C33	-2.45	115.67	121.17
27	T	101	BCR	C35-C13-C14	-2.45	118.85	122.82
25	D	403	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
36	V	201	HEC	CHB-C1B-NB	2.44	127.05	124.42
25	B	608	CLA	C3B-C4B-NB	-2.44	108.35	110.53
27	t	101	BCR	C3-C4-C5	-2.44	109.70	114.06
32	a	617	DGD	C1G-C2G-C3G	-2.44	106.17	111.80
28	D	406	PL9	C20-C19-C21	2.44	119.46	115.23
27	c	514	BCR	C33-C5-C6	-2.44	121.82	124.48
29	b	622	LMG	O2-C2-C1	-2.44	104.27	110.08
30	B	622	LHG	C20-C19-C18	-2.44	102.06	114.37
25	C	504	CLA	C3B-C4B-NB	-2.44	108.36	110.53
31	b	619	SQD	O9-S-C6	2.43	110.39	106.76
25	c	506	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
29	c	521	LMG	O6-C1-O1	-2.43	104.30	110.04
25	a	613	CLA	C3B-C4B-NB	-2.43	108.36	110.53
25	c	509	CLA	O1D-CGD-CBD	2.43	129.31	124.52
25	B	616	CLA	CHC-C4B-NB	2.43	127.69	124.05
25	b	607	CLA	O2D-CGD-CBD	2.42	115.47	111.23
25	b	613	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
32	c	516	DGD	CAB-C9B-C8B	-2.42	102.13	114.37
32	C	516	DGD	CDB-CCB-CBB	-2.42	102.13	114.37
25	c	506	CLA	CHB-C4A-NA	2.42	127.89	124.40
28	A	611	PL9	O1-C4-C3	-2.42	118.18	120.73
25	d	403	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
25	c	505	CLA	C11-C10-C8	-2.41	107.94	115.97
25	B	612	CLA	C3B-C4B-NB	-2.41	108.38	110.53
28	A	611	PL9	C12-C13-C14	-2.41	122.11	127.62
27	b	618	BCR	C7-C8-C9	-2.41	122.67	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	612	CLA	C11-C12-C13	-2.41	107.96	115.97
25	b	605	CLA	CHC-C4B-NB	2.40	127.66	124.05
25	B	607	CLA	C3B-C4B-NB	-2.40	108.39	110.53
31	B	623	SQD	O8-S-C6	2.40	110.61	105.97
25	b	613	CLA	CHB-C4A-NA	2.40	127.87	124.40
25	C	504	CLA	CED-O2D-CGD	2.40	121.36	115.92
29	C	518	LMG	O6-C1-O1	-2.40	104.37	110.04
32	a	617	DGD	C8B-C7B-C6B	-2.40	102.23	114.37
25	c	501	CLA	O2D-CGD-CBD	2.40	115.42	111.23
28	D	406	PL9	C12-C13-C14	-2.40	122.13	127.62
32	c	517	DGD	O2D-C2D-C1D	-2.40	104.36	110.08
25	b	614	CLA	CHB-C4A-NA	2.40	127.86	124.40
25	b	615	CLA	O1D-CGD-CBD	2.39	129.23	124.52
25	C	508	CLA	CHD-C4C-NC	2.39	127.94	124.23
27	K	101	BCR	C2-C1-C6	2.39	113.91	110.44
25	C	507	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
25	c	504	CLA	O2D-CGD-CBD	2.39	115.40	111.23
27	B	617	BCR	C11-C10-C9	-2.39	123.93	127.28
27	K	103	BCR	C2-C1-C6	2.38	113.90	110.44
25	b	615	CLA	CHC-C4B-NB	2.38	127.62	124.05
25	b	603	CLA	CHB-C1B-NB	2.38	127.62	124.05
31	A	615	SQD	O9-S-C6	2.38	110.31	106.76
25	c	510	CLA	CMB-C2B-C3B	2.38	132.15	126.55
30	D	408	LHG	C20-C19-C18	-2.38	102.34	114.37
25	b	607	CLA	CMB-C2B-C3B	2.38	132.14	126.55
25	b	609	CLA	CAA-CBA-CGA	-2.38	106.46	113.21
27	b	616	BCR	C29-C30-C25	2.38	113.89	110.44
25	C	506	CLA	CHB-C4A-NA	2.37	127.82	124.40
33	j	101	STE	O2-C1-C2	2.37	121.50	114.00
29	D	407	LMG	O3-C3-C2	-2.37	104.79	110.38
29	c	522	LMG	C40-C39-C38	-2.37	102.39	114.37
29	c	519	LMG	C40-C39-C38	-2.37	102.39	114.37
25	D	404	CLA	O2D-CGD-CBD	2.37	115.37	111.23
27	K	101	BCR	C15-C16-C17	-2.36	118.68	123.52
29	M	101	LMG	O6-C1-O1	-2.36	104.46	110.04
25	C	510	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
25	C	508	CLA	CHD-C1D-C2D	2.36	130.39	125.49
27	t	101	BCR	C7-C8-C9	-2.36	122.75	126.23
32	c	516	DGD	C8B-C7B-C6B	-2.36	102.45	114.37
27	t	101	BCR	C35-C13-C14	-2.36	119.00	122.82
25	B	605	CLA	C16-C15-C13	-2.36	108.14	115.97
30	E	101	LHG	C18-C17-C16	-2.36	102.46	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	601	CLA	CHD-C1D-ND	-2.35	121.49	124.80
27	A	610	BCR	C38-C26-C25	-2.35	121.92	124.48
25	A	607	CLA	C2D-C1D-ND	-2.35	107.80	110.13
25	c	504	CLA	C1-C2-C3	-2.35	122.34	126.20
28	A	611	PL9	O2-C1-C6	2.35	124.22	120.48
33	m	102	STE	C3-C2-C1	-2.35	108.37	114.51
25	D	403	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
25	b	612	CLA	C7-C6-C5	-2.35	107.00	113.26
25	B	605	CLA	O1D-CGD-CBD	2.35	129.15	124.52
25	B	613	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
25	b	604	CLA	O1A-CGA-CBA	2.34	132.95	123.78
25	C	513	CLA	CHB-C4A-NA	2.34	127.78	124.40
25	b	604	CLA	CHD-C1D-ND	-2.34	121.51	124.80
32	C	515	DGD	C6D-O5D-C1E	2.34	118.81	113.80
25	c	511	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
28	A	611	PL9	O2-C1-C2	-2.34	116.51	121.83
25	C	509	CLA	CMB-C2B-C3B	2.33	132.03	126.55
25	B	615	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
25	C	511	CLA	CHB-C4A-NA	2.33	127.76	124.40
25	B	605	CLA	C3B-C4B-NB	-2.32	108.45	110.53
27	a	611	BCR	C7-C8-C9	-2.32	122.80	126.23
32	H	102	DGD	C1D-C2D-C3D	-2.32	105.12	110.01
25	a	610	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
27	H	101	BCR	C24-C23-C22	-2.32	122.81	126.23
25	D	404	CLA	C3B-C4B-NB	-2.32	108.46	110.53
25	c	509	CLA	CHB-C4A-NA	2.32	127.74	124.40
25	B	605	CLA	CHD-C1D-ND	-2.31	121.55	124.80
27	B	617	BCR	C29-C30-C25	2.31	113.80	110.44
35	F	101	HEM	CHD-C4C-C3C	2.31	129.11	125.21
25	b	603	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
29	c	522	LMG	C38-C37-C36	-2.31	102.68	114.37
25	C	508	CLA	CHB-C4A-NA	2.31	127.73	124.40
29	d	408	LMG	O7-C10-O9	-2.31	117.39	123.33
25	C	509	CLA	CHB-C4A-NA	2.31	127.73	124.40
32	h	103	DGD	C3D-C4D-C5D	-2.31	106.05	110.23
29	A	613	LMG	C38-C37-C36	-2.31	102.70	114.37
25	a	608	CLA	C1-C2-C3	-2.31	122.42	126.20
29	d	409	LMG	O2-C2-C1	-2.31	104.58	110.08
25	c	504	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
32	a	617	DGD	CDB-CCB-CBB	-2.30	102.73	114.37
25	A	607	CLA	C1D-ND-C4D	2.30	107.93	106.31
31	a	616	SQD	O48-C23-O10	-2.30	117.88	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	608	CLA	CHC-C4B-NB	2.30	127.49	124.05
30	l	101	LHG	C11-C10-C9	-2.30	102.76	114.37
25	C	508	CLA	C1-C2-C3	-2.29	122.44	126.20
29	d	409	LMG	C40-C39-C38	-2.29	102.77	114.37
25	C	508	CLA	O1D-CGD-CBD	2.29	129.04	124.52
25	C	508	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
25	b	608	CLA	CHB-C4A-NA	2.29	127.71	124.40
25	B	602	CLA	CHA-C4D-ND	2.29	137.27	132.55
25	C	509	CLA	C16-C15-C13	-2.29	108.36	115.97
31	a	616	SQD	C9-C8-C7	-2.29	105.31	113.69
29	D	409	LMG	C38-C37-C36	-2.28	102.82	114.37
30	l	101	LHG	C20-C19-C18	-2.28	102.85	114.37
29	b	622	LMG	O8-C28-O10	-2.28	117.93	123.63
36	v	201	HEC	C4B-NB-C1B	2.28	107.91	105.21
27	C	514	BCR	C33-C5-C6	-2.28	122.00	124.48
25	B	610	CLA	C1-C2-C3	-2.28	122.47	126.20
32	h	103	DGD	O5D-C1E-C2E	2.28	111.73	108.27
29	d	409	LMG	O7-C10-O9	-2.27	118.39	123.70
25	B	609	CLA	CHB-C4A-NA	2.27	127.68	124.40
25	b	602	CLA	CHB-C1B-NB	2.27	127.46	124.05
30	E	101	LHG	C11-C10-C9	-2.27	102.88	114.37
25	b	612	CLA	CHB-C4A-NA	2.27	127.68	124.40
27	K	102	BCR	C16-C15-C14	-2.27	118.87	123.52
25	B	611	CLA	CHB-C4A-NA	2.27	127.68	124.40
29	c	519	LMG	O1-C7-C8	-2.27	105.30	110.82
25	c	513	CLA	CHB-C4A-NA	2.27	127.67	124.40
25	d	402	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
32	C	515	DGD	CBB-CAB-C9B	-2.27	102.90	114.37
32	A	617	DGD	C4E-C3E-C2E	-2.27	106.85	110.83
25	b	612	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
25	A	606	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
27	C	514	BCR	C7-C8-C9	-2.27	122.88	126.23
31	B	623	SQD	C9-C8-C7	-2.27	105.39	113.69
32	c	518	DGD	O3G-C1D-C2D	-2.27	104.83	108.27
25	b	605	CLA	CHB-C1B-NB	2.27	127.45	124.05
25	C	510	CLA	CHD-C1D-ND	-2.26	121.61	124.80
25	c	510	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
32	c	516	DGD	O5D-C6D-C5D	-2.26	104.32	109.42
32	H	102	DGD	O3E-C3E-C2E	-2.26	105.04	110.38
32	H	102	DGD	CDB-CCB-CBB	-2.26	102.93	114.37
25	B	602	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
25	c	506	CLA	CAC-C3C-C4C	2.26	127.73	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	613	CLA	C16-C15-C13	-2.26	108.45	115.97
29	c	522	LMG	O8-C28-O10	-2.26	117.97	123.63
25	b	603	CLA	CHB-C4A-NA	2.26	127.66	124.40
27	h	102	BCR	C3-C4-C5	-2.26	110.03	114.06
32	C	516	DGD	C5B-C4B-C3B	-2.26	102.96	114.37
27	C	514	BCR	C11-C10-C9	-2.26	124.11	127.28
29	C	518	LMG	C38-C37-C36	-2.26	102.96	114.37
31	F	102	SQD	C46-C45-C44	-2.25	106.39	113.67
25	B	602	CLA	CHC-C4B-NB	2.25	127.43	124.05
29	D	409	LMG	C8-O7-C10	2.25	123.19	117.80
33	b	625	STE	C3-C2-C1	-2.25	108.63	114.51
25	C	505	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
27	b	618	BCR	C15-C16-C17	-2.25	118.92	123.52
25	b	602	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
29	c	521	LMG	O2-C2-C1	-2.25	104.72	110.08
27	h	102	BCR	C16-C15-C14	-2.24	118.93	123.52
25	C	513	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
29	d	409	LMG	O3-C3-C2	-2.24	105.09	110.38
25	c	502	CLA	CHB-C1B-NB	2.24	127.41	124.05
25	c	510	CLA	C1-C2-C3	-2.24	122.52	126.20
27	t	101	BCR	C33-C5-C6	-2.24	122.04	124.48
27	a	611	BCR	C29-C30-C25	2.24	113.69	110.44
26	a	609	PHO	CMA-C3A-C4A	-2.24	109.78	114.61
28	A	611	PL9	C27-C28-C29	-2.24	122.50	127.62
25	c	508	CLA	CHD-C1D-ND	-2.24	121.65	124.80
27	A	610	BCR	C7-C8-C9	-2.24	122.93	126.23
27	B	618	BCR	C33-C5-C6	-2.24	122.05	124.48
27	b	617	BCR	C24-C23-C22	-2.23	122.93	126.23
29	c	521	LMG	C40-C39-C38	-2.23	103.10	114.37
25	D	403	CLA	CHC-C4B-NB	2.23	127.39	124.05
27	c	515	BCR	C33-C5-C6	-2.23	122.05	124.48
25	B	601	CLA	C2A-C1A-CHA	2.23	127.73	123.87
27	C	514	BCR	C27-C26-C25	2.23	125.71	122.70
30	A	614	LHG	O8-C23-C24	2.22	118.61	111.83
25	A	609	CLA	C3B-C4B-NB	-2.22	108.55	110.53
25	B	603	CLA	O2D-CGD-CBD	2.22	115.12	111.23
25	C	502	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
29	b	622	LMG	C40-C39-C38	-2.22	103.14	114.37
27	b	617	BCR	C15-C14-C13	-2.22	124.16	127.28
32	C	515	DGD	O1G-C1A-C2A	-2.22	105.07	111.83
27	a	611	BCR	C15-C16-C17	-2.22	118.98	123.52
25	b	615	CLA	C1-C2-C3	-2.22	122.56	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	101	LHG	C11-C10-C9	-2.22	103.15	114.37
32	A	617	DGD	CAB-C9B-C8B	-2.22	103.15	114.37
29	D	407	LMG	O2-C2-C1	-2.22	104.79	110.08
25	c	508	CLA	CHB-C4A-NA	2.22	127.60	124.40
29	b	622	LMG	O1-C7-C8	-2.22	105.43	110.82
25	b	612	CLA	O1D-CGD-CBD	2.22	128.89	124.52
25	b	605	CLA	C3B-C4B-NB	-2.21	108.55	110.53
36	v	201	HEC	CHD-C1D-ND	2.21	127.10	124.37
25	C	508	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
25	A	606	CLA	O1D-CGD-CBD	2.20	128.87	124.52
27	k	101	BCR	C24-C23-C22	-2.20	122.97	126.23
33	t	102	STE	O2-C1-C2	2.20	120.96	114.00
25	c	511	CLA	O2D-CGD-CBD	2.20	115.08	111.23
27	b	618	BCR	C27-C26-C25	2.20	125.68	122.70
32	C	517	DGD	CAB-C9B-C8B	-2.20	103.23	114.37
25	B	609	CLA	CHC-C4B-NB	2.20	127.35	124.05
25	B	609	CLA	CHA-C1A-NA	-2.20	121.40	126.39
25	b	605	CLA	CMB-C2B-C3B	2.20	131.73	126.55
26	a	609	PHO	O1D-CGD-CBD	2.20	128.06	124.72
25	C	513	CLA	C1-C2-C3	-2.20	122.59	126.20
27	H	101	BCR	C1-C6-C5	-2.20	119.63	122.64
25	B	615	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
28	a	612	PL9	C32-C33-C34	-2.20	122.59	127.62
30	d	406	LHG	C20-C19-C18	-2.20	103.26	114.37
25	b	610	CLA	CHD-C1D-ND	-2.20	121.71	124.80
28	d	405	PL9	C47-C48-C49	-2.20	120.32	127.64
32	c	517	DGD	O2E-C2E-C1E	-2.19	104.85	110.08
25	c	508	CLA	CHD-C4C-NC	2.19	127.63	124.23
25	C	510	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
27	D	405	BCR	C38-C26-C25	-2.19	122.09	124.48
25	c	502	CLA	C4D-CHA-C1A	2.19	123.86	121.24
25	b	604	CLA	C4-C3-C5	2.19	119.03	115.23
25	c	501	CLA	O1D-CGD-CBD	2.19	128.83	124.52
25	c	503	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
32	C	515	DGD	CAB-C9B-C8B	-2.19	103.31	114.37
25	C	505	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
27	H	101	BCR	C16-C15-C14	-2.19	119.05	123.52
25	b	602	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
36	V	201	HEC	C1D-C2D-C3D	-2.18	104.68	106.98
25	b	610	CLA	CHD-C1D-C2D	2.18	130.03	125.49
30	a	614	LHG	C20-C19-C18	-2.18	103.33	114.37
25	C	507	CLA	C2A-C1A-CHA	2.18	127.66	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	610	CLA	C1-C2-C3	-2.18	122.62	126.20
33	B	625	STE	O2-C1-C2	2.18	120.90	114.00
25	h	101	CLA	CHB-C1B-NB	2.18	127.32	124.05
27	B	618	BCR	C35-C13-C14	-2.18	119.28	122.82
29	c	519	LMG	O2-C2-C1	-2.18	104.89	110.08
25	B	601	CLA	O2A-C1-C2	-2.18	99.73	108.11
25	b	606	CLA	CMB-C2B-C1B	-2.18	122.11	125.42
25	c	510	CLA	CHB-C1B-NB	2.18	127.31	124.05
28	d	405	PL9	C27-C28-C29	-2.17	122.65	127.62
27	t	101	BCR	C29-C30-C25	2.17	113.60	110.44
32	c	518	DGD	C8B-C7B-C6B	-2.17	103.39	114.37
30	A	614	LHG	C27-C26-C25	-2.17	103.39	114.37
26	A	608	PHO	CMA-C3A-C4A	-2.17	109.93	114.61
28	d	405	PL9	C8-C7-C3	2.17	117.64	112.03
25	B	615	CLA	C7-C6-C5	-2.17	107.48	113.26
30	B	622	LHG	O8-C23-O10	-2.17	118.20	123.63
28	A	611	PL9	C20-C19-C21	2.17	118.99	115.23
26	d	401	PHO	C3D-C4D-ND	2.17	110.48	107.71
30	A	614	LHG	C11-C10-C9	-2.17	103.42	114.37
27	d	404	BCR	C1-C6-C5	-2.16	119.68	122.64
25	d	403	CLA	CMB-C2B-C3B	2.16	131.64	126.55
32	C	515	DGD	C6B-C5B-C4B	-2.16	103.44	114.37
25	c	508	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
29	c	521	LMG	C42-C41-C40	-2.16	103.44	114.37
25	b	602	CLA	CHD-C1D-ND	-2.16	121.76	124.80
25	a	613	CLA	CHB-C4A-NA	2.16	127.52	124.40
29	D	407	LMG	C38-C37-C36	-2.16	103.45	114.37
25	A	609	CLA	CHD-C4C-NC	2.16	127.58	124.23
27	B	618	BCR	C30-C25-C26	-2.16	119.68	122.64
25	B	613	CLA	CHD-C1D-ND	-2.16	121.76	124.80
32	a	617	DGD	CAB-C9B-C8B	-2.16	103.45	114.37
25	c	507	CLA	C2A-C1A-CHA	2.16	127.61	123.87
32	C	515	DGD	C8B-C7B-C6B	-2.16	103.46	114.37
32	A	617	DGD	O2D-C2D-C1D	-2.16	104.94	110.08
32	A	617	DGD	CBB-CAB-C9B	-2.16	103.47	114.37
30	E	101	LHG	C27-C26-C25	-2.16	103.47	114.37
30	a	614	LHG	O8-C6-C5	-2.15	102.19	108.40
25	c	505	CLA	CHB-C4A-NA	2.15	127.51	124.40
25	C	505	CLA	C1-C2-C3	-2.15	122.67	126.20
25	B	605	CLA	CHB-C4A-NA	2.15	127.51	124.40
32	c	516	DGD	C3G-C2G-C1G	-2.15	106.77	111.78
31	f	101	SQD	C1-O5-C5	-2.15	109.52	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	511	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
30	e	102	LHG	C20-C19-C18	-2.15	103.50	114.37
32	c	516	DGD	CBB-CAB-C9B	-2.15	103.50	114.37
25	b	603	CLA	C6-C7-C8	-2.15	108.83	115.97
25	b	612	CLA	CHA-C1A-NA	-2.15	121.53	126.39
25	h	101	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
29	c	521	LMG	O1-C1-C2	-2.14	105.02	108.27
25	B	613	CLA	CMB-C2B-C3B	2.14	131.59	126.55
25	c	507	CLA	O2D-CGD-CBD	2.14	114.97	111.23
25	c	504	CLA	CHB-C4A-NA	2.14	127.49	124.40
29	c	519	LMG	O8-C28-O10	-2.14	118.28	123.63
29	d	408	LMG	C40-C39-C38	-2.14	103.56	114.37
32	c	517	DGD	CAB-C9B-C8B	-2.14	103.56	114.37
25	B	614	CLA	C1-C2-C3	-2.14	122.69	126.20
26	d	401	PHO	C6-C7-C8	-2.14	108.86	115.97
25	c	513	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
29	b	622	LMG	C1-C2-C3	-2.14	105.52	110.01
26	A	608	PHO	OBD-CAD-C3D	2.13	131.22	127.89
32	h	103	DGD	O6E-C5E-C6E	-2.13	101.16	106.44
25	B	610	CLA	CHB-C1B-NB	2.13	127.25	124.05
27	b	617	BCR	C8-C7-C6	-2.13	121.31	127.00
33	t	104	STE	C3-C2-C1	-2.13	108.95	114.51
27	B	619	BCR	C15-C14-C13	-2.13	124.29	127.28
30	A	614	LHG	C18-C17-C16	-2.13	103.61	114.37
32	h	103	DGD	O5E-C6E-C5E	-2.13	104.09	111.33
25	B	607	CLA	CHC-C4B-NB	2.13	127.24	124.05
25	b	607	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
27	K	102	BCR	C30-C25-C26	-2.13	119.73	122.64
30	A	614	LHG	O8-C6-C5	-2.13	102.27	108.40
32	C	517	DGD	C7B-C6B-C5B	-2.12	103.63	114.37
29	B	621	LMG	O7-C10-O9	-2.12	117.87	123.33
25	a	608	CLA	C1D-ND-C4D	2.12	107.80	106.31
29	M	101	LMG	O2-C2-C1	-2.12	105.02	110.08
27	t	101	BCR	C27-C26-C25	2.12	125.57	122.70
29	d	409	LMG	C38-C37-C36	-2.12	103.64	114.37
25	c	507	CLA	CHD-C1D-ND	-2.12	121.82	124.80
29	M	101	LMG	O1-C7-C8	-2.12	105.66	110.82
29	A	613	LMG	C40-C39-C38	-2.12	103.65	114.37
25	d	403	CLA	CHC-C4B-NB	2.12	127.23	124.05
25	D	404	CLA	CHA-C1A-NA	-2.12	121.60	126.39
25	C	503	CLA	C6-C5-C3	2.12	118.62	113.47
25	B	610	CLA	O1D-CGD-CBD	2.12	128.69	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	V	201	HEC	CAD-CBD-CGD	-2.11	108.06	113.67
25	C	504	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
29	M	101	LMG	C9-C8-C7	-2.11	106.86	111.78
25	b	610	CLA	C7-C6-C5	-2.11	107.63	113.26
35	e	101	HEM	C3B-C2B-C1B	2.11	108.00	106.41
25	c	512	CLA	CHD-C1D-ND	-2.11	121.83	124.80
25	c	513	CLA	CHA-C1A-NA	-2.11	121.62	126.39
25	C	507	CLA	O2D-CGD-CBD	2.11	114.92	111.23
25	c	501	CLA	C3B-C4B-NB	-2.11	108.65	110.53
32	H	102	DGD	CAB-C9B-C8B	-2.11	103.72	114.37
25	d	403	CLA	CHD-C1D-C2D	2.11	129.87	125.49
25	d	403	CLA	CHB-C1B-NB	2.11	127.21	124.05
31	a	615	SQD	O9-S-C6	2.11	109.90	106.76
25	C	510	CLA	O2D-CGD-CBD	2.10	114.91	111.23
32	C	517	DGD	C5B-C4B-C3B	-2.10	103.73	114.37
25	c	503	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
25	B	606	CLA	CHB-C4A-NA	2.10	127.43	124.40
31	a	616	SQD	C45-O47-C7	-2.10	112.77	117.80
25	b	604	CLA	CHD-C4C-NC	2.10	127.49	124.23
29	A	613	LMG	C1-O6-C5	-2.10	109.62	113.72
32	H	102	DGD	O6E-C5E-C4E	2.10	113.48	109.70
30	B	622	LHG	C18-C17-C16	-2.10	103.76	114.37
32	a	617	DGD	CFB-CEB-CDB	-2.10	103.76	114.37
32	H	102	DGD	C7B-C6B-C5B	-2.10	103.76	114.37
25	C	506	CLA	O1D-CGD-CBD	2.10	128.66	124.52
29	m	101	LMG	C40-C39-C38	-2.10	103.77	114.37
25	B	613	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
25	B	609	CLA	CMB-C2B-C3B	2.10	131.48	126.55
32	c	517	DGD	CBB-CAB-C9B	-2.10	103.77	114.37
25	b	607	CLA	CHD-C4C-NC	2.10	127.48	124.23
29	A	613	LMG	O8-C28-O10	-2.10	118.39	123.63
25	B	616	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
32	C	516	DGD	CBB-CAB-C9B	-2.09	103.78	114.37
25	C	503	CLA	CMB-C2B-C3B	2.09	131.48	126.55
29	M	101	LMG	C1-O6-C5	-2.09	109.63	113.72
25	b	601	CLA	CHD-C4C-NC	2.09	127.48	124.23
25	b	602	CLA	CAA-CBA-CGA	-2.09	107.26	113.21
32	a	617	DGD	C5B-C4B-C3B	-2.09	103.79	114.37
27	K	102	BCR	C1-C6-C5	-2.09	119.78	122.64
33	C	520	STE	O2-C1-C2	2.09	120.61	114.00
26	a	609	PHO	O2A-CGA-O1A	-2.09	118.40	123.63
25	a	607	CLA	C7-C6-C5	-2.09	107.70	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	510	CLA	CHD-C4C-NC	2.09	127.47	124.23
25	C	504	CLA	CHD-C1D-ND	-2.09	121.86	124.80
32	C	516	DGD	CAB-C9B-C8B	-2.09	103.82	114.37
29	b	622	LMG	C42-C41-C40	-2.09	103.82	114.37
25	B	607	CLA	O2D-CGD-O1D	-2.09	119.79	123.85
35	e	101	HEM	CAB-C3B-C2B	-2.09	121.65	128.43
25	B	609	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
26	a	609	PHO	O2D-CGD-O1D	-2.08	119.79	123.85
27	D	405	BCR	C30-C25-C26	-2.08	119.79	122.64
25	D	403	CLA	C2B-C1B-NB	-2.08	108.17	110.33
27	B	618	BCR	C7-C8-C9	-2.08	123.15	126.23
25	C	505	CLA	CMB-C2B-C3B	2.08	131.45	126.55
29	D	407	LMG	C40-C39-C38	-2.08	103.85	114.37
25	B	604	CLA	O2D-CGD-CBD	2.08	114.87	111.23
25	C	507	CLA	CMB-C2B-C3B	2.08	131.44	126.55
30	l	101	LHG	C18-C17-C16	-2.08	103.86	114.37
25	b	608	CLA	CHA-C1A-NA	-2.08	121.68	126.39
29	M	101	LMG	O5-C6-C5	-2.08	104.26	111.33
25	C	506	CLA	CMB-C2B-C3B	2.07	131.43	126.55
28	D	406	PL9	C32-C33-C34	-2.07	122.88	127.62
25	B	601	CLA	CHB-C4A-NA	2.07	127.39	124.40
29	M	101	LMG	C35-C34-C33	-2.07	103.89	114.37
25	B	601	CLA	C4-C3-C5	2.07	118.83	115.23
27	k	102	BCR	C29-C30-C25	2.07	113.45	110.44
27	t	101	BCR	C28-C27-C26	-2.07	110.36	114.06
29	d	408	LMG	C38-C37-C36	-2.07	103.91	114.37
35	F	101	HEM	C4D-ND-C1D	2.07	107.66	105.21
33	j	101	STE	C3-C2-C1	-2.07	109.11	114.51
30	B	622	LHG	O8-C6-C5	-2.07	102.44	108.40
25	c	506	CLA	C4-C3-C5	2.07	118.82	115.23
28	d	405	PL9	O2-C1-C2	-2.07	117.13	121.83
25	B	614	CLA	O2D-CGD-CBD	2.07	114.84	111.23
29	c	521	LMG	O7-C10-O9	-2.07	118.87	123.70
28	d	405	PL9	C12-C13-C14	-2.07	122.89	127.62
27	B	618	BCR	C15-C16-C17	-2.07	119.29	123.52
25	D	404	CLA	CHC-C4B-NB	2.07	127.15	124.05
25	B	602	CLA	C1-C2-C3	-2.07	122.81	126.20
32	c	518	DGD	O2D-C2D-C1D	-2.07	105.15	110.08
25	B	612	CLA	O1D-CGD-CBD	2.06	128.59	124.52
25	b	611	CLA	C11-C10-C8	-2.06	109.10	115.97
27	H	101	BCR	C35-C13-C14	-2.06	119.47	122.82
29	D	407	LMG	C1-C2-C3	-2.06	105.67	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	518	LMG	O8-C28-O10	-2.06	118.47	123.63
28	A	611	PL9	C42-C43-C44	-2.06	122.91	127.62
27	h	102	BCR	C30-C25-C26	-2.06	119.82	122.64
29	m	101	LMG	O7-C10-O9	-2.06	118.89	123.70
25	C	501	CLA	CHA-C1A-NA	-2.06	121.73	126.39
25	b	605	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
25	B	608	CLA	C6-C7-C8	-2.06	109.13	115.97
25	B	609	CLA	O1D-CGD-CBD	2.06	128.57	124.52
25	A	606	CLA	C7-C6-C5	-2.06	107.78	113.26
27	B	619	BCR	C34-C9-C10	-2.06	119.48	122.82
29	b	622	LMG	O5-C6-C5	-2.06	104.33	111.33
29	b	622	LMG	C38-C37-C36	-2.05	103.98	114.37
25	C	507	CLA	CHA-C1A-NA	-2.05	121.74	126.39
25	c	502	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
29	B	621	LMG	C38-C37-C36	-2.05	104.00	114.37
25	C	512	CLA	C6-C5-C3	-2.05	108.47	113.47
27	t	101	BCR	C2-C1-C6	2.05	113.42	110.44
29	C	518	LMG	C40-C39-C38	-2.05	104.01	114.37
25	C	501	CLA	CHB-C1B-NB	2.05	127.12	124.05
32	c	518	DGD	C3E-C4E-C5E	-2.05	106.52	110.23
25	b	615	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
36	V	201	HEC	CMC-C2C-C1C	-2.05	122.30	125.42
25	A	609	CLA	CMB-C2B-C3B	2.05	131.37	126.55
25	A	607	CLA	CHD-C1D-C2D	2.05	129.74	125.49
25	B	604	CLA	C2D-C1D-ND	-2.05	108.10	110.13
25	B	616	CLA	CHB-C4A-NA	2.04	127.35	124.40
32	h	103	DGD	C6D-C5D-C4D	2.04	116.36	112.07
25	C	501	CLA	CAC-C3C-C4C	2.04	127.45	124.79
25	B	616	CLA	CHD-C1D-ND	-2.04	121.93	124.80
25	d	402	CLA	CHB-C4A-NA	2.04	127.35	124.40
30	a	614	LHG	C27-C26-C25	-2.04	104.05	114.37
25	C	506	CLA	C1-C2-C3	-2.04	122.85	126.20
29	b	622	LMG	C24-C23-C22	-2.04	104.05	114.37
25	c	513	CLA	C2A-C1A-CHA	2.04	127.40	123.87
25	b	610	CLA	CHB-C1B-NB	2.04	127.11	124.05
31	a	616	SQD	O49-C7-C8	-2.04	115.82	123.78
25	b	610	CLA	CHB-C4A-NA	2.04	127.34	124.40
25	B	601	CLA	CHA-C1A-NA	-2.03	121.78	126.39
33	a	618	STE	C3-C2-C1	-2.03	109.20	114.51
25	B	607	CLA	CMB-C2B-C3B	2.03	131.33	126.55
32	c	516	DGD	C6B-C5B-C4B	-2.03	104.10	114.37
25	b	608	CLA	CMB-C2B-C1B	-2.03	122.33	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	518	LMG	O3-C3-C2	-2.03	105.59	110.38
25	a	610	CLA	C4-C3-C5	2.03	118.75	115.23
25	B	608	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
25	B	607	CLA	CHB-C4A-NA	2.03	127.32	124.40
25	C	502	CLA	CHA-C1A-NA	-2.03	121.80	126.39
25	c	511	CLA	CHB-C1B-NB	2.03	127.09	124.05
36	v	201	HEC	C2B-C1B-NB	-2.03	107.56	109.90
33	B	625	STE	C3-C2-C1	-2.02	109.22	114.51
25	B	616	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
28	a	612	PL9	C50-C49-C48	-2.02	116.58	122.66
25	d	403	CLA	CHB-C4A-NA	2.02	127.32	124.40
33	J	101	STE	O2-C1-C2	2.02	120.39	114.00
32	c	517	DGD	O6E-C1E-O5D	-2.02	105.27	110.04
25	d	402	CLA	C1-C2-C3	-2.02	122.89	126.20
33	E	102	STE	O2-C1-C2	2.02	120.38	114.00
27	B	619	BCR	C1-C6-C5	-2.02	119.88	122.64
33	a	618	STE	O2-C1-C2	2.02	120.37	114.00
25	C	507	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
25	c	501	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
25	c	503	CLA	C11-C12-C13	-2.01	109.27	115.97
32	C	517	DGD	CBB-CAB-C9B	-2.01	104.20	114.37
25	A	609	CLA	CHD-C1D-ND	-2.01	121.97	124.80
30	e	102	LHG	C27-C26-C25	-2.01	104.20	114.37
33	M	102	STE	O2-C1-C2	2.01	120.35	114.00
25	c	504	CLA	CMB-C2B-C3B	2.01	131.28	126.55
25	C	503	CLA	C1D-ND-C4D	2.01	107.72	106.31
25	c	504	CLA	CHD-C1D-ND	-2.01	121.97	124.80
27	T	101	BCR	C4-C5-C6	2.01	125.42	122.70
30	d	406	LHG	C11-C10-C9	-2.01	104.21	114.37
25	C	507	CLA	CHD-C4C-NC	2.01	127.34	124.23
31	B	623	SQD	C25-C24-C23	-2.01	106.34	113.69
28	d	405	PL9	C36-C34-C33	-2.01	116.66	121.17
25	b	606	CLA	O1D-CGD-CBD	2.01	128.47	124.52
31	B	623	SQD	C46-C45-C44	-2.01	107.11	111.78
31	F	102	SQD	O5-C1-C2	-2.00	106.25	110.37
33	X	101	STE	C3-C2-C1	-2.00	109.28	114.51
32	h	103	DGD	O3E-C3E-C2E	-2.00	105.65	110.38
25	B	616	CLA	C4D-CHA-C1A	2.00	123.63	121.24
25	D	404	CLA	CHB-C4A-NA	2.00	127.29	124.40
25	B	608	CLA	CHB-C1B-NB	2.00	127.05	124.05
25	C	512	CLA	CHA-C1A-NA	-2.00	121.86	126.39

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	V	201	HEC	NA
36	v	201	HEC	NA

All (1722) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C2B-C3B-CAB-CBB
25	A	607	CLA	C4B-C3B-CAB-CBB
25	B	607	CLA	C14-C13-C15-C16
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	C2B-C3B-CAB-CBB
25	B	615	CLA	C4B-C3B-CAB-CBB
25	C	504	CLA	C2-C3-C5-C6
25	C	504	CLA	C4-C3-C5-C6
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	a	608	CLA	C2B-C3B-CAB-CBB
25	a	608	CLA	C4B-C3B-CAB-CBB
25	b	604	CLA	C11-C10-C8-C9
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	C2B-C3B-CAB-CBB
25	c	505	CLA	C4B-C3B-CAB-CBB
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	513	CLA	C1A-C2A-CAA-CBA
25	h	101	CLA	CBD-CGD-O2D-CED
27	B	619	BCR	C37-C22-C23-C24
27	D	405	BCR	C23-C24-C25-C26
27	D	405	BCR	C23-C24-C25-C30
27	K	101	BCR	C10-C11-C12-C13
27	K	101	BCR	C11-C12-C13-C14
27	K	101	BCR	C16-C17-C18-C36
27	K	102	BCR	C5-C6-C7-C8
27	a	611	BCR	C35-C13-C14-C15
27	c	514	BCR	C16-C17-C18-C36
27	d	404	BCR	C21-C22-C23-C24
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C21-C22-C23-C24
28	A	611	PL9	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C22-C23-C24-C26
28	A	611	PL9	C32-C33-C34-C35
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C37-C38-C39-C41
28	D	406	PL9	C32-C33-C34-C35
28	D	406	PL9	C42-C43-C44-C45
28	D	406	PL9	C42-C43-C44-C46
28	a	612	PL9	C22-C23-C24-C25
29	A	613	LMG	O6-C1-O1-C7
29	A	613	LMG	O9-C10-O7-C8
29	A	613	LMG	C11-C10-O7-C8
29	D	409	LMG	O1-C7-C8-C9
29	D	409	LMG	O1-C7-C8-O7
29	c	521	LMG	C11-C10-O7-C8
30	A	614	LHG	O1-C1-C2-C3
30	A	614	LHG	C3-O3-P-O5
30	B	622	LHG	C1-C2-C3-O3
30	B	622	LHG	C3-O3-P-O4
30	B	622	LHG	C3-O3-P-O5
30	B	622	LHG	C3-O3-P-O6
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	C3-O3-P-O5
30	D	408	LHG	C4-O6-P-O4
30	E	101	LHG	O1-C1-C2-C3
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O3
30	L	101	LHG	C4-O6-P-O4
30	a	614	LHG	O1-C1-C2-C3
30	a	614	LHG	C3-O3-P-O5
30	a	614	LHG	C3-O3-P-O6
30	d	406	LHG	C3-O3-P-O5
30	d	406	LHG	C3-O3-P-O6
30	d	406	LHG	C4-O6-P-O3
30	d	406	LHG	C4-O6-P-O4
30	d	406	LHG	C4-O6-P-O5
30	e	102	LHG	C1-C2-C3-O3
30	e	102	LHG	C3-O3-P-O5
30	e	102	LHG	C3-O3-P-O6
30	e	102	LHG	C24-C23-O8-C6
30	l	101	LHG	C4-O6-P-O3
31	B	623	SQD	C2-C1-O6-C44
31	B	623	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
31	B	623	SQD	O6-C44-C45-O47
31	B	623	SQD	O49-C7-O47-C45
31	B	623	SQD	C8-C7-O47-C45
31	a	615	SQD	O6-C44-C45-O47
31	a	616	SQD	C8-C7-O47-C45
31	b	619	SQD	C46-C45-O47-C7
31	b	619	SQD	C8-C7-O47-C45
31	f	101	SQD	C2-C1-O6-C44
31	f	101	SQD	O5-C1-O6-C44
32	A	617	DGD	C2B-C1B-O2G-C2G
32	A	617	DGD	O1B-C1B-O2G-C2G
32	A	617	DGD	O2G-C2G-C3G-O3G
25	c	513	CLA	CBD-CGD-O2D-CED
29	c	521	LMG	O10-C28-O8-C9
30	E	101	LHG	O10-C23-O8-C6
30	e	102	LHG	O10-C23-O8-C6
31	b	619	SQD	O10-C23-O48-C46
31	f	101	SQD	O10-C23-O48-C46
28	D	406	PL9	C47-C48-C49-C50
28	D	406	PL9	C47-C48-C49-C51
28	a	612	PL9	C47-C48-C49-C51
30	E	101	LHG	C24-C23-O8-C6
31	b	619	SQD	C24-C23-O48-C46
29	c	522	LMG	O10-C28-O8-C9
25	h	101	CLA	O1D-CGD-O2D-CED
29	D	409	LMG	O9-C10-O7-C8
29	c	521	LMG	O9-C10-O7-C8
31	a	616	SQD	O49-C7-O47-C45
25	B	616	CLA	C3-C5-C6-C7
25	C	509	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
29	c	522	LMG	C29-C28-O8-C9
31	f	101	SQD	C24-C23-O48-C46
25	c	511	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	613	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C40-C39-C41-C42
28	a	612	PL9	C35-C34-C36-C37
25	b	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	b	613	CLA	C2-C3-C5-C6
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C33-C34-C36-C37
28	A	611	PL9	C43-C44-C46-C47
25	B	605	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7
25	h	101	CLA	C3-C5-C6-C7
29	c	521	LMG	C29-C28-O8-C9
28	A	611	PL9	C12-C13-C14-C16
28	D	406	PL9	C32-C33-C34-C36
29	M	101	LMG	O10-C28-O8-C9
31	b	619	SQD	O49-C7-O47-C45
29	c	519	LMG	C11-C10-O7-C8
25	b	615	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
30	d	406	LHG	O2-C2-C3-O3
30	e	102	LHG	O2-C2-C3-O3
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
29	M	101	LMG	C29-C28-O8-C9
32	h	103	DGD	O6E-C5E-C6E-O5E
29	C	518	LMG	C11-C10-O7-C8
32	h	103	DGD	C4E-C5E-C6E-O5E
31	a	615	SQD	C11-C12-C13-C14
25	B	614	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	B	614	CLA	C2-C3-C5-C6
25	b	603	CLA	C2-C3-C5-C6
25	B	601	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	O1A-CGA-O2A-C1
29	c	522	LMG	O6-C5-C6-O5
32	C	515	DGD	O6E-C5E-C6E-O5E
28	A	611	PL9	C9-C11-C12-C13
28	A	611	PL9	C19-C21-C22-C23
28	A	611	PL9	C44-C46-C47-C48
28	D	406	PL9	C34-C36-C37-C38
28	a	612	PL9	C24-C26-C27-C28
28	a	612	PL9	C39-C41-C42-C43
32	c	518	DGD	O1A-C1A-O1G-C1G
29	b	622	LMG	O6-C1-O1-C7
29	c	522	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
31	A	615	SQD	C30-C31-C32-C33
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
29	A	613	LMG	O6-C5-C6-O5
30	d	407	LHG	C24-C25-C26-C27
28	a	612	PL9	C22-C23-C24-C26
36	V	201	HEC	C2C-C3C-CAC-CBC
25	C	512	CLA	CBD-CGD-O2D-CED
29	d	409	LMG	C10-C11-C12-C13
30	d	406	LHG	C1-C2-C3-O3
25	A	609	CLA	C4-C3-C5-C6
28	A	611	PL9	C45-C44-C46-C47
25	A	609	CLA	C2-C3-C5-C6
28	A	611	PL9	C38-C39-C41-C42
25	b	601	CLA	C3-C5-C6-C7
25	b	603	CLA	C3-C5-C6-C7
25	c	508	CLA	CBD-CGD-O2D-CED
26	d	401	PHO	CBD-CGD-O2D-CED
25	B	601	CLA	C6-C7-C8-C9
25	B	601	CLA	C14-C13-C15-C16
25	B	605	CLA	C6-C7-C8-C9
25	B	615	CLA	C11-C10-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	D	404	CLA	C11-C12-C13-C14
25	a	608	CLA	C11-C12-C13-C14
25	b	605	CLA	C14-C13-C15-C16
25	b	612	CLA	C6-C7-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	512	CLA	C6-C7-C8-C9
29	M	101	LMG	O6-C5-C6-O5
29	c	522	LMG	C4-C5-C6-O5
29	b	622	LMG	C2-C1-O1-C7
29	c	522	LMG	C2-C1-O1-C7
30	B	622	LHG	O2-C2-C3-O3
27	B	618	BCR	C7-C8-C9-C34
27	B	619	BCR	C7-C8-C9-C34
27	C	514	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	D	405	BCR	C37-C22-C23-C24
27	K	101	BCR	C11-C12-C13-C35
27	K	102	BCR	C37-C22-C23-C24
27	T	101	BCR	C37-C22-C23-C24
27	d	404	BCR	C37-C22-C23-C24
25	b	605	CLA	C2A-CAA-CBA-CGA
33	a	618	STE	C1-C2-C3-C4
32	a	617	DGD	C2B-C3B-C4B-C5B
29	A	613	LMG	C4-C5-C6-O5
25	a	610	CLA	C13-C15-C16-C17
33	B	624	STE	C1-C2-C3-C4
25	c	511	CLA	O1D-CGD-O2D-CED
33	b	621	STE	C3-C4-C5-C6
25	b	607	CLA	C2C-C3C-CAC-CBC
25	B	614	CLA	C13-C15-C16-C17
25	c	511	CLA	C13-C15-C16-C17
25	c	512	CLA	O1D-CGD-O2D-CED
25	C	508	CLA	C12-C13-C15-C16
25	C	513	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C12-C13-C15
25	c	510	CLA	C11-C10-C8-C7
25	c	513	CLA	C6-C7-C8-C10
25	a	607	CLA	C15-C16-C17-C18
29	C	518	LMG	O9-C10-O7-C8
28	A	611	PL9	C29-C31-C32-C33
28	A	611	PL9	C34-C36-C37-C38
28	A	611	PL9	C39-C41-C42-C43
25	B	613	CLA	C8-C10-C11-C12
30	a	614	LHG	C28-C29-C30-C31
29	b	622	LMG	O6-C5-C6-O5
29	B	621	LMG	C28-C29-C30-C31
29	D	409	LMG	C28-C29-C30-C31
29	d	409	LMG	C28-C29-C30-C31
30	a	614	LHG	C7-C8-C9-C10
30	a	614	LHG	C23-C24-C25-C26
30	e	102	LHG	C23-C24-C25-C26
31	A	615	SQD	C7-C8-C9-C10
25	B	609	CLA	C13-C15-C16-C17
25	B	606	CLA	C2A-CAA-CBA-CGA
36	V	201	HEC	C4C-C3C-CAC-CBC
25	C	506	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	b	612	CLA	C13-C15-C16-C17
25	b	613	CLA	C5-C6-C7-C8
25	b	615	CLA	C10-C11-C12-C13
25	c	507	CLA	C8-C10-C11-C12
25	c	508	CLA	C10-C11-C12-C13
25	d	403	CLA	C10-C11-C12-C13
29	M	101	LMG	C10-C11-C12-C13
30	d	407	LHG	C23-C24-C25-C26
31	b	619	SQD	C23-C24-C25-C26
33	b	625	STE	C1-C2-C3-C4
25	B	615	CLA	C3-C5-C6-C7
25	b	615	CLA	O1D-CGD-O2D-CED
25	A	612	CLA	C15-C16-C17-C18
25	B	601	CLA	C15-C16-C17-C18
25	B	606	CLA	C13-C15-C16-C17
25	C	503	CLA	C5-C6-C7-C8
25	C	506	CLA	C8-C10-C11-C12
25	C	513	CLA	C15-C16-C17-C18
25	b	604	CLA	C5-C6-C7-C8
25	b	606	CLA	C5-C6-C7-C8
25	c	505	CLA	C13-C15-C16-C17
25	c	510	CLA	C10-C11-C12-C13
31	a	616	SQD	C24-C23-O48-C46
30	E	101	LHG	C23-C24-C25-C26
32	c	518	DGD	C1A-C2A-C3A-C4A
25	b	614	CLA	C5-C6-C7-C8
25	A	606	CLA	C15-C16-C17-C18
25	B	615	CLA	C5-C6-C7-C8
25	b	606	CLA	C10-C11-C12-C13
25	c	512	CLA	C10-C11-C12-C13
25	c	507	CLA	C2-C3-C5-C6
29	c	521	LMG	C10-C11-C12-C13
30	l	101	LHG	C7-C8-C9-C10
25	B	606	CLA	C8-C10-C11-C12
25	B	611	CLA	C13-C15-C16-C17
33	x	101	STE	C1-C2-C3-C4
25	c	511	CLA	C15-C16-C17-C18
32	c	518	DGD	O6E-C5E-C6E-O5E
32	A	617	DGD	C2A-C1A-O1G-C1G
32	a	617	DGD	C2A-C1A-O1G-C1G
25	B	613	CLA	C5-C6-C7-C8
25	B	615	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	C10-C11-C12-C13
25	b	606	CLA	C8-C10-C11-C12
25	b	610	CLA	C15-C16-C17-C18
25	c	503	CLA	C5-C6-C7-C8
25	c	503	CLA	C8-C10-C11-C12
25	c	507	CLA	C5-C6-C7-C8
29	m	101	LMG	C38-C39-C40-C41
33	C	519	STE	C1-C2-C3-C4
25	A	612	CLA	C13-C15-C16-C17
25	B	614	CLA	C8-C10-C11-C12
25	C	506	CLA	C13-C15-C16-C17
25	a	610	CLA	C5-C6-C7-C8
25	b	614	CLA	C8-C10-C11-C12
25	c	512	CLA	C8-C10-C11-C12
29	c	521	LMG	O6-C5-C6-O5
25	B	616	CLA	C5-C6-C7-C8
25	b	604	CLA	C10-C11-C12-C13
25	b	608	CLA	C13-C15-C16-C17
25	b	610	CLA	C13-C15-C16-C17
25	c	506	CLA	C8-C10-C11-C12
25	c	509	CLA	C13-C15-C16-C17
25	c	512	CLA	C5-C6-C7-C8
29	c	519	LMG	O6-C5-C6-O5
28	A	611	PL9	C23-C24-C26-C27
25	B	602	CLA	C13-C15-C16-C17
25	C	510	CLA	C15-C16-C17-C18
25	d	403	CLA	C6-C7-C8-C9
28	a	612	PL9	C32-C33-C34-C35
32	C	516	DGD	C2E-C1E-O5D-C6D
32	c	517	DGD	C2E-C1E-O5D-C6D
30	D	408	LHG	O2-C2-C3-O3
25	c	512	CLA	CBA-CGA-O2A-C1
32	c	518	DGD	C2A-C1A-O1G-C1G
25	C	502	CLA	C16-C17-C18-C19
25	a	610	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
25	c	511	CLA	C16-C17-C18-C19
25	d	402	CLA	C16-C17-C18-C20
27	B	618	BCR	C20-C21-C22-C37
27	H	101	BCR	C16-C17-C18-C36
27	K	101	BCR	C35-C13-C14-C15
27	K	102	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
27	K	102	BCR	C20-C21-C22-C37
27	b	618	BCR	C20-C21-C22-C37
27	c	514	BCR	C11-C10-C9-C34
29	M	101	LMG	C4-C5-C6-O5
27	b	618	BCR	C37-C22-C23-C24
27	c	515	BCR	C11-C12-C13-C35
27	t	101	BCR	C7-C8-C9-C34
32	C	516	DGD	CCA-CDA-CEA-CFA
32	C	515	DGD	C4E-C5E-C6E-O5E
25	b	614	CLA	C15-C16-C17-C18
30	d	407	LHG	O1-C1-C2-C3
25	d	402	CLA	C16-C17-C18-C19
25	c	501	CLA	O1D-CGD-O2D-CED
25	c	510	CLA	C3-C5-C6-C7
27	B	618	BCR	C11-C10-C9-C8
27	K	103	BCR	C11-C10-C9-C8
27	T	101	BCR	C12-C13-C14-C15
32	a	617	DGD	O1B-C1B-O2G-C2G
32	c	517	DGD	O6E-C1E-O5D-C6D
25	b	610	CLA	C8-C10-C11-C12
32	A	617	DGD	C1B-C2B-C3B-C4B
25	B	603	CLA	C16-C17-C18-C20
25	C	502	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C20
29	d	408	LMG	C35-C36-C37-C38
30	A	614	LHG	C29-C30-C31-C32
30	d	406	LHG	C28-C29-C30-C31
32	a	617	DGD	C5A-C6A-C7A-C8A
32	c	517	DGD	C8A-C9A-CAA-CBA
33	X	101	STE	C6-C7-C8-C9
30	E	101	LHG	C33-C34-C35-C36
30	d	406	LHG	C26-C27-C28-C29
30	l	101	LHG	C15-C16-C17-C18
31	B	623	SQD	C11-C12-C13-C14
32	C	515	DGD	C4B-C5B-C6B-C7B
32	C	516	DGD	CAB-CBB-CCB-CDB
32	h	103	DGD	CBA-CCA-CDA-CEA
33	t	104	STE	C5-C6-C7-C8
25	c	506	CLA	C13-C15-C16-C17
29	b	622	LMG	C13-C14-C15-C16
29	c	521	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
29	m	101	LMG	C15-C16-C17-C18
30	a	614	LHG	C25-C26-C27-C28
30	e	102	LHG	C26-C27-C28-C29
31	a	615	SQD	C29-C30-C31-C32
31	a	616	SQD	C12-C13-C14-C15
32	h	103	DGD	C6B-C7B-C8B-C9B
33	E	102	STE	C3-C4-C5-C6
33	b	624	STE	C12-C13-C14-C15
33	c	520	STE	C9-C10-C11-C12
33	d	410	STE	C10-C11-C12-C13
33	t	102	STE	C6-C7-C8-C9
29	b	622	LMG	C23-C24-C25-C26
29	c	521	LMG	C30-C31-C32-C33
30	L	101	LHG	C10-C11-C12-C13
30	a	614	LHG	C16-C17-C18-C19
30	d	407	LHG	C29-C30-C31-C32
32	c	516	DGD	C4B-C5B-C6B-C7B
33	E	102	STE	C4-C5-C6-C7
33	I	101	STE	C11-C10-C9-C8
33	a	618	STE	C5-C6-C7-C8
30	A	614	LHG	O1-C1-C2-O2
30	D	408	LHG	O1-C1-C2-O2
30	a	614	LHG	O1-C1-C2-O2
29	D	407	LMG	C31-C32-C33-C34
30	l	101	LHG	C13-C14-C15-C16
30	l	101	LHG	C29-C30-C31-C32
31	a	616	SQD	C17-C18-C19-C20
32	A	617	DGD	C5B-C6B-C7B-C8B
32	C	517	DGD	C5A-C6A-C7A-C8A
33	b	621	STE	C14-C15-C16-C17
25	C	502	CLA	C4B-C3B-CAB-CBB
30	e	102	LHG	C7-C8-C9-C10
29	b	622	LMG	C39-C40-C41-C42
32	A	617	DGD	CCB-CDB-CEB-CFB
32	A	617	DGD	CDB-CEB-CFB-CGB
32	C	515	DGD	C3A-C4A-C5A-C6A
25	B	603	CLA	C16-C17-C18-C19
25	B	612	CLA	C16-C17-C18-C20
25	c	505	CLA	C16-C17-C18-C19
32	a	617	DGD	O1A-C1A-O1G-C1G
29	A	613	LMG	C14-C15-C16-C17
29	C	518	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
30	a	614	LHG	C17-C18-C19-C20
33	H	103	STE	C7-C8-C9-C10
33	M	102	STE	C11-C10-C9-C8
33	a	618	STE	C2-C3-C4-C5
25	b	613	CLA	C8-C10-C11-C12
29	D	409	LMG	C11-C10-O7-C8
29	d	408	LMG	C37-C38-C39-C40
31	A	616	SQD	C9-C10-C11-C12
31	a	615	SQD	C25-C26-C27-C28
32	C	516	DGD	CAA-CBA-CCA-CDA
32	c	518	DGD	C6A-C7A-C8A-C9A
33	t	103	STE	C5-C6-C7-C8
30	B	622	LHG	C23-C24-C25-C26
29	c	521	LMG	C13-C14-C15-C16
29	c	522	LMG	C11-C12-C13-C14
30	D	408	LHG	C11-C12-C13-C14
31	b	619	SQD	C24-C25-C26-C27
32	h	103	DGD	C5B-C6B-C7B-C8B
33	I	101	STE	C6-C7-C8-C9
33	b	625	STE	C7-C8-C9-C10
33	b	626	STE	C5-C6-C7-C8
31	a	616	SQD	O10-C23-O48-C46
25	c	513	CLA	C3A-C2A-CAA-CBA
28	A	611	PL9	C35-C34-C36-C37
29	A	613	LMG	C13-C14-C15-C16
31	A	615	SQD	C11-C12-C13-C14
25	a	610	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C20
32	A	617	DGD	CEB-CFB-CGB-CHB
33	b	624	STE	C13-C14-C15-C16
29	c	521	LMG	C31-C32-C33-C34
30	L	101	LHG	C18-C19-C20-C21
30	a	614	LHG	C18-C19-C20-C21
32	A	617	DGD	C6B-C7B-C8B-C9B
32	c	517	DGD	CBA-CCA-CDA-CEA
33	H	103	STE	C3-C4-C5-C6
29	D	407	LMG	C36-C37-C38-C39
31	A	616	SQD	C14-C15-C16-C17
31	A	616	SQD	C16-C17-C18-C19
32	A	617	DGD	CCA-CDA-CEA-CFA
32	c	516	DGD	C3B-C4B-C5B-C6B
33	b	623	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	b	624	STE	C11-C12-C13-C14
33	b	625	STE	C4-C5-C6-C7
29	D	407	LMG	C33-C34-C35-C36
29	m	101	LMG	C30-C31-C32-C33
30	E	101	LHG	C16-C17-C18-C19
30	E	101	LHG	C32-C33-C34-C35
30	L	101	LHG	C27-C28-C29-C30
30	d	406	LHG	C32-C33-C34-C35
31	A	616	SQD	C24-C25-C26-C27
31	b	619	SQD	C26-C27-C28-C29
32	H	102	DGD	C9A-CAA-CBA-CCA
32	c	518	DGD	C5A-C6A-C7A-C8A
32	h	103	DGD	C2B-C3B-C4B-C5B
33	b	621	STE	C4-C5-C6-C7
33	b	625	STE	C3-C4-C5-C6
33	t	104	STE	C9-C10-C11-C12
36	v	201	HEC	C2C-C3C-CAC-CBC
25	c	512	CLA	O1A-CGA-O2A-C1
29	D	407	LMG	C35-C36-C37-C38
31	a	616	SQD	C10-C11-C12-C13
32	A	617	DGD	C4B-C5B-C6B-C7B
32	c	518	DGD	CBA-CCA-CDA-CEA
33	j	101	STE	C2-C3-C4-C5
25	C	512	CLA	O1D-CGD-O2D-CED
30	A	614	LHG	C32-C33-C34-C35
30	d	406	LHG	C30-C31-C32-C33
33	H	103	STE	C5-C6-C7-C8
25	B	607	CLA	C13-C15-C16-C17
25	b	611	CLA	C13-C15-C16-C17
29	c	519	LMG	C31-C32-C33-C34
30	l	101	LHG	C27-C28-C29-C30
32	C	517	DGD	C4B-C5B-C6B-C7B
33	C	520	STE	C5-C6-C7-C8
33	t	102	STE	C3-C4-C5-C6
33	t	103	STE	C3-C4-C5-C6
33	x	101	STE	C4-C5-C6-C7
28	D	406	PL9	C12-C13-C14-C15
28	a	612	PL9	C42-C43-C44-C45
25	c	503	CLA	C16-C17-C18-C20
33	c	520	STE	C1-C2-C3-C4
27	K	102	BCR	C1-C6-C7-C8
27	b	616	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	k	101	BCR	C1-C6-C7-C8
30	A	614	LHG	C34-C35-C36-C37
30	d	406	LHG	C29-C30-C31-C32
30	d	407	LHG	C26-C27-C28-C29
31	B	623	SQD	C17-C18-C19-C20
31	a	616	SQD	C11-C12-C13-C14
33	X	101	STE	C9-C10-C11-C12
33	x	101	STE	C12-C13-C14-C15
25	C	509	CLA	O1D-CGD-O2D-CED
29	m	101	LMG	C29-C28-O8-C9
32	A	617	DGD	C4A-C5A-C6A-C7A
32	C	517	DGD	CBB-CCB-CDB-CEB
33	t	103	STE	C6-C7-C8-C9
30	A	614	LHG	C9-C10-C11-C12
31	F	102	SQD	C25-C26-C27-C28
32	A	617	DGD	CAA-CBA-CCA-CDA
32	C	517	DGD	CCA-CDA-CEA-CFA
30	B	622	LHG	C13-C14-C15-C16
29	D	407	LMG	C17-C18-C19-C20
30	E	101	LHG	C25-C26-C27-C28
30	e	102	LHG	C27-C28-C29-C30
31	f	101	SQD	C33-C34-C35-C36
33	X	101	STE	C4-C5-C6-C7
33	X	101	STE	C7-C8-C9-C10
29	M	101	LMG	C34-C35-C36-C37
30	A	614	LHG	C11-C12-C13-C14
33	H	103	STE	C12-C13-C14-C15
33	t	104	STE	C7-C8-C9-C10
27	T	101	BCR	C18-C19-C20-C21
27	c	514	BCR	C10-C11-C12-C13
25	B	602	CLA	C16-C17-C18-C20
29	A	613	LMG	C34-C35-C36-C37
29	D	407	LMG	C37-C38-C39-C40
29	b	622	LMG	C32-C33-C34-C35
30	L	101	LHG	C32-C33-C34-C35
30	a	614	LHG	C10-C11-C12-C13
31	A	616	SQD	C15-C16-C17-C18
33	b	621	STE	C10-C11-C12-C13
33	b	625	STE	C5-C6-C7-C8
31	a	615	SQD	C7-C8-C9-C10
25	B	606	CLA	C11-C10-C8-C9
25	b	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	M	101	LMG	C14-C15-C16-C17
30	e	102	LHG	C12-C13-C14-C15
29	m	101	LMG	C11-C12-C13-C14
30	a	614	LHG	C31-C32-C33-C34
30	l	101	LHG	C32-C33-C34-C35
31	B	623	SQD	C13-C14-C15-C16
32	H	102	DGD	C7A-C8A-C9A-CAA
32	C	516	DGD	O6E-C1E-O5D-C6D
29	B	621	LMG	C29-C30-C31-C32
29	B	621	LMG	C36-C37-C38-C39
31	a	615	SQD	C14-C15-C16-C17
32	c	516	DGD	C4A-C5A-C6A-C7A
25	B	605	CLA	C8-C10-C11-C12
25	C	512	CLA	C13-C15-C16-C17
29	M	101	LMG	C13-C14-C15-C16
29	b	622	LMG	C41-C42-C43-C44
32	C	515	DGD	C5B-C6B-C7B-C8B
32	H	102	DGD	C1A-C2A-C3A-C4A
29	M	101	LMG	C37-C38-C39-C40
30	A	614	LHG	C25-C26-C27-C28
30	L	101	LHG	C12-C13-C14-C15
31	a	616	SQD	C15-C16-C17-C18
32	h	103	DGD	C3A-C4A-C5A-C6A
33	C	519	STE	C6-C7-C8-C9
31	f	101	SQD	C29-C30-C31-C32
32	c	516	DGD	C5B-C6B-C7B-C8B
33	l	102	STE	C4-C5-C6-C7
25	A	607	CLA	C16-C17-C18-C20
25	C	510	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C19
32	A	617	DGD	C7A-C8A-C9A-CAA
31	f	101	SQD	C8-C7-O47-C45
32	a	617	DGD	C2B-C1B-O2G-C2G
30	a	614	LHG	C15-C16-C17-C18
33	C	519	STE	C3-C4-C5-C6
25	B	604	CLA	C10-C11-C12-C13
29	D	407	LMG	C20-C21-C22-C23
33	k	103	STE	C2-C3-C4-C5
29	C	518	LMG	C33-C34-C35-C36
30	E	101	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	H	101	BCR	C11-C12-C13-C35
27	k	101	BCR	C7-C8-C9-C34
32	c	517	DGD	CAA-CBA-CCA-CDA
33	b	621	STE	C1-C2-C3-C4
29	c	519	LMG	C38-C39-C40-C41
30	a	614	LHG	C27-C28-C29-C30
33	b	620	STE	C11-C12-C13-C14
25	b	607	CLA	C4C-C3C-CAC-CBC
25	B	602	CLA	C16-C17-C18-C19
36	V	201	HEC	C2B-C3B-CAB-CBB
29	A	613	LMG	C18-C19-C20-C21
29	D	407	LMG	C21-C22-C23-C24
29	M	101	LMG	C15-C16-C17-C18
31	B	623	SQD	C16-C17-C18-C19
32	c	518	DGD	C5B-C6B-C7B-C8B
25	B	613	CLA	C4-C3-C5-C6
33	X	101	STE	C3-C4-C5-C6
25	c	508	CLA	C13-C15-C16-C17
25	c	512	CLA	C13-C15-C16-C17
32	C	517	DGD	C7B-C8B-C9B-CAB
30	L	101	LHG	C30-C31-C32-C33
32	H	102	DGD	CCA-CDA-CEA-CFA
33	b	621	STE	C13-C14-C15-C16
25	B	605	CLA	C15-C16-C17-C18
25	B	608	CLA	C15-C16-C17-C18
31	B	623	SQD	C9-C10-C11-C12
30	D	408	LHG	C15-C16-C17-C18
30	E	101	LHG	C15-C16-C17-C18
30	L	101	LHG	C31-C32-C33-C34
33	b	624	STE	C5-C6-C7-C8
25	a	608	CLA	C10-C11-C12-C13
25	b	602	CLA	C10-C11-C12-C13
25	c	505	CLA	C15-C16-C17-C18
25	c	509	CLA	C10-C11-C12-C13
25	c	503	CLA	C16-C17-C18-C19
29	D	407	LMG	C19-C20-C21-C22
30	l	101	LHG	C10-C11-C12-C13
25	C	504	CLA	C11-C12-C13-C14
29	C	518	LMG	C31-C32-C33-C34
30	A	614	LHG	C24-C25-C26-C27
32	h	103	DGD	C8A-C9A-CAA-CBA
33	E	102	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	b	623	STE	C9-C10-C11-C12
32	a	617	DGD	C1B-C2B-C3B-C4B
25	B	612	CLA	C10-C11-C12-C13
29	c	522	LMG	C12-C13-C14-C15
29	d	408	LMG	C38-C39-C40-C41
32	h	103	DGD	C3B-C4B-C5B-C6B
33	b	625	STE	C9-C10-C11-C12
29	A	613	LMG	O1-C7-C8-O7
32	C	516	DGD	C4A-C5A-C6A-C7A
25	a	610	CLA	CBA-CGA-O2A-C1
31	a	616	SQD	C18-C19-C20-C21
32	C	516	DGD	C6A-C7A-C8A-C9A
29	d	409	LMG	O6-C5-C6-O5
29	c	522	LMG	C18-C19-C20-C21
30	a	614	LHG	C32-C33-C34-C35
32	H	102	DGD	C7B-C8B-C9B-CAB
33	b	624	STE	C11-C10-C9-C8
33	x	101	STE	C3-C4-C5-C6
29	c	521	LMG	C11-C12-C13-C14
30	l	101	LHG	C12-C13-C14-C15
31	A	615	SQD	C11-C10-C9-C8
25	c	506	CLA	C2-C1-O2A-CGA
25	c	512	CLA	C16-C17-C18-C20
25	b	604	CLA	C15-C16-C17-C18
25	c	504	CLA	C8-C10-C11-C12
28	d	405	PL9	C47-C48-C49-C50
30	E	101	LHG	C9-C10-C11-C12
32	h	103	DGD	C6A-C7A-C8A-C9A
33	d	410	STE	C5-C6-C7-C8
33	m	102	STE	C4-C5-C6-C7
25	C	501	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	C4-C3-C5-C6
28	a	612	PL9	C45-C44-C46-C47
25	C	506	CLA	C2-C3-C5-C6
30	E	101	LHG	O9-C7-O7-C5
25	b	612	CLA	C10-C11-C12-C13
29	d	408	LMG	C32-C33-C34-C35
30	a	614	LHG	C33-C34-C35-C36
30	d	406	LHG	C12-C13-C14-C15
25	b	609	CLA	C2A-CAA-CBA-CGA
25	B	604	CLA	CBD-CGD-O2D-CED
30	E	101	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	A	613	LMG	C16-C17-C18-C19
29	b	622	LMG	C29-C30-C31-C32
29	d	408	LMG	C31-C32-C33-C34
33	B	626	STE	C9-C10-C11-C12
33	t	104	STE	C4-C5-C6-C7
29	c	521	LMG	C38-C39-C40-C41
29	D	407	LMG	C15-C16-C17-C18
31	a	615	SQD	C35-C36-C37-C38
30	d	407	LHG	O1-C1-C2-O2
33	c	520	STE	C11-C12-C13-C14
25	c	508	CLA	C1A-C2A-CAA-CBA
25	h	101	CLA	C1A-C2A-CAA-CBA
29	M	101	LMG	C29-C30-C31-C32
29	b	622	LMG	C22-C23-C24-C25
30	B	622	LHG	C27-C28-C29-C30
29	M	101	LMG	C39-C40-C41-C42
30	D	408	LHG	C17-C18-C19-C20
33	H	103	STE	C11-C10-C9-C8
25	C	507	CLA	C5-C6-C7-C8
31	f	101	SQD	O49-C7-O47-C45
31	B	623	SQD	C31-C32-C33-C34
33	l	102	STE	C3-C4-C5-C6
33	E	102	STE	C1-C2-C3-C4
25	B	604	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C7
25	B	606	CLA	C6-C7-C8-C10
25	B	606	CLA	C11-C12-C13-C15
25	B	611	CLA	C11-C10-C8-C7
25	B	615	CLA	C11-C10-C8-C7
25	B	616	CLA	C6-C7-C8-C10
25	C	503	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C10-C8-C7
25	C	509	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	C	510	CLA	C12-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C12-C13-C15
25	D	404	CLA	C6-C7-C8-C10
25	a	608	CLA	C6-C7-C8-C10
25	a	608	CLA	C12-C13-C15-C16
25	b	601	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C10-C8-C7
25	b	606	CLA	C6-C7-C8-C10
25	b	614	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C15
25	d	402	CLA	C11-C12-C13-C15
25	d	403	CLA	C11-C12-C13-C15
33	J	101	STE	C1-C2-C3-C4
31	A	615	SQD	C16-C17-C18-C19
25	C	510	CLA	C2-C3-C5-C6
33	H	103	STE	C2-C3-C4-C5
31	F	102	SQD	C32-C33-C34-C35
30	e	102	LHG	C8-C7-O7-C5
25	b	606	CLA	O1D-CGD-O2D-CED
25	B	604	CLA	C11-C12-C13-C14
25	B	606	CLA	C11-C12-C13-C14
25	B	616	CLA	C6-C7-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C9
25	C	508	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	b	601	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C10-C8-C9
25	b	613	CLA	C11-C12-C13-C14
25	b	614	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
30	e	102	LHG	C16-C17-C18-C19
31	A	615	SQD	C13-C14-C15-C16
29	b	622	LMG	C16-C17-C18-C19
32	H	102	DGD	CBB-CCB-CDB-CEB
31	B	623	SQD	C24-C23-O48-C46
25	b	601	CLA	C13-C15-C16-C17
32	a	617	DGD	CAA-CBA-CCA-CDA
29	D	407	LMG	O6-C5-C6-O5
32	c	516	DGD	O6E-C5E-C6E-O5E
29	M	101	LMG	C7-C8-C9-O8
29	b	622	LMG	C7-C8-C9-O8
30	e	102	LHG	C4-C5-C6-O8
31	B	623	SQD	O6-C44-C45-C46
31	a	615	SQD	O6-C44-C45-C46
32	A	617	DGD	C1G-C2G-C3G-O3G
32	a	617	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
33	j	101	STE	C5-C6-C7-C8
25	A	607	CLA	C10-C11-C12-C13
25	h	101	CLA	C8-C10-C11-C12
26	d	401	PHO	O1D-CGD-O2D-CED
33	b	623	STE	C1-C2-C3-C4
25	C	508	CLA	C16-C17-C18-C20
29	c	522	LMG	C15-C16-C17-C18
29	d	409	LMG	C37-C38-C39-C40
30	B	622	LHG	C29-C30-C31-C32
32	A	617	DGD	CBA-CCA-CDA-CEA
29	A	613	LMG	C38-C39-C40-C41
25	c	513	CLA	C8-C10-C11-C12
29	d	409	LMG	C36-C37-C38-C39
30	D	408	LHG	C25-C26-C27-C28
31	A	616	SQD	C7-C8-C9-C10
25	a	610	CLA	O1A-CGA-O2A-C1
32	c	518	DGD	CCA-CDA-CEA-CFA
25	C	506	CLA	C4-C3-C5-C6
25	C	510	CLA	C4-C3-C5-C6
25	B	603	CLA	C5-C6-C7-C8
25	A	607	CLA	C16-C17-C18-C19
28	a	612	PL9	C47-C48-C49-C50
30	d	406	LHG	C33-C34-C35-C36
31	A	616	SQD	C10-C11-C12-C13
32	A	617	DGD	CEA-CFA-CGA-CHA
25	C	513	CLA	C13-C15-C16-C17
29	c	522	LMG	C30-C31-C32-C33
31	A	616	SQD	C11-C12-C13-C14
31	a	615	SQD	C9-C10-C11-C12
33	B	620	STE	C11-C12-C13-C14
25	c	510	CLA	C8-C10-C11-C12
29	b	622	LMG	C17-C18-C19-C20
32	A	617	DGD	C2B-C3B-C4B-C5B
33	b	623	STE	C3-C4-C5-C6
29	D	409	LMG	C7-C8-O7-C10
31	F	102	SQD	C27-C28-C29-C30
32	h	103	DGD	C7A-C8A-C9A-CAA
33	l	102	STE	C13-C14-C15-C16
33	m	102	STE	C3-C4-C5-C6
25	B	603	CLA	C13-C15-C16-C17
25	c	503	CLA	C15-C16-C17-C18
29	d	409	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	A	616	SQD	C32-C33-C34-C35
33	B	620	STE	C9-C10-C11-C12
33	M	102	STE	C5-C6-C7-C8
33	b	620	STE	C4-C5-C6-C7
33	x	101	STE	C11-C10-C9-C8
36	v	201	HEC	C4C-C3C-CAC-CBC
30	D	408	LHG	C13-C14-C15-C16
33	C	521	STE	C7-C8-C9-C10
33	H	103	STE	C1-C2-C3-C4
27	K	101	BCR	C16-C17-C18-C19
27	h	102	BCR	C16-C17-C18-C19
29	A	613	LMG	C36-C37-C38-C39
33	H	103	STE	C11-C12-C13-C14
29	D	409	LMG	C29-C28-O8-C9
30	A	614	LHG	C11-C10-C9-C8
29	D	409	LMG	C12-C13-C14-C15
32	a	617	DGD	C3B-C4B-C5B-C6B
33	M	102	STE	C2-C3-C4-C5
25	c	506	CLA	C4-C3-C5-C6
29	c	522	LMG	C32-C33-C34-C35
31	a	615	SQD	C32-C33-C34-C35
31	a	616	SQD	C11-C10-C9-C8
32	C	517	DGD	C2B-C3B-C4B-C5B
33	j	101	STE	C4-C5-C6-C7
29	d	408	LMG	C34-C35-C36-C37
32	C	516	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C9B-CAB-CBB-CCB
33	t	102	STE	C11-C10-C9-C8
31	a	616	SQD	C31-C32-C33-C34
33	B	625	STE	C7-C8-C9-C10
28	d	405	PL9	C32-C33-C34-C36
33	B	624	STE	C5-C6-C7-C8
33	X	101	STE	C11-C12-C13-C14
29	M	101	LMG	O1-C7-C8-O7
29	b	622	LMG	O7-C8-C9-O8
31	b	619	SQD	C27-C28-C29-C30
32	C	516	DGD	C8B-C9B-CAB-CBB
30	B	622	LHG	C10-C11-C12-C13
33	B	620	STE	C2-C3-C4-C5
29	c	522	LMG	C40-C41-C42-C43
29	d	408	LMG	C30-C31-C32-C33
33	k	103	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	L	101	LHG	C19-C20-C21-C22
31	A	615	SQD	C17-C18-C19-C20
32	a	617	DGD	CFB-CGB-CHB-CIB
32	A	617	DGD	C4E-C5E-C6E-O5E
31	a	615	SQD	C12-C13-C14-C15
29	c	519	LMG	C40-C41-C42-C43
33	x	101	STE	C5-C6-C7-C8
32	H	102	DGD	CDB-CEB-CFB-CGB
29	D	407	LMG	C28-C29-C30-C31
29	D	409	LMG	C34-C35-C36-C37
30	d	406	LHG	C11-C12-C13-C14
29	C	518	LMG	C17-C18-C19-C20
30	B	622	LHG	C28-C29-C30-C31
32	C	517	DGD	CBA-CCA-CDA-CEA
31	a	615	SQD	C19-C20-C21-C22
32	c	516	DGD	CDA-CEA-CFA-CGA
29	c	522	LMG	C14-C15-C16-C17
25	C	506	CLA	C3-C5-C6-C7
31	a	615	SQD	C15-C16-C17-C18
32	C	516	DGD	C2B-C3B-C4B-C5B
29	b	622	LMG	C28-C29-C30-C31
25	c	510	CLA	C15-C16-C17-C18
29	c	521	LMG	C33-C34-C35-C36
25	B	615	CLA	C4-C3-C5-C6
30	l	101	LHG	C9-C10-C11-C12
29	C	518	LMG	C29-C28-O8-C9
25	c	511	CLA	C8-C10-C11-C12
33	d	410	STE	C12-C13-C14-C15
29	b	622	LMG	C15-C16-C17-C18
29	m	101	LMG	O6-C5-C6-O5
30	A	614	LHG	C27-C28-C29-C30
30	A	614	LHG	C30-C31-C32-C33
32	h	103	DGD	CAB-CBB-CCB-CDB
30	E	101	LHG	O1-C1-C2-O2
25	B	604	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C9
25	C	504	CLA	C11-C10-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C9
25	C	510	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	D	404	CLA	C6-C7-C8-C9
25	a	608	CLA	C6-C7-C8-C9
25	a	608	CLA	C14-C13-C15-C16
25	b	603	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	b	606	CLA	C11-C12-C13-C14
25	b	608	CLA	C14-C13-C15-C16
25	c	507	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C10-C8-C9
25	d	402	CLA	C11-C12-C13-C14
25	B	606	CLA	C4B-C3B-CAB-CBB
25	c	512	CLA	C4B-C3B-CAB-CBB
25	d	402	CLA	C4B-C3B-CAB-CBB
25	h	101	CLA	C4B-C3B-CAB-CBB
30	B	622	LHG	C17-C18-C19-C20
30	L	101	LHG	C11-C12-C13-C14
25	c	508	CLA	O1D-CGD-O2D-CED
32	C	517	DGD	C3A-C4A-C5A-C6A
25	C	505	CLA	C10-C11-C12-C13
25	C	513	CLA	C8-C10-C11-C12
25	c	505	CLA	C5-C6-C7-C8
25	b	613	CLA	C16-C17-C18-C19
30	e	102	LHG	C28-C29-C30-C31
32	C	517	DGD	CDB-CEB-CFB-CGB
29	A	613	LMG	C2-C1-O1-C7
31	A	615	SQD	C26-C27-C28-C29
32	C	517	DGD	CAB-CBB-CCB-CDB
30	l	101	LHG	O6-C4-C5-C6
29	d	409	LMG	C34-C35-C36-C37
32	C	517	DGD	CCB-CDB-CEB-CFB
32	a	617	DGD	C4B-C5B-C6B-C7B
25	B	604	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C12-C13-C15
25	B	605	CLA	C6-C7-C8-C10
25	B	607	CLA	C12-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C10
25	B	615	CLA	C6-C7-C8-C10
25	C	506	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	b	603	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C15
25	b	608	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C10-C8-C7
25	c	508	CLA	C11-C10-C8-C7
29	b	622	LMG	C24-C25-C26-C27
25	C	508	CLA	C8-C10-C11-C12
30	L	101	LHG	C9-C10-C11-C12
26	d	401	PHO	C2C-C3C-CAC-CBC
25	c	512	CLA	C3A-C2A-CAA-CBA
30	d	406	LHG	C35-C36-C37-C38
29	d	408	LMG	C33-C34-C35-C36
25	B	606	CLA	C15-C16-C17-C18
25	C	509	CLA	C16-C17-C18-C20
25	B	611	CLA	C8-C10-C11-C12
27	c	515	BCR	C7-C8-C9-C34
31	B	623	SQD	O10-C23-O48-C46
29	D	409	LMG	C13-C14-C15-C16
32	a	617	DGD	C8B-C9B-CAB-CBB
32	c	518	DGD	CCB-CDB-CEB-CFB
29	d	409	LMG	C38-C39-C40-C41
29	m	101	LMG	C19-C20-C21-C22
31	A	615	SQD	C10-C11-C12-C13
32	a	617	DGD	C8A-C9A-CAA-CBA
33	j	101	STE	C1-C2-C3-C4
32	A	617	DGD	CFA-CGA-CHA-CIA
29	c	521	LMG	C15-C16-C17-C18
30	E	101	LHG	C18-C19-C20-C21
33	a	618	STE	C4-C5-C6-C7
29	A	613	LMG	O1-C7-C8-C9
29	C	518	LMG	O1-C7-C8-C9
29	M	101	LMG	O1-C7-C8-C9
29	c	521	LMG	C7-C8-C9-O8
30	E	101	LHG	C4-C5-C6-O8
31	a	616	SQD	C44-C45-C46-O48
32	C	515	DGD	O1G-C1G-C2G-C3G
25	B	608	CLA	C3-C5-C6-C7
29	D	409	LMG	C16-C17-C18-C19
33	m	102	STE	C5-C6-C7-C8
25	b	613	CLA	C16-C17-C18-C20
30	A	614	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
30	a	614	LHG	C29-C30-C31-C32
30	d	407	LHG	C28-C29-C30-C31
26	A	608	PHO	C8-C10-C11-C12
33	X	101	STE	C14-C15-C16-C17
33	d	410	STE	C11-C12-C13-C14
25	c	505	CLA	C4-C3-C5-C6
25	B	615	CLA	C2-C3-C5-C6
25	c	513	CLA	C5-C6-C7-C8
32	a	617	DGD	CFA-CGA-CHA-CIA
25	B	612	CLA	C16-C17-C18-C19
25	D	404	CLA	C16-C17-C18-C19
30	e	102	LHG	O6-C4-C5-O7
30	l	101	LHG	O6-C4-C5-O7
30	d	407	LHG	C27-C28-C29-C30
25	c	512	CLA	C2B-C3B-CAB-CBB
25	h	101	CLA	C2B-C3B-CAB-CBB
27	b	616	BCR	C5-C6-C7-C8
32	c	518	DGD	C4A-C5A-C6A-C7A
33	C	521	STE	C3-C4-C5-C6
29	c	519	LMG	C33-C34-C35-C36
32	c	516	DGD	C8B-C9B-CAB-CBB
30	l	101	LHG	C35-C36-C37-C38
29	C	518	LMG	C38-C39-C40-C41
33	H	103	STE	C6-C7-C8-C9
32	c	517	DGD	C4E-C5E-C6E-O5E
29	d	408	LMG	C36-C37-C38-C39
31	F	102	SQD	C31-C32-C33-C34
25	C	508	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C20
29	C	518	LMG	O1-C7-C8-O7
29	M	101	LMG	O7-C8-C9-O8
29	c	522	LMG	O1-C7-C8-O7
31	A	615	SQD	O6-C44-C45-O47
32	c	518	DGD	C6B-C7B-C8B-C9B
28	A	611	PL9	C4-C3-C7-C8
28	a	612	PL9	C4-C3-C7-C8
31	A	616	SQD	C29-C30-C31-C32
33	C	519	STE	C4-C5-C6-C7
29	A	613	LMG	C35-C36-C37-C38
30	B	622	LHG	C7-C8-C9-C10
32	C	515	DGD	CCA-CDA-CEA-CFA
33	B	620	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	B	618	BCR	C10-C11-C12-C13
33	l	102	STE	C9-C10-C11-C12
25	B	616	CLA	C11-C12-C13-C15
25	D	404	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
29	C	518	LMG	C37-C38-C39-C40
30	D	408	LHG	C32-C33-C34-C35
32	C	515	DGD	C3B-C4B-C5B-C6B
33	k	103	STE	C3-C4-C5-C6
33	x	101	STE	C10-C11-C12-C13
32	c	517	DGD	C1A-C2A-C3A-C4A
25	c	513	CLA	CBA-CGA-O2A-C1
30	l	101	LHG	C30-C31-C32-C33
25	D	404	CLA	C3-C5-C6-C7
25	C	501	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
31	A	615	SQD	C14-C15-C16-C17
32	c	517	DGD	C7A-C8A-C9A-CAA
33	b	624	STE	C9-C10-C11-C12
33	C	520	STE	C6-C7-C8-C9
27	c	514	BCR	C14-C15-C16-C17
33	J	101	STE	C5-C6-C7-C8
28	D	406	PL9	C39-C41-C42-C43
28	D	406	PL9	C44-C46-C47-C48
30	E	101	LHG	C24-C25-C26-C27
30	e	102	LHG	C11-C10-C9-C8
31	f	101	SQD	C30-C31-C32-C33
30	E	101	LHG	C29-C30-C31-C32
32	c	518	DGD	C7A-C8A-C9A-CAA
33	b	626	STE	C1-C2-C3-C4
31	B	623	SQD	C23-C24-C25-C26
31	b	619	SQD	C19-C20-C21-C22
31	A	616	SQD	C24-C23-O48-C46
32	H	102	DGD	O2G-C1B-C2B-C3B
33	E	102	STE	C7-C8-C9-C10
25	c	505	CLA	C2-C3-C5-C6
25	C	509	CLA	C15-C16-C17-C18
30	B	622	LHG	C24-C25-C26-C27
31	A	616	SQD	C27-C28-C29-C30
32	h	103	DGD	C5A-C6A-C7A-C8A
27	B	619	BCR	C35-C13-C14-C15
27	K	103	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
27	b	616	BCR	C20-C21-C22-C37
27	k	101	BCR	C16-C17-C18-C36
25	b	602	CLA	C13-C15-C16-C17
32	H	102	DGD	C2B-C3B-C4B-C5B
25	C	509	CLA	C16-C17-C18-C19
25	c	513	CLA	O1A-CGA-O2A-C1
25	a	613	CLA	C10-C11-C12-C13
25	b	601	CLA	C8-C10-C11-C12
25	c	510	CLA	C13-C15-C16-C17
27	b	617	BCR	C7-C8-C9-C34
25	A	607	CLA	C11-C12-C13-C15
25	B	601	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	b	613	CLA	C12-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C10
25	c	505	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C12-C13-C15
25	d	403	CLA	C12-C13-C15-C16
29	D	407	LMG	C10-C11-C12-C13
29	b	622	LMG	C18-C19-C20-C21
29	c	521	LMG	C40-C41-C42-C43
33	d	410	STE	C3-C4-C5-C6
29	c	522	LMG	C38-C39-C40-C41
30	D	408	LHG	C33-C34-C35-C36
30	d	406	LHG	C25-C26-C27-C28
33	b	620	STE	C3-C4-C5-C6
27	b	616	BCR	C21-C22-C23-C24
25	B	616	CLA	CBA-CGA-O2A-C1
30	d	406	LHG	C15-C16-C17-C18
32	C	516	DGD	C5D-C6D-O5D-C1E
32	c	517	DGD	C5D-C6D-O5D-C1E
25	c	512	CLA	C15-C16-C17-C18
25	C	501	CLA	C2A-CAA-CBA-CGA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	d	403	CLA	C16-C17-C18-C19
29	c	522	LMG	C31-C32-C33-C34
33	b	625	STE	C11-C10-C9-C8
25	c	512	CLA	C4-C3-C5-C6
29	c	519	LMG	O9-C10-O7-C8
29	A	613	LMG	C9-C8-O7-C10
25	B	616	CLA	O1A-CGA-O2A-C1
29	m	101	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	E	101	LHG	C28-C29-C30-C31
25	a	610	CLA	C15-C16-C17-C18
27	b	618	BCR	C14-C15-C16-C17
29	D	409	LMG	C33-C34-C35-C36
30	B	622	LHG	C25-C26-C27-C28
25	B	610	CLA	C16-C17-C18-C19
31	A	616	SQD	C19-C20-C21-C22
32	H	102	DGD	C3A-C4A-C5A-C6A
32	C	515	DGD	O1A-C1A-O1G-C1G
27	B	619	BCR	C11-C10-C9-C8
27	H	101	BCR	C11-C10-C9-C8
27	K	101	BCR	C12-C13-C14-C15
33	x	101	STE	C15-C16-C17-C18
30	E	101	LHG	C11-C12-C13-C14
29	b	622	LMG	O1-C7-C8-C9
31	A	615	SQD	O6-C44-C45-C46
36	V	201	HEC	C4B-C3B-CAB-CBB
33	d	410	STE	C1-C2-C3-C4
35	F	101	HEM	C4C-C3C-CAC-CBC
35	e	101	HEM	C4B-C3B-CAB-CBB
30	D	408	LHG	C29-C30-C31-C32
25	c	505	CLA	C10-C11-C12-C13
33	b	624	STE	C10-C11-C12-C13
33	b	624	STE	C6-C7-C8-C9
29	b	622	LMG	O1-C7-C8-O7
30	E	101	LHG	O7-C5-C6-O8
31	f	101	SQD	O47-C45-C46-O48
32	C	515	DGD	O1G-C1G-C2G-O2G
25	B	608	CLA	C6-C7-C8-C9
25	B	614	CLA	C6-C7-C8-C9
25	B	615	CLA	C11-C12-C13-C14
25	C	505	CLA	C14-C13-C15-C16
25	b	602	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C9
32	c	517	DGD	C9A-CAA-CBA-CCA
32	h	103	DGD	CAA-CBA-CCA-CDA
29	A	613	LMG	C33-C34-C35-C36
29	C	518	LMG	C14-C15-C16-C17
30	D	408	LHG	C14-C15-C16-C17
31	A	616	SQD	C26-C27-C28-C29
32	c	516	DGD	CBB-CCB-CDB-CEB
33	C	520	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	b	623	STE	C7-C8-C9-C10
29	D	409	LMG	O10-C28-O8-C9
30	A	614	LHG	C17-C18-C19-C20
29	C	518	LMG	C15-C16-C17-C18
33	t	103	STE	C4-C5-C6-C7
33	C	521	STE	C10-C11-C12-C13
29	D	409	LMG	C31-C32-C33-C34
33	C	521	STE	C12-C13-C14-C15
29	D	409	LMG	C36-C37-C38-C39
30	E	101	LHG	C30-C31-C32-C33
32	c	516	DGD	O6D-C5D-C6D-O5D
25	B	601	CLA	C3-C5-C6-C7
31	a	615	SQD	C23-C24-C25-C26
25	c	512	CLA	C2-C3-C5-C6
25	D	404	CLA	C10-C11-C12-C13
25	c	504	CLA	C11-C12-C13-C15
31	A	616	SQD	O10-C23-O48-C46
29	D	409	LMG	C37-C38-C39-C40
29	A	613	LMG	C11-C12-C13-C14
29	m	101	LMG	C37-C38-C39-C40
25	B	616	CLA	C11-C12-C13-C14
31	A	616	SQD	C11-C10-C9-C8
31	a	615	SQD	C24-C25-C26-C27
29	D	407	LMG	C12-C13-C14-C15
25	B	601	CLA	C4B-C3B-CAB-CBB
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
33	c	520	STE	C4-C5-C6-C7
25	B	603	CLA	C8-C10-C11-C12
32	c	516	DGD	C6A-C7A-C8A-C9A
32	H	102	DGD	CCB-CDB-CEB-CFB
25	c	513	CLA	C2A-CAA-CBA-CGA
33	k	103	STE	C7-C8-C9-C10
32	c	517	DGD	C3A-C4A-C5A-C6A
29	b	622	LMG	C36-C37-C38-C39
25	B	605	CLA	C12-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C15
25	C	509	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	c	501	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
26	a	609	PHO	C6-C7-C8-C10
32	H	102	DGD	C3B-C4B-C5B-C6B
33	H	103	STE	C4-C5-C6-C7
29	c	519	LMG	C36-C37-C38-C39
32	c	517	DGD	C5A-C6A-C7A-C8A
33	c	520	STE	C11-C10-C9-C8
28	d	405	PL9	C33-C34-C36-C37
25	c	504	CLA	C5-C6-C7-C8
29	b	622	LMG	C11-C10-O7-C8
25	C	511	CLA	C6-C7-C8-C9
25	b	613	CLA	C6-C7-C8-C9
25	b	613	CLA	C14-C13-C15-C16
25	c	513	CLA	C6-C7-C8-C9
25	d	403	CLA	C14-C13-C15-C16
32	C	517	DGD	C3B-C4B-C5B-C6B
33	C	521	STE	C11-C12-C13-C14
25	B	602	CLA	C10-C11-C12-C13
32	c	518	DGD	C2A-C3A-C4A-C5A
33	C	521	STE	C4-C5-C6-C7
29	D	407	LMG	C11-C12-C13-C14
33	k	103	STE	C6-C7-C8-C9
29	D	409	LMG	O7-C8-C9-O8
29	c	521	LMG	O7-C8-C9-O8
31	a	616	SQD	O47-C45-C46-O48
25	C	505	CLA	C15-C16-C17-C18
29	D	407	LMG	C34-C35-C36-C37
29	c	522	LMG	O1-C7-C8-C9
29	c	522	LMG	C7-C8-C9-O8
33	c	520	STE	C15-C16-C17-C18
32	A	617	DGD	O6E-C5E-C6E-O5E
33	d	410	STE	C2-C3-C4-C5
33	m	102	STE	C6-C7-C8-C9
25	B	612	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
31	A	616	SQD	C28-C29-C30-C31
32	c	516	DGD	C4D-C5D-C6D-O5D
30	l	101	LHG	C26-C27-C28-C29
29	b	622	LMG	C10-C11-C12-C13
29	D	407	LMG	C16-C17-C18-C19
29	c	522	LMG	C17-C18-C19-C20
29	c	521	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	b	620	STE	C13-C14-C15-C16
25	B	612	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	b	615	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O1D
30	D	408	LHG	C3-O3-P-O6
30	L	101	LHG	C3-O3-P-O6
30	L	101	LHG	C4-O6-P-O5
30	d	406	LHG	C3-O3-P-O4
30	e	102	LHG	C3-O3-P-O4
30	l	101	LHG	C4-O6-P-O5
28	A	611	PL9	C30-C29-C31-C32
25	B	601	CLA	C2B-C3B-CAB-CBB
25	C	502	CLA	C2B-C3B-CAB-CBB
27	d	404	BCR	C23-C24-C25-C30
25	B	613	CLA	C2-C3-C5-C6
31	F	102	SQD	O6-C44-C45-C46
25	b	603	CLA	C8-C10-C11-C12
27	K	103	BCR	C37-C22-C23-C24
33	a	618	STE	C7-C8-C9-C10
29	C	518	LMG	C19-C20-C21-C22
32	C	515	DGD	C4D-C5D-C6D-O5D
31	B	623	SQD	C35-C36-C37-C38
32	C	516	DGD	C3A-C4A-C5A-C6A
32	A	617	DGD	C2A-C3A-C4A-C5A
25	C	502	CLA	C15-C16-C17-C18
31	b	619	SQD	C11-C12-C13-C14
25	B	607	CLA	C8-C10-C11-C12
25	d	403	CLA	C16-C17-C18-C20
30	d	407	LHG	C30-C31-C32-C33
25	B	604	CLA	O2A-C1-C2-C3
29	m	101	LMG	C9-C8-O7-C10
32	a	617	DGD	C6A-C7A-C8A-C9A
25	A	607	CLA	C15-C16-C17-C18
25	B	616	CLA	C2-C3-C5-C6
32	c	518	DGD	C7B-C8B-C9B-CAB
29	m	101	LMG	C21-C22-C23-C24
27	k	102	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	I	101	STE	C7-C8-C9-C10
30	e	102	LHG	O6-C4-C5-C6
33	B	625	STE	C2-C3-C4-C5
33	b	621	STE	C5-C6-C7-C8
30	a	614	LHG	C19-C20-C21-C22
25	A	607	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C10-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C10-C8-C9
25	c	505	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	c	511	CLA	C14-C13-C15-C16
25	h	101	CLA	C11-C10-C8-C9
25	h	101	CLA	C14-C13-C15-C16
33	b	623	STE	C10-C11-C12-C13
33	x	101	STE	C11-C12-C13-C14
25	B	606	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C12-C13-C15
27	c	514	BCR	C16-C17-C18-C19
27	k	101	BCR	C11-C10-C9-C8
29	c	522	LMG	C13-C14-C15-C16
31	b	619	SQD	O5-C1-O6-C44
25	h	101	CLA	C16-C17-C18-C19
30	e	102	LHG	C24-C25-C26-C27
32	h	103	DGD	C2A-C3A-C4A-C5A
33	c	520	STE	C12-C13-C14-C15
33	M	103	STE	C7-C8-C9-C10
32	C	517	DGD	C6A-C7A-C8A-C9A
33	k	103	STE	C5-C6-C7-C8
30	e	102	LHG	O7-C5-C6-O8
31	b	619	SQD	O6-C44-C45-O47
31	b	619	SQD	O47-C45-C46-O48
29	d	408	LMG	C29-C30-C31-C32
33	B	624	STE	C7-C8-C9-C10
29	d	409	LMG	C14-C15-C16-C17
25	D	403	CLA	C16-C17-C18-C20
33	b	626	STE	C7-C8-C9-C10
32	C	515	DGD	O6D-C5D-C6D-O5D
30	e	102	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	B	610	CLA	C16-C17-C18-C20
25	c	509	CLA	CAA-CBA-CGA-O2A
31	A	616	SQD	C30-C31-C32-C33
31	a	615	SQD	C34-C35-C36-C37
25	B	613	CLA	C15-C16-C17-C18
30	l	101	LHG	C17-C18-C19-C20
31	B	623	SQD	C34-C35-C36-C37
33	b	620	STE	C14-C15-C16-C17
33	t	102	STE	C2-C3-C4-C5
25	b	609	CLA	C16-C17-C18-C20
25	c	509	CLA	C16-C17-C18-C19
30	E	101	LHG	C12-C13-C14-C15
32	C	515	DGD	C8A-C9A-CAA-CBA
32	C	516	DGD	C5B-C6B-C7B-C8B
30	E	101	LHG	C17-C18-C19-C20
29	m	101	LMG	C28-C29-C30-C31
32	h	103	DGD	O2G-C1B-C2B-C3B
31	B	623	SQD	C29-C30-C31-C32
33	B	620	STE	C10-C11-C12-C13
33	C	521	STE	C5-C6-C7-C8
32	c	518	DGD	C4E-C5E-C6E-O5E
29	B	621	LMG	C10-C11-C12-C13
32	A	617	DGD	O1A-C1A-O1G-C1G
25	c	510	CLA	C16-C17-C18-C19
25	B	614	CLA	C14-C13-C15-C16
29	b	622	LMG	C4-C5-C6-O5
25	C	512	CLA	C4B-C3B-CAB-CBB
25	b	613	CLA	C4B-C3B-CAB-CBB
29	C	518	LMG	C16-C17-C18-C19
29	c	519	LMG	C29-C28-O8-C9
25	D	404	CLA	C13-C15-C16-C17
29	m	101	LMG	O10-C28-O8-C9
25	B	601	CLA	C4-C3-C5-C6
25	c	506	CLA	C2-C3-C5-C6
29	M	101	LMG	C17-C18-C19-C20
25	c	509	CLA	C3-C5-C6-C7
31	A	615	SQD	C25-C26-C27-C28
25	D	403	CLA	C16-C17-C18-C19
29	c	519	LMG	C39-C40-C41-C42
29	d	409	LMG	C13-C14-C15-C16
25	b	605	CLA	C12-C13-C15-C16
33	x	101	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	I	101	STE	C9-C10-C11-C12
29	b	622	LMG	C35-C36-C37-C38
30	E	101	LHG	C26-C27-C28-C29
29	c	522	LMG	O7-C8-C9-O8
25	c	508	CLA	C4-C3-C5-C6
33	l	102	STE	C5-C6-C7-C8
29	D	407	LMG	C14-C15-C16-C17
27	B	618	BCR	C16-C17-C18-C36
27	k	101	BCR	C35-C13-C14-C15
29	c	519	LMG	C37-C38-C39-C40
25	C	511	CLA	C8-C10-C11-C12
25	a	613	CLA	C2C-C3C-CAC-CBC
33	l	102	STE	C14-C15-C16-C17
31	F	102	SQD	C44-C45-C46-O48
31	a	616	SQD	C9-C10-C11-C12
29	D	409	LMG	C29-C30-C31-C32
31	b	619	SQD	C12-C13-C14-C15
33	c	520	STE	C7-C8-C9-C10
27	c	514	BCR	C15-C16-C17-C18
25	B	615	CLA	C16-C17-C18-C19
25	b	609	CLA	C15-C16-C17-C18
33	c	520	STE	O2-C1-C2-C3
33	t	104	STE	O1-C1-C2-C3
33	t	104	STE	O2-C1-C2-C3
30	l	101	LHG	C16-C17-C18-C19
32	C	517	DGD	C8A-C9A-CAA-CBA
31	A	616	SQD	C23-C24-C25-C26
31	B	623	SQD	C7-C8-C9-C10
30	E	101	LHG	C11-C10-C9-C8
25	b	607	CLA	C4-C3-C5-C6
33	d	410	STE	C4-C5-C6-C7
33	c	520	STE	O1-C1-C2-C3
33	d	410	STE	O1-C1-C2-C3
31	b	619	SQD	C30-C31-C32-C33
25	A	607	CLA	C14-C13-C15-C16
25	C	502	CLA	C14-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	b	610	CLA	C11-C12-C13-C14
25	c	502	CLA	C6-C7-C8-C9
25	c	504	CLA	C11-C10-C8-C9
25	c	505	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	510	CLA	C14-C13-C15-C16
25	c	511	CLA	C11-C10-C8-C9
26	a	609	PHO	C11-C10-C8-C9
25	A	612	CLA	C16-C17-C18-C19
32	H	102	DGD	O1B-C1B-C2B-C3B
29	m	101	LMG	C17-C18-C19-C20
29	b	622	LMG	C9-C8-O7-C10
32	c	516	DGD	CBA-CCA-CDA-CEA
33	l	102	STE	C10-C11-C12-C13
33	B	626	STE	C7-C8-C9-C10
25	B	603	CLA	C4-C3-C5-C6
33	b	626	STE	C6-C7-C8-C9
31	b	619	SQD	C16-C17-C18-C19
25	B	610	CLA	C15-C16-C17-C18
29	C	518	LMG	C39-C40-C41-C42
25	C	513	CLA	C1A-C2A-CAA-CBA
27	h	102	BCR	C11-C10-C9-C8
25	b	605	CLA	C16-C17-C18-C20
32	C	517	DGD	O6D-C5D-C6D-O5D
32	C	516	DGD	C9A-CAA-CBA-CCA
33	I	101	STE	C4-C5-C6-C7
25	B	605	CLA	C2B-C3B-CAB-CBB
25	B	606	CLA	C2B-C3B-CAB-CBB
25	C	512	CLA	C2B-C3B-CAB-CBB
25	d	402	CLA	C2B-C3B-CAB-CBB
27	B	617	BCR	C1-C6-C7-C8
27	H	101	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
27	K	103	BCR	C1-C6-C7-C8
27	b	617	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
27	d	404	BCR	C23-C24-C25-C26
27	k	102	BCR	C1-C6-C7-C8
35	e	101	HEM	CAD-CBD-CGD-O1D
33	B	624	STE	C2-C3-C4-C5
30	E	101	LHG	C2-C3-O3-P
29	b	622	LMG	C31-C32-C33-C34
32	A	617	DGD	C7B-C8B-C9B-CAB
33	B	625	STE	O2-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O2D
28	A	611	PL9	C12-C11-C9-C10
28	d	405	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C2-C3-C5-C6
32	c	517	DGD	C8B-C9B-CAB-CBB
32	C	517	DGD	C9A-CAA-CBA-CCA
33	d	410	STE	O2-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
27	K	101	BCR	C15-C16-C17-C18
25	B	603	CLA	C6-C7-C8-C10
25	C	505	CLA	C6-C7-C8-C10
25	C	505	CLA	C12-C13-C15-C16
25	b	605	CLA	C11-C12-C13-C15
25	c	512	CLA	C6-C7-C8-C10
32	c	518	DGD	CBB-CCB-CDB-CEB
32	h	103	DGD	C9A-CAA-CBA-CCA
32	c	516	DGD	O1G-C1G-C2G-O2G
29	b	622	LMG	C34-C35-C36-C37
31	F	102	SQD	C29-C30-C31-C32
31	a	616	SQD	C13-C14-C15-C16
33	C	519	STE	C5-C6-C7-C8
36	v	201	HEC	CAD-CBD-CGD-O2D
25	b	602	CLA	CBD-CGD-O2D-CED
29	M	101	LMG	C12-C13-C14-C15
32	c	517	DGD	C7B-C8B-C9B-CAB
33	B	624	STE	C3-C4-C5-C6
27	b	616	BCR	C37-C22-C23-C24
29	c	521	LMG	C16-C17-C18-C19
25	B	601	CLA	C2-C3-C5-C6
28	D	406	PL9	C33-C34-C36-C37
25	C	506	CLA	C2-C1-O2A-CGA
33	C	521	STE	C11-C10-C9-C8
25	C	512	CLA	C16-C17-C18-C20
33	X	101	STE	C5-C6-C7-C8
31	b	619	SQD	C10-C11-C12-C13
33	c	520	STE	C14-C15-C16-C17
29	c	521	LMG	C32-C33-C34-C35
33	B	625	STE	O1-C1-C2-C3
29	b	622	LMG	C42-C43-C44-C45
33	b	621	STE	C7-C8-C9-C10
30	d	407	LHG	C2-C3-O3-P
25	b	607	CLA	C2-C3-C5-C6
32	C	515	DGD	C6A-C7A-C8A-C9A
25	C	509	CLA	C5-C6-C7-C8
26	d	401	PHO	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	c	516	DGD	O1G-C1G-C2G-C3G
35	e	101	HEM	CAD-CBD-CGD-O2D
32	a	617	DGD	O2G-C2G-C3G-O3G
30	L	101	LHG	C25-C26-C27-C28
33	B	624	STE	C4-C5-C6-C7
25	B	603	CLA	C2A-CAA-CBA-CGA
29	m	101	LMG	C33-C34-C35-C36
30	d	406	LHG	C14-C15-C16-C17
32	C	516	DGD	C7A-C8A-C9A-CAA
30	L	101	LHG	C17-C18-C19-C20
30	l	101	LHG	C14-C15-C16-C17
33	b	621	STE	O2-C1-C2-C3
25	C	505	CLA	C16-C17-C18-C19
29	D	407	LMG	C13-C14-C15-C16
32	c	516	DGD	C6B-C7B-C8B-C9B
33	b	620	STE	C5-C6-C7-C8
33	B	624	STE	O2-C1-C2-C3
29	m	101	LMG	C40-C41-C42-C43
32	C	515	DGD	O1G-C1A-C2A-C3A
32	c	516	DGD	O1G-C1A-C2A-C3A
25	b	607	CLA	C16-C17-C18-C19
26	d	401	PHO	CHA-CBD-CGD-O1D
26	d	401	PHO	CHA-CBD-CGD-O2D
27	T	101	BCR	C16-C17-C18-C36
27	b	618	BCR	C16-C17-C18-C36
36	v	201	HEC	CAD-CBD-CGD-O1D
33	b	626	STE	C3-C4-C5-C6
31	a	615	SQD	O47-C45-C46-O48
31	f	101	SQD	O6-C44-C45-O47
29	C	518	LMG	O6-C1-O1-C7
29	M	101	LMG	O6-C1-O1-C7
32	C	516	DGD	O6D-C1D-O3G-C3G
25	b	611	CLA	C15-C16-C17-C18
33	H	103	STE	C10-C11-C12-C13
25	B	601	CLA	C11-C10-C8-C7
30	L	101	LHG	C11-C10-C9-C8
29	B	621	LMG	C30-C31-C32-C33
29	c	519	LMG	C34-C35-C36-C37
30	A	614	LHG	C13-C14-C15-C16
32	A	617	DGD	CBB-CCB-CDB-CEB
25	B	604	CLA	O1D-CGD-O2D-CED
27	h	102	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C11-C10-C8-C9
25	C	502	CLA	C11-C12-C13-C14
25	a	608	CLA	C11-C10-C8-C9
25	h	101	CLA	C11-C12-C13-C14
32	C	516	DGD	CDB-CEB-CFB-CGB
29	b	622	LMG	C8-C7-O1-C1
31	b	619	SQD	C45-C44-O6-C1
32	C	515	DGD	C5D-C6D-O5D-C1E
33	l	102	STE	C11-C12-C13-C14
33	B	624	STE	O1-C1-C2-C3
33	b	621	STE	O1-C1-C2-C3
25	B	613	CLA	C2-C1-O2A-CGA
28	d	405	PL9	C47-C48-C49-C51
25	b	605	CLA	C16-C17-C18-C19
28	a	612	PL9	C23-C24-C26-C27
26	A	608	PHO	C16-C17-C18-C20
26	a	609	PHO	O2A-C1-C2-C3
29	b	622	LMG	C7-C8-O7-C10
32	a	617	DGD	C1G-C2G-O2G-C1B
29	c	522	LMG	C19-C20-C21-C22
30	l	101	LHG	C33-C34-C35-C36
25	C	510	CLA	C8-C10-C11-C12
25	a	610	CLA	C10-C11-C12-C13
32	a	617	DGD	C6B-C7B-C8B-C9B
30	e	102	LHG	C11-C12-C13-C14
36	V	201	HEC	CAD-CBD-CGD-O1D
32	a	617	DGD	C7B-C8B-C9B-CAB
31	A	616	SQD	C13-C14-C15-C16
33	M	102	STE	O1-C1-C2-C3
30	e	102	LHG	C14-C15-C16-C17
33	b	624	STE	C7-C8-C9-C10
29	A	613	LMG	C7-C8-C9-O8
31	b	619	SQD	C44-C45-C46-O48
31	f	101	SQD	C44-C45-C46-O48
32	c	516	DGD	C1G-C2G-C3G-O3G
25	C	510	CLA	CBD-CGD-O2D-CED
31	b	619	SQD	C11-C10-C9-C8
33	b	620	STE	C7-C8-C9-C10
31	a	615	SQD	C27-C28-C29-C30
31	b	619	SQD	C7-C8-C9-C10
25	b	613	CLA	C13-C15-C16-C17
29	M	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	CBA-CCA-CDA-CEA
25	C	512	CLA	C16-C17-C18-C19
25	c	508	CLA	C15-C16-C17-C18
31	a	615	SQD	C13-C14-C15-C16
25	B	601	CLA	C10-C11-C12-C13
30	a	614	LHG	C26-C27-C28-C29
36	V	201	HEC	CAD-CBD-CGD-O2D
30	l	101	LHG	C19-C20-C21-C22
33	c	520	STE	C2-C3-C4-C5
30	B	622	LHG	C26-C27-C28-C29
27	K	101	BCR	C14-C15-C16-C17
25	B	605	CLA	C14-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C14
25	b	601	CLA	C11-C10-C8-C9
25	b	608	CLA	C11-C12-C13-C14
25	c	501	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C10-C8-C9
25	c	510	CLA	C6-C7-C8-C9
26	a	609	PHO	C14-C13-C15-C16
25	c	506	CLA	C16-C17-C18-C20
29	m	101	LMG	O8-C28-C29-C30
30	L	101	LHG	C35-C36-C37-C38
32	c	517	DGD	O6E-C5E-C6E-O5E
32	H	102	DGD	C9B-CAB-CBB-CCB
25	h	101	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	C12-C13-C15-C16
25	a	608	CLA	C11-C12-C13-C15
25	b	608	CLA	C11-C12-C13-C15
25	b	612	CLA	C6-C7-C8-C10
25	c	504	CLA	C11-C10-C8-C7
25	c	510	CLA	C12-C13-C15-C16
32	C	517	DGD	O1A-C1A-O1G-C1G
25	b	613	CLA	C2B-C3B-CAB-CBB
27	B	617	BCR	C5-C6-C7-C8
27	H	101	BCR	C23-C24-C25-C26
27	K	101	BCR	C5-C6-C7-C8
27	K	103	BCR	C5-C6-C7-C8
27	b	617	BCR	C23-C24-C25-C26
27	c	514	BCR	C5-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
29	d	409	LMG	O7-C10-C11-C12
32	c	518	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
33	b	620	STE	C11-C10-C9-C8
25	D	403	CLA	C2-C1-O2A-CGA
25	a	607	CLA	C2-C1-O2A-CGA
25	b	606	CLA	C16-C17-C18-C20
25	C	503	CLA	C10-C11-C12-C13
30	d	407	LHG	C32-C33-C34-C35
31	a	615	SQD	O47-C7-C8-C9
32	a	617	DGD	CCA-CDA-CEA-CFA
25	b	608	CLA	C4-C3-C5-C6
30	D	408	LHG	C1-C2-C3-O3
25	B	611	CLA	C10-C11-C12-C13
29	d	408	LMG	O7-C10-C11-C12
33	M	103	STE	C4-C5-C6-C7
31	a	616	SQD	C14-C15-C16-C17
25	b	608	CLA	C2-C3-C5-C6
28	a	612	PL9	C43-C44-C46-C47
33	x	101	STE	C2-C3-C4-C5
32	H	102	DGD	CAB-CBB-CCB-CDB
25	B	610	CLA	C2A-CAA-CBA-CGA
29	b	622	LMG	O7-C10-C11-C12
32	c	516	DGD	O2G-C1B-C2B-C3B
29	c	522	LMG	C36-C37-C38-C39
25	B	603	CLA	C6-C7-C8-C9
25	B	613	CLA	C11-C12-C13-C14
27	K	102	BCR	C7-C8-C9-C34
27	k	101	BCR	C37-C22-C23-C24
30	A	614	LHG	C2-C3-O3-P
31	f	101	SQD	O48-C23-C24-C25
32	C	515	DGD	C1G-C2G-C3G-O3G
25	B	602	CLA	C1A-C2A-CAA-CBA
25	B	605	CLA	C4B-C3B-CAB-CBB
25	B	610	CLA	C4B-C3B-CAB-CBB
25	C	512	CLA	C1A-C2A-CAA-CBA
25	b	614	CLA	C4B-C3B-CAB-CBB
25	a	608	CLA	C3-C5-C6-C7
25	b	610	CLA	C4-C3-C5-C6
25	c	509	CLA	C4-C3-C5-C6
28	D	406	PL9	C30-C29-C31-C32
32	c	517	DGD	O6D-C1D-O3G-C3G
29	m	101	LMG	O7-C10-C11-C12
25	b	610	CLA	C2-C3-C5-C6
32	A	617	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
33	M	102	STE	C6-C7-C8-C9
25	D	403	CLA	C2C-C3C-CAC-CBC
25	B	613	CLA	CAA-CBA-CGA-O2A
29	A	613	LMG	C10-C11-C12-C13
29	B	621	LMG	O7-C10-C11-C12
29	c	519	LMG	C32-C33-C34-C35
26	d	401	PHO	C8-C10-C11-C12
25	b	611	CLA	CAA-CBA-CGA-O2A
25	A	607	CLA	C11-C10-C8-C7
25	B	615	CLA	C12-C13-C15-C16
25	D	404	CLA	C12-C13-C15-C16
25	a	608	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C12-C13-C15
32	c	517	DGD	CDA-CEA-CFA-CGA
29	M	101	LMG	C28-C29-C30-C31
30	a	614	LHG	C30-C31-C32-C33
32	A	617	DGD	C8B-C9B-CAB-CBB
25	B	616	CLA	O2A-C1-C2-C3
29	m	101	LMG	C7-C8-O7-C10
25	B	612	CLA	CAA-CBA-CGA-O2A
33	J	101	STE	C6-C7-C8-C9
25	b	613	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	A	612	CLA	C16-C17-C18-C20
28	d	405	PL9	C11-C12-C13-C14
25	B	605	CLA	C10-C11-C12-C13
25	b	602	CLA	C8-C10-C11-C12
29	A	613	LMG	C17-C18-C19-C20
33	c	520	STE	C10-C11-C12-C13
33	M	102	STE	O2-C1-C2-C3
29	M	101	LMG	C22-C23-C24-C25
25	B	601	CLA	C3A-C2A-CAA-CBA
25	B	602	CLA	C3A-C2A-CAA-CBA
28	D	406	PL9	C40-C39-C41-C42
33	t	104	STE	C12-C13-C14-C15
25	b	611	CLA	C8-C10-C11-C12
28	a	612	PL9	C33-C34-C36-C37
31	a	615	SQD	C33-C34-C35-C36
32	h	103	DGD	CDA-CEA-CFA-CGA
33	M	103	STE	C1-C2-C3-C4
25	B	602	CLA	C11-C12-C13-C14
25	B	615	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C11-C10-C8-C9
25	C	513	CLA	C14-C13-C15-C16
26	a	609	PHO	C6-C7-C8-C9
33	m	102	STE	C7-C8-C9-C10
25	C	510	CLA	C13-C15-C16-C17
25	C	505	CLA	C4-C3-C5-C6
32	C	515	DGD	O1B-C1B-C2B-C3B
25	h	101	CLA	CAA-CBA-CGA-O2A
25	C	505	CLA	C2-C3-C5-C6
31	B	623	SQD	O5-C5-C6-S
28	a	612	PL9	C37-C38-C39-C40
25	B	612	CLA	CAA-CBA-CGA-O1A
27	c	515	BCR	C7-C8-C9-C10
29	m	101	LMG	C8-C7-O1-C1
31	a	615	SQD	O49-C7-C8-C9
25	c	509	CLA	C2A-CAA-CBA-CGA
30	L	101	LHG	O10-C23-O8-C6
31	b	619	SQD	O6-C44-C45-C46
31	f	101	SQD	O6-C44-C45-C46
25	a	613	CLA	C4C-C3C-CAC-CBC
29	c	521	LMG	C36-C37-C38-C39
29	D	409	LMG	C17-C18-C19-C20
25	b	608	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O2D
26	a	609	PHO	CAD-CBD-CGD-O2D
30	D	408	LHG	C11-C10-C9-C8
30	d	406	LHG	C23-C24-C25-C26
29	c	521	LMG	C14-C15-C16-C17
25	A	606	CLA	C2-C1-O2A-CGA
25	c	510	CLA	CAA-CBA-CGA-O2A
29	D	409	LMG	C11-C12-C13-C14
25	d	403	CLA	C6-C7-C8-C10
33	B	625	STE	C5-C6-C7-C8
33	E	102	STE	O2-C1-C2-C3
25	B	613	CLA	CAA-CBA-CGA-O1A
25	b	611	CLA	CAA-CBA-CGA-O1A
29	b	622	LMG	O9-C10-C11-C12
32	h	103	DGD	O1B-C1B-C2B-C3B
32	c	516	DGD	CCB-CDB-CEB-CFB
30	L	101	LHG	O7-C7-C8-C9
31	A	615	SQD	O47-C7-C8-C9
32	C	515	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	O1D-CGD-O2D-CED
25	h	101	CLA	CAA-CBA-CGA-O1A
32	c	517	DGD	O1B-C1B-C2B-C3B
32	c	517	DGD	CCB-CDB-CEB-CFB
29	c	521	LMG	C42-C43-C44-C45

There are no ring outliers.

133 monomers are involved in 233 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	101	STE	2	0
25	c	511	CLA	3	0
29	c	521	LMG	3	0
25	a	610	CLA	4	0
25	B	615	CLA	1	0
25	C	502	CLA	1	0
29	D	407	LMG	2	0
27	B	617	BCR	1	0
33	b	625	STE	2	0
31	B	623	SQD	2	0
25	B	612	CLA	1	0
25	b	603	CLA	3	0
25	b	604	CLA	3	0
33	H	103	STE	2	0
32	C	517	DGD	2	0
31	A	615	SQD	2	0
27	B	619	BCR	4	0
32	c	518	DGD	3	0
36	v	201	HEC	1	0
27	C	514	BCR	4	0
25	b	613	CLA	3	0
35	e	101	HEM	2	0
30	B	622	LHG	1	0
25	C	508	CLA	3	0
25	B	602	CLA	3	0
27	K	101	BCR	1	0
27	h	102	BCR	2	0
25	b	609	CLA	2	0
27	b	616	BCR	2	0
29	M	101	LMG	2	0
25	B	616	CLA	2	0
25	b	601	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	620	STE	1	0
25	B	606	CLA	5	0
25	C	512	CLA	2	0
25	A	612	CLA	4	0
25	B	609	CLA	1	0
25	A	607	CLA	1	0
30	d	406	LHG	4	0
33	C	519	STE	1	0
35	F	101	HEM	3	0
25	c	508	CLA	2	0
25	C	504	CLA	3	0
32	A	617	DGD	4	0
25	b	615	CLA	3	0
25	c	503	CLA	4	0
25	b	614	CLA	2	0
30	a	614	LHG	2	0
33	b	623	STE	1	0
26	a	609	PHO	1	0
25	b	602	CLA	2	0
25	C	505	CLA	4	0
33	x	101	STE	2	0
33	c	520	STE	1	0
33	B	625	STE	1	0
25	b	611	CLA	2	0
25	B	604	CLA	4	0
27	B	618	BCR	2	0
25	c	513	CLA	5	0
26	d	401	PHO	1	0
31	F	102	SQD	1	0
25	C	511	CLA	1	0
25	h	101	CLA	1	0
25	b	608	CLA	2	0
25	B	607	CLA	2	0
25	c	501	CLA	3	0
22	A	602[A]	OEY	1	0
30	d	407	LHG	1	0
32	c	517	DGD	3	0
25	c	512	CLA	2	0
25	C	506	CLA	1	0
30	A	614	LHG	3	0
31	b	619	SQD	2	0
30	L	101	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	k	102	BCR	1	0
25	a	613	CLA	4	0
27	t	101	BCR	3	0
27	c	514	BCR	2	0
27	A	610	BCR	2	0
29	A	613	LMG	1	0
29	c	519	LMG	1	0
25	B	611	CLA	2	0
25	c	510	CLA	4	0
25	c	505	CLA	3	0
33	b	621	STE	4	0
27	a	611	BCR	1	0
30	D	408	LHG	1	0
25	B	601	CLA	4	0
30	E	101	LHG	2	0
31	f	101	SQD	1	0
30	e	102	LHG	2	0
28	d	405	PL9	1	0
33	I	101	STE	1	0
33	j	101	STE	1	0
27	c	515	BCR	3	0
27	K	102	BCR	2	0
25	b	612	CLA	2	0
32	h	103	DGD	2	0
25	D	403	CLA	1	0
22	a	602[A]	OEY	1	0
25	b	607	CLA	3	0
25	c	507	CLA	3	0
31	a	615	SQD	1	0
31	A	616	SQD	4	0
32	C	516	DGD	3	0
25	c	504	CLA	1	0
25	d	403	CLA	1	0
27	T	101	BCR	3	0
30	l	101	LHG	1	0
25	a	607	CLA	4	0
27	K	103	BCR	1	0
26	D	402	PHO	1	0
33	m	102	STE	1	0
25	B	613	CLA	1	0
25	b	605	CLA	2	0
25	D	404	CLA	1	0

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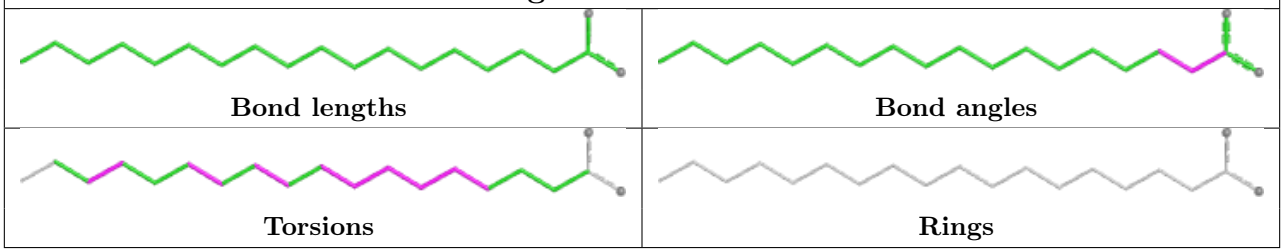
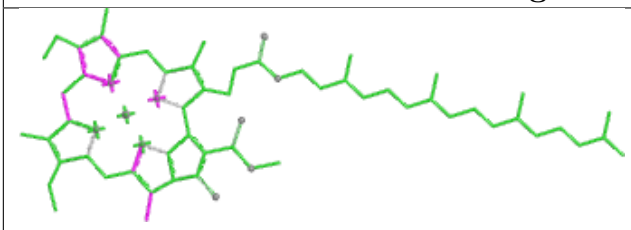
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	C	515	DGD	1	0
27	H	101	BCR	2	0
25	A	606	CLA	3	0
27	D	405	BCR	1	0
29	m	101	LMG	2	0
25	C	507	CLA	1	0
28	A	611	PL9	4	0
25	B	603	CLA	1	0
33	l	102	STE	3	0
25	C	509	CLA	1	0
27	b	617	BCR	2	0
32	H	102	DGD	2	0
28	D	406	PL9	2	0
29	C	518	LMG	1	0
29	D	409	LMG	2	0
28	a	612	PL9	2	0
25	B	614	CLA	3	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.

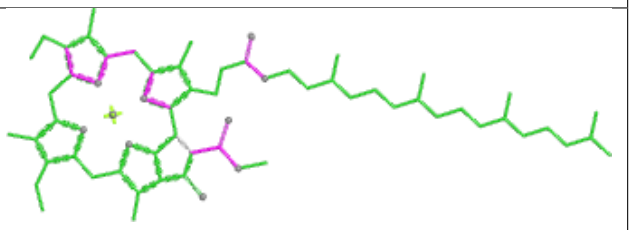
Ligand STE X 101



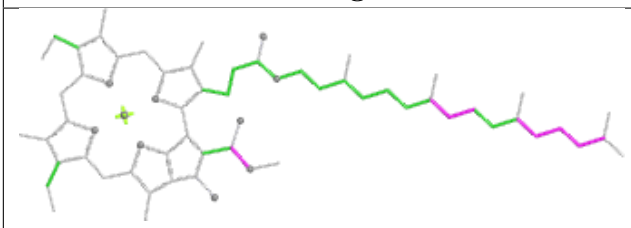
Ligand CLA c 511



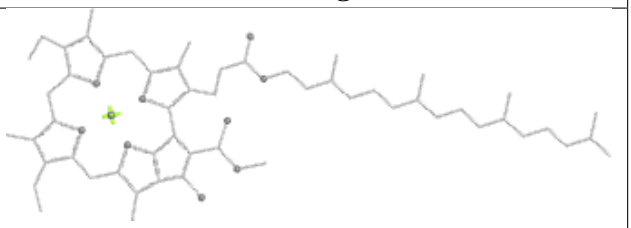
Bond lengths



Bond angles

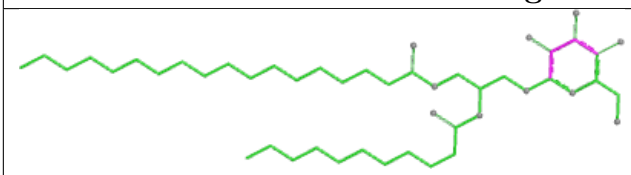


Torsions

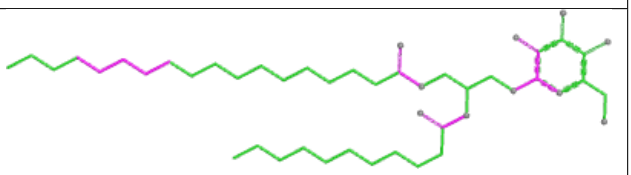


Rings

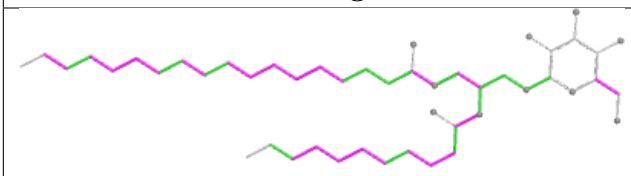
Ligand LMG c 521



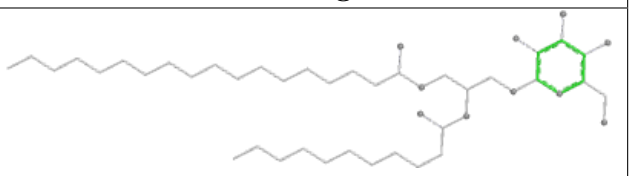
Bond lengths



Bond angles

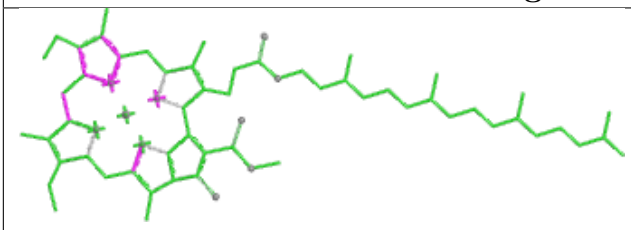


Torsions

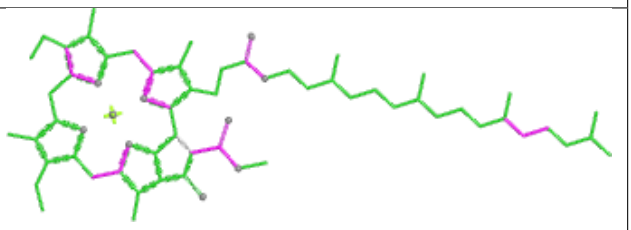


Rings

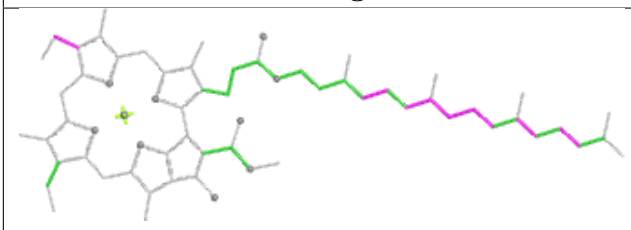
Ligand CLA B 605



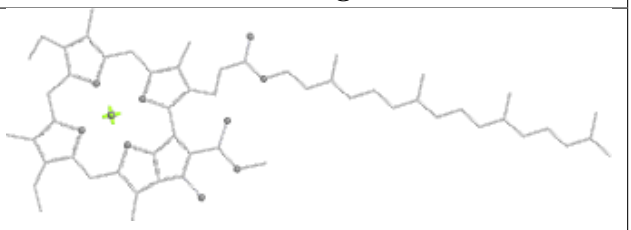
Bond lengths



Bond angles

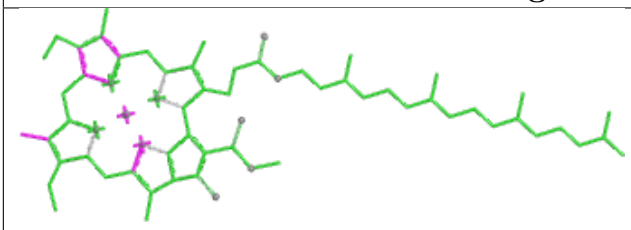


Torsions

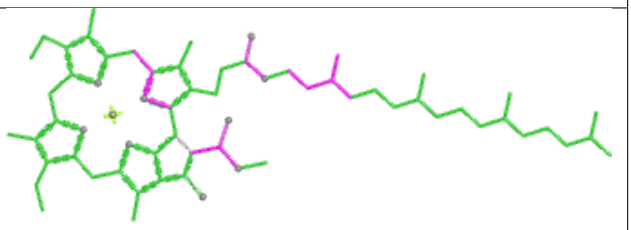


Rings

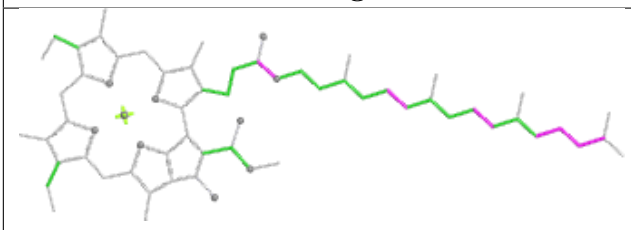
Ligand CLA a 610



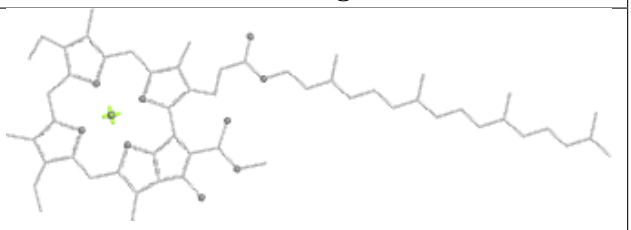
Bond lengths



Bond angles

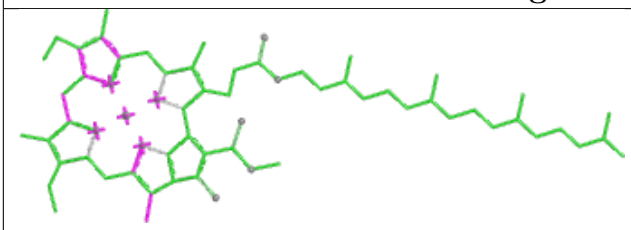


Torsions

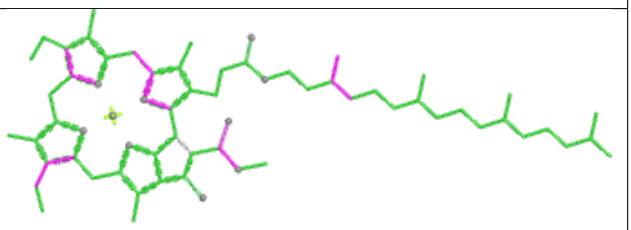


Rings

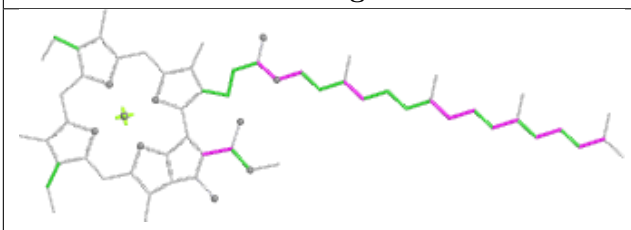
Ligand CLA c 506



Bond lengths



Bond angles



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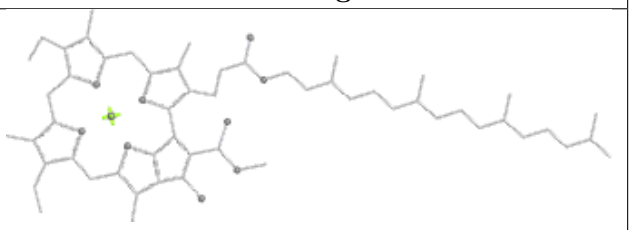
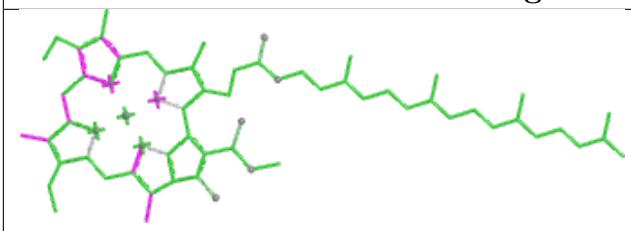
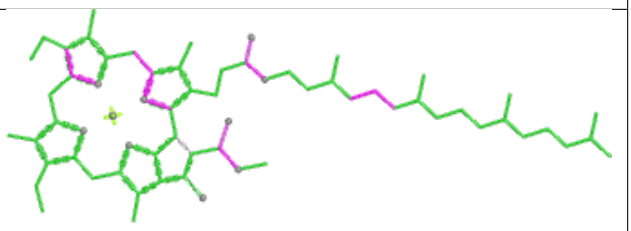


Rings

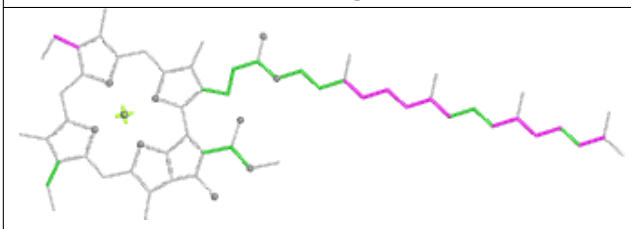
Ligand CLA B 615



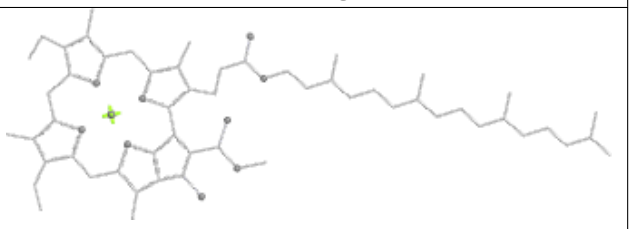
Bond lengths



Bond angles

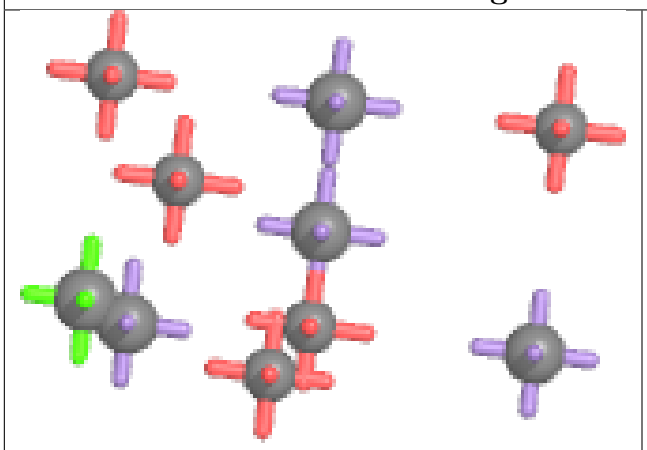


Torsions

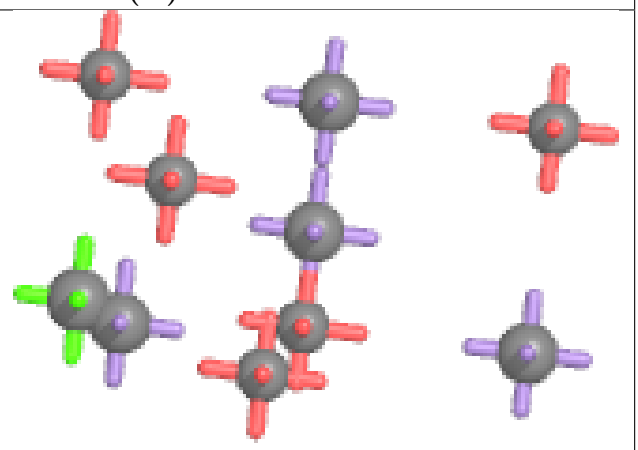


Rings

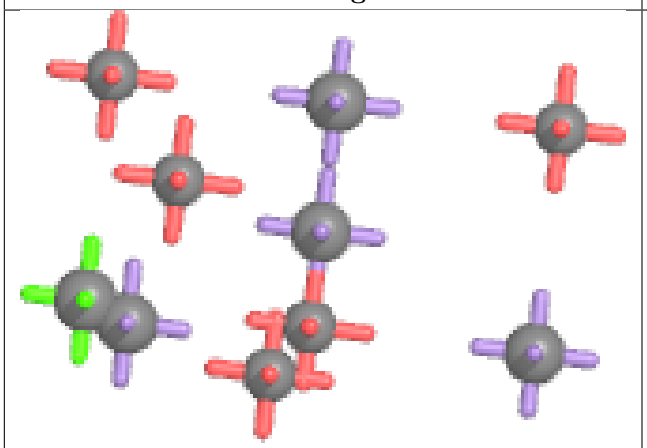
Ligand OEX A 601 (C)



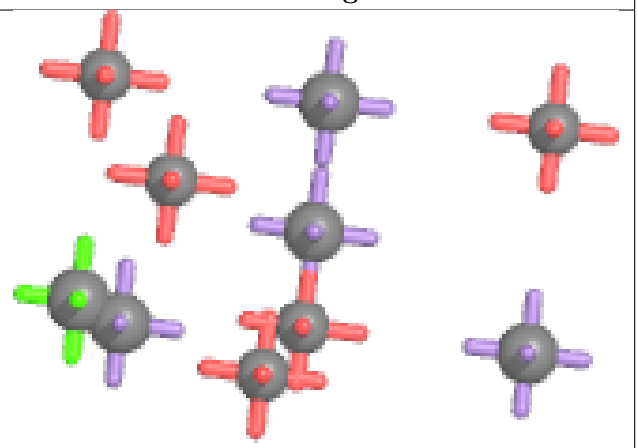
Bond lengths



Bond angles

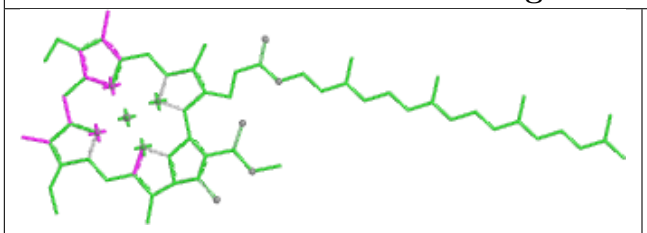


Torsions

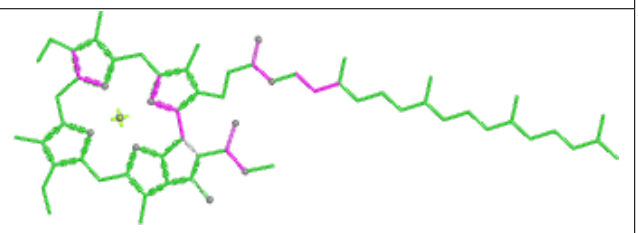


Rings

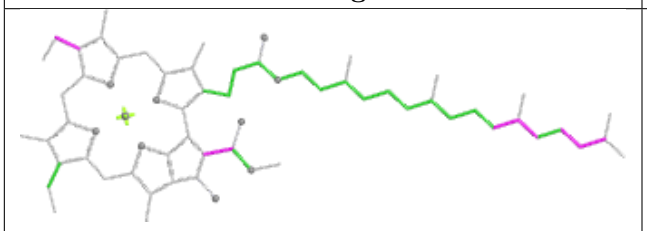
Ligand CLA C 502



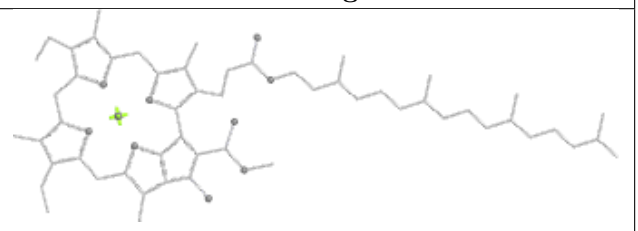
Bond lengths



Bond angles

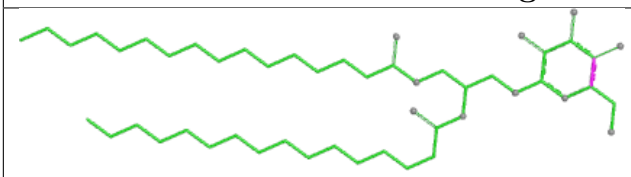


Torsions

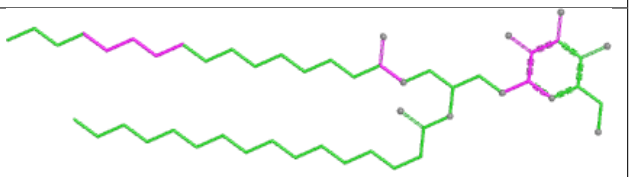


Rings

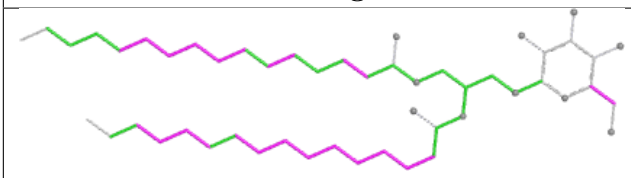
Ligand LMG D 407



Bond lengths



Bond angles



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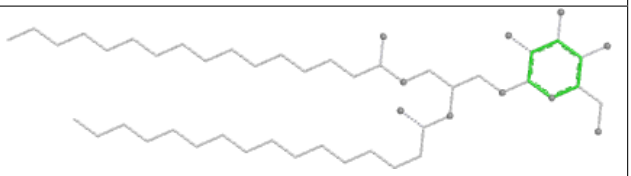
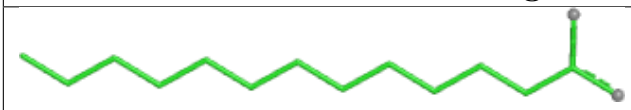


Rings

Ligand STE M 102



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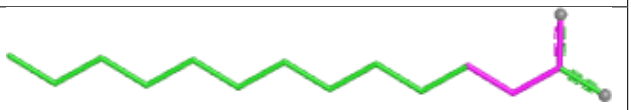
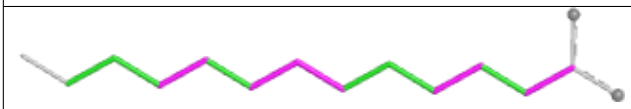


Bond angles



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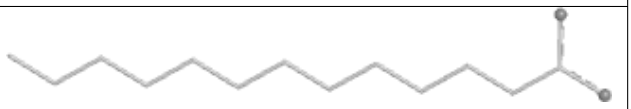
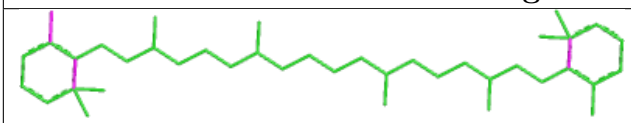


Rings

Ligand BCR B 617



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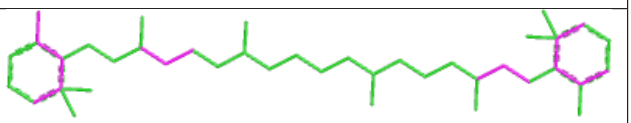
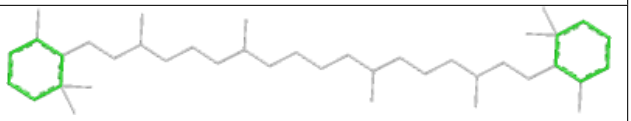


Bond angles

Torsions

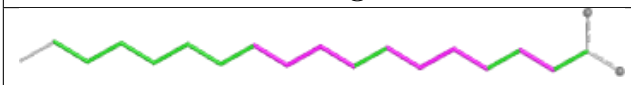


Rings

Ligand STE b 625

Bond lengths

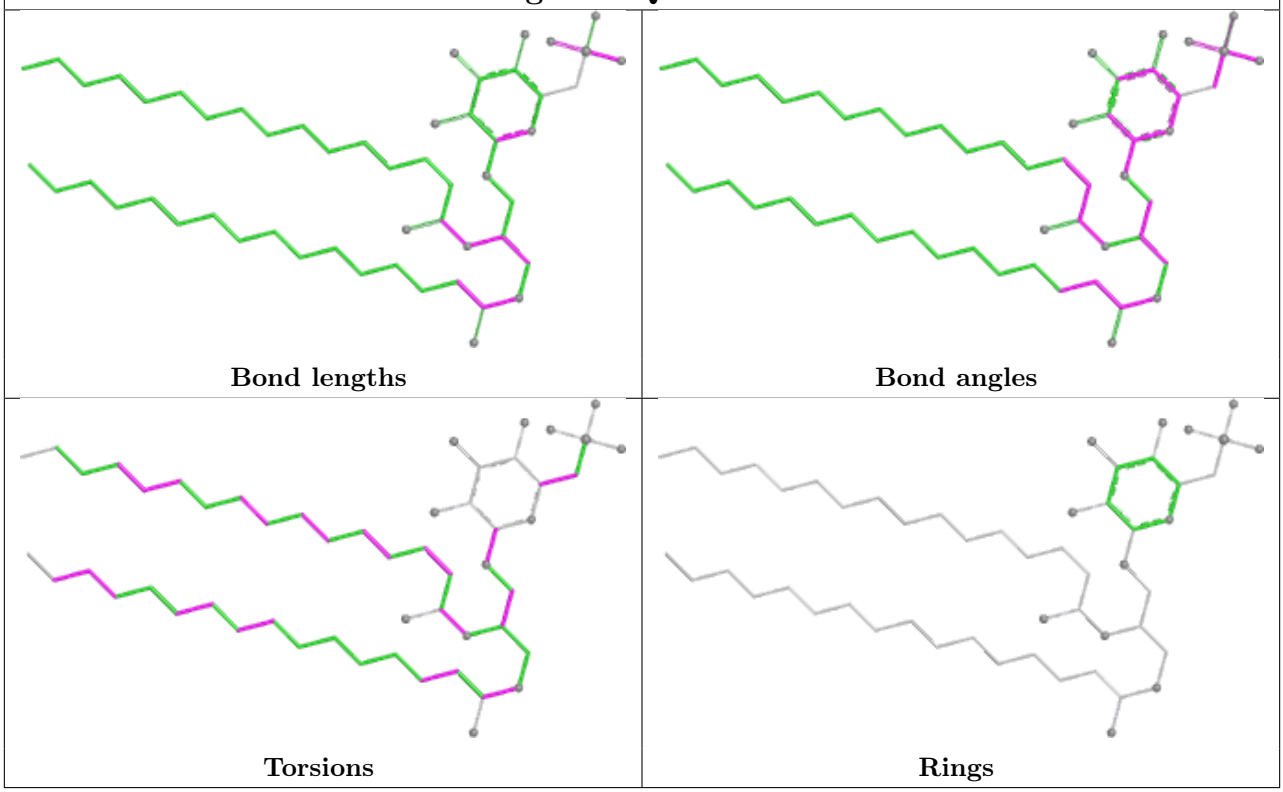
Bond angles



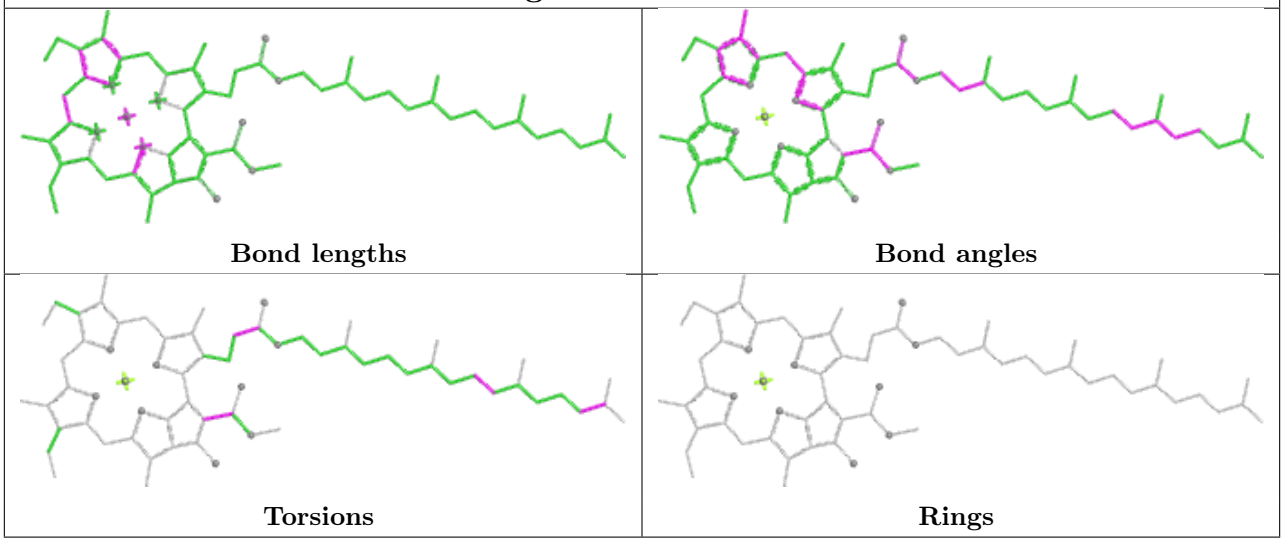
Torsions

Rings

Ligand SQD B 623



Ligand CLA B 612



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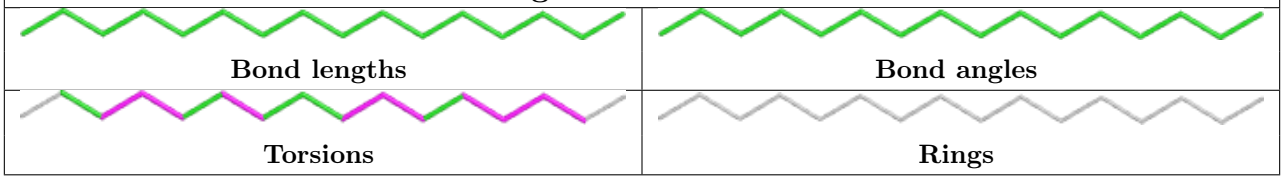
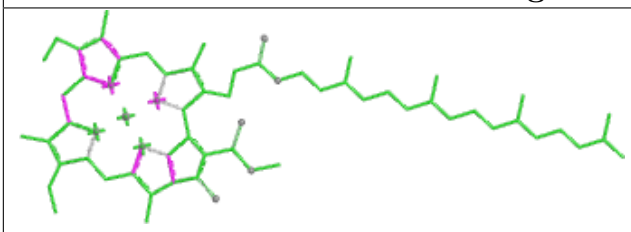
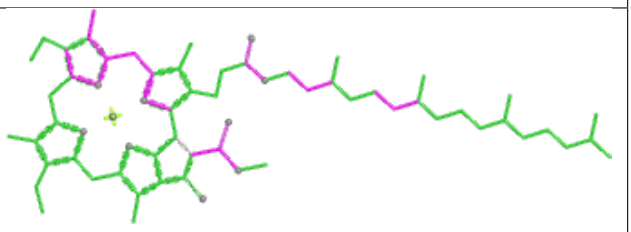


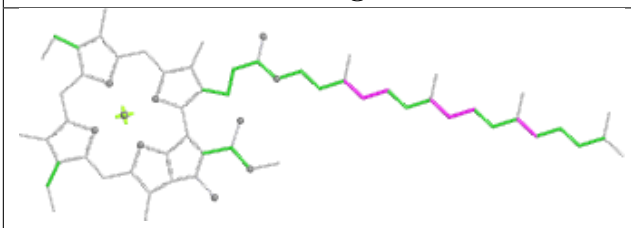
Ligand CLA b 603



Bond lengths



Bond angles



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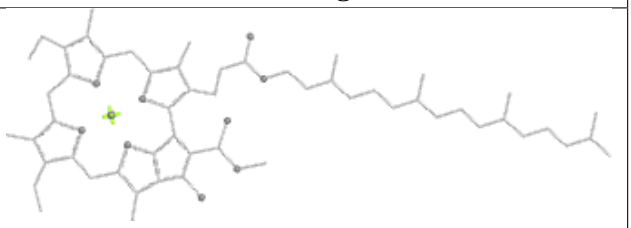
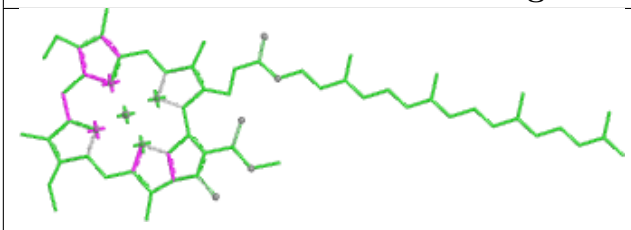


Rings

Ligand CLA b 604



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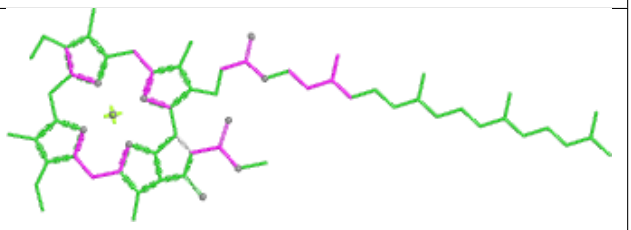
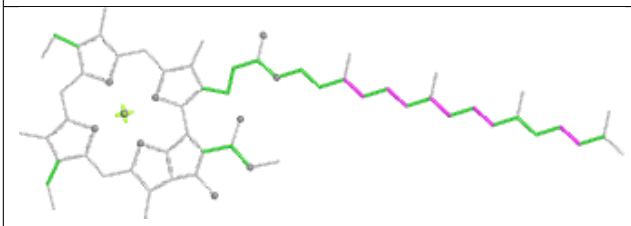


Bond angles



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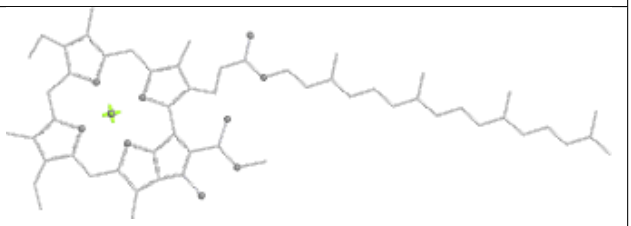
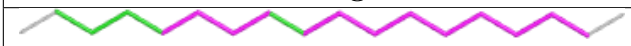


Rings

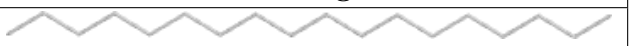
Ligand STE H 103

Bond lengths

Bond angles

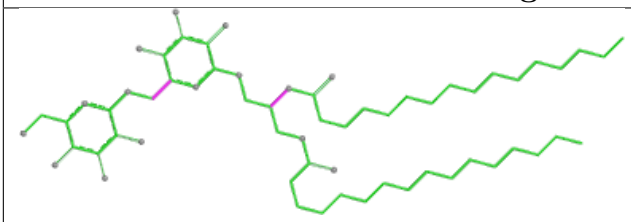


Torsions



Rings

Ligand DGD C 517



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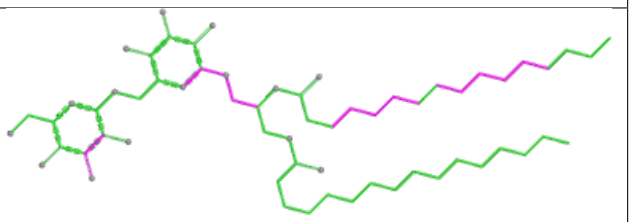
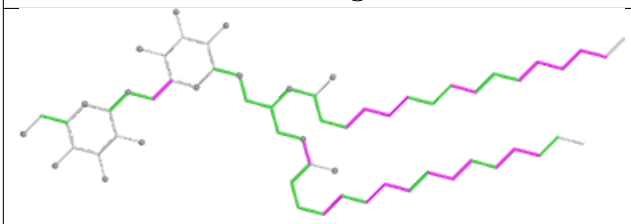


Bond angles



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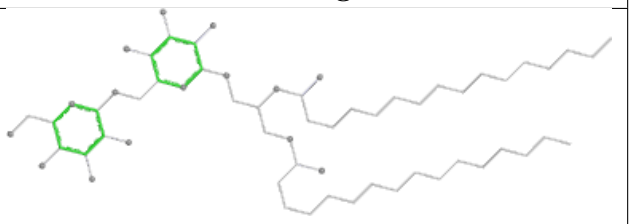
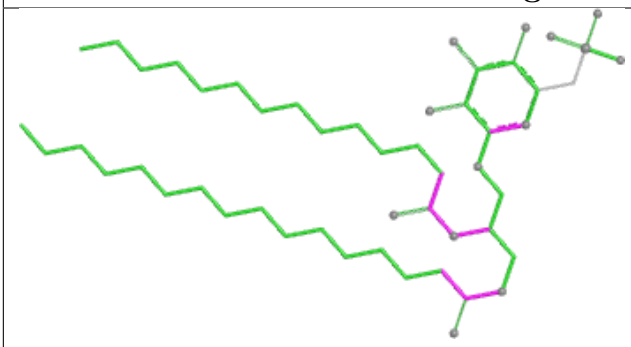


Rings

Ligand SQD A 615



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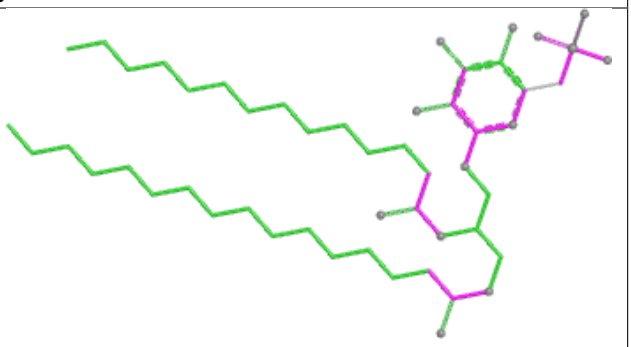
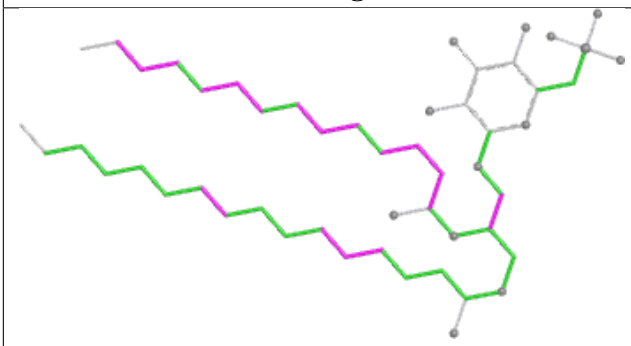


Bond angles



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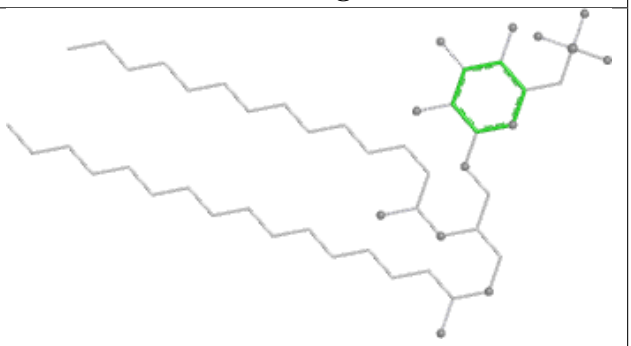
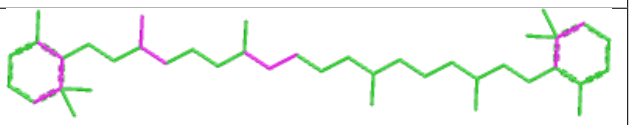


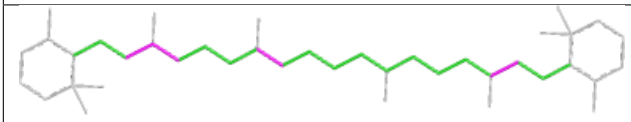
Rings

Ligand BCR B 619

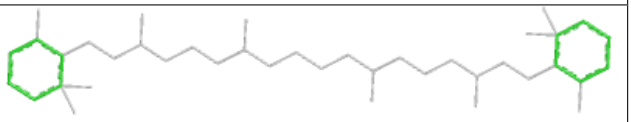
Bond lengths



Bond angles

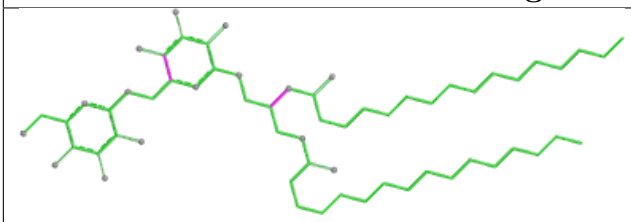


Torsions

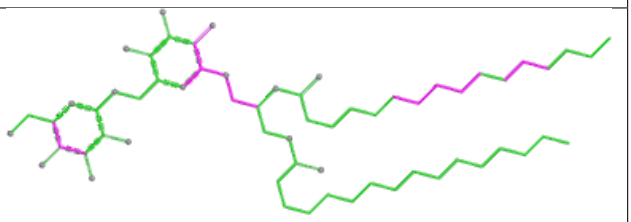


Rings

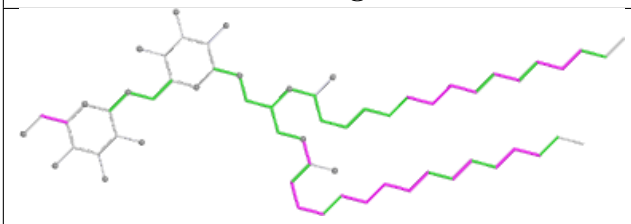
Ligand DGD c 518



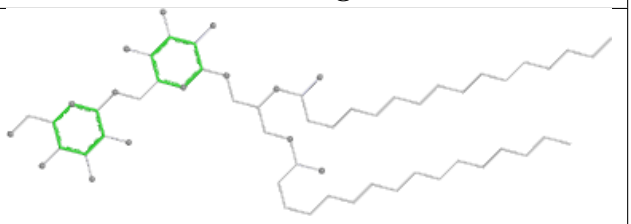
Bond lengths



Bond angles

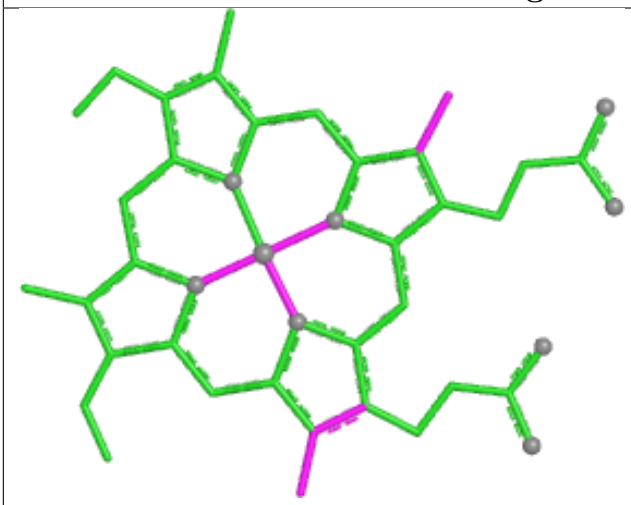


Torsions

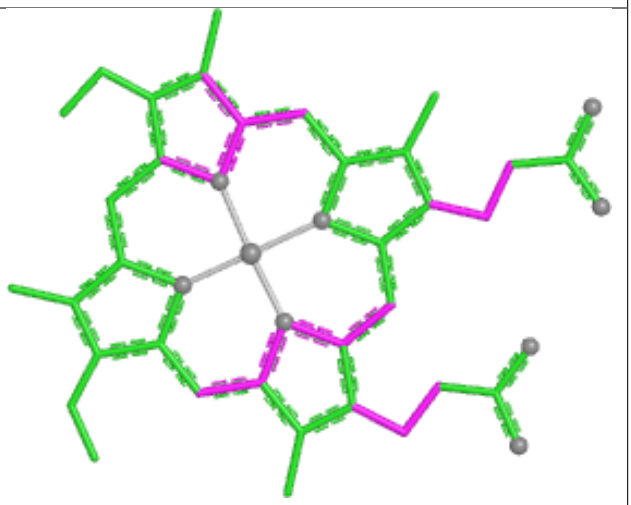


Rings

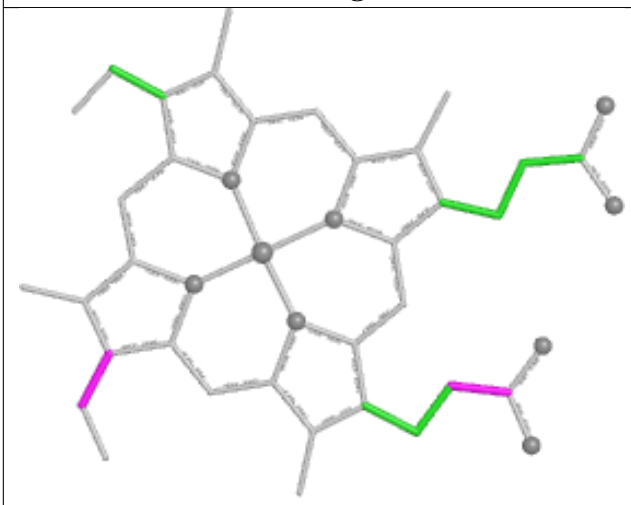
Ligand HEC v 201



Bond lengths



Bond angles



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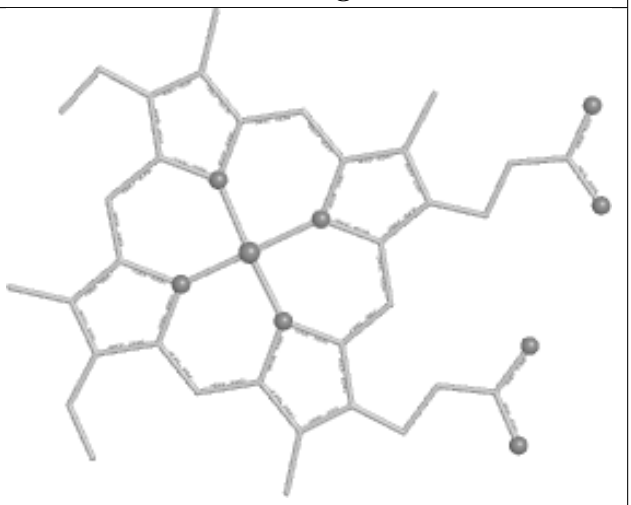
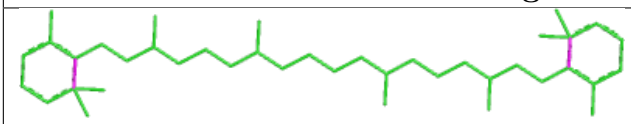
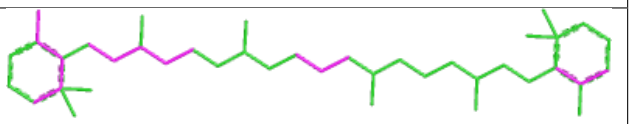


Rings

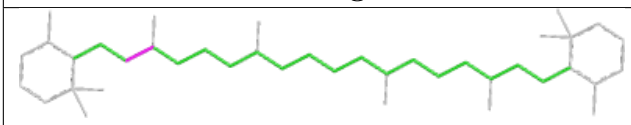
Ligand BCR C 514



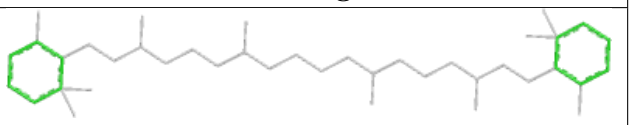
Bond lengths



Bond angles

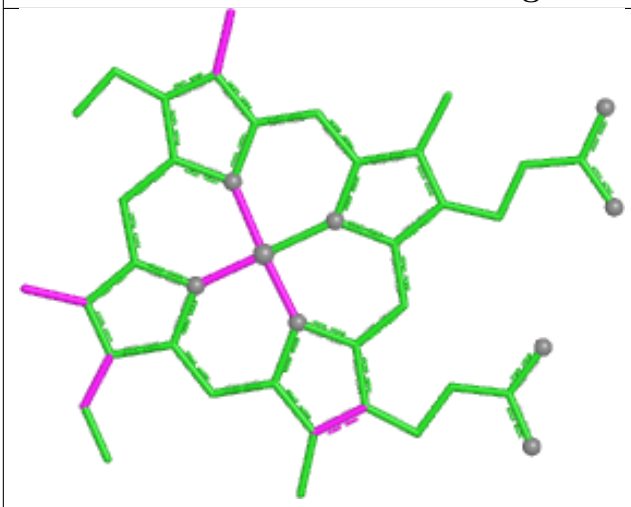


Torsions

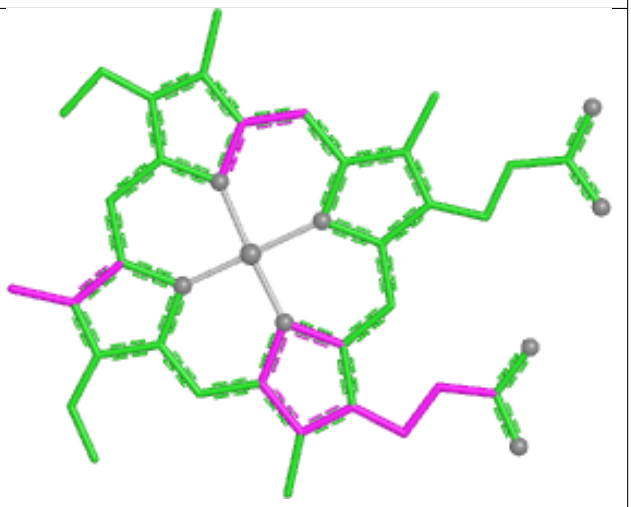


Rings

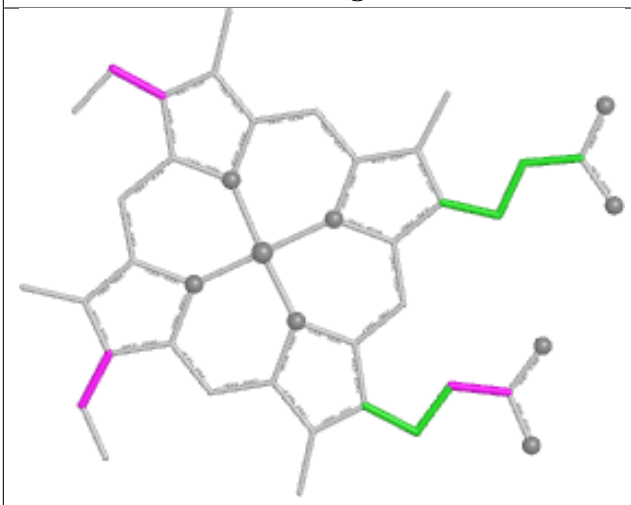
Ligand HEC V 201



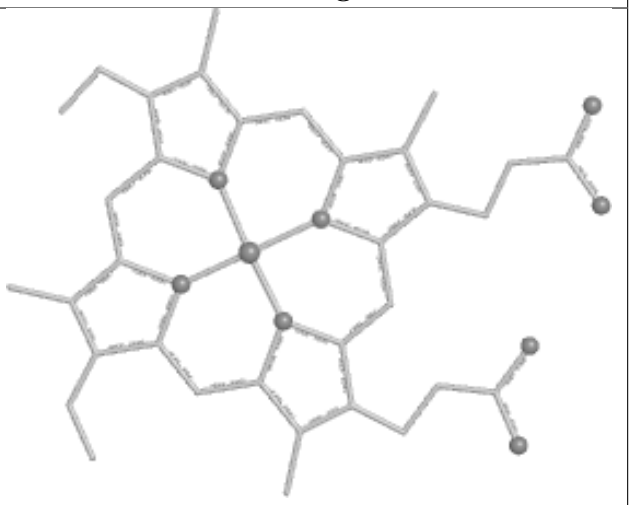
Bond lengths



Bond angles

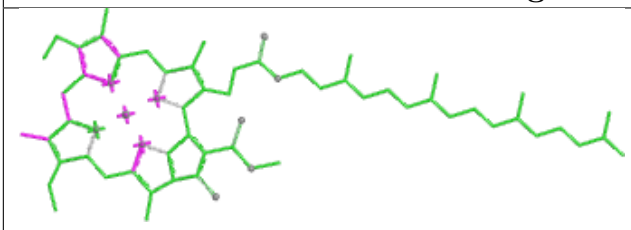


Torsions



Rings

Ligand CLA b 613



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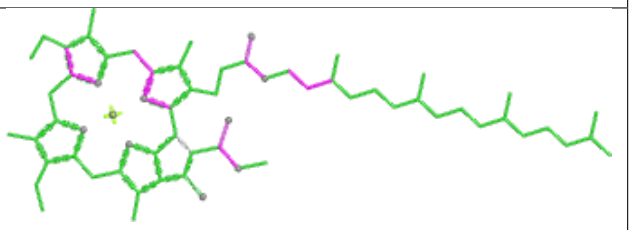
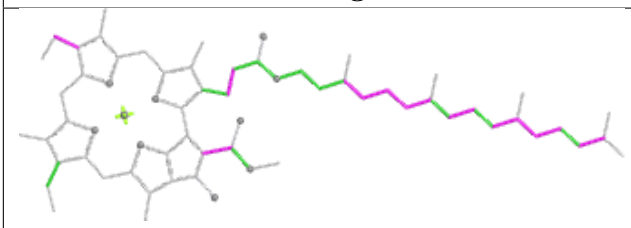
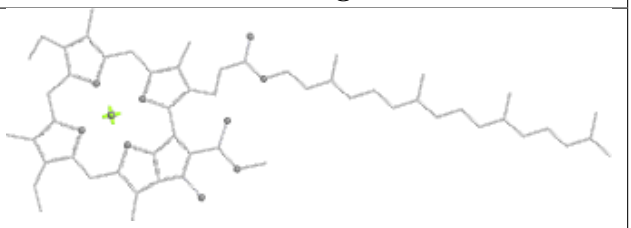


Bond angles

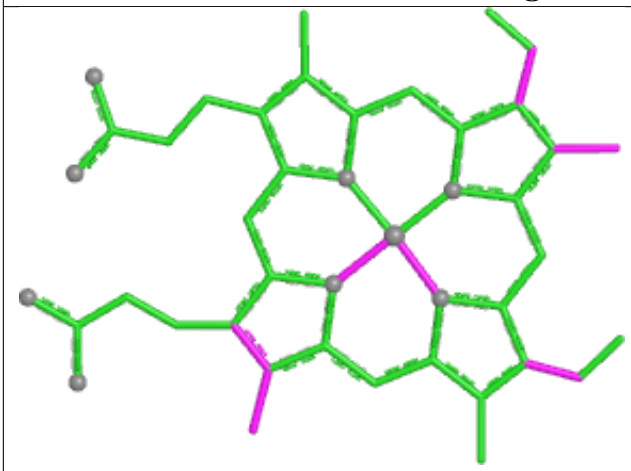


Torsions



Rings

Ligand HEM e 101



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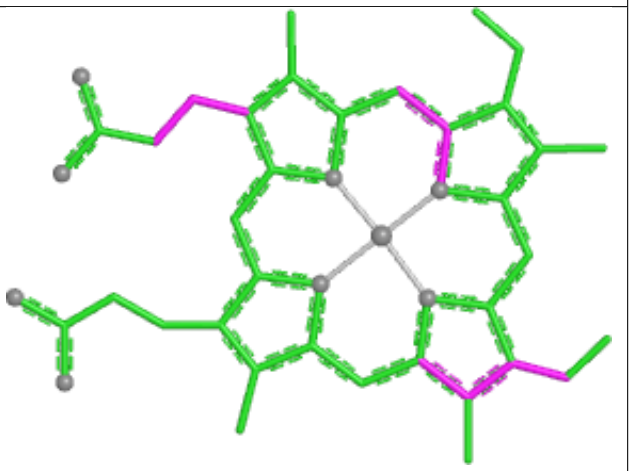

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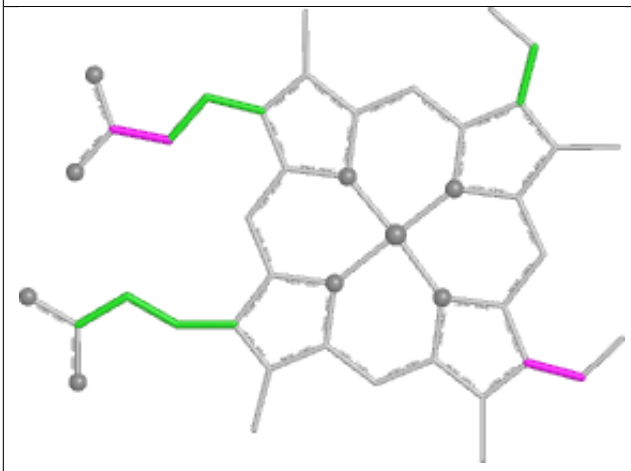

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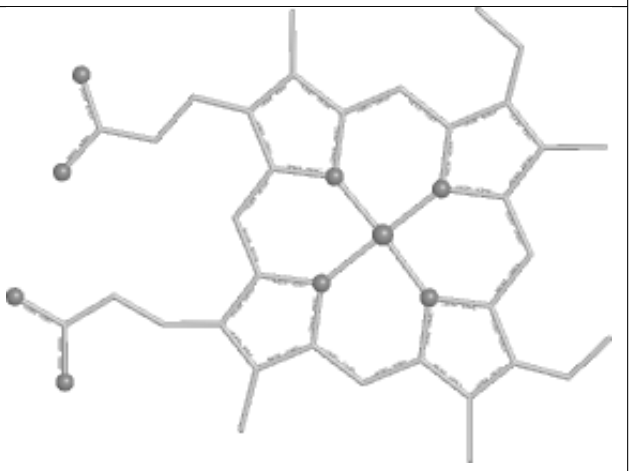
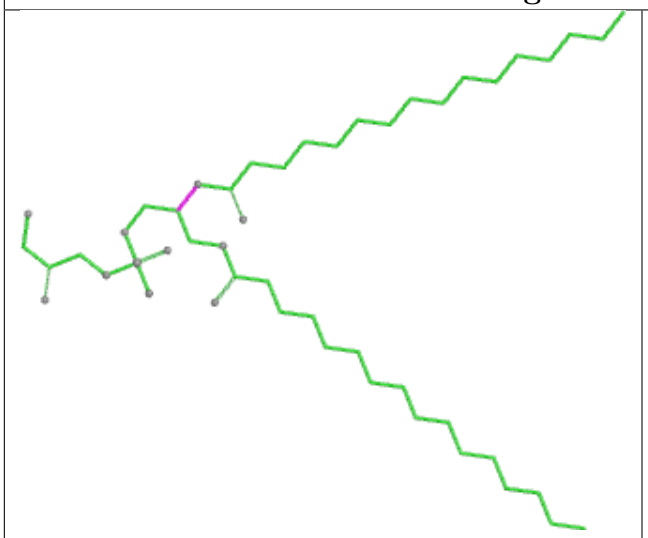


Rings

Ligand LHG B 622



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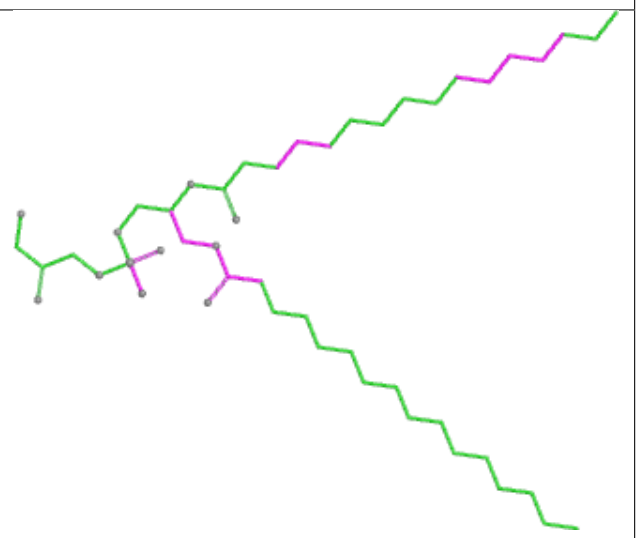
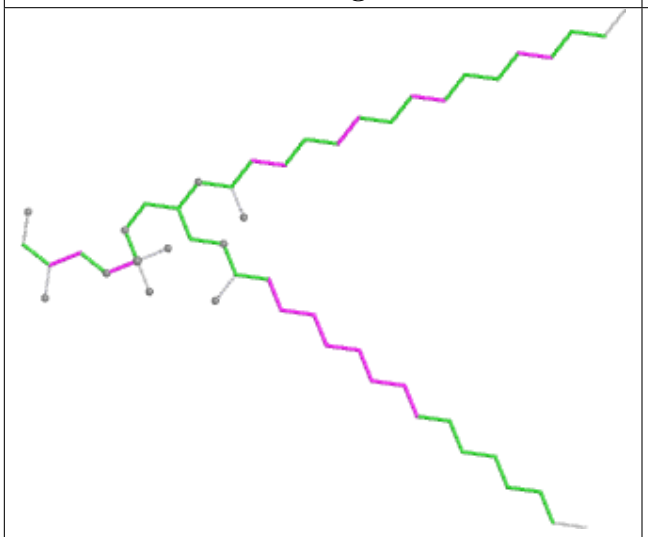


Bond angles



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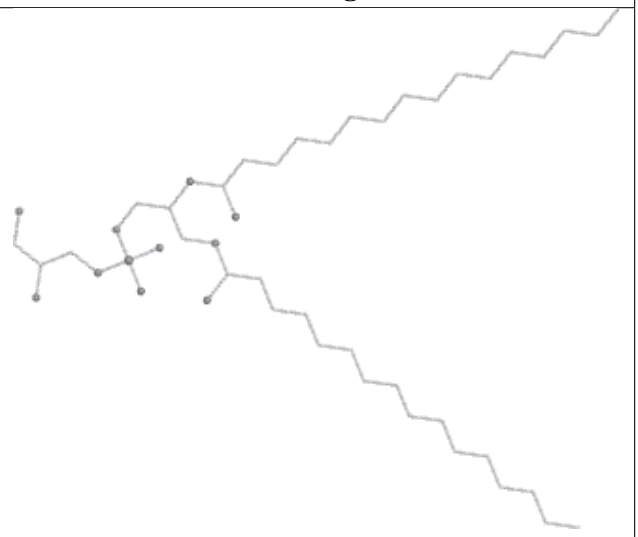
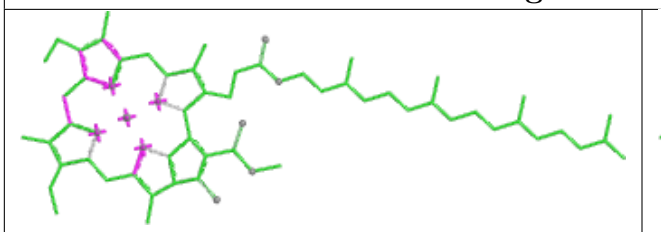


Rings

Ligand CLA C 508



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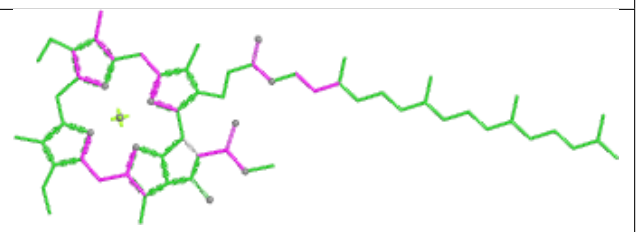

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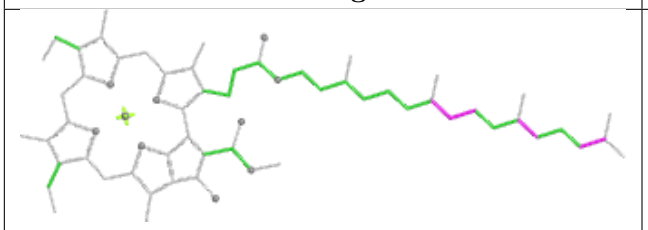

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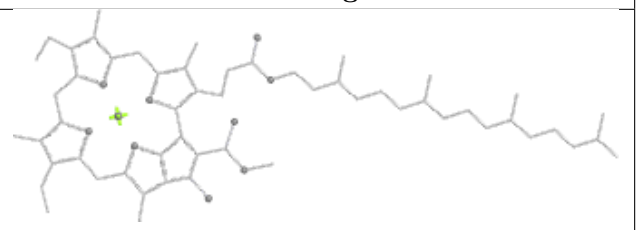
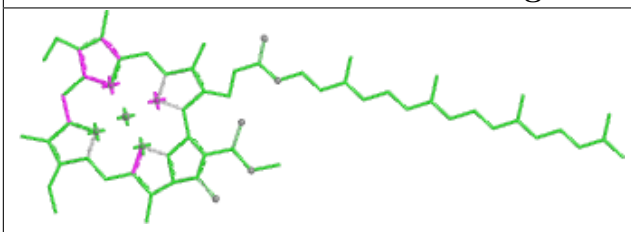
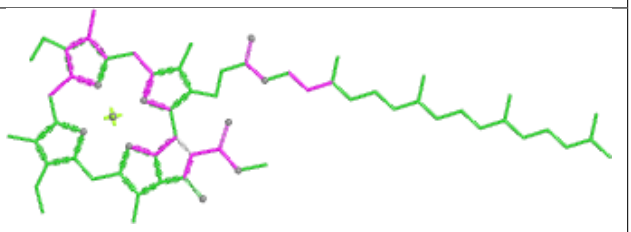


Rings

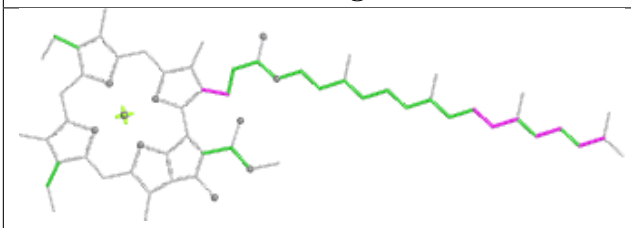
Ligand CLA B 602



Bond lengths



Bond angles



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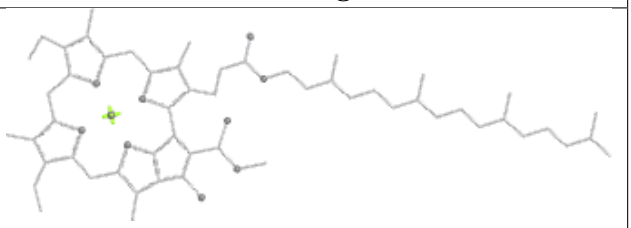
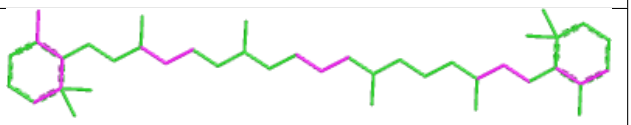


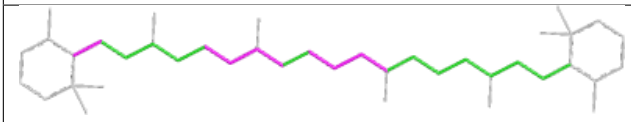
Rings

Ligand BCR K 101

Bond lengths



Bond angles



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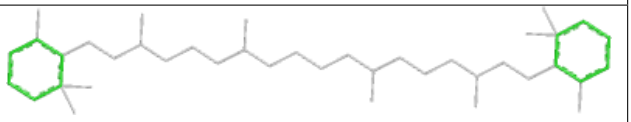
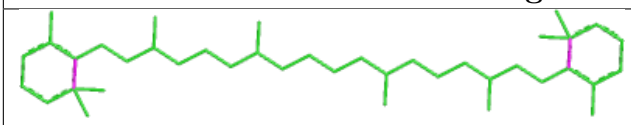


Rings

Ligand BCR h 102



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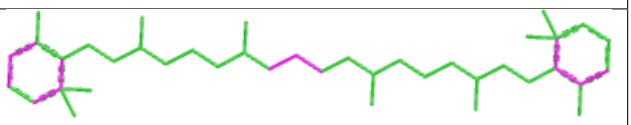
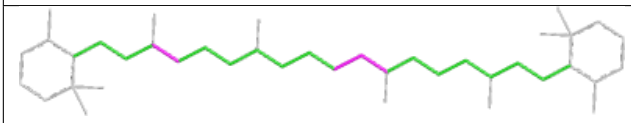


Bond angles



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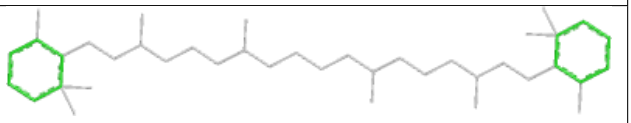
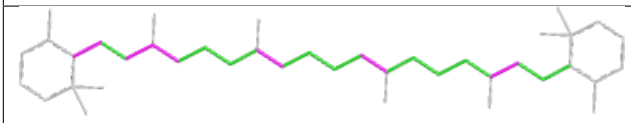


Rings

Ligand BCR k 101

Bond lengths

Bond angles



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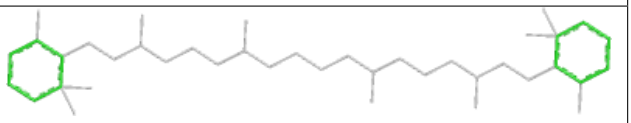
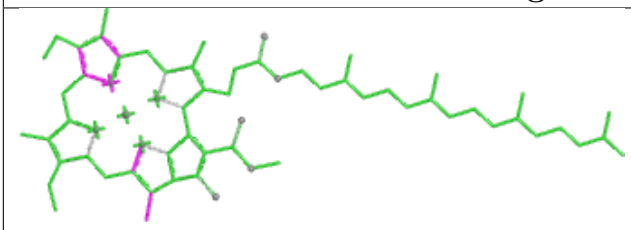
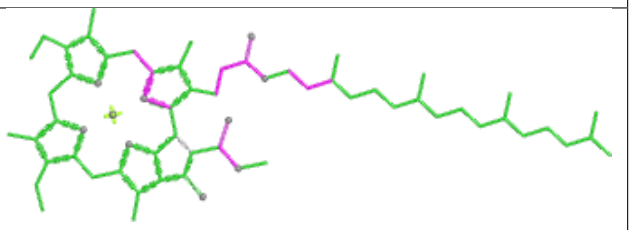


Rings

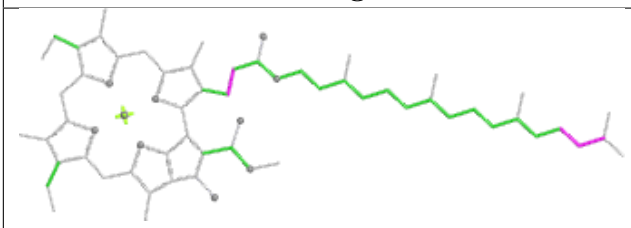
Ligand CLA b 609



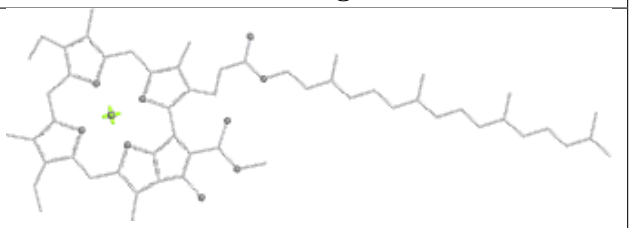
Bond lengths



Bond angles

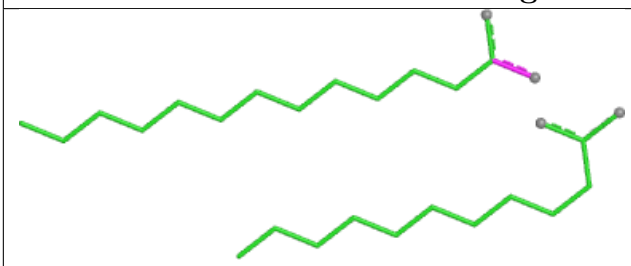


Torsions

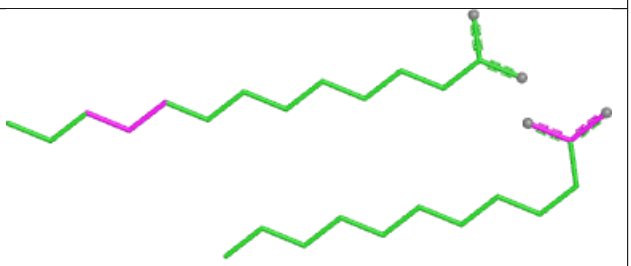


Rings

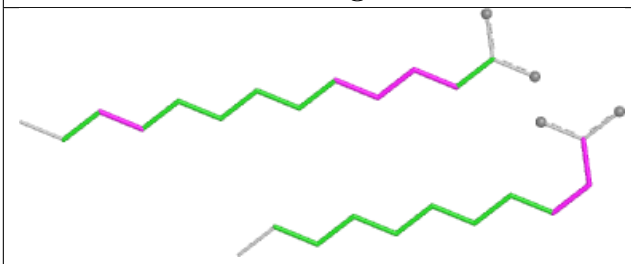
Ligand LMG B 621



Bond lengths



Bond angles



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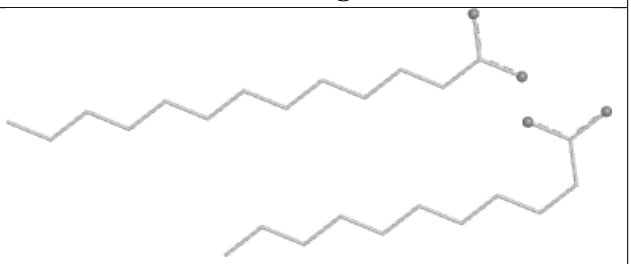
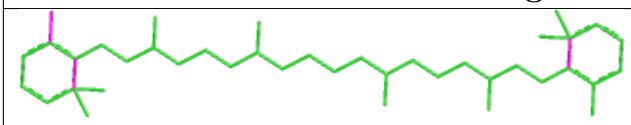
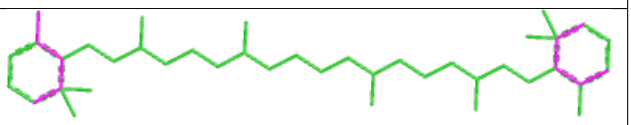


Rings

Ligand BCR b 616

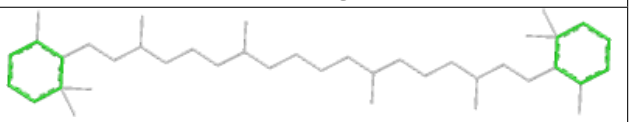


Bond lengths

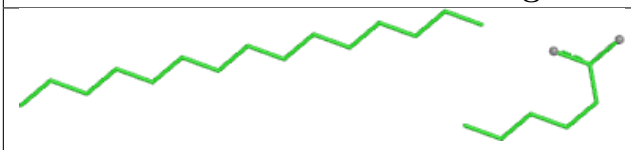
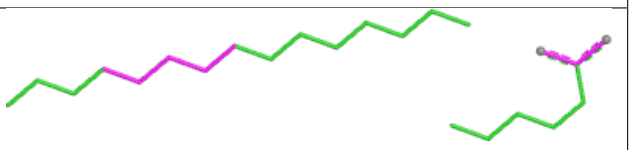
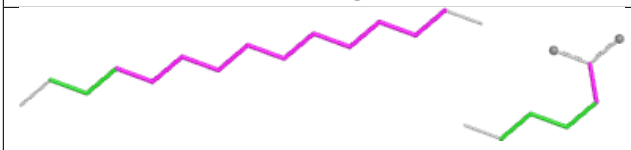
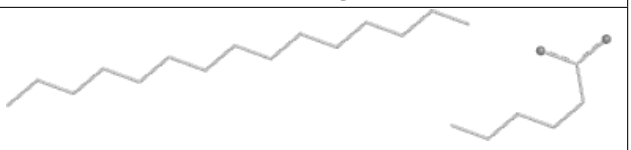


Bond angles

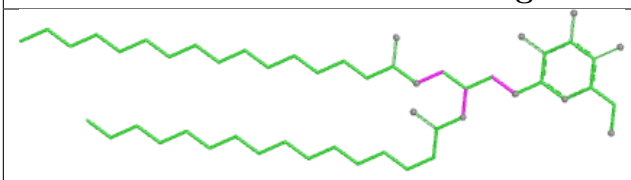
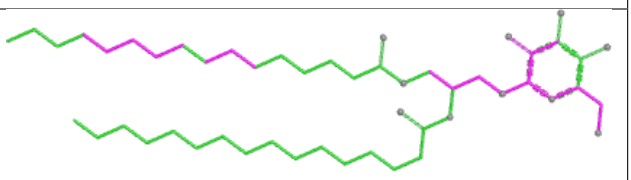
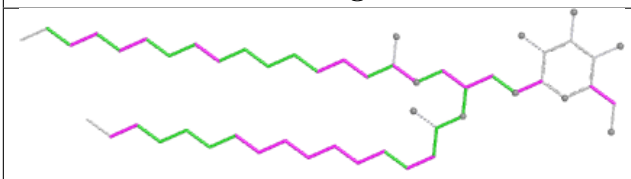
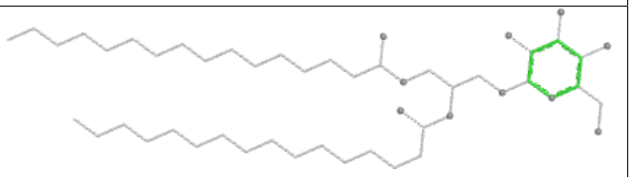
Torsions



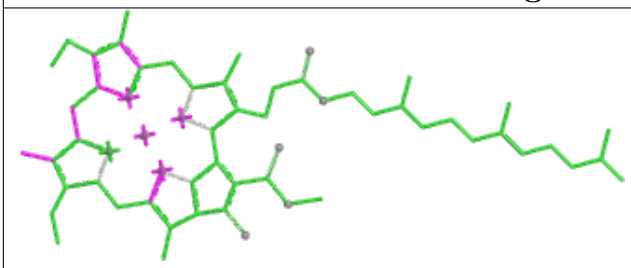
Rings

Ligand LMG d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

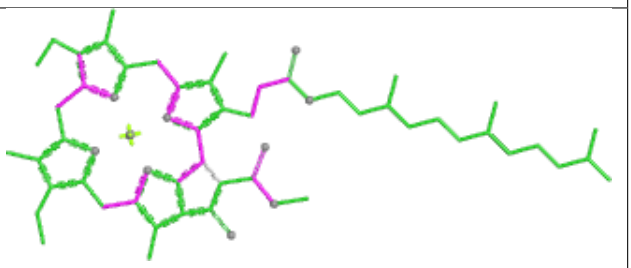
Ligand STE b 626	
Bond lengths	Bond angles
Torsions	Rings

Ligand LMG M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

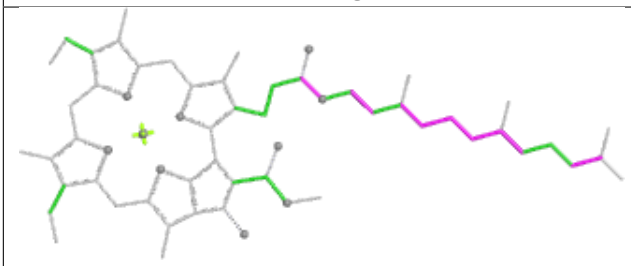
Ligand CLA B 616



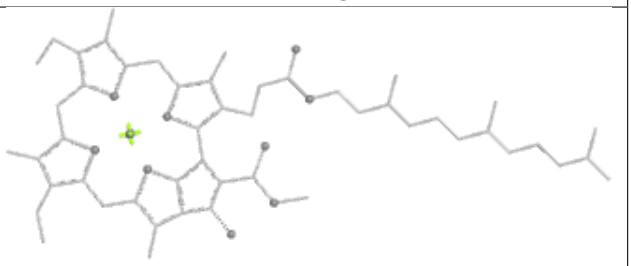
Bond lengths



Bond angles

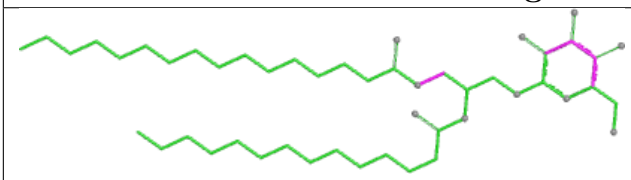


Torsions

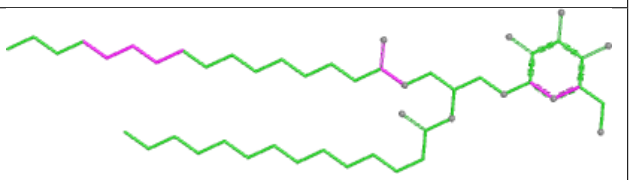


Rings

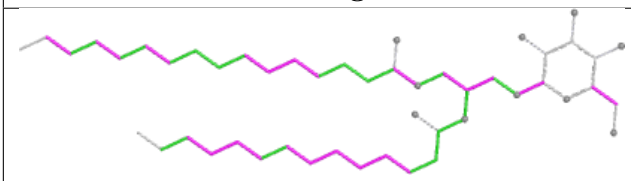
Ligand LMG c 522



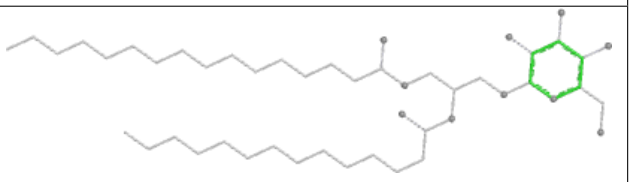
Bond lengths



Bond angles

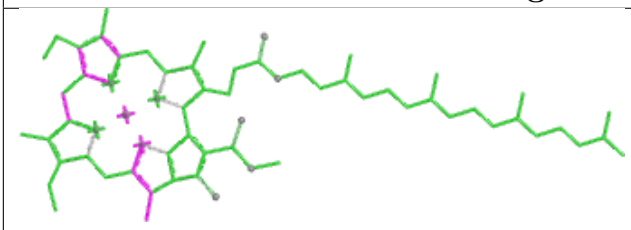


Torsions



Rings

Ligand CLA b 601



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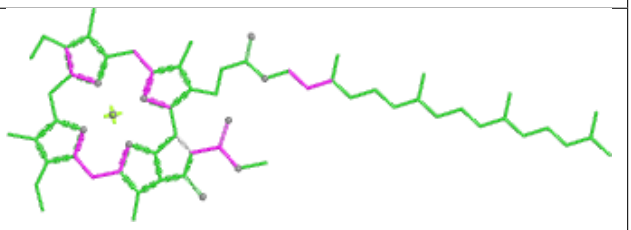
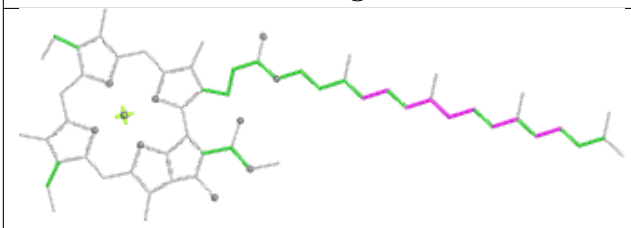


Bond angles



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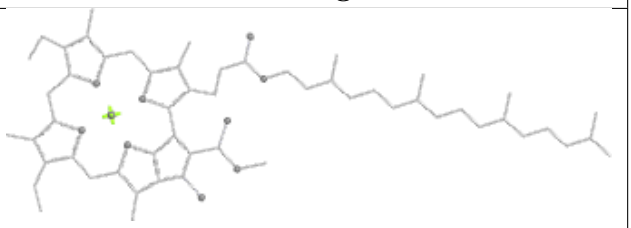
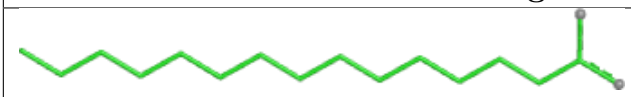


Rings

Ligand STE B 620



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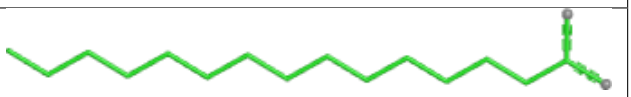
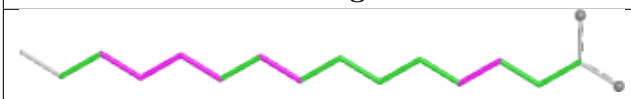


Bond angles



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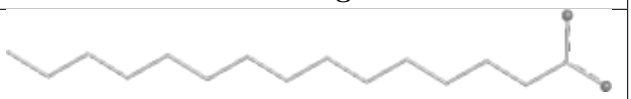
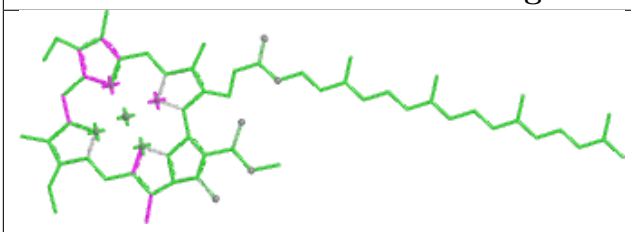


Rings

Ligand CLA B 606



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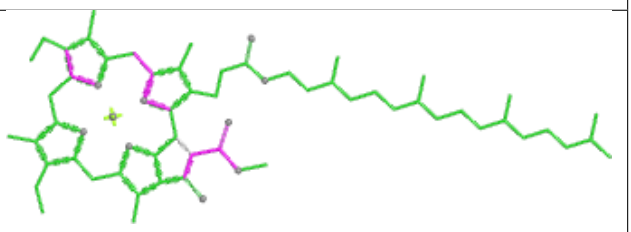
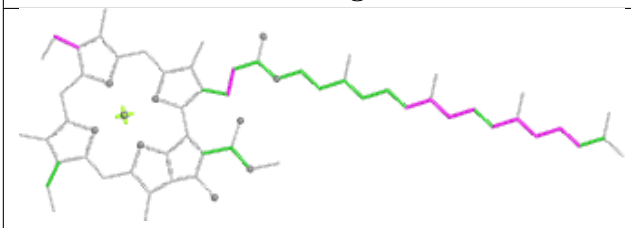


Bond angles



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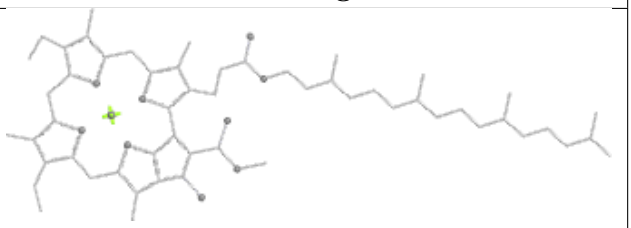
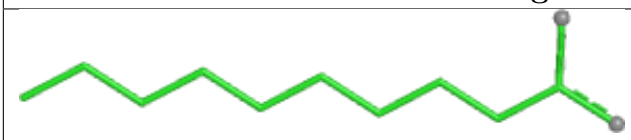


Rings

Ligand STE J 101



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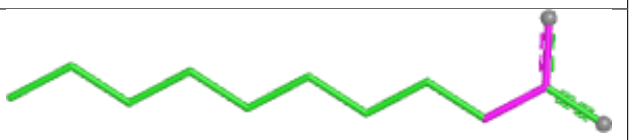
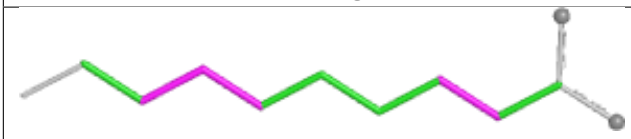


Bond angles



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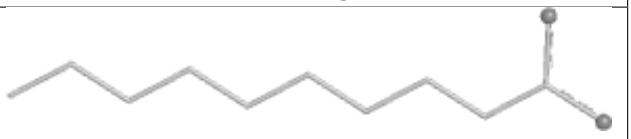
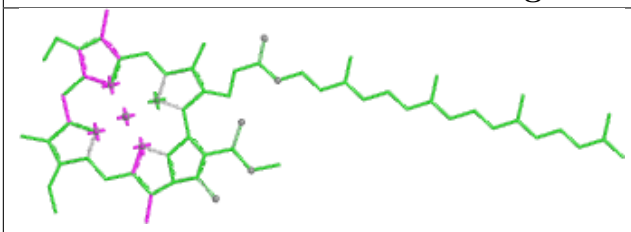


Rings

Ligand CLA C 512



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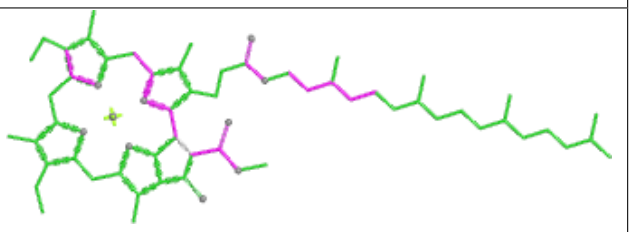
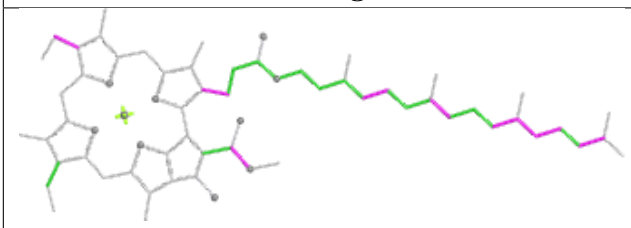


Bond angles



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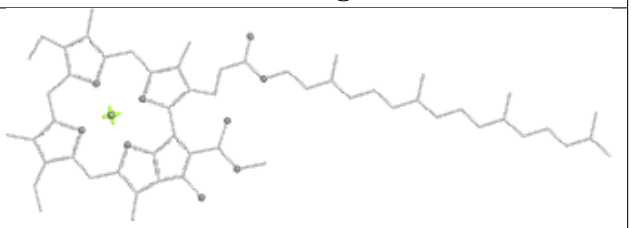
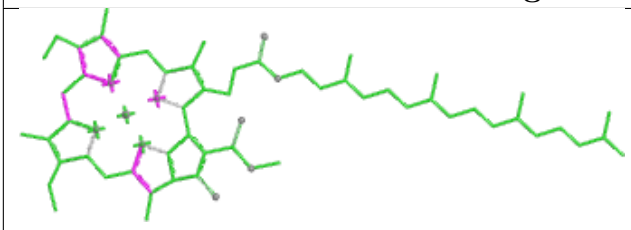


Rings

Ligand CLA A 612



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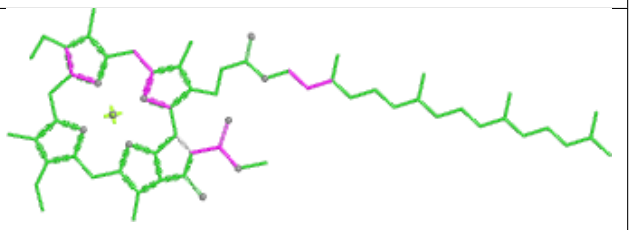
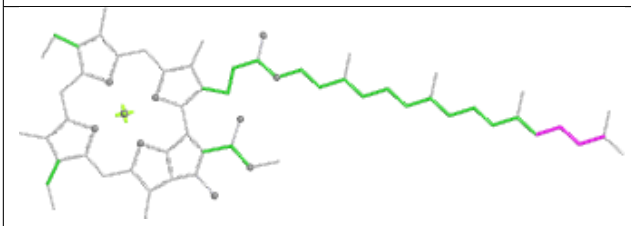


Bond angles



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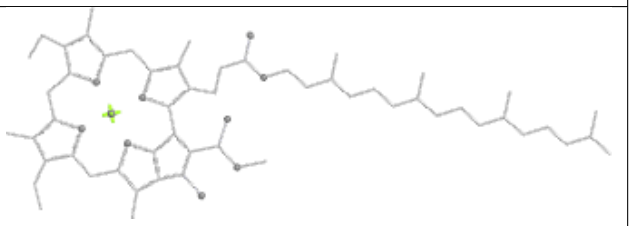
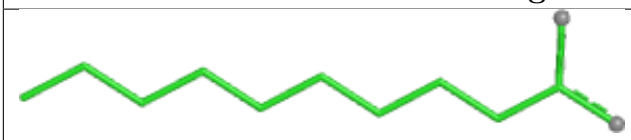


Rings

Ligand STE E 102



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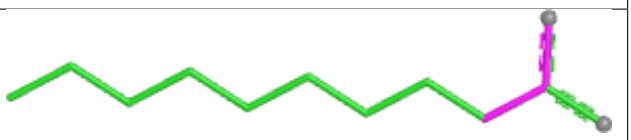
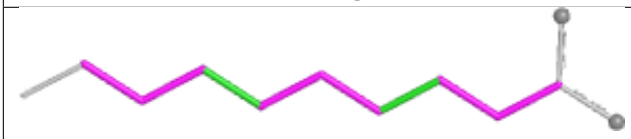


Bond angles



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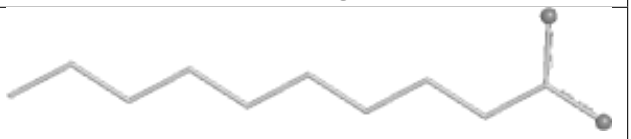
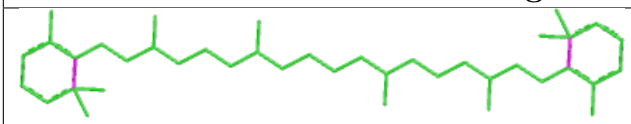


Rings

Ligand BCR b 618



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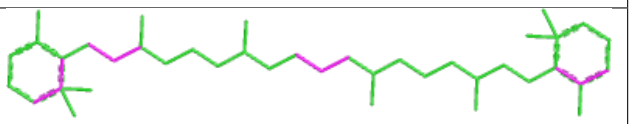
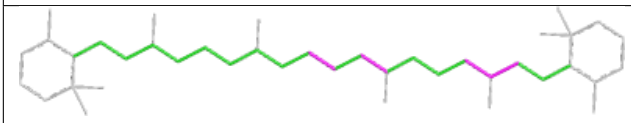


Bond angles



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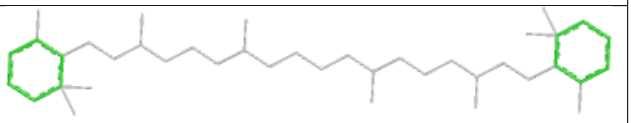
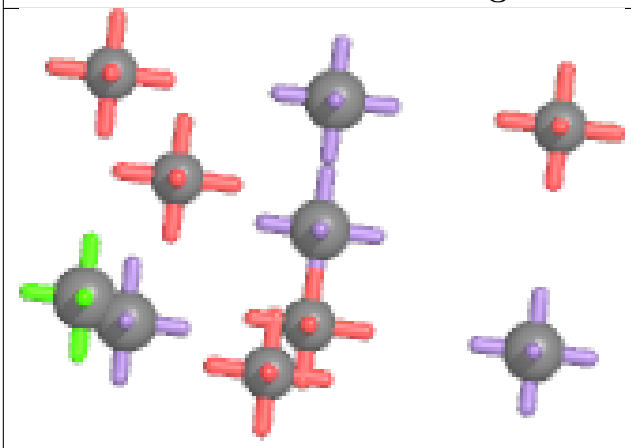


Rings

Ligand OEX A 601 (B)



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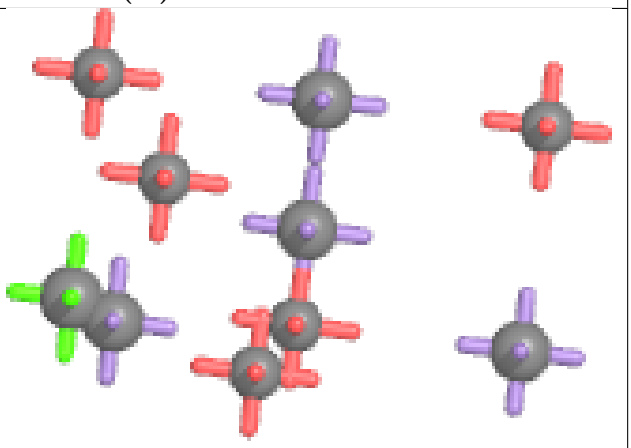

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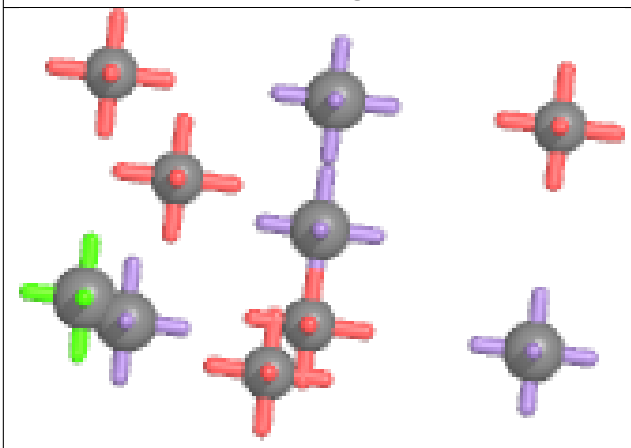
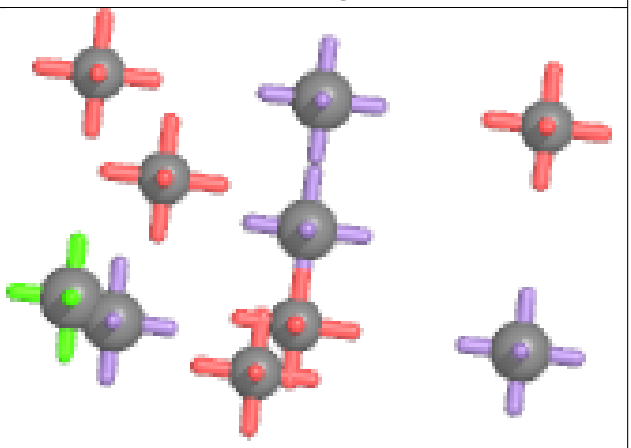
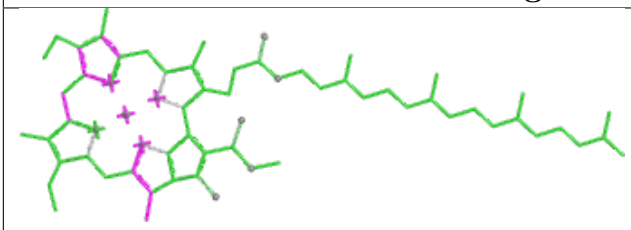


Torsions



Rings

Ligand CLA C 501



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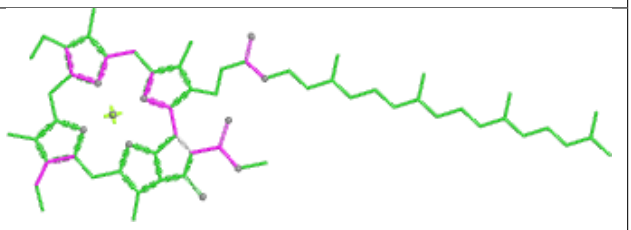
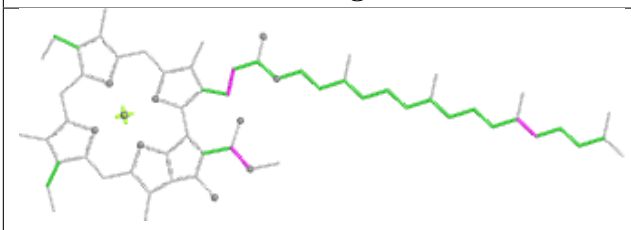


Bond angles



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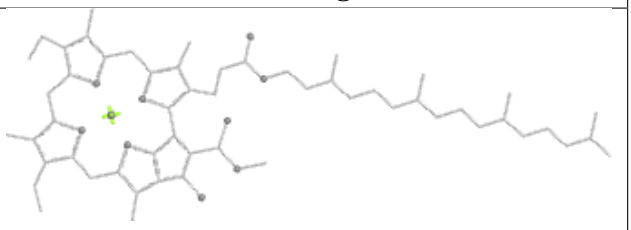
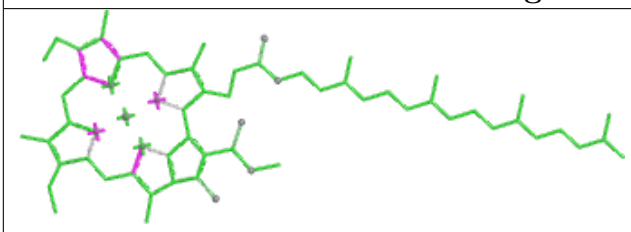


Rings

Ligand CLA B 609



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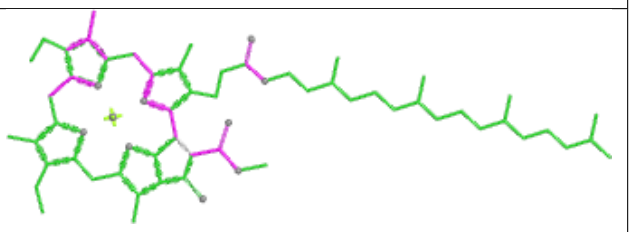
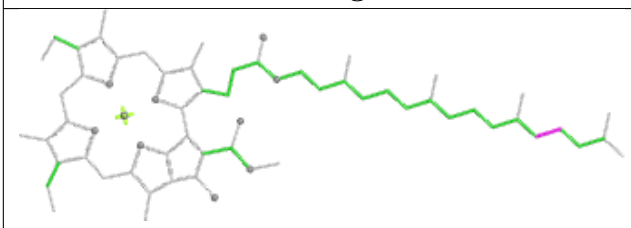


Bond angles



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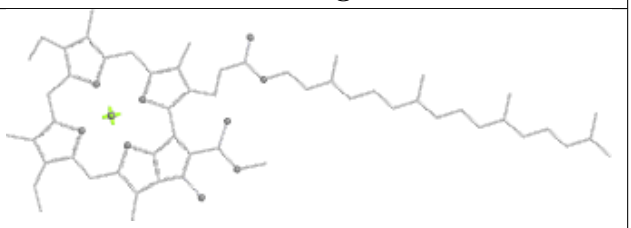
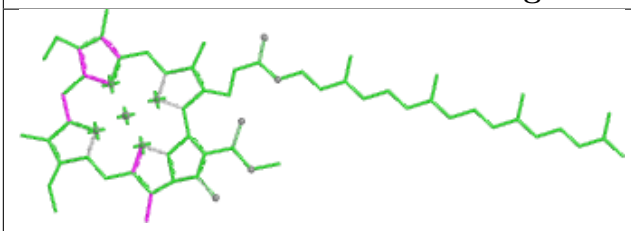


Rings

Ligand CLA A 607



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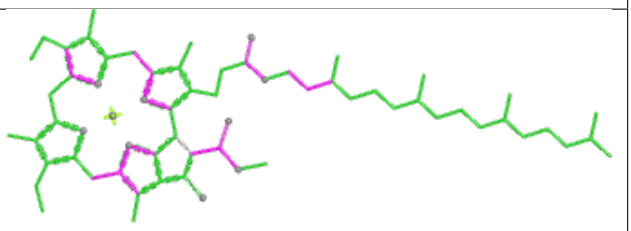
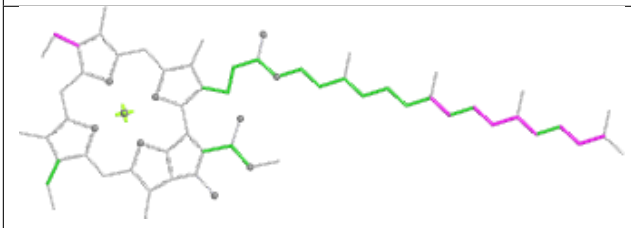
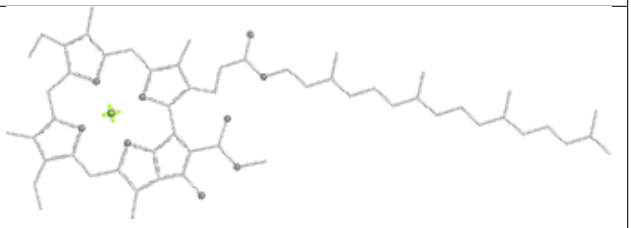


Bond angles

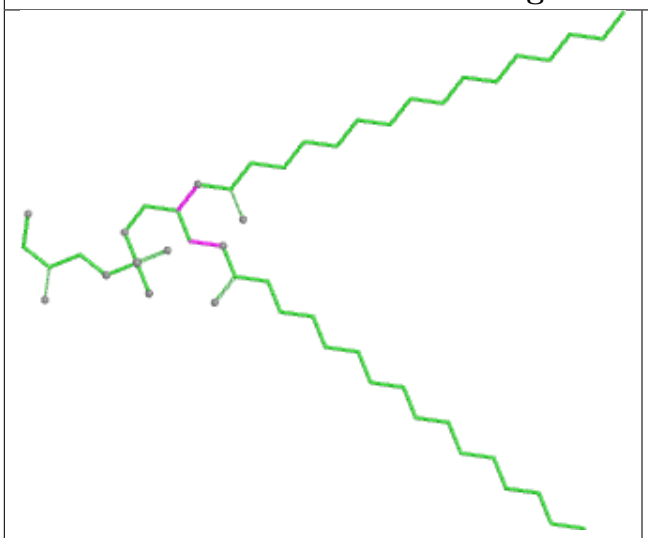


Torsions



Rings

Ligand LHG d 406



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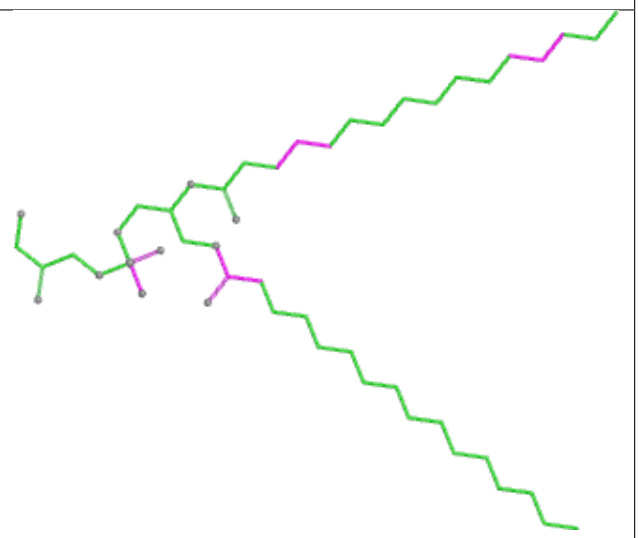
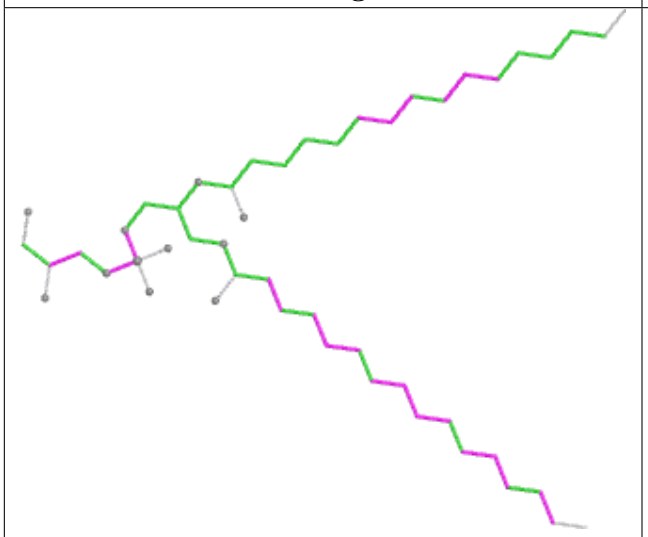


Bond angles



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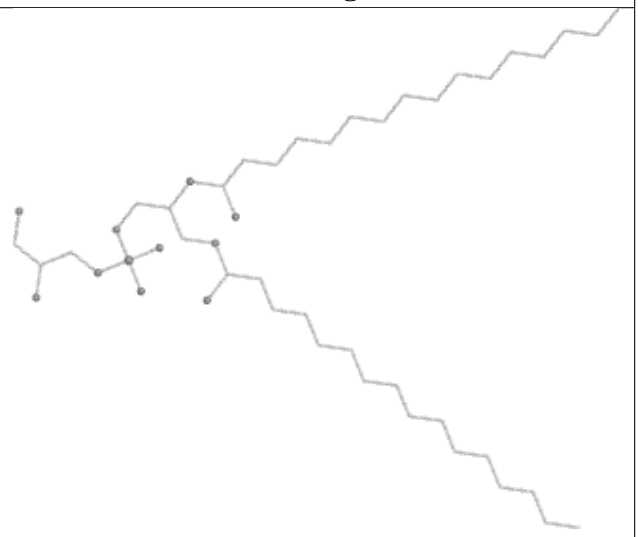
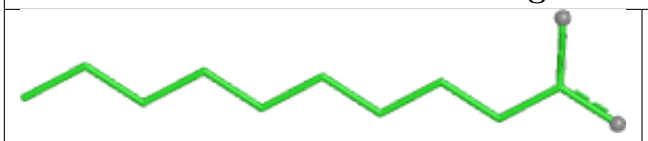


Rings

Ligand STE C 519



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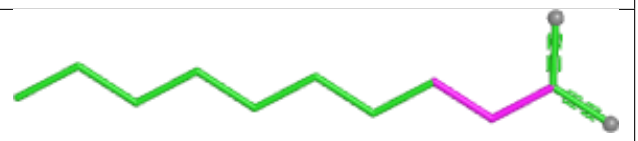
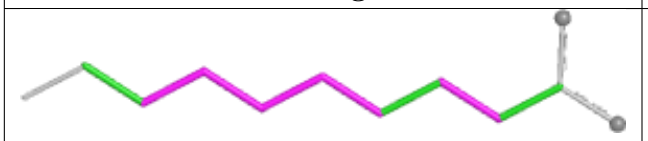
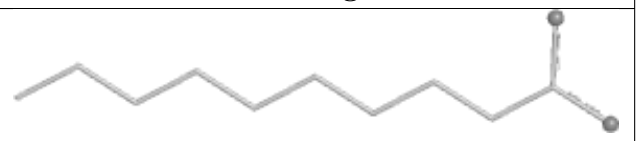


Bond angles

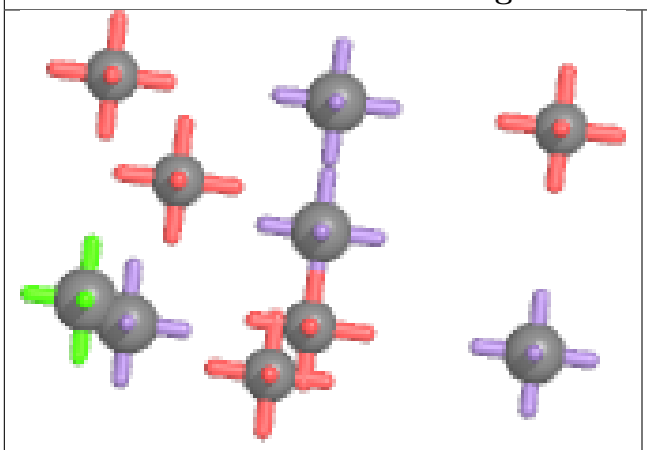


Torsions

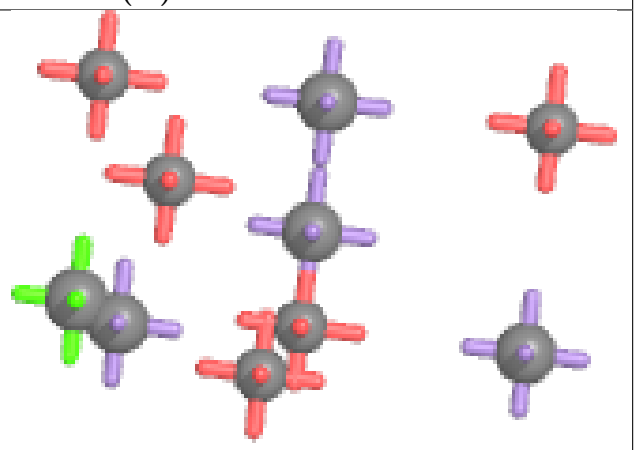


Rings

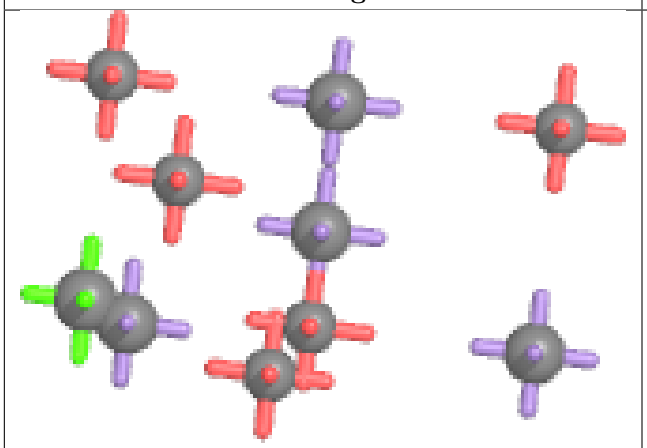
Ligand OEX a 601 (C)



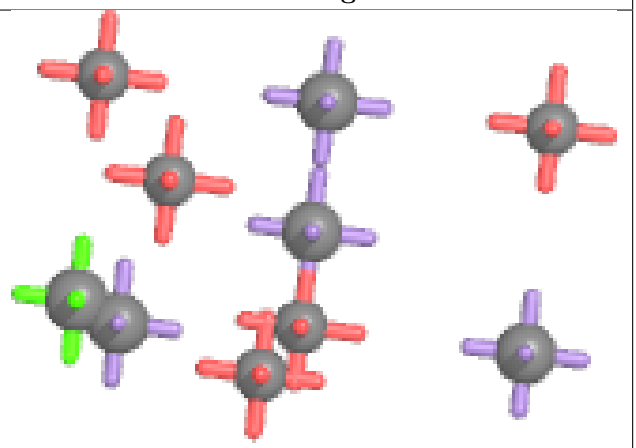
Bond lengths



Bond angles

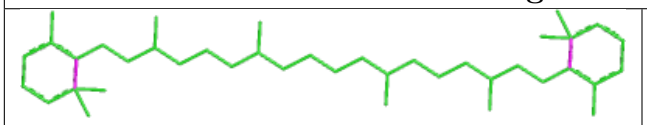


Torsions

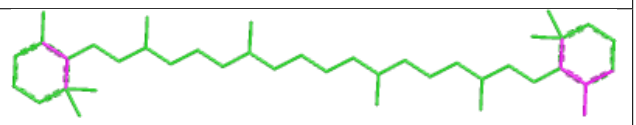


Rings

Ligand BCR d 404

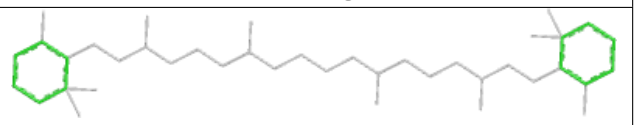


Bond lengths



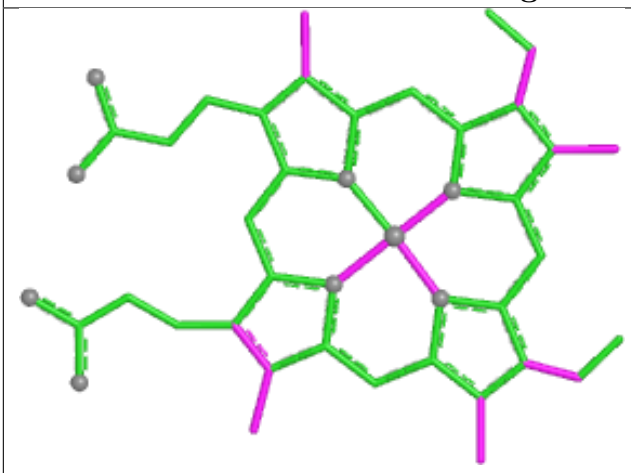
Bond angles

Torsions

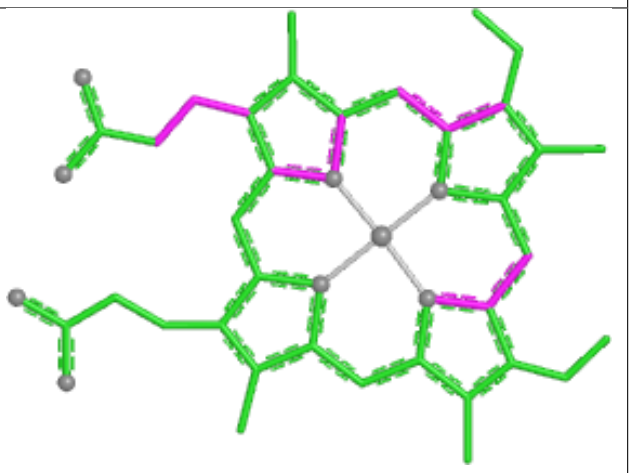


Rings

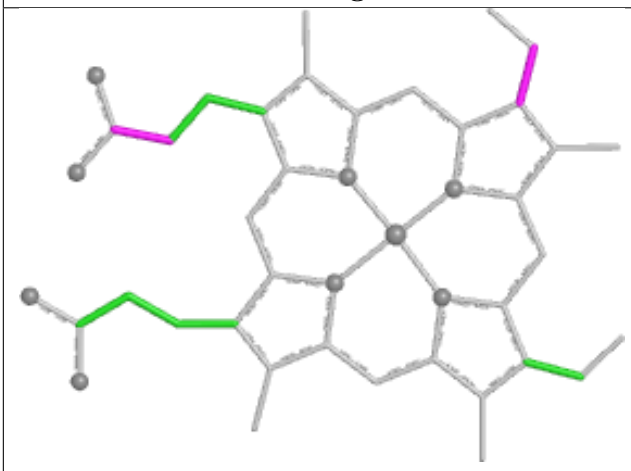
Ligand HEM F 101



Bond lengths



Bond angles



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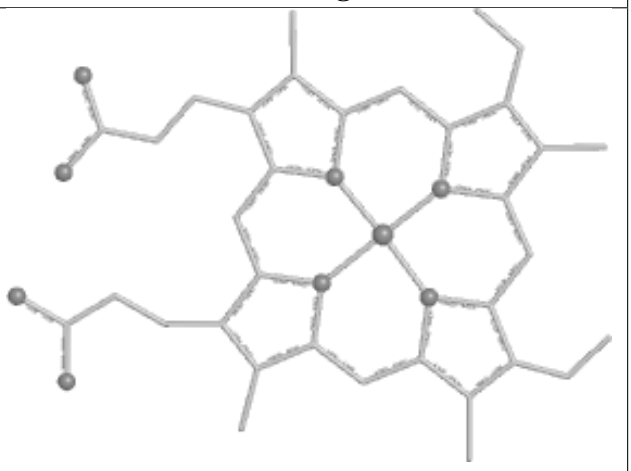
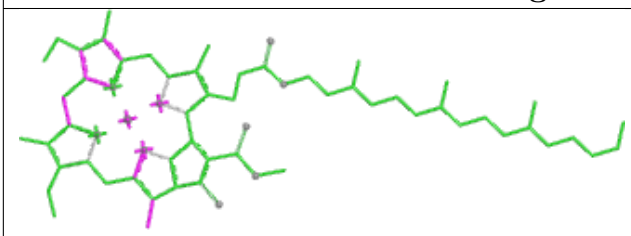


Rings

Ligand CLA c 508



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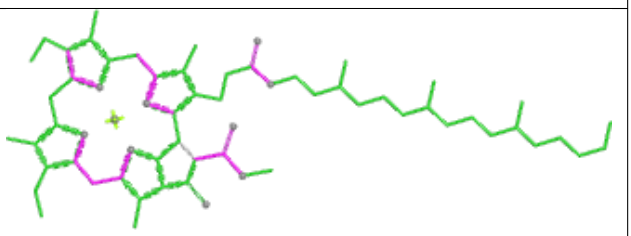
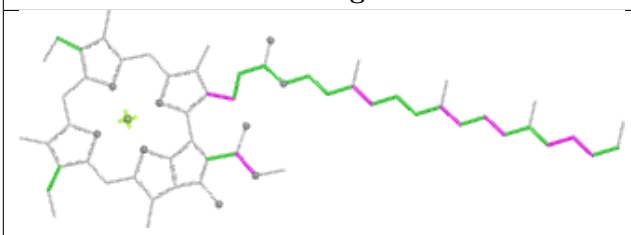


Bond angles



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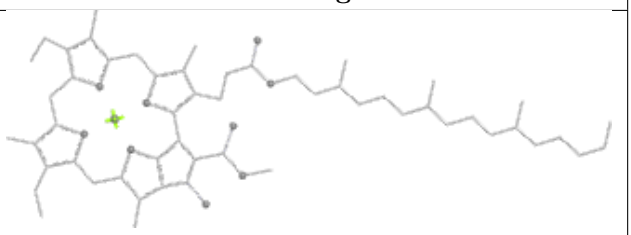
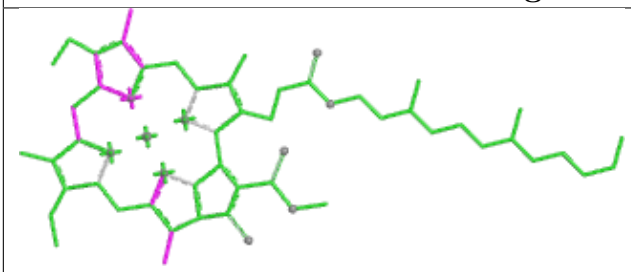
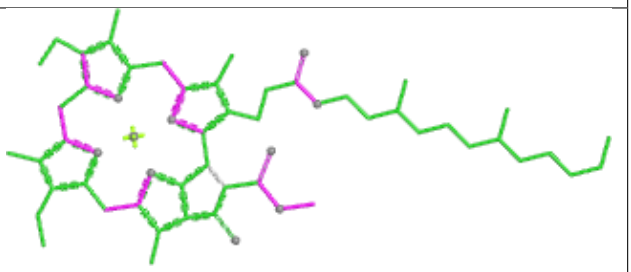
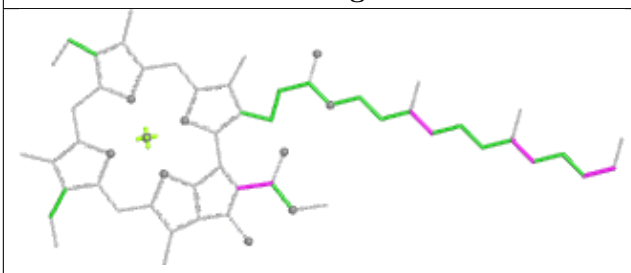
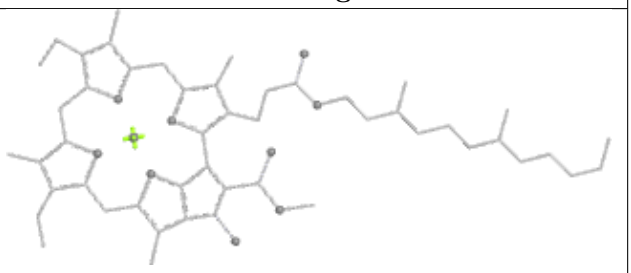
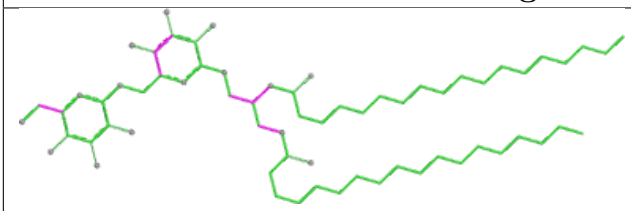
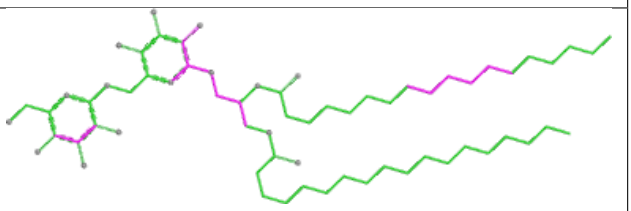
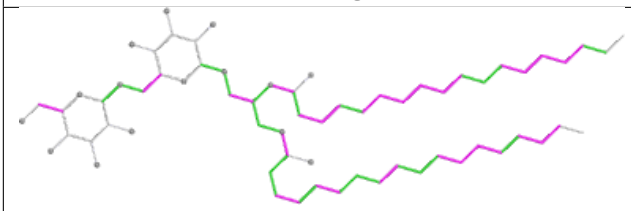
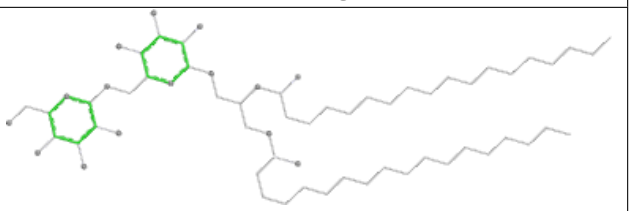
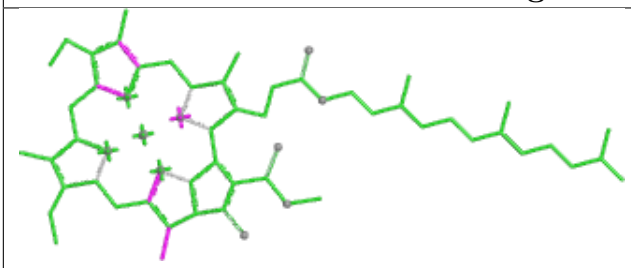
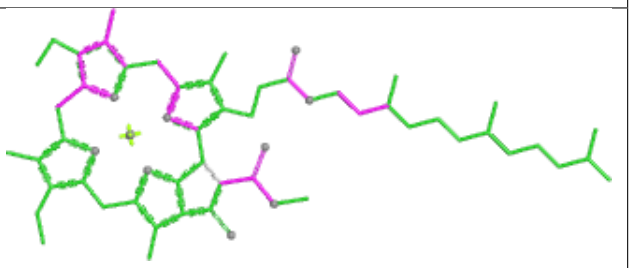
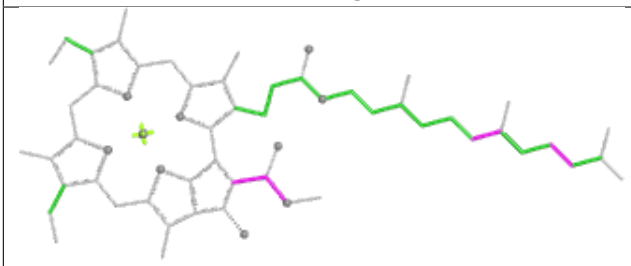
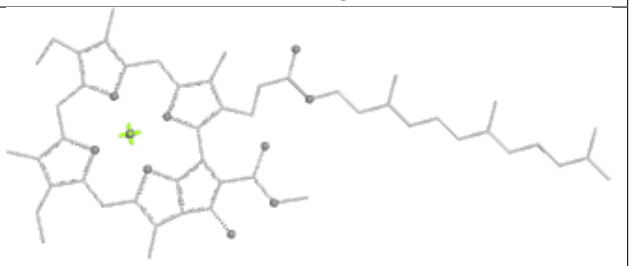
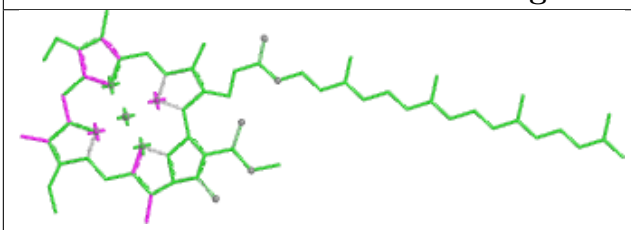
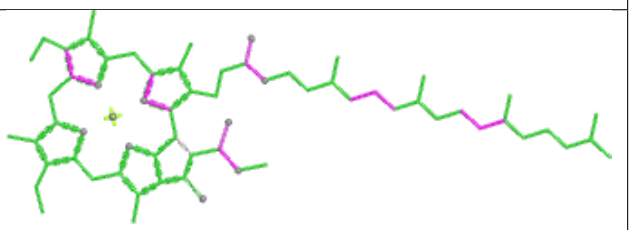
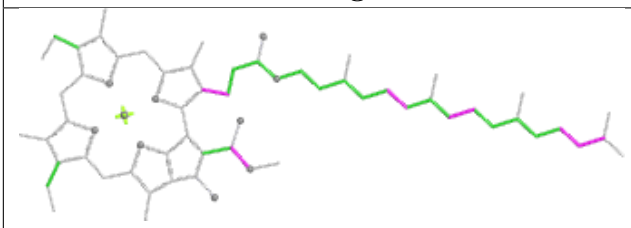
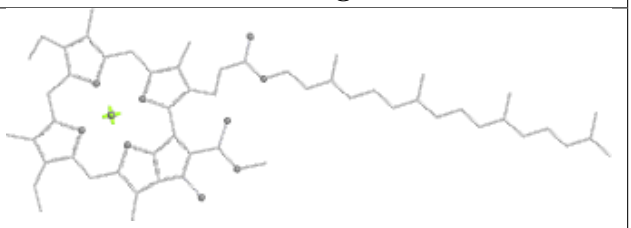


Rings

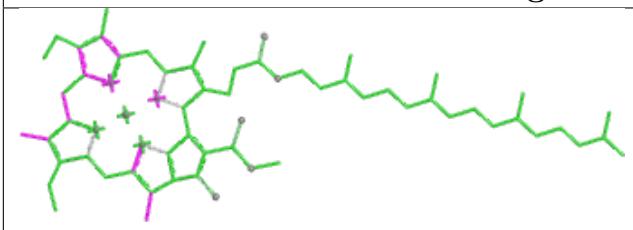
Ligand CLA C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD A 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

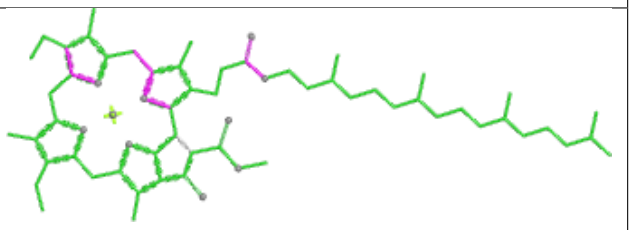
Ligand CLA b 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

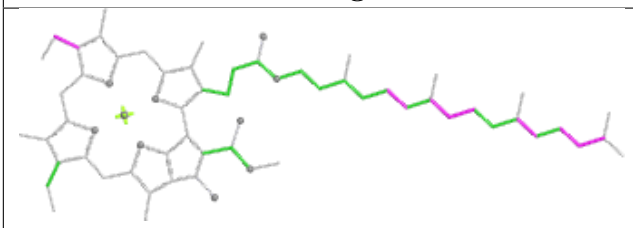
Ligand CLA b 614



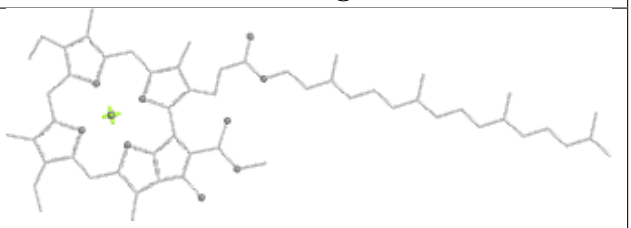
Bond lengths



Bond angles

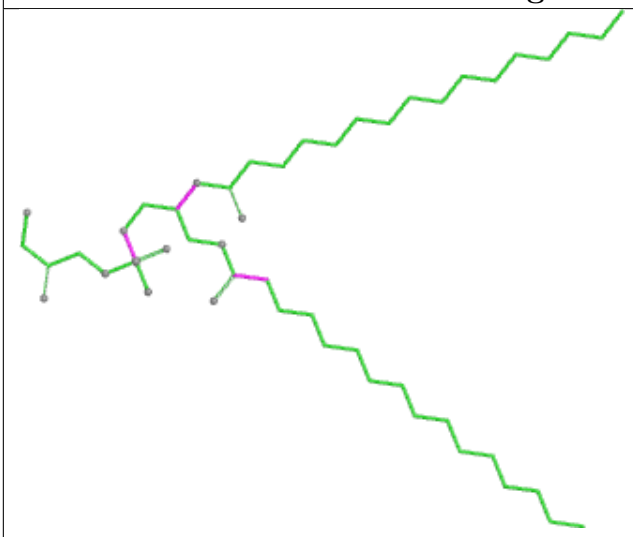


Torsions

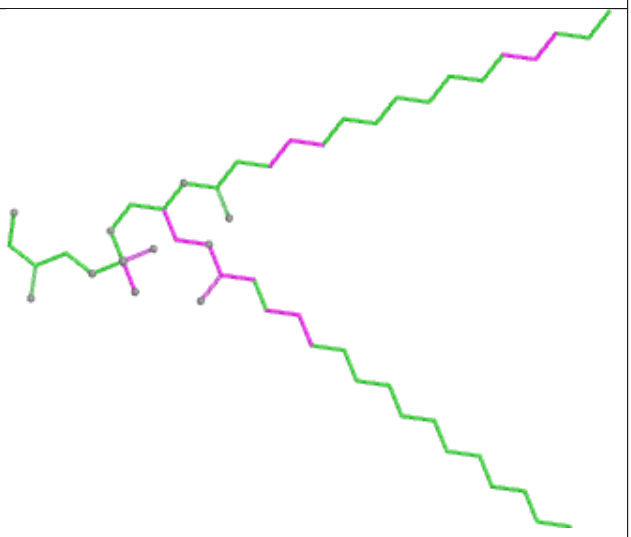


Rings

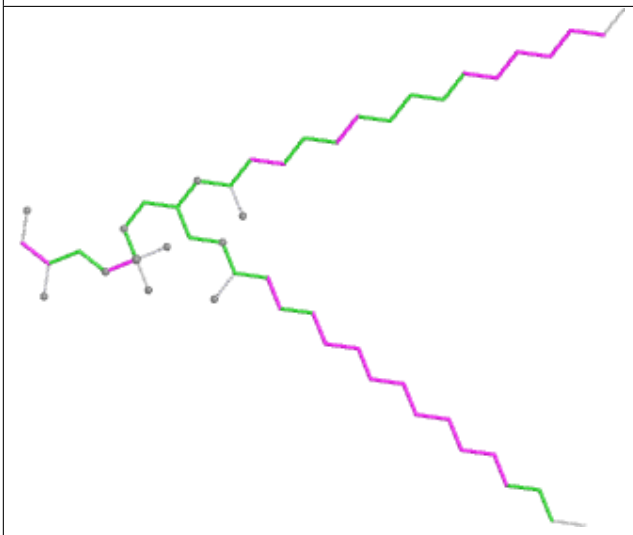
Ligand LHG a 614



Bond lengths



Bond angles



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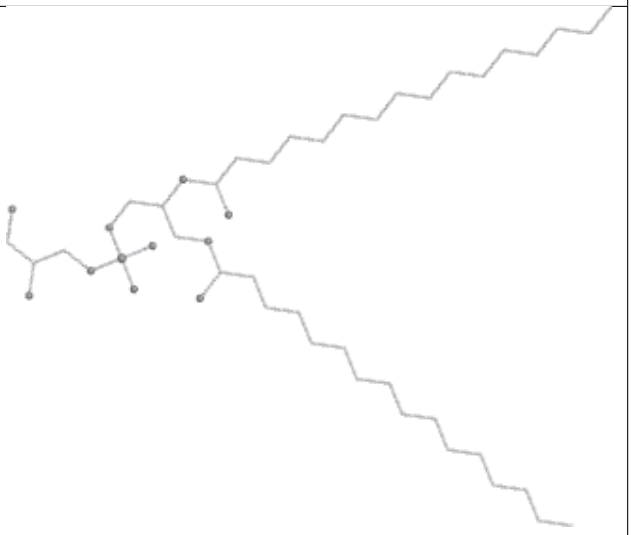
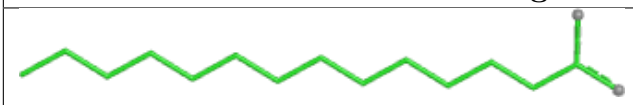


Rings

Ligand STE b 623



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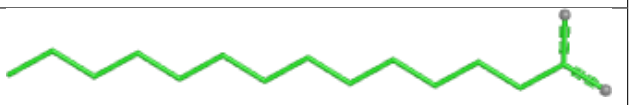

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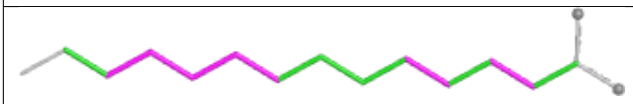

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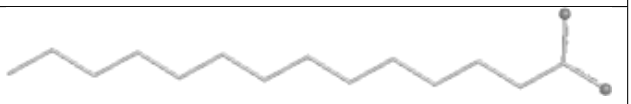
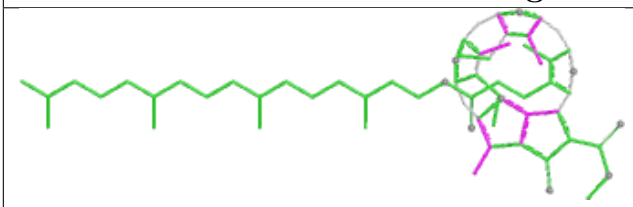


Rings

Ligand PHO a 609



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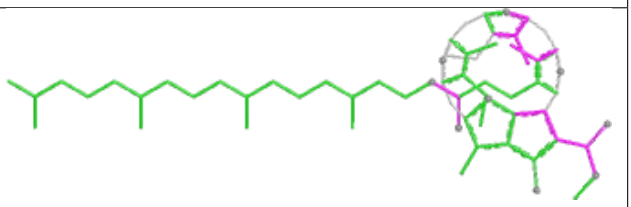
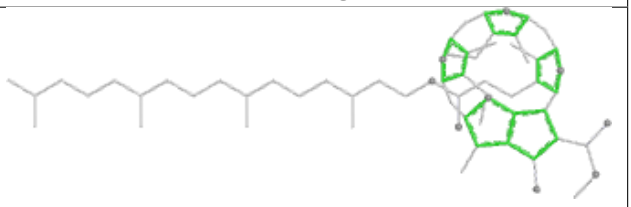


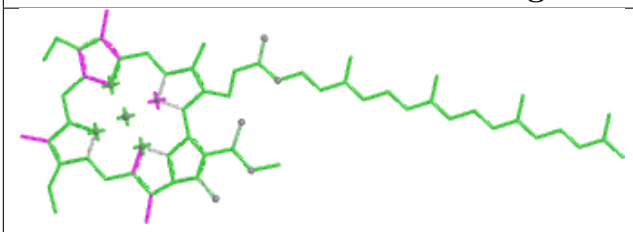
Bond angles

Torsions

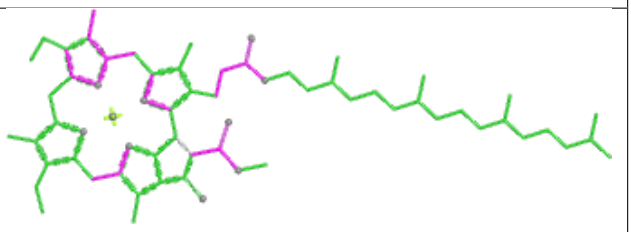


Rings

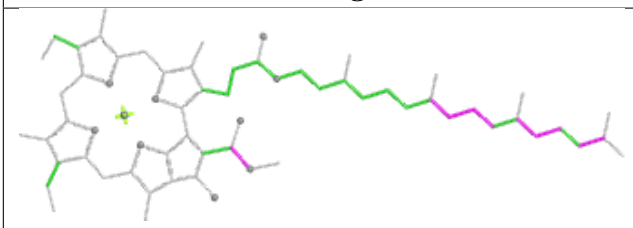
Ligand CLA b 602



Bond lengths



Bond angles



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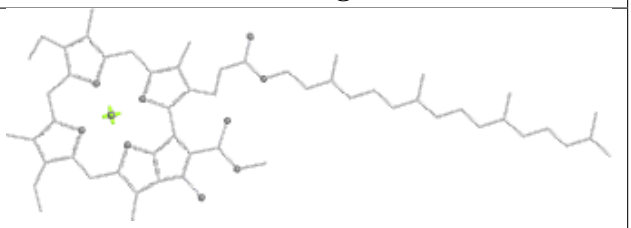
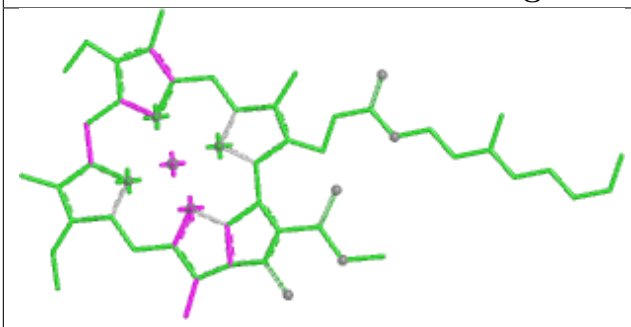
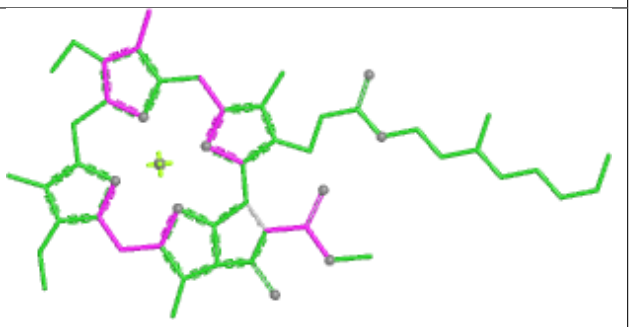


Rings

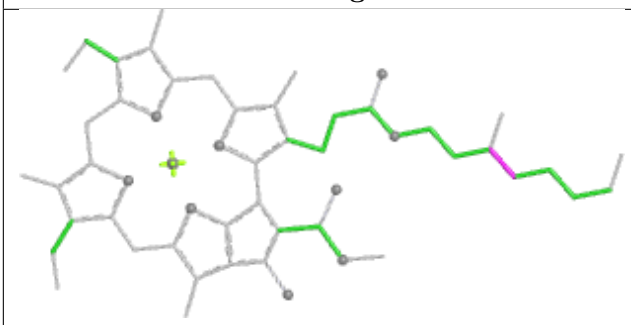
Ligand CLA A 609



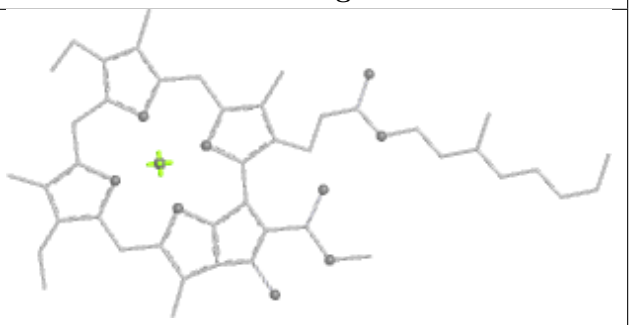
Bond lengths



Bond angles

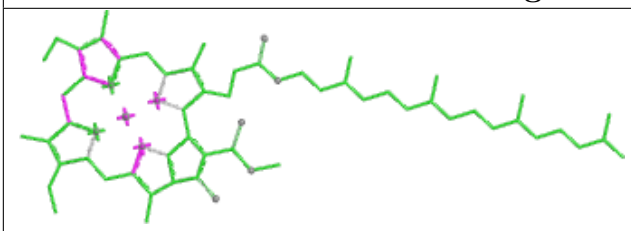


Torsions

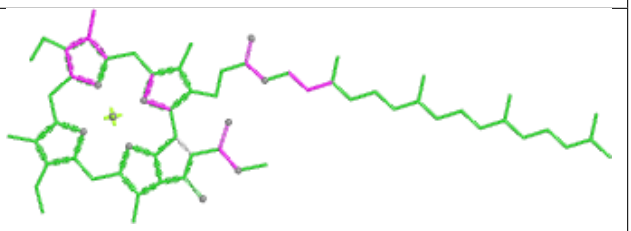


Rings

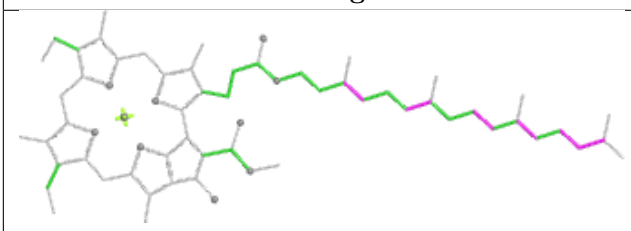
Ligand CLA C 505



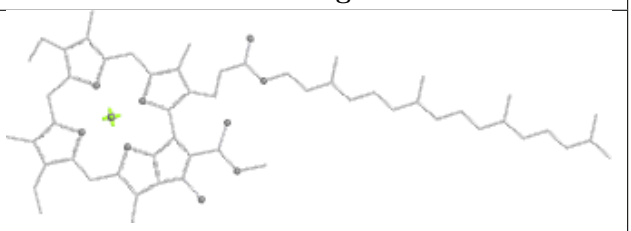
Bond lengths



Bond angles

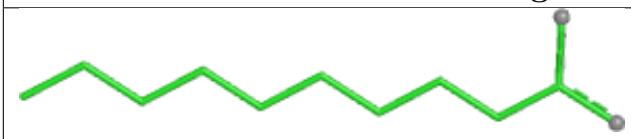


Torsions



Rings

Ligand STE k 103



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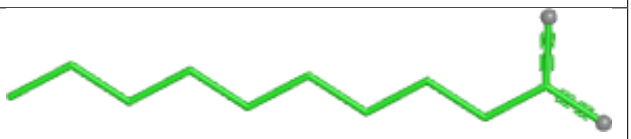
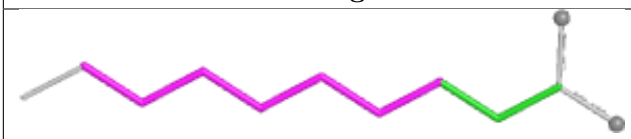


Bond angles



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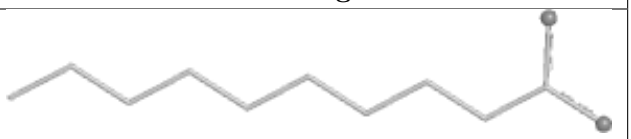
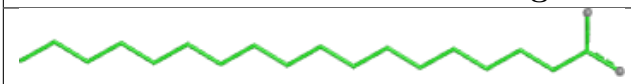


Rings

Ligand STE x 101



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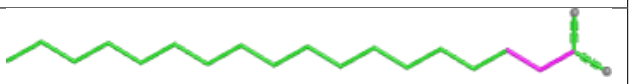


Bond angles

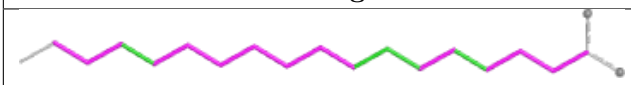
Torsions

Rings

Ligand STE c 520

Bond lengths

Bond angles



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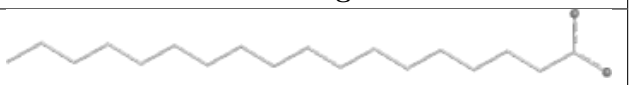
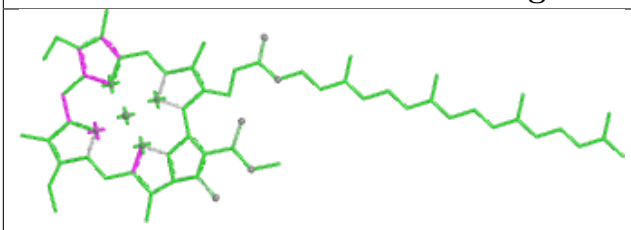


Rings

Ligand CLA a 608



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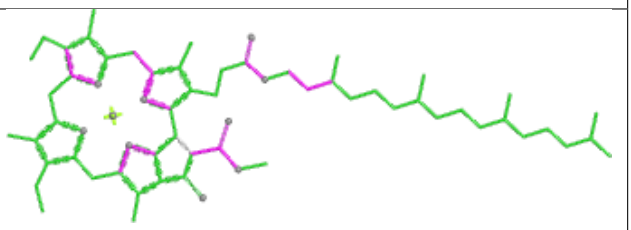

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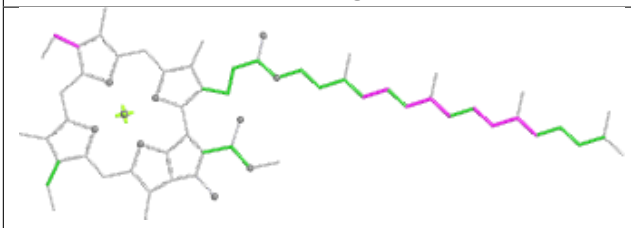

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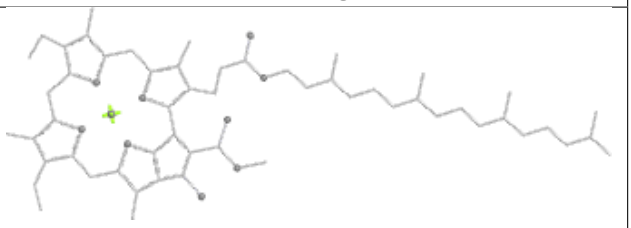

Rings

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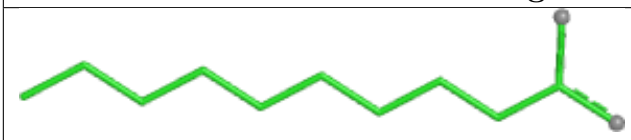

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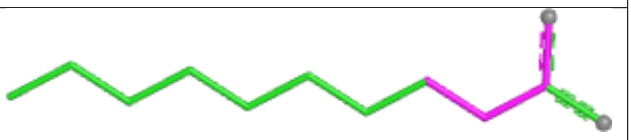
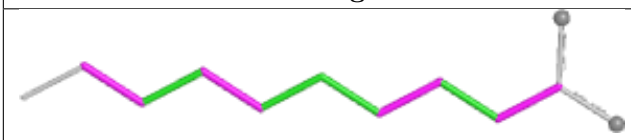


Bond angles



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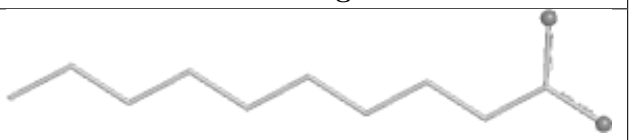

Rings

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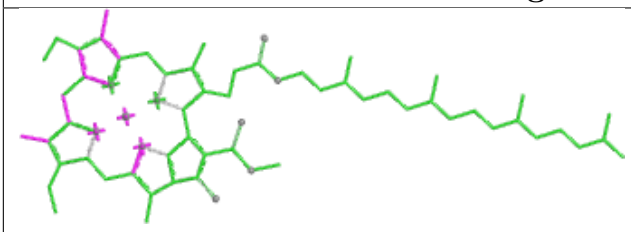

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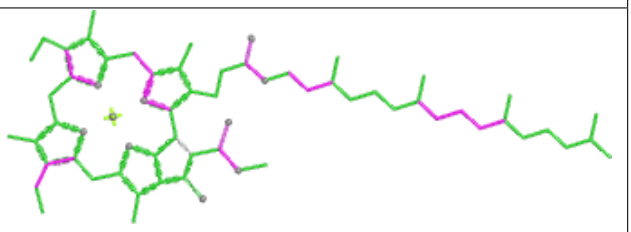

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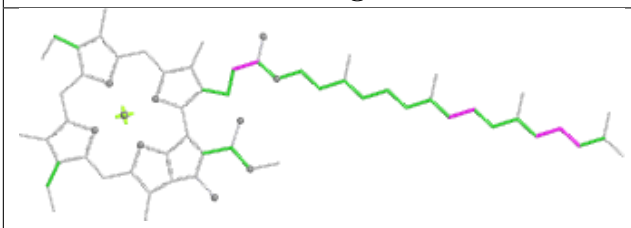

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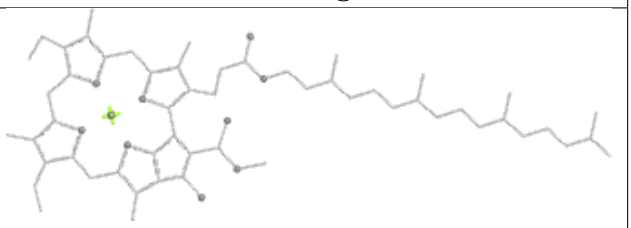
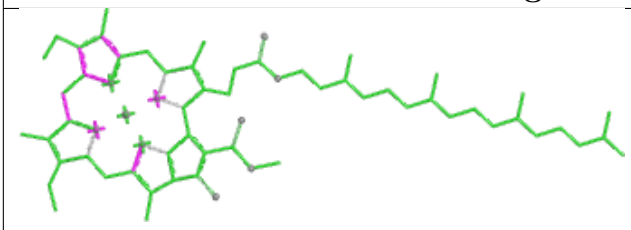


Rings

Ligand CLA B 604



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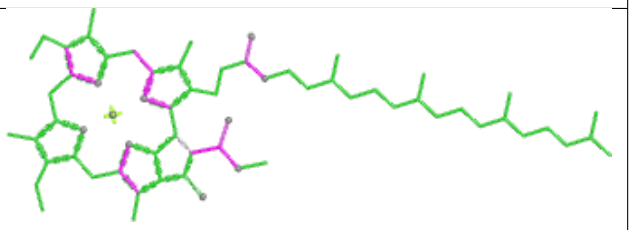
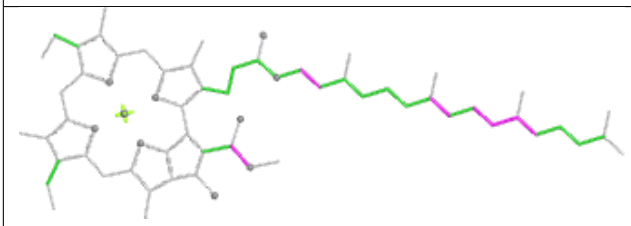


Bond angles



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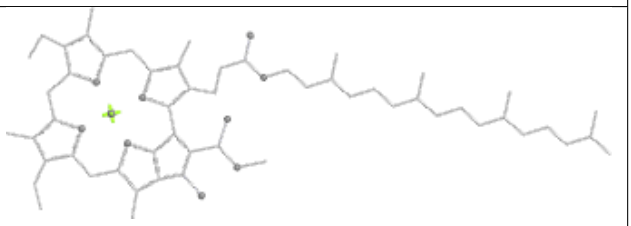
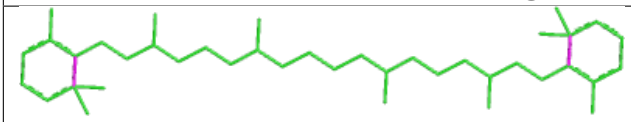


Rings

Ligand BCR B 618



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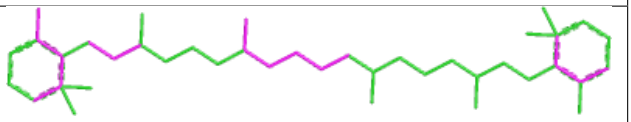

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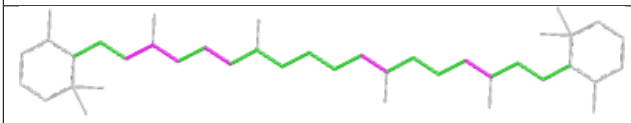

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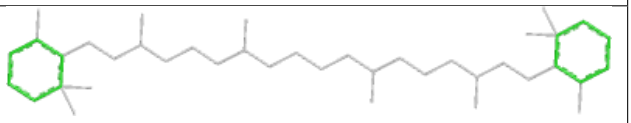
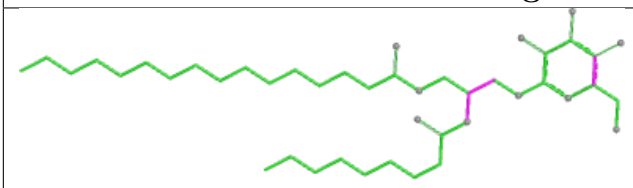


Rings

Ligand LMG d 409



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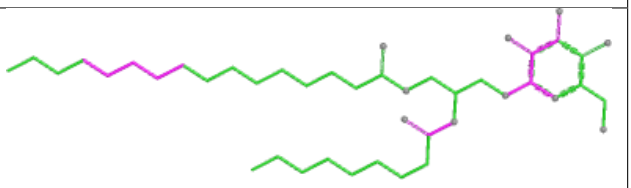
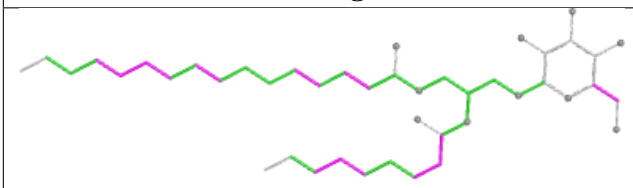


Bond angles



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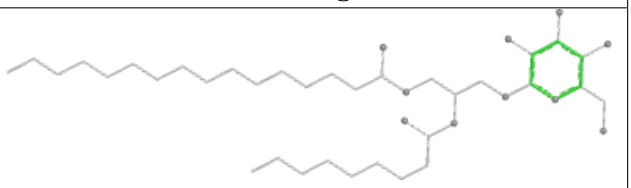
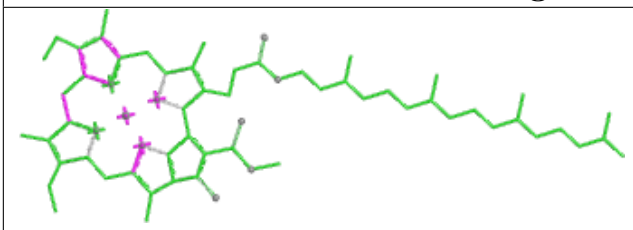


Rings

Ligand CLA c 513



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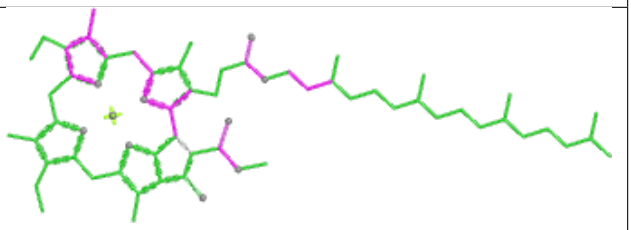

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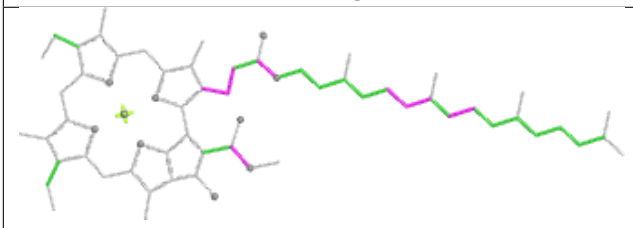

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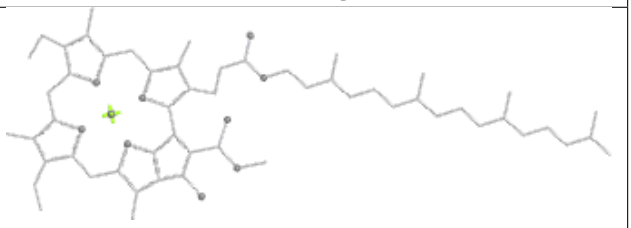
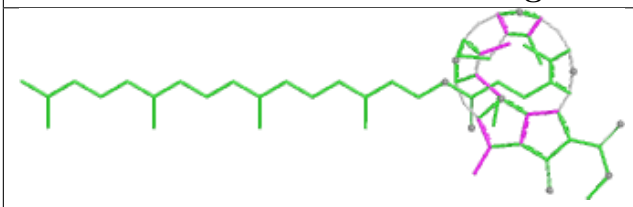


Rings

Ligand PHO d 401



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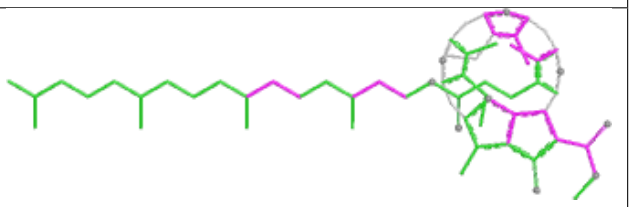
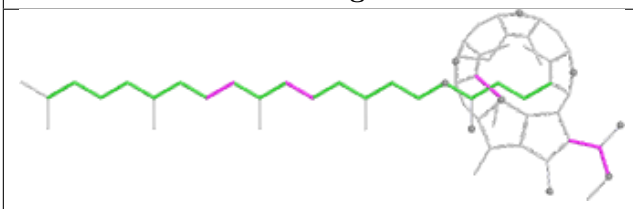


Bond angles



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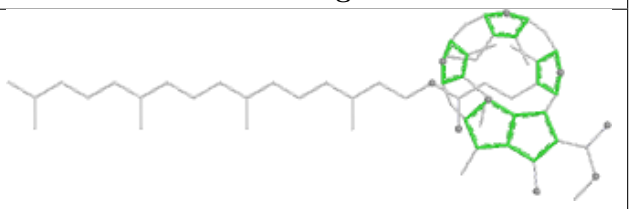
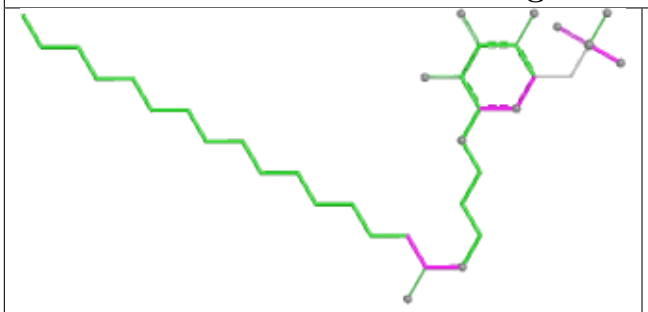


Rings

Ligand SQD F 102



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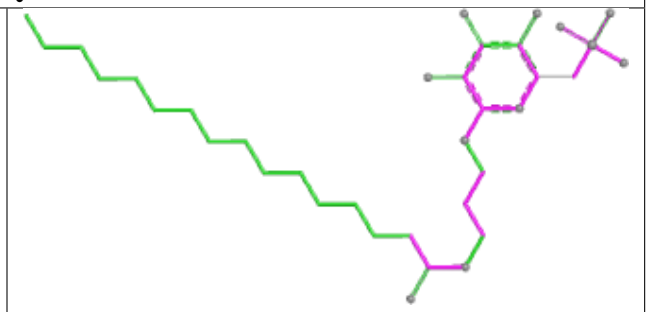

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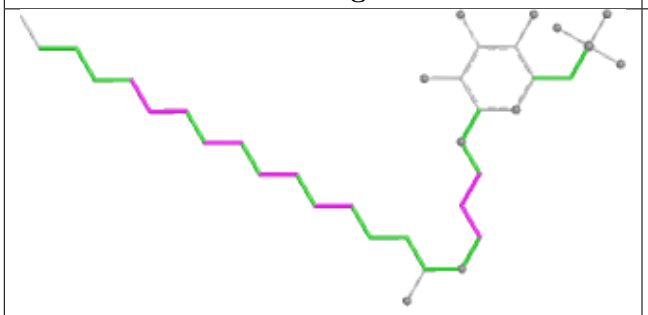

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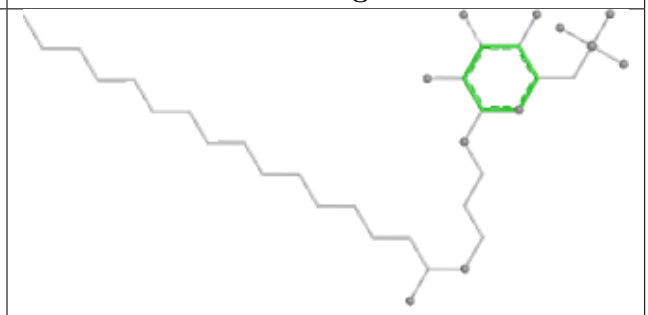
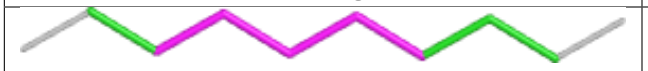


Rings

Ligand STE t 103

Bond lengths

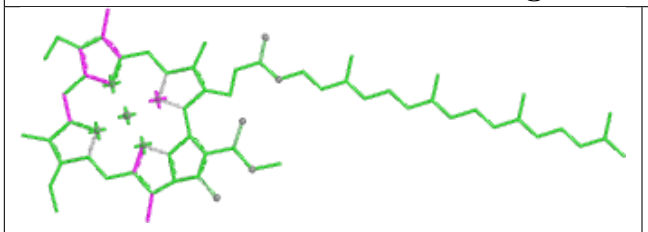
Bond angles



Torsions

Rings

Ligand CLA C 511



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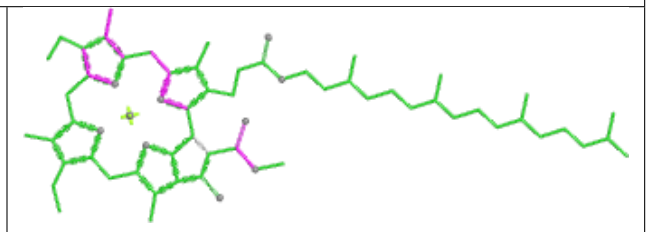
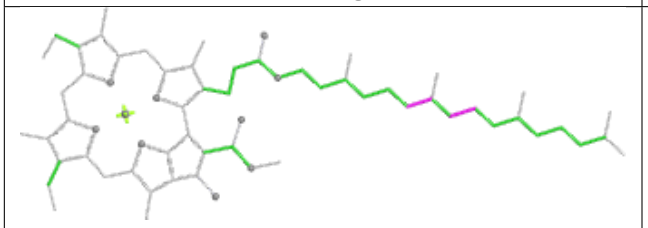


Bond angles



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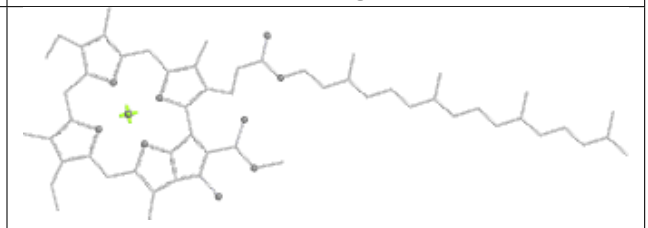
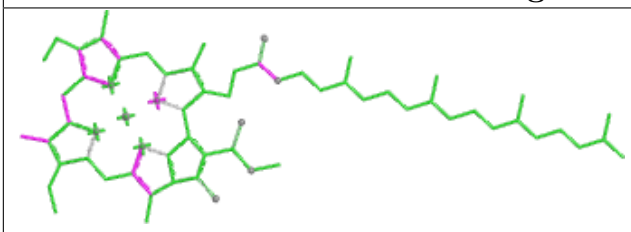


Rings

Ligand CLA h 101



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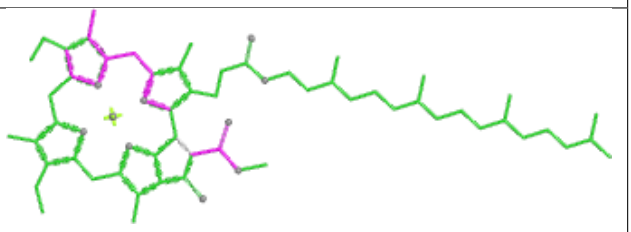

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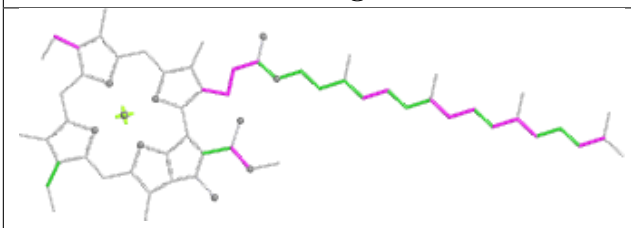

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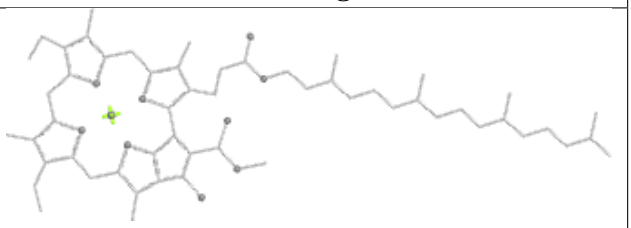
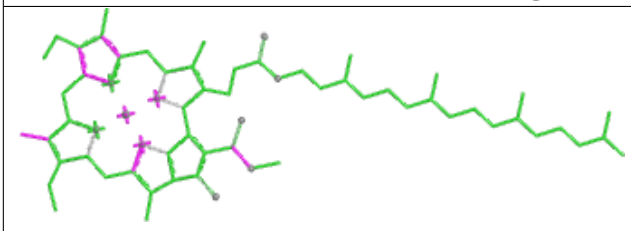
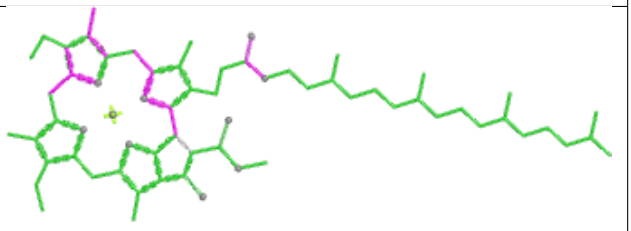


Rings

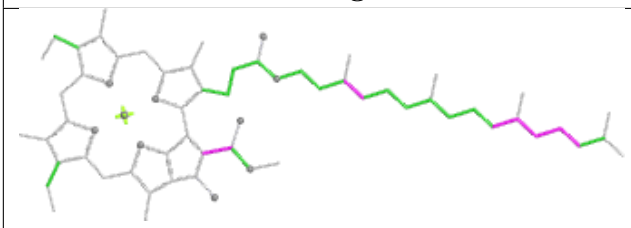
Ligand CLA b 608



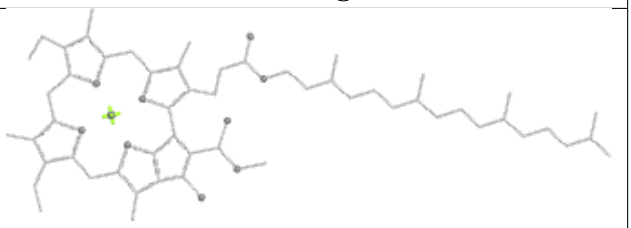
Bond lengths



Bond angles

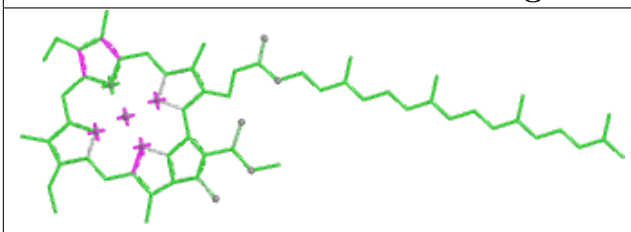


Torsions

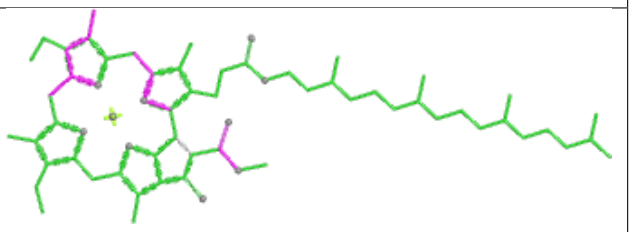


Rings

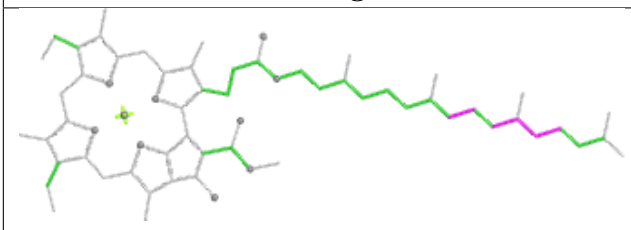
Ligand CLA B 607



Bond lengths



Bond angles



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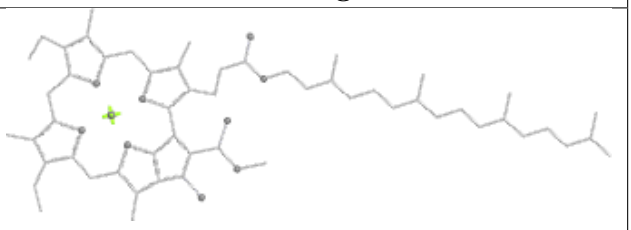
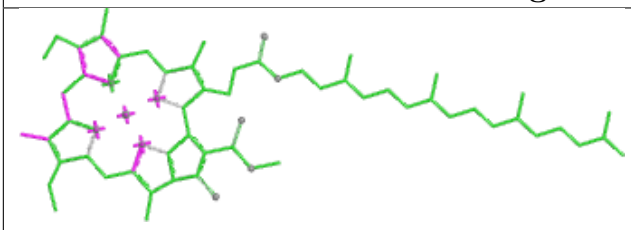
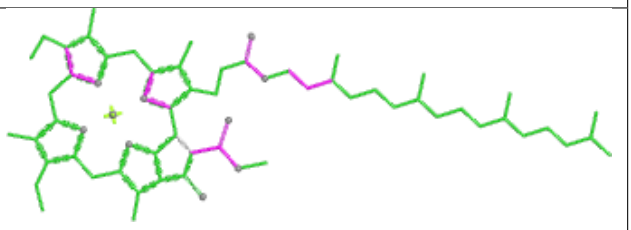


Rings

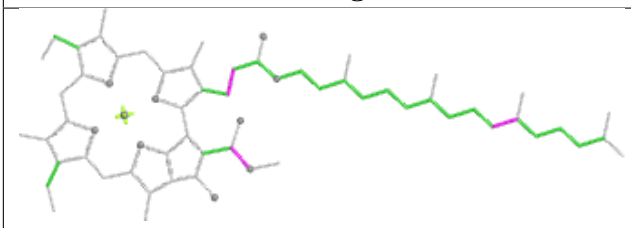
Ligand CLA c 501



Bond lengths



Bond angles



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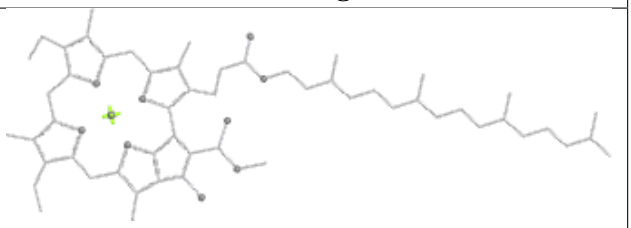
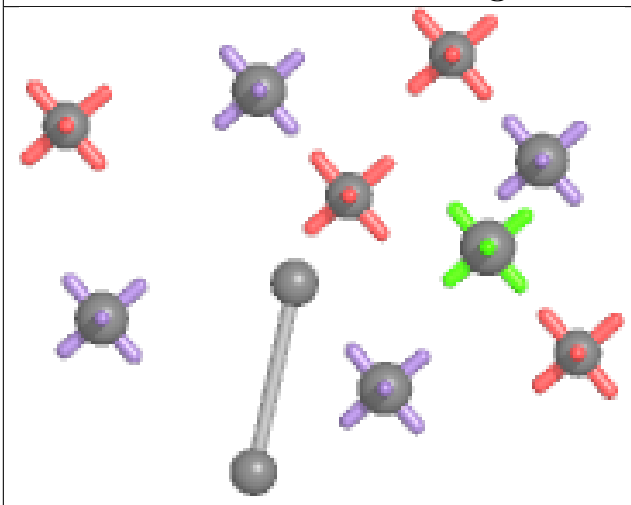


Rings

Ligand OEY A 602 (A)



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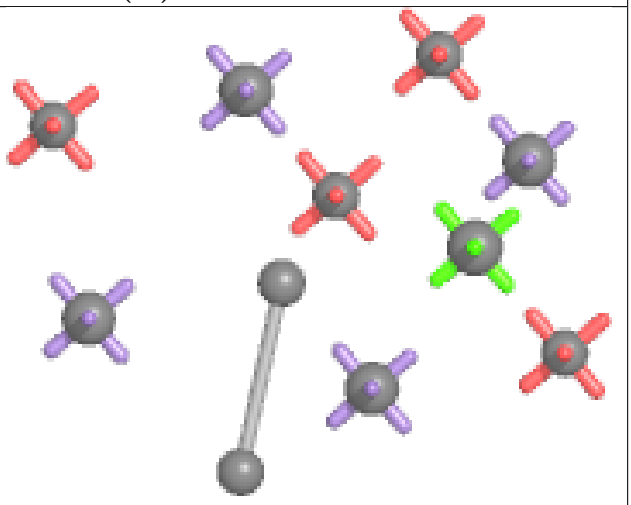
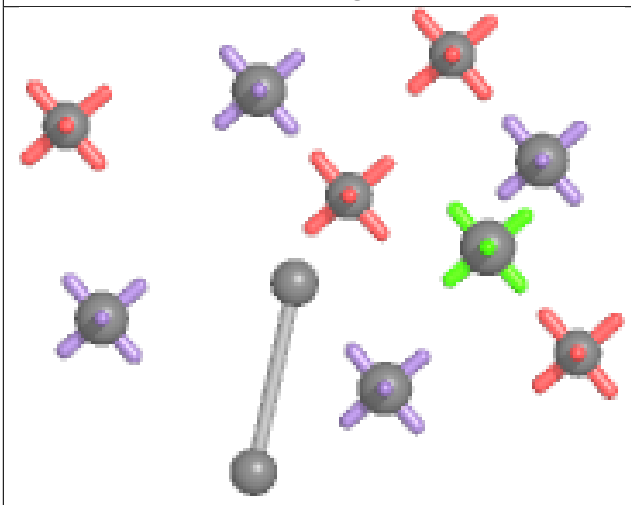


Bond angles



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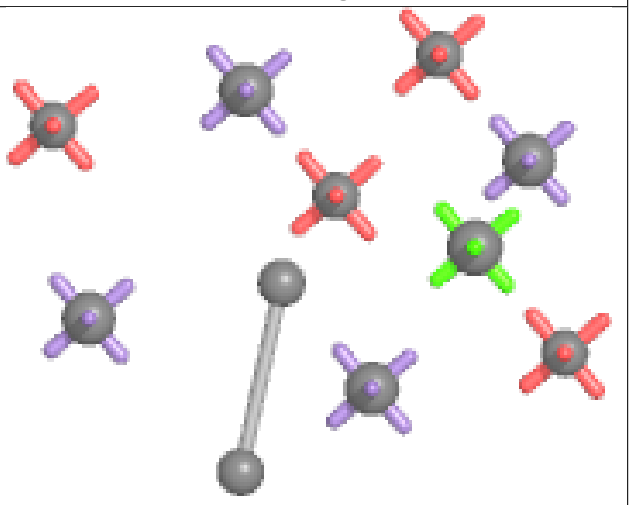
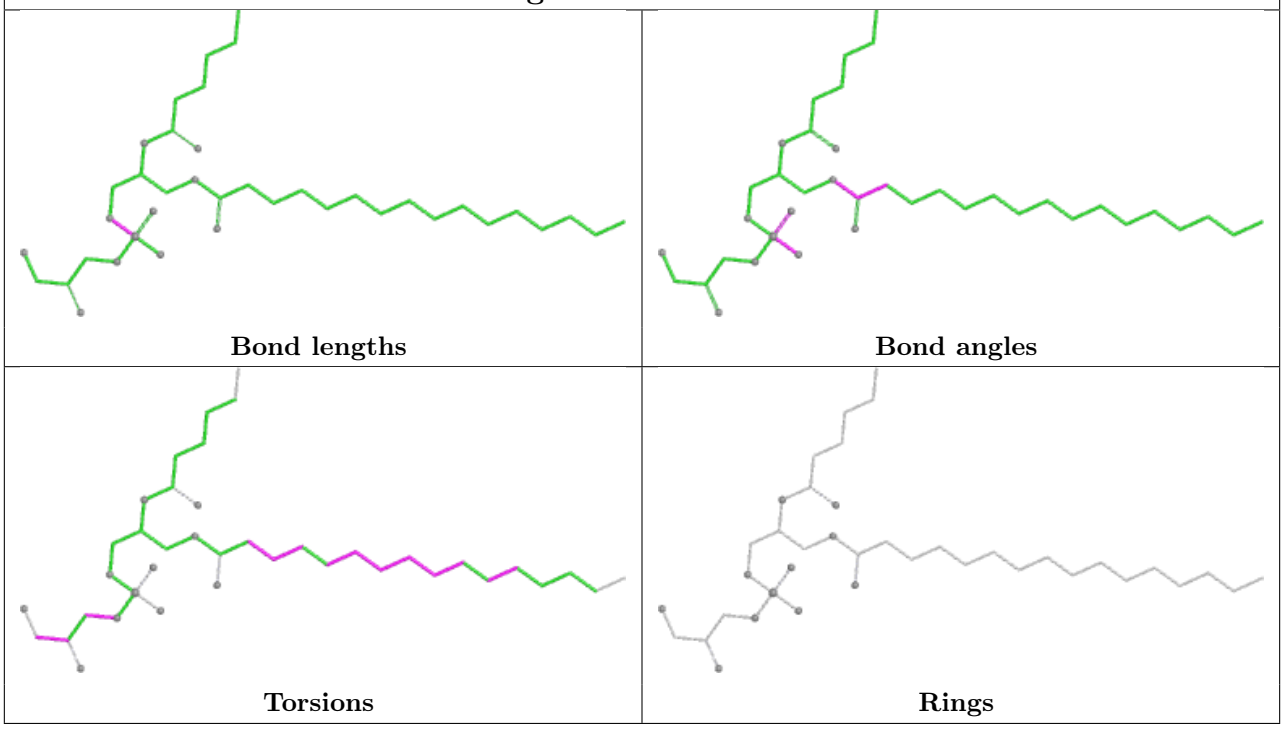
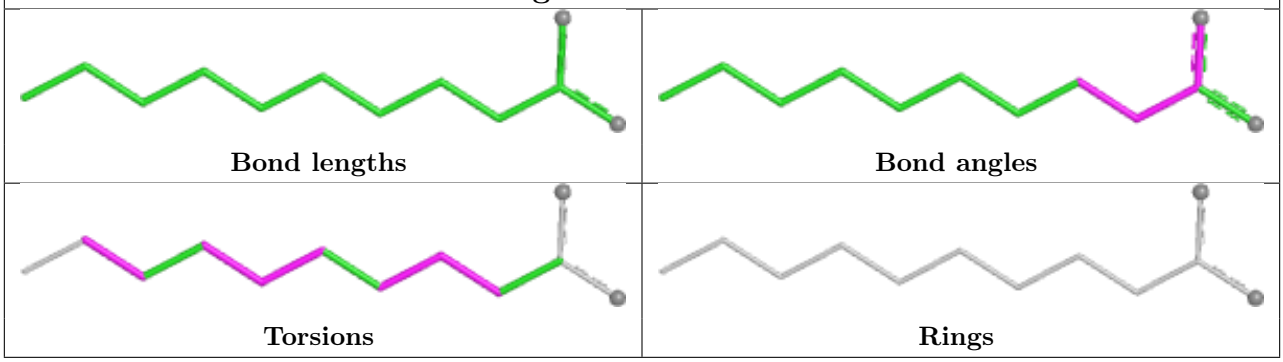


Rings

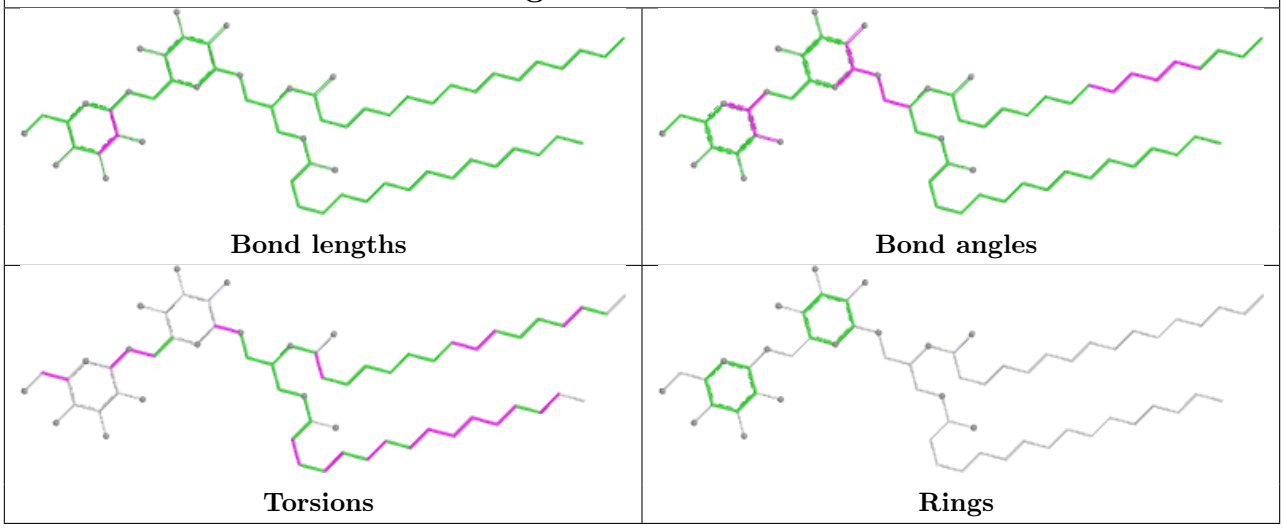
Ligand LHG d 407

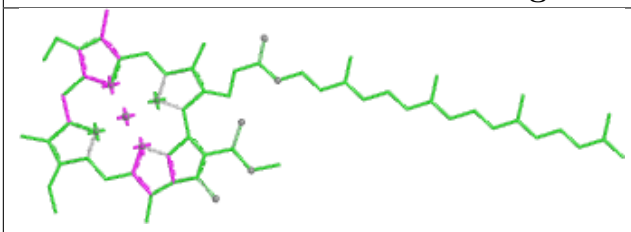
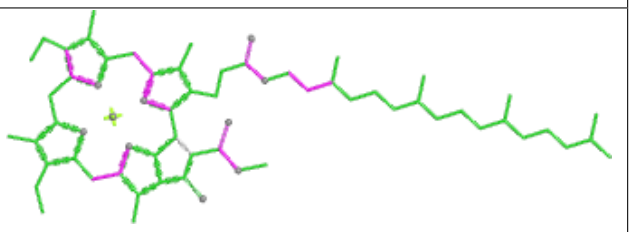
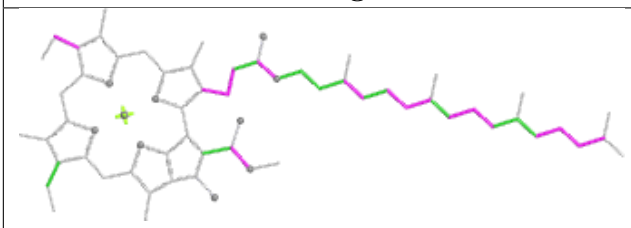
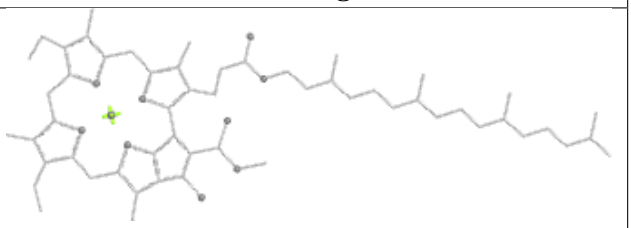


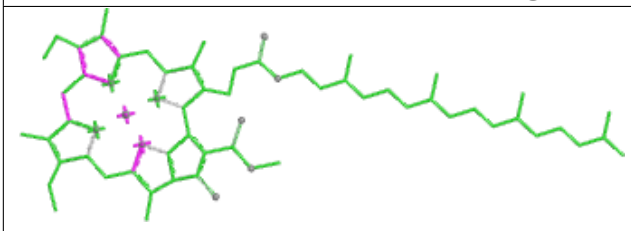
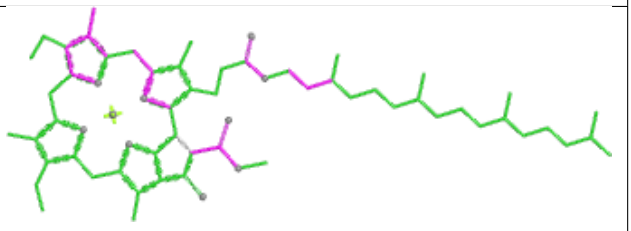
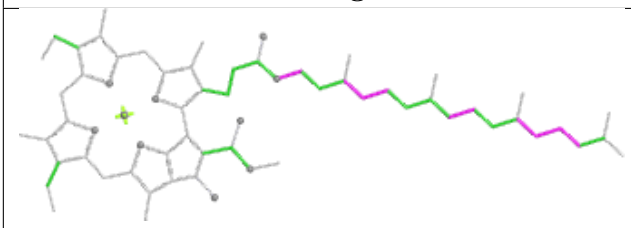
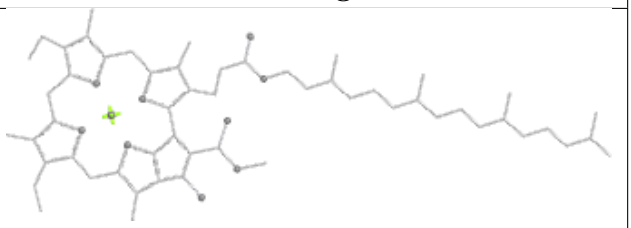
Ligand STE a 618



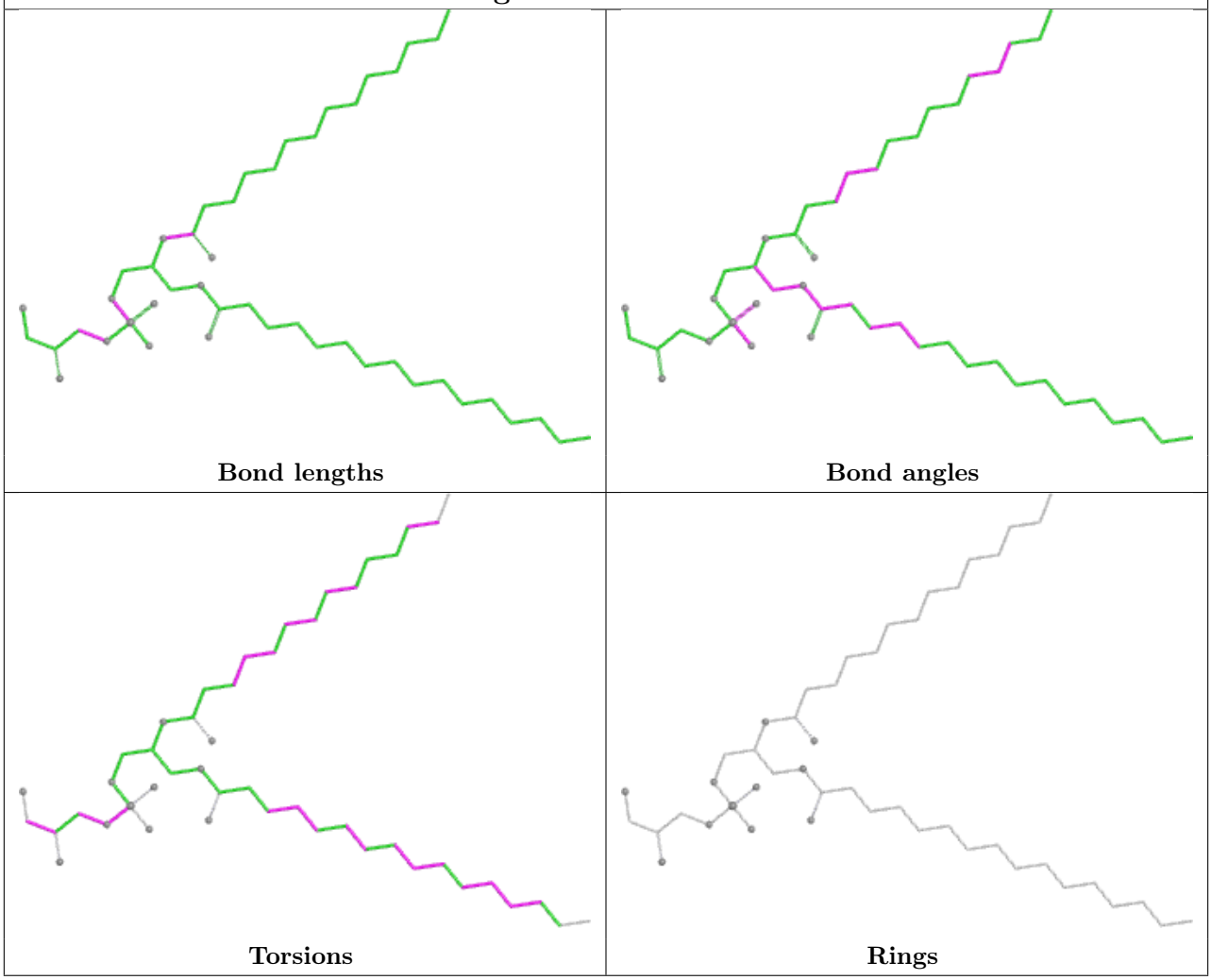
Ligand DGD c 517



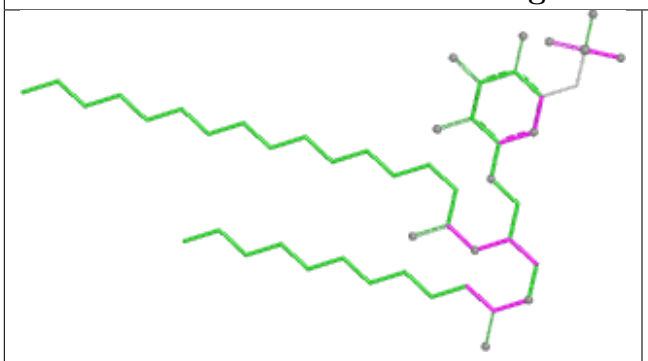
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

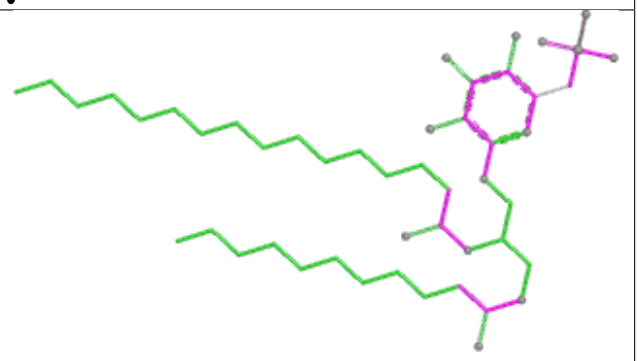
Ligand LHG A 614



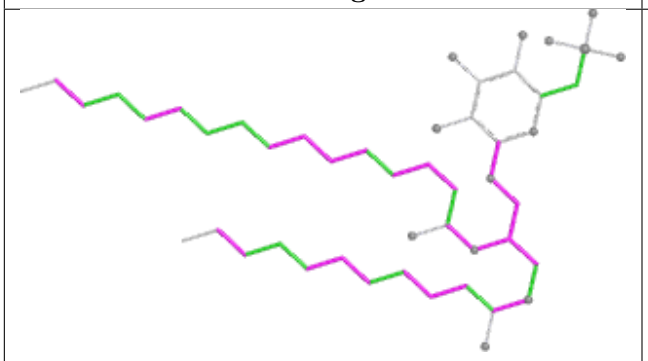
Ligand SQD b 619



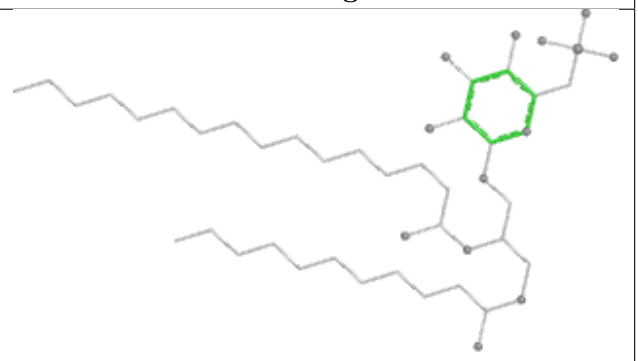
Bond lengths



Bond angles

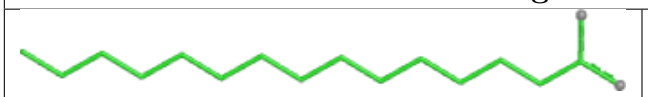


Torsions

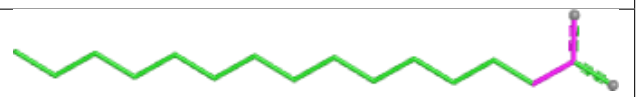


Rings

Ligand STE d 410

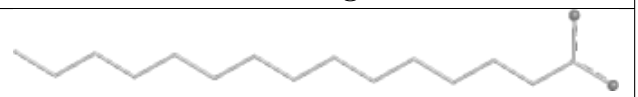


Bond lengths



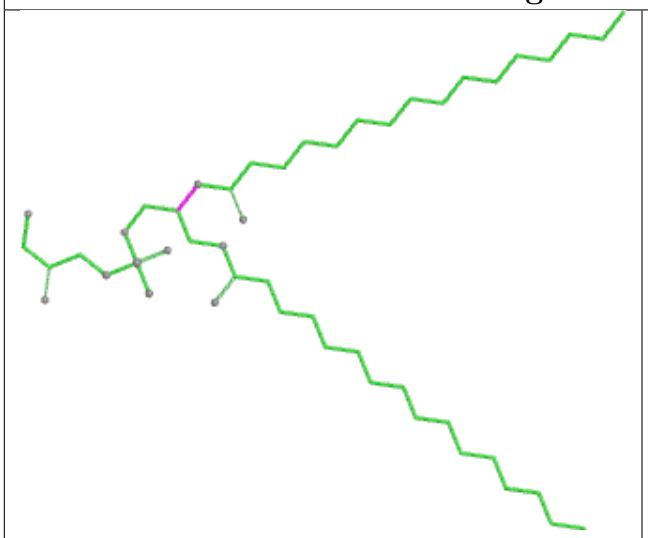
Bond angles

Torsions

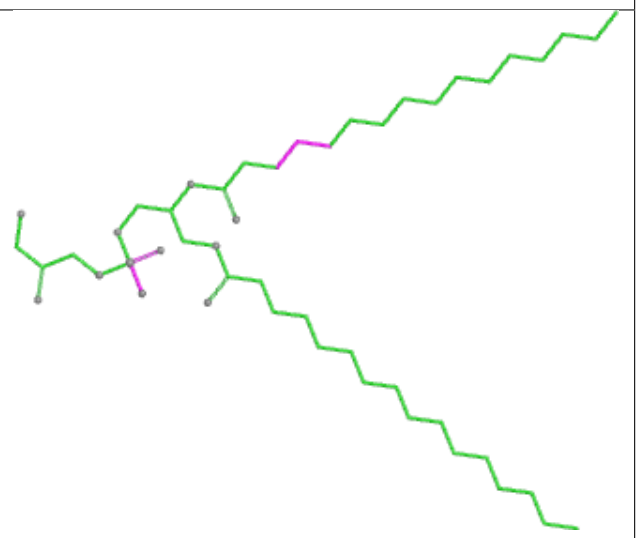


Rings

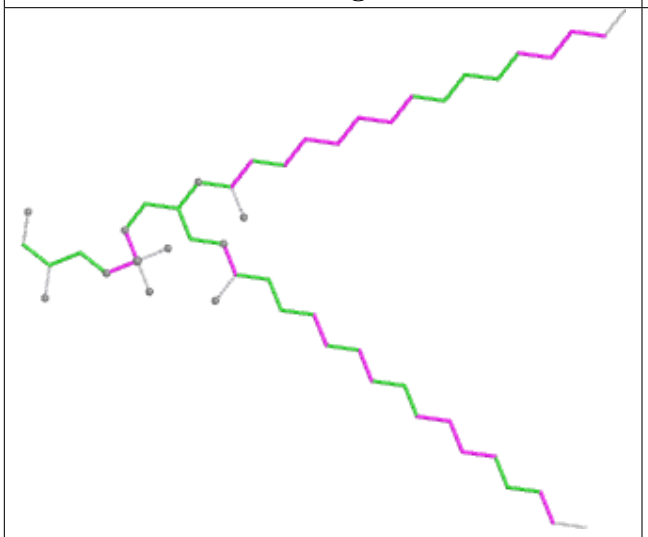
Ligand LHG L 101



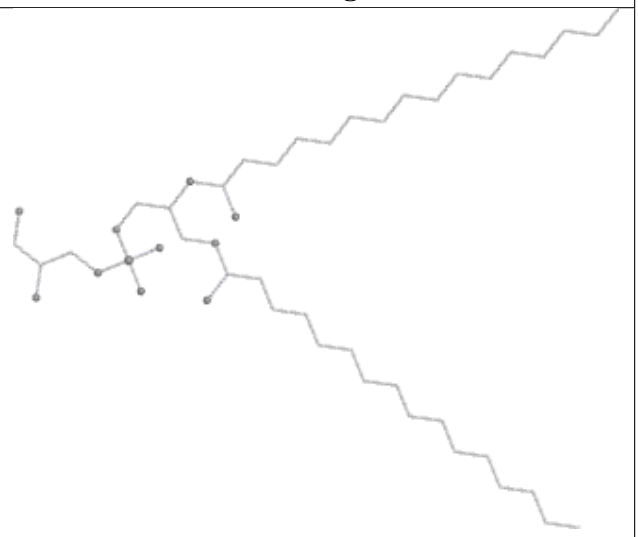
Bond lengths



Bond angles



Torsions

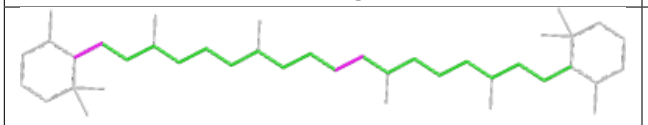


Rings

Ligand BCR k 102

Bond lengths

Bond angles



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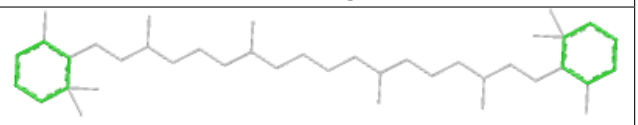
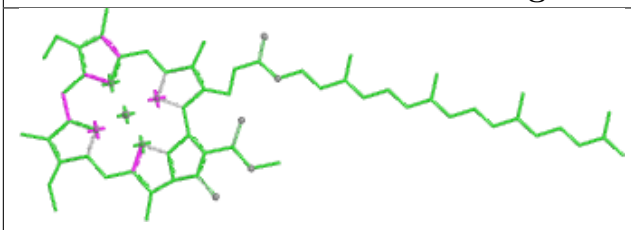


Rings

Ligand CLA a 613



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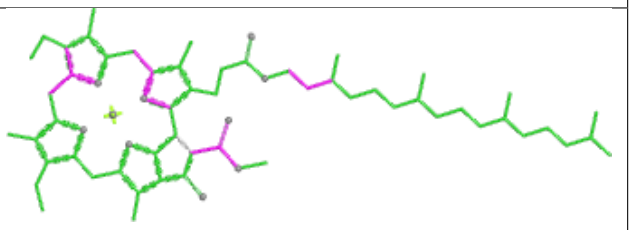
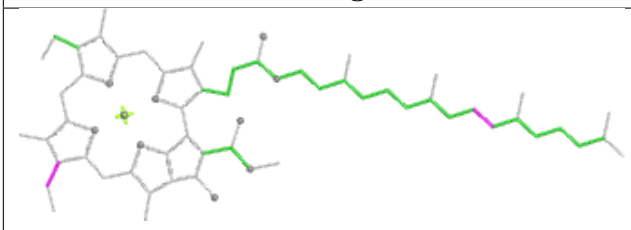


Bond angles



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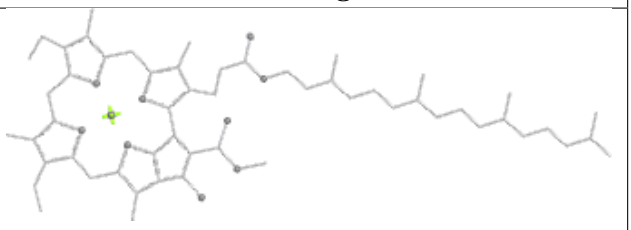
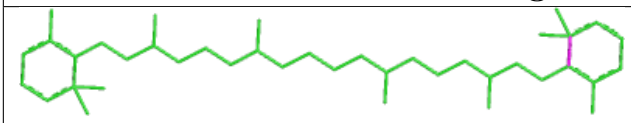


Rings

Ligand BCR t 101



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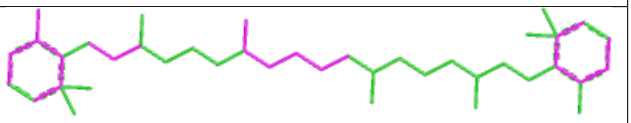
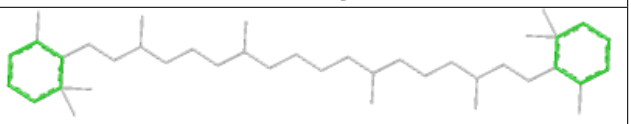


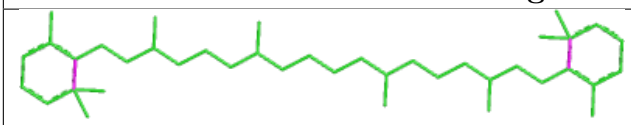
Bond angles

Torsions



Rings

Ligand BCR c 514



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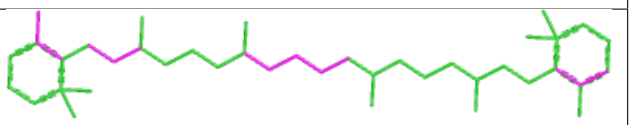
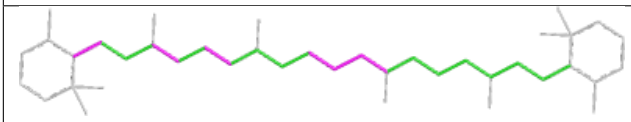


Bond angles



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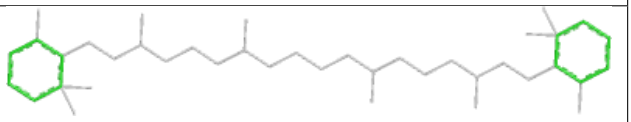
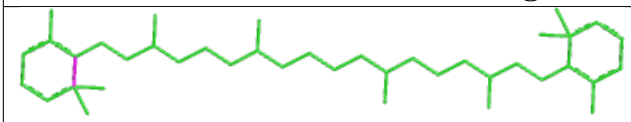


Rings

Ligand BCR A 610



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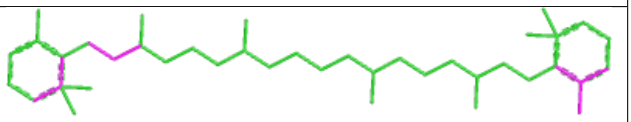
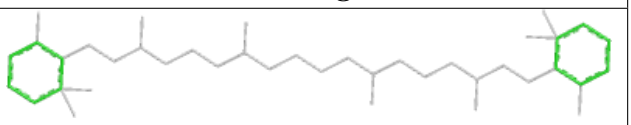


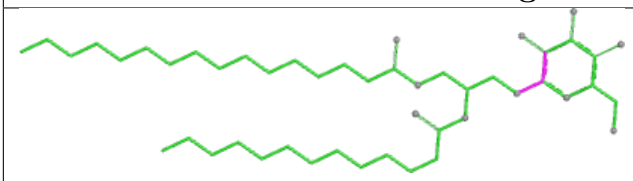
Bond angles

Torsions



Rings

Ligand LMG A 613



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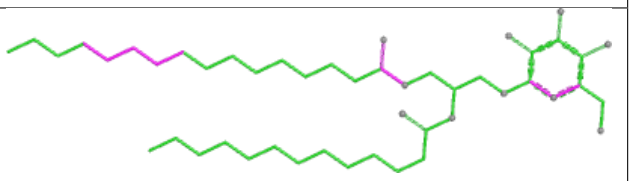
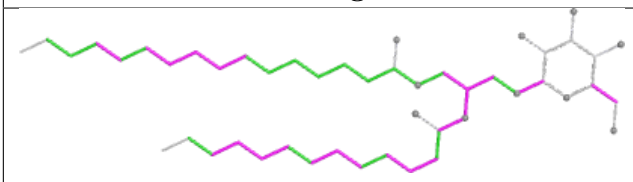
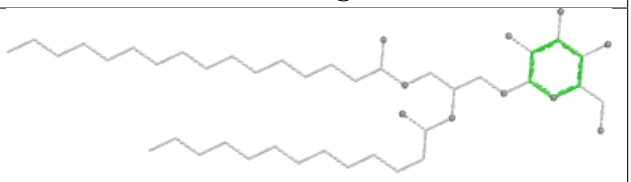


Bond angles

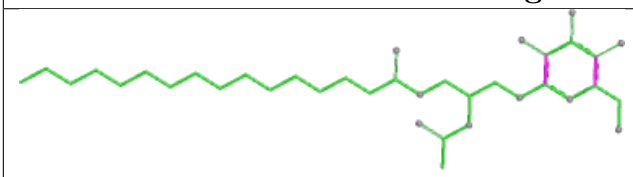


Torsions



Rings

Ligand LMG c 519



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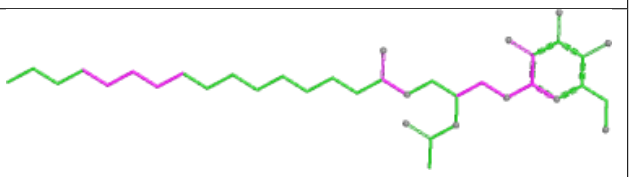
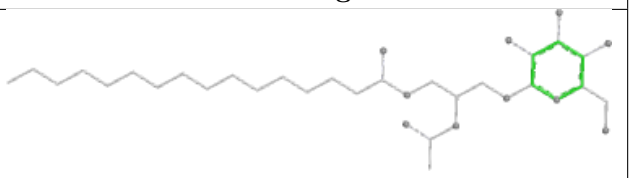


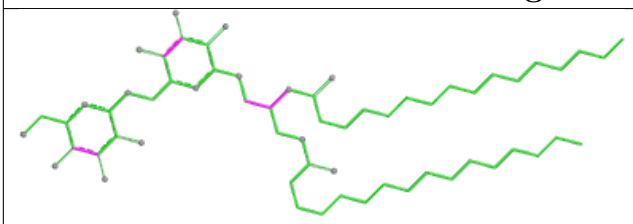
Bond angles

Torsions



Rings

Ligand DGD c 516



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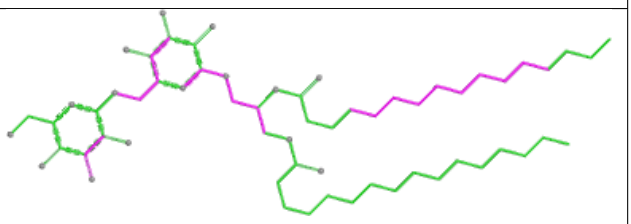
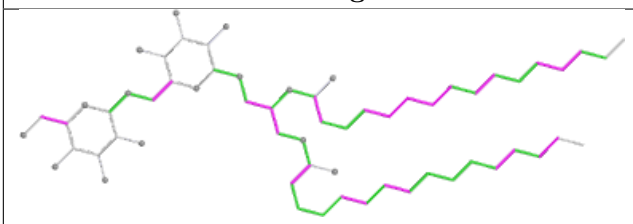


Bond angles



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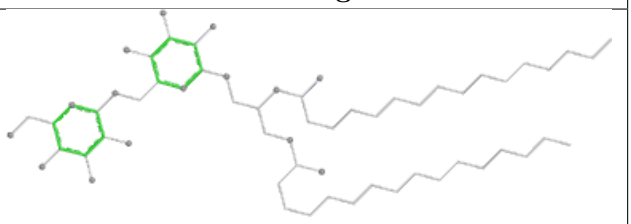
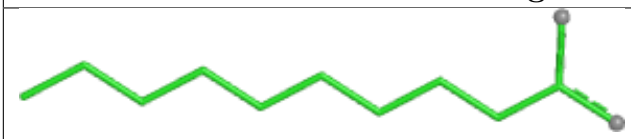


Rings

Ligand STE B 624



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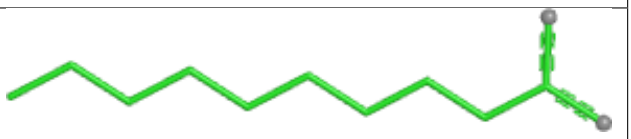

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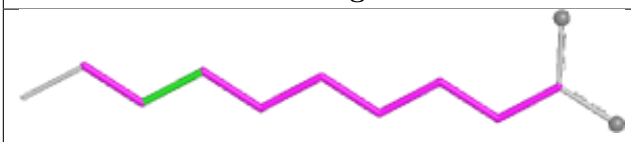

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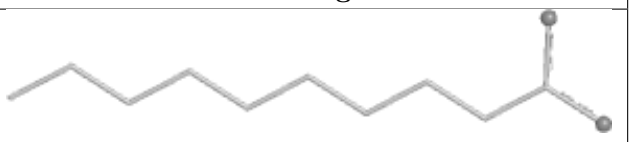
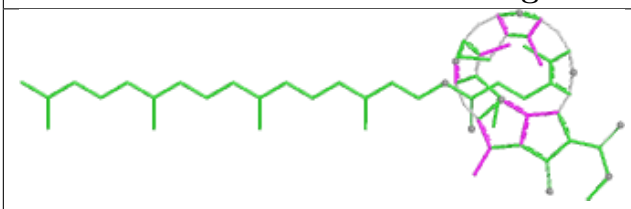


Rings

Ligand PHO A 608



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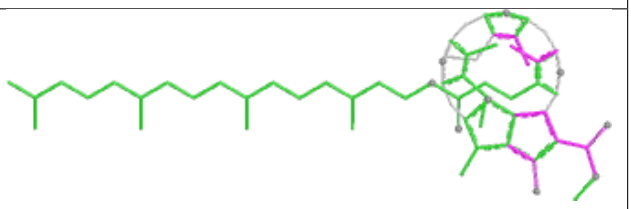
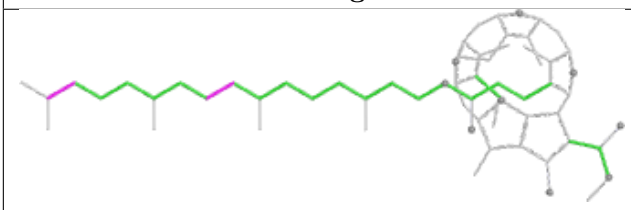


Bond angles



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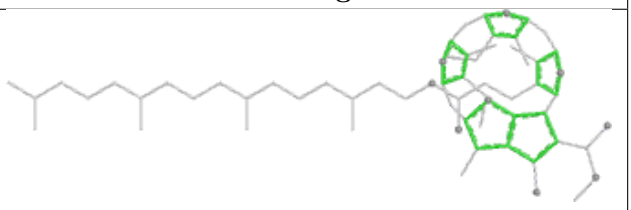
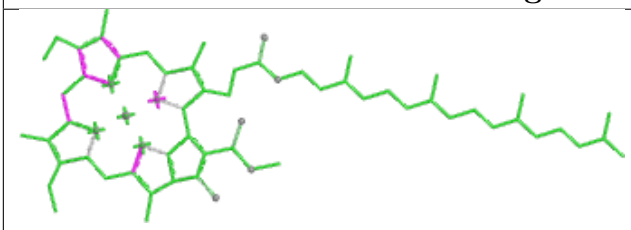


Rings

Ligand CLA B 611



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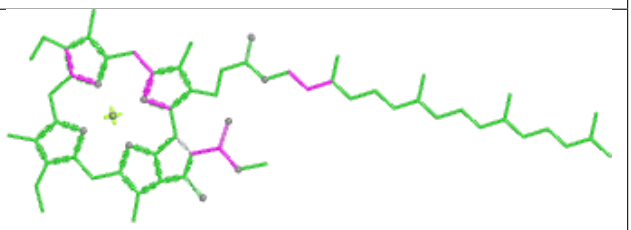

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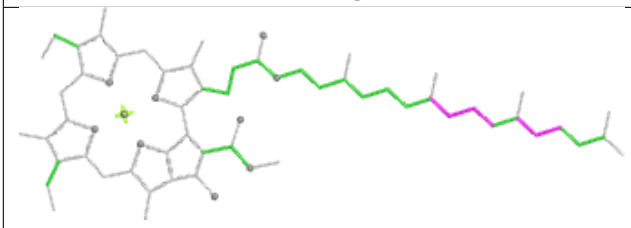

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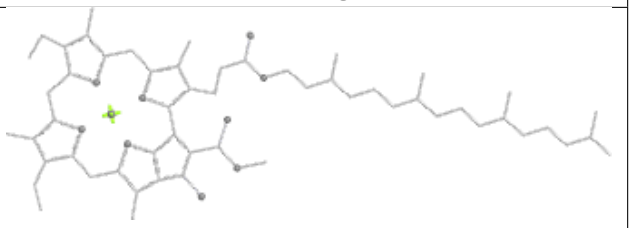
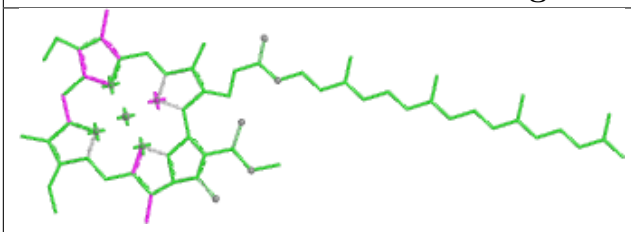


Rings

Ligand CLA c 510



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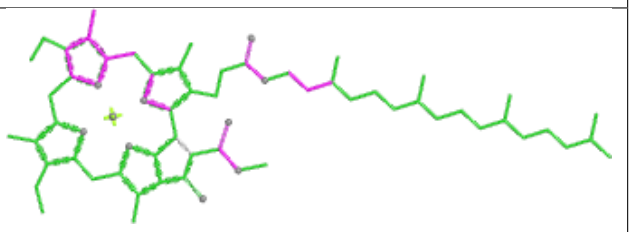
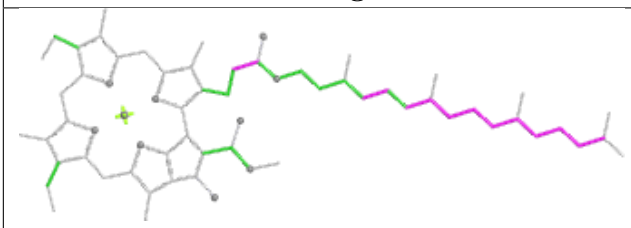


Bond angles



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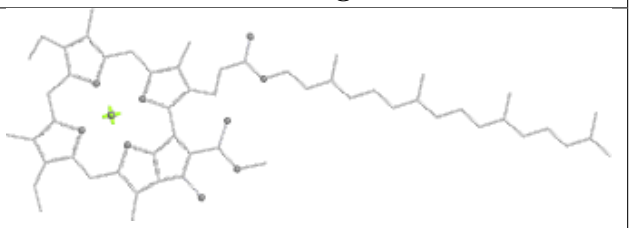
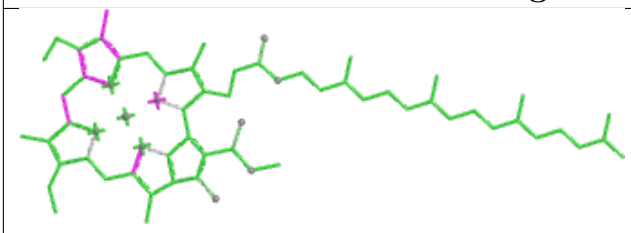


Rings

Ligand CLA c 505



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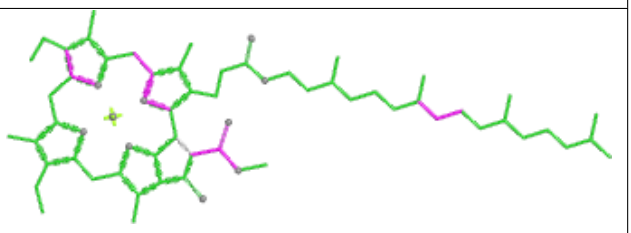

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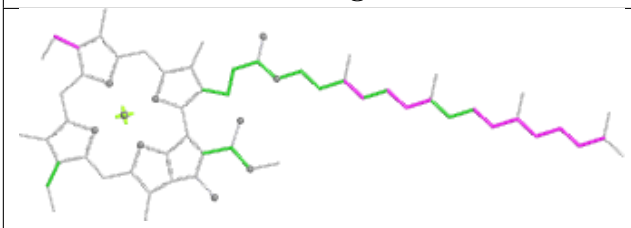

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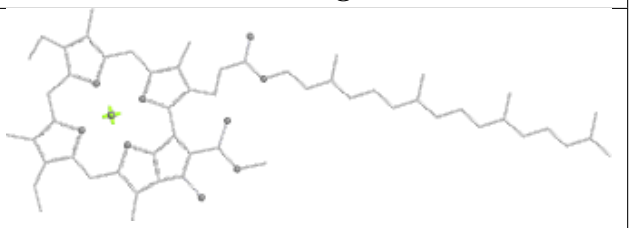
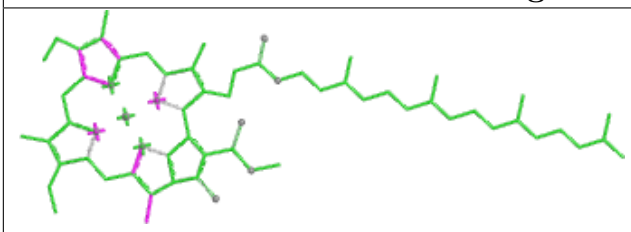


Rings

Ligand CLA b 606



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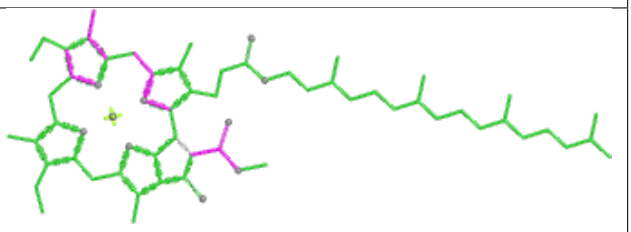
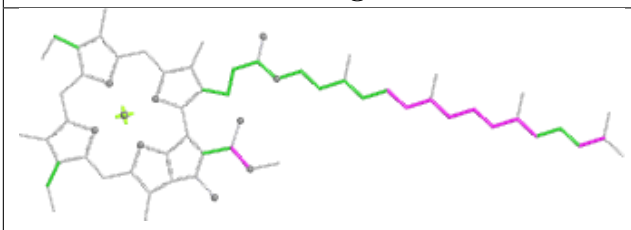


Bond angles



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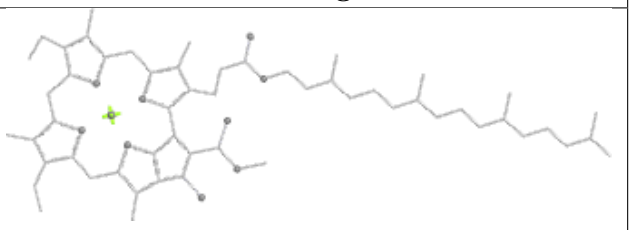
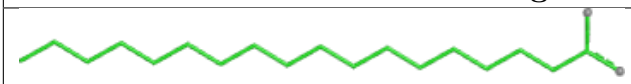


Rings

Ligand STE b 621



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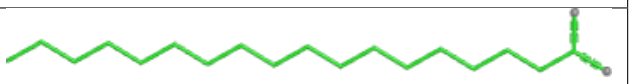


Bond angles

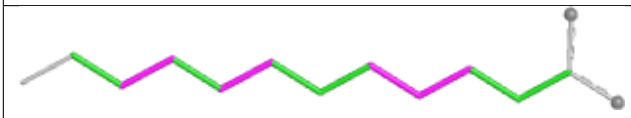
Torsions

Rings

Ligand STE t 102

Bond lengths

Bond angles



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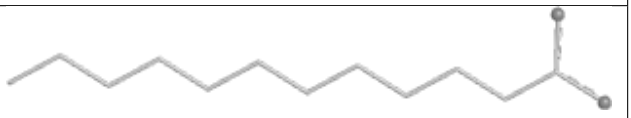
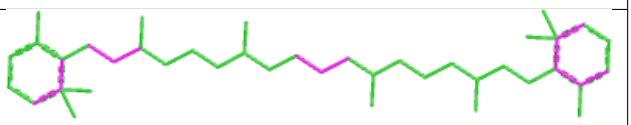


Rings

Ligand BCR a 611

Bond lengths



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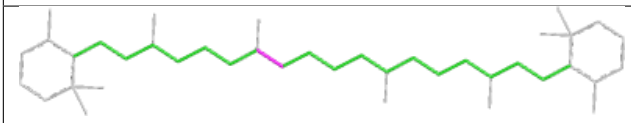

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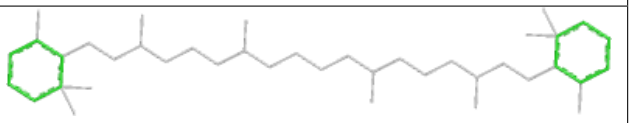
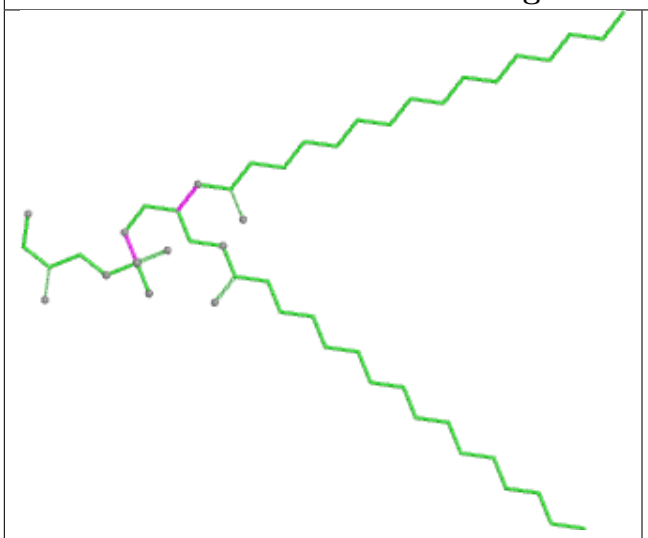


Rings

Ligand LHG D 408



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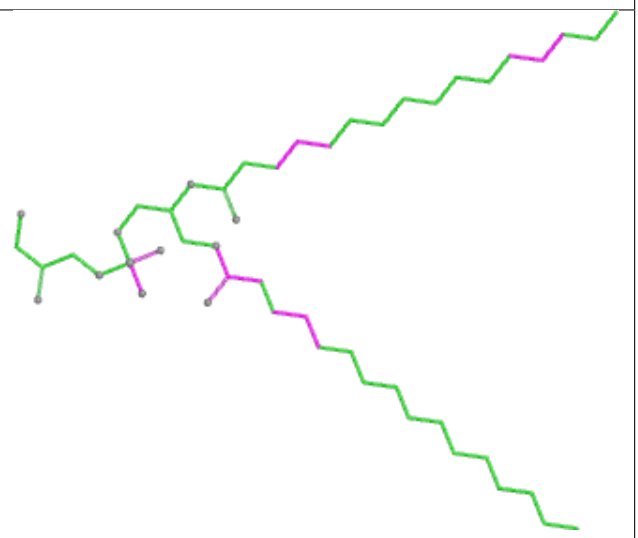

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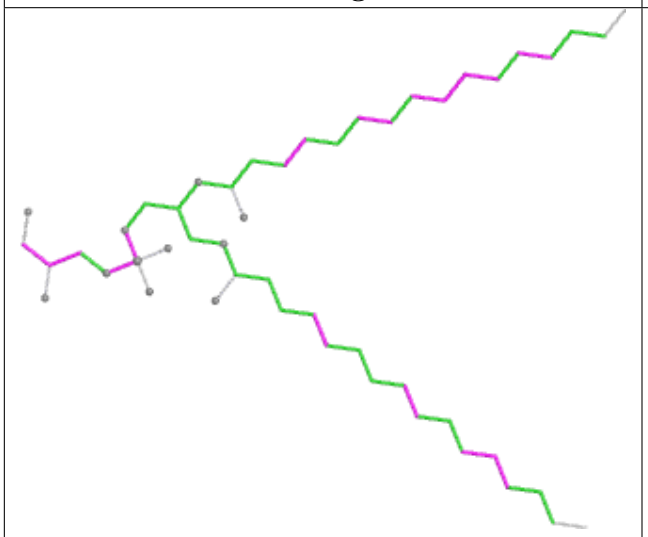

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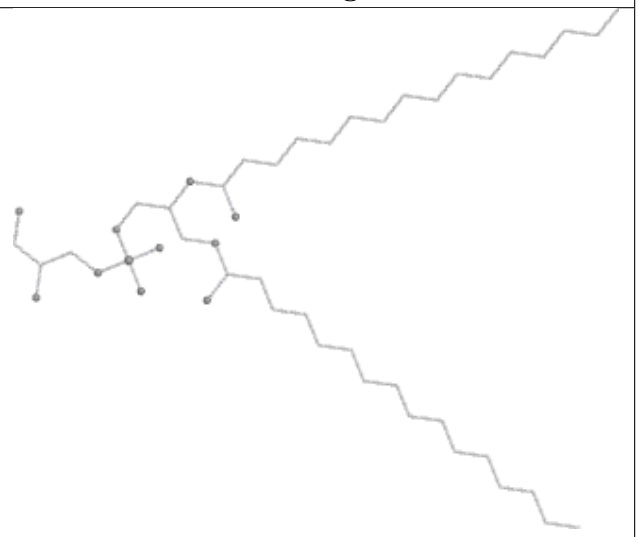
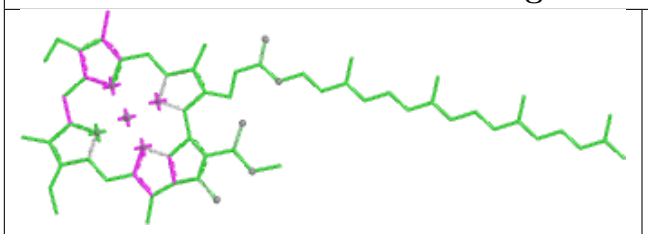


Rings

Ligand CLA B 601



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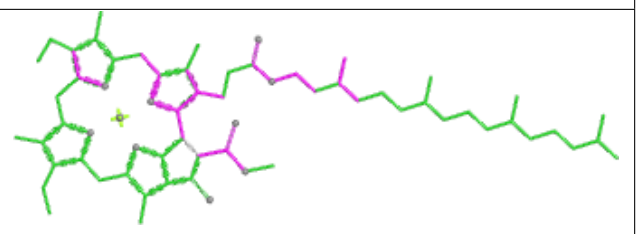
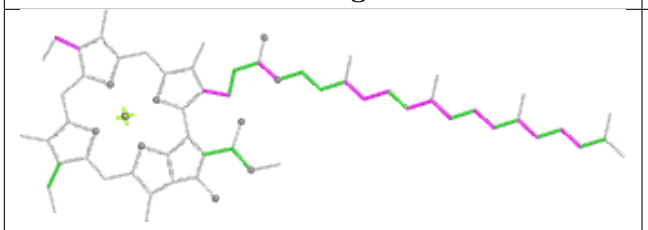


Bond angles



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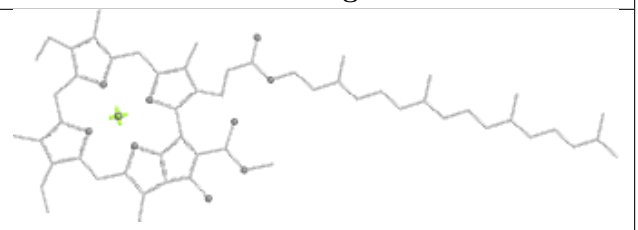
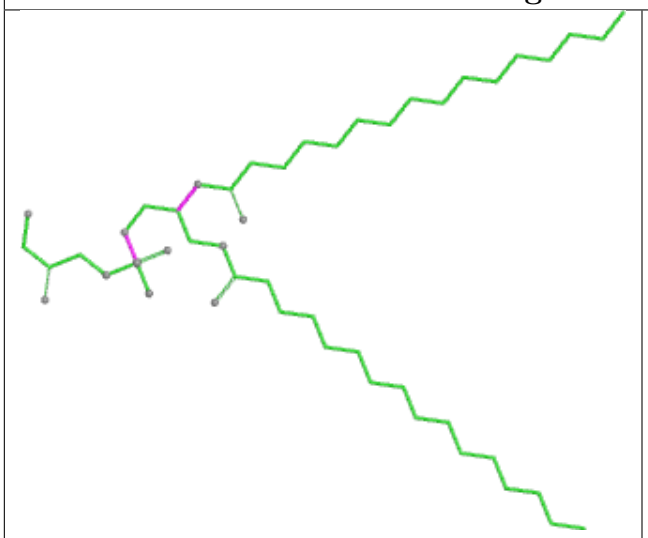


Rings

Ligand LHG E 101



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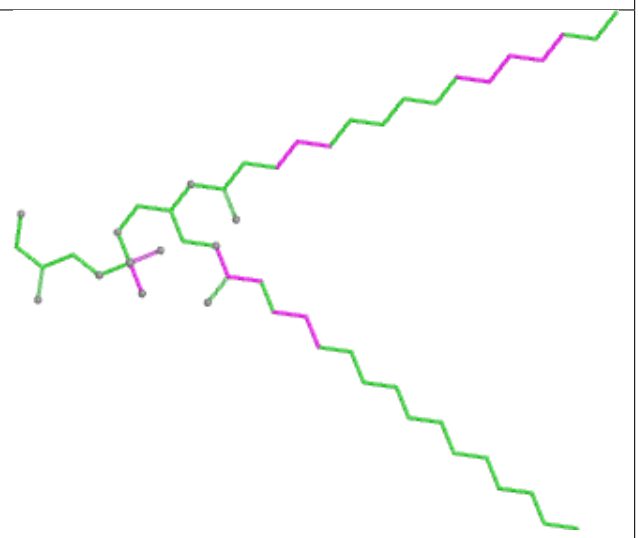
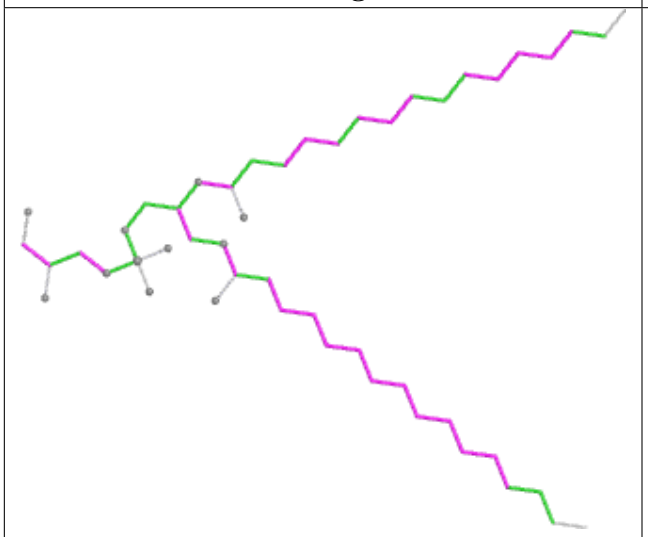


Bond angles



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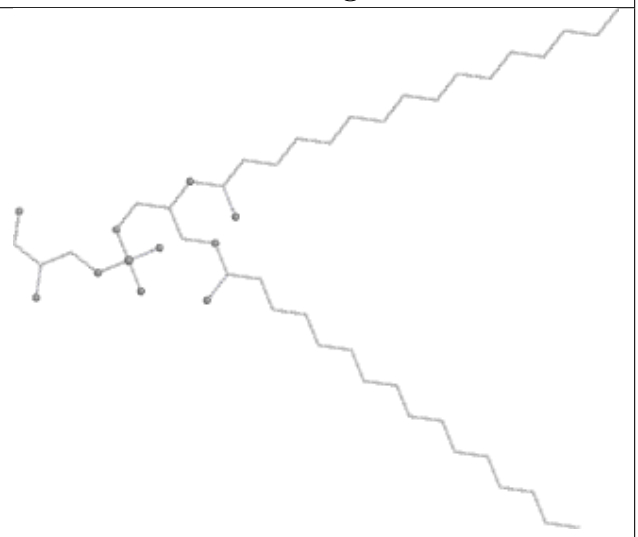
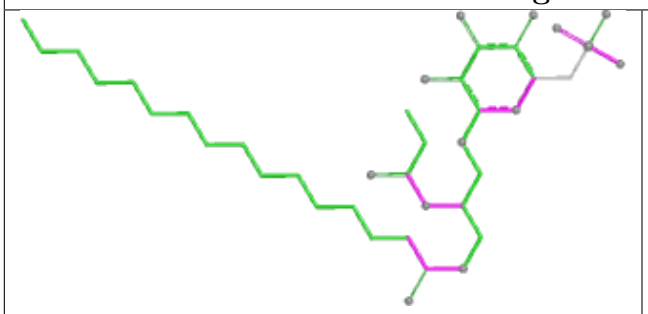


Rings

Ligand SQD f 101



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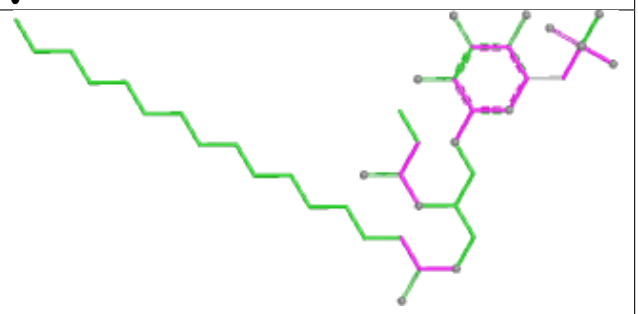
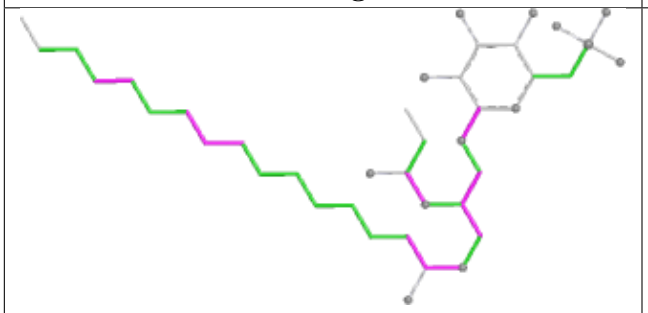


Bond angles



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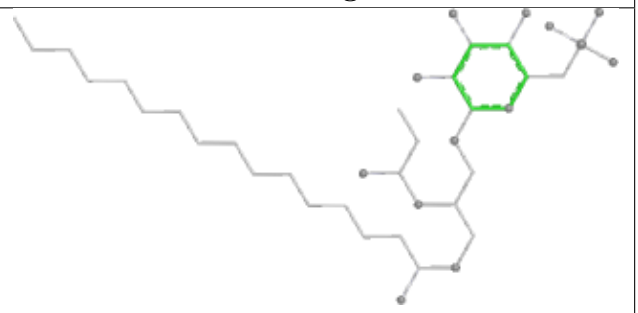
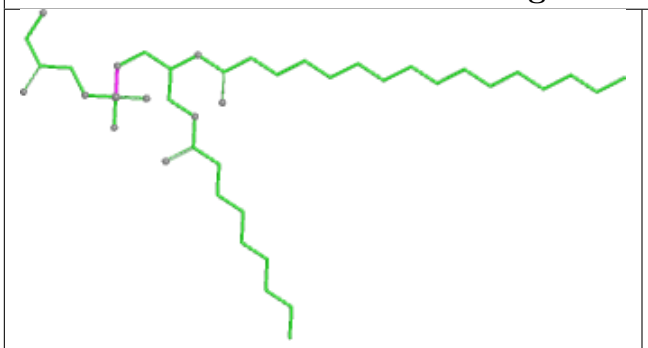
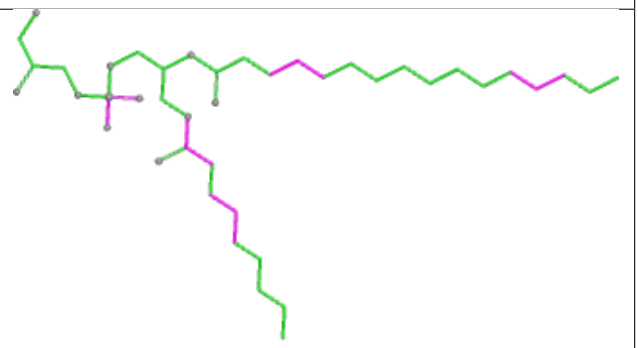


Rings

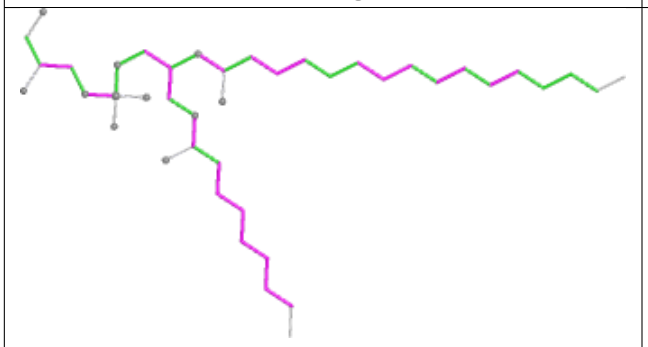
Ligand LHG e 102



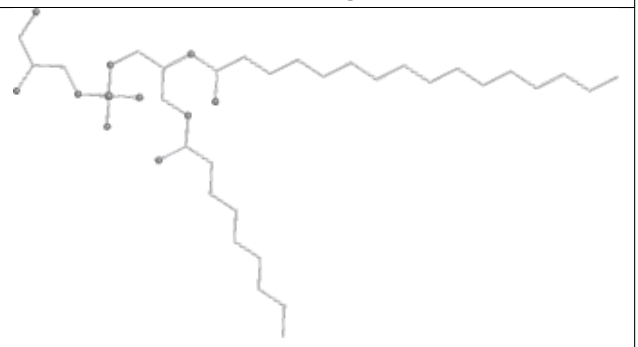
Bond lengths



Bond angles

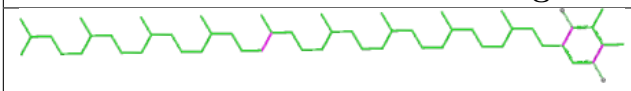


Torsions



Rings

Ligand PL9 d 405



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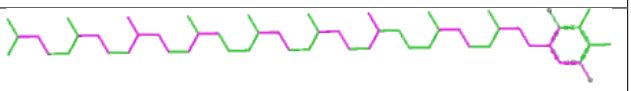
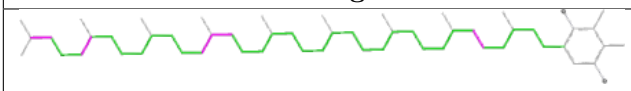


Bond angles



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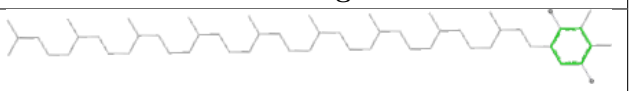
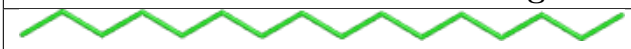


Rings

Ligand STE B 626



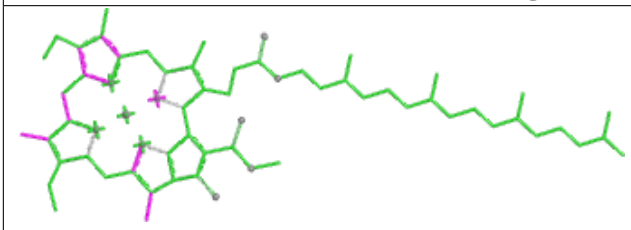
Bond lengths

Bond angles

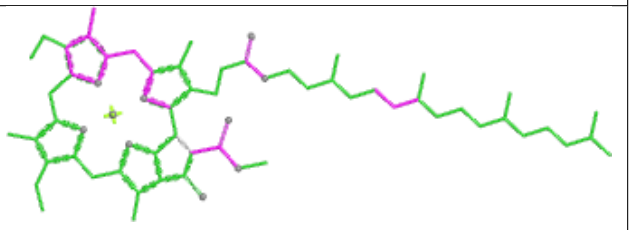
Torsions

Rings

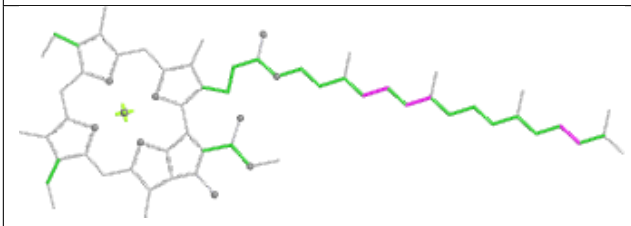
Ligand CLA B 608



Bond lengths



Bond angles



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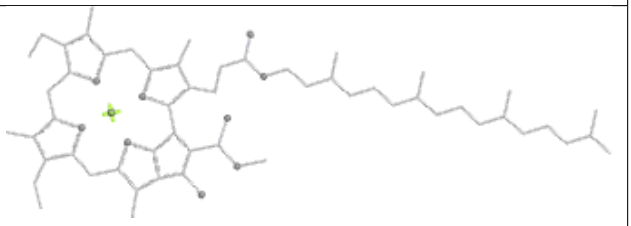
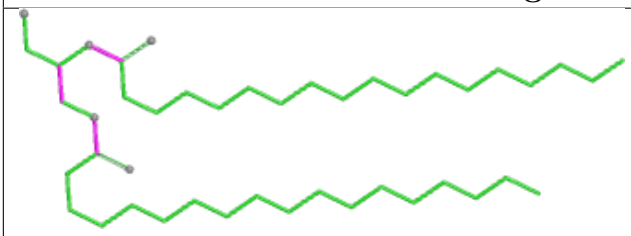


Rings

Ligand DGD a 617



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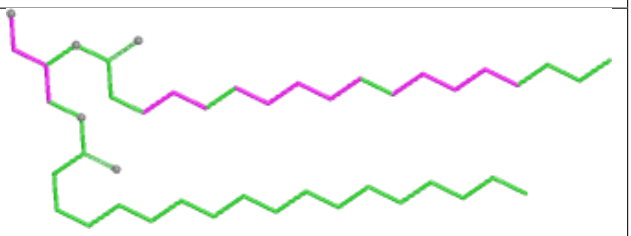
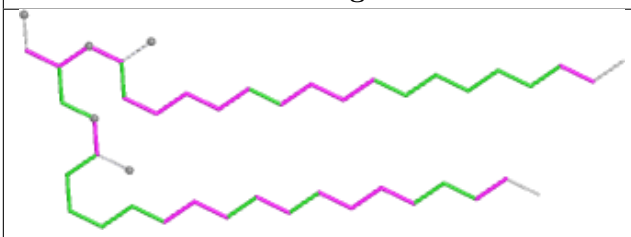


Bond angles



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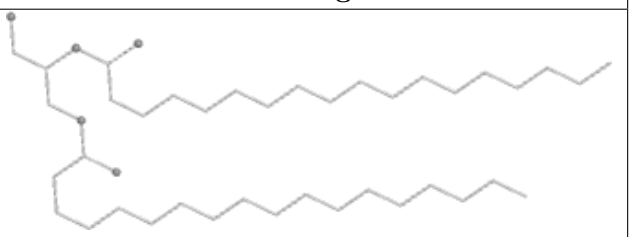
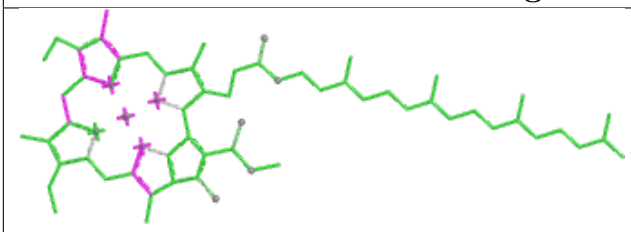


Rings

Ligand CLA B 610



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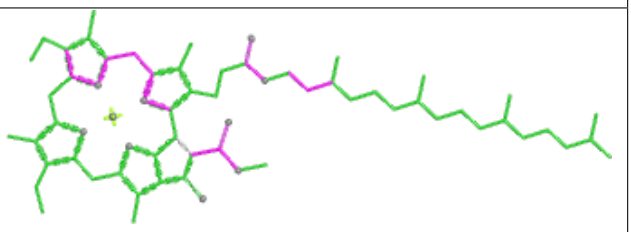
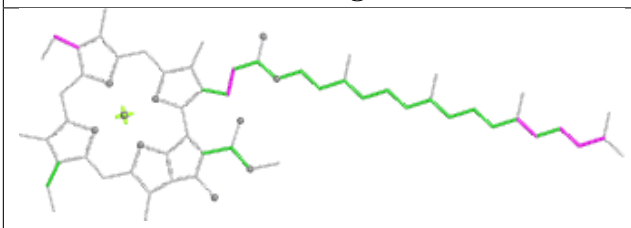


Bond angles



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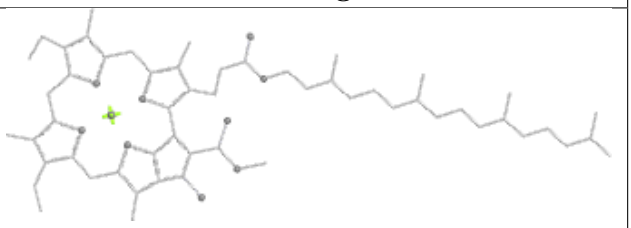


Rings

Ligand STE I 101

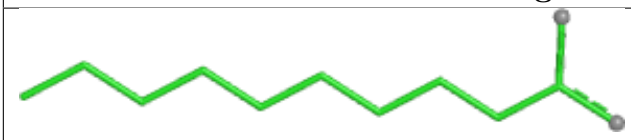
Bond lengths

Bond angles

Torsions

Rings

Ligand STE j 101



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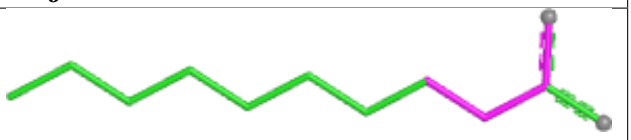
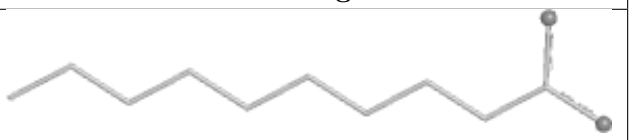


Bond angles

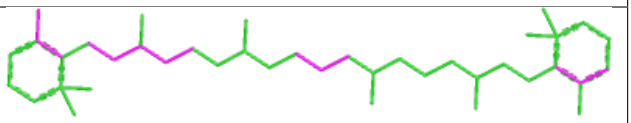
Torsions



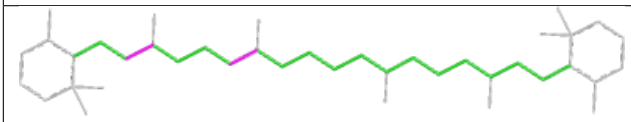
Rings

Ligand BCR c 515

Bond lengths



Bond angles



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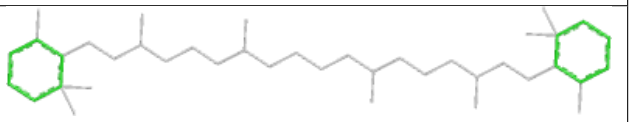
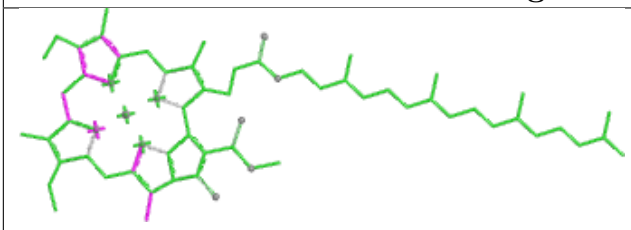


Rings

Ligand CLA d 402



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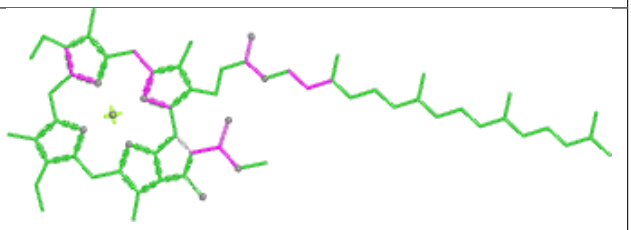
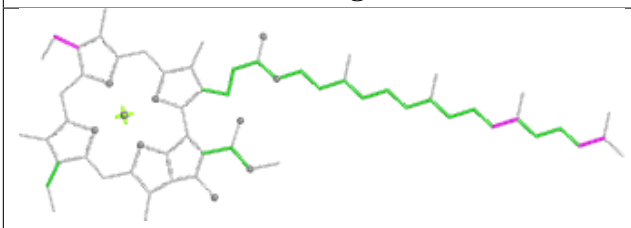


Bond angles



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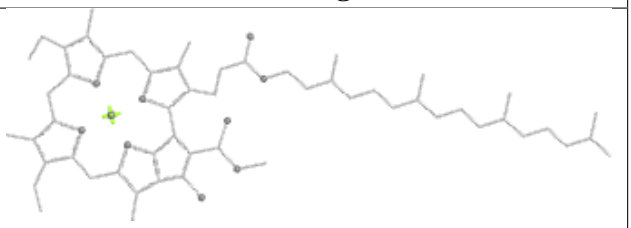
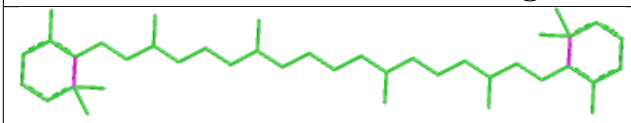
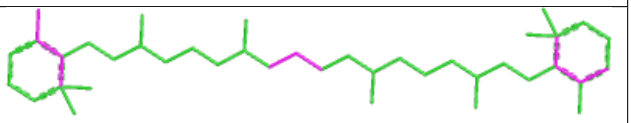


Rings

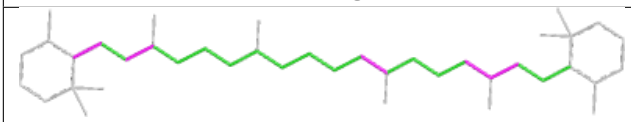
Ligand BCR K 102



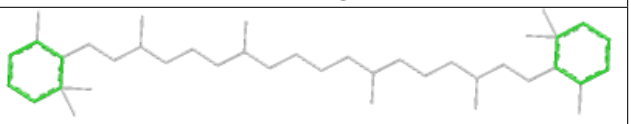
Bond lengths



Bond angles

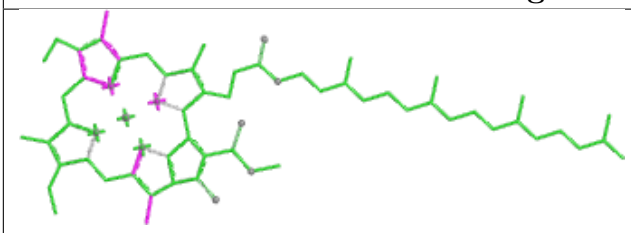


Torsions

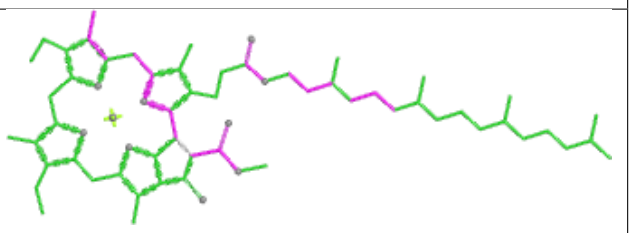


Rings

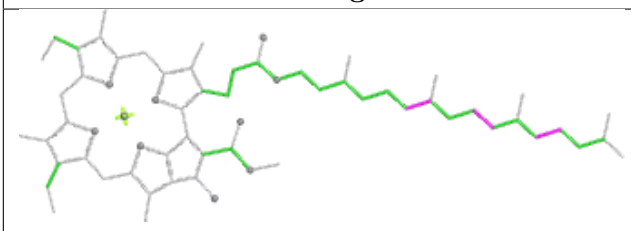
Ligand CLA b 612



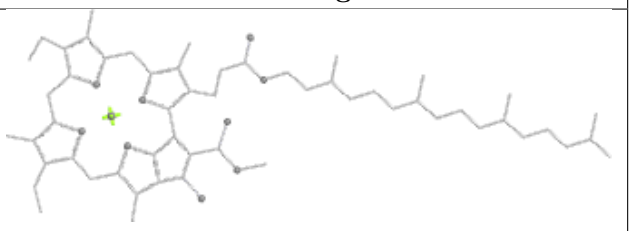
Bond lengths



Bond angles

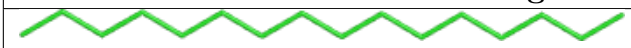


Torsions



Rings

Ligand STE C 521



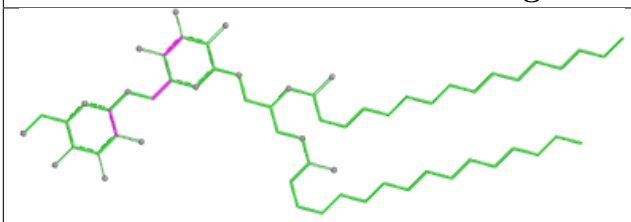
Bond lengths

Bond angles

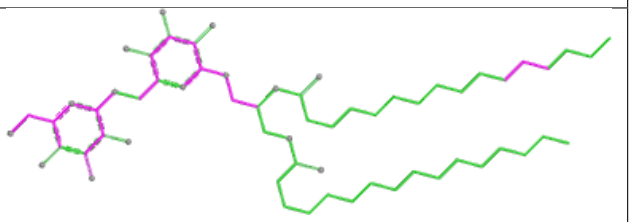
Torsions

Rings

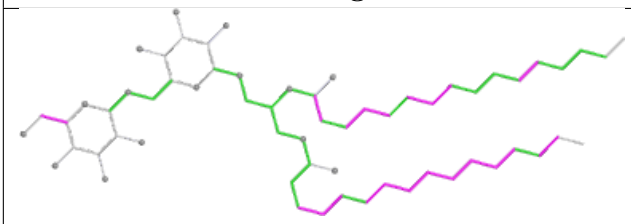
Ligand DGD h 103



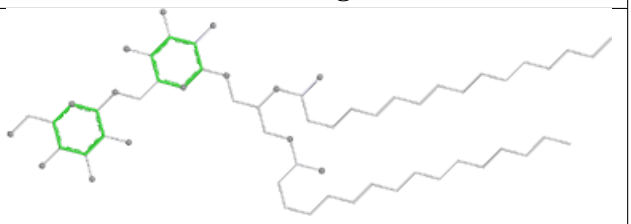
Bond lengths



Bond angles

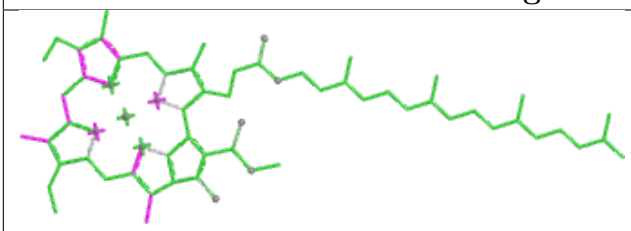


Torsions

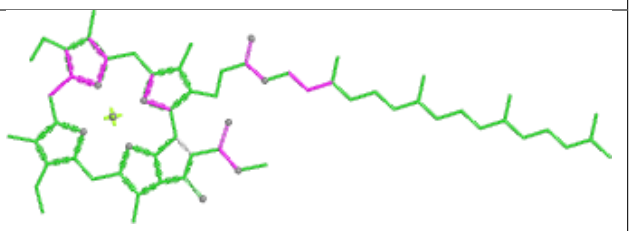


Rings

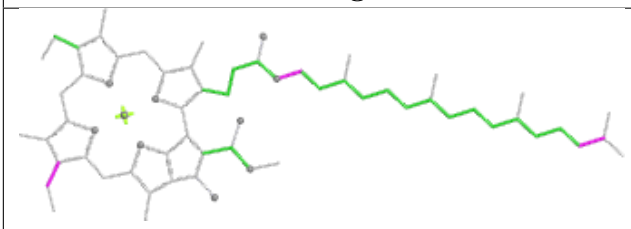
Ligand CLA D 403



Bond lengths



Bond angles



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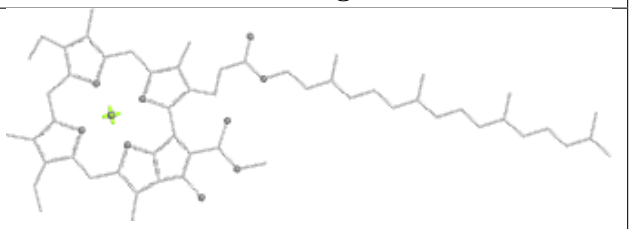
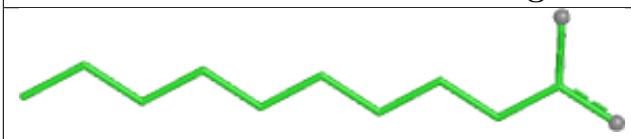
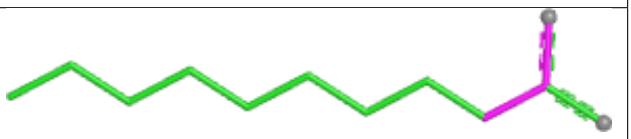


Rings

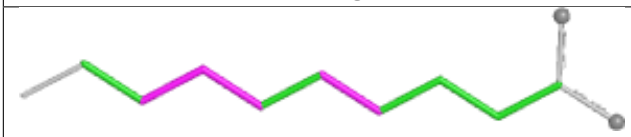
Ligand STE C 520



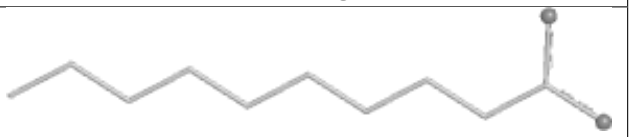
Bond lengths



Bond angles

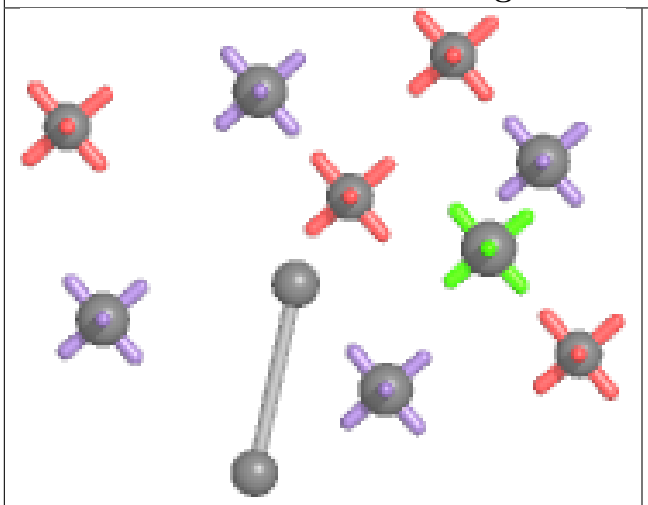


Torsions

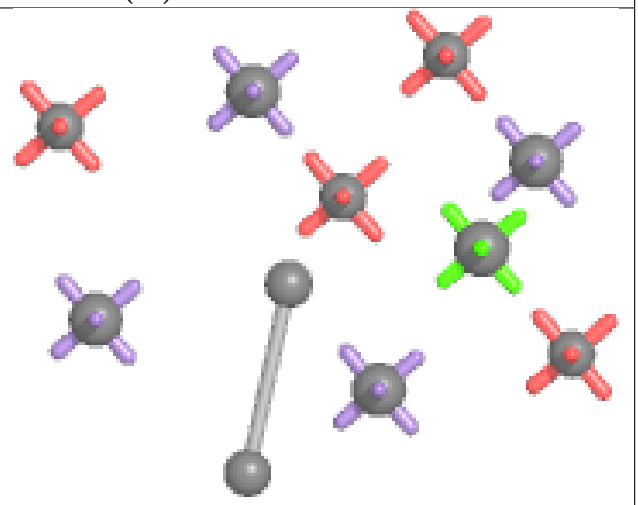


Rings

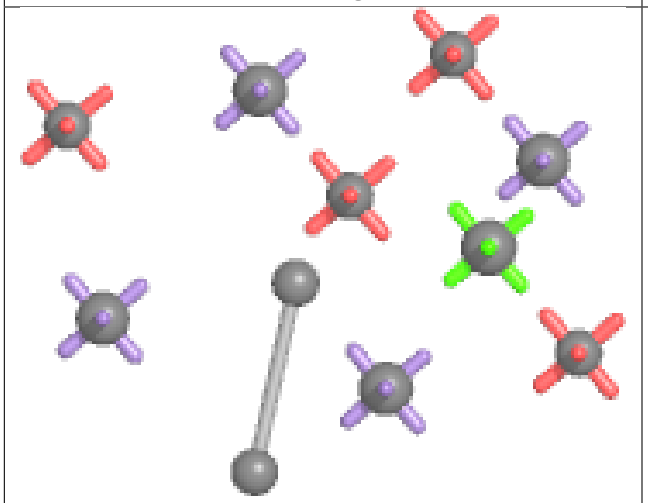
Ligand OEY a 602 (A)



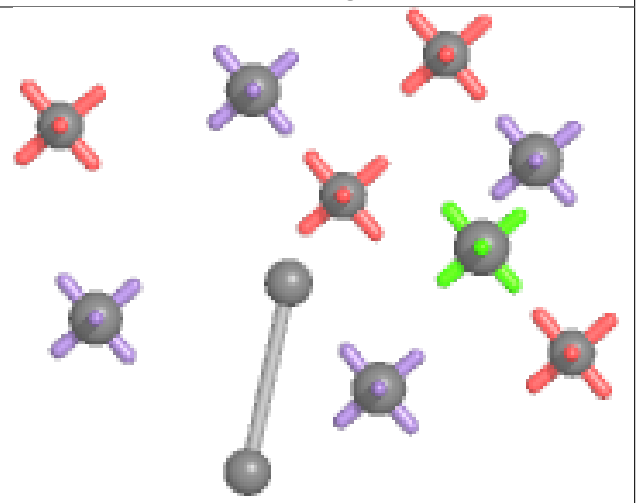
Bond lengths



Bond angles

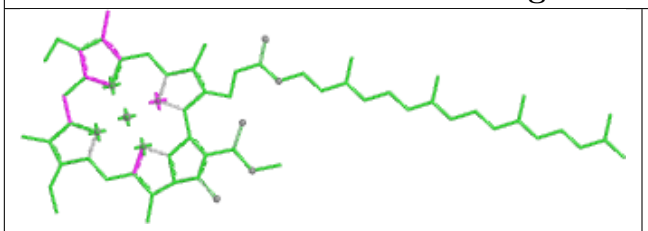


Torsions

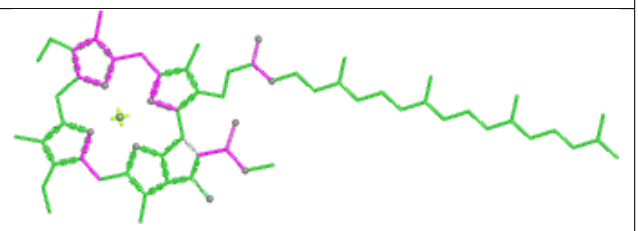


Rings

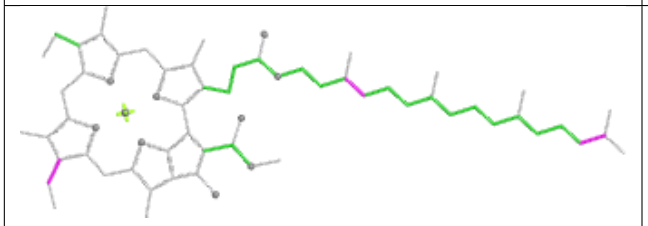
Ligand CLA b 607



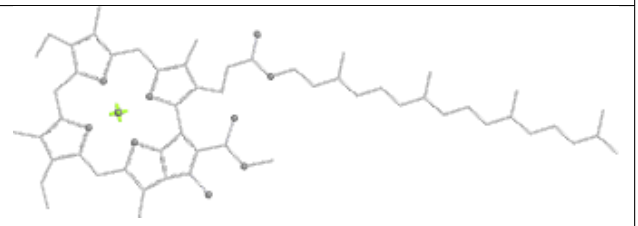
Bond lengths



Bond angles

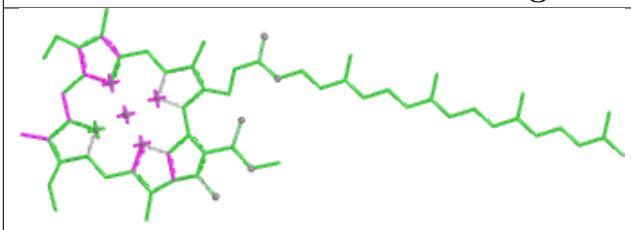


Torsions



Rings

Ligand CLA c 507



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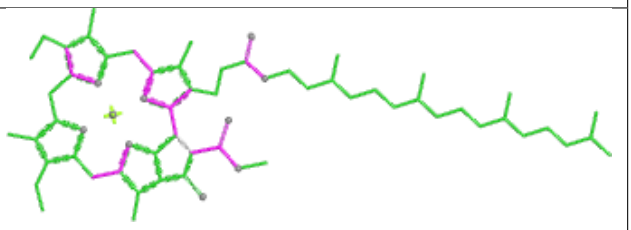

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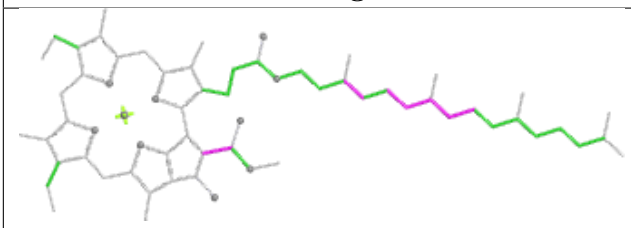

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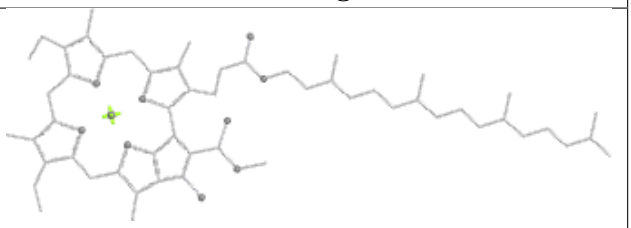
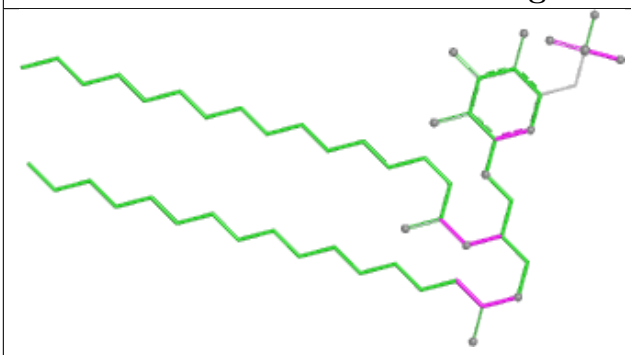


Rings

Ligand SQD a 615



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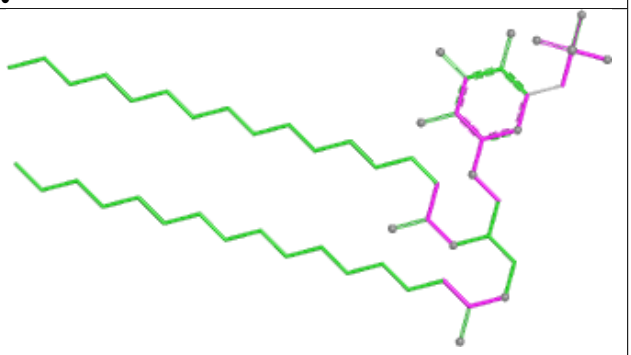
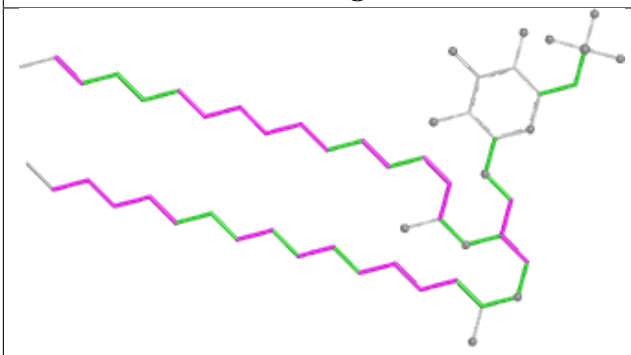


Bond angles



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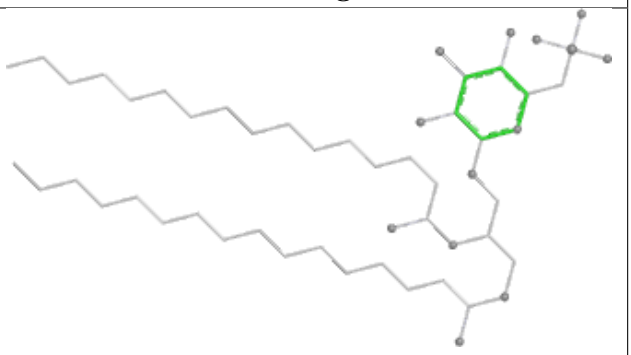

Rings

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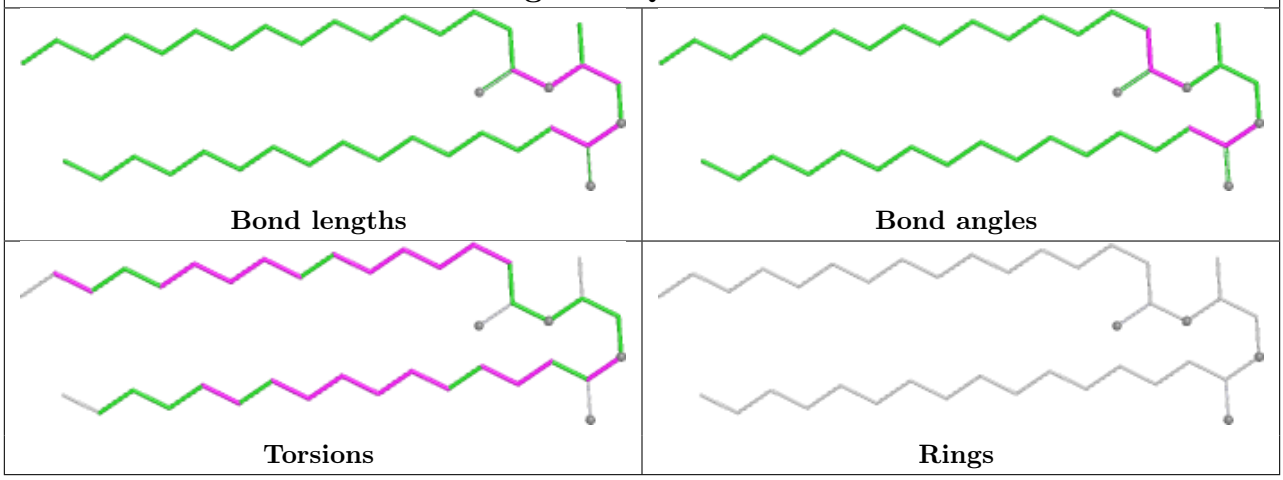

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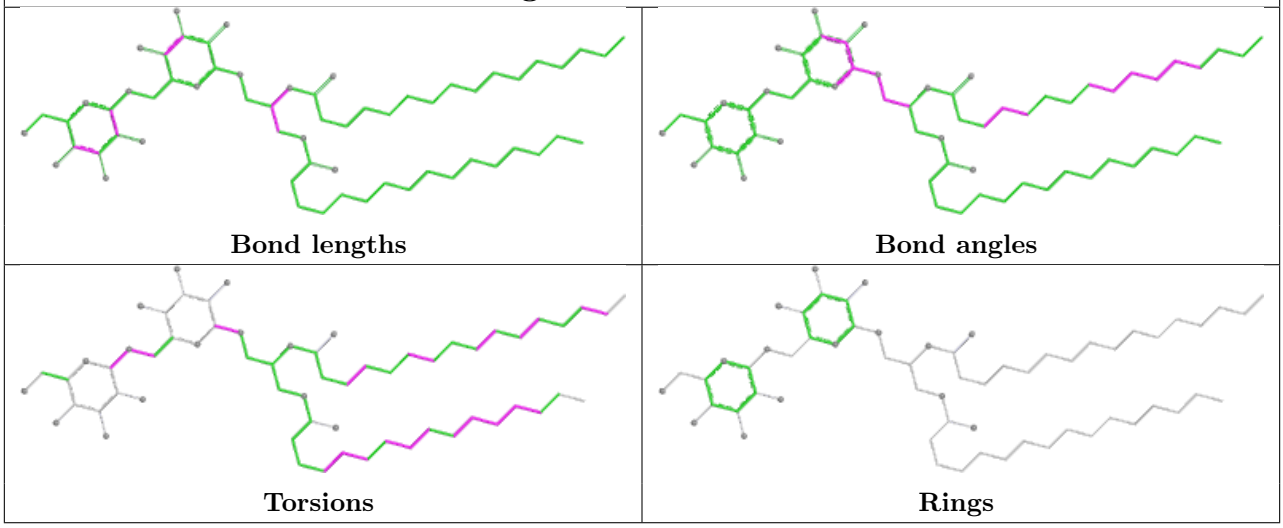
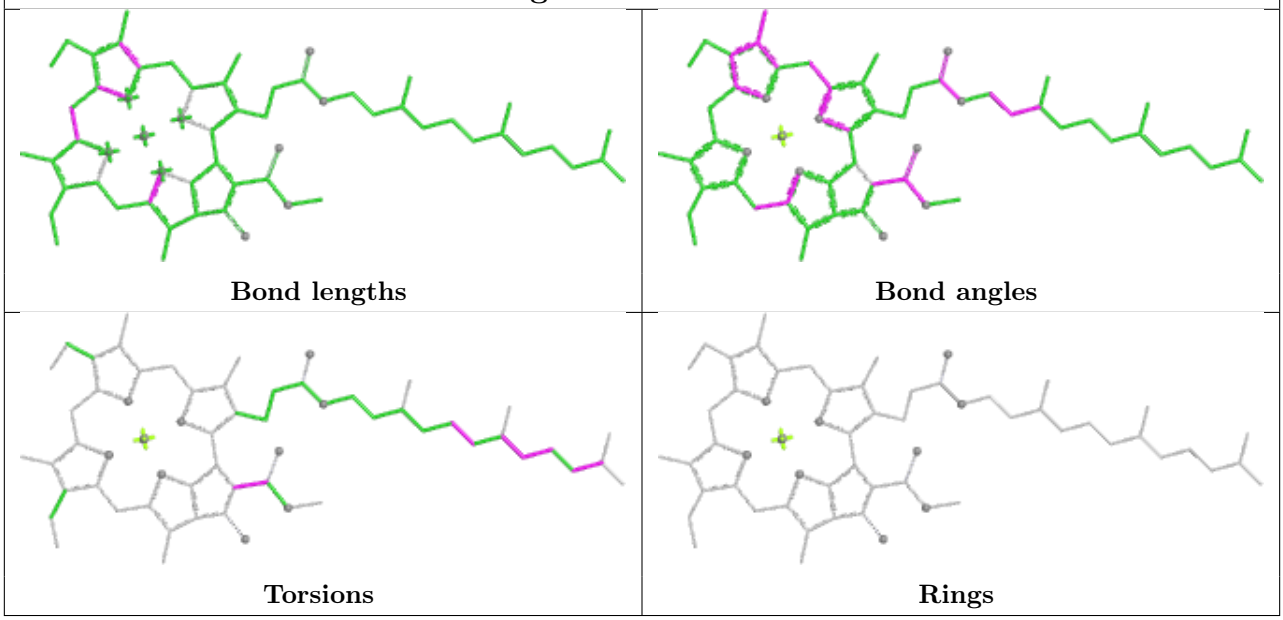


Ligand CLA c 504



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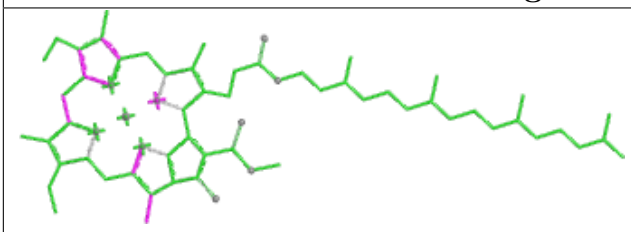
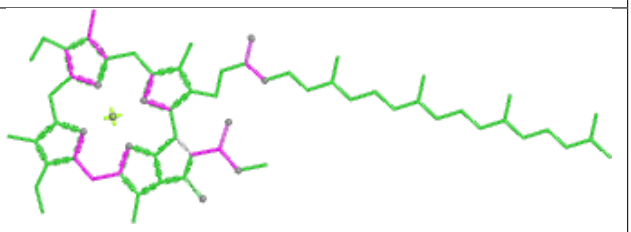
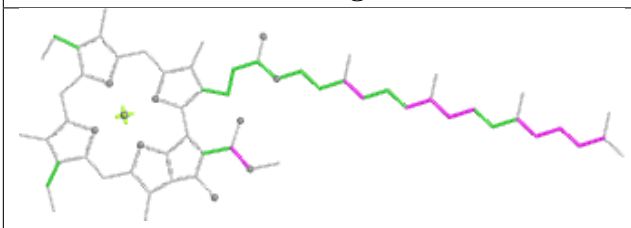


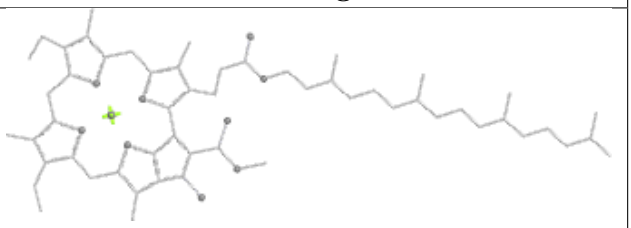
Bond lengths



Bond angles

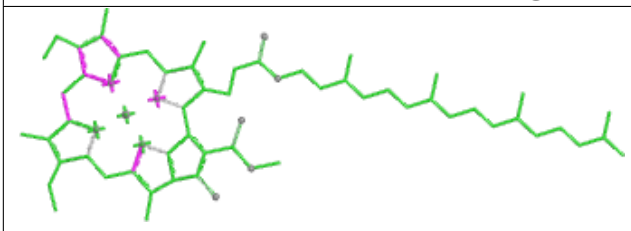


Torsions



Rings

Ligand CLA d 403



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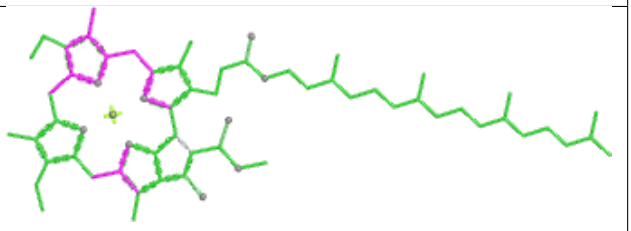

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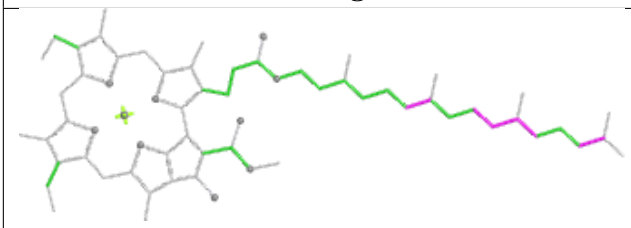

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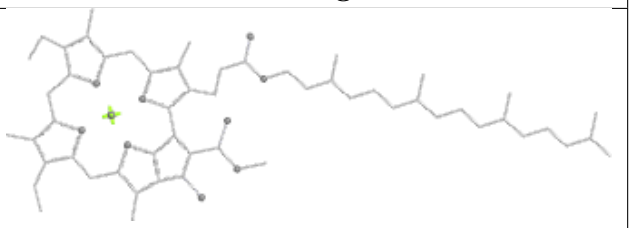
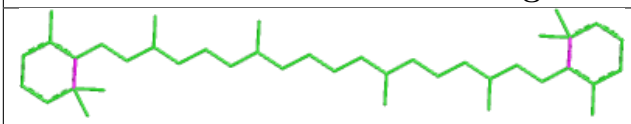


Rings

Ligand BCR T 101



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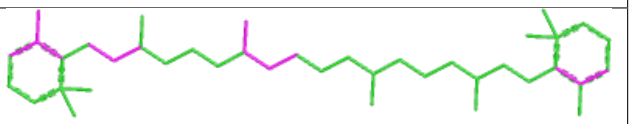
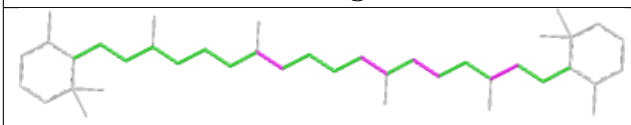


Bond angles



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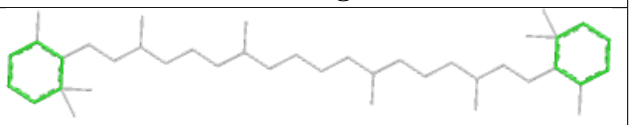
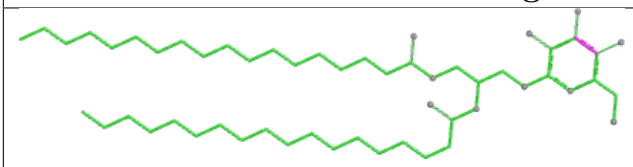


Rings

Ligand LMG b 622



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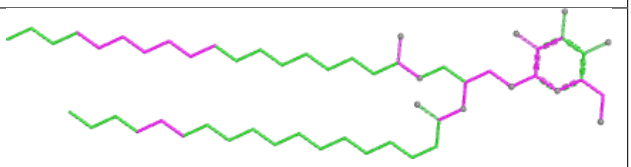

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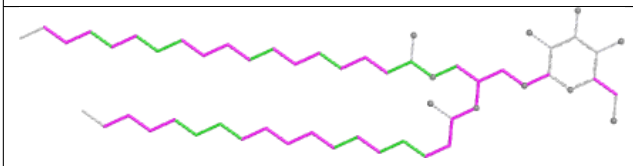

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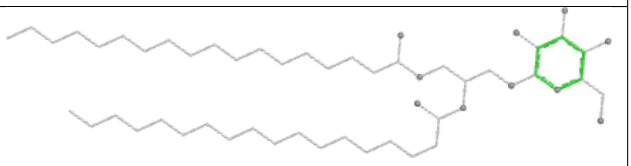
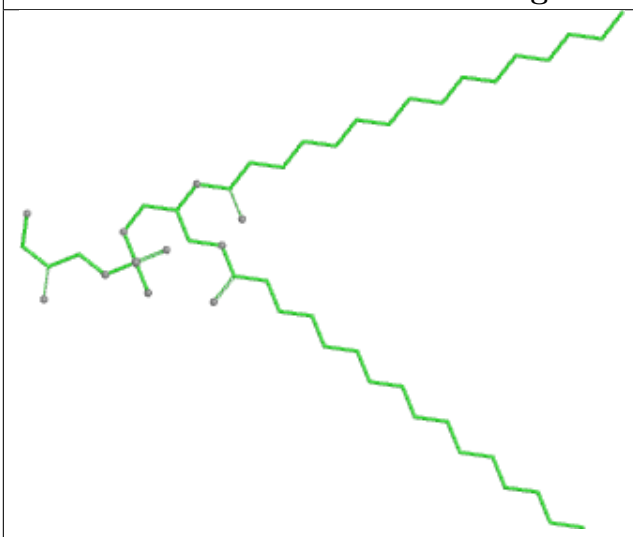


Rings

Ligand LHG l 101



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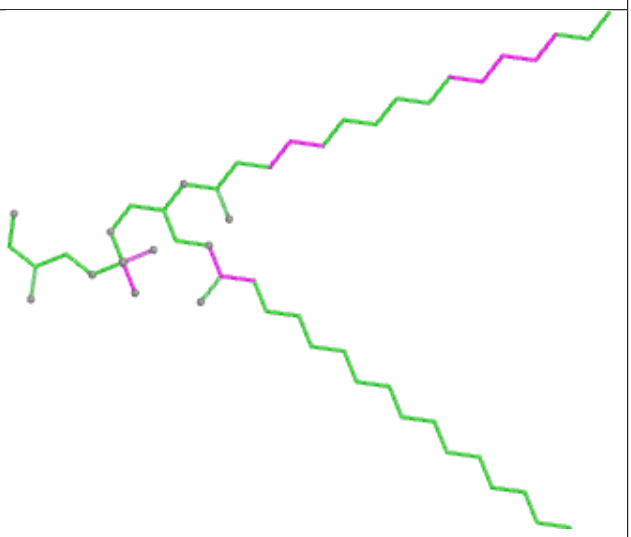

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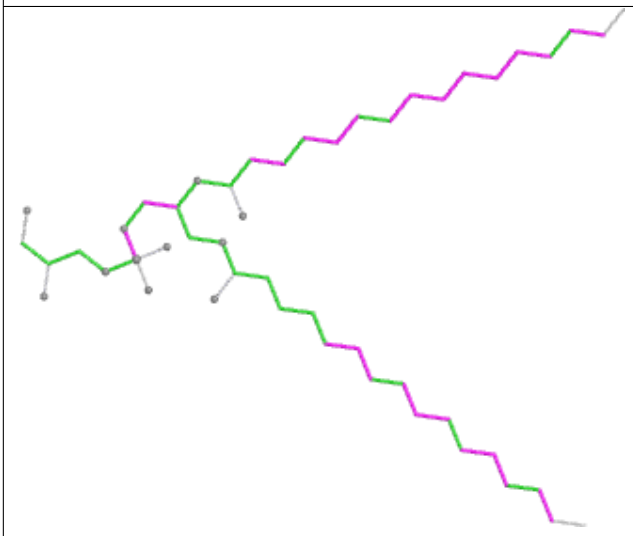

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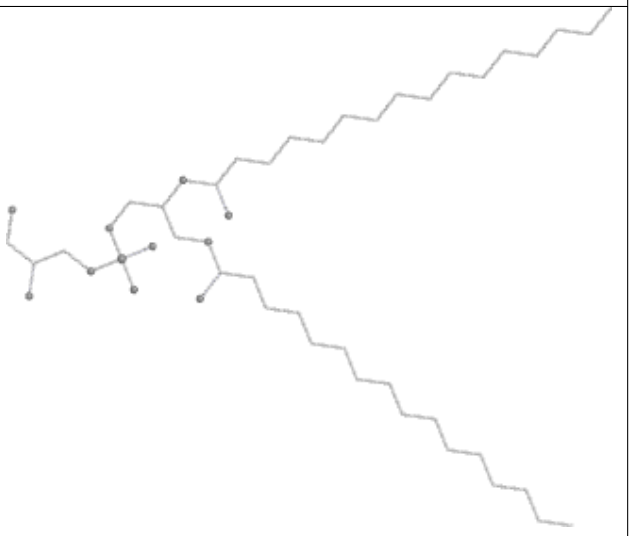
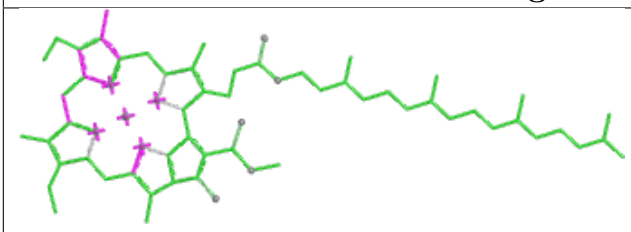


Rings

Ligand CLA a 607



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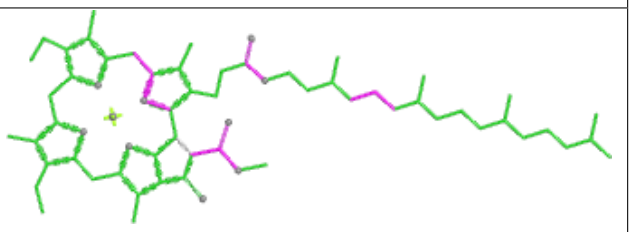

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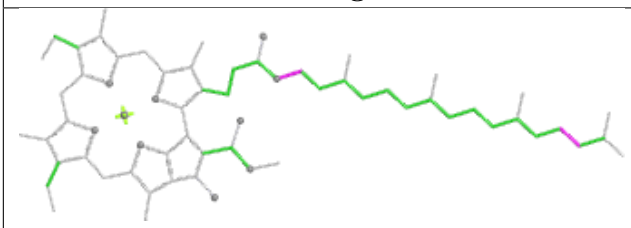

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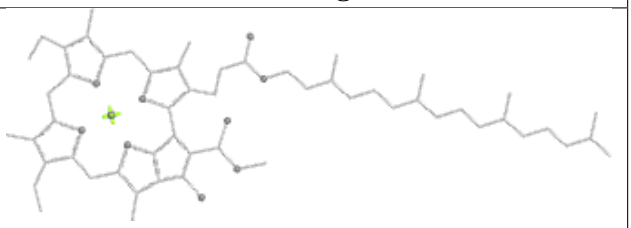
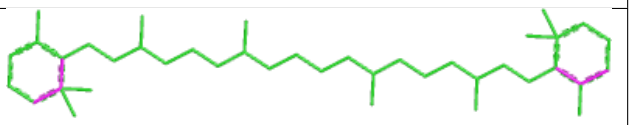


Rings

Ligand BCR K 103

Bond lengths



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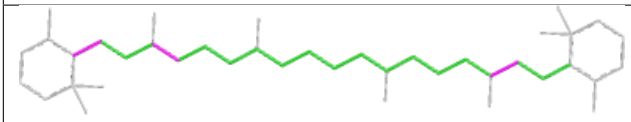

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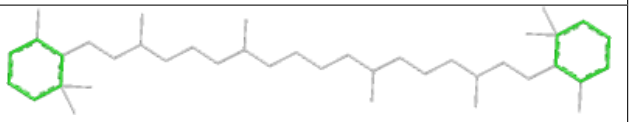
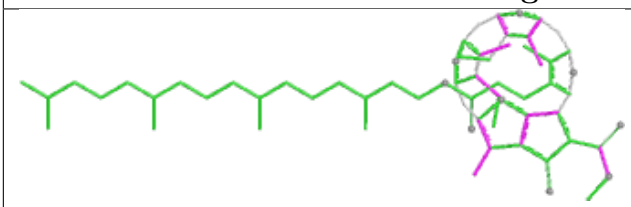


Rings

Ligand PHO D 402



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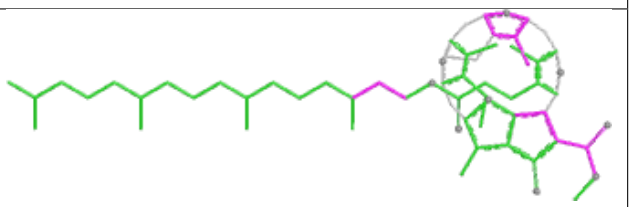
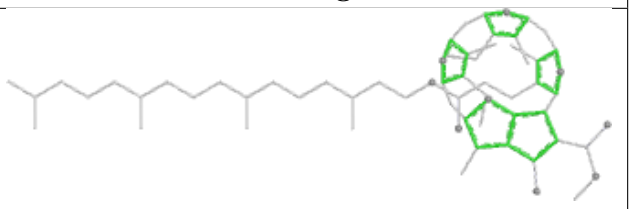


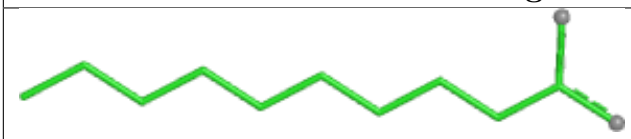
Bond angles

Torsions



Rings

Ligand STE m 102



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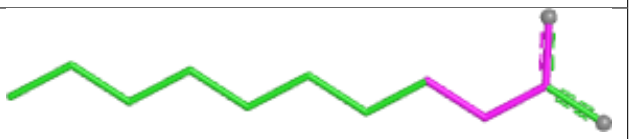
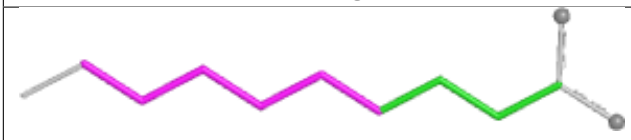


Bond angles



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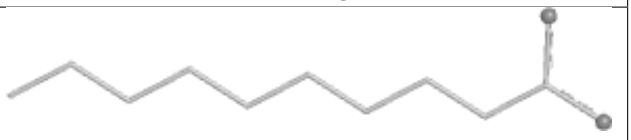
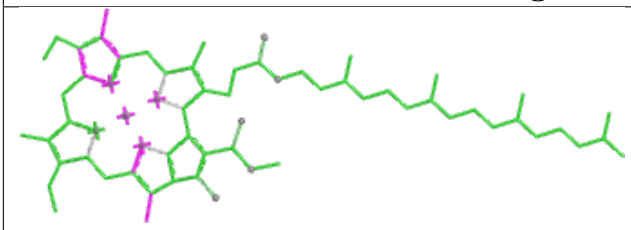


Rings

Ligand CLA c 509



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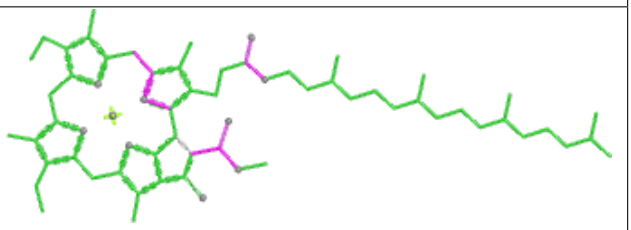
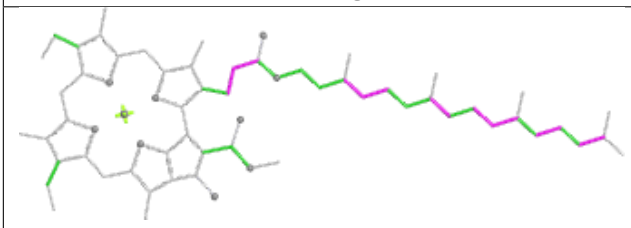


Bond angles



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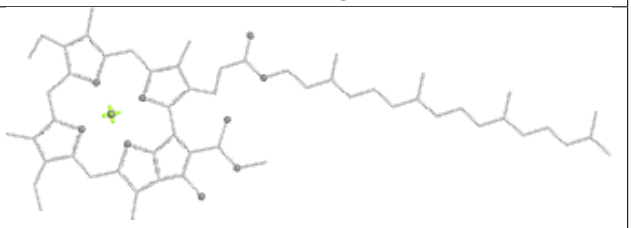
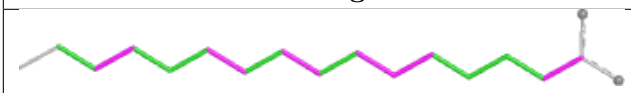


Rings

Ligand STE t 104

Bond lengths

Bond angles



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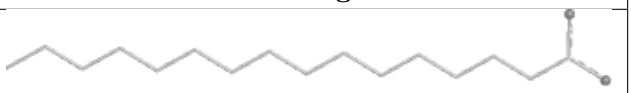
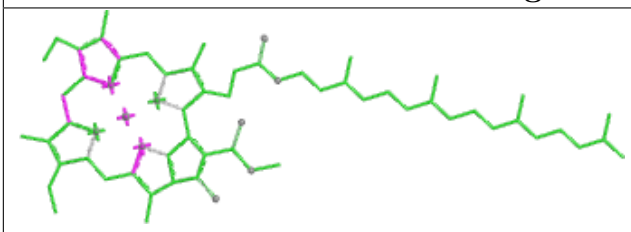


Rings

Ligand CLA B 613



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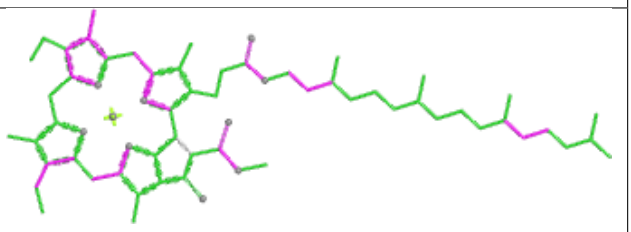
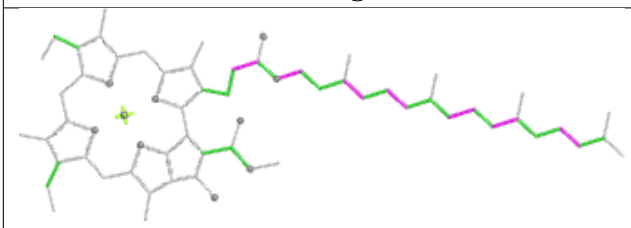
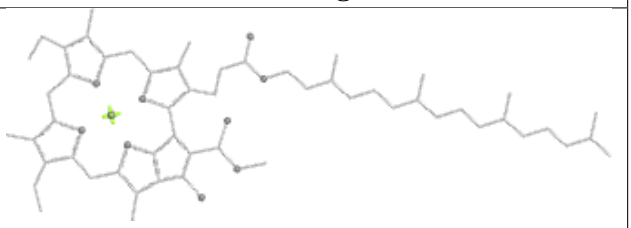


Bond angles

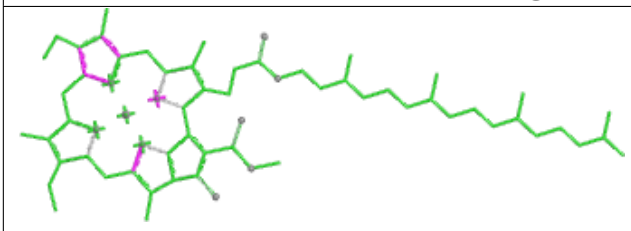


Torsions



Rings

Ligand CLA b 605



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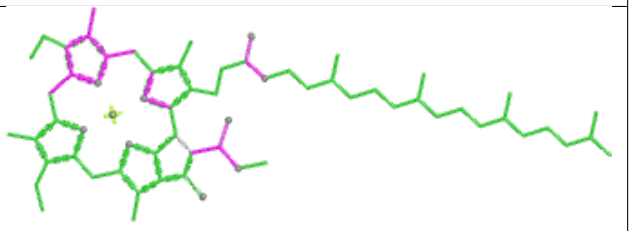
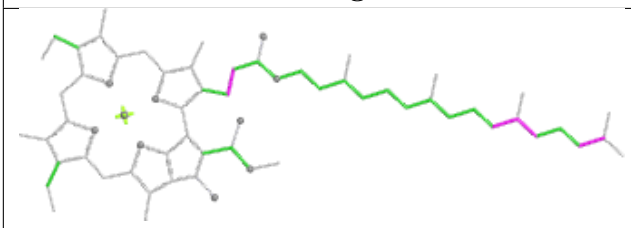


Bond angles



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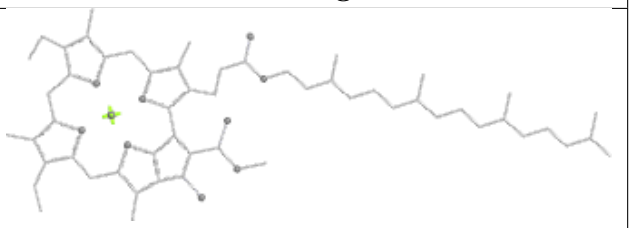
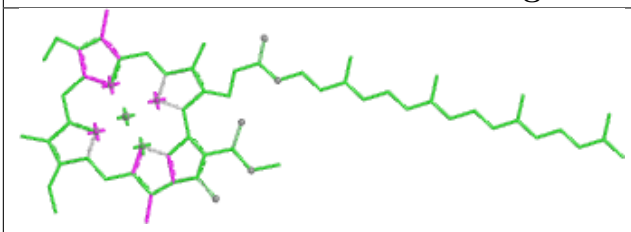


Rings

Ligand CLA D 404



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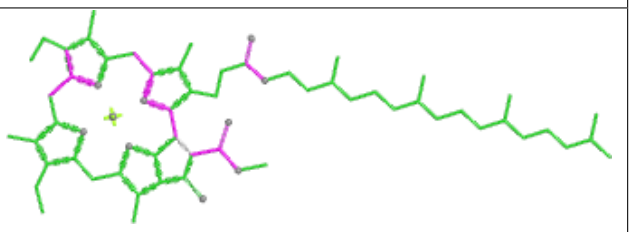
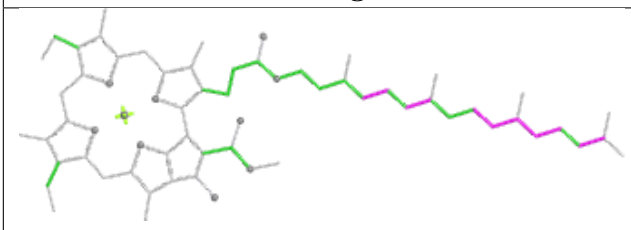


Bond angles



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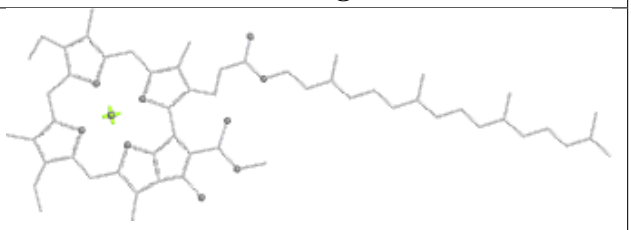
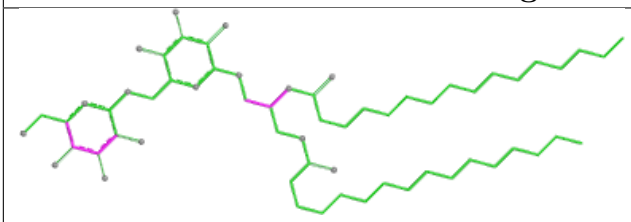


Rings

Ligand DGD C 515



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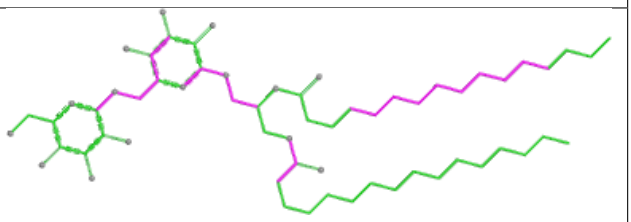
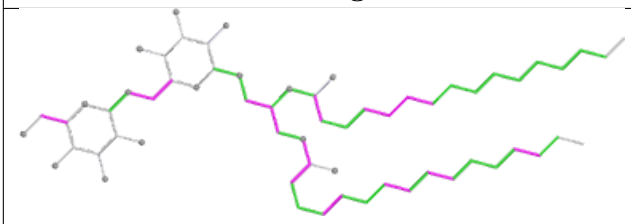


Bond angles



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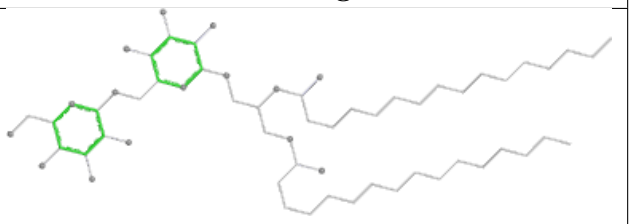
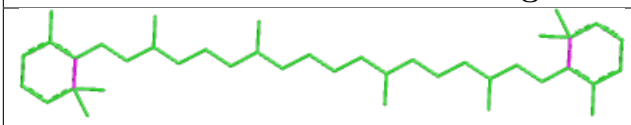


Rings

Ligand BCR H 101



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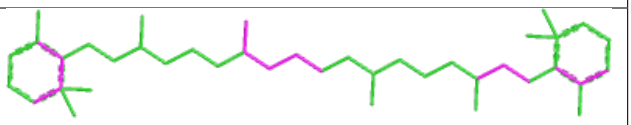
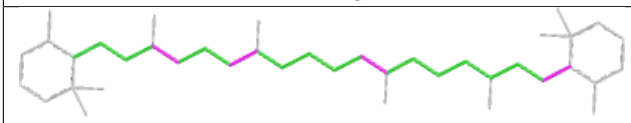


Bond angles



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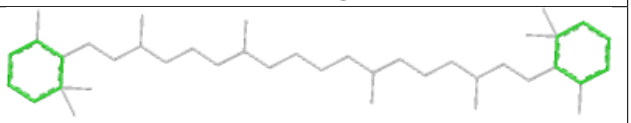
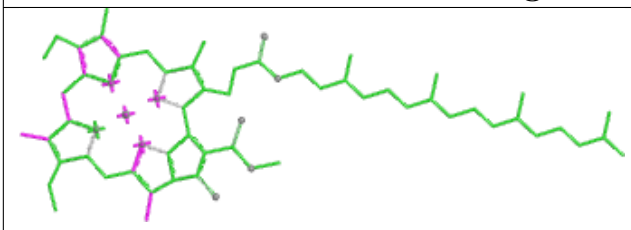


Rings

Ligand CLA A 606



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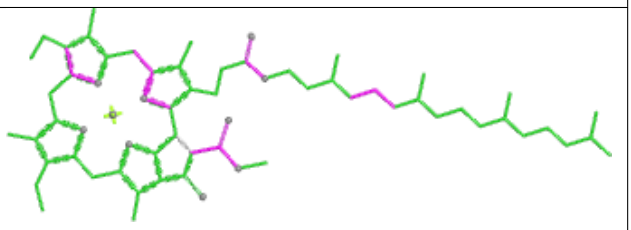
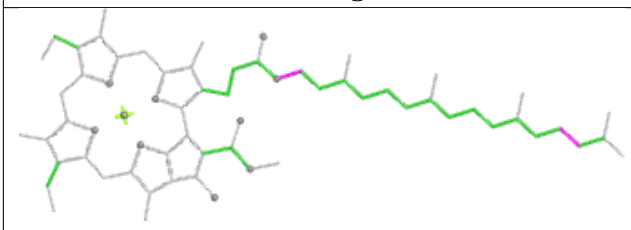


Bond angles



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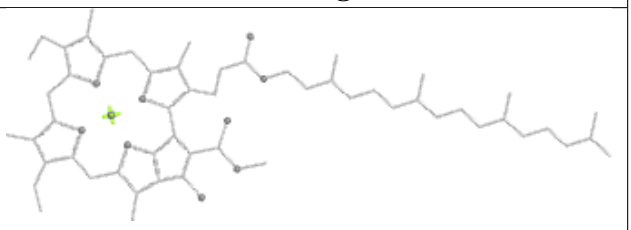
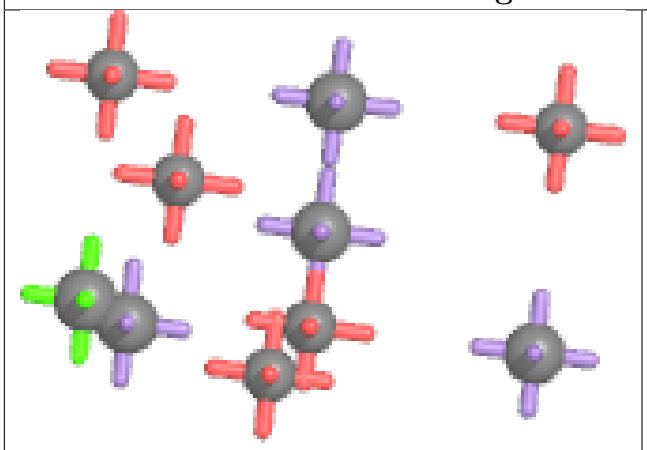


Rings

Ligand OEX a 601 (B)



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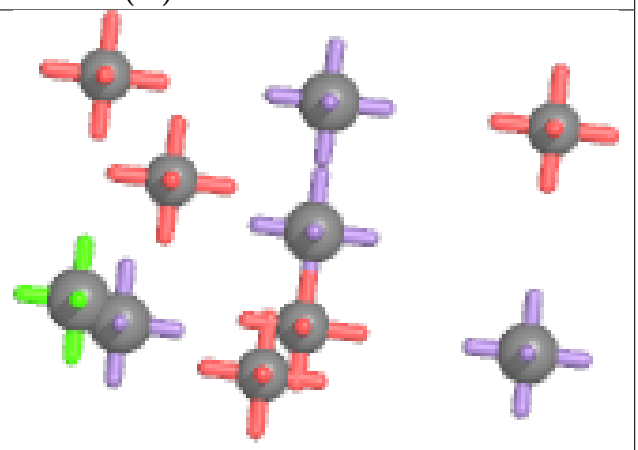
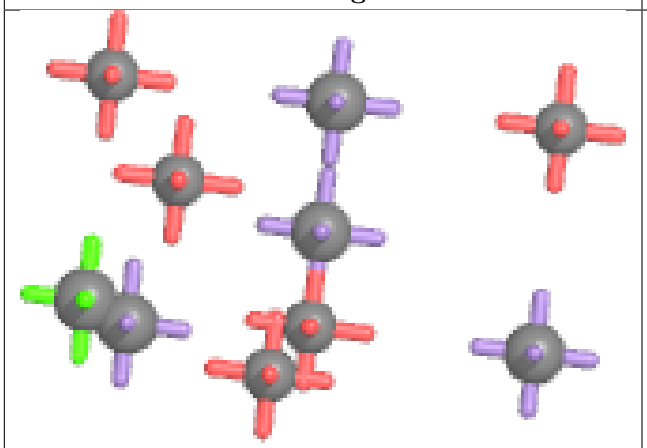


Bond angles



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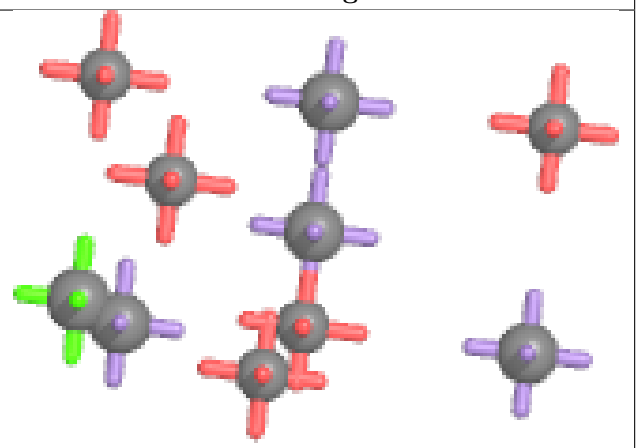
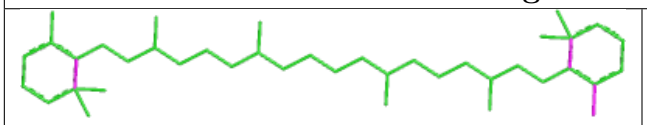


Rings

Ligand BCR D 405



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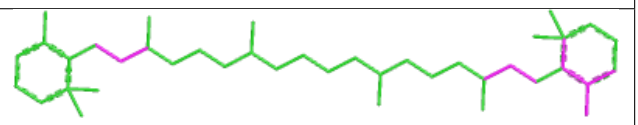
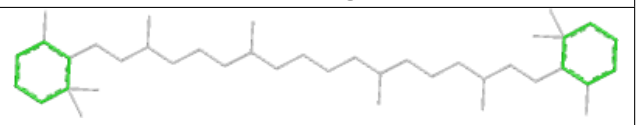


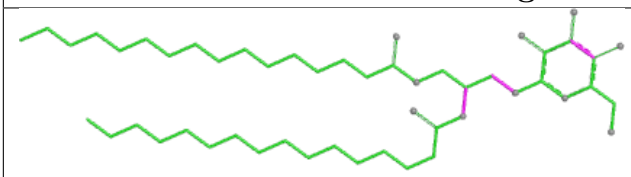
Bond angles

Torsions



Rings

Ligand LMG m 101



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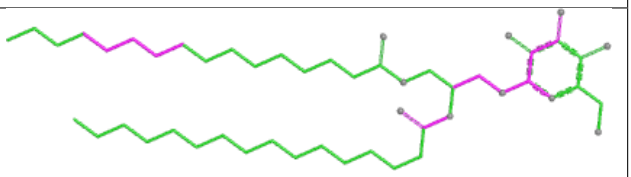
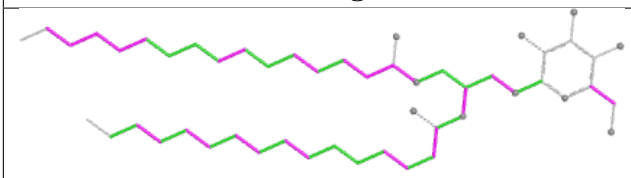


Bond angles



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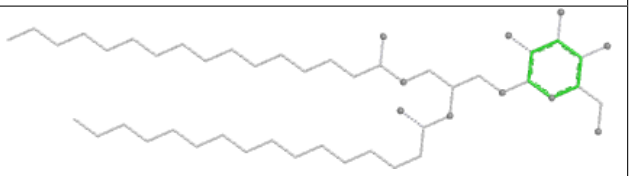
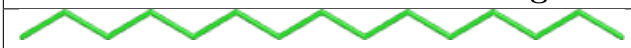


Rings

Ligand STE b 624



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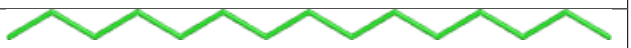
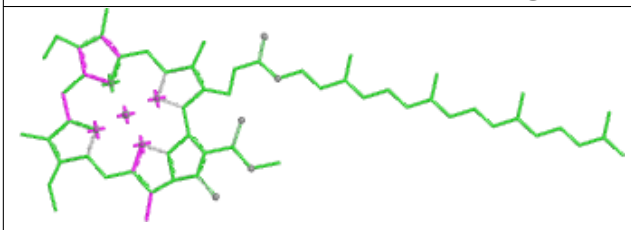


Bond angles

Torsions

Rings

Ligand CLA C 503



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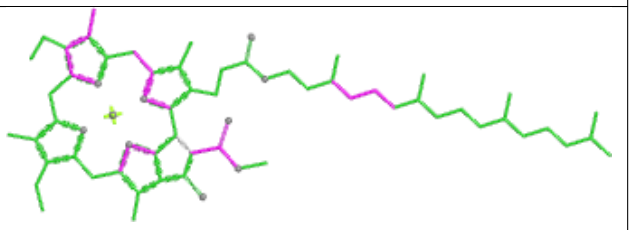

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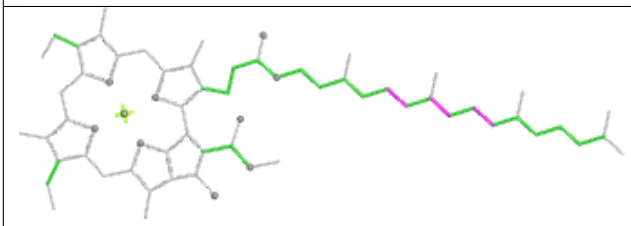

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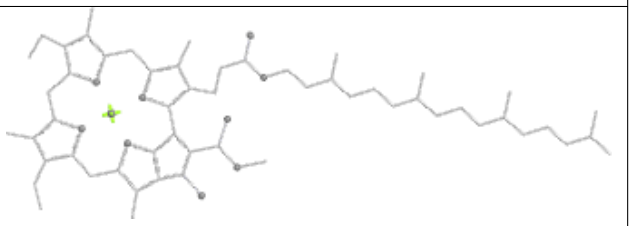
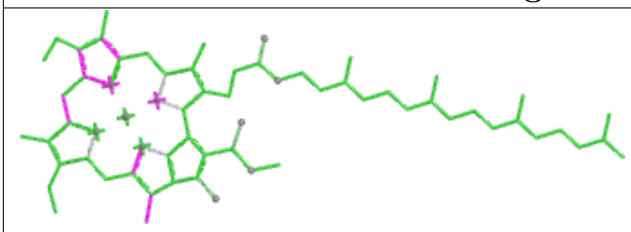


Rings

Ligand CLA C 507



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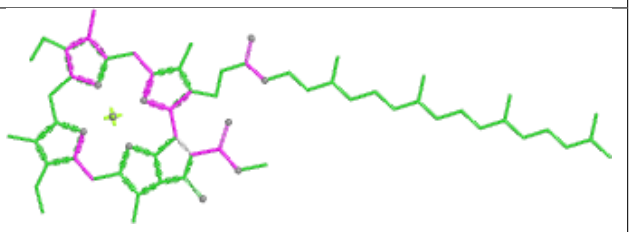
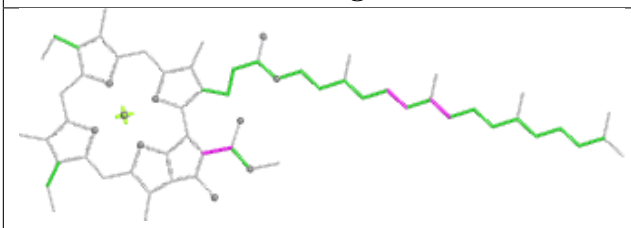


Bond angles



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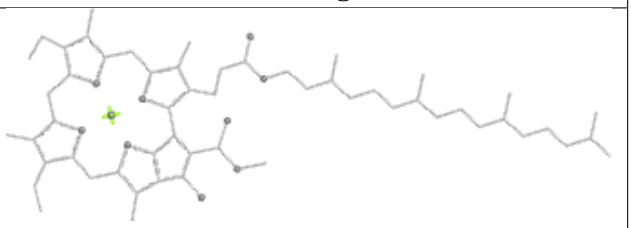
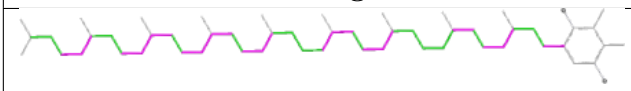


Rings

Ligand PL9 A 611

Bond lengths

Bond angles



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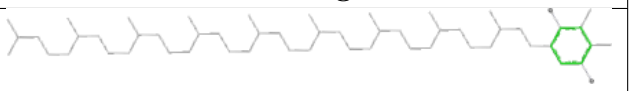
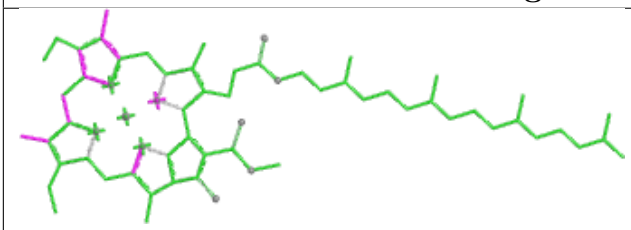


Rings

Ligand CLA B 603



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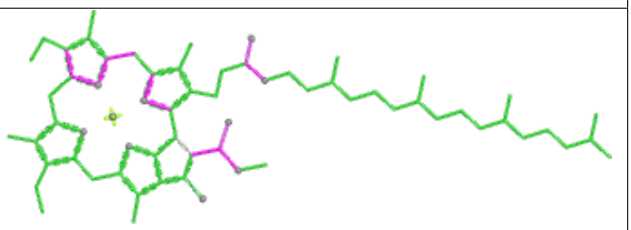
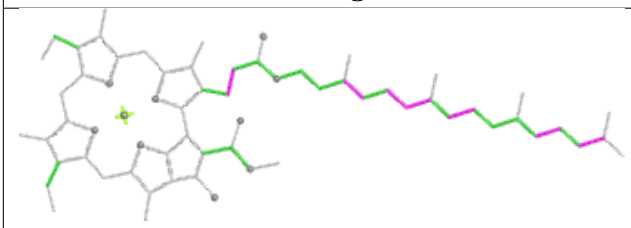


Bond angles



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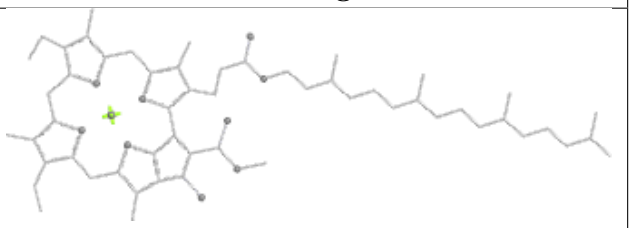
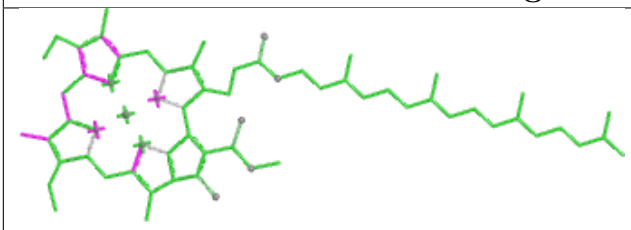


Rings

Ligand CLA C 513



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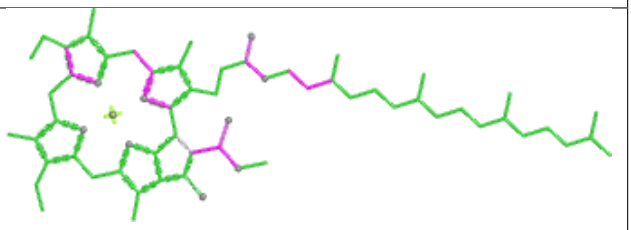
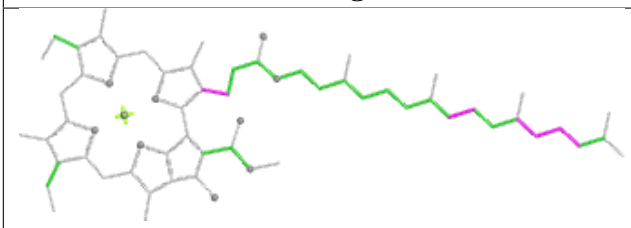


Bond angles



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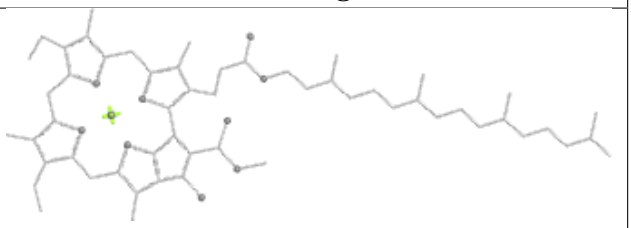
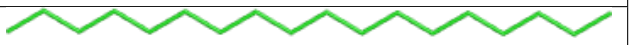


Rings

Ligand STE l 102

Bond lengths

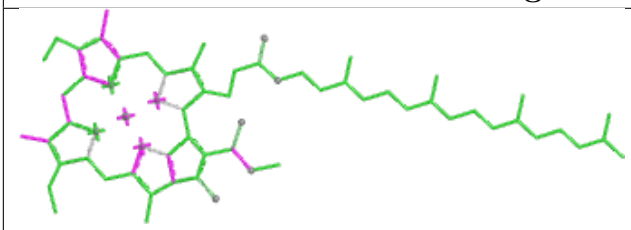


Bond angles

Torsions

Rings

Ligand CLA C 509



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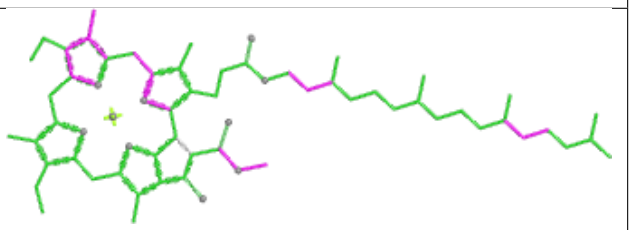
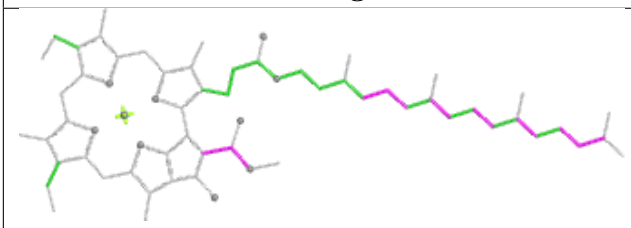
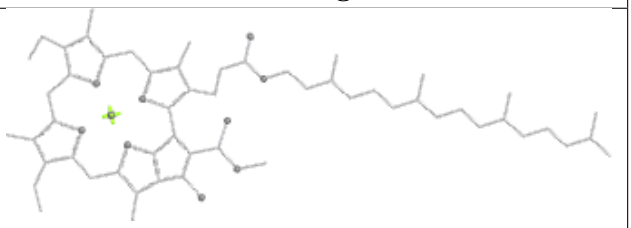


Bond angles

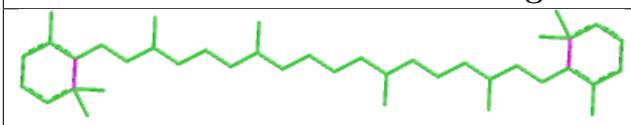


Torsions

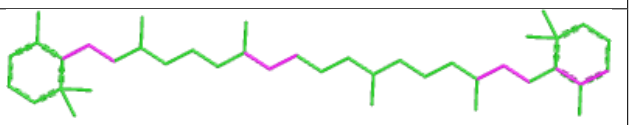


Rings

Ligand BCR b 617

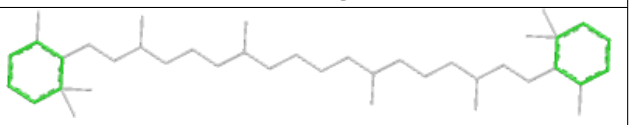


Bond lengths



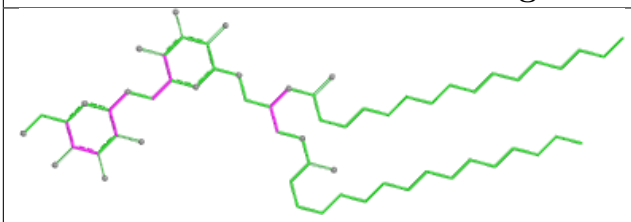
Bond angles

Torsions

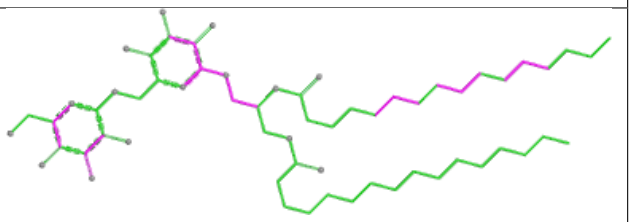


Rings

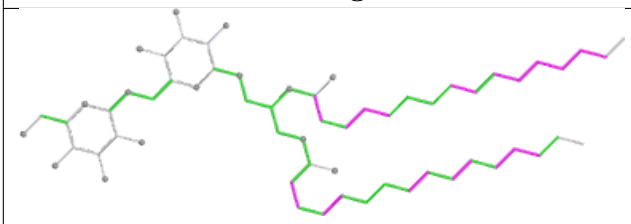
Ligand DGD H 102



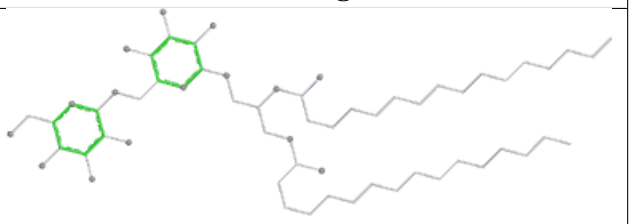
Bond lengths



Bond angles

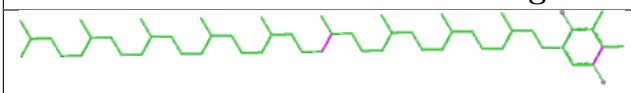


Torsions

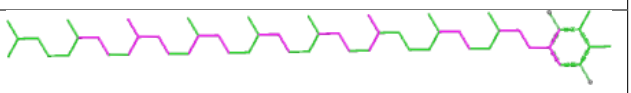


Rings

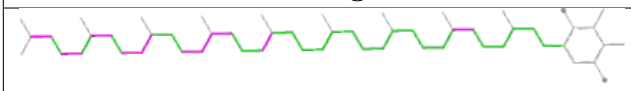
Ligand PL9 D 406



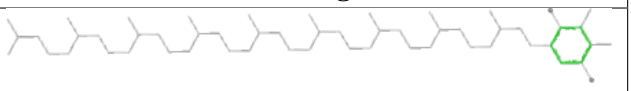
Bond lengths



Bond angles

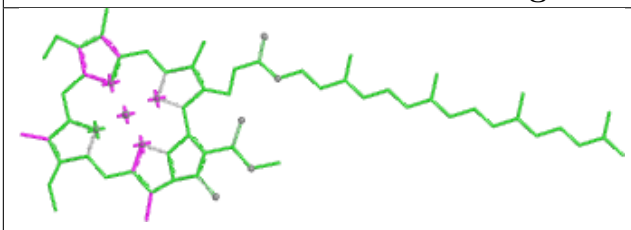


Torsions

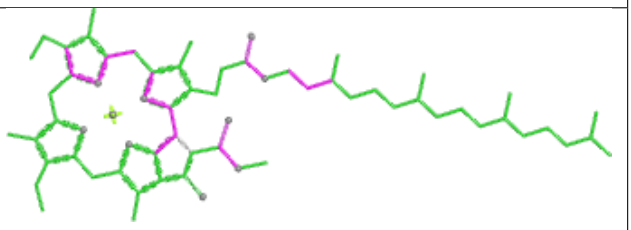


Rings

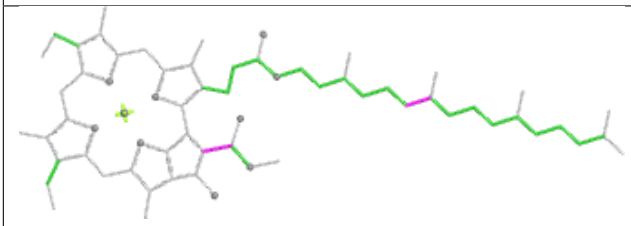
Ligand CLA c 502



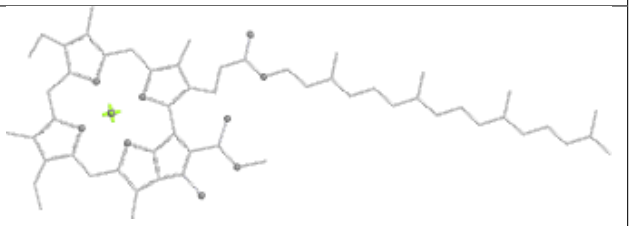
Bond lengths



Bond angles

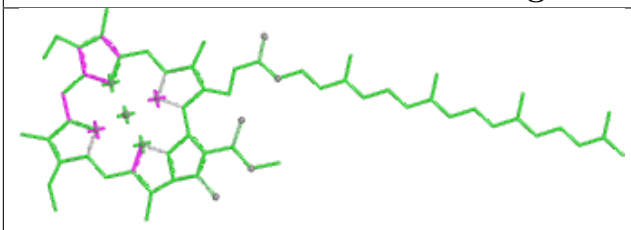


Torsions

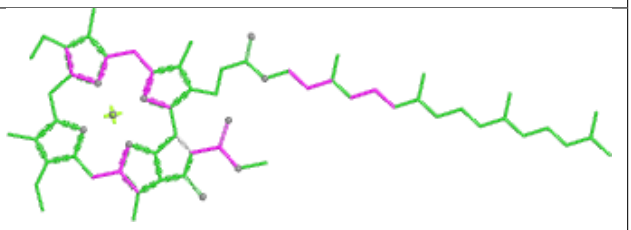


Rings

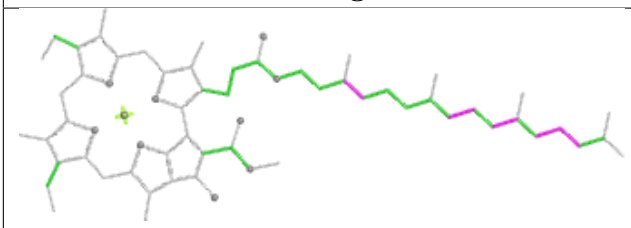
Ligand CLA b 610



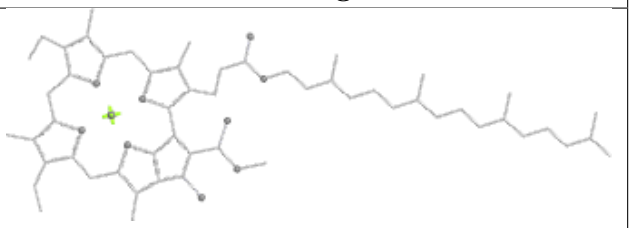
Bond lengths



Bond angles

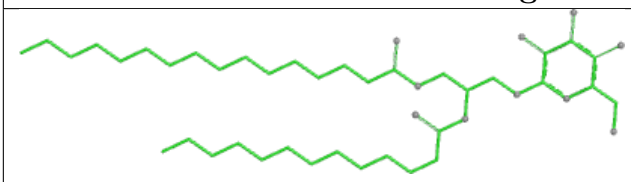


Torsions

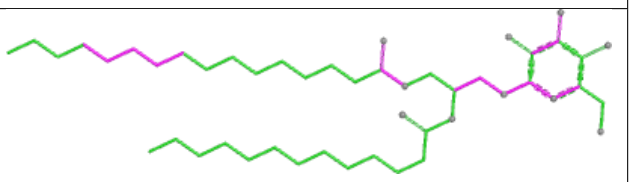


Rings

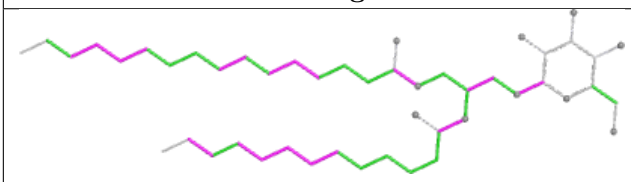
Ligand LMG C 518



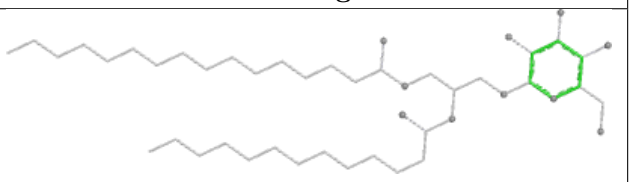
Bond lengths



Bond angles

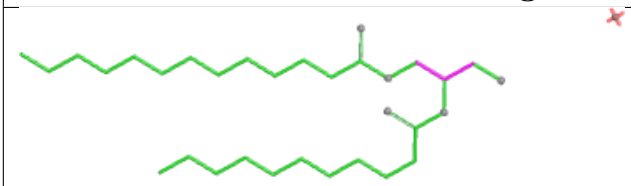


Torsions

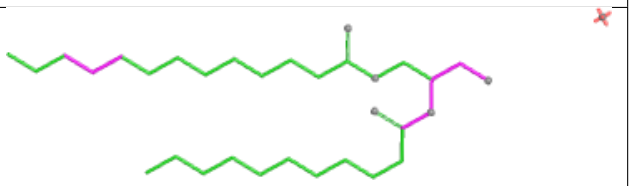


Rings

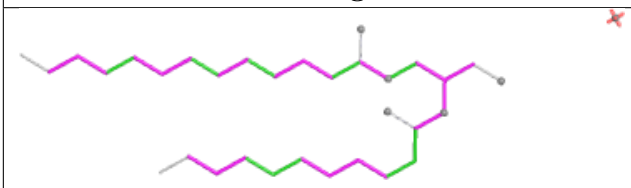
Ligand LMG D 409



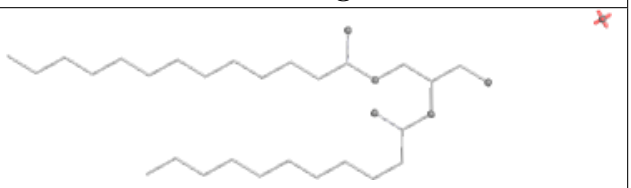
Bond lengths



Bond angles

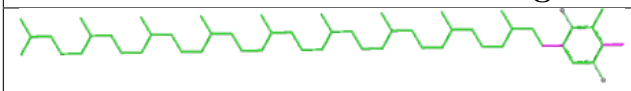


Torsions

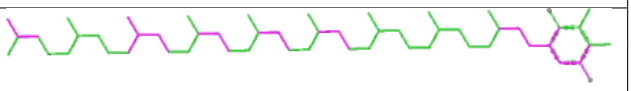


Rings

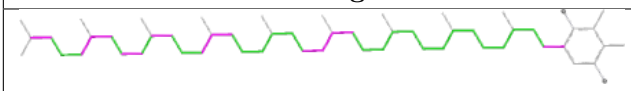
Ligand PL9 a 612



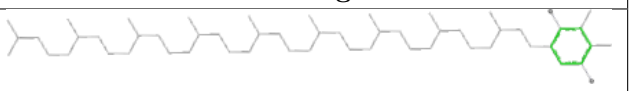
Bond lengths



Bond angles



Torsions



Rings

Ligand STE M 103

Bond lengths

Bond angles

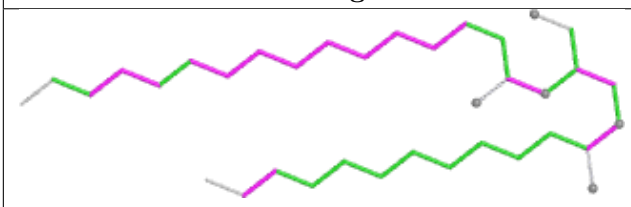
Torsions

Rings

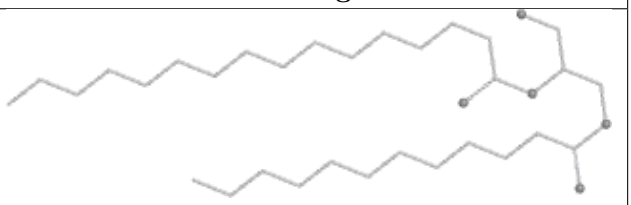
Ligand SQD a 616

Bond lengths

Bond angles

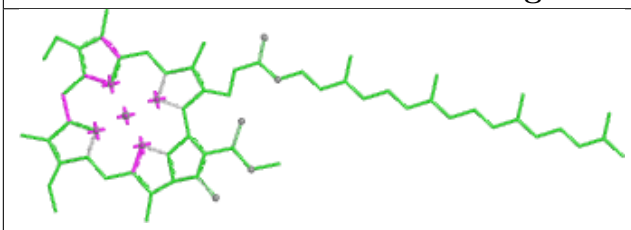


Torsions

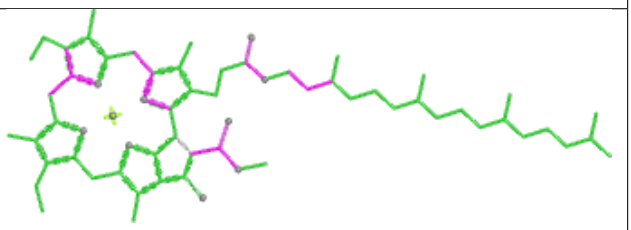


Rings

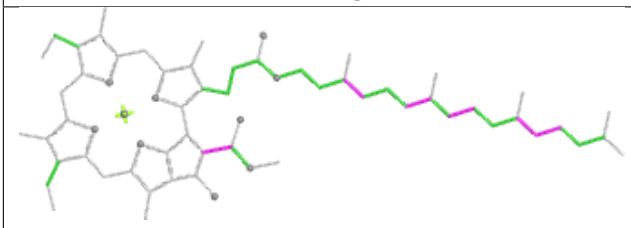
Ligand CLA B 614



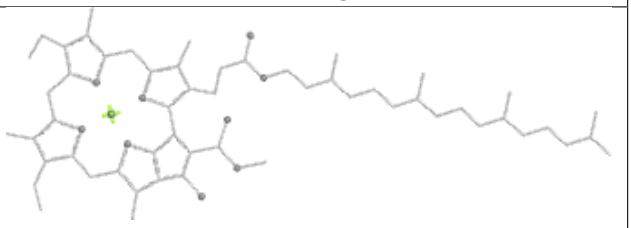
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.70	1 (0%)	90	89	8, 28, 47, 76	64 (19%)
1	a	334/344 (97%)	-0.58	0	100	100	8, 30, 56, 76	64 (19%)
2	B	505/510 (99%)	-0.59	0	100	100	17, 32, 60, 90	4 (0%)
2	b	505/510 (99%)	-0.48	2 (0%)	88	88	25, 35, 68, 105	0
3	C	442/461 (95%)	-0.59	0	100	100	9, 35, 50, 70	11 (2%)
3	c	451/461 (97%)	-0.45	1 (0%)	91	90	9, 39, 57, 91	12 (2%)
4	D	341/352 (96%)	-0.73	0	100	100	10, 29, 45, 78	2 (0%)
4	d	341/352 (96%)	-0.60	0	100	100	10, 33, 56, 82	3 (0%)
5	E	82/84 (97%)	-0.02	0	100	100	31, 48, 67, 83	1 (1%)
5	e	82/84 (97%)	0.11	0	100	100	37, 56, 76, 82	0
6	F	34/45 (75%)	-0.30	1 (2%)	53	52	35, 41, 58, 88	0
6	f	34/45 (75%)	-0.14	0	100	100	39, 48, 74, 88	0
7	H	65/66 (98%)	-0.35	0	100	100	32, 40, 54, 68	0
7	h	63/66 (95%)	-0.12	0	100	100	39, 49, 60, 63	0
8	I	35/38 (92%)	-0.43	0	100	100	32, 38, 62, 81	0
8	i	35/38 (92%)	-0.45	0	100	100	31, 39, 67, 81	0
9	J	36/40 (90%)	-0.25	0	100	100	33, 46, 71, 84	0
9	j	36/40 (90%)	-0.08	1 (2%)	55	54	38, 52, 83, 93	0
10	K	37/46 (80%)	-0.26	0	100	100	40, 47, 62, 70	0
10	k	37/46 (80%)	-0.06	0	100	100	46, 51, 66, 78	0
11	L	37/37 (100%)	-0.61	1 (2%)	56	55	24, 28, 60, 64	0
11	l	36/37 (97%)	-0.63	0	100	100	26, 31, 63, 87	0
12	M	32/36 (88%)	-0.54	0	100	100	27, 33, 57, 70	0
12	m	31/36 (86%)	-0.59	0	100	100	28, 32, 50, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.33	4 (1%)	70	70	25, 41, 77, 126	1 (0%)
13	o	244/272 (89%)	-0.35	1 (0%)	88	88	26, 39, 78, 115	0
14	T	29/32 (90%)	-0.74	0	100	100	26, 30, 54, 67	0
14	t	29/32 (90%)	-0.57	0	100	100	26, 31, 67, 81	0
15	U	97/134 (72%)	-0.43	0	100	100	30, 41, 66, 89	0
15	u	97/134 (72%)	-0.46	1 (1%)	79	79	31, 39, 55, 85	0
16	V	137/163 (84%)	-0.50	0	100	100	29, 38, 55, 71	0
16	v	137/163 (84%)	-0.35	0	100	100	33, 44, 63, 75	0
17	Y	27/46 (58%)	0.46	1 (3%)	45	44	49, 66, 76, 85	0
17	y	30/46 (65%)	0.23	0	100	100	56, 68, 77, 93	0
18	X	38/41 (92%)	-0.13	0	100	100	39, 48, 65, 74	0
18	x	39/41 (95%)	0.21	1 (2%)	57	56	47, 60, 80, 92	0
19	Z	62/62 (100%)	0.54	2 (3%)	50	49	52, 63, 101, 111	0
19	z	62/62 (100%)	0.26	1 (1%)	70	70	55, 64, 100, 109	0
20	R	34/41 (82%)	0.48	1 (2%)	53	52	57, 66, 78, 84	0
20	r	31/41 (75%)	0.92	1 (3%)	50	49	68, 80, 97, 101	0
All	All	5302/5700 (93%)	-0.44	20 (0%)	88	88	8, 37, 69, 126	162 (3%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	3.6
18	x	37	VAL	3.5
13	O	59	LYS	3.2
20	R	35	LEU	3.1
13	o	58	ASN	3.1
19	Z	33	TRP	2.9
15	u	53	ALA	2.8
2	b	495	PHE	2.8
13	O	60	ARG	2.7
3	c	23	ALA	2.6
13	O	4	THR	2.5
11	L	2	GLU	2.3
17	Y	20	ALA	2.3
20	r	12	VAL	2.2
19	z	33	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
9	j	6	GLY	2.1
1	A	11	ALA	2.1
13	O	56	PRO	2.0
2	b	496	TYR	2.0
6	F	13	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.93	0.09	35,47,63,65	0
14	FME	T	1	10/11	0.94	0.08	34,39,49,63	0
14	FME	t	1	10/11	0.94	0.07	30,38,53,58	0
8	FME	I	1	10/11	0.96	0.07	39,44,52,53	0
12	FME	m	1	10/11	0.97	0.06	32,46,60,66	0
8	FME	i	1	10/11	0.97	0.07	37,46,50,53	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	STE	H	103	18/20	0.72	0.13	56,69,71,71	0
33	STE	k	103	12/20	0.75	0.13	55,65,72,77	0
29	LMG	b	622	55/55	0.76	0.14	51,63,76,78	0
30	LHG	e	102	42/49	0.77	0.12	60,76,86,97	0
33	STE	B	625	12/20	0.77	0.13	51,56,71,74	0
29	LMG	c	521	48/55	0.77	0.13	48,66,83,91	0
33	STE	a	618	12/20	0.77	0.11	49,63,71,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LHG	E	101	49/49	0.77	0.12	43,73,89,90	0
33	STE	E	102	12/20	0.79	0.11	58,68,81,81	0
29	LMG	d	408	23/55	0.79	0.12	48,61,69,73	0
28	PL9	A	611	55/55	0.80	0.12	39,56,70,72	0
29	LMG	D	409	33/55	0.80	0.10	32,50,67,78	0
32	DGD	a	617	44/66	0.81	0.12	36,49,71,74	0
28	PL9	a	612	55/55	0.81	0.12	41,61,74,80	0
33	STE	B	626	16/20	0.81	0.12	47,54,60,64	0
33	STE	b	623	16/20	0.81	0.10	52,57,74,79	0
33	STE	C	520	12/20	0.81	0.11	45,52,59,59	0
33	STE	B	620	17/20	0.82	0.11	32,46,61,64	0
32	DGD	A	617	66/66	0.82	0.10	47,56,65,72	0
33	STE	b	625	20/20	0.82	0.10	46,55,62,63	0
33	STE	J	101	12/20	0.82	0.11	45,52,59,63	0
33	STE	t	104	18/20	0.82	0.12	45,52,78,78	0
31	SQD	a	616	36/54	0.83	0.10	37,52,65,73	0
33	STE	t	103	10/20	0.83	0.11	46,50,56,60	0
33	STE	b	621	20/20	0.83	0.12	38,50,67,71	0
33	STE	X	101	20/20	0.84	0.12	35,44,63,75	0
29	LMG	A	613	48/55	0.84	0.10	36,54,67,76	0
33	STE	m	102	12/20	0.84	0.12	46,56,66,66	0
33	STE	t	102	14/20	0.84	0.10	41,45,59,59	0
31	SQD	A	616	39/54	0.84	0.10	41,51,73,74	0
25	CLA	h	101	65/65	0.84	0.10	46,62,82,86	0
33	STE	c	520	20/20	0.85	0.10	40,51,78,80	0
29	LMG	c	519	37/55	0.85	0.09	43,57,66,68	0
29	LMG	c	522	49/55	0.85	0.10	37,50,75,84	0
33	STE	b	624	15/20	0.85	0.11	45,51,65,66	0
33	STE	C	519	12/20	0.85	0.12	38,43,55,55	0
33	STE	b	626	10/20	0.85	0.10	43,51,58,60	0
33	STE	b	620	16/20	0.86	0.11	34,46,57,58	0
29	LMG	B	621	28/55	0.86	0.09	35,47,57,65	0
33	STE	I	101	15/20	0.86	0.11	40,50,60,63	0
31	SQD	B	623	54/54	0.86	0.10	36,59,78,86	0
29	LMG	m	101	51/55	0.86	0.09	34,48,59,63	0
31	SQD	f	101	41/54	0.86	0.11	57,75,85,87	0
33	STE	x	101	20/20	0.86	0.12	41,50,59,62	0
31	SQD	b	619	49/54	0.87	0.10	40,55,78,82	0
33	STE	j	101	12/20	0.87	0.10	47,53,56,56	0
29	LMG	C	518	48/55	0.88	0.09	39,58,70,76	0
27	BCR	k	101	40/40	0.88	0.10	44,52,60,62	0
33	STE	B	624	12/20	0.88	0.10	41,48,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	STE	l	102	18/20	0.89	0.10	37,44,64,64	0
33	STE	d	410	17/20	0.89	0.09	43,48,62,62	0
33	STE	C	521	16/20	0.90	0.09	34,43,57,57	0
33	STE	M	103	10/20	0.90	0.09	41,45,51,57	0
31	SQD	F	102	36/54	0.90	0.10	44,61,69,70	0
27	BCR	d	404	40/40	0.90	0.08	38,47,72,79	0
27	BCR	K	102	40/40	0.90	0.09	37,45,55,58	0
27	BCR	h	102	40/40	0.91	0.08	37,49,62,64	0
25	CLA	B	601	65/65	0.91	0.09	31,52,75,81	0
32	DGD	H	102	62/66	0.91	0.08	32,41,48,52	0
31	SQD	a	615	54/54	0.91	0.09	37,54,68,70	0
32	DGD	h	103	62/66	0.91	0.08	38,43,53,57	0
29	LMG	M	101	51/55	0.91	0.08	33,47,59,63	0
27	BCR	D	405	40/40	0.91	0.08	28,38,67,71	0
29	LMG	D	407	51/55	0.92	0.09	31,44,68,69	0
27	BCR	c	514	40/40	0.92	0.08	44,50,57,58	0
25	CLA	C	513	65/65	0.92	0.08	38,50,72,76	0
31	SQD	A	615	52/54	0.92	0.09	34,48,69,73	0
27	BCR	b	618	40/40	0.92	0.07	31,43,56,59	0
27	BCR	B	618	40/40	0.93	0.06	26,34,40,43	0
30	LHG	a	614	49/49	0.93	0.08	30,46,60,63	0
33	STE	M	102	15/20	0.93	0.07	38,44,55,64	0
25	CLA	c	512	65/65	0.93	0.08	44,52,73,80	0
27	BCR	H	101	40/40	0.93	0.07	31,41,51,53	0
27	BCR	K	101	40/40	0.93	0.07	38,47,54,56	0
32	DGD	C	516	62/66	0.93	0.07	32,42,80,88	0
25	CLA	B	606	65/65	0.93	0.07	22,32,58,64	0
27	BCR	A	610	40/40	0.93	0.06	24,31,41,42	0
32	DGD	c	517	62/66	0.93	0.07	34,44,72,76	0
32	DGD	c	518	62/66	0.93	0.08	30,42,65,70	0
27	BCR	b	616	40/40	0.94	0.06	27,37,42,45	0
27	BCR	b	617	40/40	0.94	0.06	26,34,43,46	0
25	CLA	c	506	65/65	0.94	0.07	33,41,71,75	0
27	BCR	B	617	40/40	0.94	0.06	25,33,42,43	0
27	BCR	c	515	40/40	0.94	0.06	29,42,50,53	0
25	CLA	c	508	64/65	0.94	0.07	32,38,69,88	0
27	BCR	B	619	40/40	0.94	0.06	28,38,50,53	0
25	CLA	c	511	65/65	0.94	0.08	40,47,57,62	0
27	BCR	k	102	40/40	0.94	0.08	38,47,55,58	0
32	DGD	C	515	62/66	0.94	0.07	25,33,65,72	0
25	CLA	C	506	65/65	0.94	0.07	27,37,69,71	0
25	CLA	c	513	65/65	0.94	0.08	41,55,78,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	b	605	65/65	0.94	0.07	28,36,59,62	0
32	DGD	c	516	62/66	0.94	0.07	25,35,58,68	0
27	BCR	T	101	40/40	0.94	0.06	29,35,43,46	0
30	LHG	l	101	49/49	0.94	0.07	30,39,48,54	0
34	BCT	a	606	4/4	0.94	0.08	30,36,40,46	0
29	LMG	d	409	44/55	0.95	0.07	37,44,66,73	0
27	BCR	a	611	40/40	0.95	0.05	23,31,42,44	0
30	LHG	A	614	47/49	0.95	0.08	27,38,64,73	0
30	LHG	B	622	49/49	0.95	0.07	29,39,54,57	0
25	CLA	c	504	60/65	0.95	0.06	29,37,64,68	0
25	CLA	B	609	65/65	0.95	0.06	26,34,50,54	0
25	CLA	B	616	60/65	0.95	0.07	24,32,66,70	0
25	CLA	c	509	65/65	0.95	0.07	32,39,53,57	0
25	CLA	c	510	65/65	0.95	0.06	29,41,50,54	0
25	CLA	C	503	65/65	0.95	0.06	30,36,41,46	0
25	CLA	B	602	65/65	0.95	0.06	26,32,48,53	0
25	CLA	C	508	65/65	0.95	0.06	29,34,74,85	0
25	CLA	d	403	65/65	0.95	0.08	30,39,72,76	0
27	BCR	t	101	40/40	0.95	0.05	25,32,45,47	0
25	CLA	C	510	65/65	0.95	0.06	29,36,47,53	0
26	PHO	d	401	64/64	0.95	0.06	23,34,40,44	0
28	PL9	d	405	55/55	0.95	0.06	22,31,38,39	0
25	CLA	C	511	65/65	0.95	0.07	27,42,51,56	0
25	CLA	C	512	65/65	0.95	0.07	34,44,75,80	0
32	DGD	C	517	62/66	0.95	0.07	25,39,64,71	0
25	CLA	B	604	65/65	0.95	0.07	22,28,57,61	0
25	CLA	a	608	65/65	0.95	0.07	26,35,73,78	0
27	BCR	C	514	40/40	0.95	0.07	29,36,46,48	0
25	CLA	A	607	65/65	0.95	0.07	24,29,76,83	0
25	CLA	b	608	65/65	0.95	0.07	30,39,55,68	0
25	CLA	b	613	65/65	0.95	0.06	27,35,63,67	0
25	CLA	b	615	60/65	0.95	0.07	30,39,77,82	0
27	BCR	K	103	40/40	0.95	0.07	32,43,51,57	0
34	BCT	D	401	4/4	0.95	0.08	35,36,39,40	0
25	CLA	c	503	65/65	0.95	0.06	31,39,45,49	0
30	LHG	d	407	39/49	0.96	0.07	31,40,56,62	0
25	CLA	b	601	65/65	0.96	0.06	30,37,51,53	0
25	CLA	B	611	65/65	0.96	0.05	21,28,40,42	0
25	CLA	d	402	65/65	0.96	0.06	23,29,49,60	0
25	CLA	b	607	65/65	0.96	0.06	29,36,52,56	0
25	CLA	C	507	65/65	0.96	0.06	26,33,46,51	0
26	PHO	D	402	64/64	0.96	0.05	20,29,34,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	PL9	D	406	55/55	0.96	0.05	21,28,36,40	0
26	PHO	a	609	64/64	0.96	0.05	21,28,33,38	0
25	CLA	b	609	65/65	0.96	0.06	28,34,41,48	0
25	CLA	b	610	65/65	0.96	0.06	22,31,46,52	0
25	CLA	b	611	65/65	0.96	0.06	21,30,42,45	0
25	CLA	b	612	65/65	0.96	0.06	20,28,59,63	0
25	CLA	B	614	65/65	0.96	0.06	22,32,62,69	0
25	CLA	b	614	65/65	0.96	0.06	28,36,51,59	0
25	CLA	C	509	65/65	0.96	0.07	27,35,49,53	0
25	CLA	c	501	65/65	0.96	0.06	28,35,43,49	0
25	CLA	c	502	65/65	0.96	0.06	26,34,51,56	0
25	CLA	B	607	65/65	0.96	0.06	19,26,51,53	0
25	CLA	C	502	65/65	0.96	0.06	27,32,44,50	0
25	CLA	c	505	65/65	0.96	0.06	27,36,54,57	0
25	CLA	B	610	65/65	0.96	0.06	22,30,36,40	0
25	CLA	c	507	65/65	0.96	0.06	28,37,49,52	0
25	CLA	C	504	59/65	0.96	0.06	29,35,63,69	0
25	CLA	a	607	65/65	0.96	0.06	22,27,37,44	0
25	CLA	C	505	65/65	0.96	0.06	25,33,55,61	0
25	CLA	a	610	65/65	0.96	0.08	22,28,65,69	0
25	CLA	B	605	65/65	0.97	0.05	22,28,38,40	0
30	LHG	D	408	49/49	0.97	0.06	27,34,44,48	0
25	CLA	A	612	65/65	0.97	0.04	17,25,39,45	0
30	LHG	L	101	49/49	0.97	0.06	29,36,47,53	0
25	CLA	D	403	65/65	0.97	0.05	20,25,45,51	0
30	LHG	d	406	49/49	0.97	0.06	29,36,42,51	0
25	CLA	D	404	65/65	0.97	0.07	25,32,81,91	0
25	CLA	B	612	65/65	0.97	0.05	21,28,38,41	0
25	CLA	B	613	65/65	0.97	0.06	21,27,54,65	0
25	CLA	B	603	65/65	0.97	0.05	22,27,51,59	0
26	PHO	A	608	64/64	0.97	0.05	18,25,32,36	0
25	CLA	a	613	65/65	0.97	0.05	19,27,38,43	0
25	CLA	B	615	65/65	0.97	0.05	25,32,49,54	0
25	CLA	b	602	65/65	0.97	0.06	24,31,52,61	0
25	CLA	b	603	65/65	0.97	0.06	22,31,64,72	0
25	CLA	b	604	65/65	0.97	0.05	22,30,40,44	0
25	CLA	B	608	65/65	0.97	0.05	25,30,46,51	0
25	CLA	b	606	65/65	0.97	0.06	23,30,55,59	0
25	CLA	C	501	65/65	0.97	0.05	26,30,40,44	0
25	CLA	A	606	65/65	0.97	0.05	18,24,35,45	0
35	HEM	e	101	43/43	0.97	0.09	46,55,66,78	0
35	HEM	F	101	43/43	0.98	0.08	38,43,51,63	0

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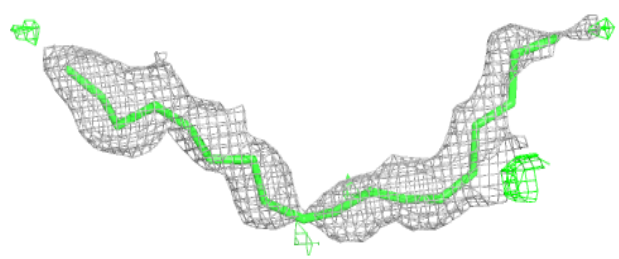
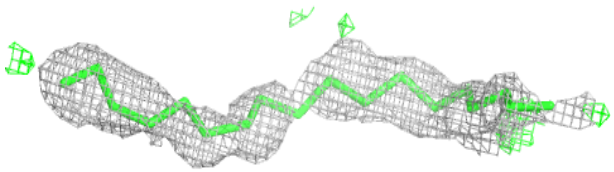
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	A	609	54/65	0.98	0.05	20,26,54,60	0
23	FE2	A	603	1/1	0.99	0.02	30,30,30,30	0
24	CL	A	604	1/1	0.99	0.03	28,28,28,28	0
24	CL	a	604	1/1	0.99	0.08	27,27,27,27	0
24	CL	a	605	1/1	0.99	0.06	29,29,29,29	0
21	OEX	A	601[B]	10/10	0.99	0.03	25,29,33,33	10
21	OEX	A	601[C]	10/10	0.99	0.03	22,25,28,28	10
21	OEX	a	601[B]	10/10	0.99	0.02	26,29,32,32	10
21	OEX	a	601[C]	10/10	0.99	0.02	21,23,25,25	10
22	OEY	A	602[A]	11/11	0.99	0.03	26,29,32,32	11
22	OEY	a	602[A]	11/11	0.99	0.03	28,30,34,34	11
36	HEC	V	201	43/43	0.99	0.05	23,30,38,42	0
36	HEC	v	201	43/43	0.99	0.05	28,33,37,43	0
23	FE2	a	603	1/1	1.00	0.01	34,34,34,34	0
24	CL	A	605	1/1	1.00	0.04	29,29,29,29	0

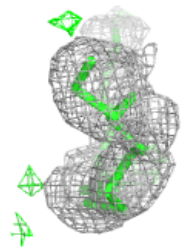
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE H 103:

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

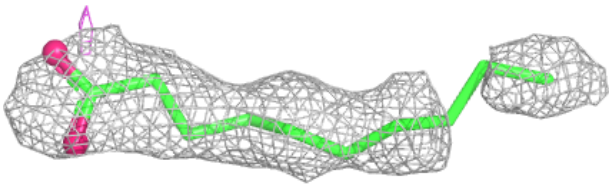


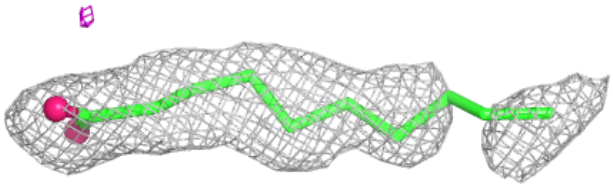


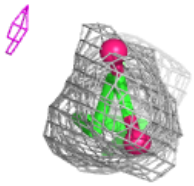


Electron density around STE k 103:

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

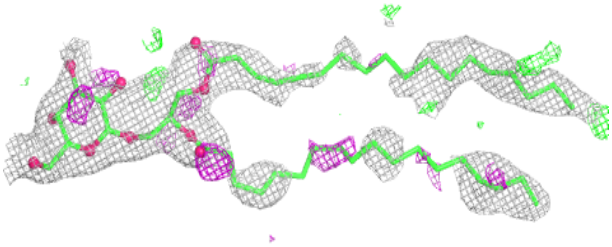


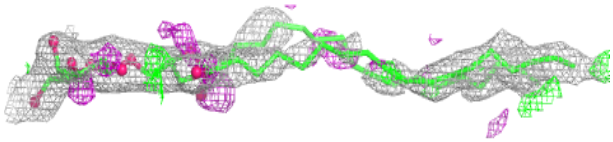


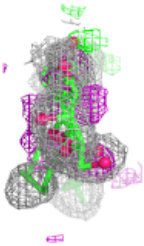


Electron density around LMG b 622:

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

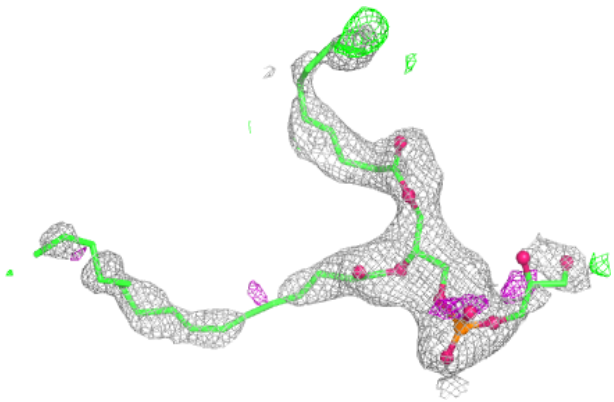


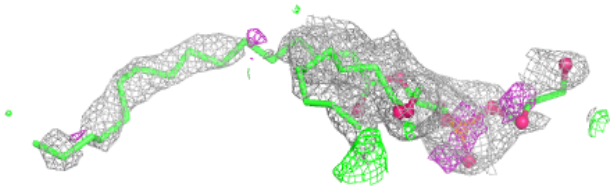


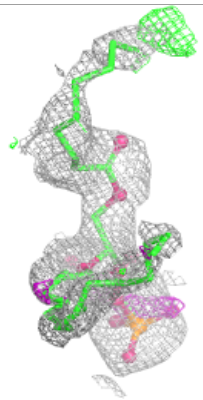


Electron density around LHG e 102:

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

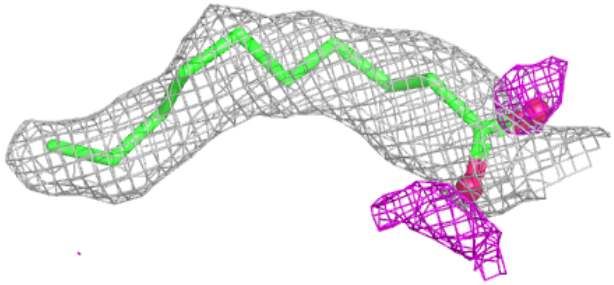


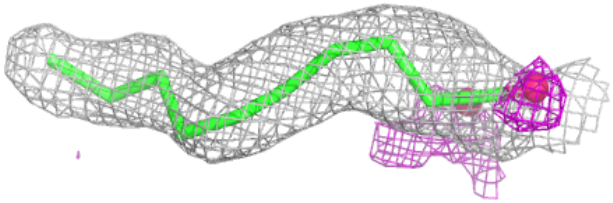


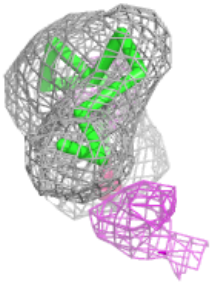


Electron density around STE B 625:

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

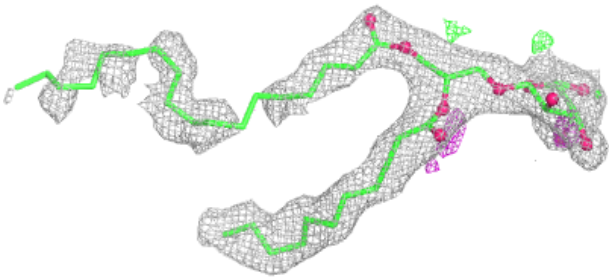


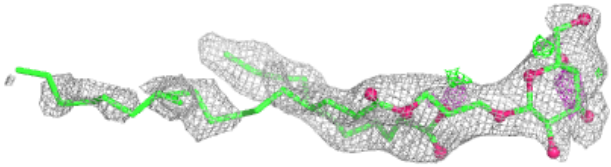


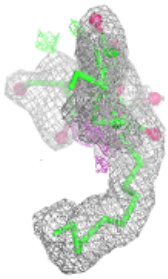


Electron density around LMG c 521:

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

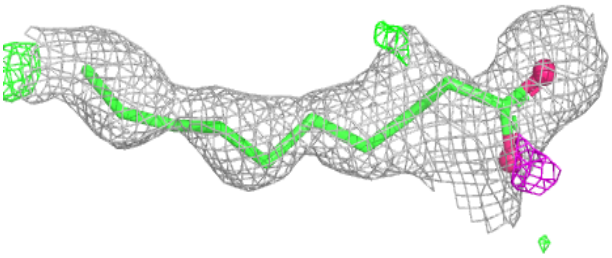


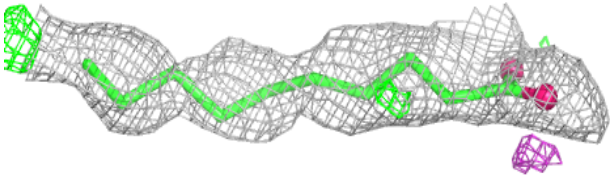


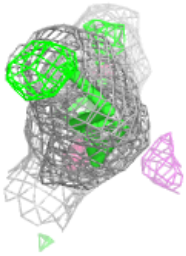


Electron density around STE a 618:

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

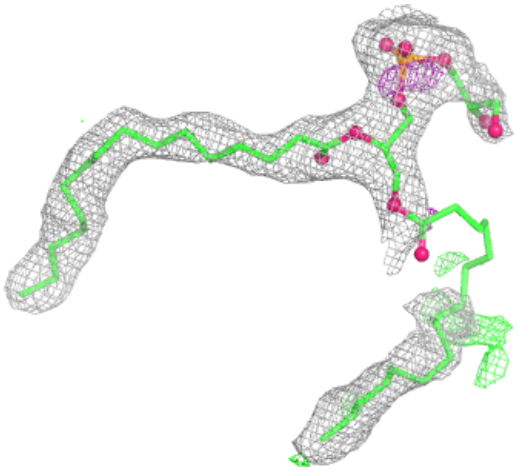


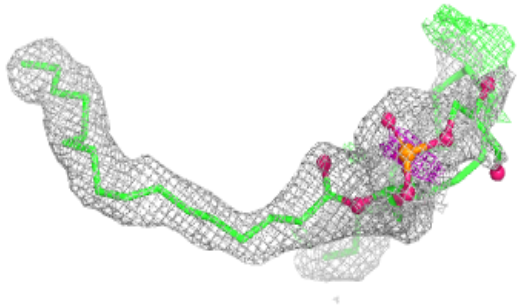


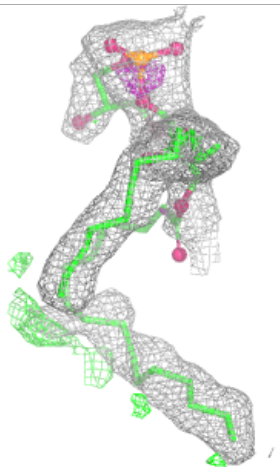


Electron density around LHG E 101:

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

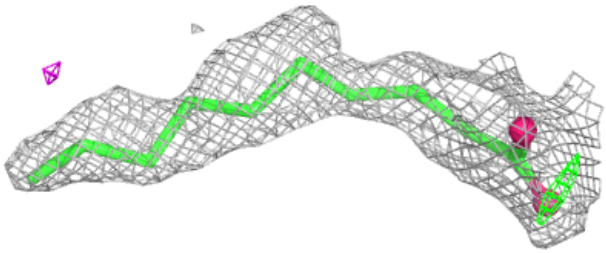


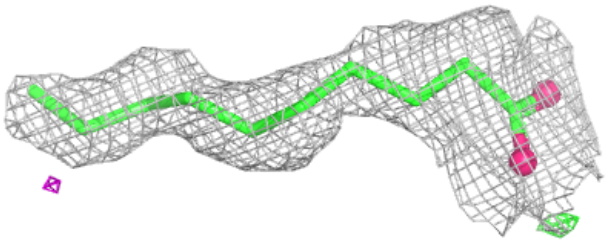


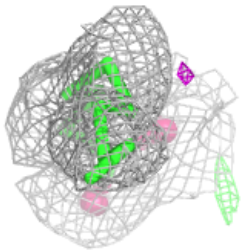


Electron density around STE E 102:

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

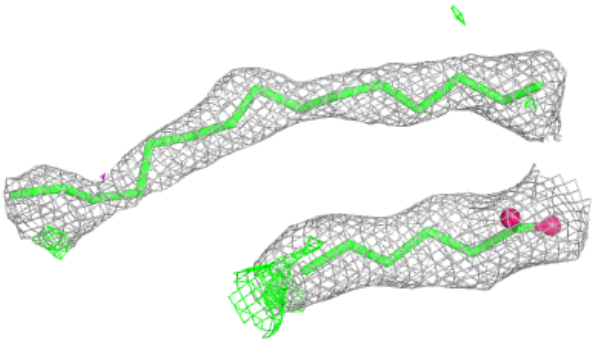


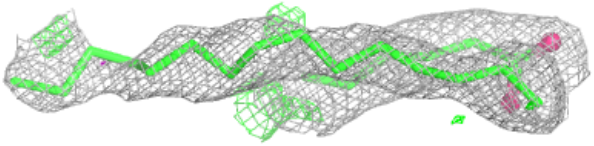


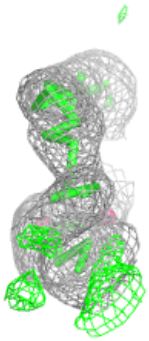


Electron density around LMG d 408:

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

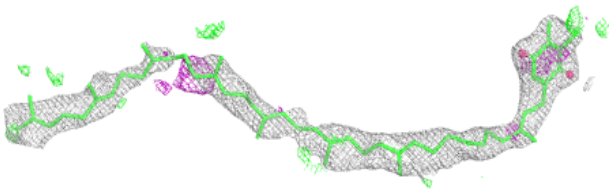


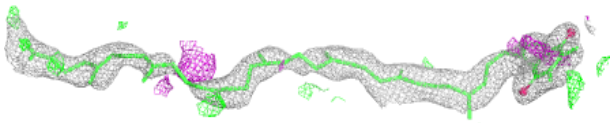




Electron density around PL9 A 611:

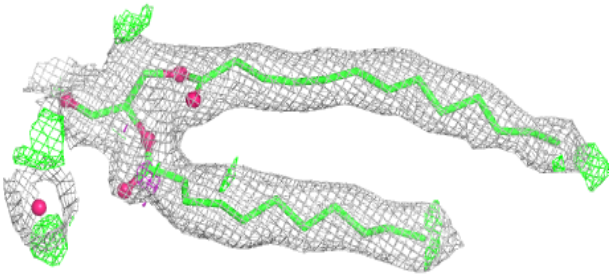
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

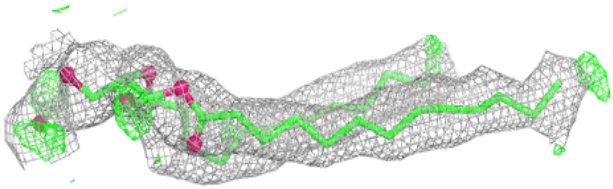


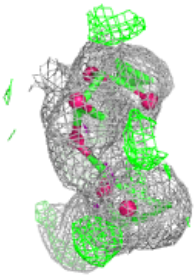


Electron density around LMG D 409:

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

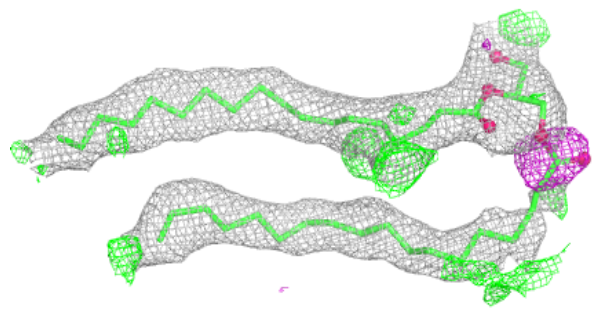


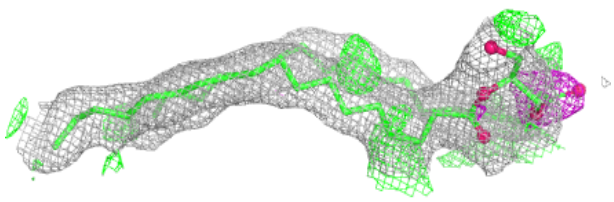


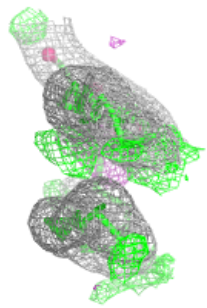


Electron density around DGD a 617:

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

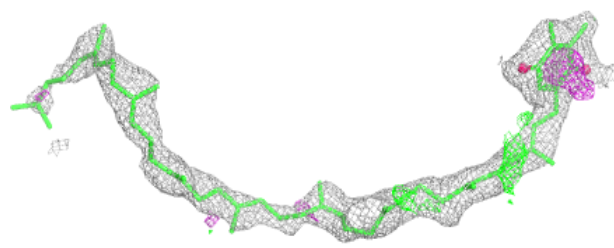


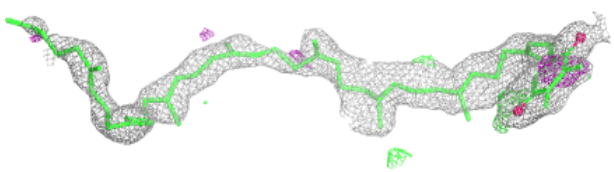


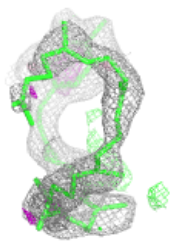


Electron density around PL9 a 612:

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

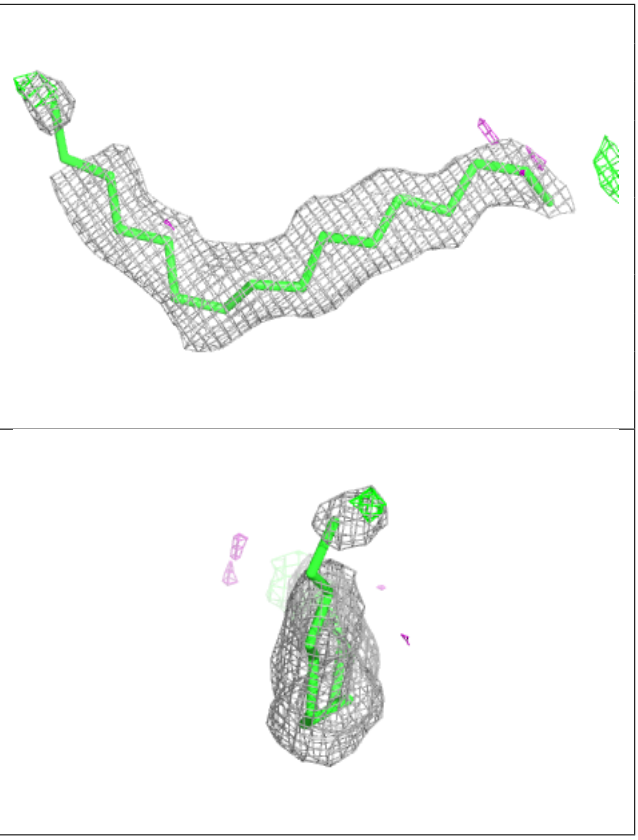






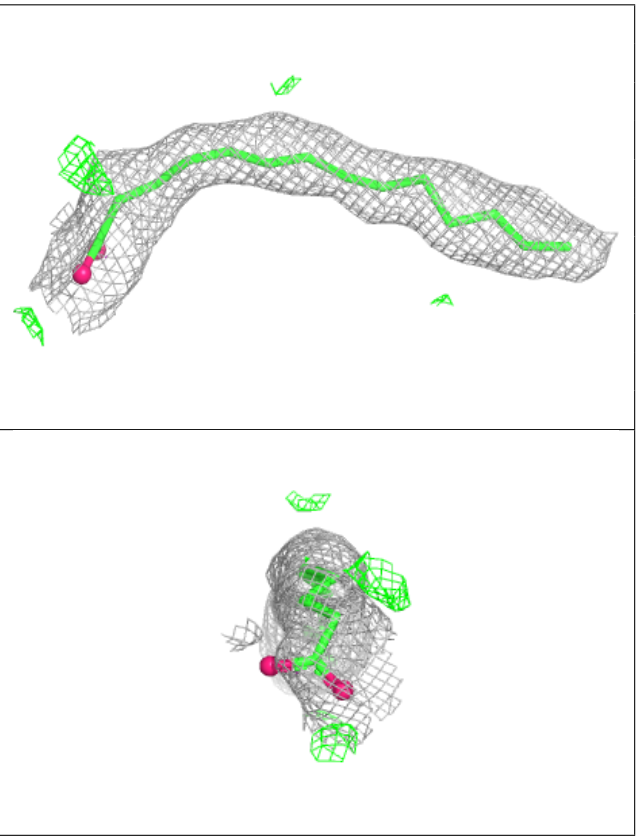
Electron density around STE B 626:

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



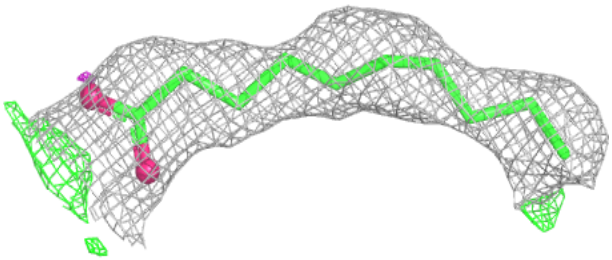
Electron density around STE b 623:

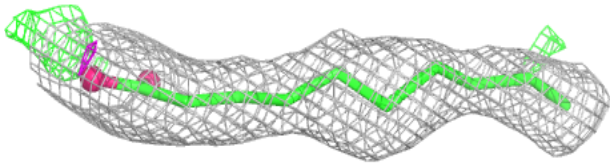
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

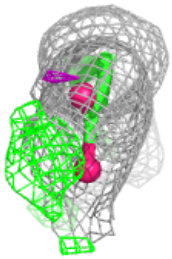


Electron density around STE C 520:

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

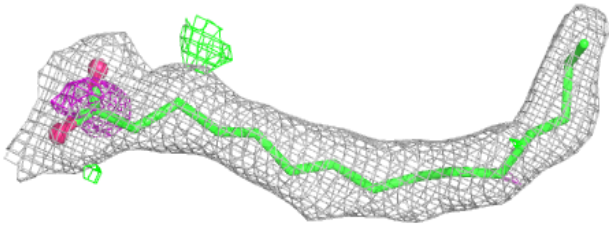


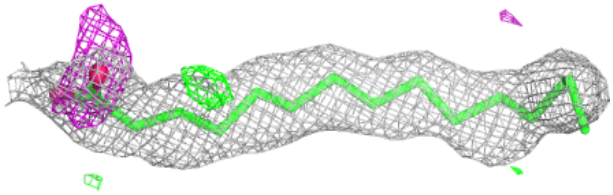


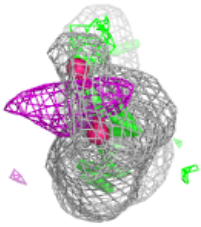


Electron density around STE B 620:

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

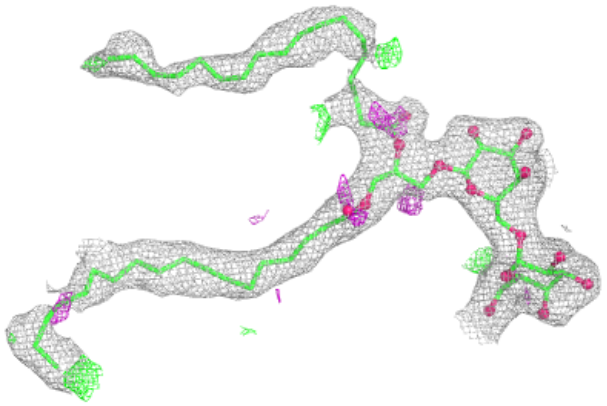


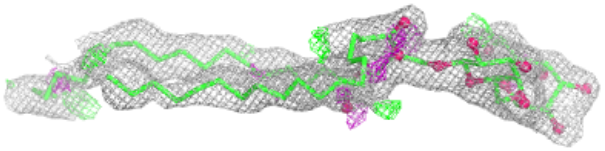


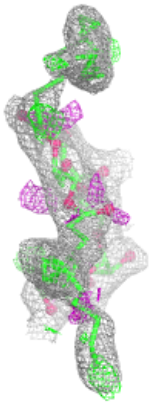


Electron density around DGD A 617:

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

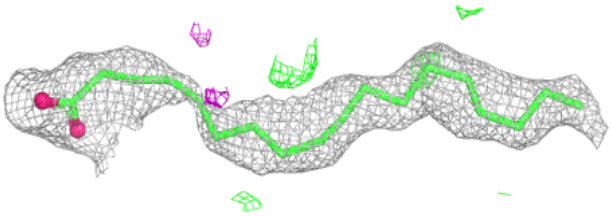


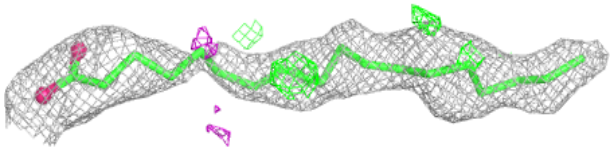


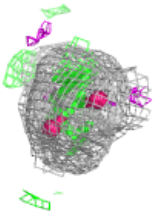


Electron density around STE b 625:

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

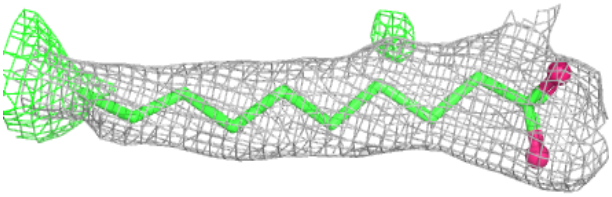


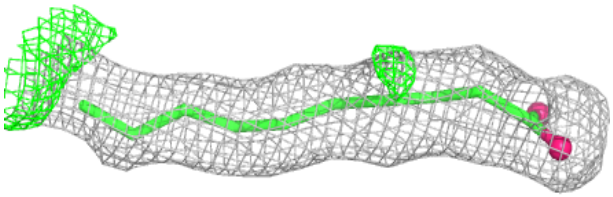


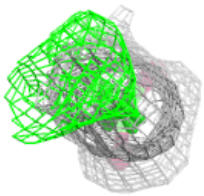


Electron density around STE J 101:

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

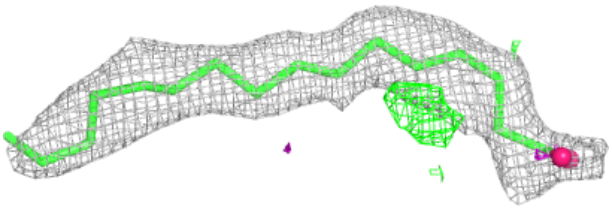


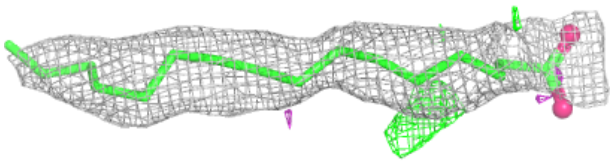


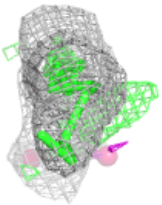


Electron density around STE t 104:

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

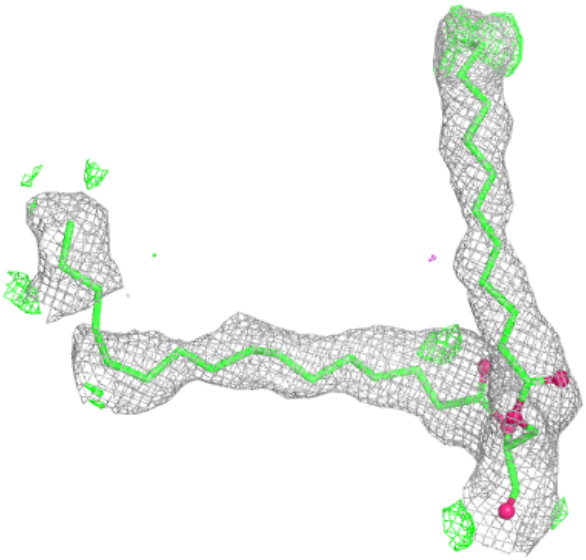


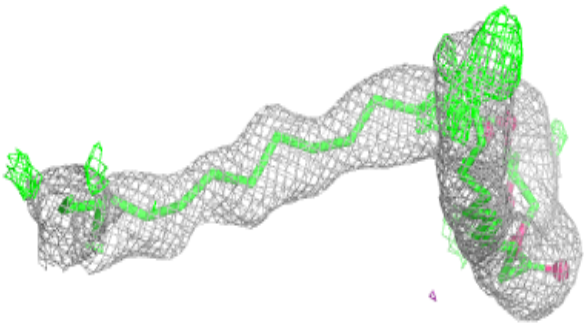


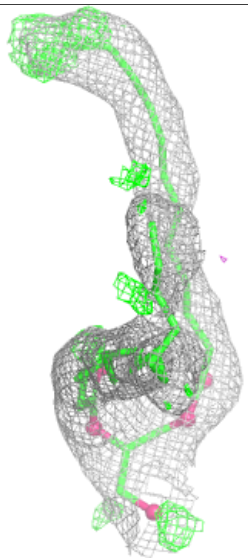


Electron density around SQD a 616:

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

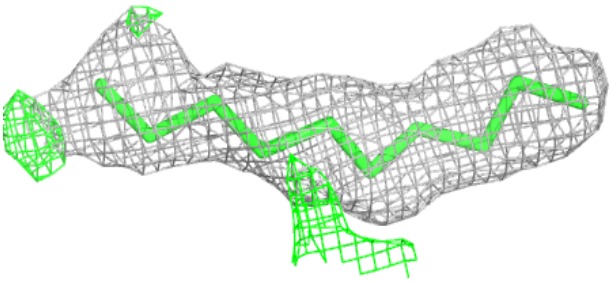


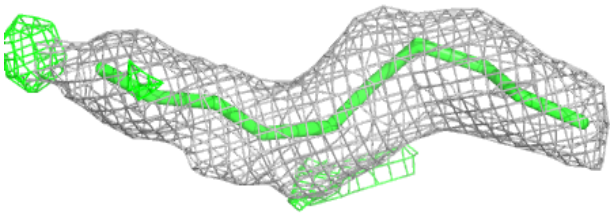


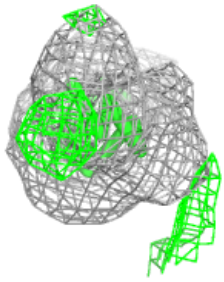


Electron density around STE t 103:

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

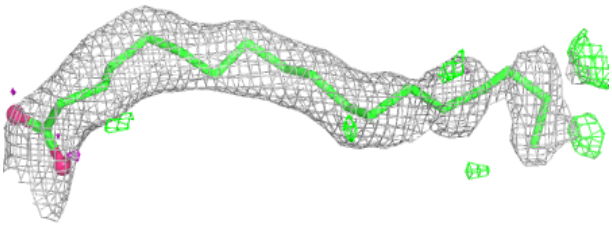


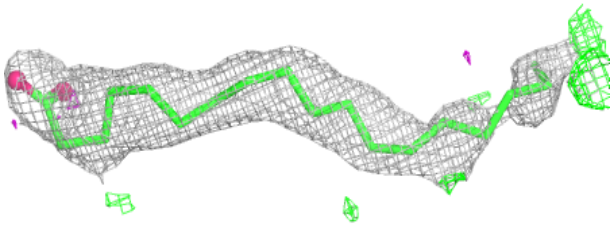


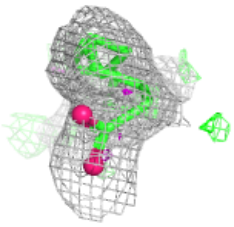


Electron density around STE b 621:

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

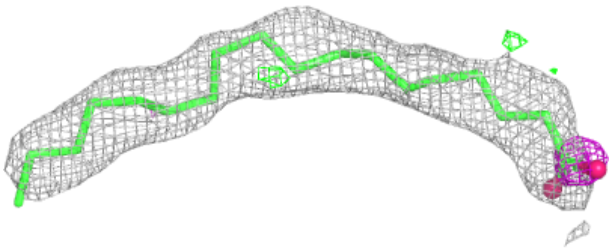


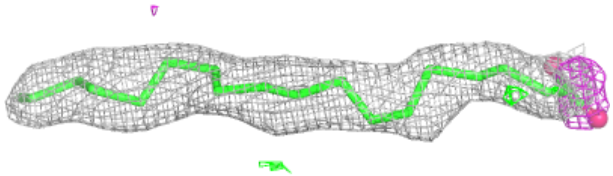


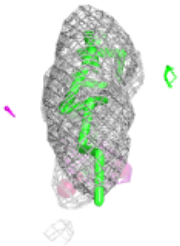


Electron density around STE X 101:

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

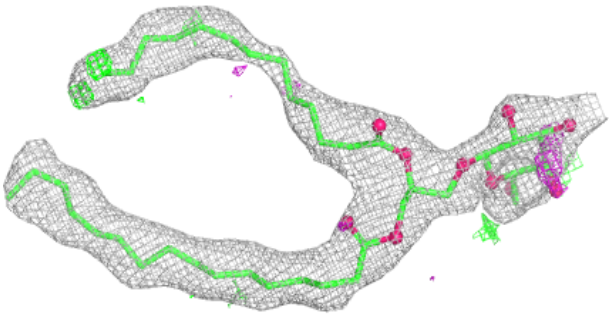


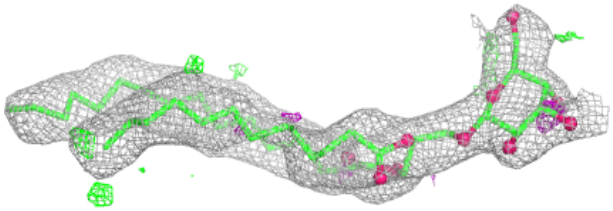


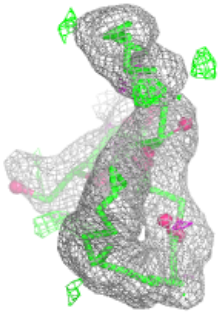


Electron density around LMG A 613:

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

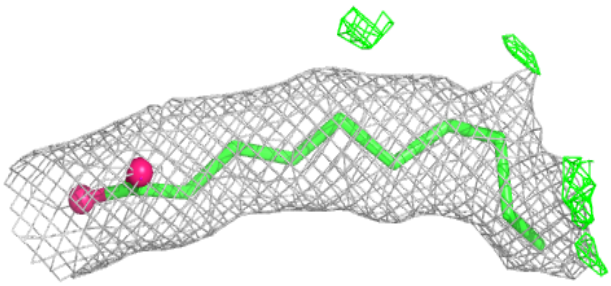


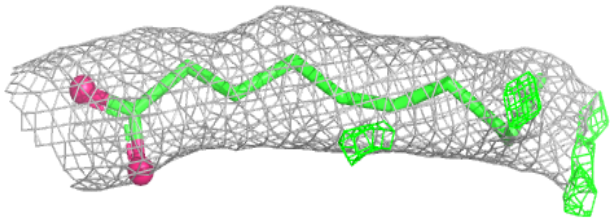


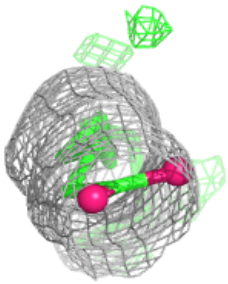


Electron density around STE m 102:

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

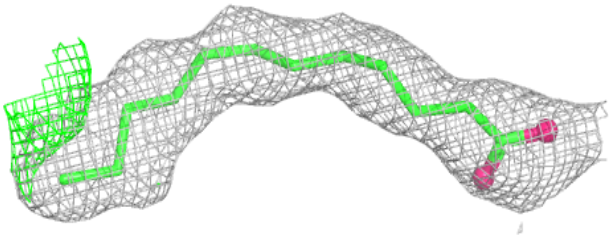


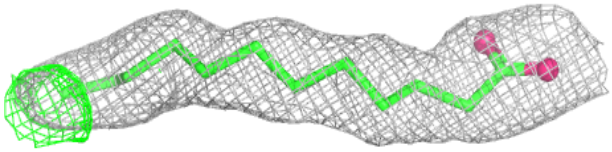


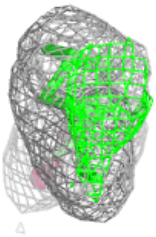


Electron density around STE t 102:

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

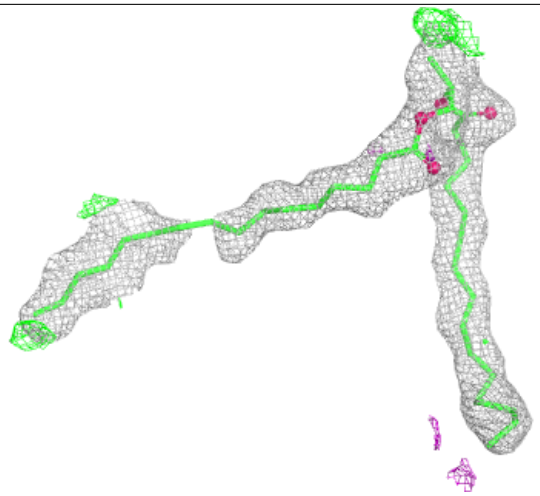


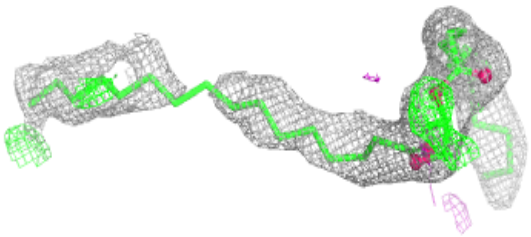


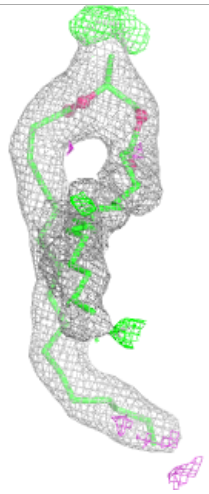


Electron density around SQD A 616:

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

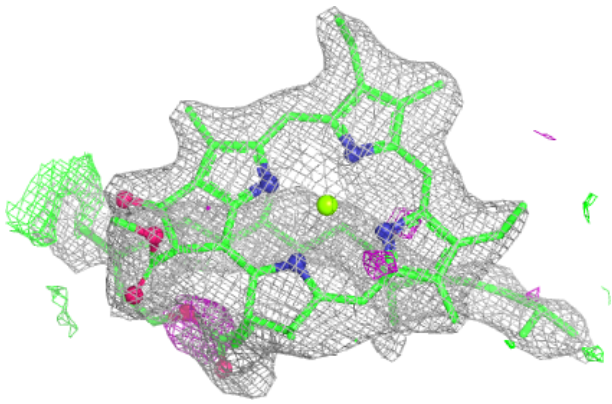


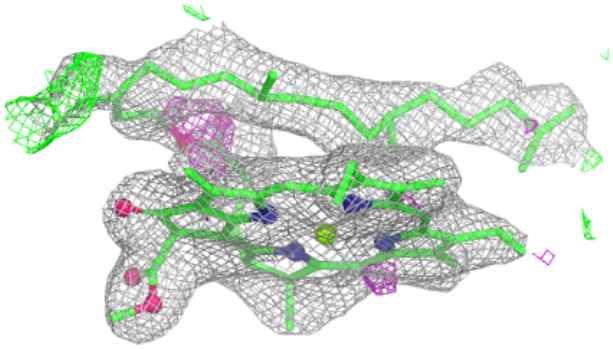


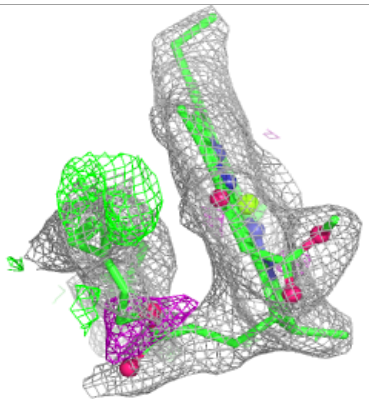


Electron density around CLA h 101:

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

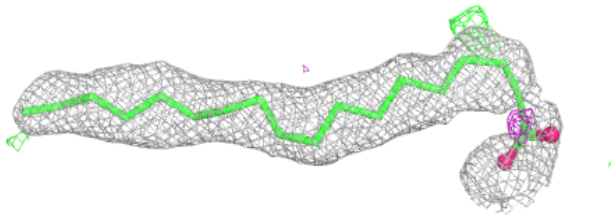


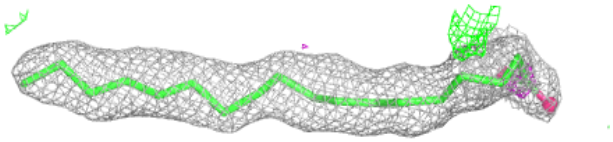


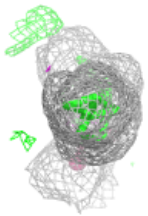


Electron density around STE c 520:

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

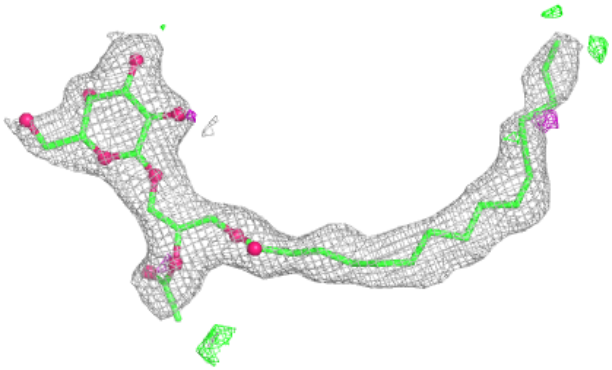


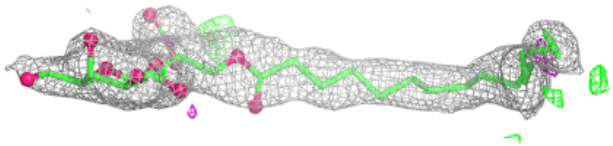


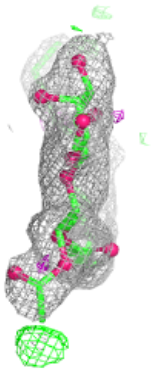


Electron density around LMG c 519:

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

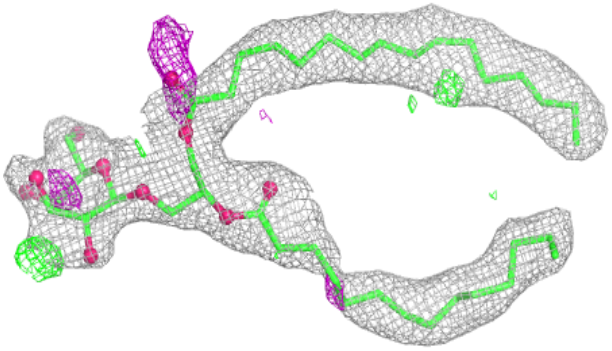


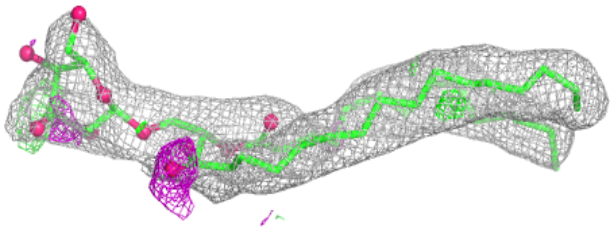


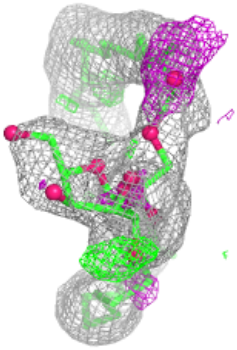


Electron density around LMG c 522:

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

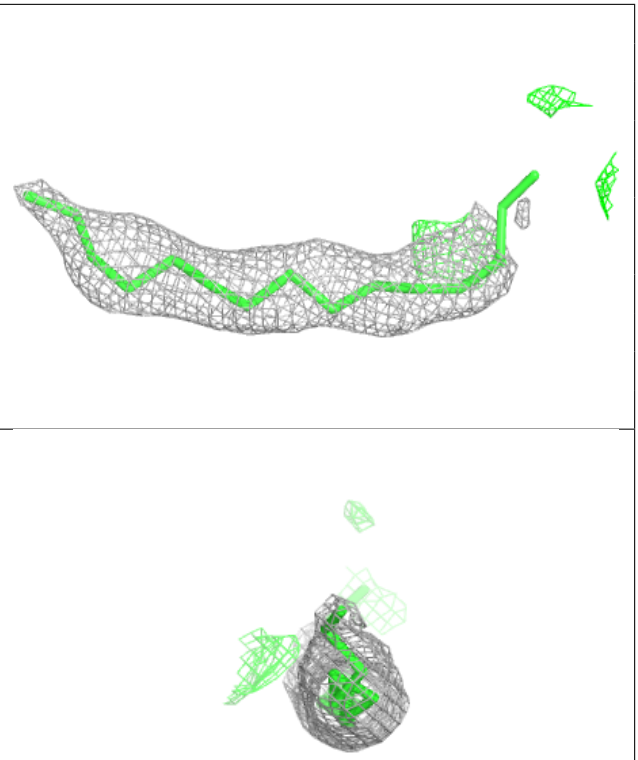






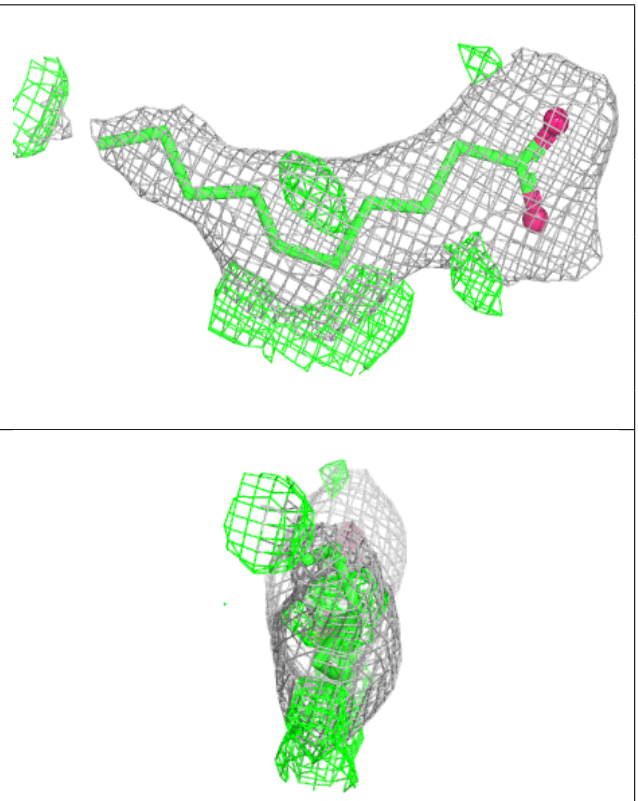
Electron density around STE b 624:

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



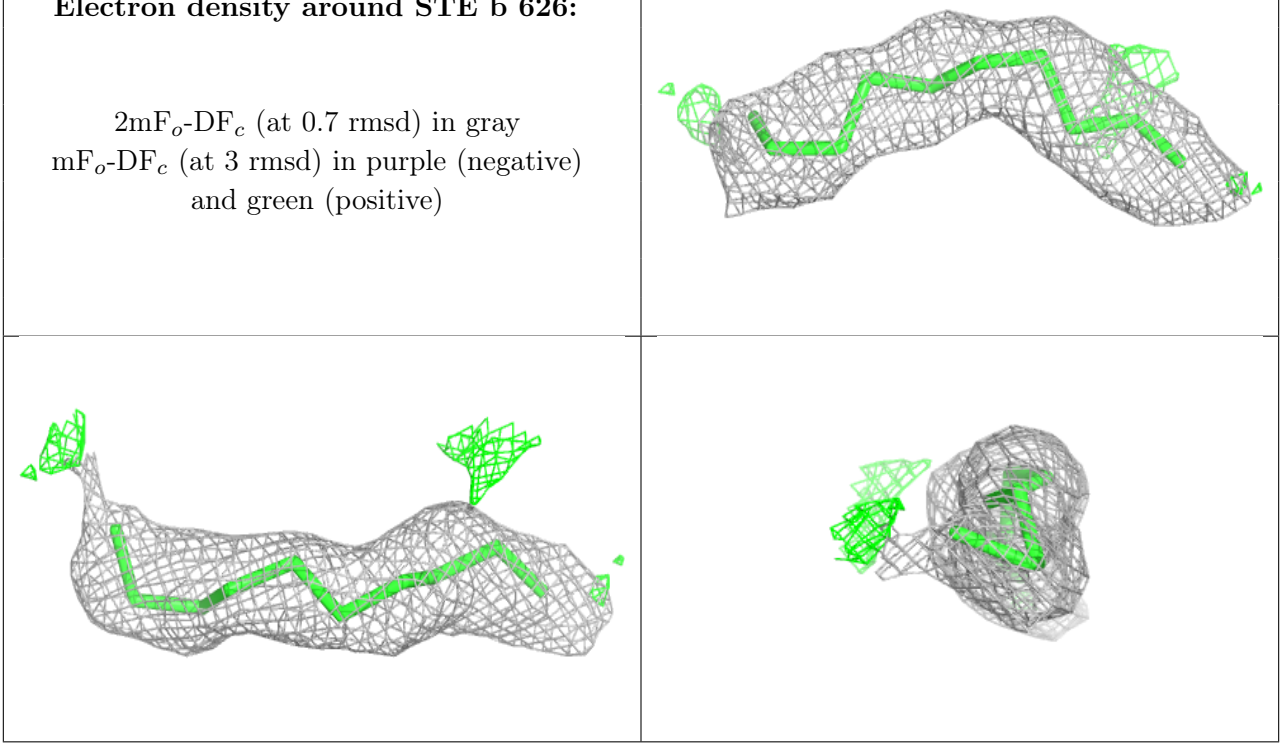
Electron density around STE C 519:

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



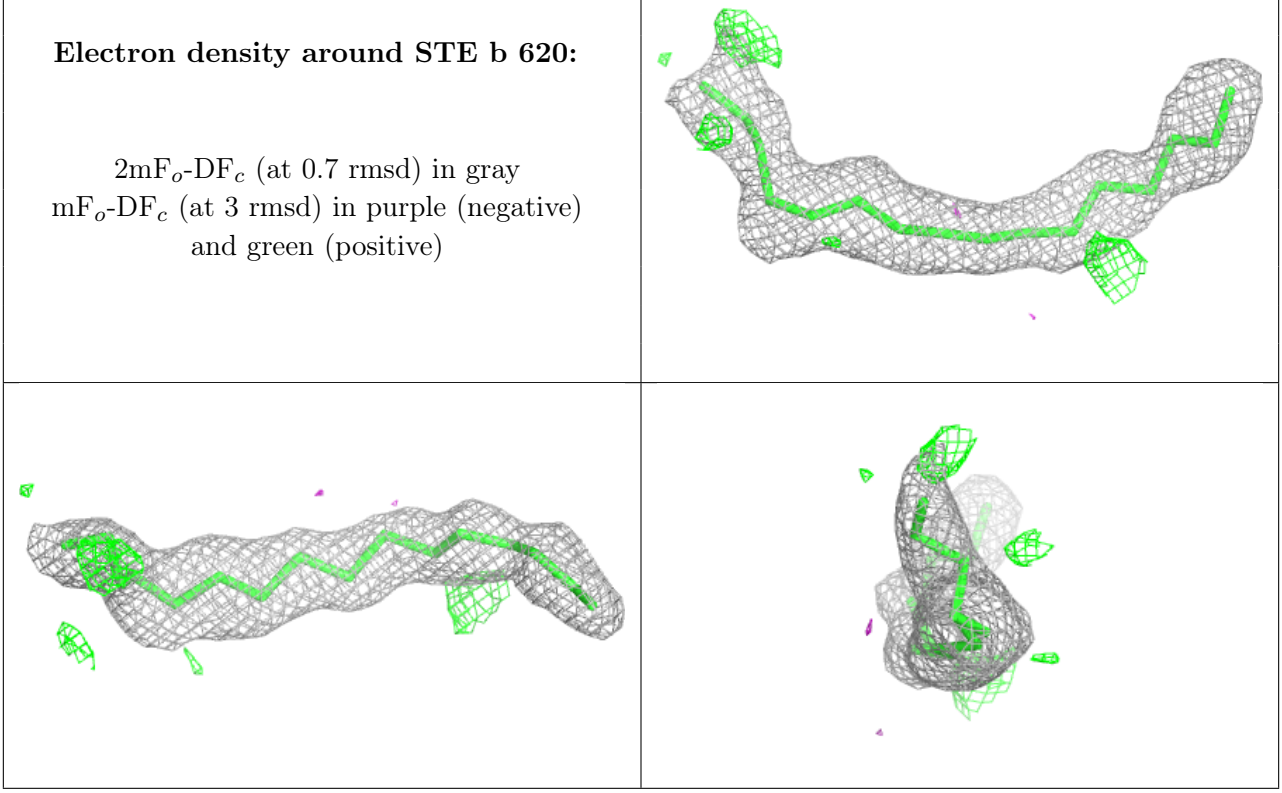
Electron density around STE b 626:

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



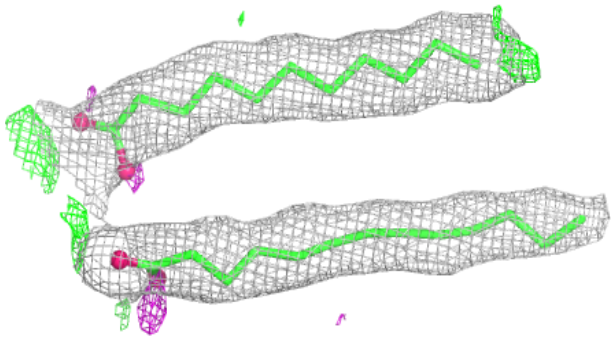
Electron density around STE b 620:

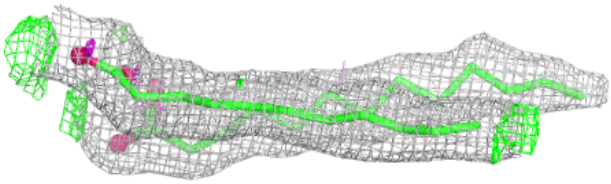
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

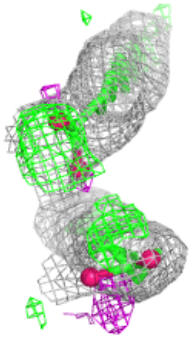


Electron density around LMG B 621:

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

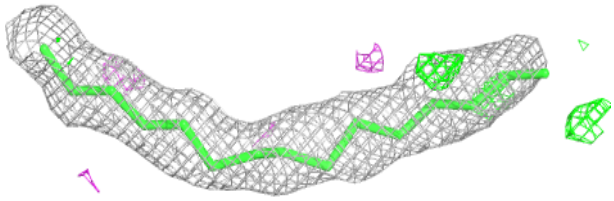


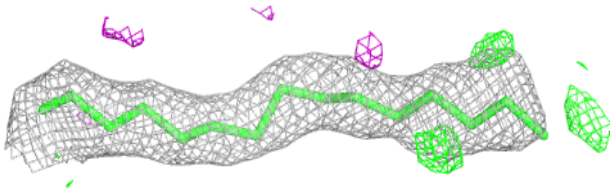


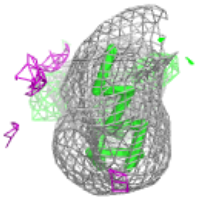


Electron density around STE I 101:

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

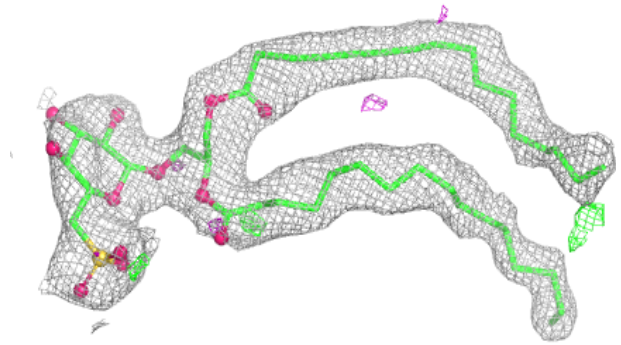


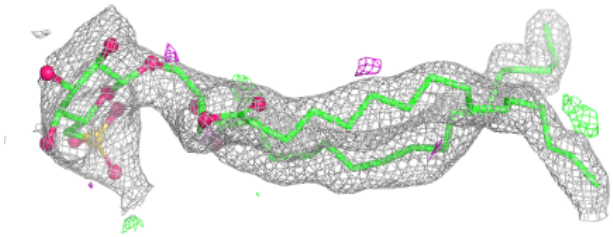


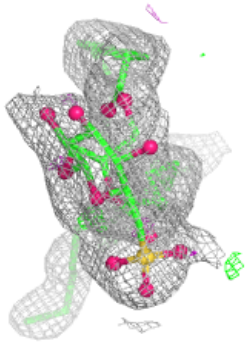


Electron density around SQD B 623:

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

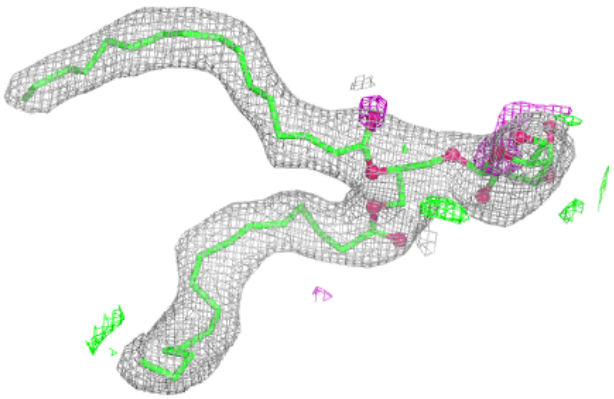


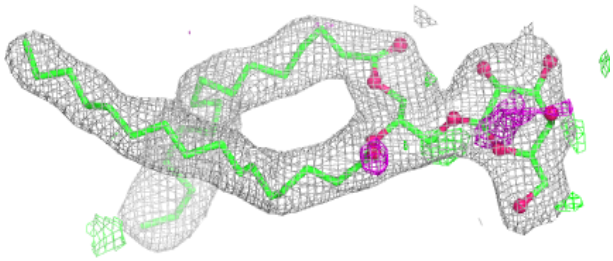


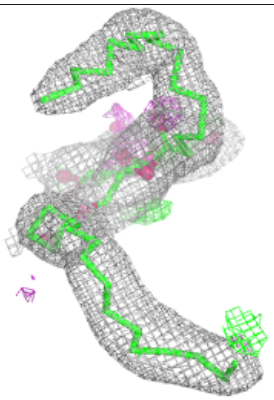


Electron density around LMG m 101:

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

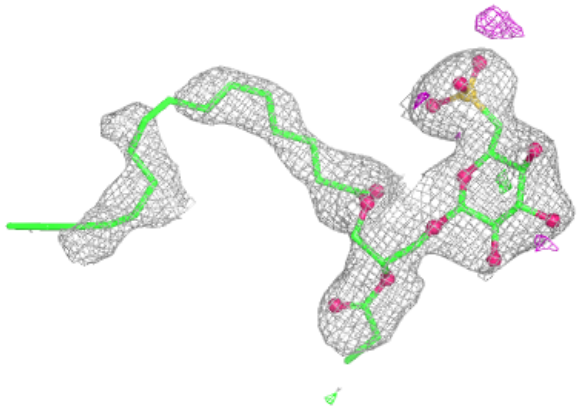


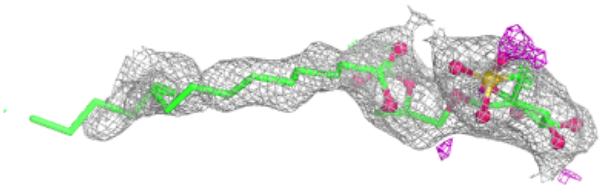


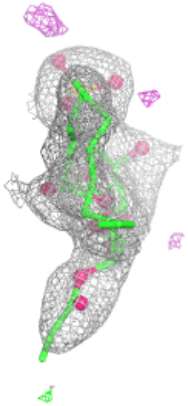


Electron density around SQD f 101:

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

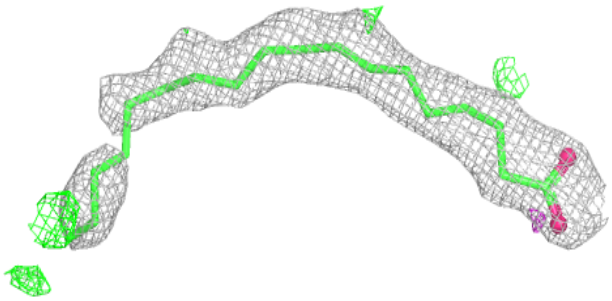


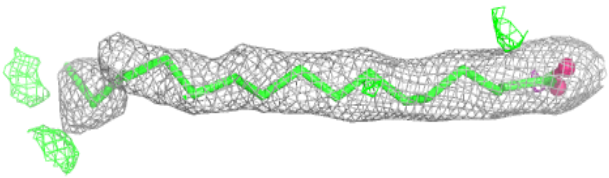


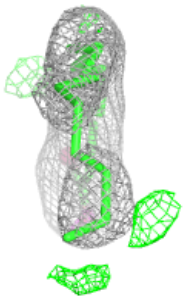


Electron density around STE x 101:

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

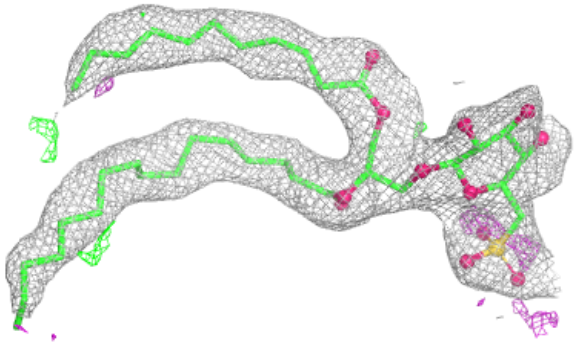


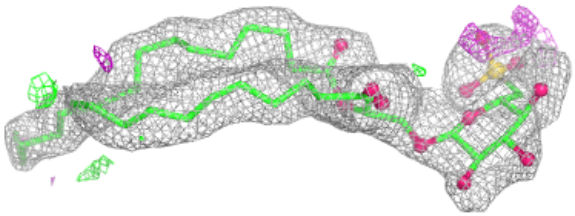




Electron density around SQD b 619:

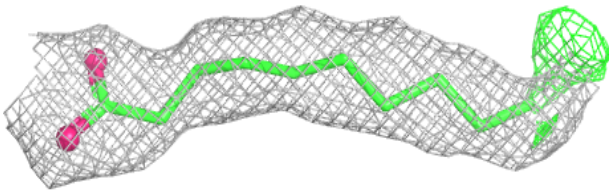
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

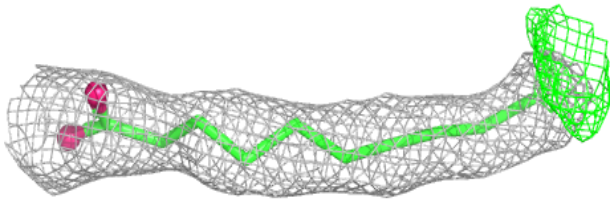


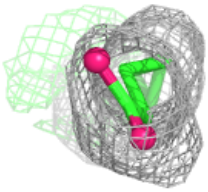


Electron density around STE j 101:

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

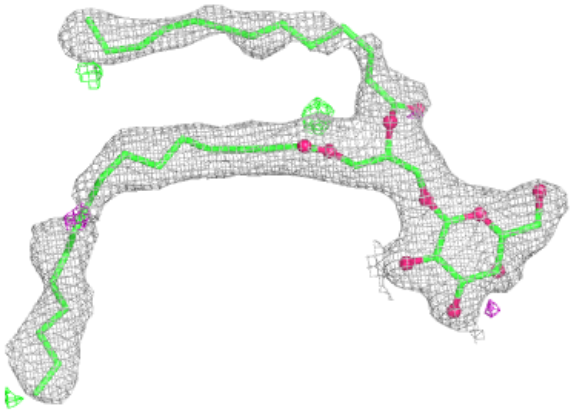


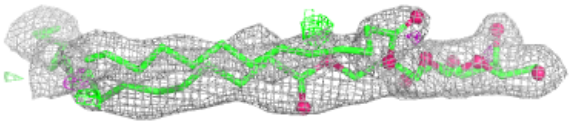


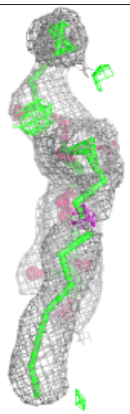


Electron density around LMG C 518:

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

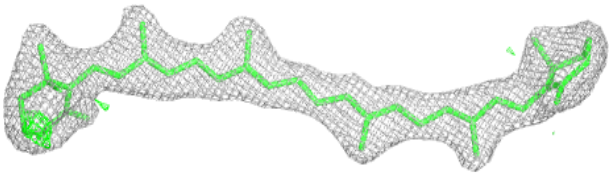


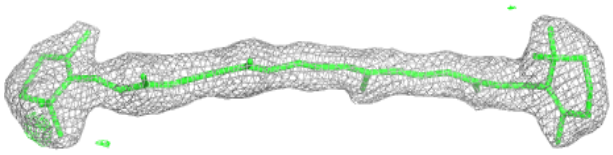


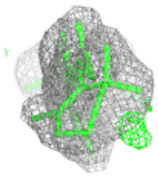


Electron density around BCR k 101:

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

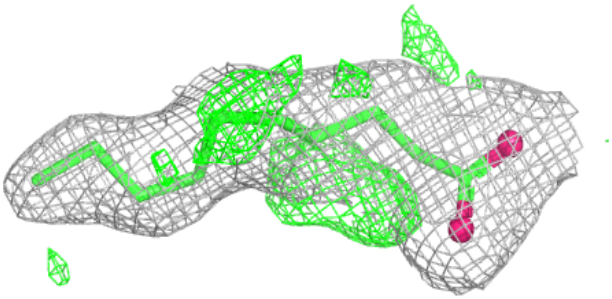


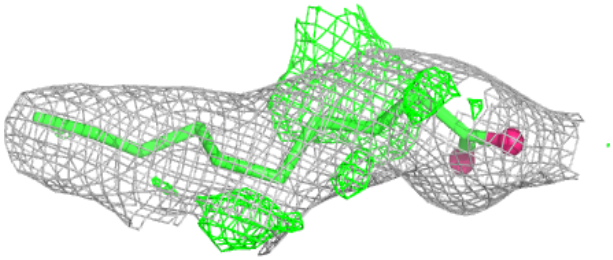


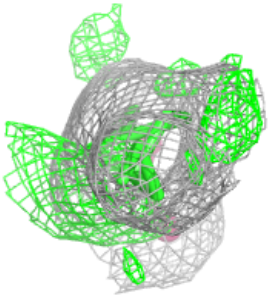


Electron density around STE B 624:

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

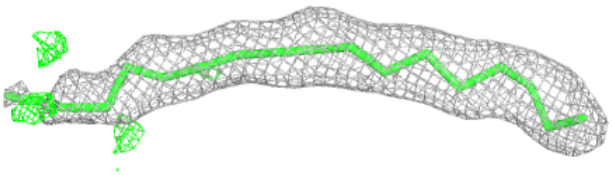


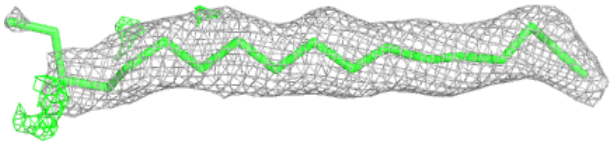


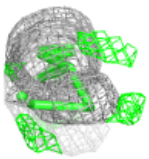


Electron density around STE l 102:

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

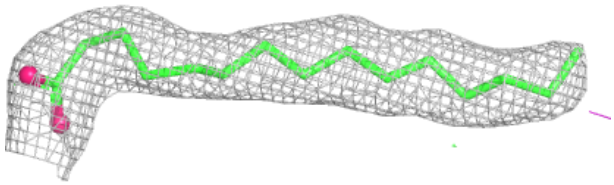


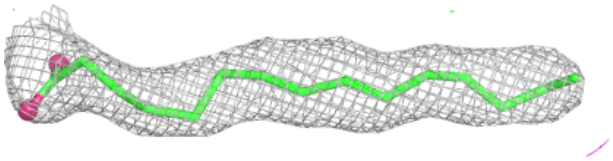


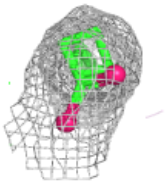


Electron density around STE d 410:

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

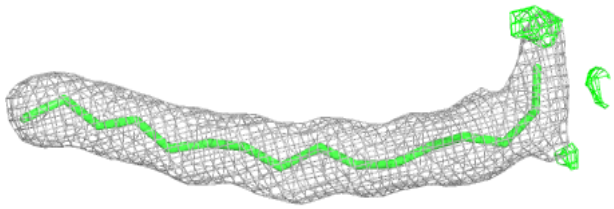


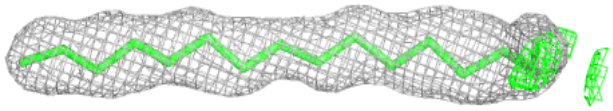


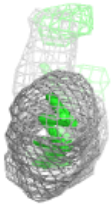


Electron density around STE C 521:

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

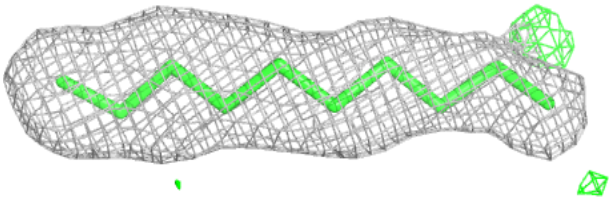


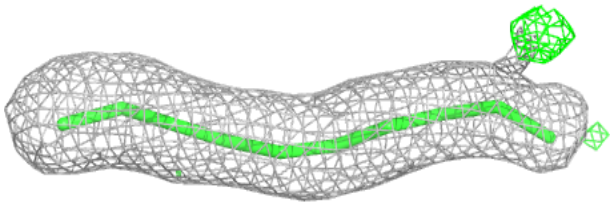


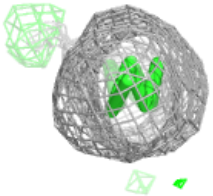


Electron density around STE M 103:

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

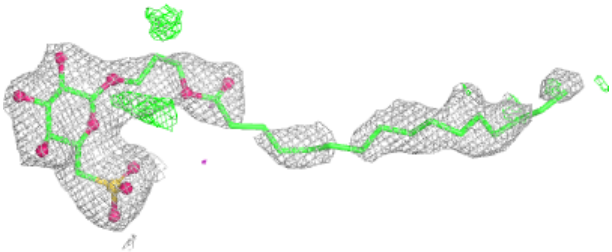


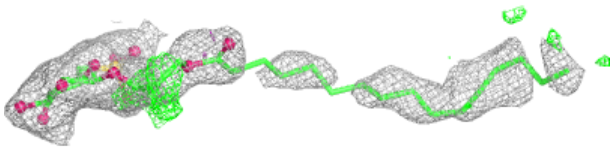


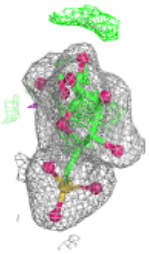


Electron density around SQD F 102:

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

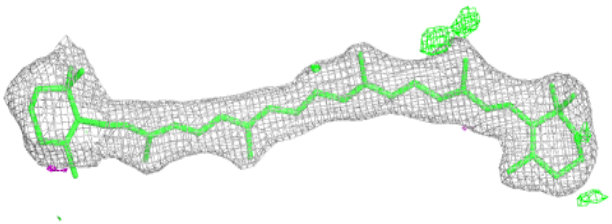


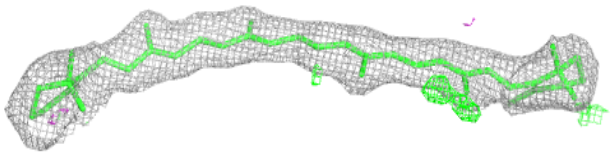


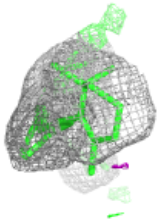


Electron density around BCR d 404:

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

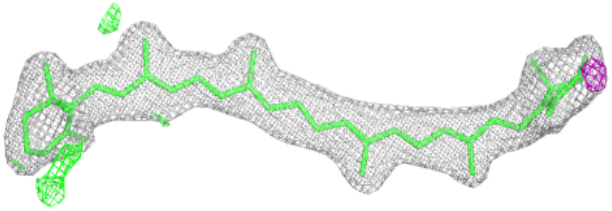


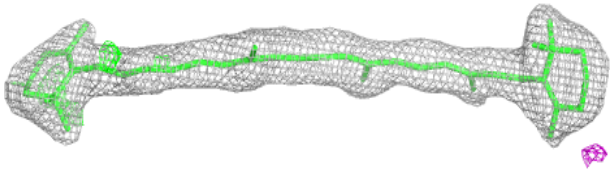


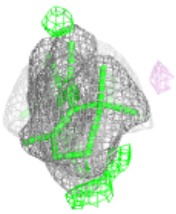


Electron density around BCR K 102:

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

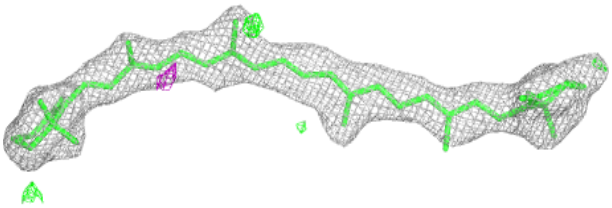


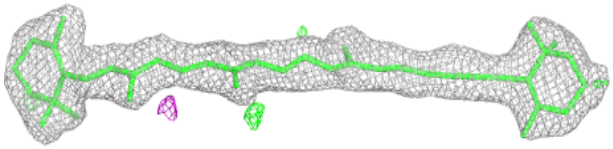


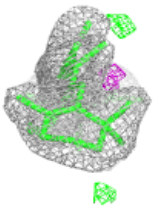


Electron density around BCR h 102:

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

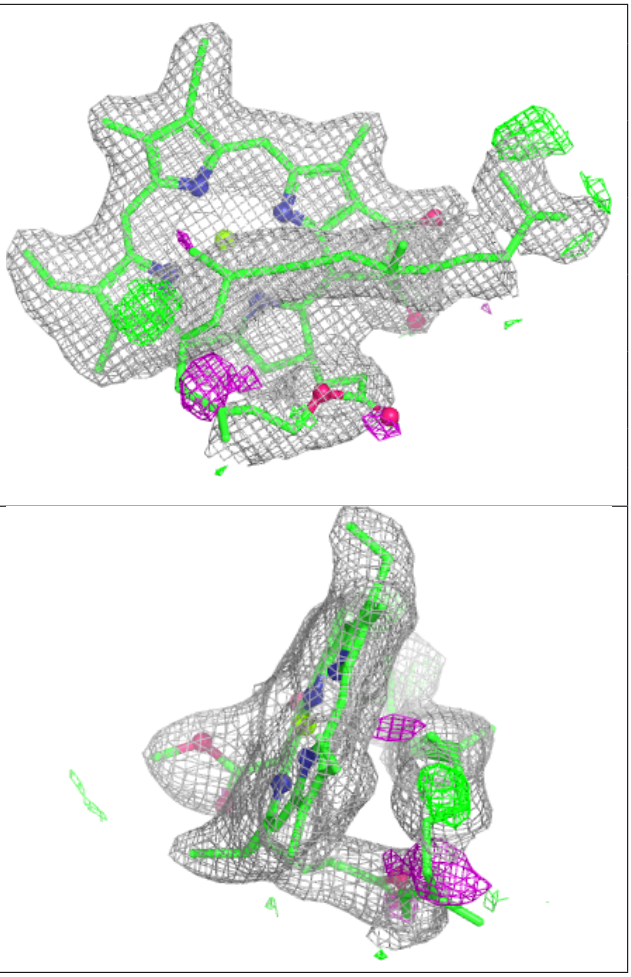


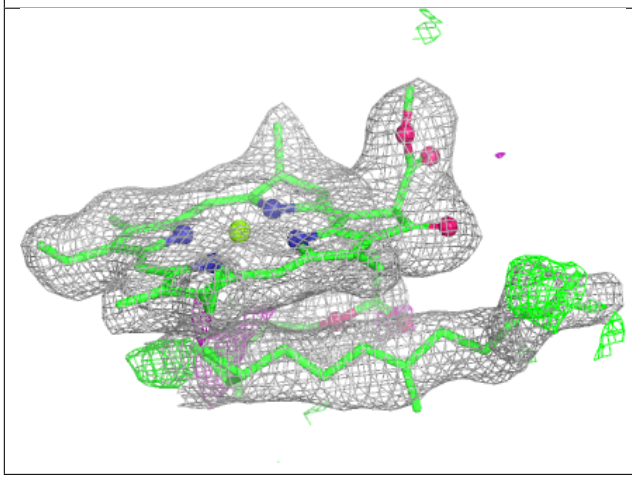




Electron density around CLA B 601:

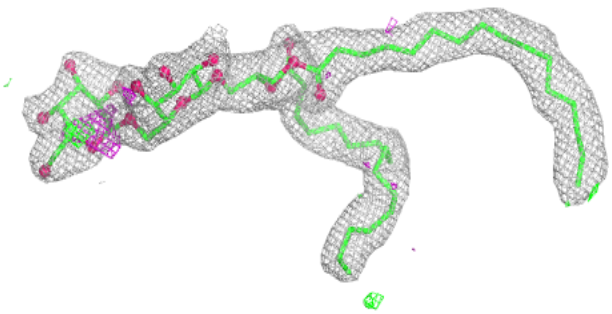
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

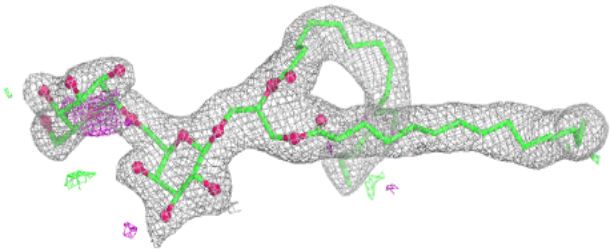


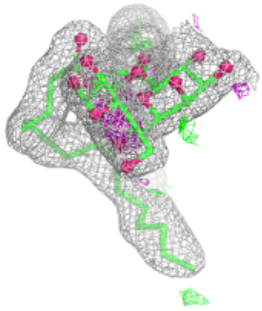


Electron density around DGD H 102:

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

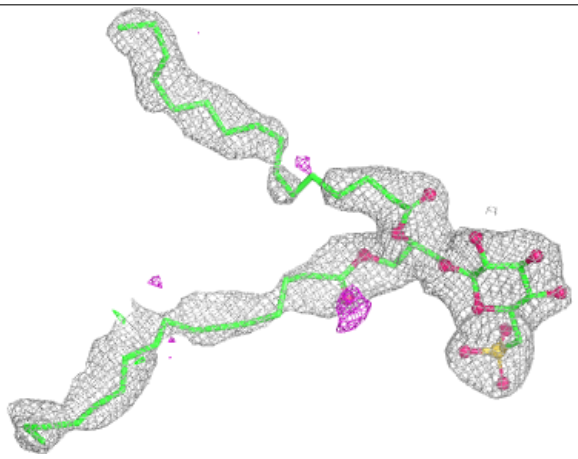


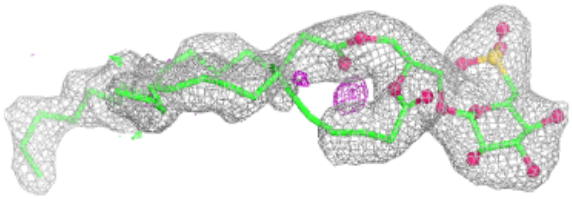


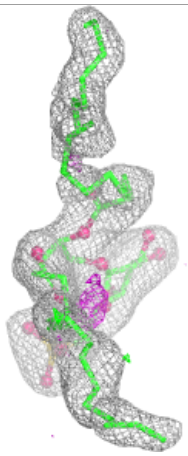


Electron density around SQD a 615:

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

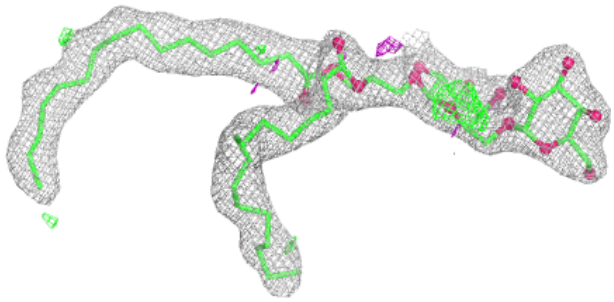


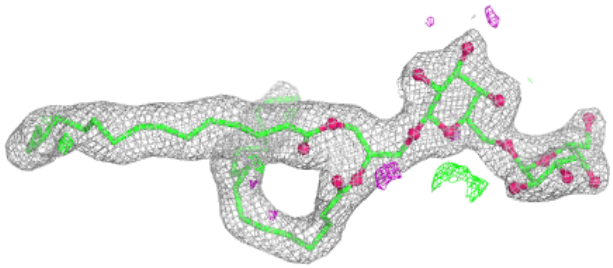


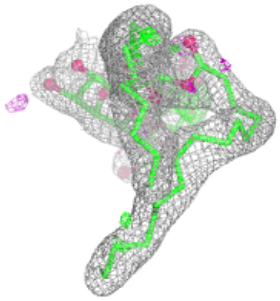


Electron density around DGD h 103:

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

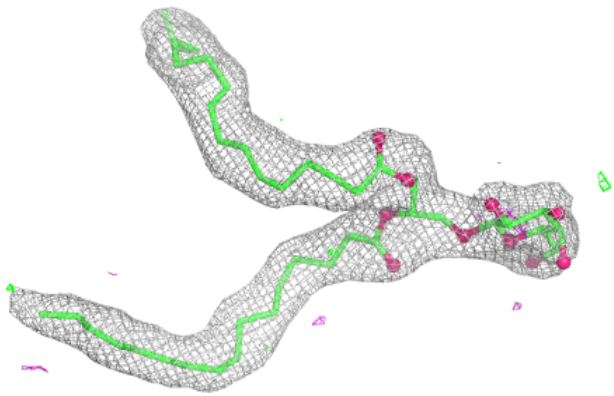


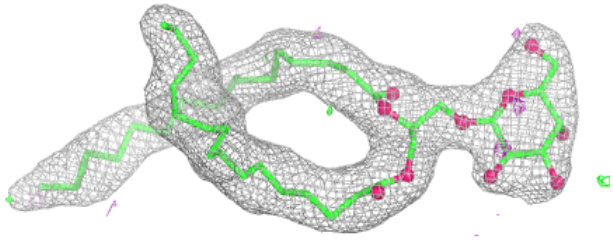


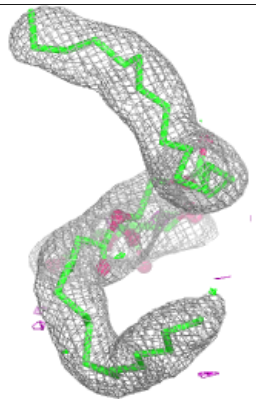


Electron density around LMG M 101:

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

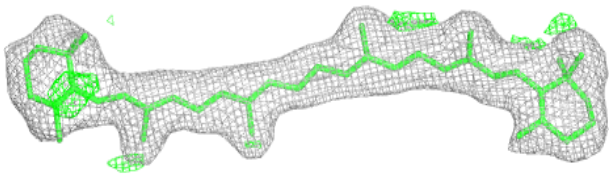


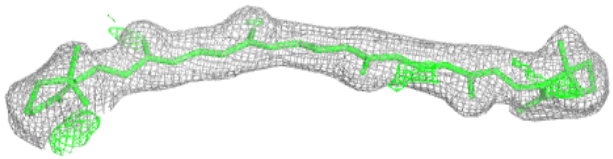


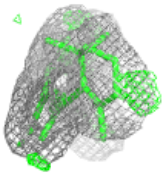


Electron density around BCR D 405:

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

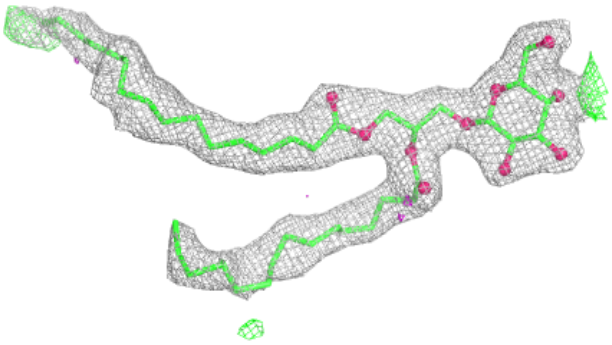


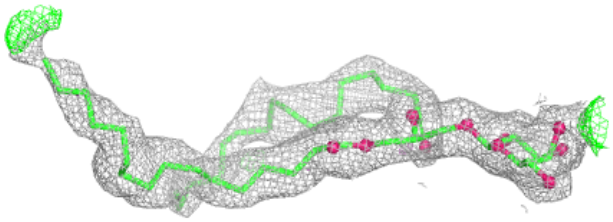


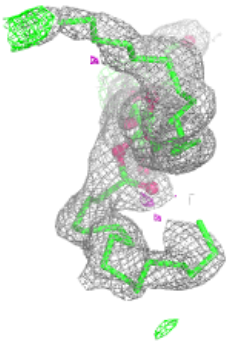


Electron density around LMG D 407:

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

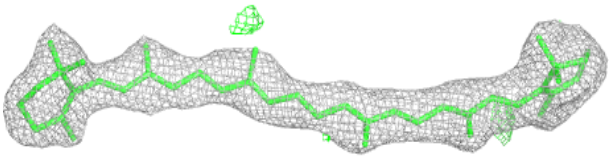


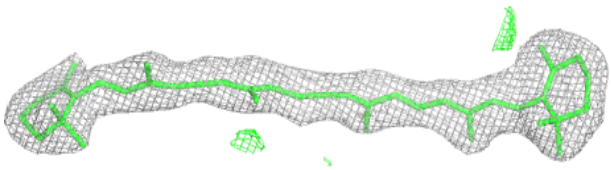


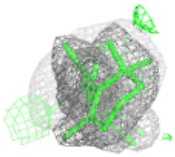


Electron density around BCR c 514:

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

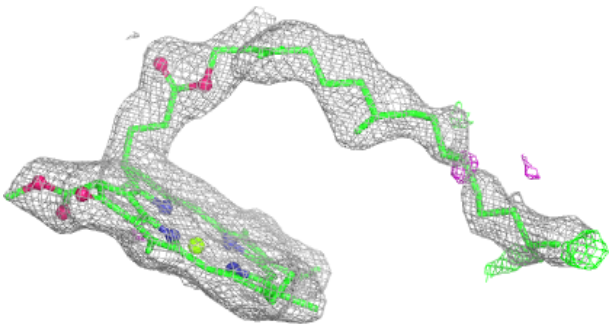


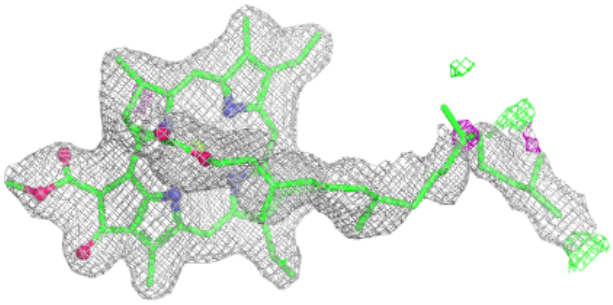


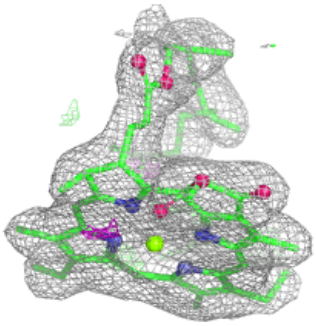


Electron density around CLA C 513:

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

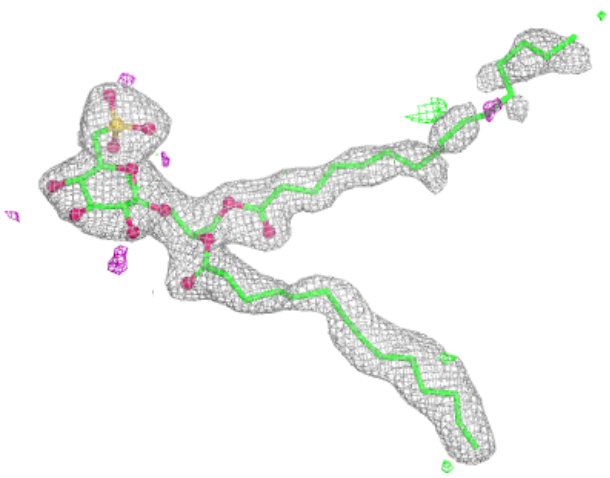


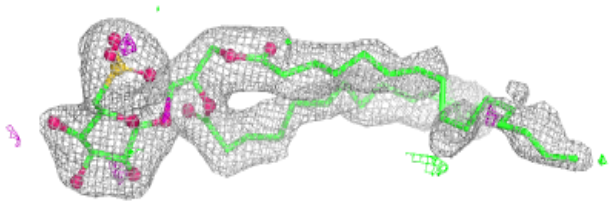


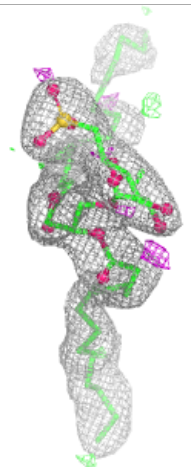


Electron density around SQD A 615:

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

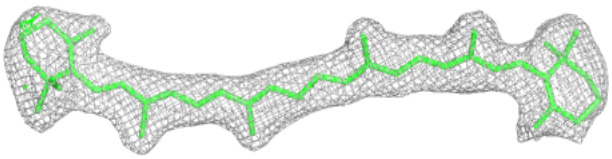


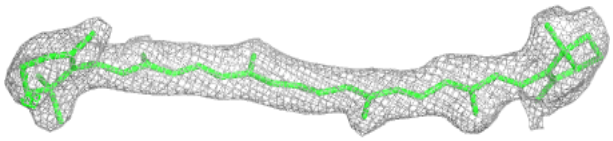


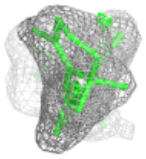


Electron density around BCR b 618:

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

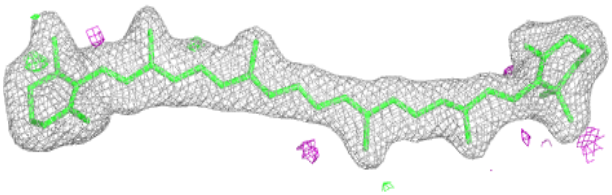


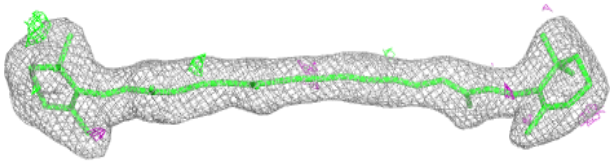


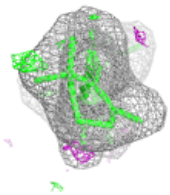


Electron density around BCR B 618:

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

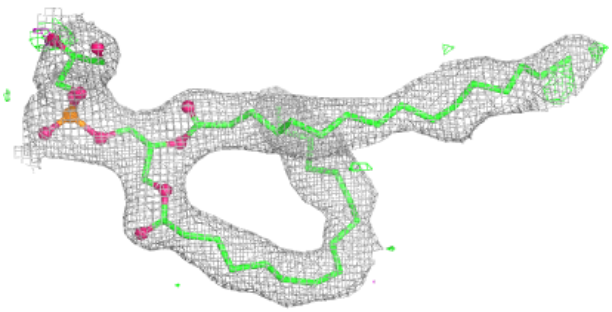


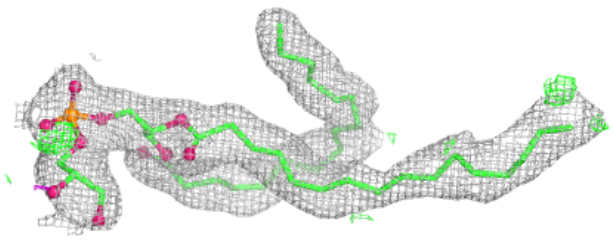


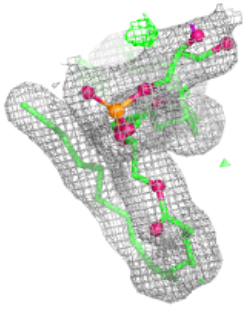


Electron density around LHG a 614:

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

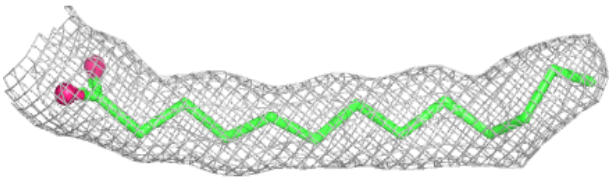


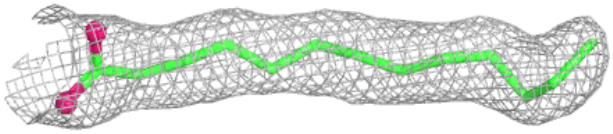


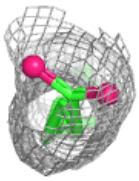


Electron density around STE M 102:

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

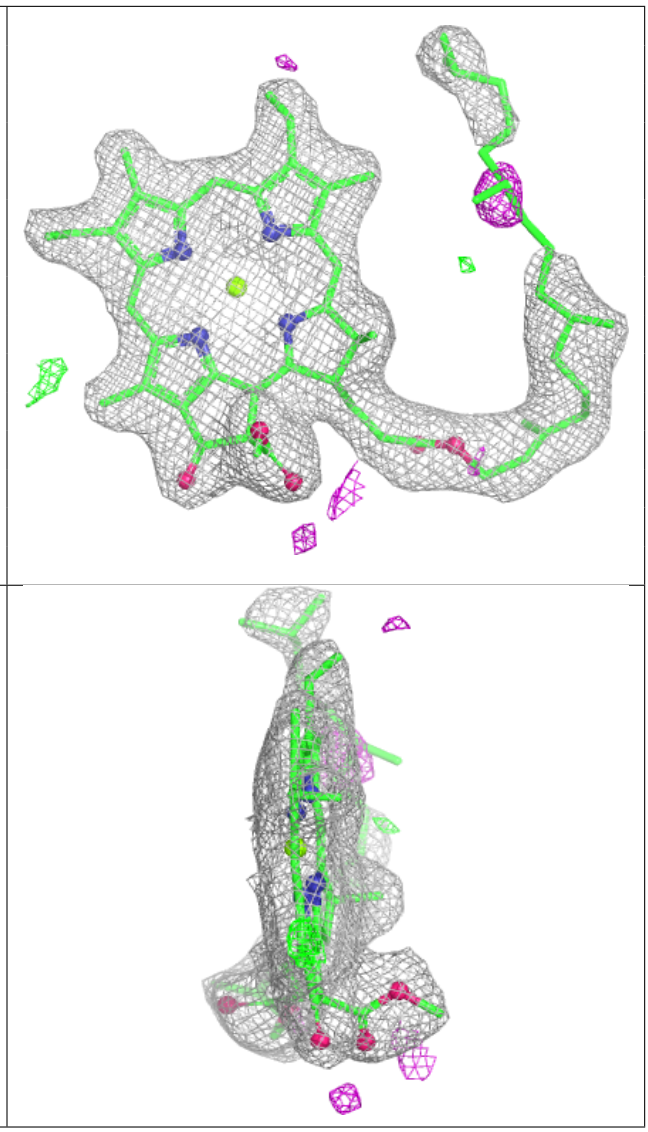






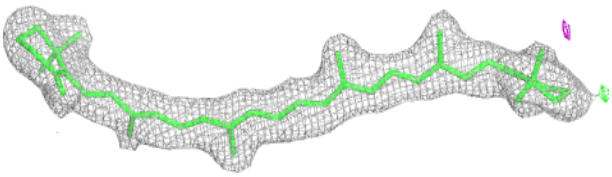
Electron density around CLA c 512:

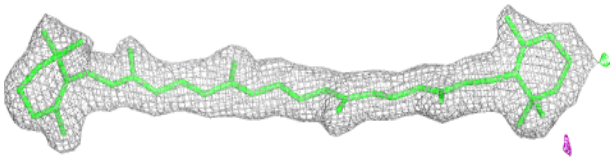
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

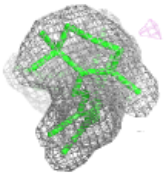


Electron density around BCR H 101:

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

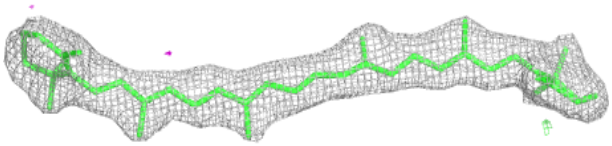


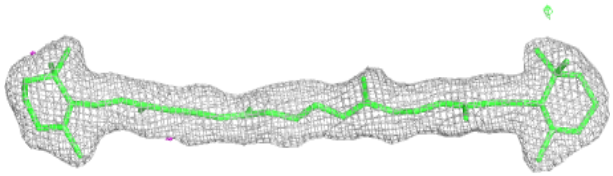


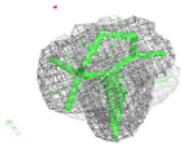


Electron density around BCR K 101:

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

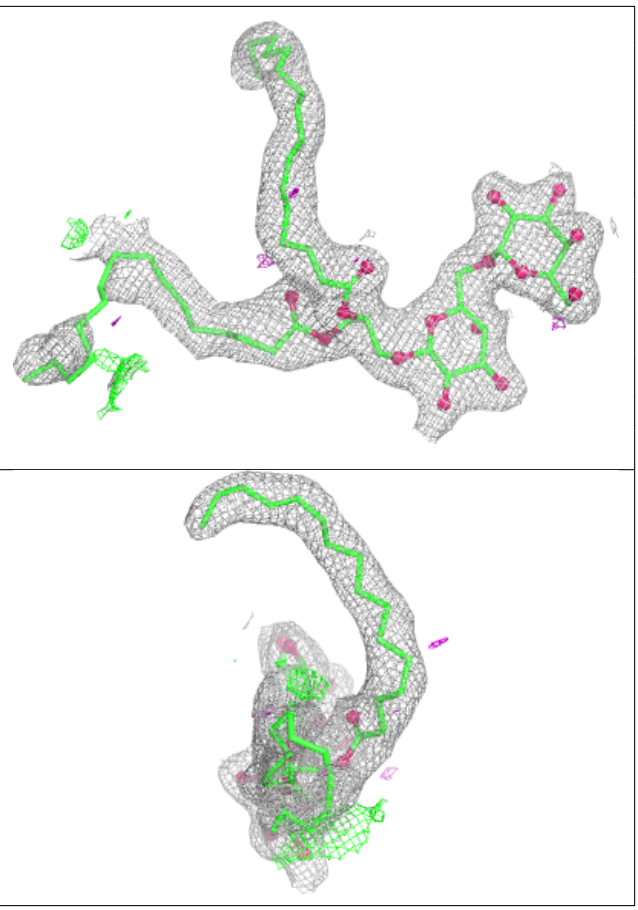






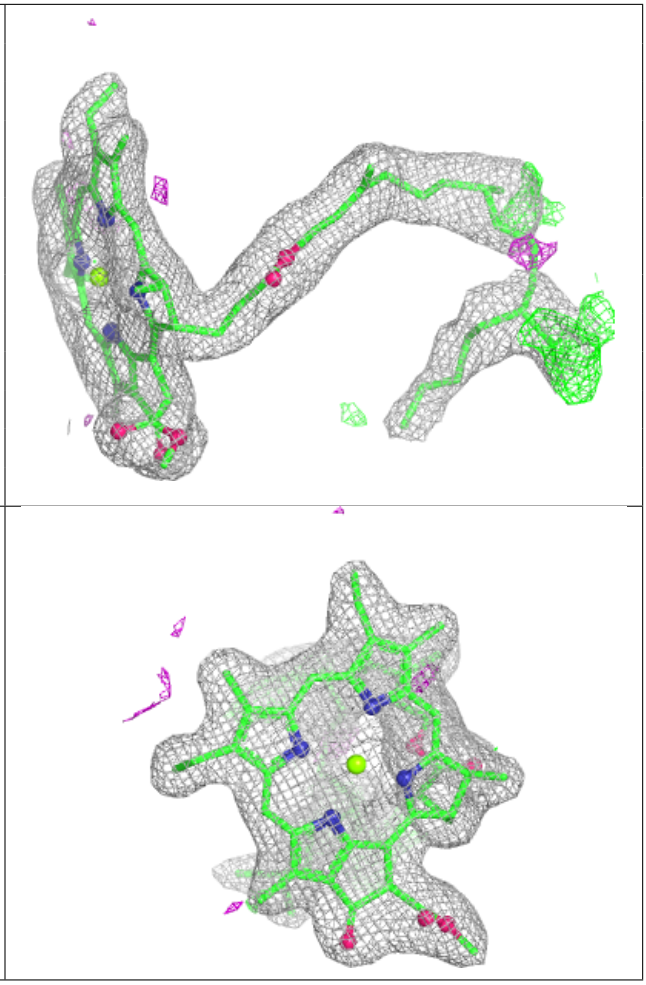
Electron density around DGD C 516:

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



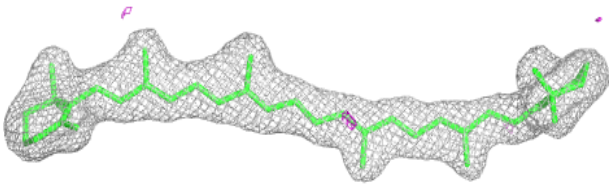
Electron density around CLA B 606:

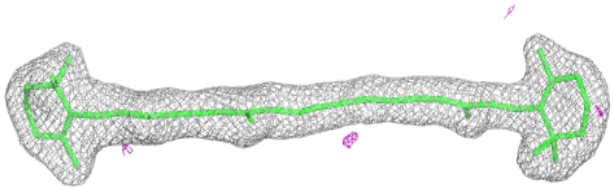
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

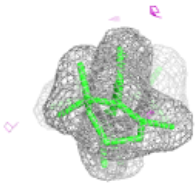


Electron density around BCR A 610:

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

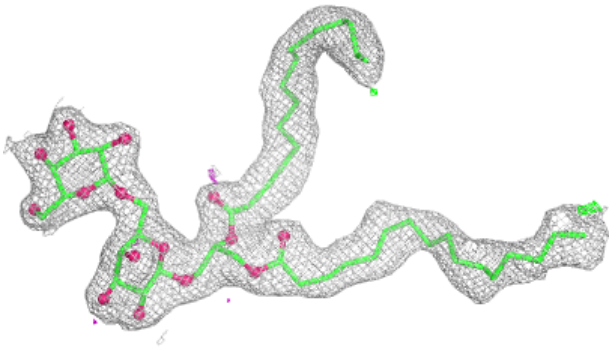


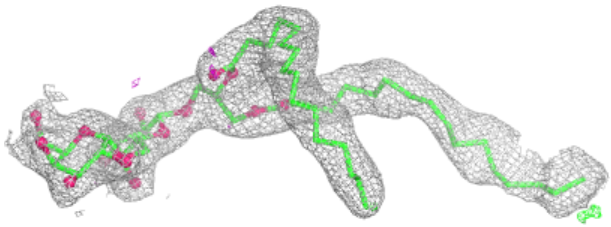


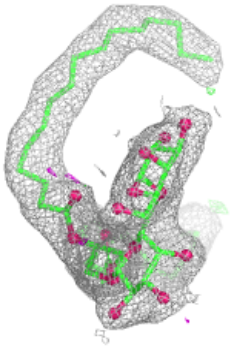


Electron density around DGD c 517:

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

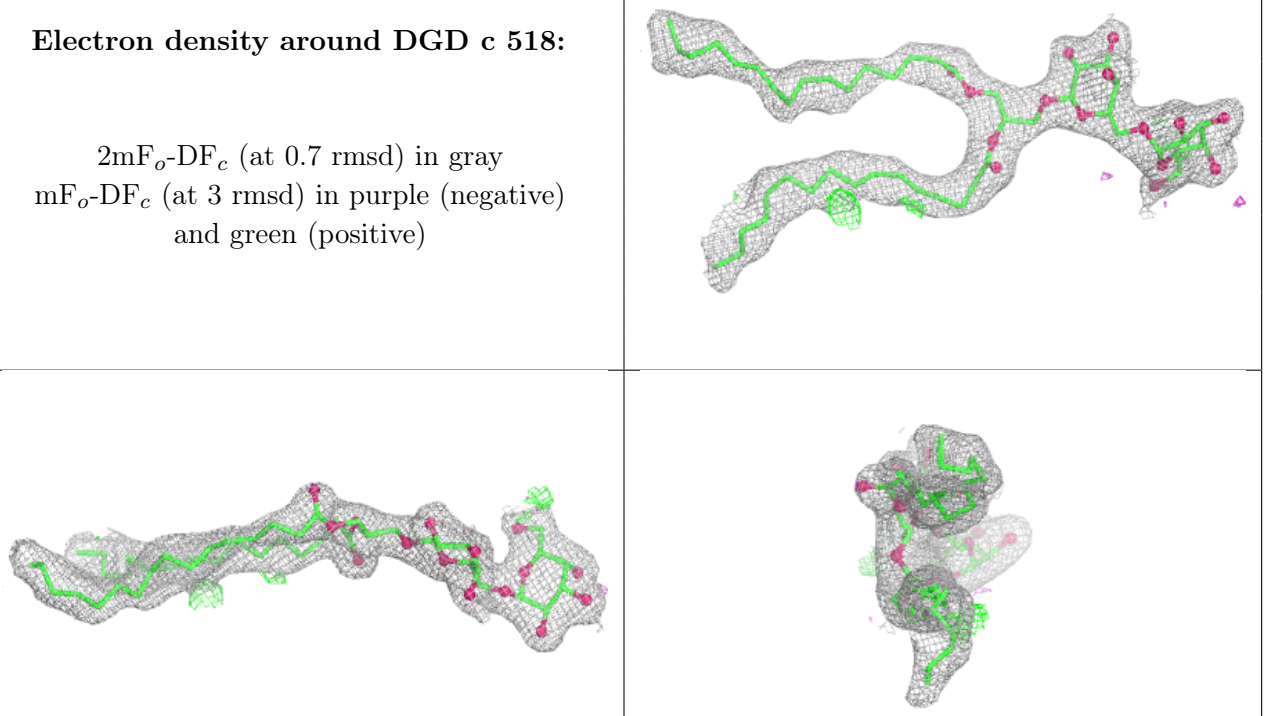






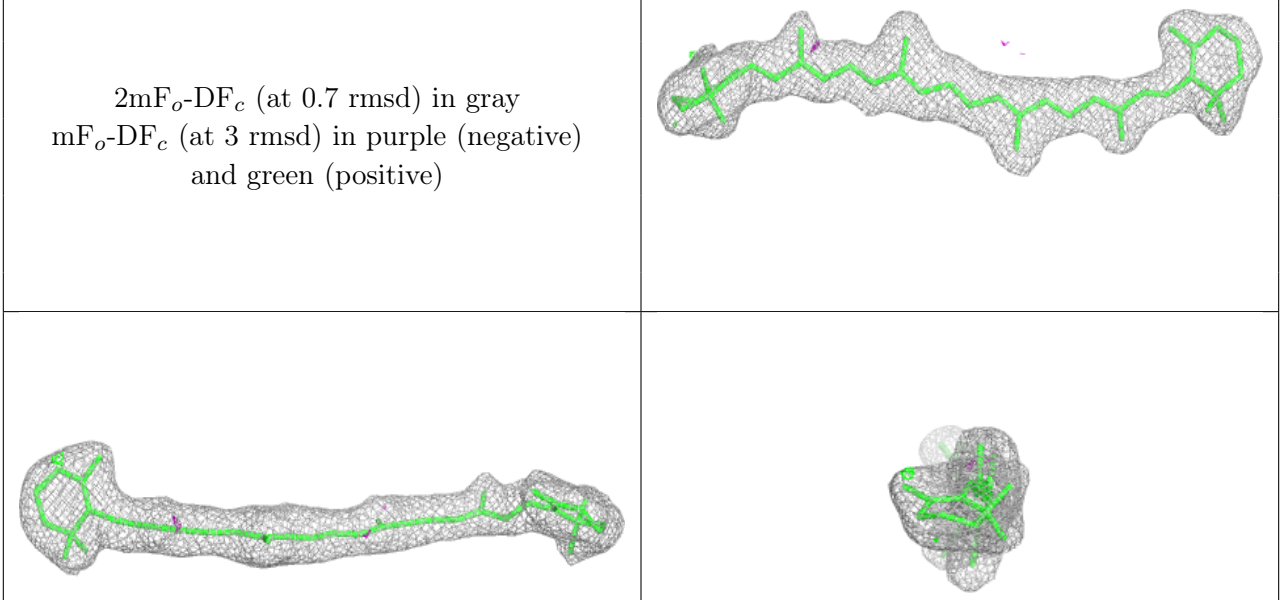
Electron density around DGD c 518:

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



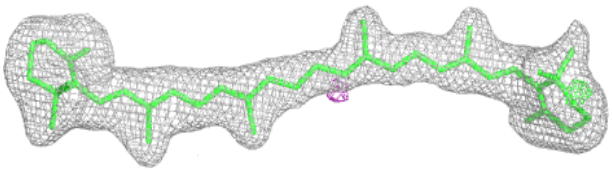
Electron density around BCR b 616:

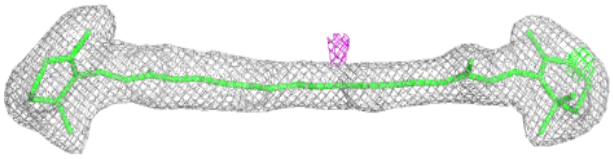
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

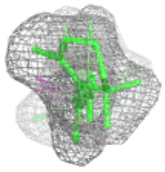


Electron density around BCR b 617:

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

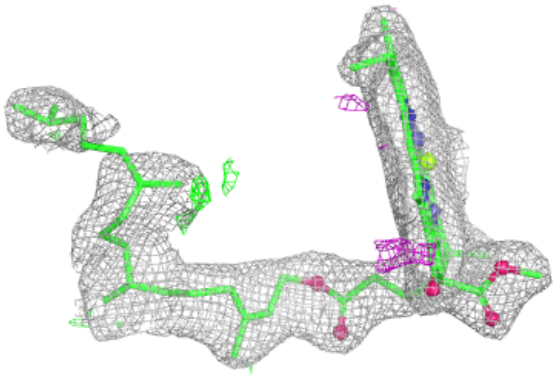


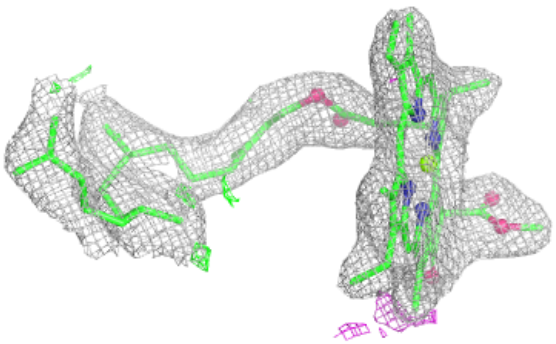


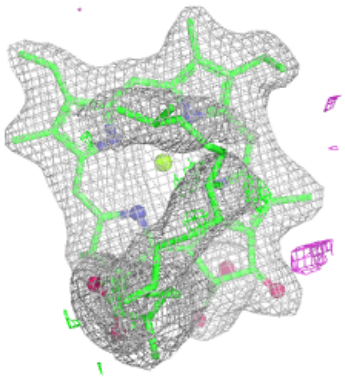


Electron density around CLA c 506:

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

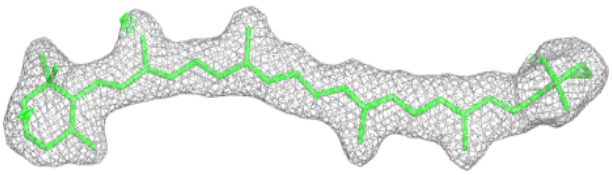


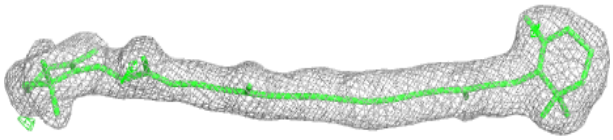


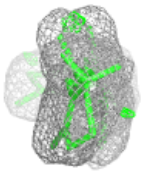


Electron density around BCR B 617:

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

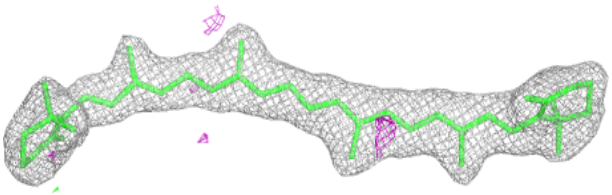


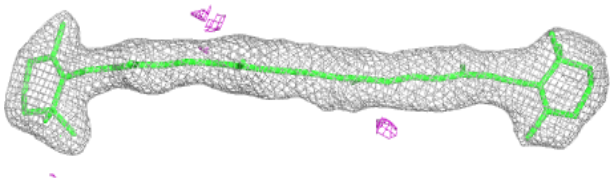


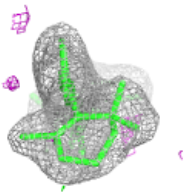


Electron density around BCR c 515:

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

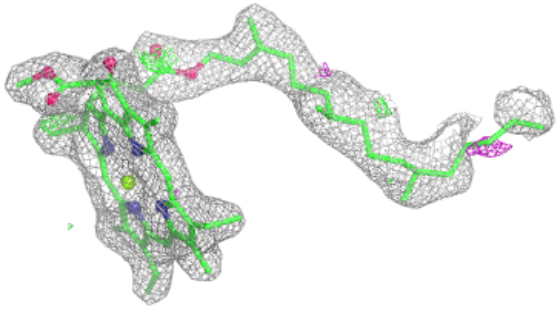


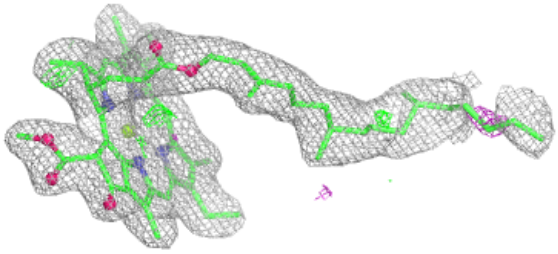


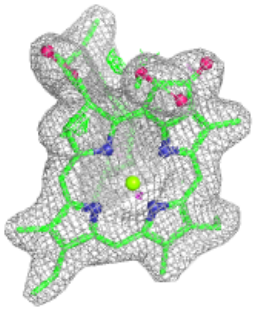


Electron density around CLA c 508:

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

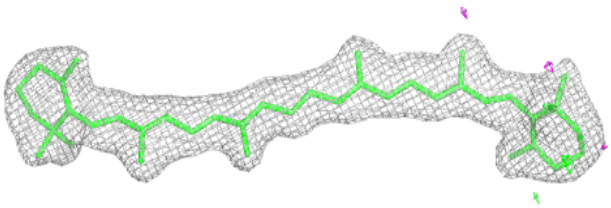


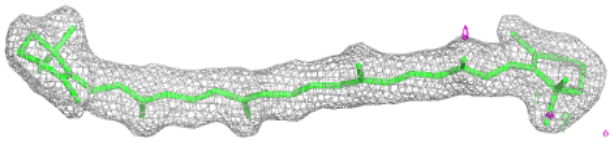


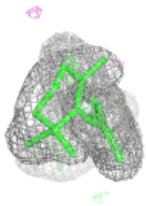


Electron density around BCR B 619:

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

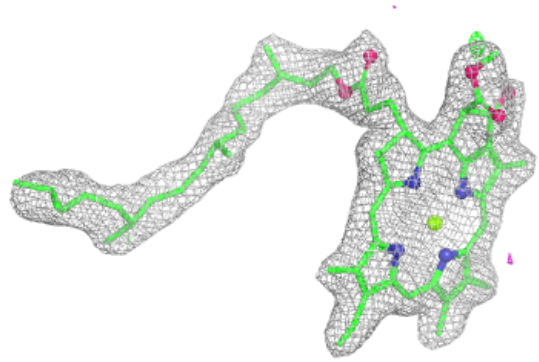


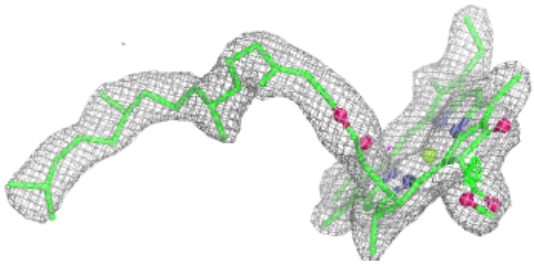


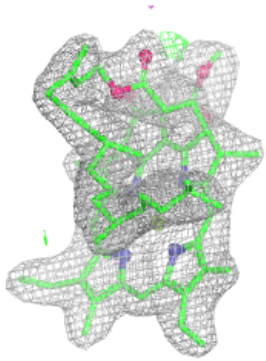


Electron density around CLA c 511:

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

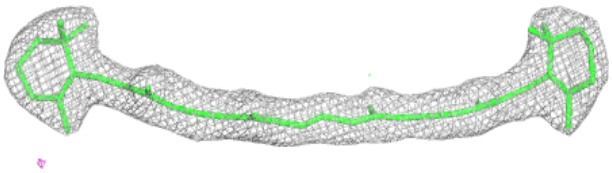


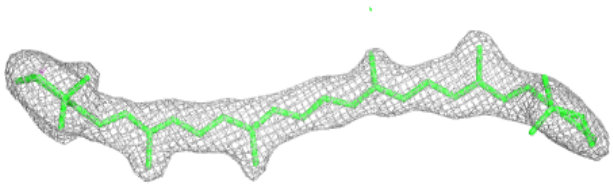


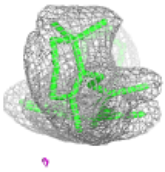


Electron density around BCR k 102:

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

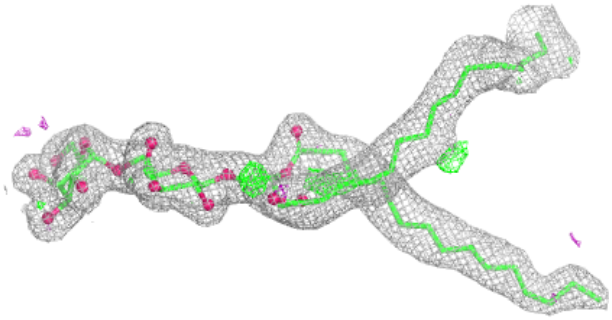


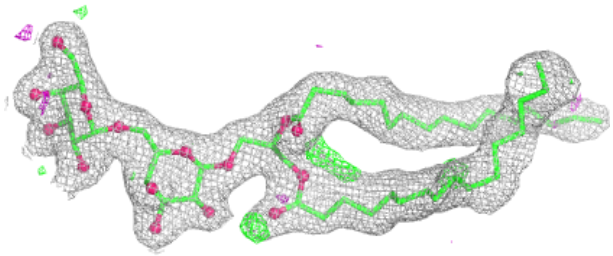


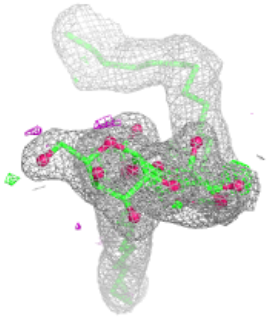


Electron density around DGD C 515:

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

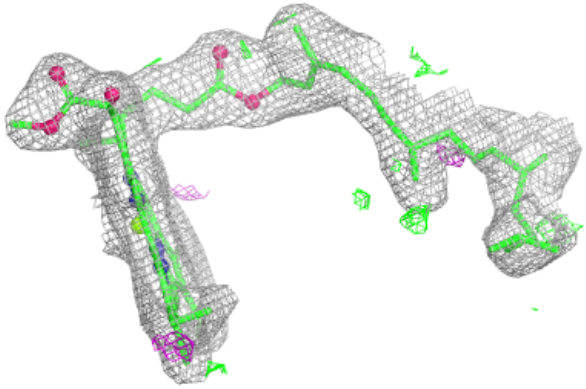


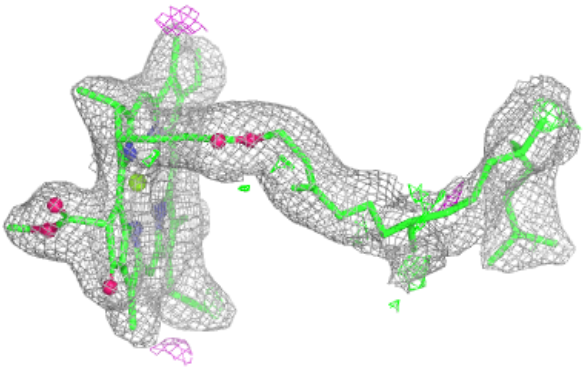


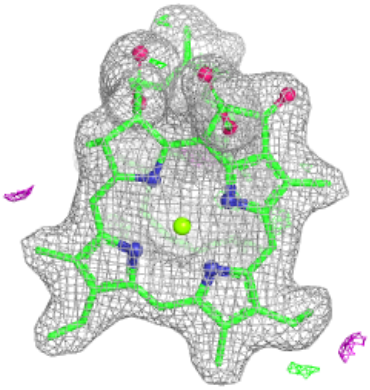


Electron density around CLA C 506:

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

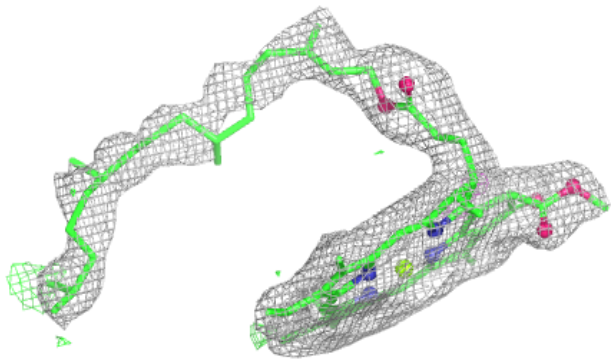


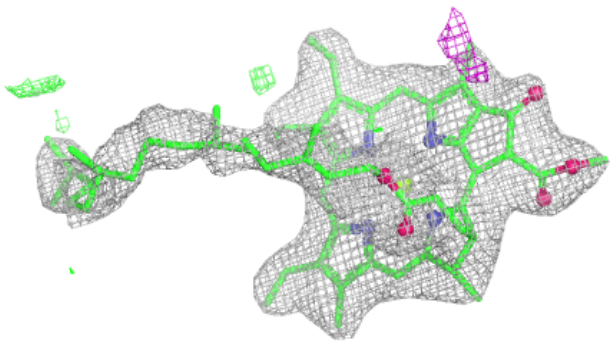


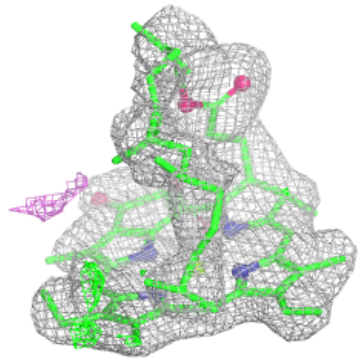


Electron density around CLA c 513:

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

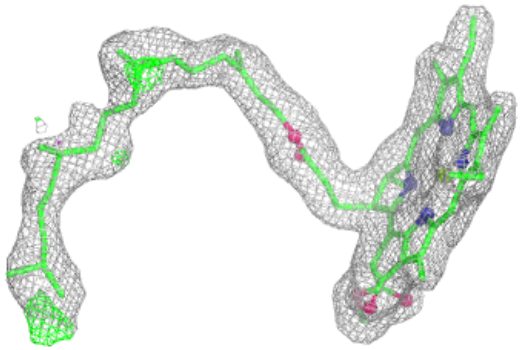


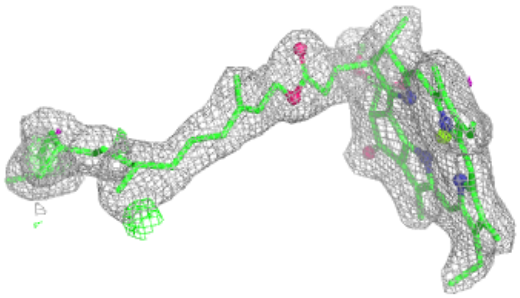


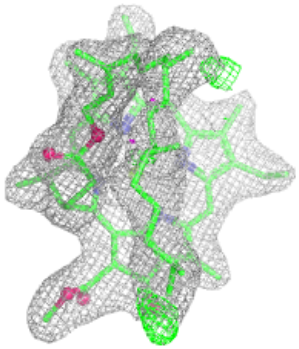


Electron density around CLA b 605:

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

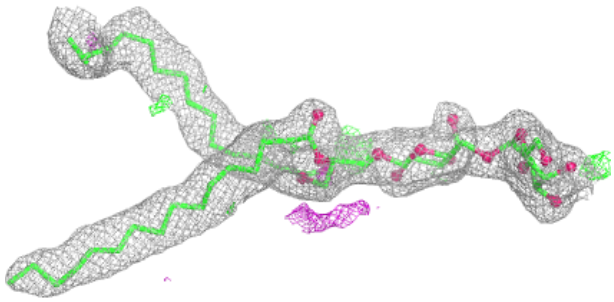


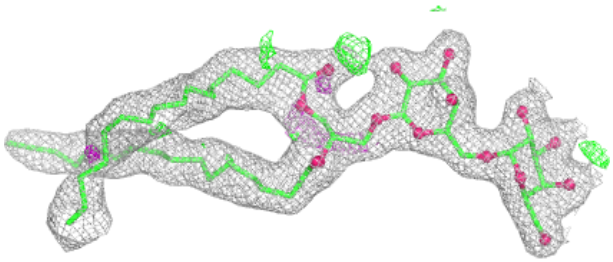


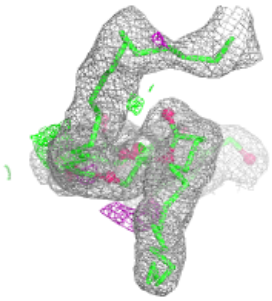


Electron density around DGD c 516:

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

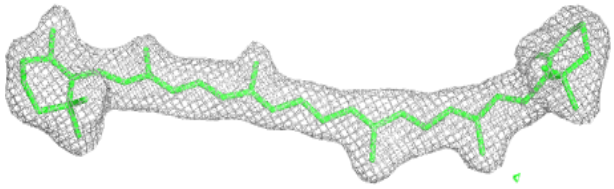


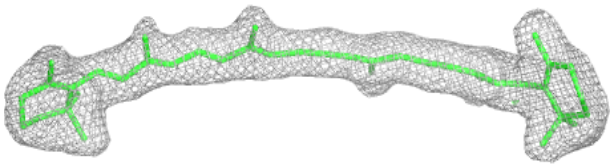


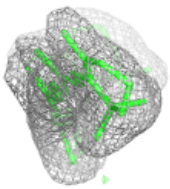


Electron density around BCR T 101:

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

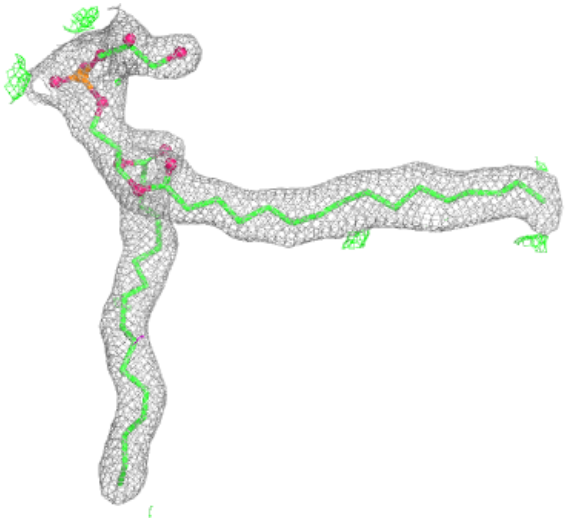


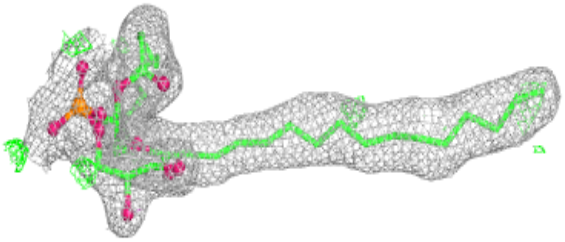


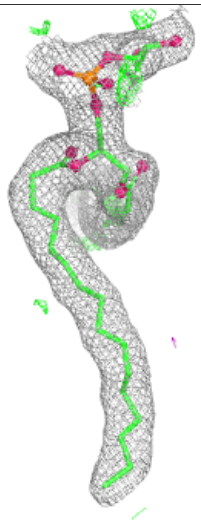


Electron density around LHG l 101:

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

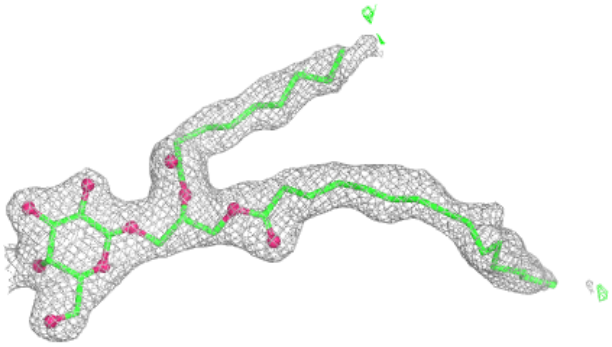


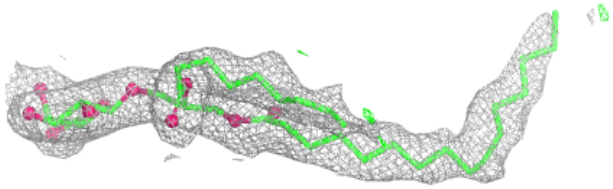


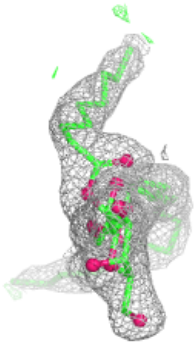


Electron density around LMG d 409:

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

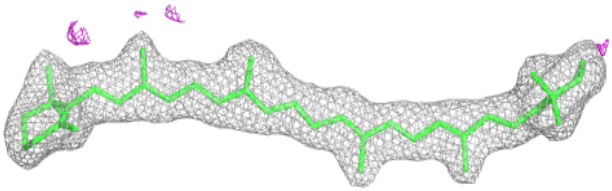


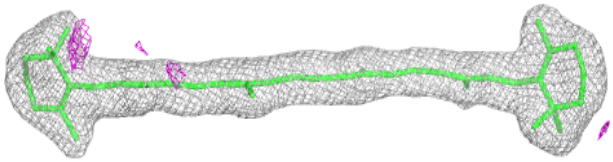


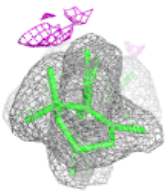


Electron density around BCR a 611:

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

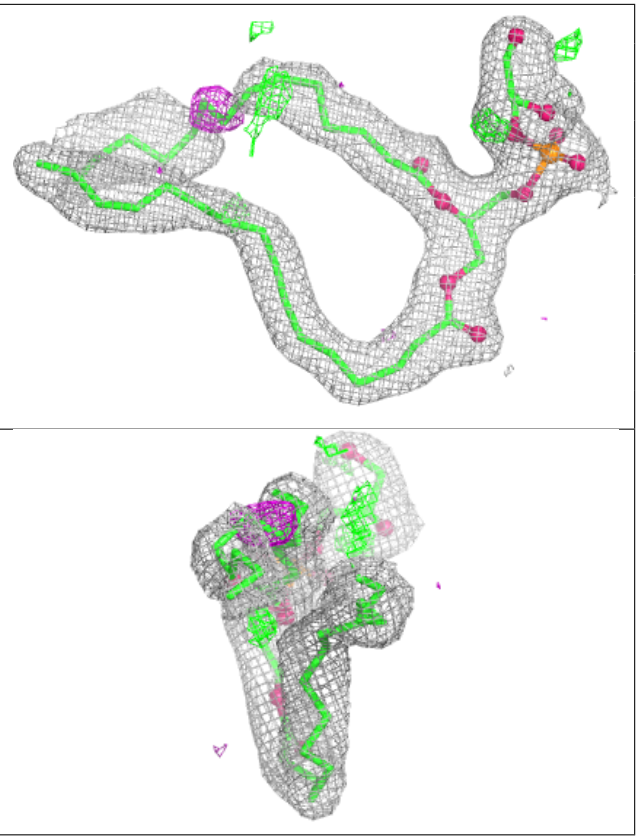


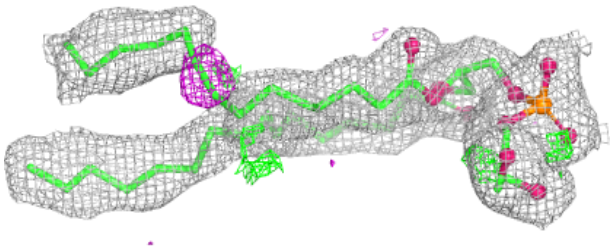




Electron density around LHG A 614:

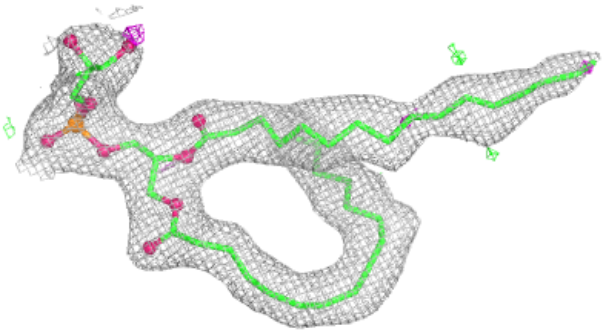
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

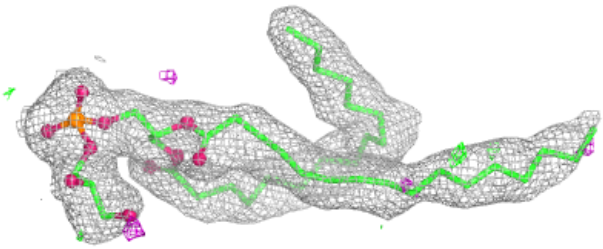


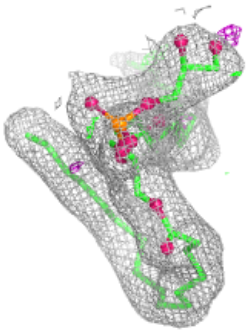


Electron density around LHG B 622:

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

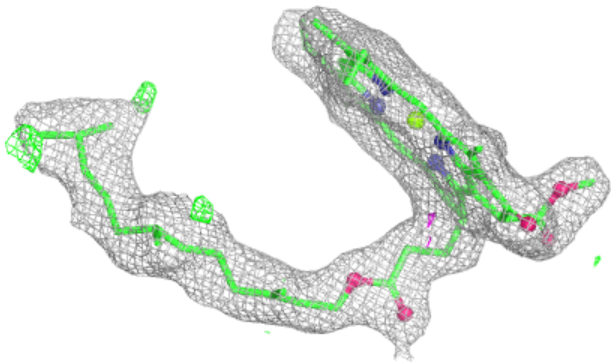


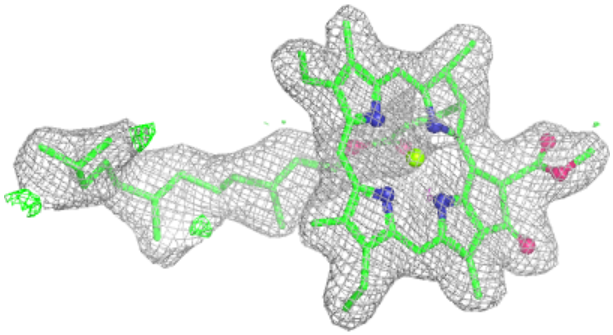


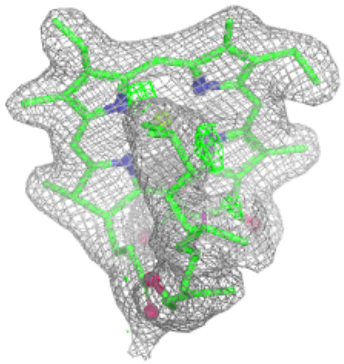


Electron density around CLA c 504:

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

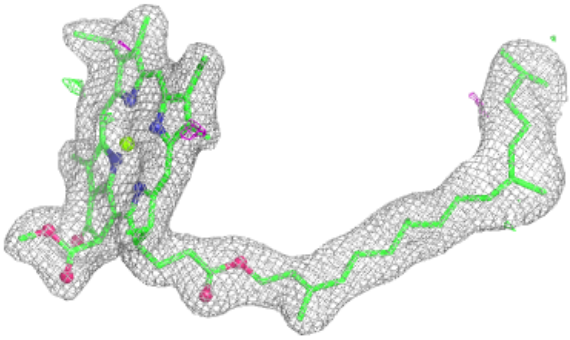


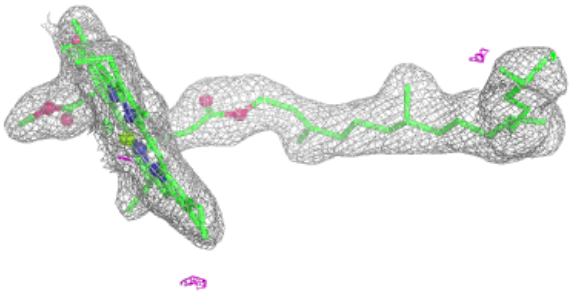


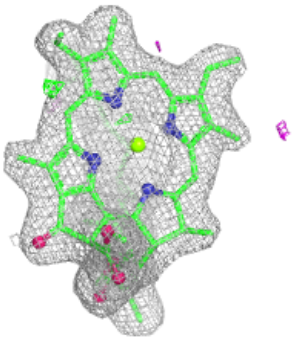


Electron density around CLA B 609:

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

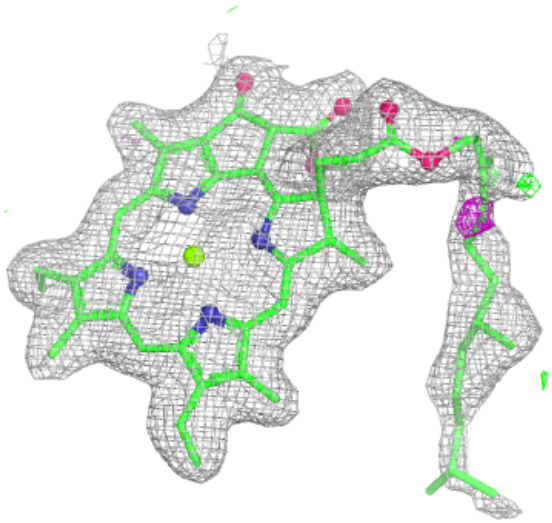


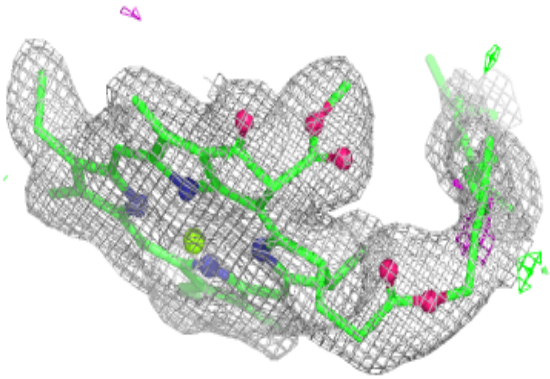


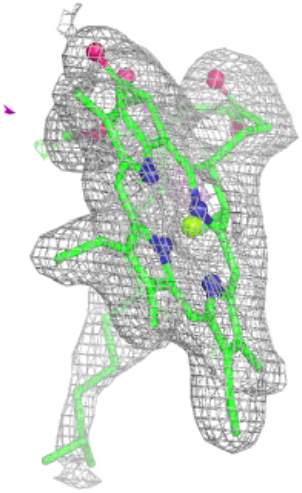


Electron density around CLA B 616:

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

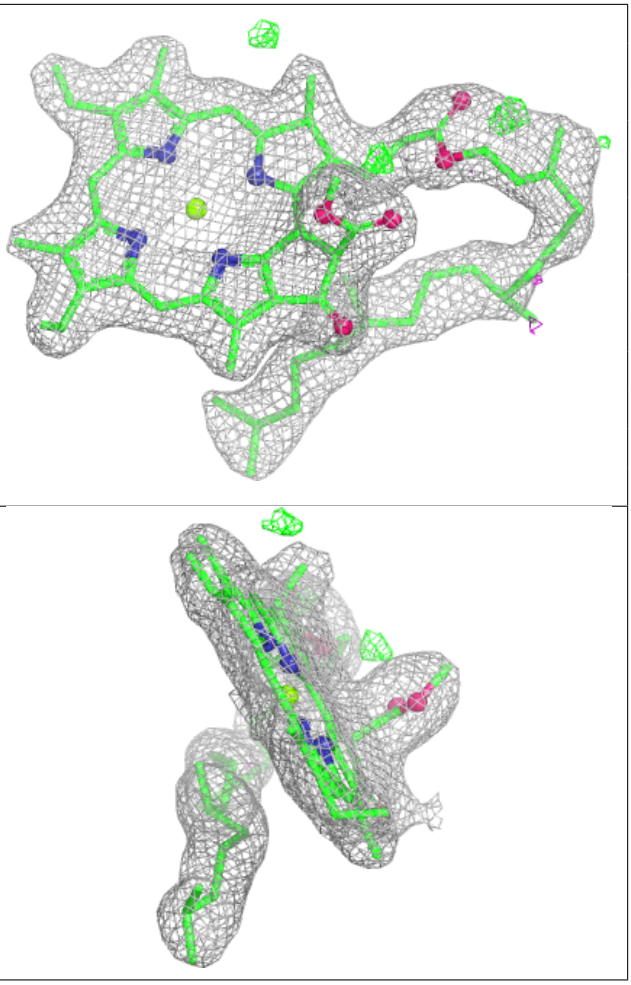






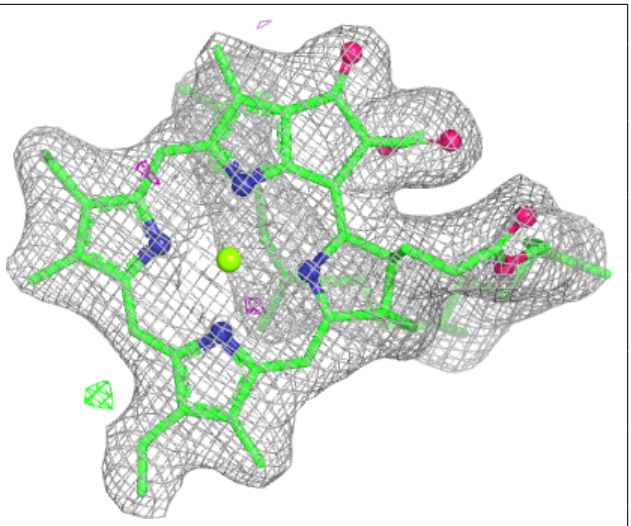
Electron density around CLA c 509:

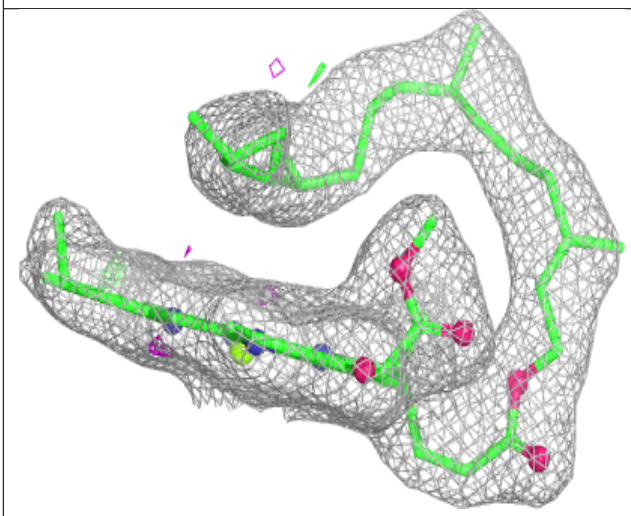
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

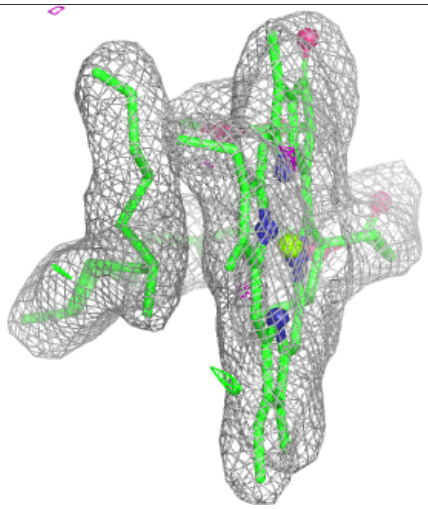


Electron density around CLA c 510:

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

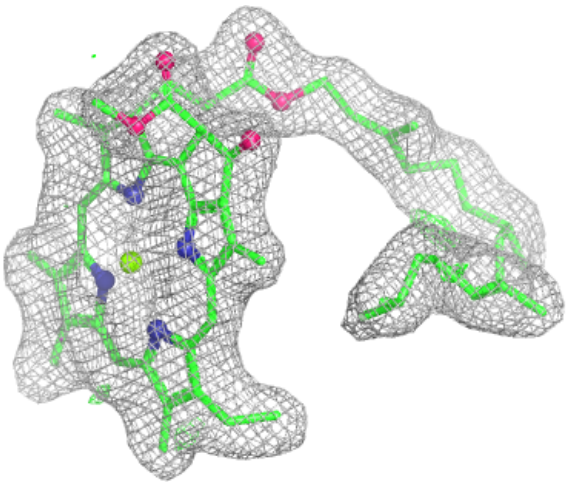


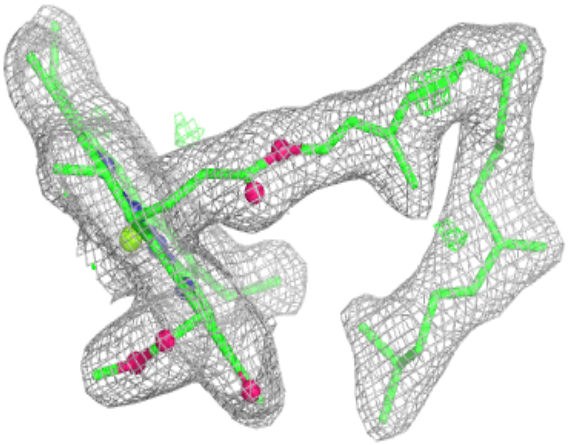


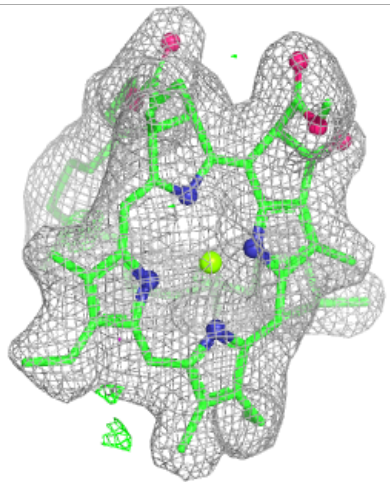


Electron density around CLA C 503:

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

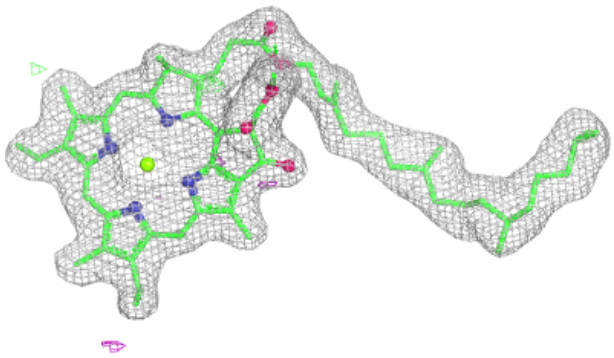


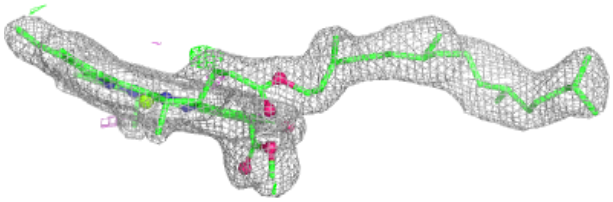


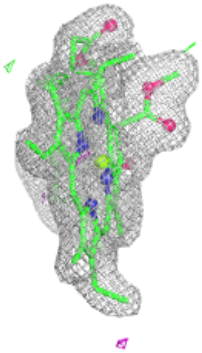


Electron density around CLA B 602:

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

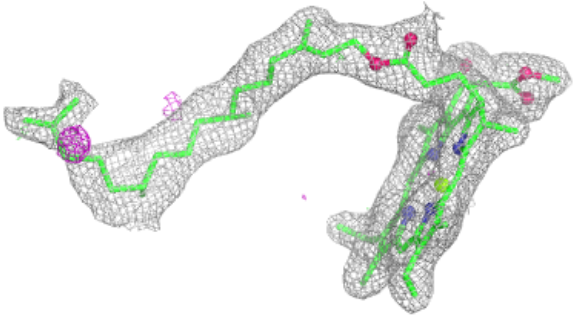


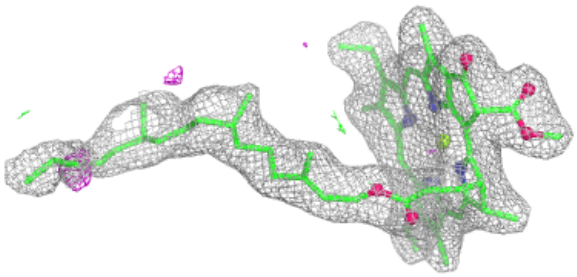


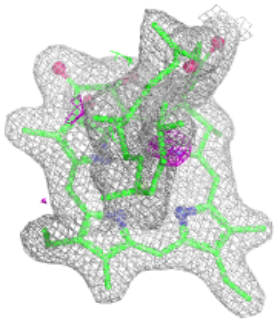


Electron density around CLA C 508:

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

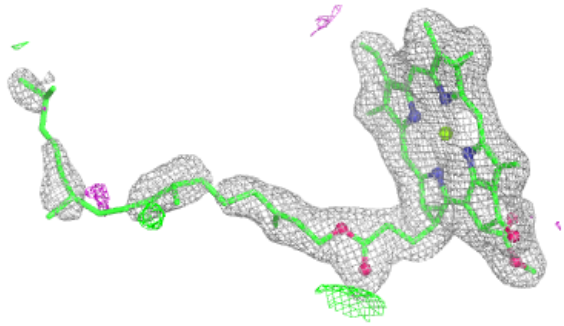


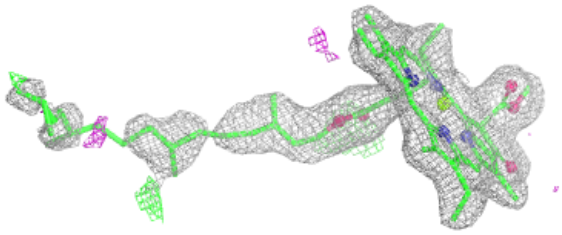


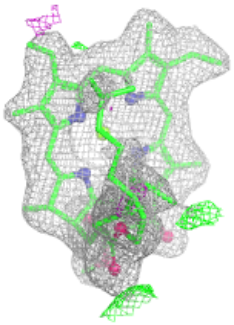


Electron density around CLA d 403:

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

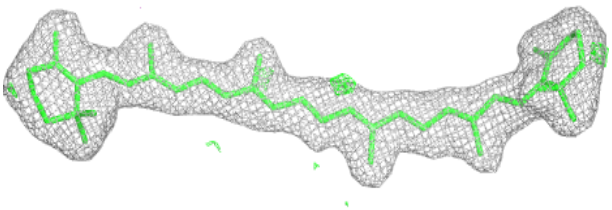


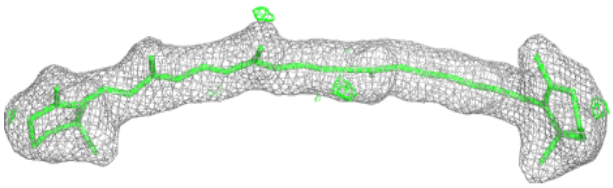


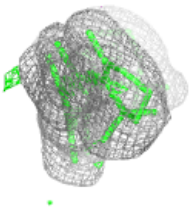


Electron density around BCR t 101:

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

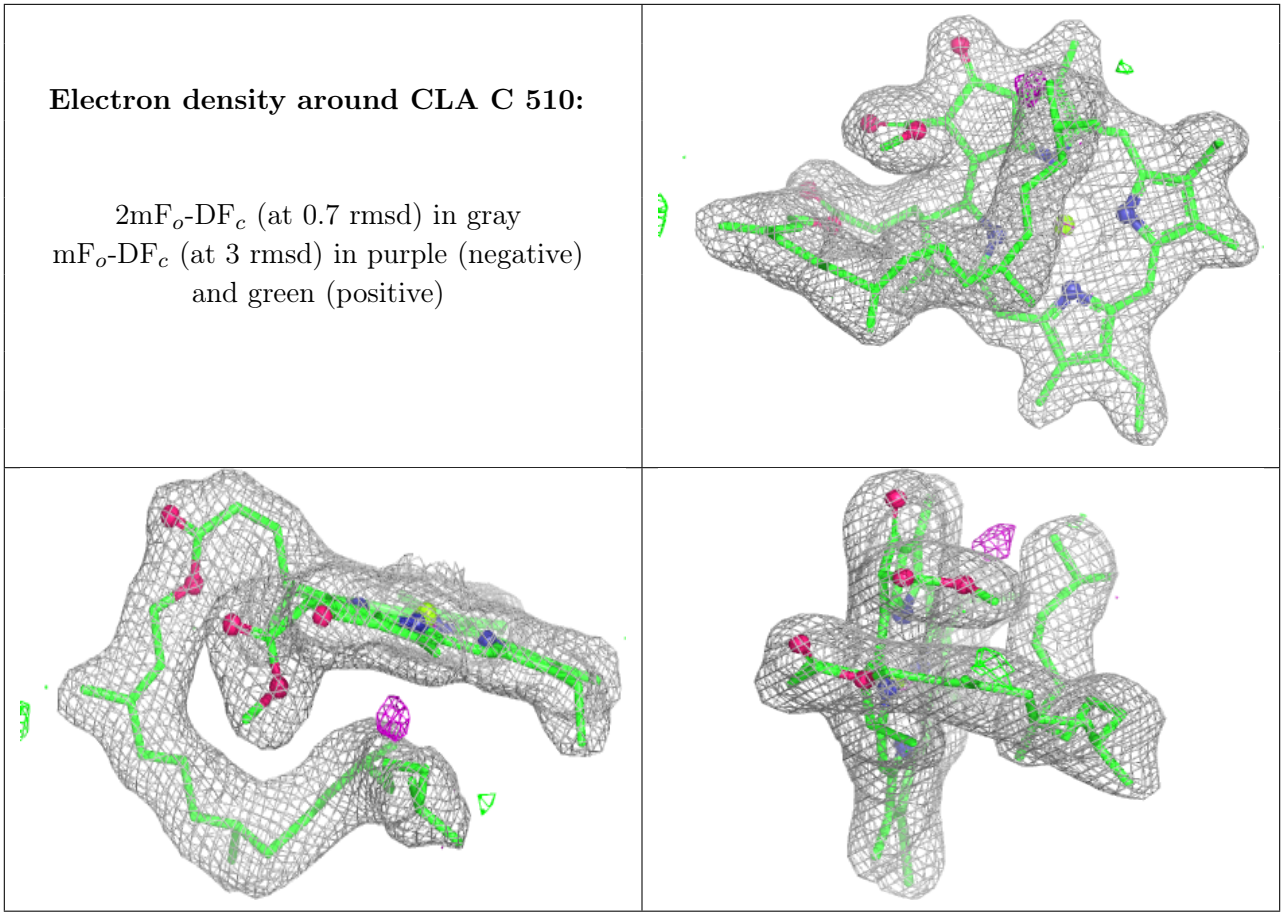






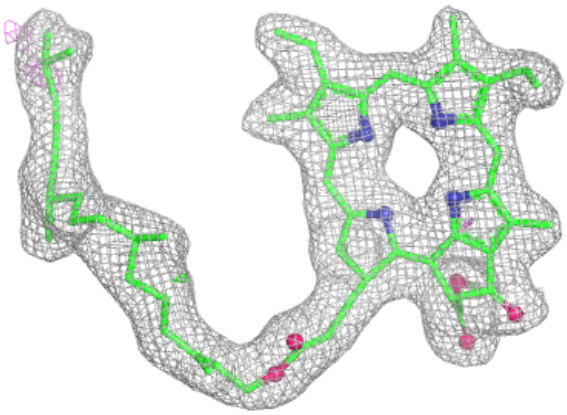
Electron density around CLA C 510:

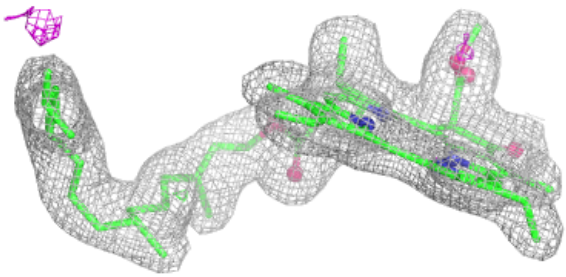
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

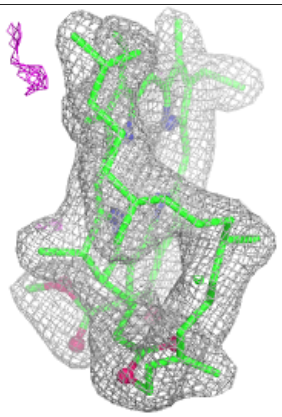


Electron density around PHO d 401:

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

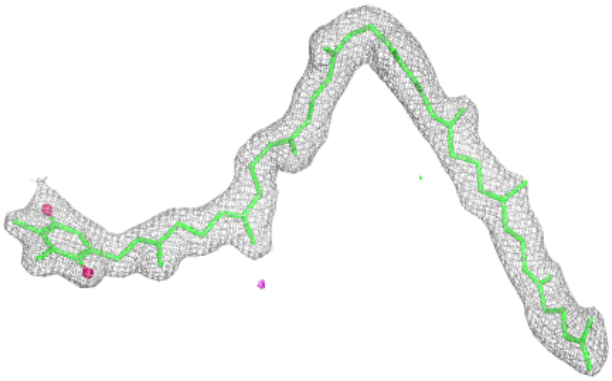


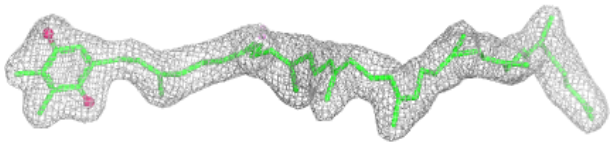


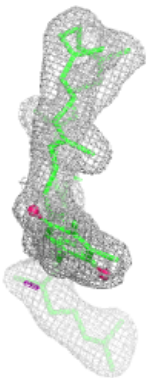


Electron density around PL9 d 405:

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

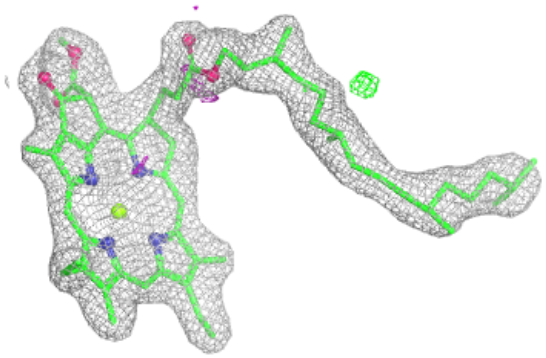


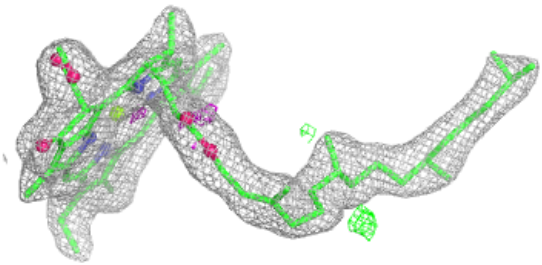


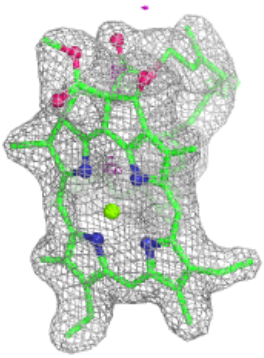


Electron density around CLA C 511:

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

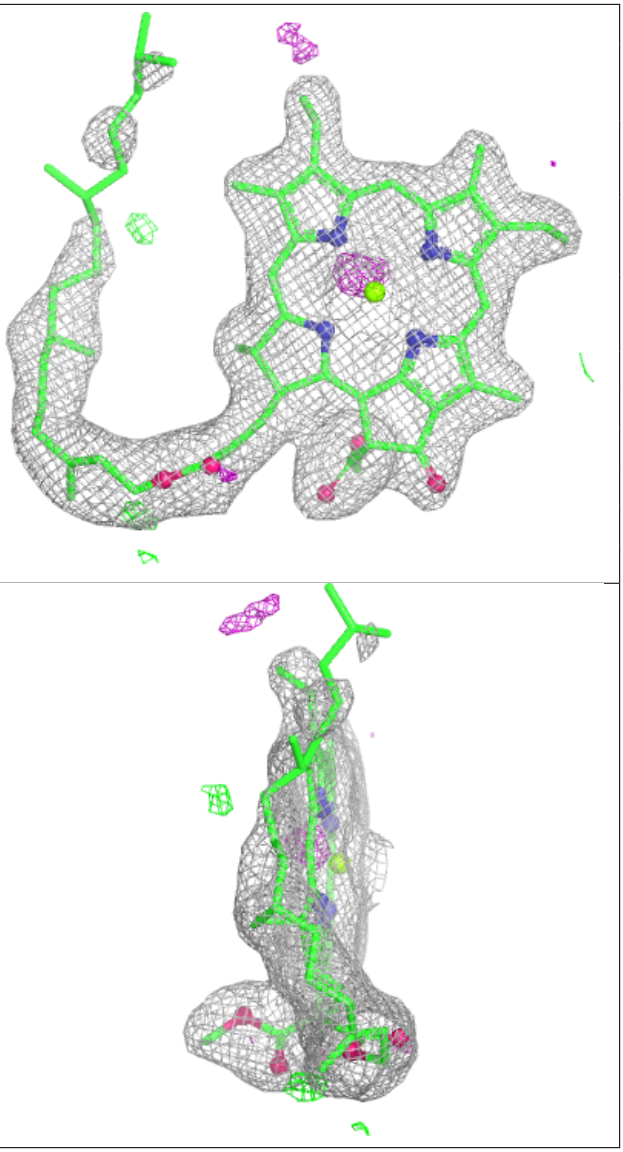






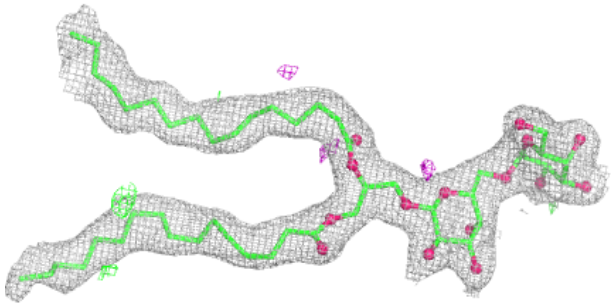
Electron density around CLA C 512:

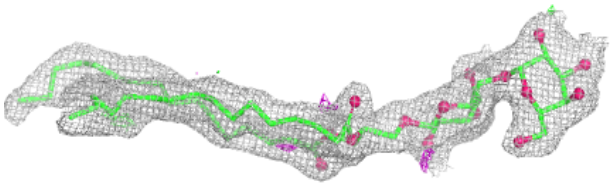
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

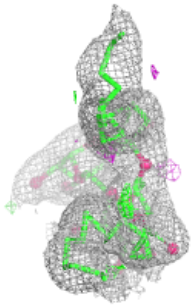


Electron density around DGD C 517:

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

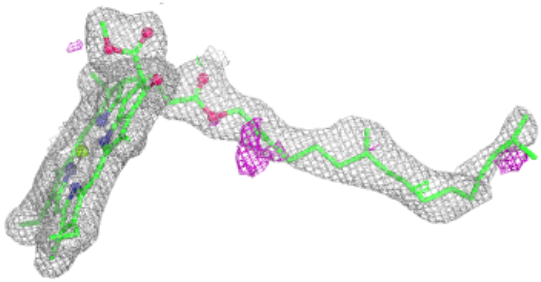


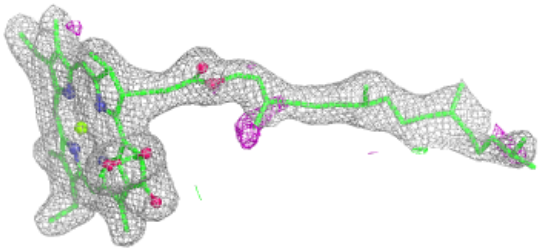


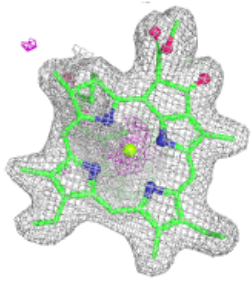


Electron density around CLA B 604:

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

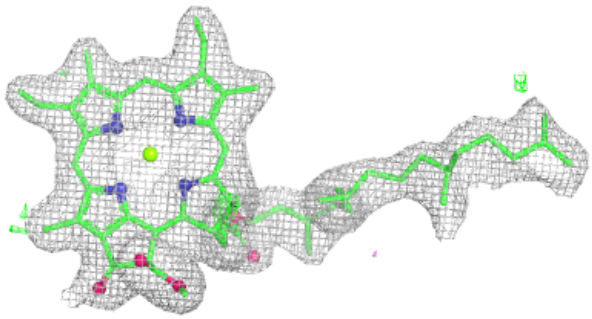


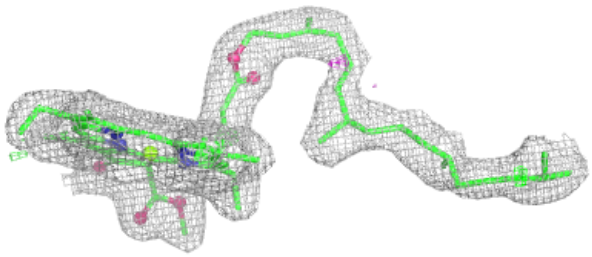


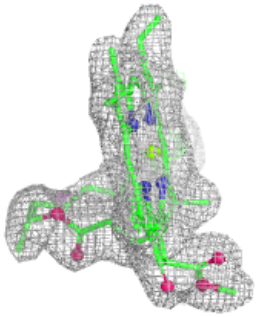


Electron density around CLA a 608:

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

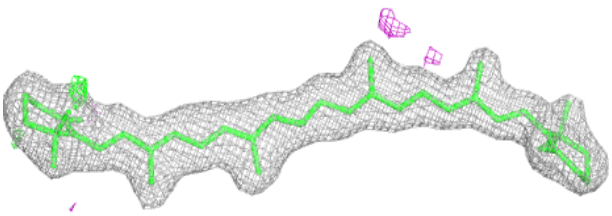


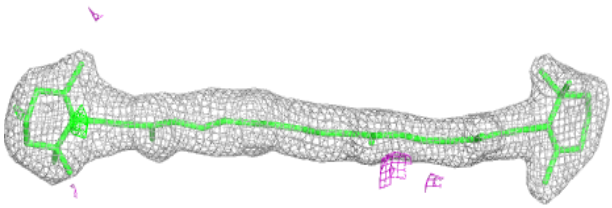


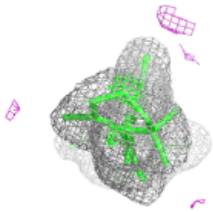


Electron density around BCR C 514:

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

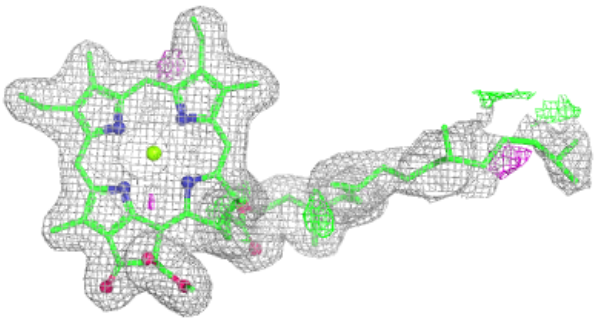


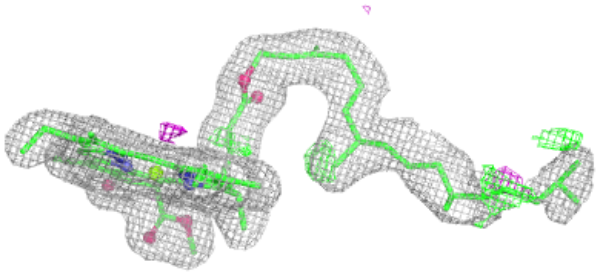


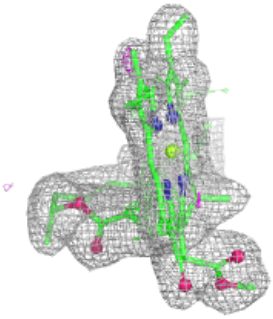


Electron density around CLA A 607:

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

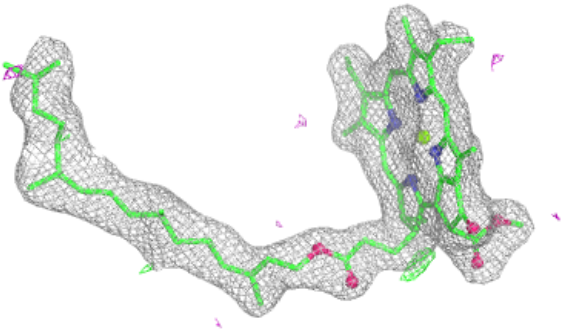


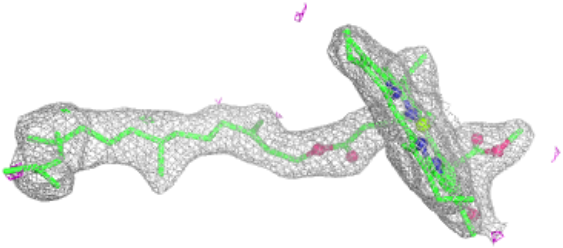


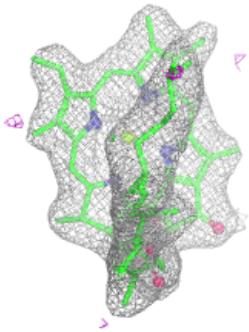


Electron density around CLA b 608:

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

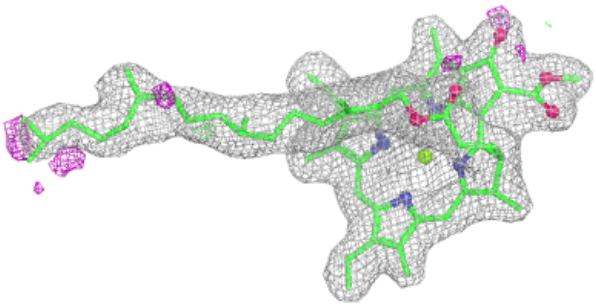


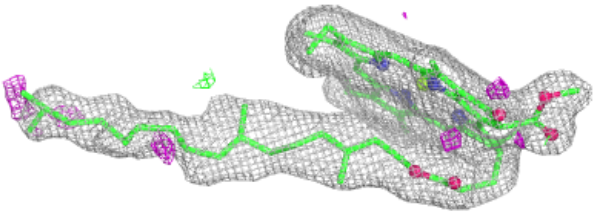


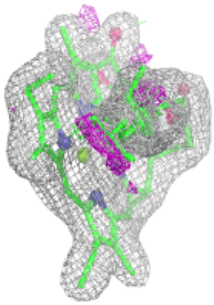


Electron density around CLA b 613:

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

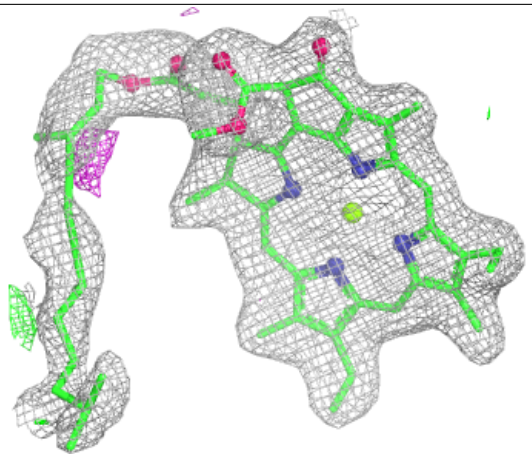


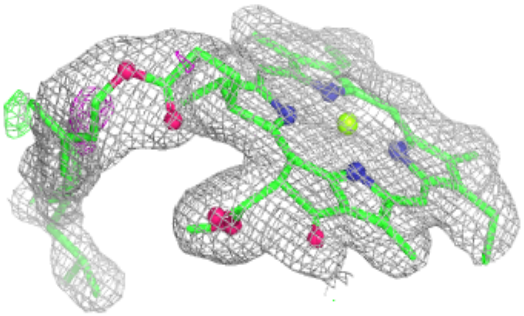




Electron density around CLA b 615:

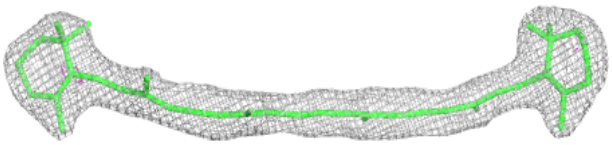
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

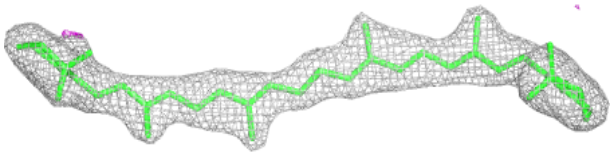


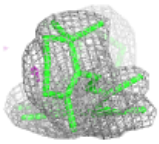


Electron density around BCR K 103:

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

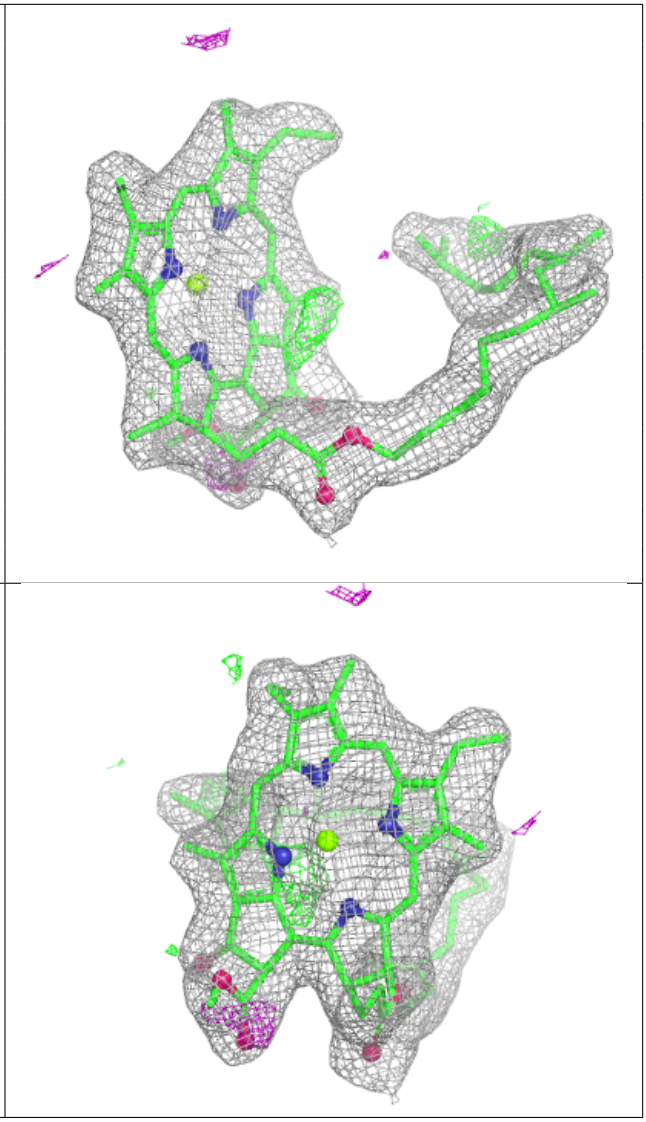






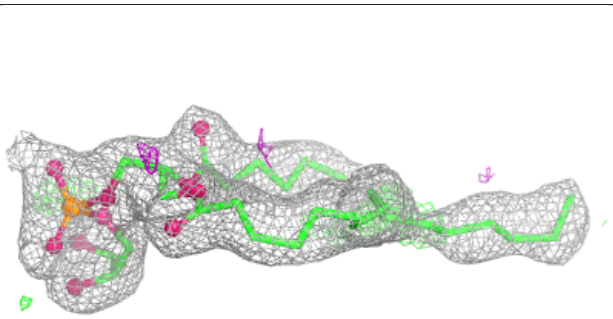
Electron density around CLA c 503:

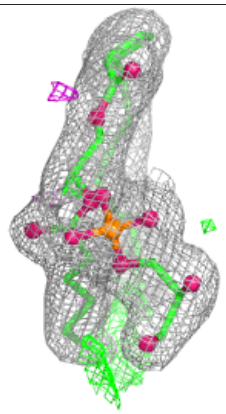
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LHG d 407:

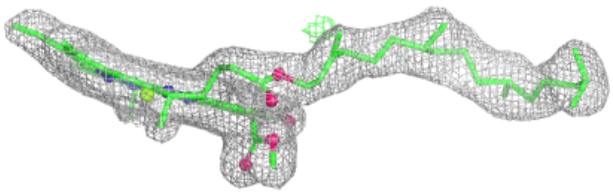
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

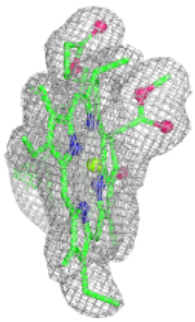




Electron density around CLA b 601:

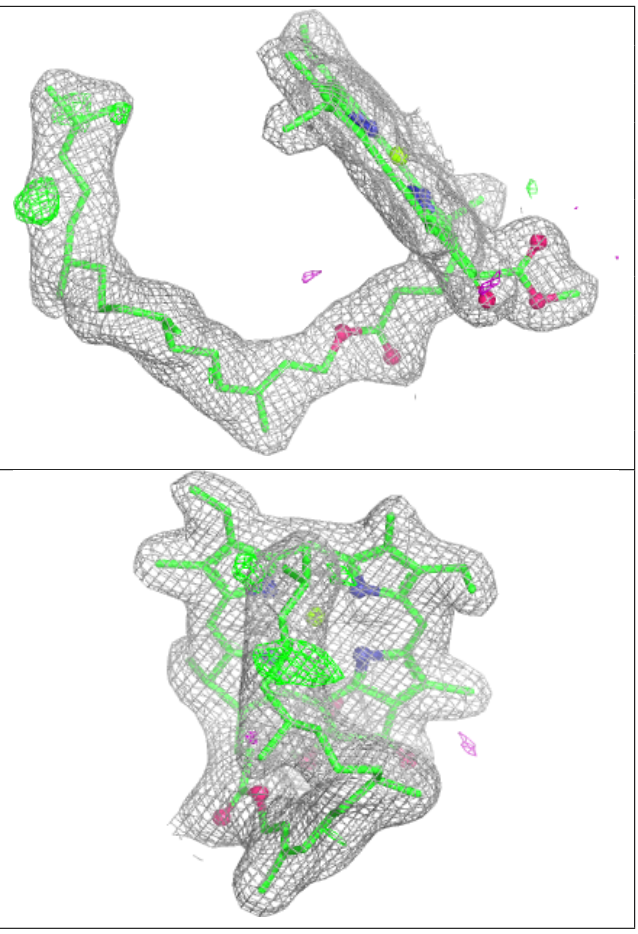
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





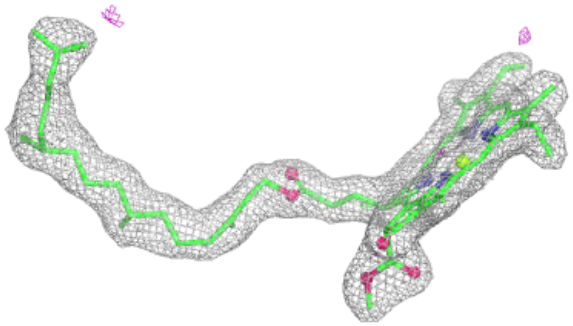
Electron density around CLA B 611:

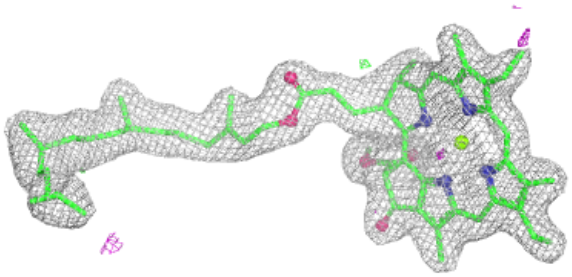
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

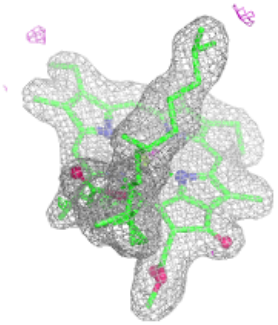


Electron density around CLA d 402:

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

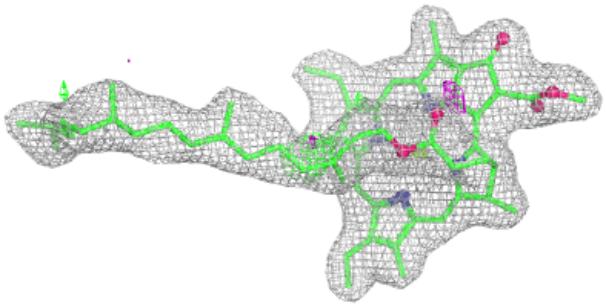


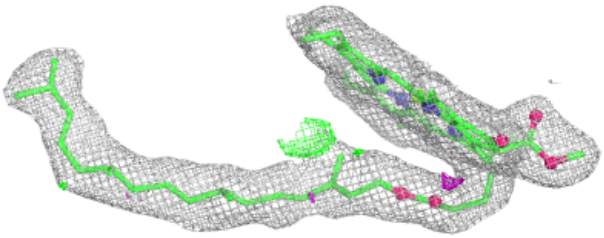


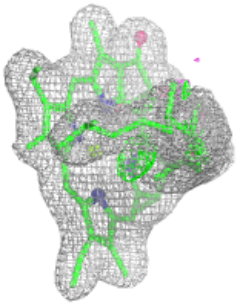


Electron density around CLA b 607:

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

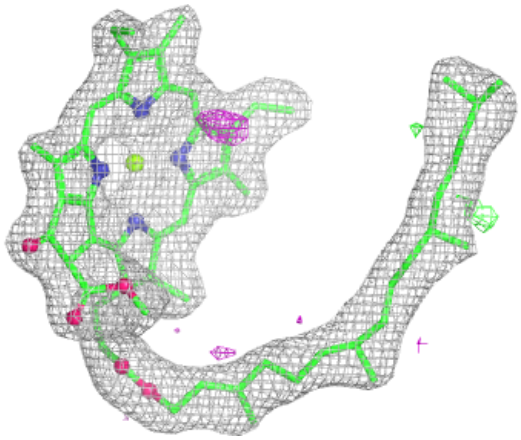


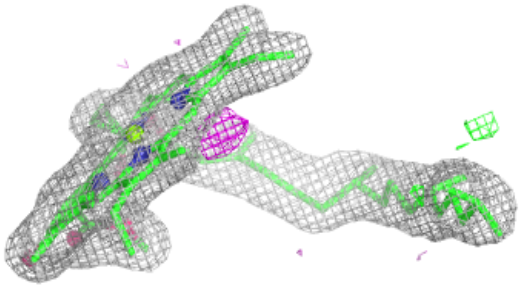


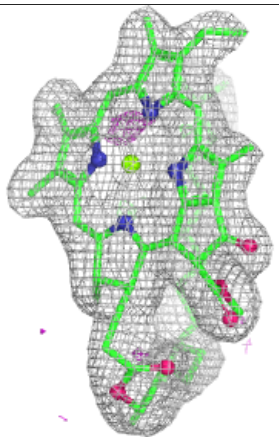


Electron density around CLA C 507:

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

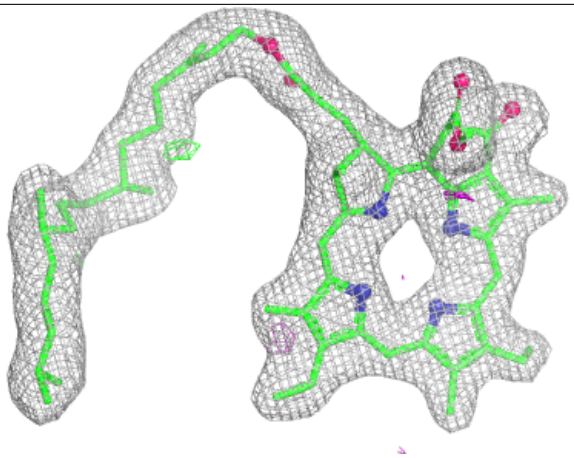


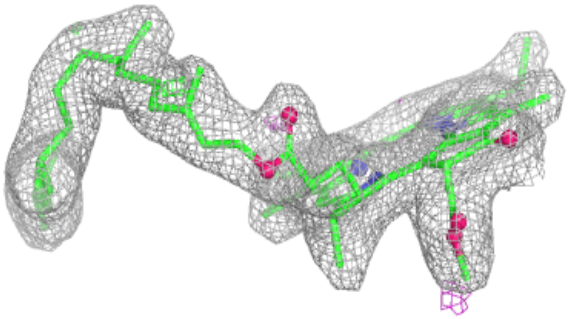


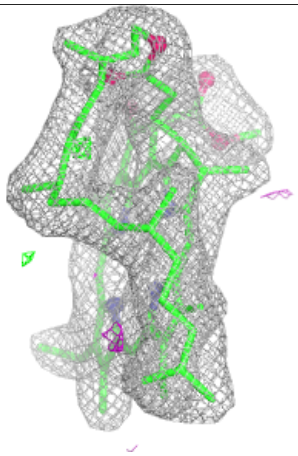


Electron density around PHO D 402:

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

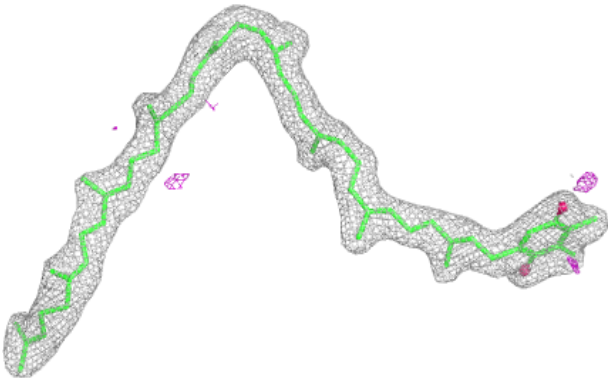


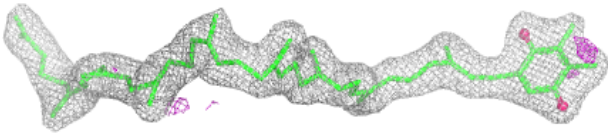


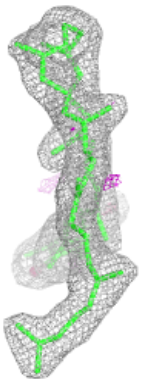


Electron density around PL9 D 406:

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

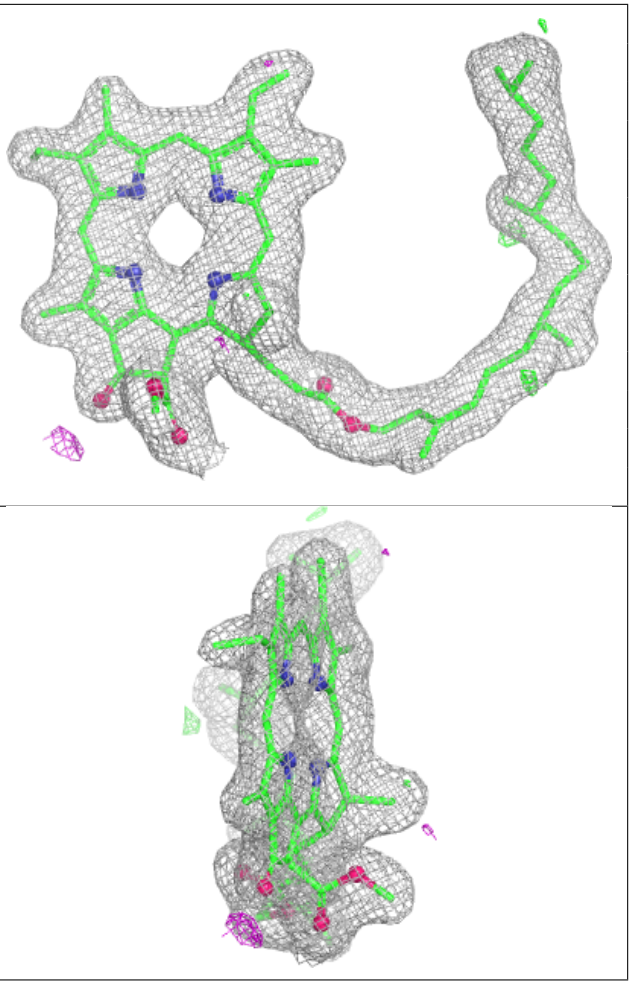






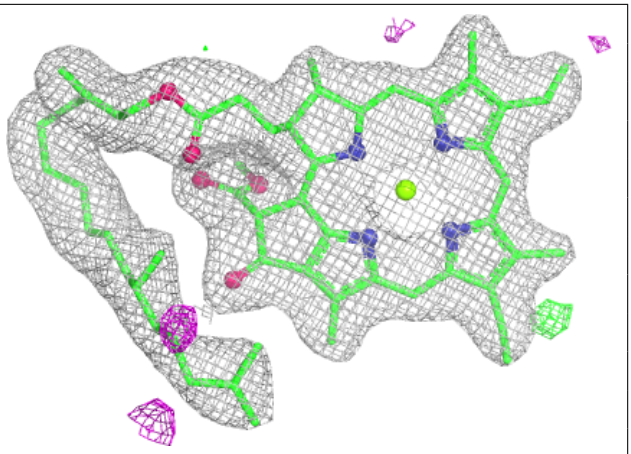
Electron density around PHO a 609:

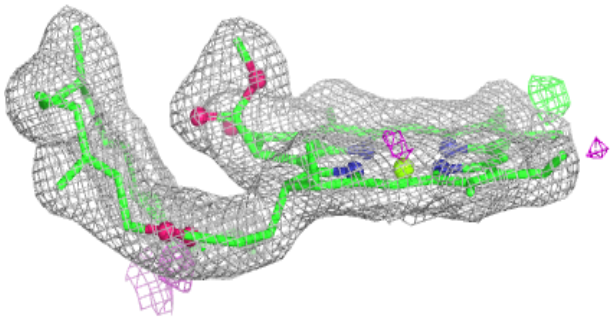
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

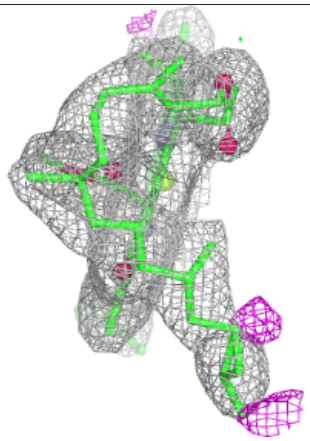


Electron density around CLA b 609:

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

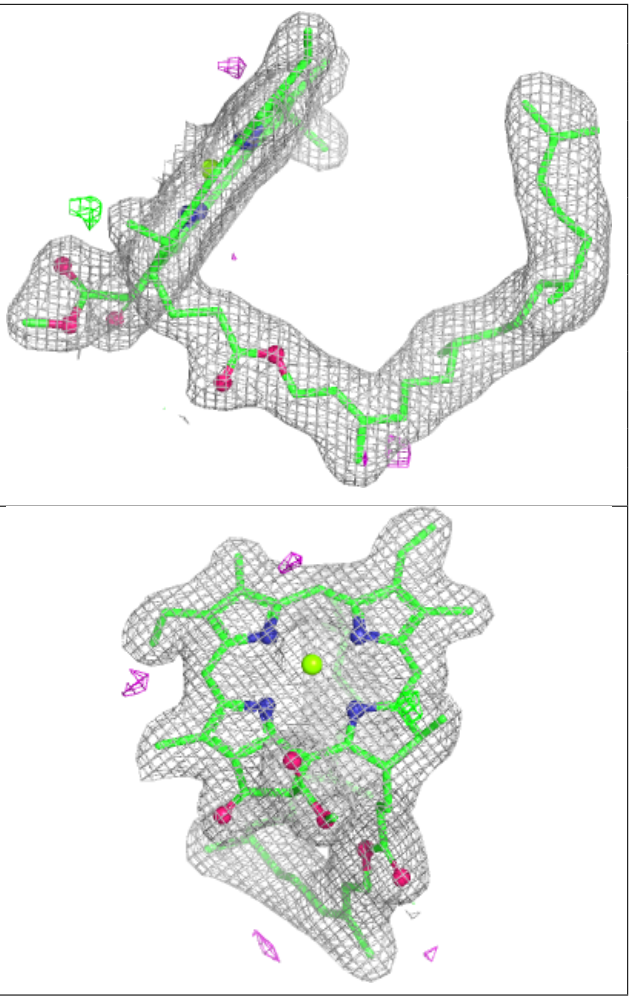






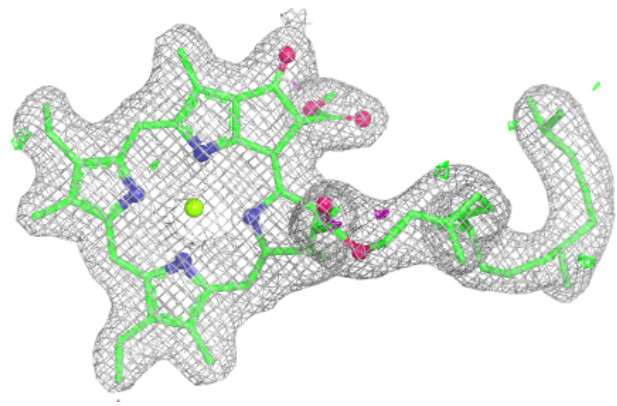
Electron density around CLA b 610:

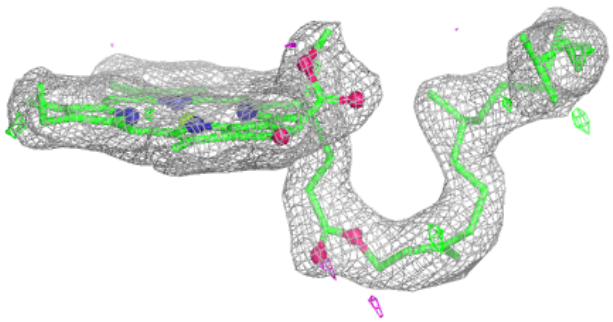
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

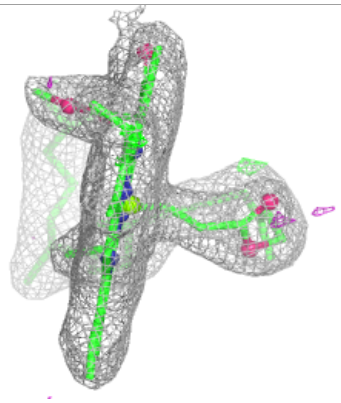


Electron density around CLA b 611:

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

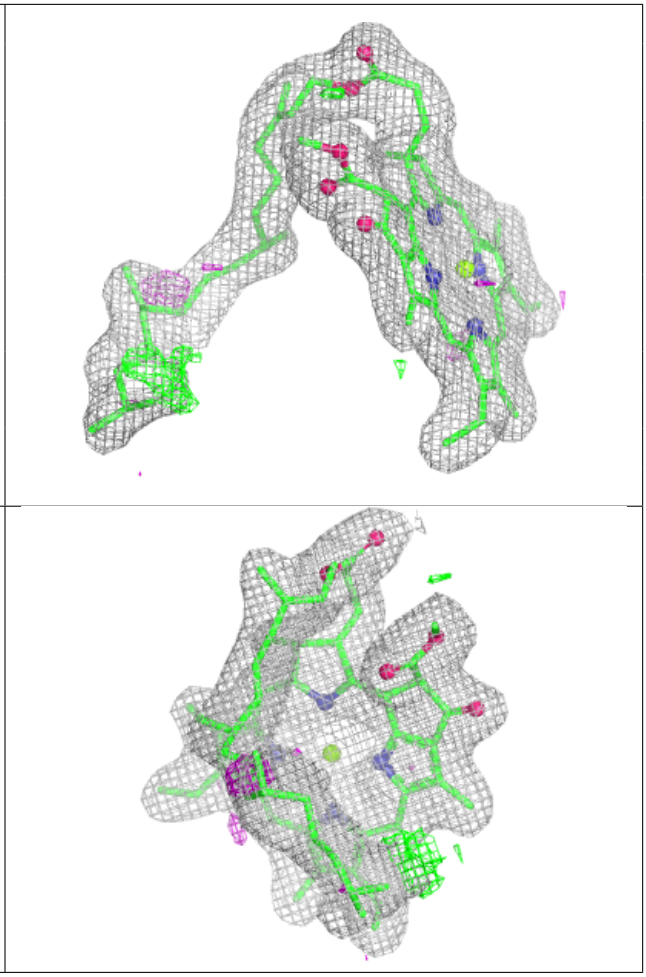






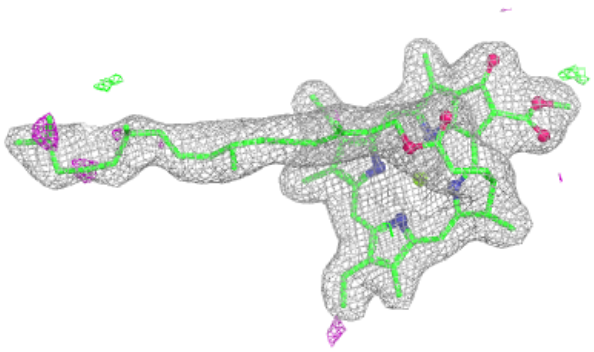
Electron density around CLA b 612:

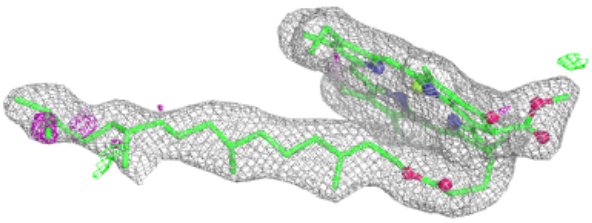
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

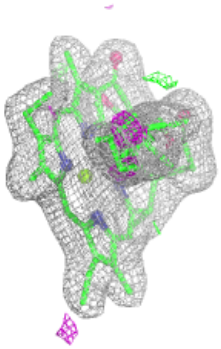


Electron density around CLA B 614:

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

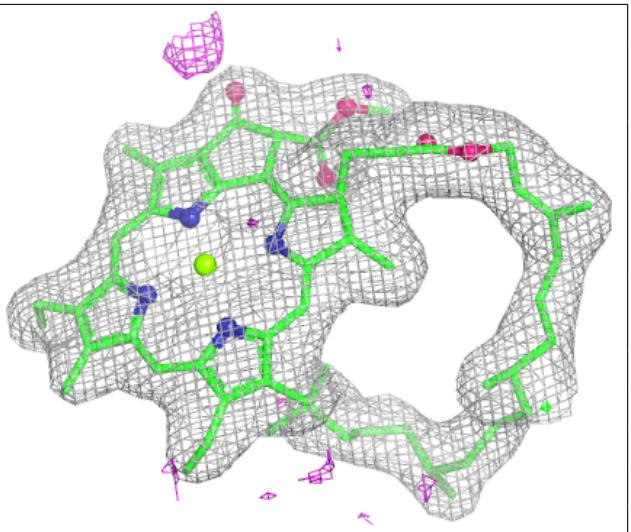


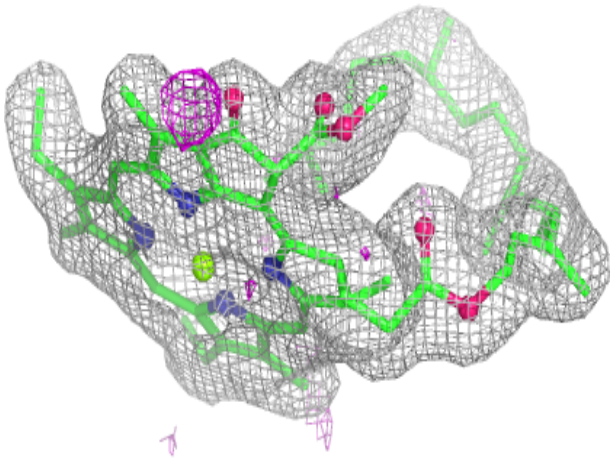


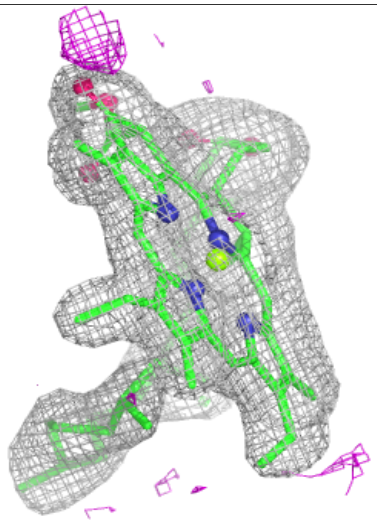


Electron density around CLA b 614:

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

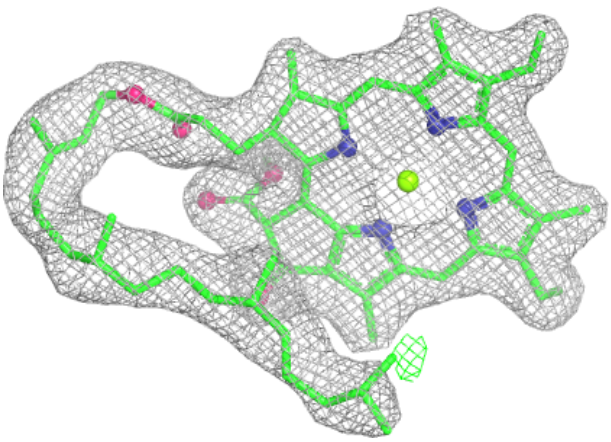


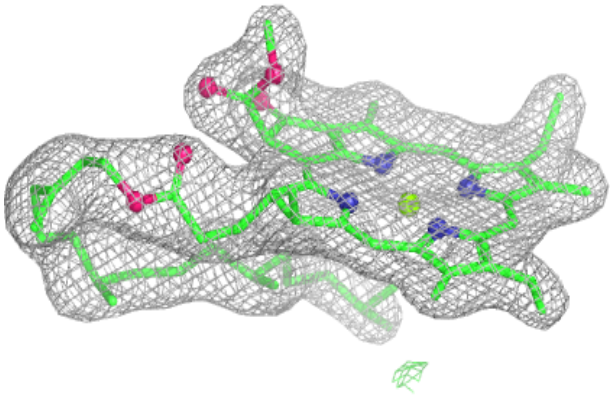


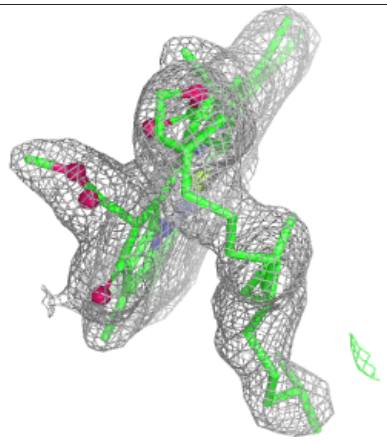


Electron density around CLA C 509:

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

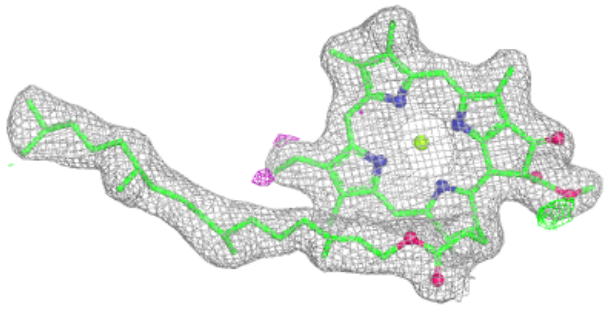


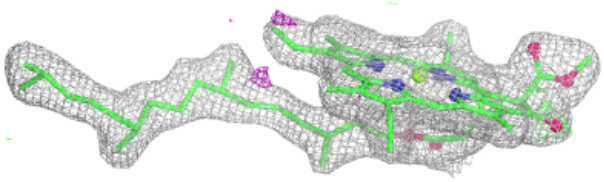


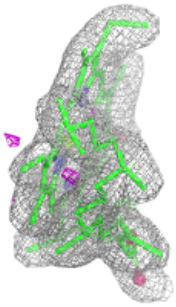


Electron density around CLA c 501:

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

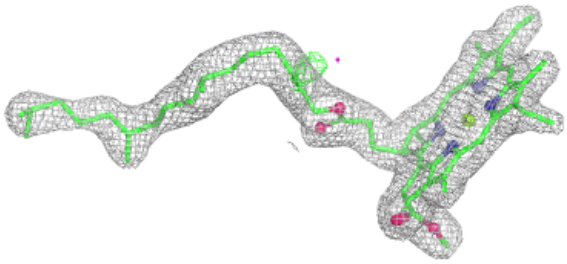


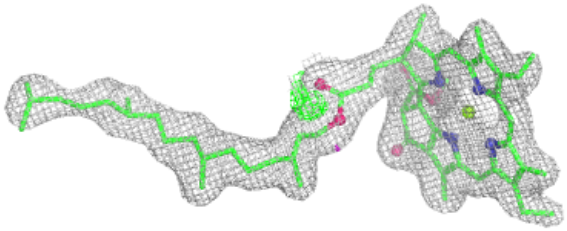


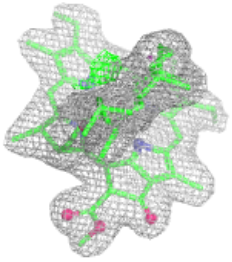


Electron density around CLA c 502:

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

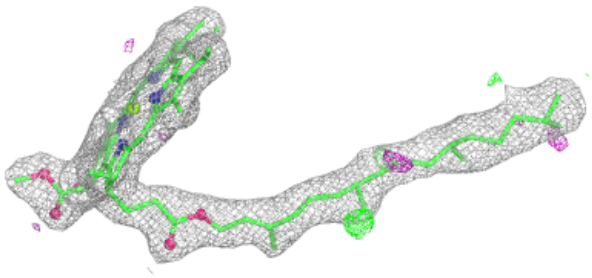


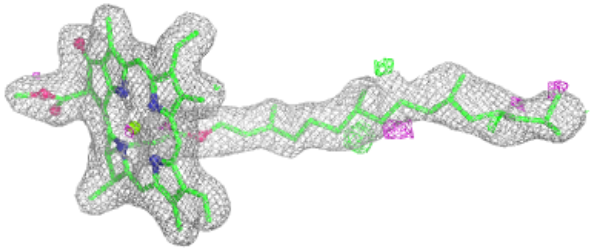


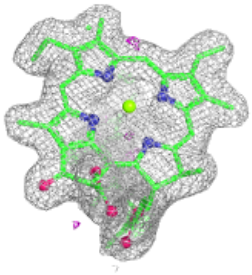


Electron density around CLA B 607:

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

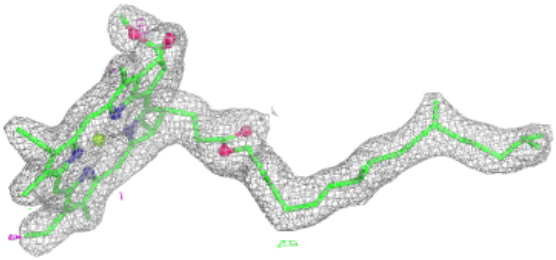


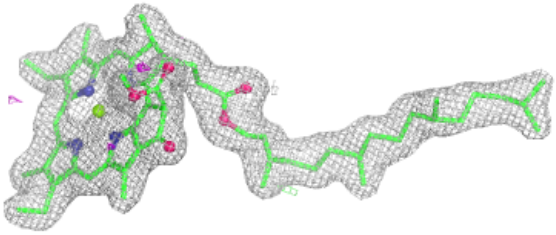


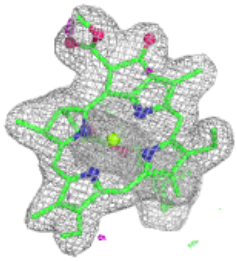


Electron density around CLA C 502:

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

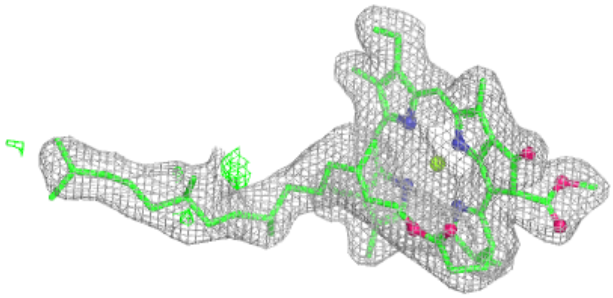


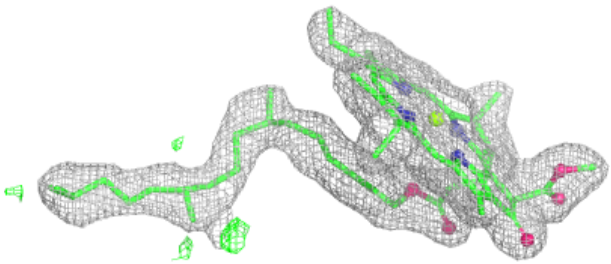


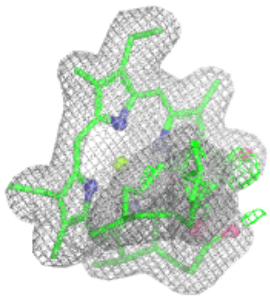


Electron density around CLA c 505:

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

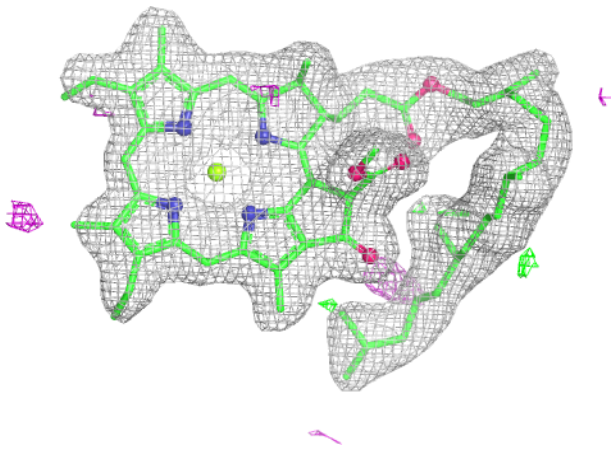


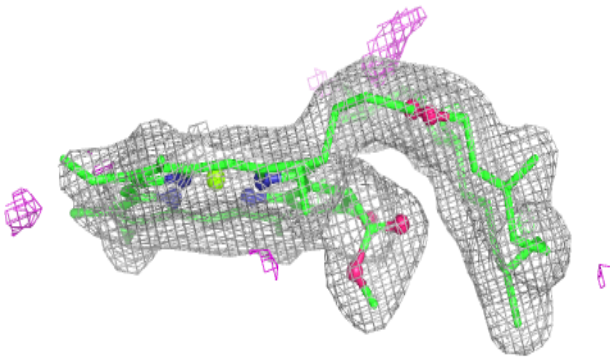


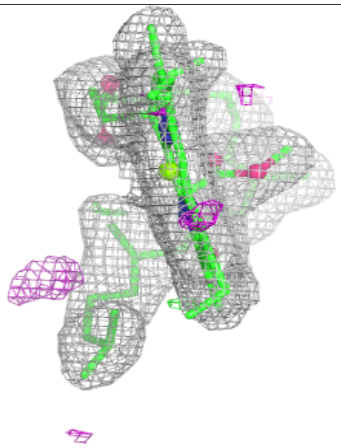


Electron density around CLA B 610:

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

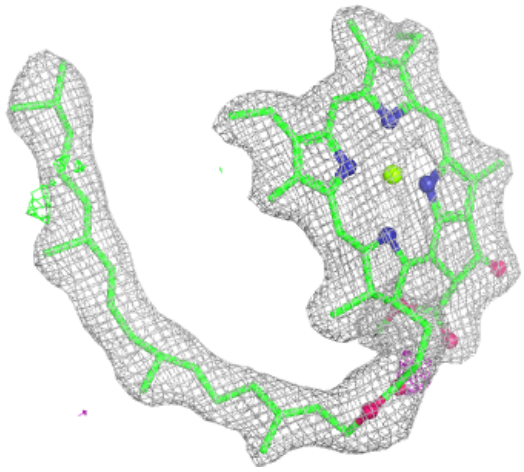


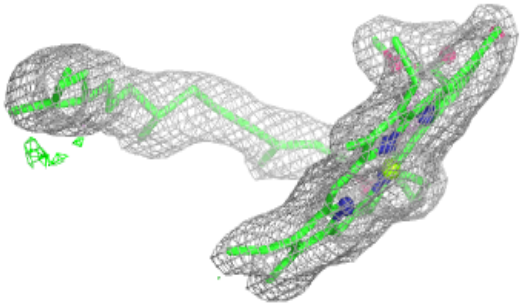


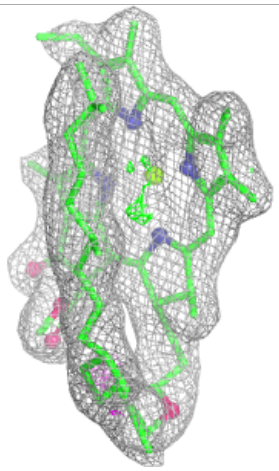


Electron density around CLA c 507:

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

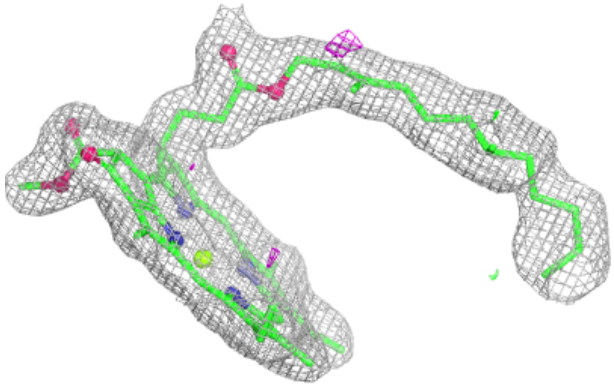


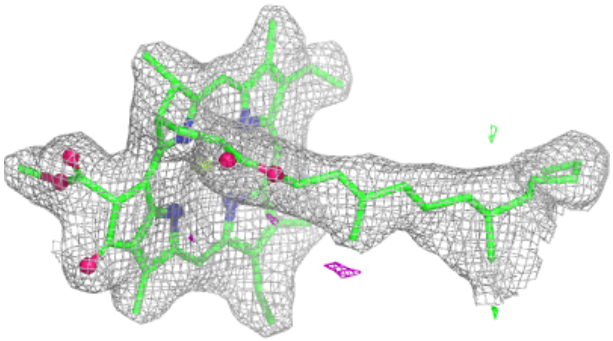


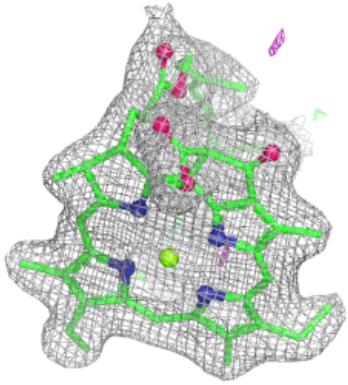


Electron density around CLA C 504:

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

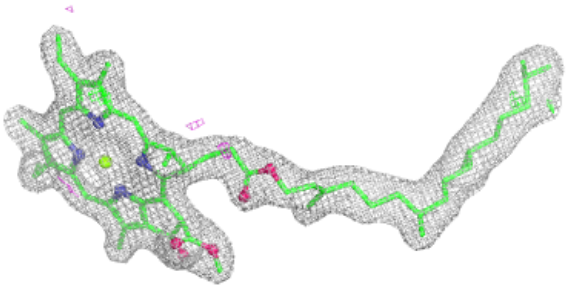


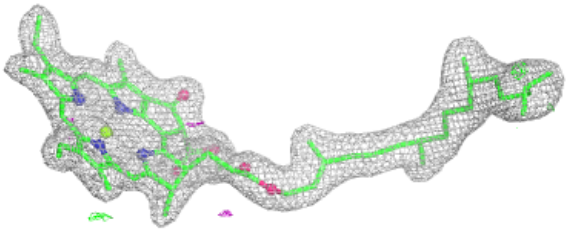


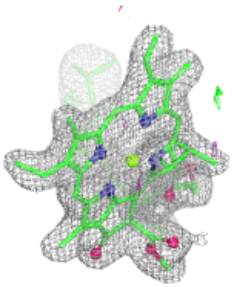


Electron density around CLA a 607:

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

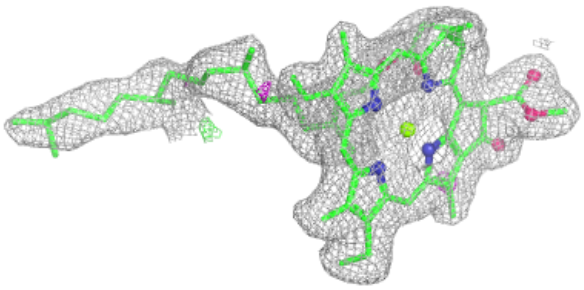


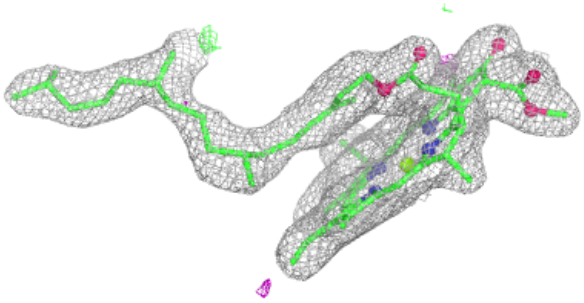


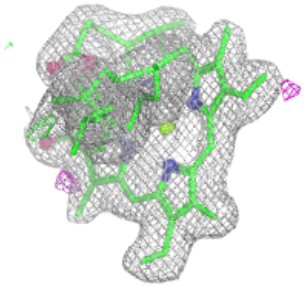


Electron density around CLA C 505:

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

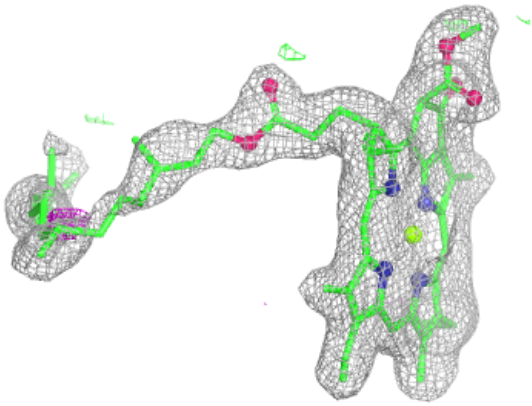


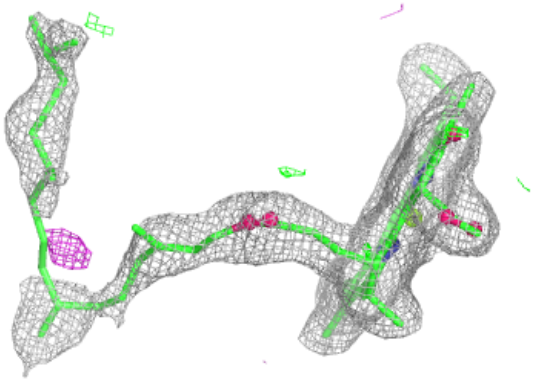


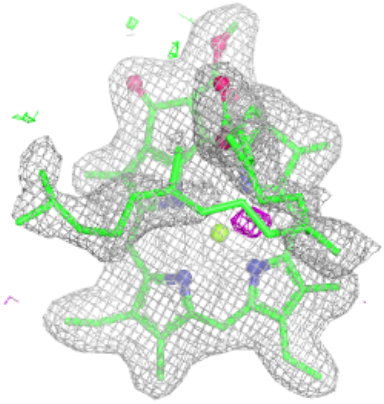


Electron density around CLA a 610:

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

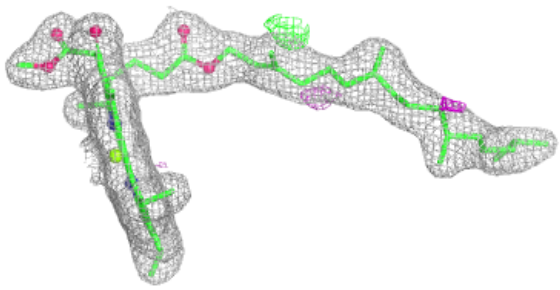


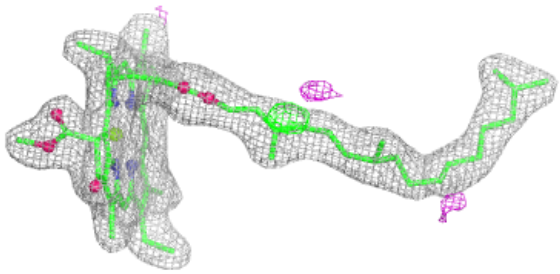


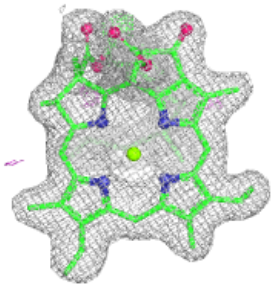


Electron density around CLA B 605:

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

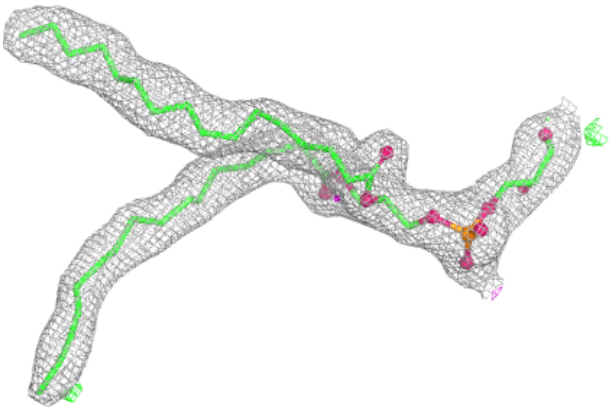


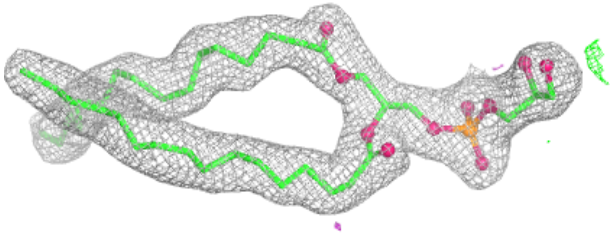


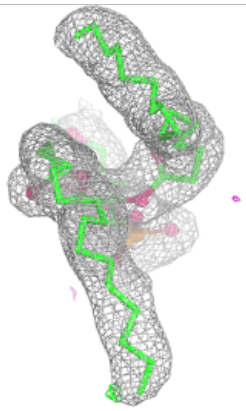


Electron density around LHG D 408:

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

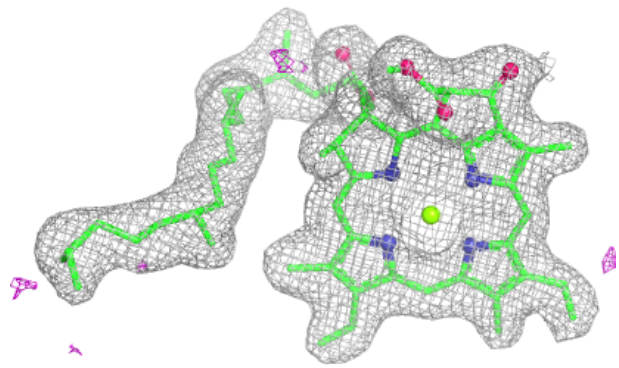


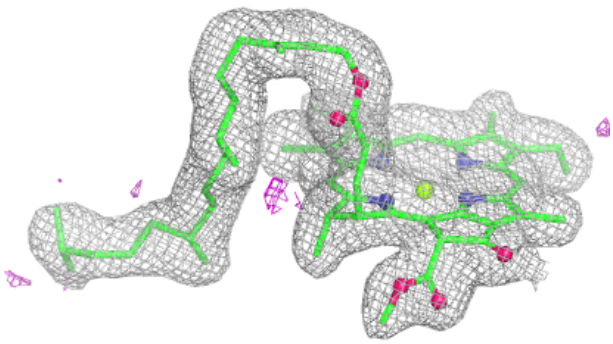


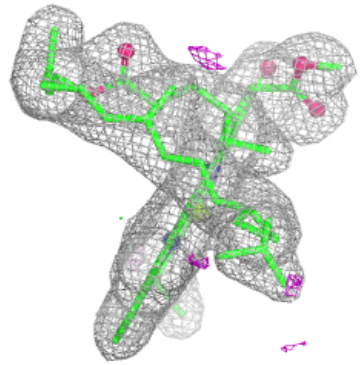


Electron density around CLA A 612:

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

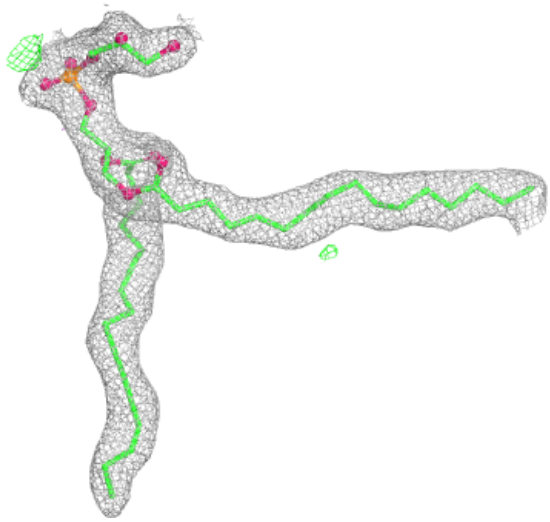


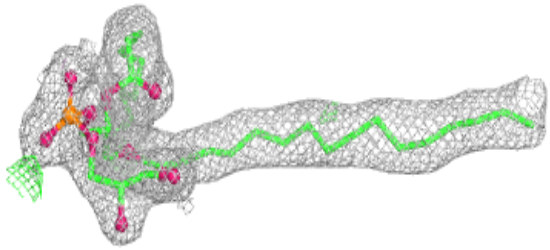


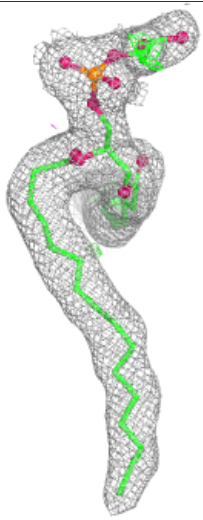


Electron density around LHG L 101:

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

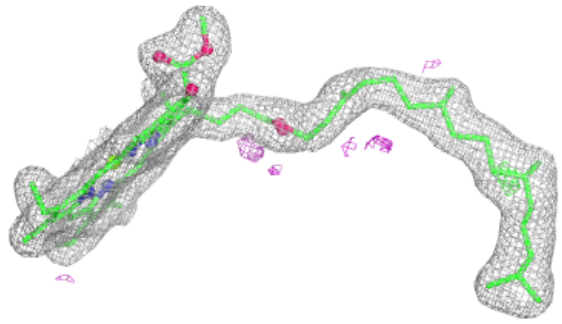


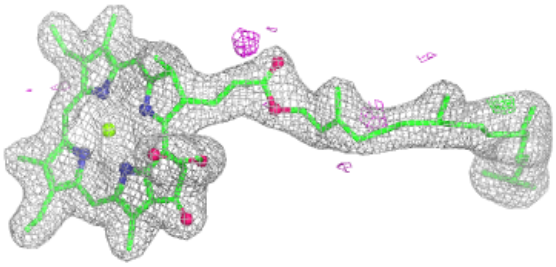


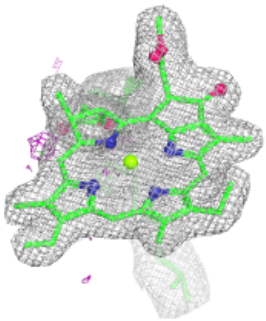


Electron density around CLA D 403:

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

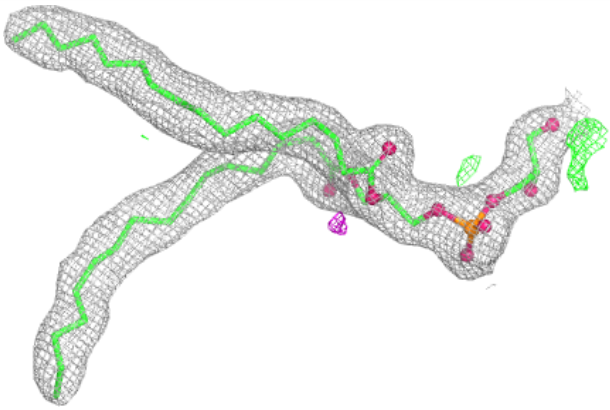


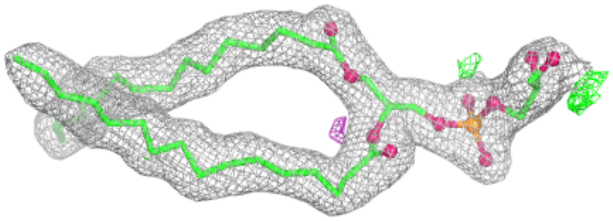


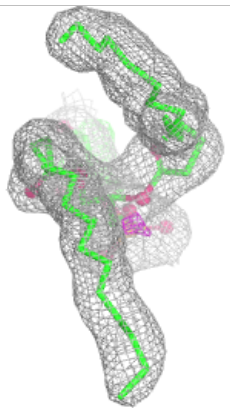


Electron density around LHG d 406:

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

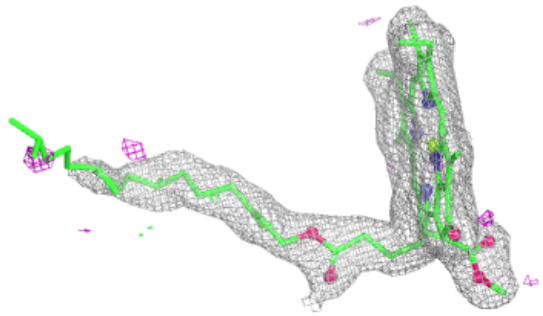


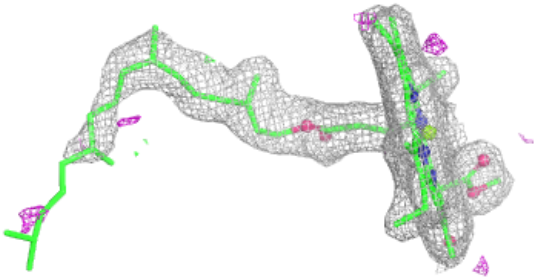


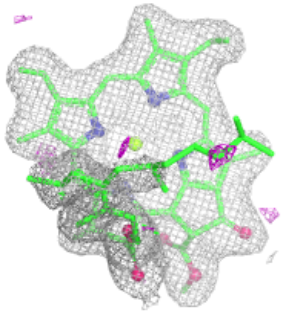


Electron density around CLA D 404:

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

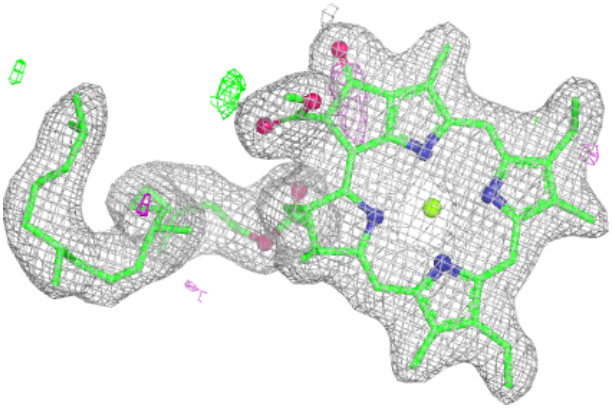


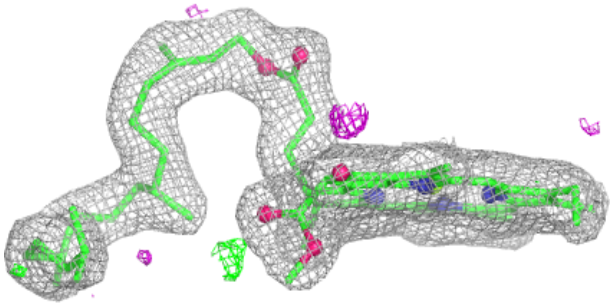


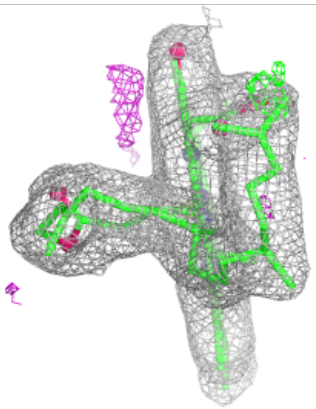


Electron density around CLA B 612:

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

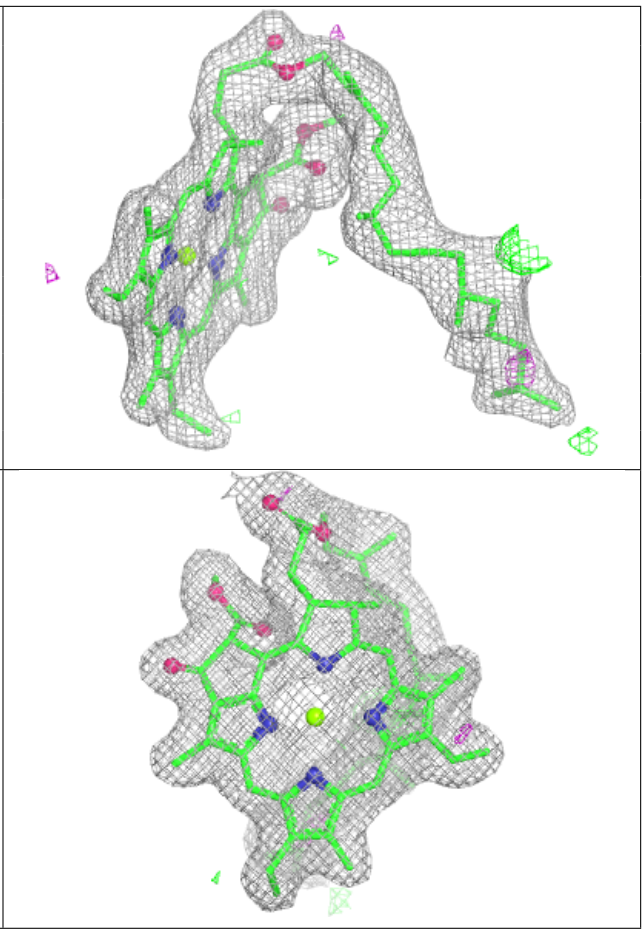






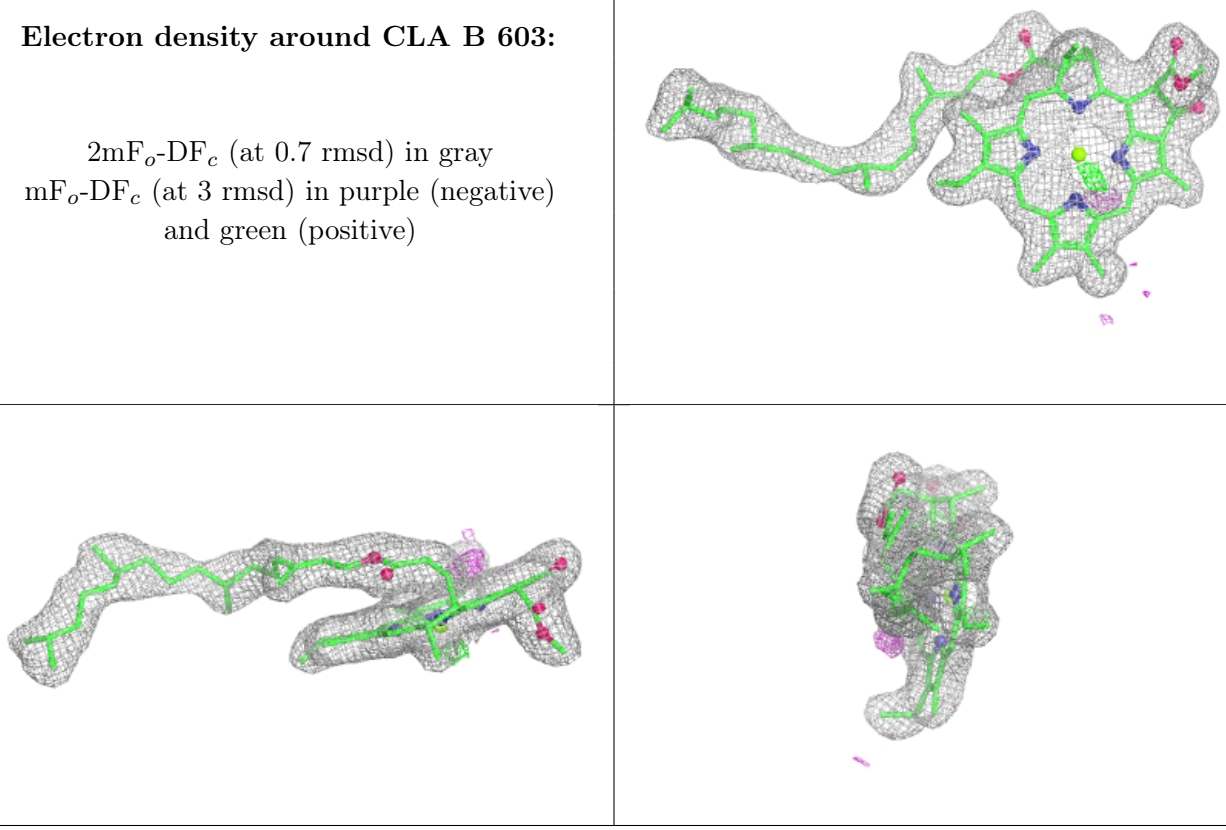
Electron density around CLA B 613:

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



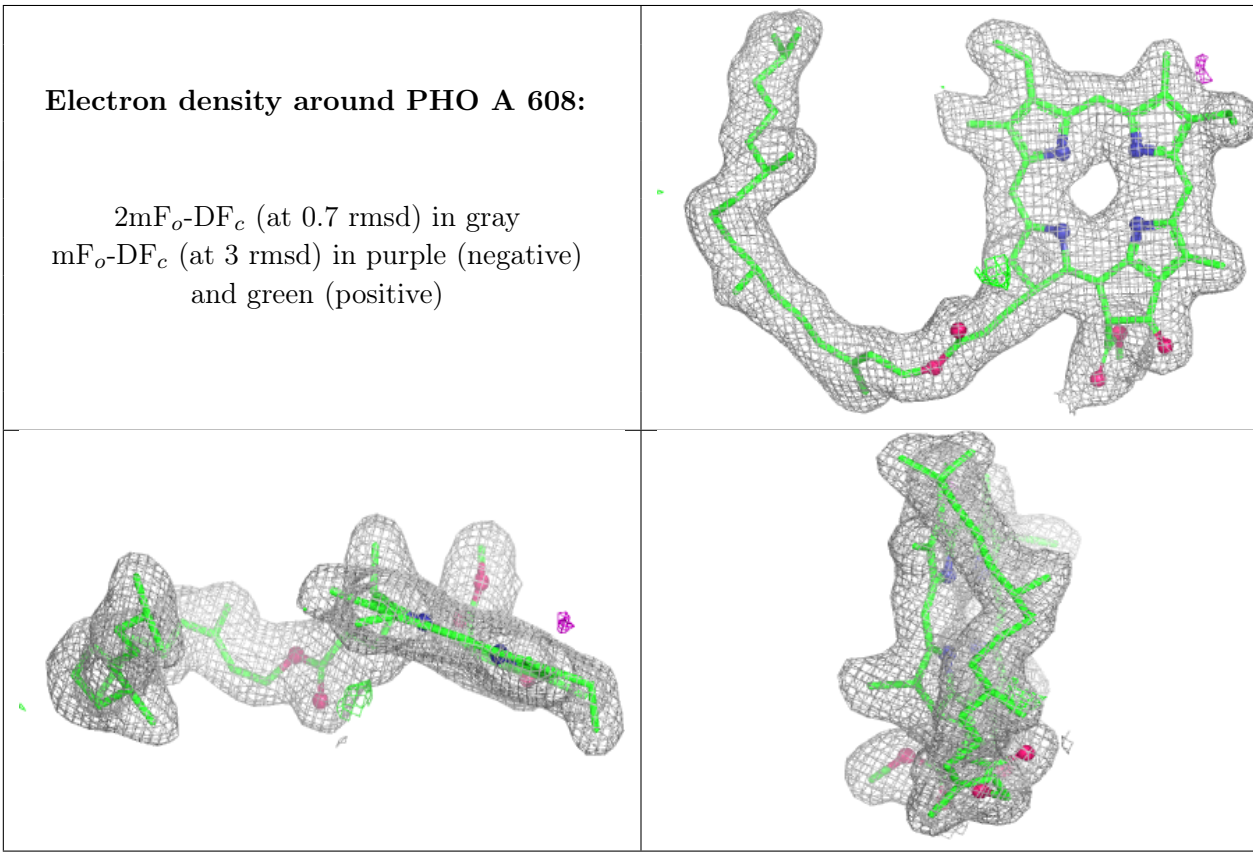
Electron density around CLA B 603:

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



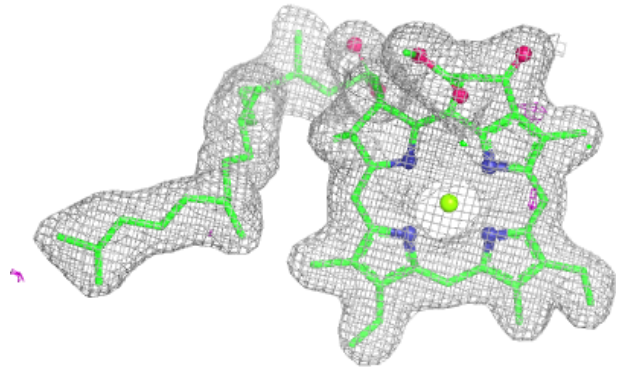
Electron density around PHO A 608:

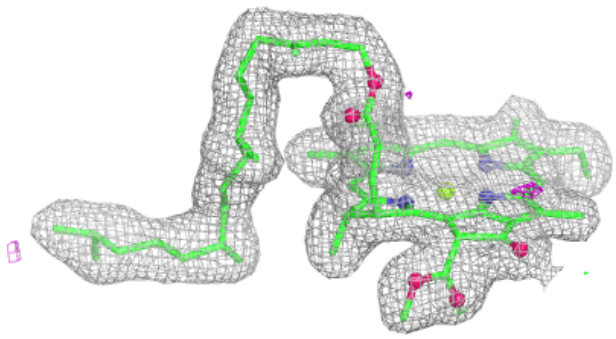
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

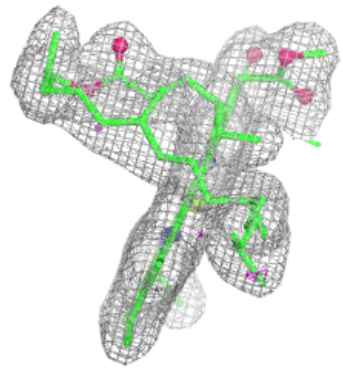


Electron density around CLA a 613:

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

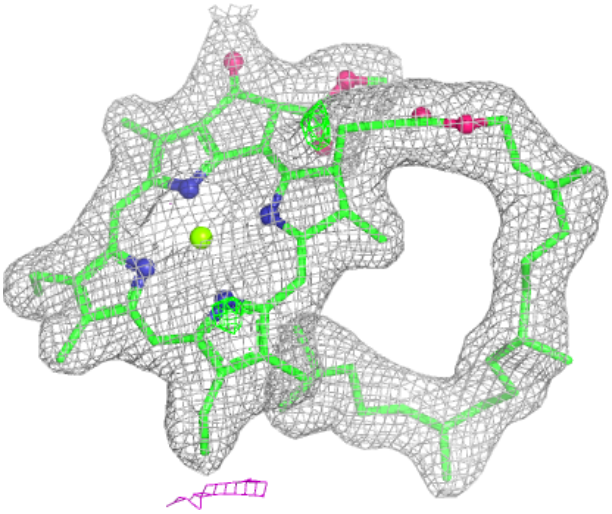


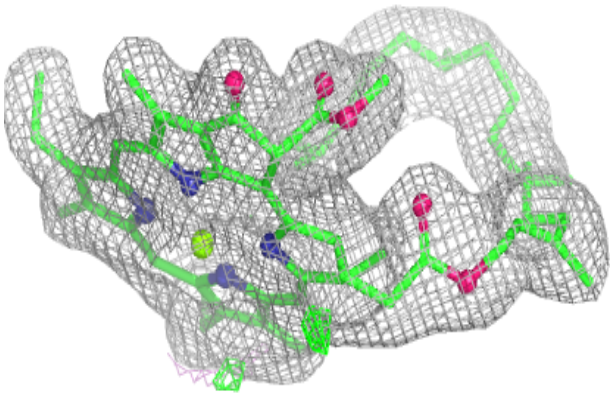


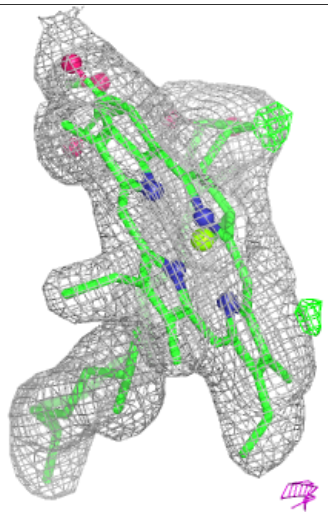


Electron density around CLA B 615:

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

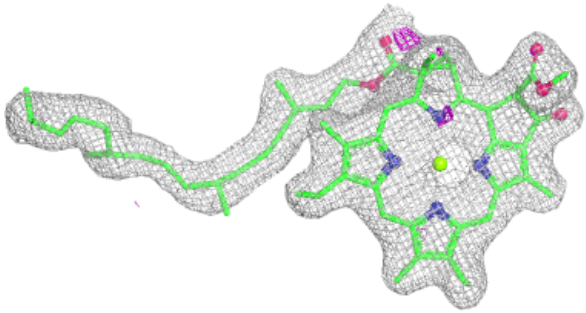


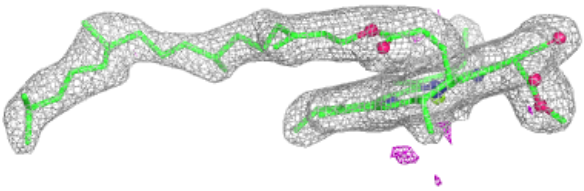


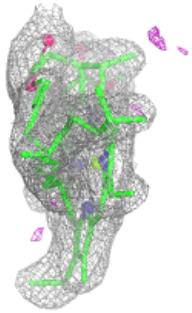


Electron density around CLA b 602:

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

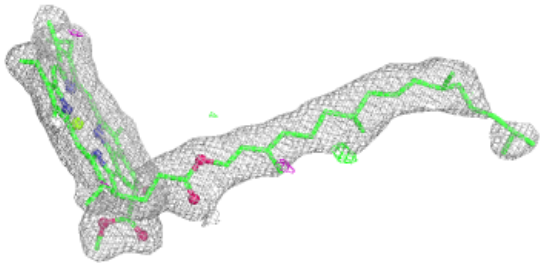


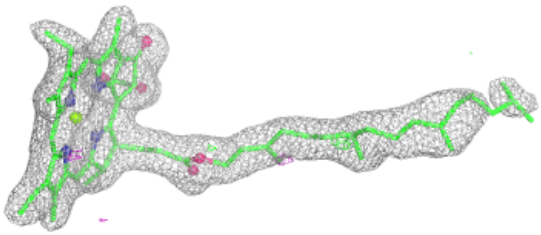


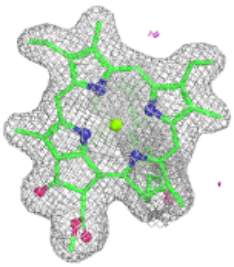


Electron density around CLA b 603:

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

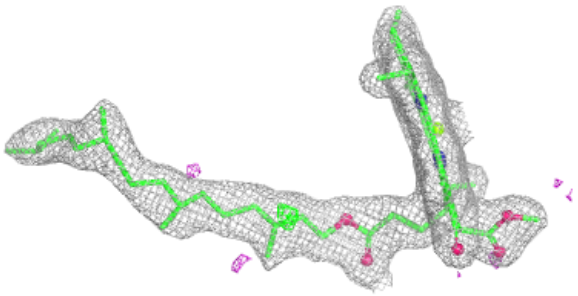


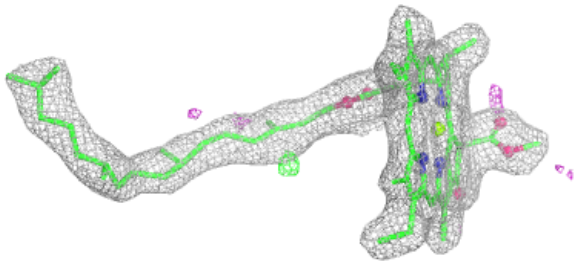


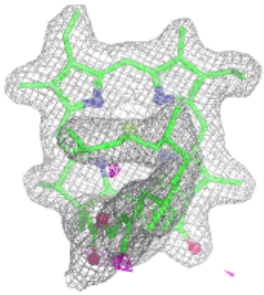


Electron density around CLA b 604:

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

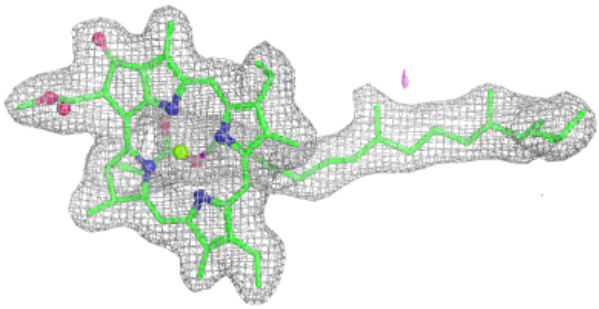


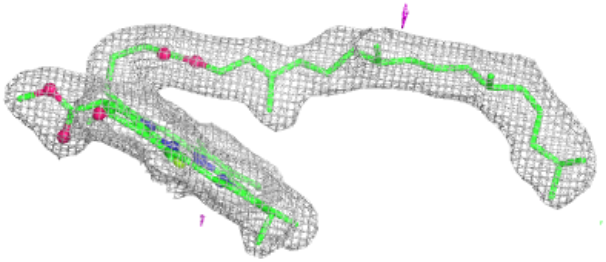


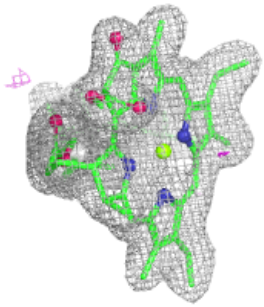


Electron density around CLA B 608:

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

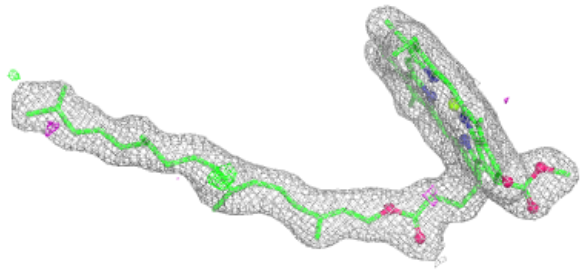


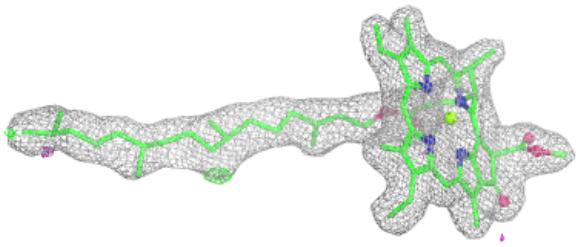


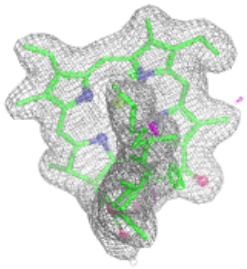


Electron density around CLA b 606:

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

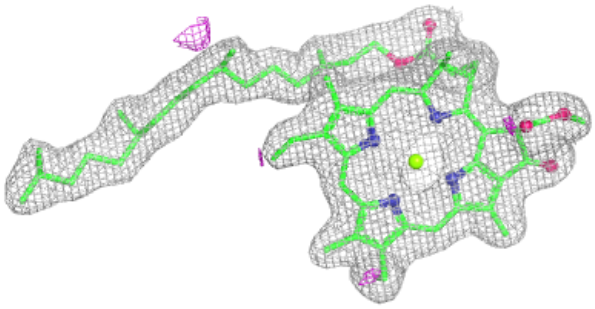


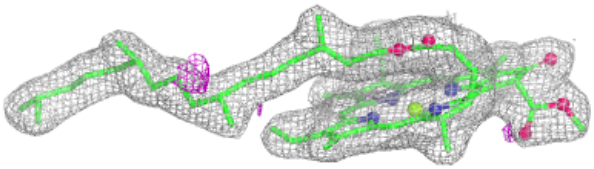


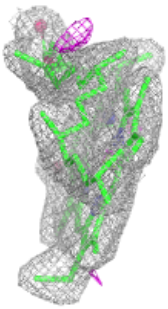


Electron density around CLA C 501:

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

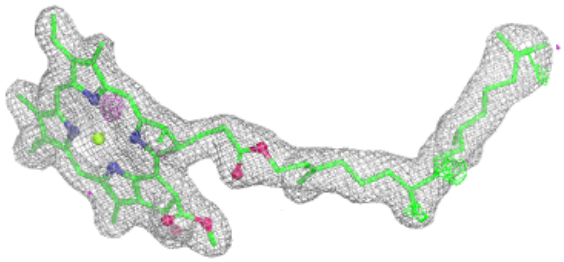


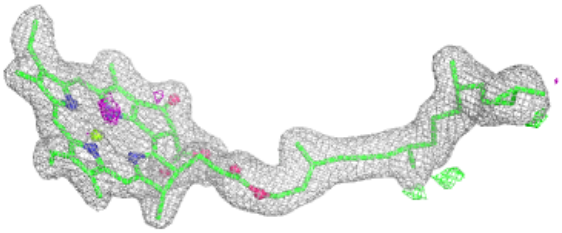


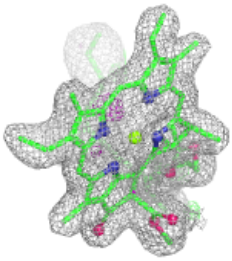


Electron density around CLA A 606:

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

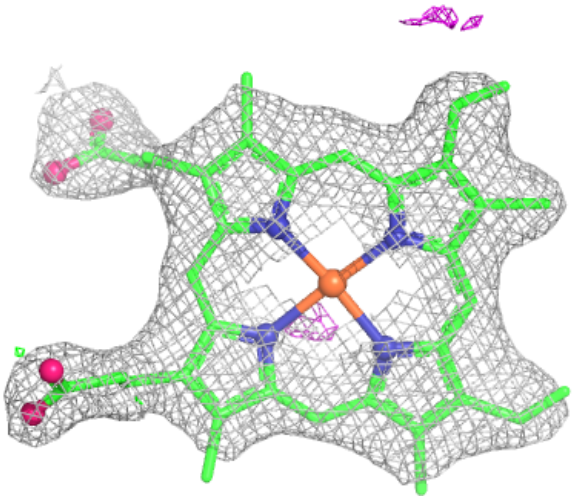


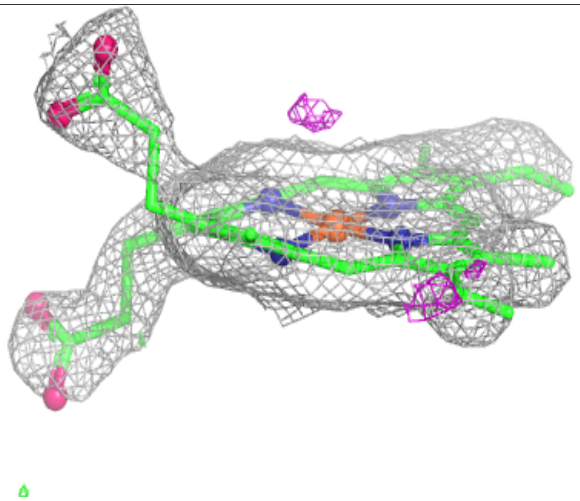


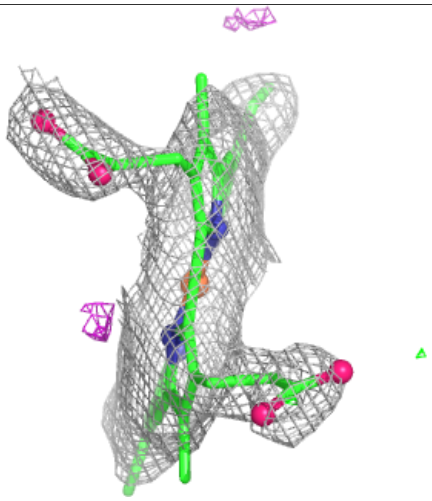


Electron density around HEM e 101:

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

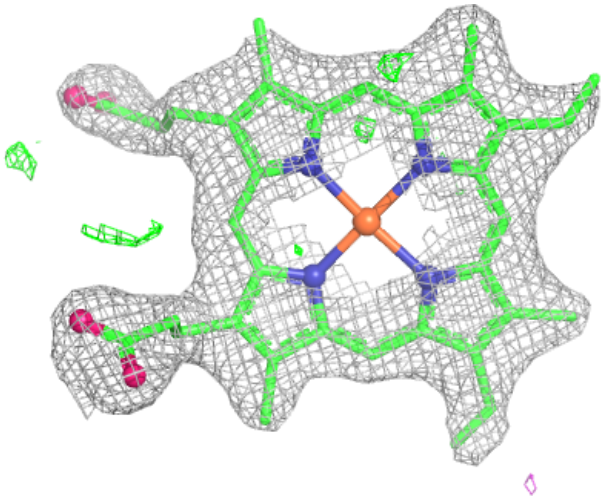


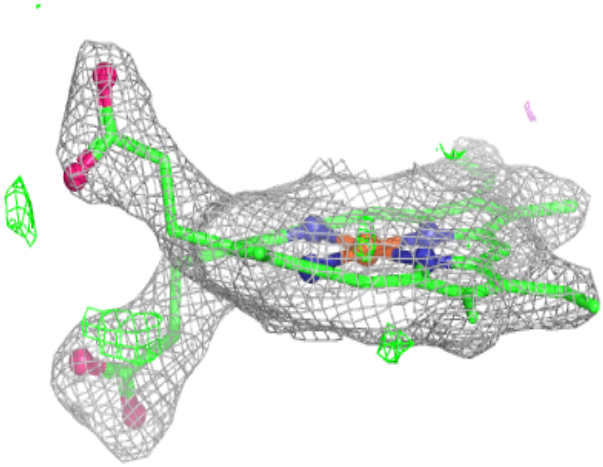


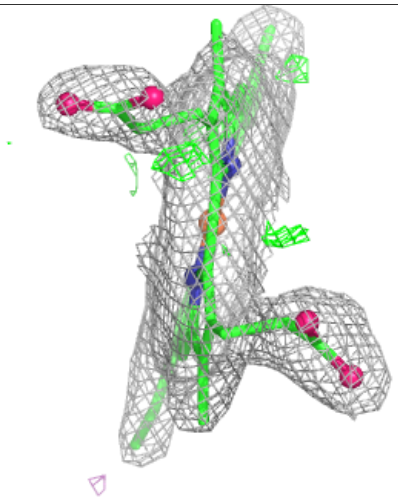


Electron density around HEM F 101:

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

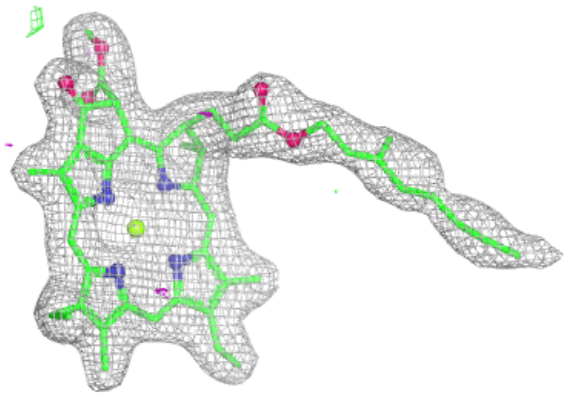


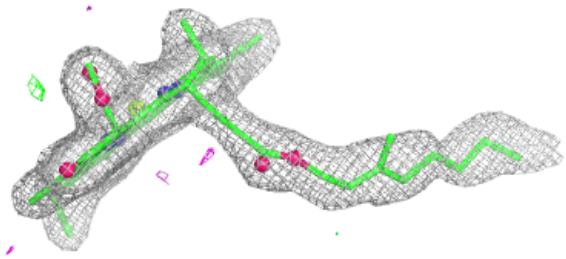


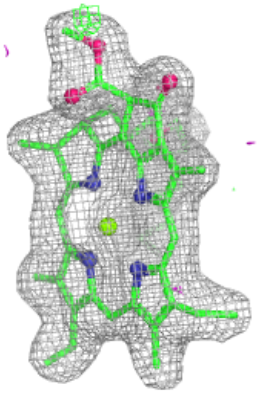


Electron density around CLA A 609:

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

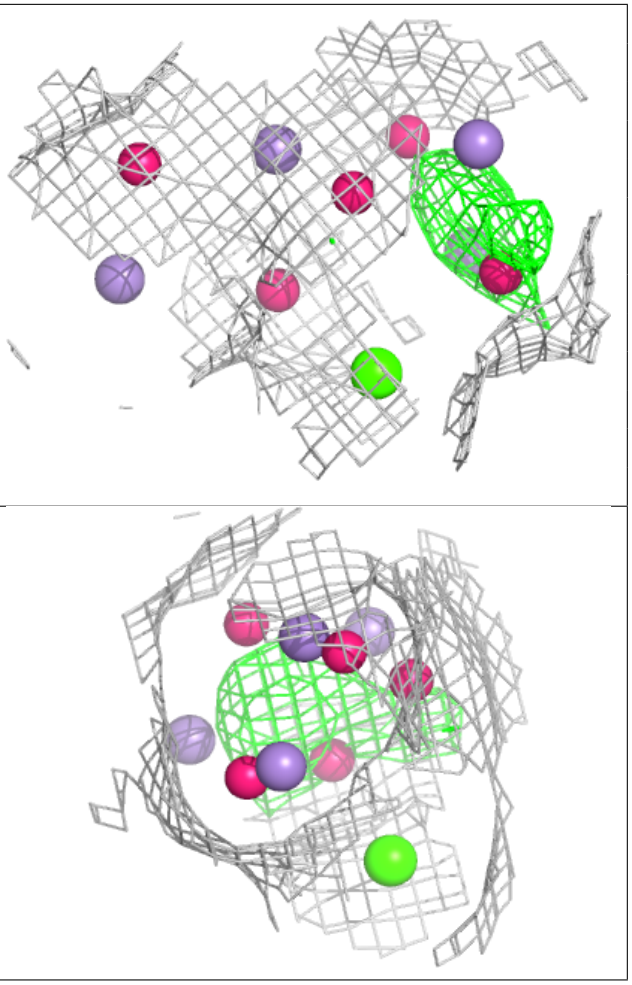






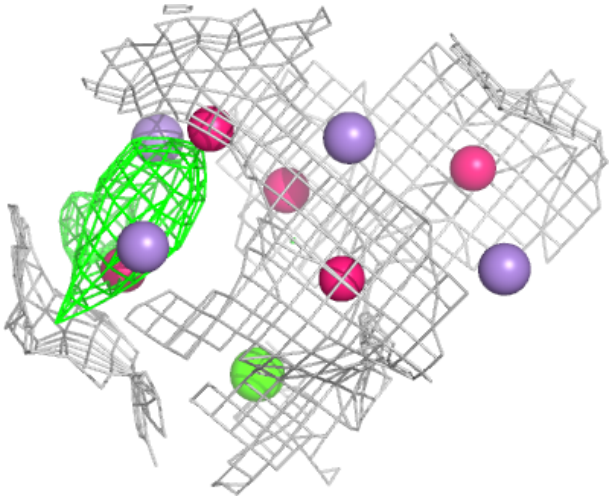
Electron density around OEX A 601 (B):

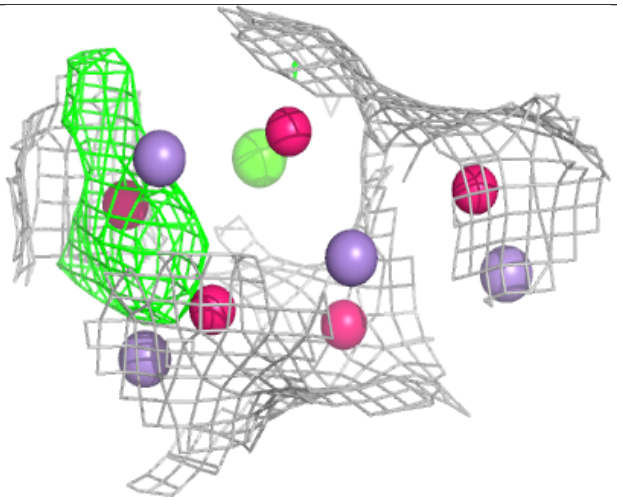
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

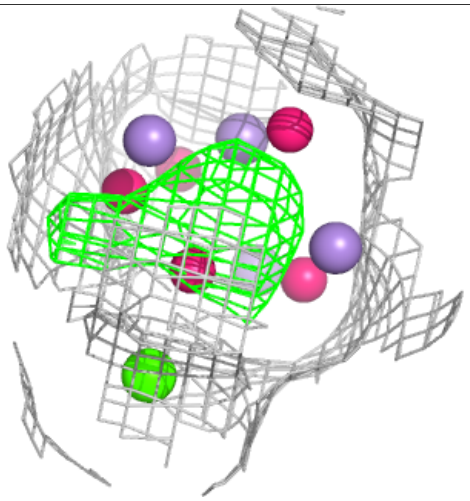


Electron density around OEX A 601 (C):

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

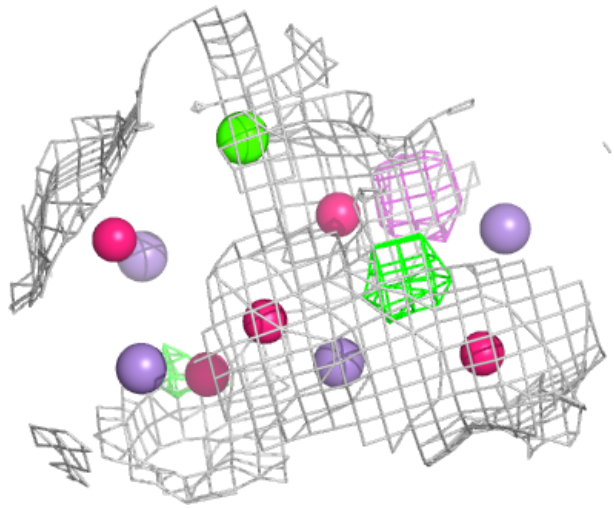


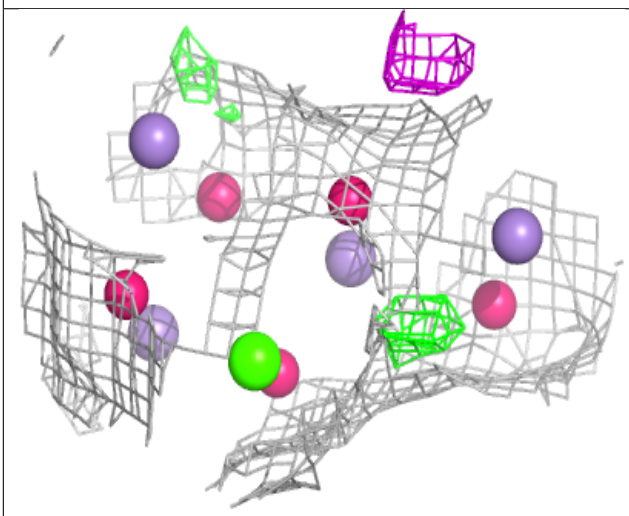


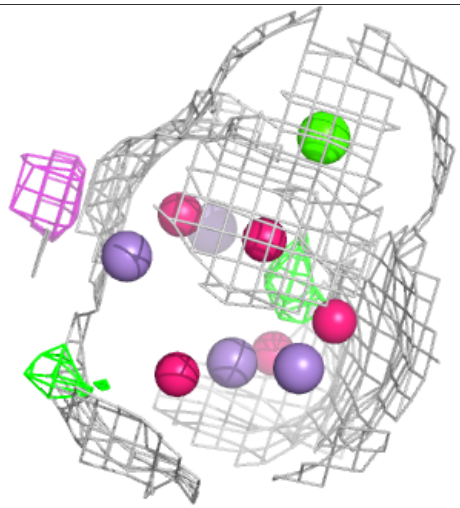


Electron density around OEX a 601 (B):

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

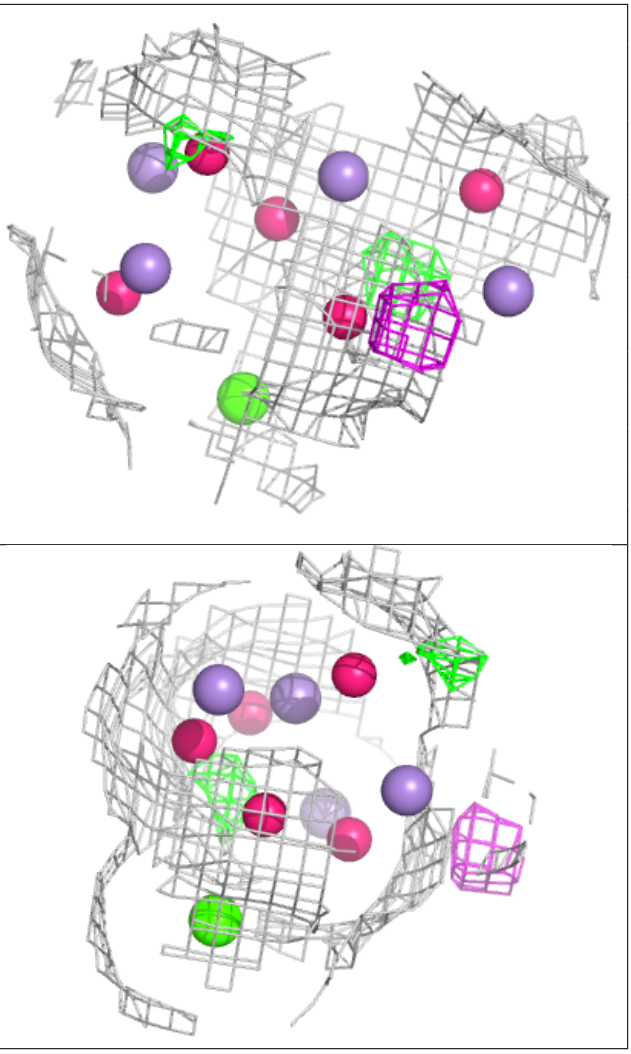






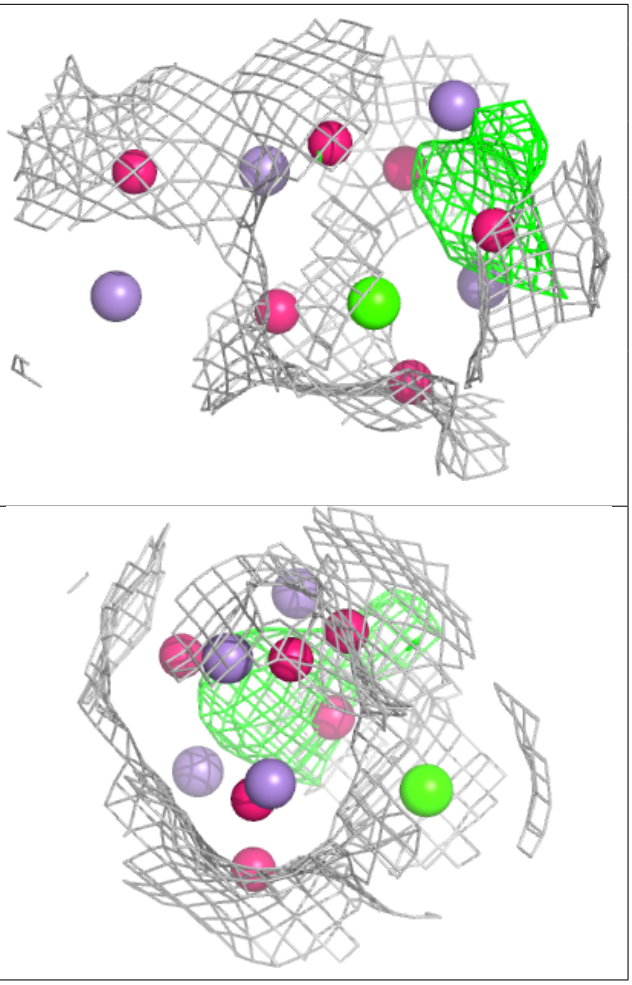
Electron density around OEX a 601 (C):

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



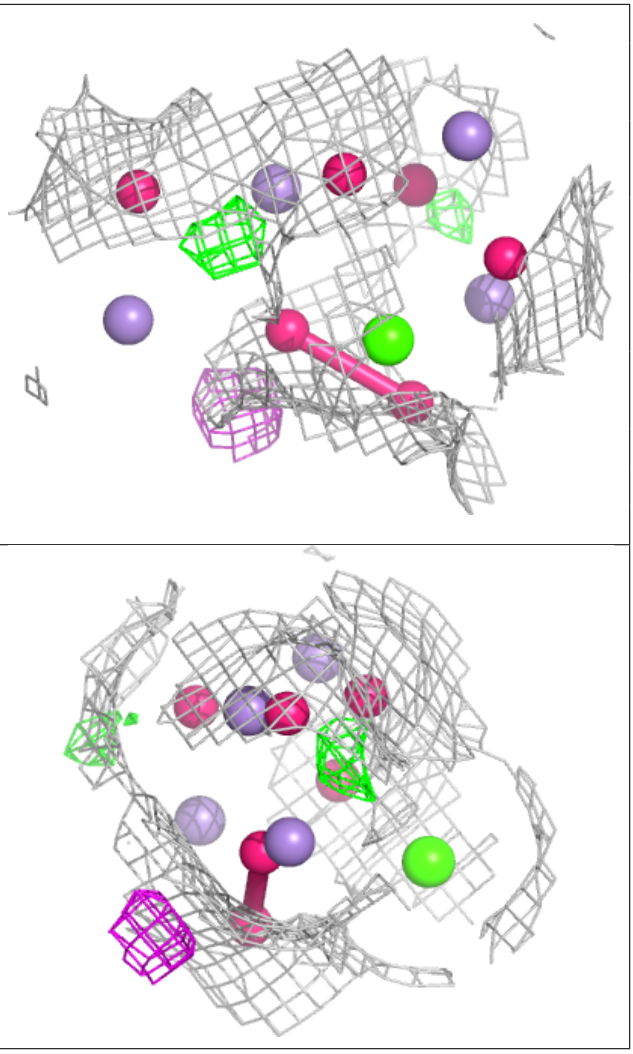
Electron density around OEY A 602 (A):

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



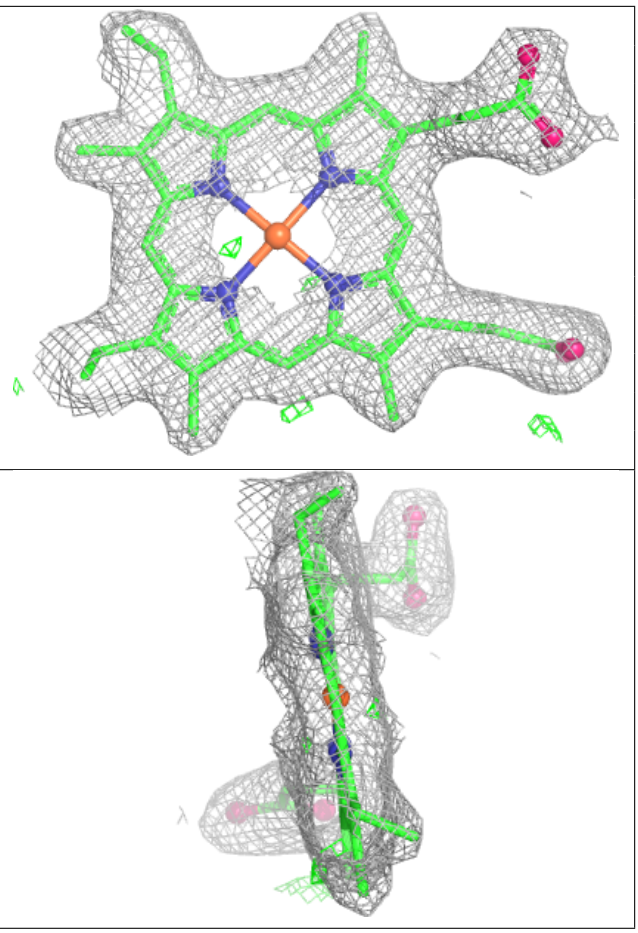
Electron density around OEY a 602 (A):

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



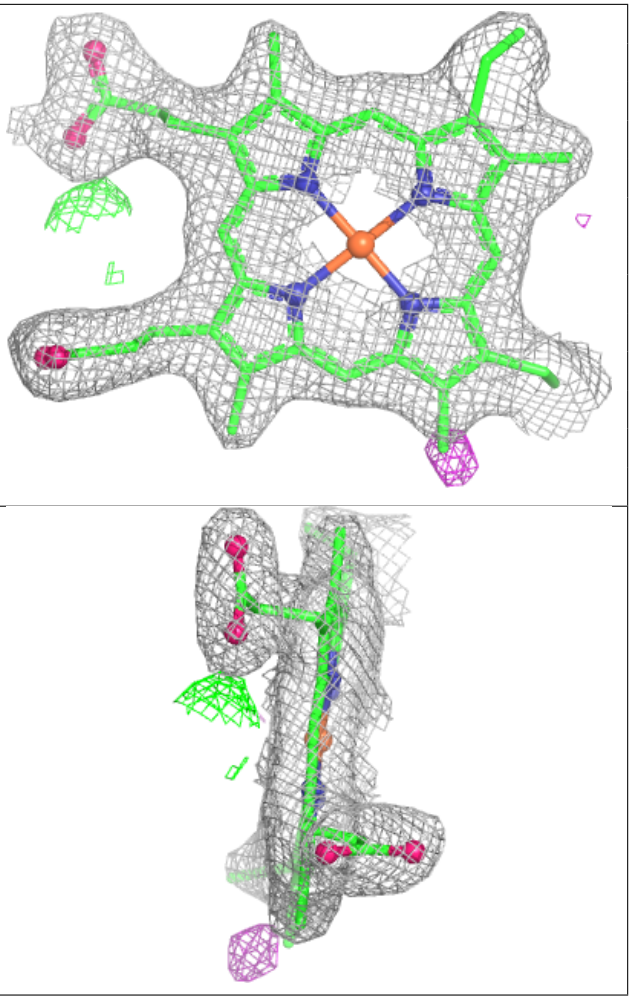
Electron density around HEC V 201:

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



Electron density around HEC v 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.