Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2026 – 01:14 AM UTC

PDB ID	:	7RF1 / pdb_00007rf1
Title	:	RT XFEL structure of Photosystem II averaged across all S-states at 1.89 Angstrom resolution
Authors	:	Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovski, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on	:	2021-07-13
Resolution	:	1.89 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:

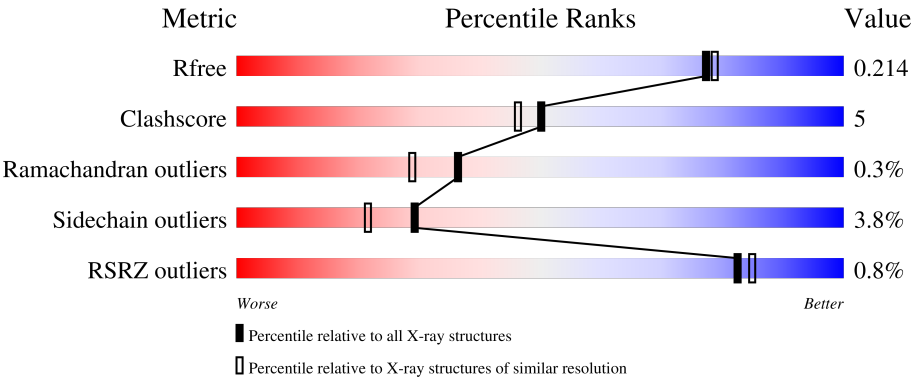
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)

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 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	92% 5%
1	a	344	% 87% 9%

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

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Mol	Chain	Length	Quality of chain
2	B	510	91% 8%
2	b	510	89% 9%
3	C	461	89% 6%
3	c	461	87% 10%
4	D	352	87% 10%
4	d	352	86% 10%
5	E	84	77% 19%
5	e	84	75% 23%
6	F	45	69% 7% 24%
6	f	45	60% 16% 24%
7	H	66	5% 91% 8%
7	h	66	5% 80% 14% 5%
8	I	38	79% 16% 5%
8	i	38	79% 16% 5%
9	J	40	75% 15% 10%
9	j	40	72% 15% 10%
10	K	46	70% 11% 20%
10	k	46	52% 28% 20%
11	L	37	92% 8%
11	l	37	81% 11% 5%
12	M	36	78% 14% 8%
12	m	36	64% 22% 11%
13	O	272	79% 9% 10%
13	o	272	82% 7% 10%
14	T	32	6% 84% 9% 6%

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Mol	Chain	Length	Quality of chain
14	t	32	6% 88% 6% 6%
15	U	134	63% 9% 28%
15	u	134	68% 28%
16	V	163	74% 9% 16%
16	v	163	63% 20% 16%
17	Y	46	7% 39% 17% 41%
17	y	46	43% 20% 35%
18	X	41	85% 5% 7%
18	x	41	73% 17% 5% 5%
19	Z	62	6% 73% 24%
19	z	62	74% 19% 6%
20	R	41	51% 15% 32%
20	r	41	22% 41% 20% 7% 32%

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
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	501	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	h	101	X	-	-	-
27	STE	A	417	-	-	X	-
27	STE	b	624	-	-	X	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 104284 atoms, of which 51760 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5140	1717	2518	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	1	0
			7824	2614	3840	665	692	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6775	2248	3350	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			557	187	282	45	42	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3700	1168	1830	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3720	1170	1846	317	383	4			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2137	675	1073	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2137	675	1073	177	208	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			
20	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

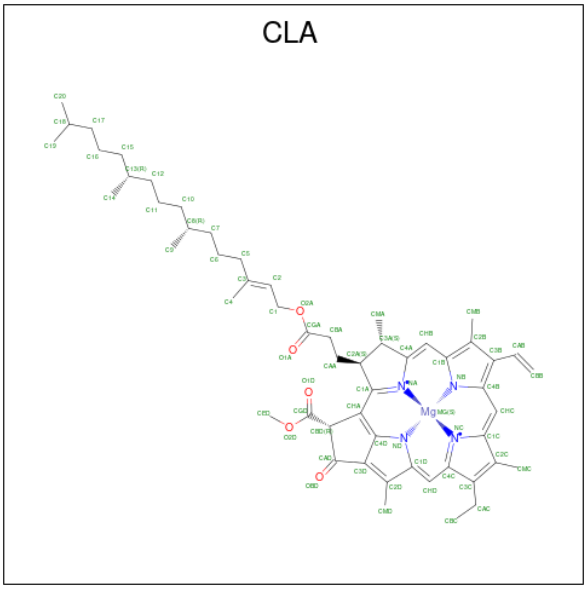
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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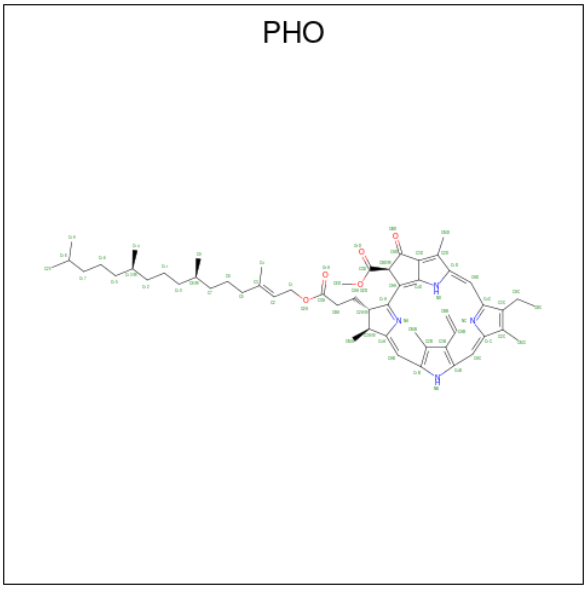
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

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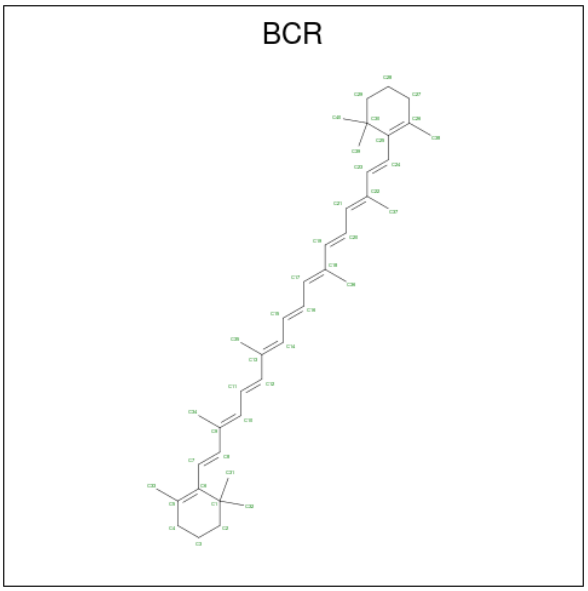
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	h	1	Total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

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



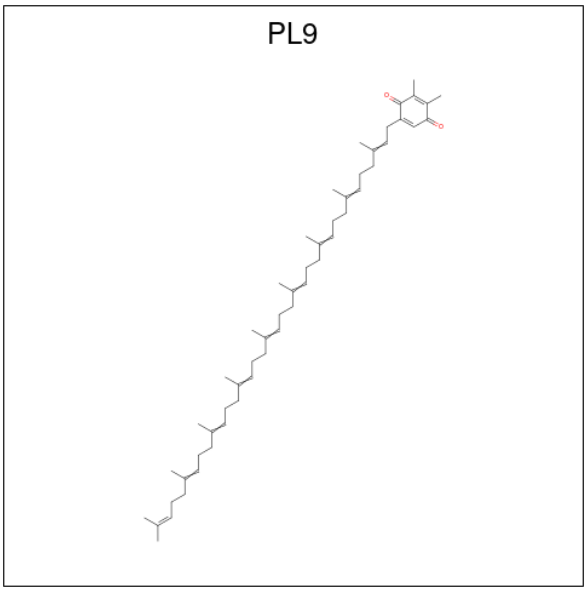
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	D	1	Total C H 96 40 56	0	0
25	H	1	Total C H 96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

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

- Molecule 26 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: $C_{53}H_{80}O_2$).



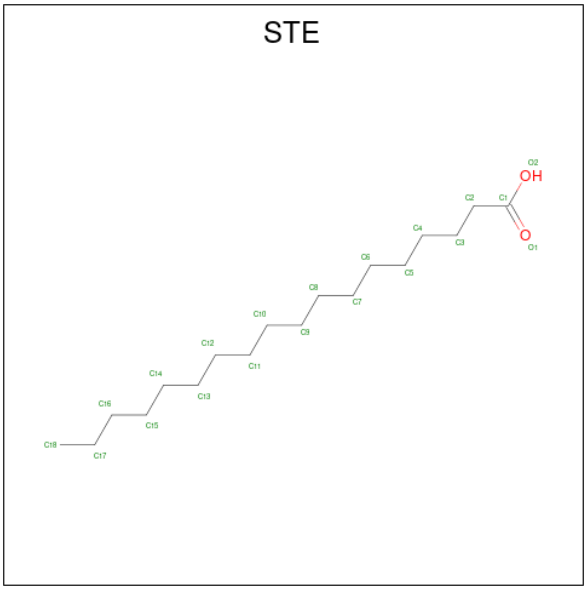
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C H O 135 53 80 2	0	0
26	D	1	Total C H O 135 53 80 2	0	0

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

- Molecule 27 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 9 9	0	0
27	A	1	Total C 8 8	0	0
27	A	1	Total C H 52 17 35	0	0
27	A	1	Total C 11 11	0	0
27	B	1	Total C H O 43 15 26 2	0	0
27	B	1	Total C H O 28 10 16 2	0	0
27	B	1	Total C H 41 15 26	0	0
27	C	1	Total C H O 35 12 21 2	0	0
27	C	1	Total C H 15 5 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C 7 7	0	0
27	C	1	Total C H O 28 10 16 2	0	0
27	C	1	Total C H 47 16 31	0	0
27	C	1	Total C 8 8	0	0
27	C	1	Total C 14 14	0	0
27	C	1	Total C H 43 14 29	0	0
27	D	1	Total C H O 55 18 35 2	0	0
27	D	1	Total C 9 9	0	0
27	E	1	Total C H O 28 10 16 2	0	0
27	E	1	Total C 12 12	0	0
27	E	1	Total C H O 55 18 35 2	0	0
27	H	1	Total C H 53 18 35	0	0
27	I	1	Total C H 41 15 26	0	0
27	I	1	Total C H O 45 15 28 2	0	0
27	J	1	Total C H O 28 10 16 2	0	0
27	M	1	Total C H O 37 13 22 2	0	0
27	M	1	Total C H 26 10 16	0	0
27	T	1	Total C H 46 16 30	0	0
27	Z	1	Total C H 52 17 35	0	0
27	a	1	Total C H 26 10 16	0	0
27	a	1	Total C H O 28 10 16 2	0	0

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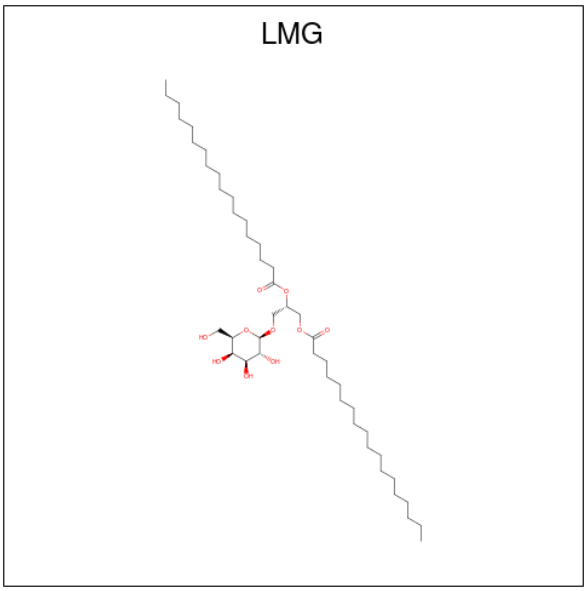
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C H O 55 18 35 2	0	0
27	b	1	Total C O 20 18 2	0	0
27	b	1	Total C H O 40 14 24 2	0	0
27	b	1	Total C H 26 10 16	0	0
27	b	1	Total C 11 11	0	0
27	c	1	Total C H 37 13 24	0	0
27	c	1	Total C H 53 18 35	0	0
27	d	1	Total C H O 43 15 26 2	0	0
27	d	1	Total C H O 28 10 16 2	0	0
27	d	1	Total C 10 10	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C 8 8	0	0
27	e	1	Total C 9 9	0	0
27	e	1	Total C O 13 11 2	0	0
27	i	1	Total C O 12 10 2	0	0
27	i	1	Total C H 18 6 12	0	0
27	j	1	Total C H O 28 10 16 2	0	0
27	j	1	Total C 16 16	0	0
27	l	1	Total C H 53 18 35	0	0
27	m	1	Total C H O 28 10 16 2	0	0
27	m	1	Total C H 44 15 29	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	t	1	Total C H O 34 12 20 2	0	0
27	t	1	Total C H O 46 16 28 2	0	0
27	x	1	Total C H O 55 18 35 2	0	0
27	z	1	Total C H 24 9 15	0	0

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



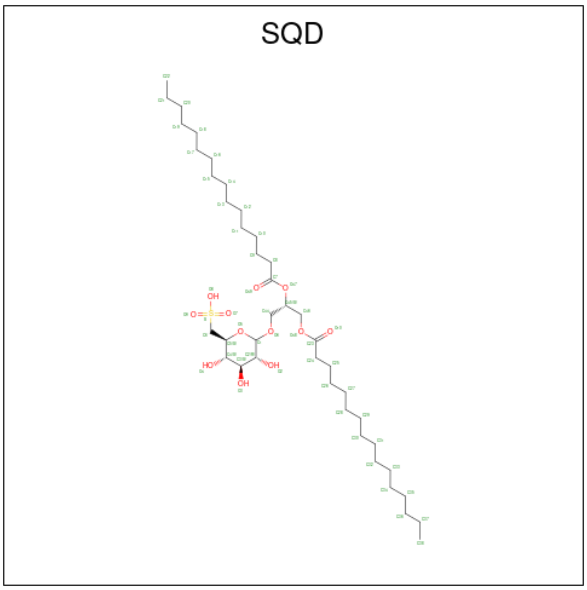
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H O 114 38 66 10	0	0
28	B	1	Total C H O 109 35 64 10	0	0
28	C	1	Total C H O 83 26 47 10	0	0
28	C	1	Total C H O 114 38 66 10	0	0
28	D	1	Total C H O 124 40 74 10	0	0
28	D	1	Total C H O 123 41 72 10	0	0
28	M	1	Total C H O 123 41 72 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	a	1	Total C H O 141 45 86 10	0	0
28	b	1	Total C O 24 20 4	0	0
28	b	1	Total C H O 123 41 72 10	0	0
28	b	1	Total C H O 141 45 86 10	0	0
28	c	1	Total C H O 75 25 45 5	0	0
28	c	1	Total C H O 110 36 64 10	0	0
28	c	1	Total C H O 117 38 69 10	0	0
28	c	1	Total C H O 117 39 68 10	0	0
28	d	1	Total C H O 102 34 58 10	0	0

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



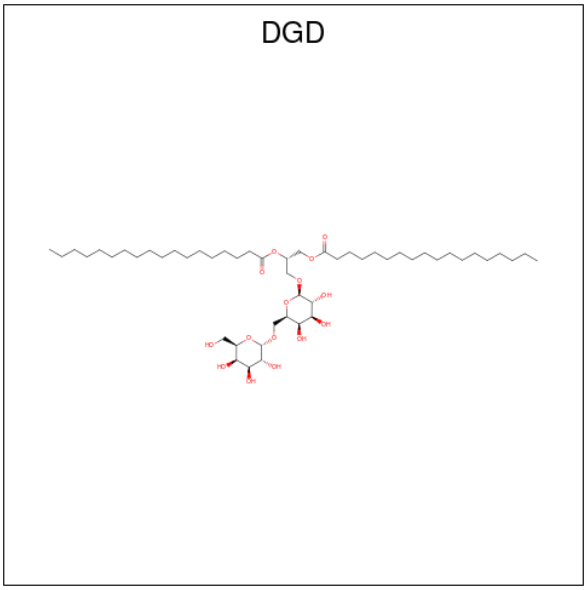
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C H O S 122 39 70 12 1	0	0
29	A	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total C H O S 81 25 45 10 1	0	0
29	a	1	Total C H O S 131 41 77 12 1	0	0
29	a	1	Total C O S 54 41 12 1	0	0
29	b	1	Total C H O S 113 36 64 12 1	0	0
29	f	1	Total C H O S 89 28 48 12 1	0	0
29	l	1	Total C H O S 131 41 77 12 1	0	0

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



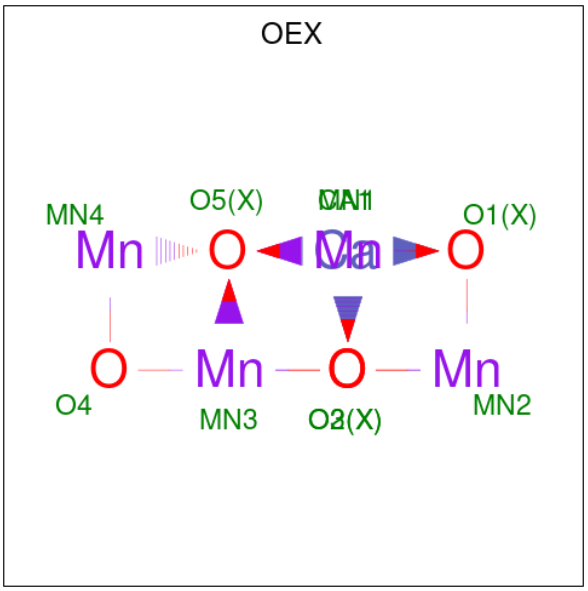
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C H O 162 51 96 15	0	0
30	C	1	Total C H O 144 47 82 15	0	0
30	C	1	Total C H O 144 47 82 15	0	0
30	C	1	Total C H O 144 47 82 15	0	0
30	H	1	Total C H O 144 47 82 15	0	0

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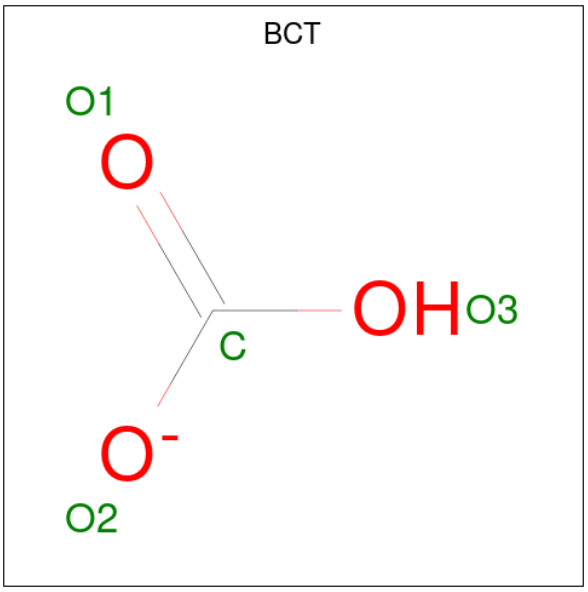
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	1	Total C H O 144 47 82 15	0	0
30	c	1	Total C H O 144 47 82 15	0	0
30	c	1	Total C H O 144 47 82 15	0	0
30	h	1	Total C H O 144 47 82 15	0	0

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



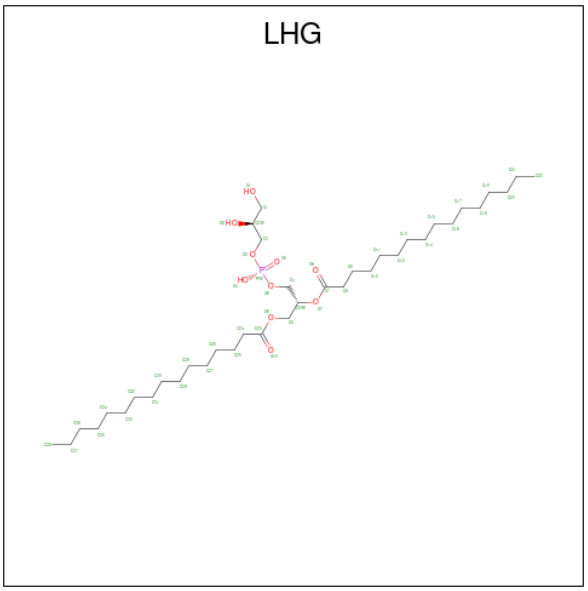
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total Ca Mn O 10 1 4 5	0	0
31	a	1	Total Ca Mn O 10 1 4 5	0	0

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



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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



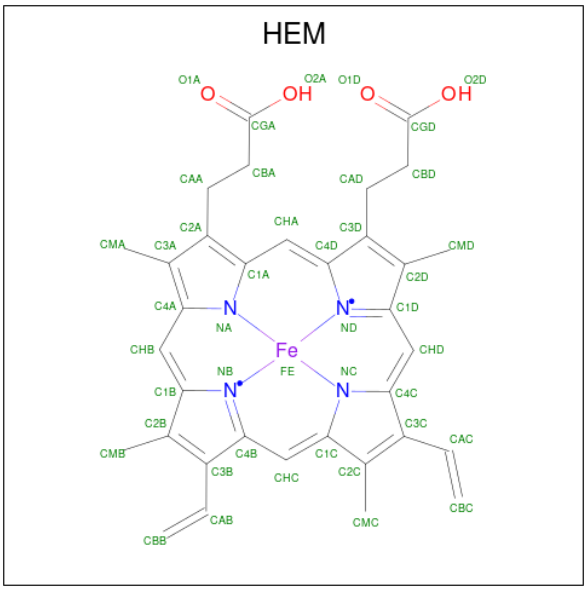
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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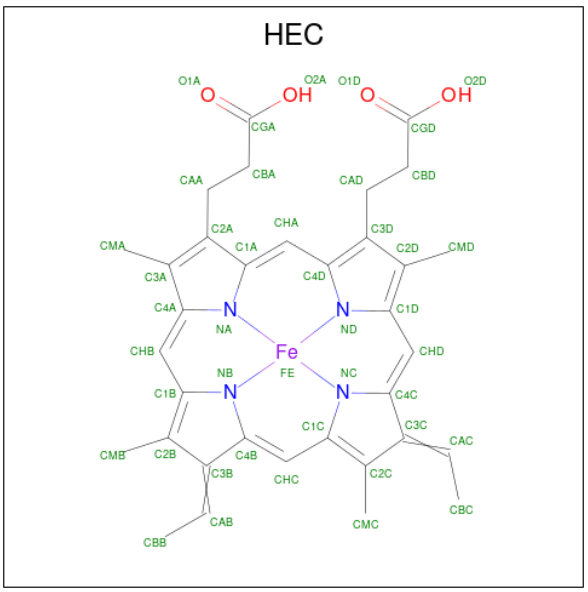
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	a	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	d	1	Total	C	H	O	P	0	0
			123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

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



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

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



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	202	Total	O	0	0
			202	202		
36	C	180	Total	O	0	0
			180	180		
36	D	137	Total	O	0	0
			137	137		
36	E	20	Total	O	0	0
			20	20		
36	F	11	Total	O	0	0
			11	11		
36	H	26	Total	O	0	0
			26	26		
36	I	9	Total	O	0	0
			9	9		
36	J	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	K	4	Total O 4 4	0	0
36	L	10	Total O 10 10	0	0
36	M	7	Total O 7 7	0	0
36	O	104	Total O 104 104	0	0
36	T	9	Total O 9 9	0	0
36	U	45	Total O 45 45	0	0
36	V	82	Total O 82 82	0	0
36	Y	1	Total O 1 1	0	0
36	X	12	Total O 12 12	0	0
36	a	115	Total O 115 115	0	0
36	b	200	Total O 200 200	0	0
36	c	171	Total O 171 171	0	0
36	d	125	Total O 125 125	0	0
36	e	10	Total O 10 10	0	0
36	f	10	Total O 10 10	0	0
36	h	23	Total O 23 23	0	0
36	i	5	Total O 5 5	0	0
36	j	6	Total O 6 6	0	0
36	k	5	Total O 5 5	0	0
36	l	15	Total O 15 15	0	0
36	m	7	Total O 7 7	0	0

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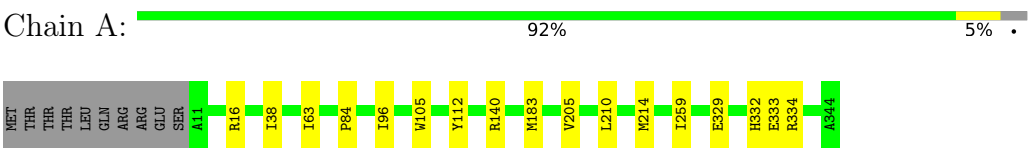
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	o	110	Total O 110 110	0	0
36	t	12	Total O 12 12	0	0
36	u	61	Total O 61 61	0	0
36	v	59	Total O 59 59	0	0
36	y	2	Total O 2 2	0	0
36	x	7	Total O 7 7	0	0
36	z	1	Total O 1 1	0	0

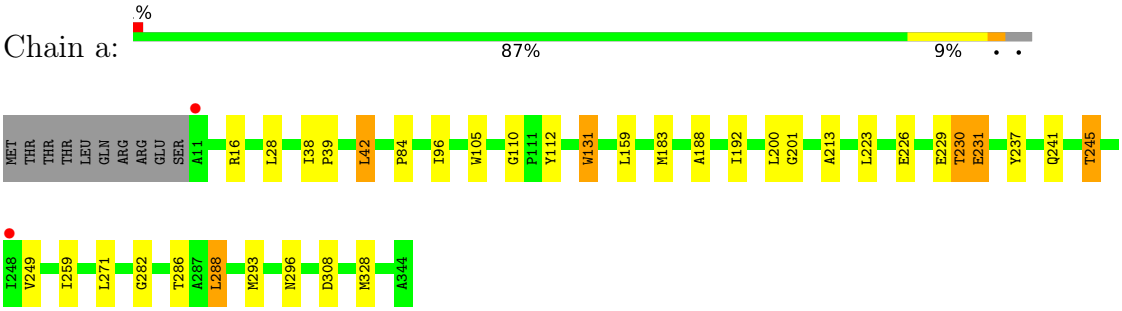
3 Residue-property plots (i)

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

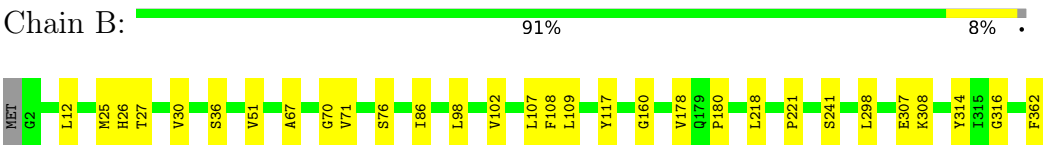
• Molecule 1: Photosystem II protein D1 1

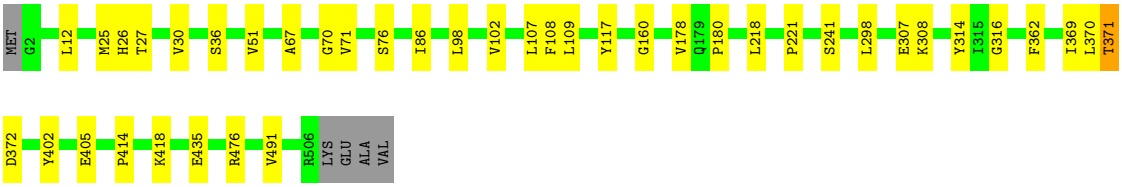


• Molecule 1: Photosystem II protein D1 1

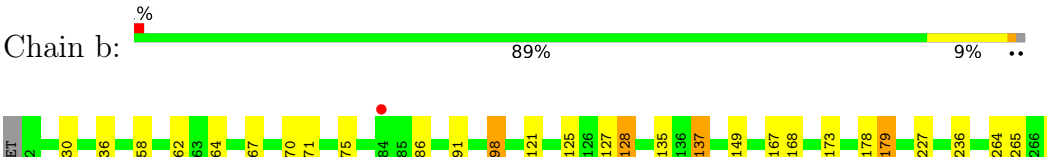


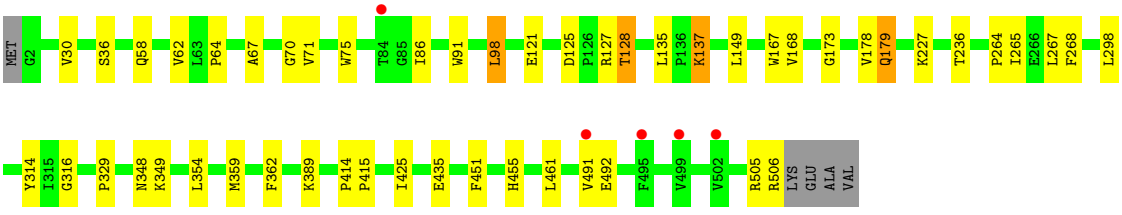
• Molecule 2: Photosystem II CP47 reaction center protein





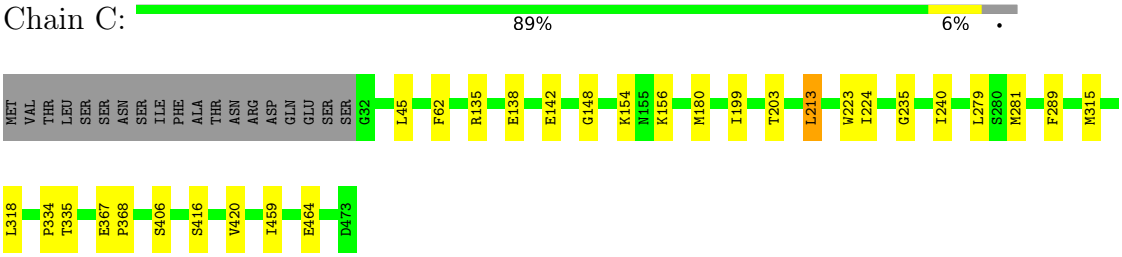
• Molecule 2: Photosystem II CP47 reaction center protein





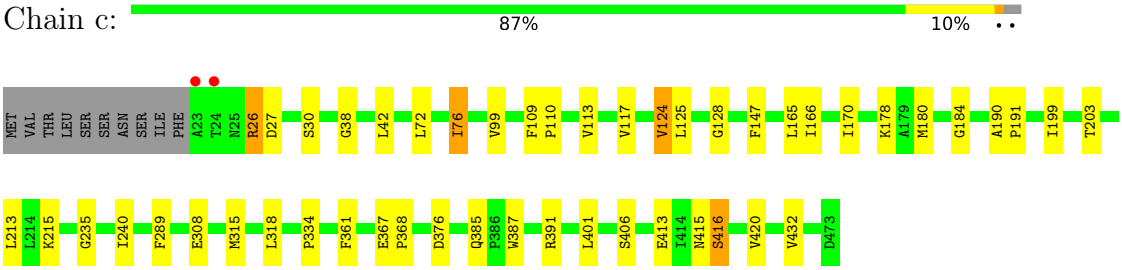
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



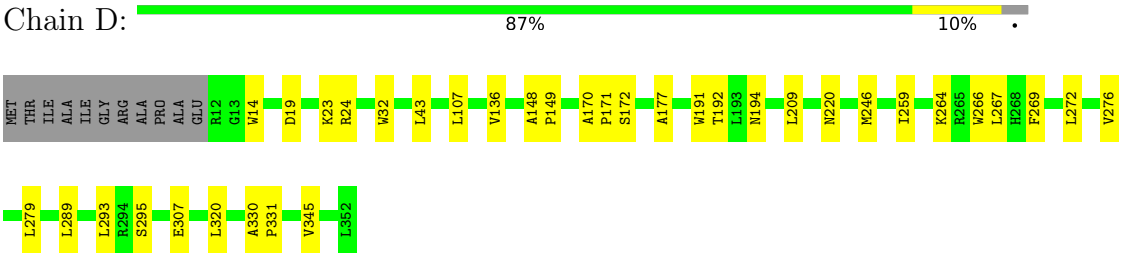
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



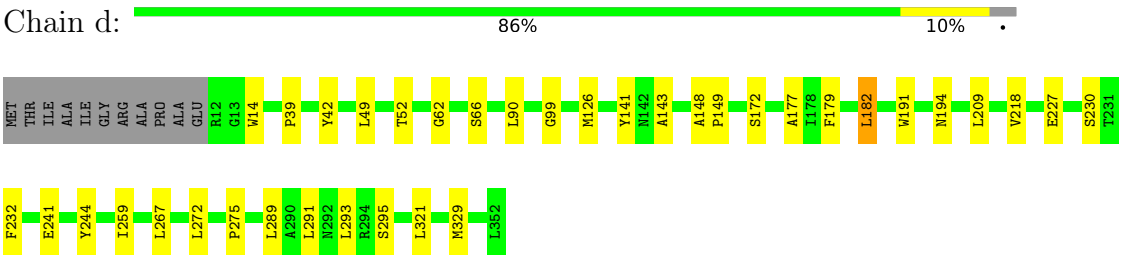
• Molecule 4: Photosystem II D2 protein

Chain D:



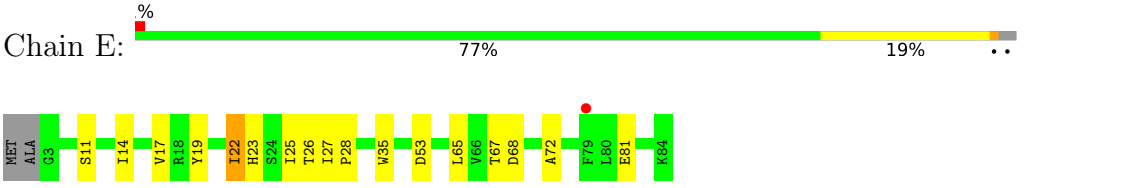
• Molecule 4: Photosystem II D2 protein

Chain d:



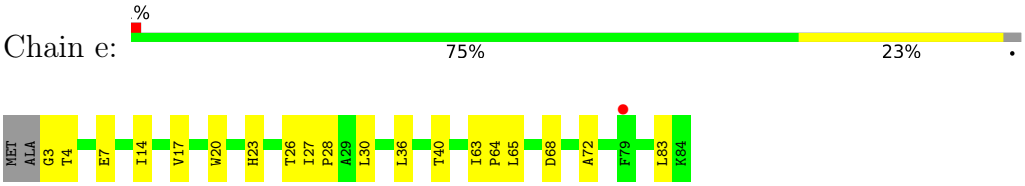
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



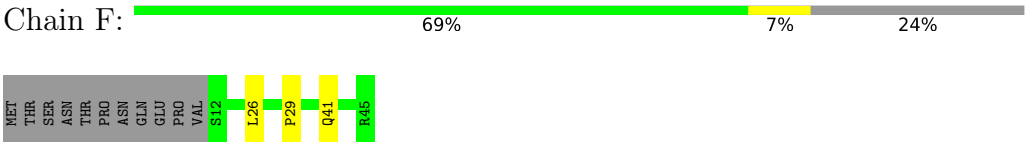
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



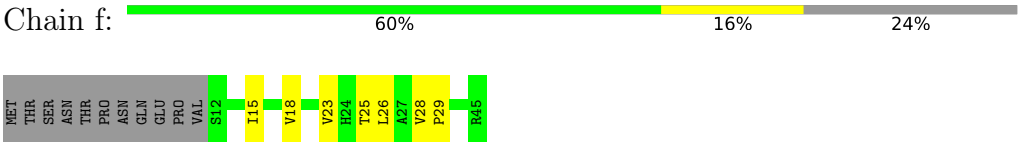
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



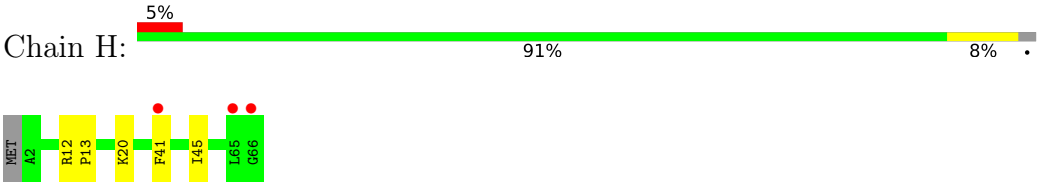
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



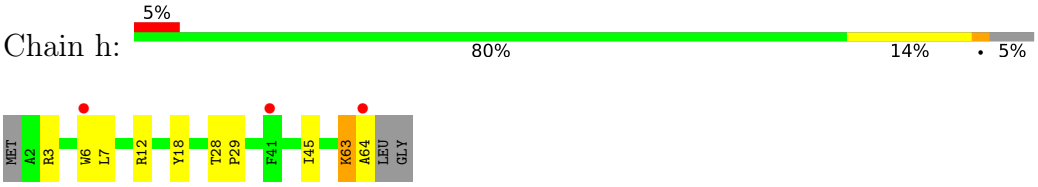
• Molecule 7: Photosystem II reaction center protein H

Chain H:



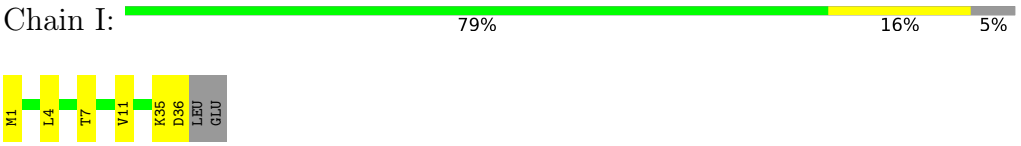
• Molecule 7: Photosystem II reaction center protein H

Chain h:



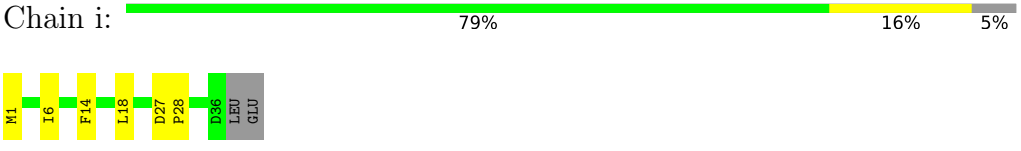
• Molecule 8: Photosystem II reaction center protein I

Chain I:



• Molecule 8: Photosystem II reaction center protein I

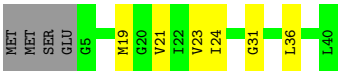
Chain i:



• Molecule 9: Photosystem II reaction center protein J

Chain J:

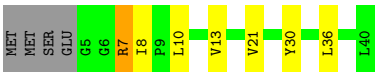




• Molecule 9: Photosystem II reaction center protein J

Chain j:

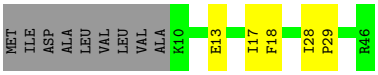




• Molecule 10: Photosystem II reaction center protein K

Chain K:

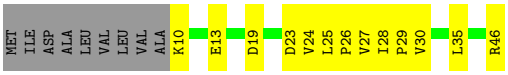




• Molecule 10: Photosystem II reaction center protein K

Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:

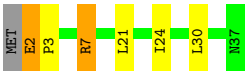




• Molecule 11: Photosystem II reaction center protein L

Chain l:

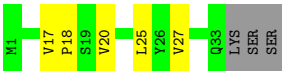




• Molecule 12: Photosystem II reaction center protein M

Chain M:





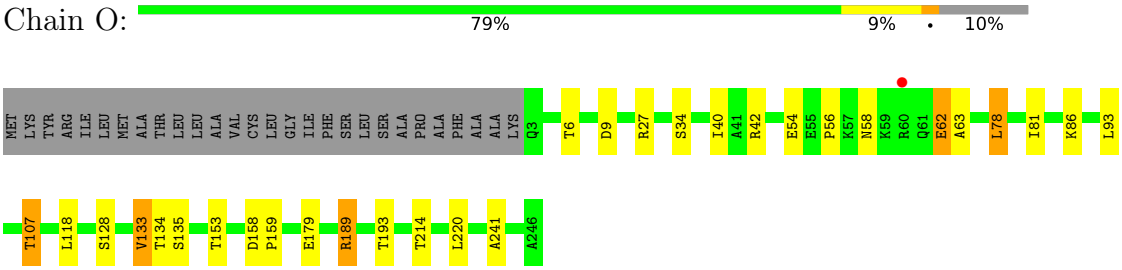
• Molecule 12: Photosystem II reaction center protein M

Chain m:



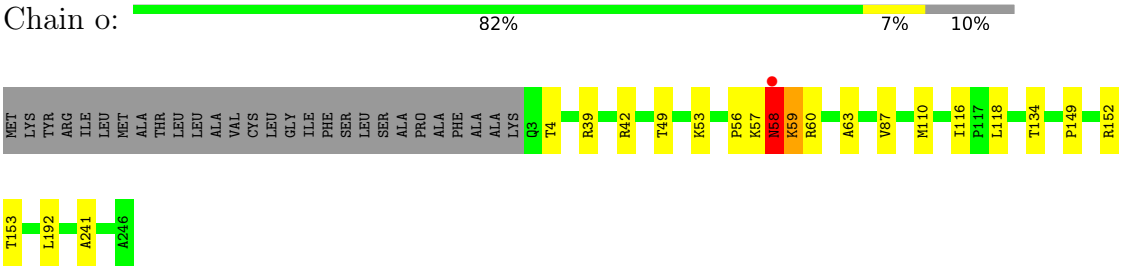
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



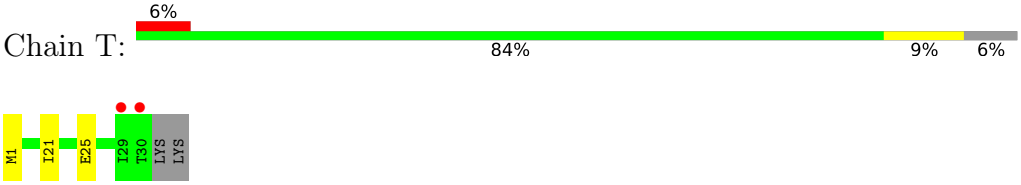
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



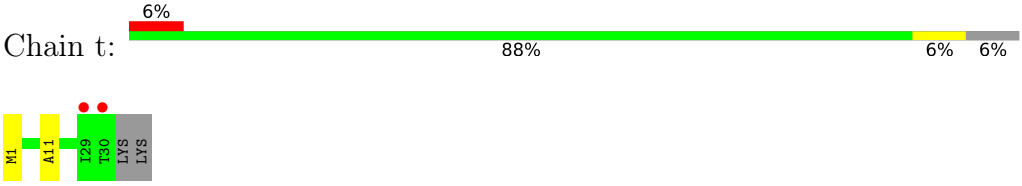
• Molecule 14: Photosystem II reaction center protein T

Chain T:



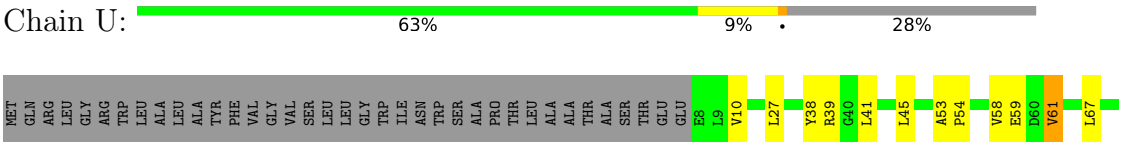
• Molecule 14: Photosystem II reaction center protein T

Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

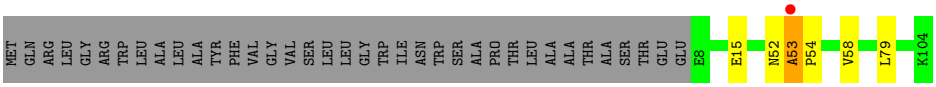




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:

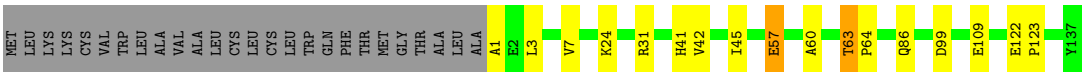




• Molecule 16: Cytochrome c-550

Chain V:





• Molecule 16: Cytochrome c-550

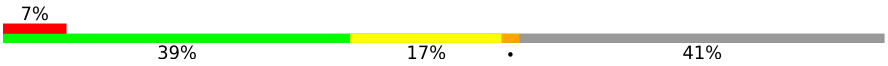
Chain v:

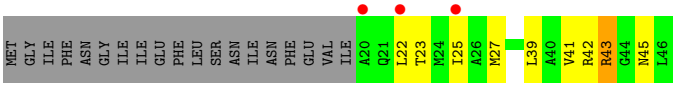




• Molecule 17: Photosystem II reaction center protein Ycf12

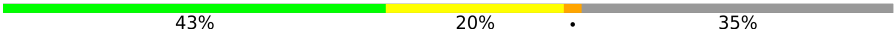
Chain Y:

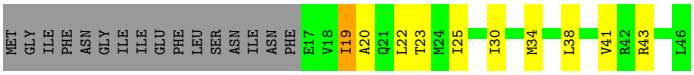




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:

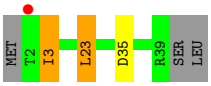




• Molecule 18: Photosystem II reaction center X protein

Chain X:

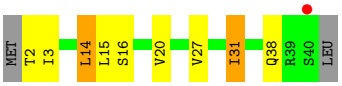




• Molecule 18: Photosystem II reaction center X protein

Chain x:

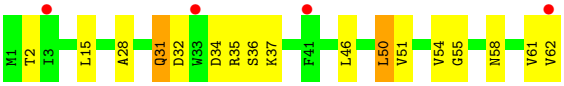




• Molecule 19: Photosystem II reaction center protein Z

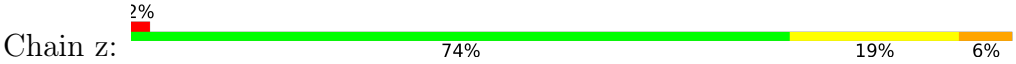
Chain Z:

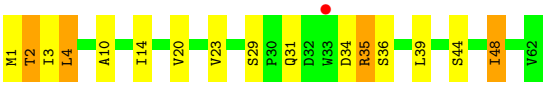




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

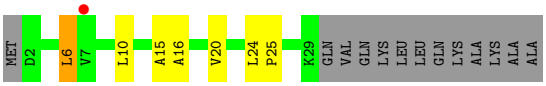




• Molecule 20: Photosystem II protein Y

Chain R:

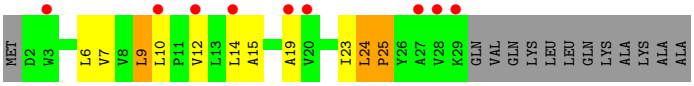




• Molecule 20: Photosystem II protein Y

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	117.00Å 221.60Å 307.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.67 – 1.89 33.67 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.67-1.89) 89.2 (33.67-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.42 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.214 0.171 , 0.214	Depositor DCC
R_{free} test set	5621 reflections (0.65%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	104284	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: SQD, PHO, STE, FE2, CLA, LHG, HEM, DGD, CL, LMG, BCT, OEX, PL9, FME, BCR, HEC

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	0.63	1/2707 (0.0%)	0.68	0/3692
1	a	0.58	1/2704 (0.0%)	0.70	2/3688 (0.1%)
2	B	0.54	1/4161 (0.0%)	0.62	0/5669
2	b	0.52	0/4127	0.60	0/5623
3	C	0.52	0/3546	0.61	0/4828
3	c	0.48	0/3619	0.58	0/4926
4	D	0.59	0/2812	0.63	0/3832
4	d	0.53	0/2821	0.62	0/3844
5	E	0.53	0/688	0.59	0/940
5	e	0.45	0/683	0.57	0/932
6	F	0.59	0/284	0.64	0/387
6	f	0.55	0/284	0.66	0/387
7	H	0.67	0/523	0.69	0/713
7	h	0.54	0/511	0.65	0/697
8	I	0.63	0/293	0.63	0/396
8	i	0.64	0/293	0.65	0/396
9	J	0.48	0/263	0.59	0/356
9	j	0.55	0/263	0.54	0/356
10	K	0.47	0/303	0.66	0/416
10	k	0.57	1/303 (0.3%)	0.55	0/416
11	L	0.72	0/311	0.74	0/422
11	l	0.64	0/303	0.68	0/412
12	M	0.64	0/249	0.71	0/341
12	m	0.68	0/244	0.71	0/334
13	O	0.62	0/1904	0.69	0/2585
13	o	0.61	0/1905	0.69	0/2583
14	T	0.69	0/257	0.74	0/349
14	t	0.70	0/255	0.67	0/346
15	U	0.53	0/785	0.63	0/1064
15	u	0.62	0/785	0.73	0/1064
16	V	0.62	0/1085	0.69	1/1473 (0.1%)
16	v	0.57	0/1085	0.66	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.46	0/197	0.58	0/264
17	y	0.42	0/219	0.56	0/294
18	X	0.48	0/284	0.60	0/384
18	x	0.42	0/289	0.52	0/391
19	Z	0.43	0/490	0.58	0/669
19	z	0.55	1/488 (0.2%)	0.56	0/666
20	R	0.35	0/227	0.54	0/313
20	r	0.33	0/227	0.44	0/313
All	All	0.56	5/42777 (0.0%)	0.64	3/58234 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1
15	u	0	1
16	V	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	ILE	CA-CB	13.22	1.61	1.54
19	z	23	VAL	CA-CB	-7.81	1.50	1.54
1	a	110	GLY	CA-C	6.98	1.56	1.51
10	k	28	ILE	CA-CB	-6.30	1.50	1.54
2	B	221	PRO	CA-C	6.26	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	110	GLY	O-C-N	12.76	125.66	121.07
1	a	131	TRP	CA-CB-CG	-5.03	104.05	113.60
16	V	63	THR	C-N-CD	-5.00	104.49	125.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide
13	o	152	ARG	Sidechain
15	u	52	ASN	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	2622	2518	2519	14	0
1	a	2619	2510	2510	21	0
2	B	4005	3873	3867	22	0
2	b	3984	3840	3842	42	0
3	C	3425	3350	3339	19	0
3	c	3500	3426	3426	31	0
4	D	2717	2621	2621	28	0
4	d	2723	2627	2627	21	0
5	E	666	651	651	11	0
5	e	664	648	648	16	0
6	F	275	282	282	2	0
6	f	275	282	282	8	0
7	H	510	532	532	4	0
7	h	498	518	518	6	0
8	I	296	311	311	2	0
8	i	296	311	311	2	0
9	J	257	268	268	7	0
9	j	257	268	268	6	0
10	K	293	305	305	2	0
10	k	293	305	305	6	0
11	L	304	316	316	2	0
11	l	296	304	304	4	0
12	M	256	269	269	3	0
12	m	251	267	267	7	0
13	O	1870	1830	1830	17	0
13	o	1874	1846	1846	10	0
14	T	258	261	261	1	0
14	t	256	256	256	1	0
15	U	774	773	773	7	0
15	u	774	773	773	6	0
16	V	1064	1073	1073	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	v	1064	1073	1073	18	0
17	Y	196	217	217	5	0
17	y	218	241	241	6	0
18	X	281	312	312	3	0
18	x	286	316	314	4	0
19	Z	479	516	516	8	0
19	z	477	509	509	9	0
20	R	221	238	238	4	0
20	r	221	238	238	7	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	184	192	192	3	0
23	B	1035	1139	1139	14	0
23	C	839	922	922	20	0
23	D	195	216	216	4	0
23	a	260	288	288	2	0
23	b	970	1067	1067	18	0
23	c	839	919	919	19	0
23	d	130	144	144	3	0
23	h	65	72	72	2	0
24	A	64	74	74	3	0
24	D	64	74	74	1	0
24	a	64	74	74	1	0
24	d	64	74	74	1	0
25	A	40	56	56	0	0
25	B	120	168	168	8	0
25	C	120	168	168	4	0
25	D	40	56	56	6	0
25	H	40	56	56	3	0
25	K	40	56	56	3	0
25	T	40	56	56	4	0
25	a	40	56	56	3	0
25	b	120	168	168	6	0
25	c	80	112	112	7	0
25	d	40	56	56	2	0
25	k	80	112	112	1	0
25	t	40	56	56	4	0
25	x	40	56	56	3	0
26	A	55	80	80	0	0
26	D	55	80	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	a	55	80	80	2	0
26	d	55	80	80	0	0
27	A	45	35	83	11	0
27	B	44	68	68	1	0
27	C	90	107	152	5	0
27	D	29	35	52	2	0
27	E	44	51	74	6	0
27	H	18	35	35	0	0
27	I	32	54	52	2	0
27	J	12	16	16	2	0
27	M	25	38	38	0	0
27	T	16	30	31	0	0
27	Z	17	35	33	0	0
27	a	22	32	32	0	0
27	b	77	75	131	14	0
27	c	31	59	57	1	0
27	d	39	42	61	4	0
27	e	39	0	67	5	0
27	i	18	12	24	3	0
27	j	28	16	44	4	0
27	l	18	35	35	3	0
27	m	27	45	45	0	0
27	t	32	48	48	0	0
27	x	20	35	35	1	0
27	z	9	15	14	0	0
28	A	48	66	66	2	0
28	B	45	64	60	1	0
28	C	84	113	106	3	0
28	D	101	146	142	5	0
28	M	51	72	71	0	0
28	a	55	86	86	1	0
28	b	130	158	179	14	0
28	c	173	246	240	3	0
28	d	44	58	58	1	0
29	A	106	70	149	12	0
29	F	36	45	45	2	0
29	a	108	77	156	10	0
29	b	49	64	65	1	0
29	f	41	48	49	2	0
29	l	54	77	78	0	0
30	A	66	96	96	7	0
30	C	186	246	245	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	H	62	82	80	1	0
30	c	186	246	242	4	0
30	h	62	82	80	0	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	D	4	1	1	0	0
32	a	4	1	1	0	0
33	D	145	215	215	4	0
33	E	49	74	74	4	0
33	L	49	74	74	0	0
33	a	42	57	57	1	0
33	d	137	199	199	7	0
33	l	49	74	74	1	0
34	F	43	30	30	2	0
34	f	43	30	30	7	0
35	V	43	32	30	0	0
35	v	43	32	30	3	0
36	A	144	0	0	2	0
36	B	202	0	0	2	0
36	C	180	0	0	2	0
36	D	137	0	0	4	0
36	E	20	0	0	0	0
36	F	11	0	0	0	0
36	H	26	0	0	0	0
36	I	9	0	0	1	0
36	J	13	0	0	1	0
36	K	4	0	0	0	0
36	L	10	0	0	0	0
36	M	7	0	0	0	0
36	O	104	0	0	3	0
36	T	9	0	0	0	0
36	U	45	0	0	2	0
36	V	82	0	0	1	0
36	X	12	0	0	0	0
36	Y	1	0	0	0	0
36	a	115	0	0	2	0
36	b	200	0	0	1	0
36	c	171	0	0	4	0
36	d	125	0	0	1	0
36	e	10	0	0	1	0
36	f	10	0	0	1	0
36	h	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	i	5	0	0	0	0
36	j	6	0	0	1	0
36	k	5	0	0	2	0
36	l	15	0	0	0	0
36	m	7	0	0	0	0
36	o	110	0	0	0	0
36	t	12	0	0	0	0
36	u	61	0	0	0	0
36	v	59	0	0	1	0
36	x	7	0	0	0	0
36	y	2	0	0	0	0
36	z	1	0	0	0	0
All	All	52524	51760	52200	549	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 (549) 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)
16:v:40:CYS:SG	35:v:201:HEC:CAC	2.05	1.45
2:b:267:LEU:HD13	28:b:619:LMG:C2	1.94	0.98
2:b:267:LEU:HD22	28:b:619:LMG:C1	1.95	0.96
28:C:517:LMG:HO4	28:C:517:LMG:HO5	1.17	0.93
16:v:76:MET:HE2	16:v:112:LEU:HD22	1.50	0.91
7:h:64:ALA:HB2	36:h:201:HOH:O	1.72	0.90
27:j:102:STE:H21	27:j:102:STE:H71	1.56	0.86
2:b:167:TRP:CE2	2:b:267:LEU:HD11	2.10	0.86
28:D:408:LMG:O5	36:D:501:HOH:O	1.94	0.85
28:b:623:LMG:O5	36:b:701:HOH:O	1.92	0.85
10:k:19:ASP:OD2	36:k:201:HOH:O	1.95	0.84
27:i:101:STE:H32	27:i:101:STE:H91	1.60	0.83
28:C:517:LMG:O5	28:C:517:LMG:O4	1.93	0.81
16:v:40:CYS:SG	35:v:201:HEC:C3C	2.69	0.80
27:i:101:STE:H91	27:i:101:STE:C3	2.12	0.79
30:c:519:DGD:O1A	36:c:601:HOH:O	2.02	0.77
13:O:6:THR:HG22	13:O:9:ASP:OD2	1.85	0.76
27:b:624:STE:H61	27:b:627:STE:C17	2.15	0.76
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.69	0.75
29:a:414:SQD:H361	25:t:101:BCR:H332	1.70	0.74
29:A:413:SQD:H322	27:A:416:STE:H61	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.23	0.72
15:u:53:ALA:HB1	15:u:54:PRO:CD	2.18	0.72
5:e:68:ASP:O	5:e:72:ALA:HB2	1.90	0.72
23:b:612:CLA:H203	33:d:406:LHG:H223	1.72	0.72
3:c:376:ASP:OD2	36:c:602:HOH:O	2.08	0.72
9:J:36:LEU:O	36:J:201:HOH:O	2.09	0.71
13:O:179:GLU:OE1	36:O:301:HOH:O	2.09	0.71
4:d:141:TYR:OH	33:d:406:LHG:O4	2.05	0.71
27:A:416:STE:C18	27:A:417:STE:H141	2.22	0.70
23:C:504:CLA:H91	23:C:508:CLA:H172	1.74	0.69
2:B:241:SER:HB3	23:B:612:CLA:HED3	1.72	0.69
17:Y:23:THR:HG22	17:Y:27:MET:HE3	1.73	0.69
13:o:57:LYS:O	13:o:59:LYS:N	2.26	0.69
25:D:406:BCR:H392	25:D:406:BCR:H23C	1.74	0.69
27:b:624:STE:H61	27:b:627:STE:H171	1.74	0.68
7:h:63:LYS:O	36:h:201:HOH:O	2.10	0.68
15:u:53:ALA:CB	15:u:54:PRO:CD	2.71	0.68
9:j:36:LEU:O	36:j:201:HOH:O	2.12	0.68
10:k:13:GLU:N	10:k:13:GLU:OE1	2.28	0.67
25:b:618:BCR:H331	25:b:618:BCR:C8	2.25	0.67
27:b:624:STE:H32	27:b:627:STE:H181	1.77	0.67
4:d:267:LEU:C	4:d:267:LEU:HD23	2.19	0.67
15:U:58:VAL:O	15:U:61:VAL:HG22	1.95	0.66
23:B:604:CLA:H43	23:B:605:CLA:H2	1.75	0.66
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.61	0.66
30:C:521:DGD:O1A	36:C:601:HOH:O	2.12	0.65
5:e:30:LEU:HD11	34:f:101:HEM:CBB	2.27	0.65
23:B:601:CLA:H142	36:B:895:HOH:O	1.95	0.65
27:b:624:STE:C3	27:b:627:STE:H181	2.27	0.65
4:D:107:LEU:O	36:D:502:HOH:O	2.15	0.64
28:b:621:LMG:O10	12:m:4:ASN:ND2	2.30	0.64
29:A:413:SQD:H352	30:A:414:DGD:HAE2	1.80	0.64
25:H:101:BCR:H331	25:H:101:BCR:C8	2.26	0.64
4:d:126:MET:HE3	4:d:143:ALA:O	1.97	0.64
13:O:189:ARG:NE	36:O:302:HOH:O	2.13	0.63
16:V:109:GLU:OE1	36:V:301:HOH:O	2.15	0.63
25:b:617:BCR:H331	25:b:617:BCR:C8	2.26	0.63
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.13	0.62
25:d:404:BCR:H331	25:d:404:BCR:C8	2.29	0.62
25:t:101:BCR:HC8	25:t:101:BCR:H311	1.82	0.62
23:c:501:CLA:H192	23:c:507:CLA:HBB1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:403:CLA:HBB1	23:d:403:CLA:HMB3	1.81	0.62
23:c:504:CLA:H91	23:c:508:CLA:C18	2.29	0.62
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.81	0.62
3:c:391[A]:ARG:NE	36:c:603:HOH:O	2.32	0.62
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.82	0.62
33:E:101:LHG:O1	27:E:103:STE:H81	2.00	0.61
10:K:17:ILE:HG23	10:K:18:PHE:CD2	2.36	0.61
2:b:267:LEU:CD2	28:b:619:LMG:C1	2.75	0.61
9:J:19:MET:HE3	25:K:101:BCR:C36	2.31	0.61
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.83	0.61
2:b:86:ILE:HD12	2:b:86:ILE:O	2.00	0.61
29:A:413:SQD:H301	30:A:414:DGD:HAN2	1.82	0.60
25:C:514:BCR:H331	25:C:514:BCR:C8	2.30	0.60
27:e:101:STE:C18	27:e:104:STE:H71	2.30	0.60
3:c:27:ASP:OD1	3:c:30:SER:OG	2.17	0.60
23:b:612:CLA:H192	33:d:406:LHG:H223	1.83	0.60
25:B:619:BCR:H331	25:B:619:BCR:C8	2.31	0.60
17:Y:39:LEU:HD21	19:Z:28:ALA:HB3	1.82	0.60
15:U:70:ARG:NH2	36:U:202:HOH:O	2.30	0.60
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.84	0.59
5:e:20:TRP:HH2	27:e:101:STE:H152	1.67	0.59
34:f:101:HEM:HHD	34:f:101:HEM:HBC2	1.84	0.59
13:O:6:THR:HG22	13:O:9:ASP:CG	2.27	0.59
20:R:16:ALA:O	20:R:20:VAL:HG23	2.03	0.59
15:u:53:ALA:HB1	15:u:54:PRO:HD3	1.84	0.59
16:v:104:MET:HA	16:v:107:LEU:HD22	1.84	0.59
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.84	0.59
5:e:7:GLU:OE2	36:e:201:HOH:O	2.15	0.59
23:C:507:CLA:H191	27:C:528:STE:H101	1.85	0.58
36:A:573:HOH:O	13:O:107:THR:HG21	2.04	0.58
4:D:272:LEU:C	4:D:272:LEU:HD23	2.29	0.58
11:l:24:ILE:HD13	12:m:18:PRO:HB2	1.86	0.58
17:y:19:ILE:HD13	17:y:20:ALA:N	2.18	0.58
4:D:264:LYS:CE	36:D:506:HOH:O	2.52	0.57
25:b:617:BCR:H331	25:b:617:BCR:HC8	1.86	0.57
15:U:59:GLU:OE1	36:U:201:HOH:O	2.17	0.57
2:b:492:GLU:OE1	5:e:3:GLY:N	2.38	0.57
27:A:416:STE:H182	27:A:417:STE:H141	1.85	0.57
24:a:407:PHO:HBB1	24:a:407:PHO:HMB3	1.86	0.57
24:A:406:PHO:HBC3	4:D:279:LEU:HD22	1.87	0.56
3:c:113:VAL:O	3:c:117:VAL:HG23	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:213:LEU:HD11	25:c:515:BCR:C20	2.35	0.56
2:b:267:LEU:HD13	28:b:619:LMG:C1	2.35	0.56
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.56
4:D:209:LEU:HD23	4:D:209:LEU:C	2.31	0.56
5:e:17:VAL:HG23	9:j:7:ARG:CD	2.36	0.56
10:k:23:ASP:OD2	36:k:201:HOH:O	2.17	0.56
5:E:11:SER:HB3	27:E:103:STE:H122	1.88	0.56
29:A:413:SQD:H381	27:I:101:STE:C15	2.36	0.56
3:c:391[A]:ARG:CZ	36:c:603:HOH:O	2.54	0.56
18:x:16:SER:O	18:x:20:VAL:HG23	2.06	0.56
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.89	0.55
2:b:267:LEU:HB2	28:b:619:LMG:C3	2.35	0.55
2:B:371:THR:HG23	2:B:372:ASP:O	2.07	0.55
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.71	0.55
19:z:10:ALA:O	19:z:14:ILE:HD13	2.07	0.55
2:b:227:LYS:CE	27:b:624:STE:H22	2.37	0.55
19:z:36:SER:HA	19:z:39:LEU:HD23	1.89	0.55
4:d:272:LEU:C	4:d:272:LEU:HD23	2.31	0.55
23:C:511:CLA:HBB1	23:C:511:CLA:HMB3	1.89	0.55
23:b:613:CLA:H171	23:b:613:CLA:H141	1.88	0.55
27:e:101:STE:H181	27:e:104:STE:H71	1.89	0.55
23:C:507:CLA:H192	27:C:528:STE:H82	1.88	0.55
28:a:415:LMG:C10	28:a:415:LMG:O8	2.54	0.55
2:b:227:LYS:NZ	27:b:624:STE:H22	2.22	0.55
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.88	0.55
25:B:618:BCR:H331	25:B:618:BCR:C8	2.36	0.54
15:u:53:ALA:CB	15:u:54:PRO:HD2	2.37	0.54
19:z:44:SER:O	19:z:48:ILE:HD12	2.07	0.54
13:O:56:PRO:O	13:O:58:ASN:N	2.41	0.54
17:y:19:ILE:HD13	17:y:19:ILE:C	2.33	0.54
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.43	0.54
3:c:406:SER:HA	3:c:420:VAL:HG23	1.89	0.54
3:C:203:THR:O	3:C:235:GLY:HA3	2.08	0.54
5:E:65:LEU:O	5:E:67:THR:HG23	2.07	0.54
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.73	0.54
2:b:227:LYS:HE3	27:b:624:STE:H22	1.90	0.54
29:F:102:SQD:O6	29:F:102:SQD:O48	2.26	0.54
2:b:125:ASP:OD2	2:b:128:THR:HG23	2.09	0.53
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.90	0.53
23:C:509:CLA:H91	23:C:512:CLA:HAA2	1.91	0.53
23:b:612:CLA:C20	33:d:406:LHG:H223	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.90	0.53
5:e:26:THR:HA	20:r:15:ALA:HB1	1.89	0.53
12:M:27:VAL:HG13	27:l:103:STE:H62	1.91	0.53
24:d:401:PHO:HBC2	24:d:401:PHO:HHD	1.90	0.53
27:A:416:STE:C18	27:A:417:STE:H121	2.39	0.53
2:b:268:PHE:CE2	28:b:619:LMG:C4	2.92	0.53
16:v:13:ASN:OD1	16:v:15:GLU:N	2.41	0.53
25:H:101:BCR:H331	25:H:101:BCR:HC8	1.89	0.53
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.91	0.53
25:K:101:BCR:H321	25:K:101:BCR:HC8	1.91	0.53
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.09	0.53
34:f:101:HEM:HMA1	20:r:23:ILE:HD12	1.91	0.53
29:A:413:SQD:H321	30:A:414:DGD:CDA	2.39	0.52
27:j:102:STE:H21	27:j:102:STE:C7	2.34	0.52
23:C:513:CLA:H202	27:C:526:STE:C17	2.40	0.52
2:b:36:SER:OG	25:b:617:BCR:H362	2.09	0.52
23:B:616:CLA:C2	23:B:616:CLA:O1A	2.57	0.52
25:D:406:BCR:H331	25:D:406:BCR:C8	2.40	0.52
23:B:606:CLA:H72	25:B:619:BCR:H311	1.91	0.52
2:b:167:TRP:CD2	2:b:267:LEU:HD11	2.44	0.52
34:F:101:HEM:HBB2	34:F:101:HEM:HMB1	1.92	0.51
17:Y:23:THR:CG2	17:Y:27:MET:HE3	2.39	0.51
16:v:12:LEU:HD23	16:v:17:LYS:HD3	1.91	0.51
17:y:34:MET:O	17:y:38:LEU:HG	2.10	0.51
29:A:413:SQD:H223	23:D:403:CLA:H201	1.93	0.51
23:C:502:CLA:H61	23:C:512:CLA:H42	1.91	0.51
29:a:414:SQD:H1	36:a:601:HOH:O	2.09	0.51
13:o:56:PRO:HD3	13:o:63:ALA:HB2	1.92	0.51
29:F:102:SQD:H342	18:X:23:LEU:HD22	1.93	0.51
1:a:42:LEU:HD21	29:a:414:SQD:H341	1.93	0.51
3:c:180:MET:HG2	3:c:199:ILE:O	2.11	0.51
23:b:603:CLA:H42	23:b:604:CLA:H2	1.93	0.51
23:c:506:CLA:O1A	23:c:506:CLA:C2	2.59	0.51
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.45	0.51
1:a:249:VAL:HG12	2:b:491:VAL:HG21	1.93	0.50
3:C:213:LEU:HG	23:C:506:CLA:H193	1.92	0.50
3:c:318:LEU:C	3:c:318:LEU:HD23	2.36	0.50
25:t:101:BCR:H23C	25:t:101:BCR:H382	1.93	0.50
9:j:10:LEU:O	9:j:13:VAL:HG22	2.11	0.50
2:B:109:LEU:HD13	29:a:414:SQD:H282	1.92	0.50
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:503:CLA:H203	23:c:510:CLA:HAB	1.92	0.50
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.50
16:v:76:MET:HE1	16:v:115:ILE:HD12	1.92	0.50
4:D:307:GLU:HG3	36:D:512:HOH:O	2.12	0.50
25:D:406:BCR:H392	25:D:406:BCR:C23	2.42	0.50
27:b:624:STE:H52	27:d:410:STE:C2	2.42	0.50
16:V:57:GLU:CD	16:V:57:GLU:H	2.19	0.49
25:k:101:BCR:H321	25:k:101:BCR:HC8	1.94	0.49
13:o:4:THR:HG22	13:o:4:THR:O	2.12	0.49
19:z:1:MET:HB3	19:z:4:LEU:HG	1.95	0.49
25:T:101:BCR:H311	25:T:101:BCR:C8	2.42	0.49
4:D:192:THR:HG23	23:D:404:CLA:HBC2	1.94	0.49
29:a:412:SQD:H462	4:d:232:PHE:CE2	2.47	0.49
23:c:509:CLA:H43	23:c:509:CLA:O1A	2.12	0.49
20:r:19:ALA:O	20:r:23:ILE:HG22	2.13	0.49
23:b:613:CLA:H121	23:b:613:CLA:H91	1.95	0.49
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.95	0.49
19:z:2:THR:HG22	19:z:3:ILE:N	2.27	0.49
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.94	0.49
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.94	0.49
5:E:53:ASP:O	16:V:1:ALA:N	2.45	0.49
5:e:17:VAL:HG23	9:j:7:ARG:HD2	1.95	0.49
16:v:40:CYS:SG	35:v:201:HEC:CBC	2.96	0.49
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.95	0.49
5:E:68:ASP:O	5:E:72:ALA:HB2	2.13	0.49
16:v:41:HIS:HA	16:v:45:ILE:O	2.13	0.49
3:C:154:LYS:NZ	36:C:608:HOH:O	2.46	0.49
3:C:180:MET:HG2	3:C:199:ILE:O	2.13	0.49
2:b:127:ARG:NH2	7:h:18:TYR:O	2.44	0.49
27:A:416:STE:H161	27:A:417:STE:H102	1.94	0.48
25:C:514:BCR:H331	25:C:514:BCR:HC8	1.93	0.48
3:c:180:MET:HE1	28:c:523:LMG:HC72	1.95	0.48
3:c:124:VAL:HG13	25:c:514:BCR:H362	1.94	0.48
3:C:45:LEU:HD22	3:C:138:GLU:HG2	1.94	0.48
27:j:102:STE:H32	27:j:102:STE:H62	1.50	0.48
25:D:406:BCR:H402	9:J:21:VAL:HG13	1.95	0.48
2:b:62:VAL:HB	23:b:604:CLA:HED3	1.95	0.48
3:C:318:LEU:C	3:C:318:LEU:HD23	2.39	0.48
9:J:19:MET:HE3	25:K:101:BCR:H361	1.94	0.48
9:j:30:TYR:OH	27:j:102:STE:H21	2.14	0.48
25:a:409:BCR:H331	25:a:409:BCR:C8	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:508:CLA:H191	30:c:520:DGD:HA71	1.96	0.48
25:c:514:BCR:H24C	25:c:514:BCR:H371	1.71	0.48
6:f:23:VAL:HG21	34:f:101:HEM:HBD2	1.95	0.48
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.49	0.48
1:A:16:ARG:HG2	27:A:417:STE:C11	2.44	0.47
30:C:522:DGD:CFA	27:J:101:STE:C10	2.92	0.47
20:r:6:LEU:O	20:r:10:LEU:HG	2.14	0.47
1:a:259:ILE:HG21	26:a:410:PL9:H202	1.95	0.47
26:a:410:PL9:H48	4:d:39:PRO:HG3	1.96	0.47
2:B:102:VAL:HA	25:B:618:BCR:C40	2.45	0.47
19:Z:51:VAL:O	19:Z:54:VAL:O	2.32	0.47
6:f:18:VAL:HG22	29:f:102:SQD:H272	1.96	0.47
13:o:58:ASN:O	13:o:60:ARG:N	2.47	0.47
6:f:15:ILE:HG13	36:f:205:HOH:O	2.14	0.47
3:C:135:ARG:O	3:C:135:ARG:HD3	2.15	0.47
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.96	0.47
5:e:36:LEU:O	5:e:40:THR:HG23	2.15	0.47
1:A:16:ARG:NH1	1:A:16:ARG:HB2	2.30	0.47
29:A:413:SQD:C38	27:I:101:STE:C15	2.93	0.47
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.97	0.47
23:b:614:CLA:H2	23:b:615:CLA:HBB2	1.97	0.47
4:d:14:TRP:HE1	27:d:412:STE:H122	1.80	0.47
4:d:49:LEU:HD13	25:d:404:BCR:C15	2.44	0.47
4:d:209:LEU:HD23	4:d:209:LEU:C	2.39	0.47
1:A:329:GLU:HG3	36:A:620:HOH:O	2.14	0.47
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.29	0.47
2:B:117:TYR:HA	11:L:1:MET:HE1	1.97	0.47
2:b:64:PRO:O	28:b:619:LMG:C4	2.63	0.46
4:d:194:ASN:HA	4:d:295:SER:OG	2.15	0.46
4:d:230:SER:HB2	36:d:550:HOH:O	2.15	0.46
25:D:406:BCR:H402	9:J:21:VAL:CG1	2.45	0.46
2:b:267:LEU:CG	28:b:619:LMG:C1	2.93	0.46
4:d:62:GLY:HA3	5:e:63:ILE:HD13	1.97	0.46
12:m:9:ILE:HG13	12:m:13:LEU:HD22	1.98	0.46
13:o:56:PRO:CD	13:o:63:ALA:HB2	2.46	0.46
1:a:183:MET:HA	23:a:405:CLA:HMD1	1.95	0.46
33:l:102:LHG:H101	33:l:102:LHG:H241	1.97	0.46
1:A:183:MET:HG2	23:D:403:CLA:HBC1	1.98	0.46
4:D:14:TRP:HE1	27:D:414:STE:H121	1.80	0.46
5:E:35:TRP:HE1	27:E:104:STE:H111	1.81	0.46
13:O:27:ARG:O	13:O:27:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:124:VAL:HG11	25:c:514:BCR:C16	2.46	0.46
23:c:513:CLA:C4B	25:c:514:BCR:H383	2.44	0.46
27:A:416:STE:C16	27:A:417:STE:H102	2.46	0.46
28:C:517:LMG:C7	28:C:517:LMG:O9	2.59	0.46
1:a:201:GLY:HA3	1:a:286:THR:HB	1.97	0.46
28:b:619:LMG:H152	28:b:619:LMG:H121	1.57	0.46
3:c:178:LYS:NZ	3:c:184:GLY:O	2.49	0.46
23:c:513:CLA:O2A	27:c:516:STE:H101	2.16	0.46
1:a:213:ALA:HB2	4:d:275:PRO:HG2	1.98	0.46
15:u:53:ALA:HB1	15:u:54:PRO:HD2	1.97	0.46
2:b:359:MET:HB2	2:b:425:ILE:HD12	1.98	0.46
6:f:28:VAL:CG2	6:f:29:PRO:HD3	2.41	0.46
16:v:64:PRO:HD2	16:v:66:ARG:NH2	2.31	0.46
1:A:84:PRO:HA	1:A:112:TYR:CG	2.51	0.46
25:C:520:BCR:C8	25:C:520:BCR:H331	2.45	0.46
2:b:98:LEU:HD11	23:b:605:CLA:H152	1.96	0.46
2:b:264:PRO:HD2	28:b:619:LMG:C3	2.46	0.46
27:d:412:STE:H101	27:d:412:STE:H131	1.80	0.46
2:B:218:LEU:HD12	27:B:622:STE:H21	1.98	0.46
2:B:307:GLU:OE1	13:o:59:LYS:HD3	2.16	0.46
23:C:504:CLA:C14	23:C:508:CLA:H141	2.46	0.46
3:c:124:VAL:HG11	25:c:514:BCR:H16C	1.98	0.46
1:a:84:PRO:HA	1:a:112:TYR:CG	2.51	0.45
1:a:308:ASP:OD1	1:a:308:ASP:C	2.60	0.45
29:A:413:SQD:H352	30:A:414:DGD:CBA	2.44	0.45
23:C:504:CLA:C13	23:C:508:CLA:H141	2.46	0.45
27:b:624:STE:C6	27:b:627:STE:H171	2.45	0.45
29:A:413:SQD:H223	23:D:403:CLA:C20	2.46	0.45
13:O:133:VAL:C	13:O:134:THR:HG23	2.41	0.45
16:V:41:HIS:O	16:V:42:VAL:C	2.60	0.45
29:a:414:SQD:H331	29:a:414:SQD:H302	1.35	0.45
27:D:414:STE:H121	27:D:414:STE:H151	1.70	0.45
13:O:107:THR:HG22	36:O:343:HOH:O	2.16	0.45
27:b:624:STE:H101	27:b:624:STE:H71	1.32	0.45
23:B:613:CLA:C10	23:B:613:CLA:H142	2.46	0.45
8:I:36:ASP:OD1	36:I:201:HOH:O	2.21	0.45
16:V:99:ASP:N	16:V:99:ASP:OD1	2.46	0.45
23:B:601:CLA:C12	23:B:601:CLA:H91	2.47	0.45
5:e:27:ILE:HB	5:e:28:PRO:CD	2.47	0.45
3:C:281:MET:HE1	23:C:505:CLA:HBC3	1.97	0.45
23:b:614:CLA:HHC	23:b:614:CLA:HBB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:14:ILE:O	5:e:20:TRP:NE1	2.49	0.45
12:m:17:VAL:HB	12:m:18:PRO:HD3	1.99	0.45
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	1.99	0.45
12:M:17:VAL:HB	12:M:18:PRO:HD3	1.98	0.45
1:a:230:THR:HG23	1:a:231:GLU:HG2	1.98	0.45
23:C:510:CLA:HMB3	23:C:510:CLA:HBB1	1.99	0.45
15:U:53:ALA:HB1	15:U:54:PRO:HA	1.98	0.45
19:Z:32:ASP:O	19:Z:36:SER:OG	2.25	0.45
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.51	0.45
27:i:101:STE:H91	27:i:101:STE:H61	1.26	0.45
10:k:25:LEU:N	10:k:26:PRO:CD	2.80	0.45
5:E:26:THR:HA	20:R:15:ALA:HB1	1.98	0.44
25:x:101:BCR:H24C	25:x:101:BCR:H371	1.87	0.44
29:A:413:SQD:H321	30:A:414:DGD:HAH2	1.99	0.44
4:D:194:ASN:HA	4:D:295:SER:OG	2.17	0.44
29:a:414:SQD:H342	29:a:414:SQD:H371	1.36	0.44
1:A:16:ARG:HD2	27:A:417:STE:H111	1.99	0.44
23:C:506:CLA:H143	30:C:521:DGD:CGA	2.48	0.44
5:E:22[A]:ILE:HD11	5:E:26:THR:HG21	1.99	0.44
15:U:39:ARG:NH2	16:V:60:ALA:O	2.51	0.44
11:l:7:ARG:NH1	27:l:103:STE:H41	2.32	0.44
29:a:412:SQD:O10	29:a:412:SQD:C26	2.65	0.44
23:b:612:CLA:H192	33:d:406:LHG:C22	2.46	0.44
10:K:28:ILE:N	10:K:29:PRO:CD	2.81	0.44
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.53	0.44
3:C:367:GLU:N	3:C:368:PRO:CD	2.80	0.44
23:C:511:CLA:HMB3	23:C:511:CLA:CBB	2.48	0.44
13:O:78:LEU:HB3	13:O:81:ILE:HD11	2.00	0.44
6:f:15:ILE:HD11	34:f:101:HEM:O2A	2.18	0.44
23:C:507:CLA:C19	27:C:528:STE:H101	2.46	0.44
33:E:101:LHG:HC82	27:E:103:STE:H152	2.00	0.44
16:V:41:HIS:HA	16:V:45:ILE:O	2.18	0.44
19:Z:61:VAL:O	19:Z:62:VAL:C	2.61	0.44
33:a:413:LHG:H252	36:a:529:HOH:O	2.16	0.44
23:h:101:CLA:CHA	23:h:101:CLA:HBA2	2.46	0.44
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.99	0.44
23:C:513:CLA:H202	27:C:526:STE:H171	2.00	0.44
15:U:27:LEU:HD13	15:U:61:VAL:CG1	2.48	0.44
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.52	0.44
1:a:282:GLY:CA	29:a:412:SQD:H223	2.48	0.44
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:412:SQD:O10	29:a:412:SQD:H262	2.18	0.43
8:i:14:PHE:CZ	8:i:18:LEU:HD11	2.52	0.43
4:D:267:LEU:C	4:D:267:LEU:HD23	2.43	0.43
10:k:26:PRO:O	10:k:29:PRO:HD2	2.18	0.43
23:B:602:CLA:HBB1	23:B:602:CLA:HMB1	2.00	0.43
16:v:122:GLU:N	16:v:123:PRO:HD2	2.34	0.43
18:x:27:VAL:O	18:x:31:ILE:HD13	2.18	0.43
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.53	0.43
13:O:93:LEU:O	13:O:128:SER:HA	2.19	0.43
25:T:101:BCR:HC8	25:T:101:BCR:H321	2.00	0.43
30:A:414:DGD:HD5	2:b:75:TRP:HB3	2.00	0.43
27:A:415:STE:H182	27:A:415:STE:H151	1.77	0.43
2:B:36:SER:OG	25:B:618:BCR:H362	2.18	0.43
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.43
9:J:19:MET:O	9:J:23:VAL:HG23	2.18	0.43
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.00	0.43
2:b:30:VAL:HG12	23:b:604:CLA:HHD	2.00	0.43
6:f:26:LEU:O	6:f:29:PRO:HD2	2.18	0.43
20:r:9:LEU:O	20:r:12:VAL:HG22	2.19	0.43
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.01	0.43
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.86	0.43
4:D:330:ALA:HB3	4:D:331:PRO:HD3	2.00	0.43
20:R:24:LEU:HB3	20:R:25:PRO:HD3	2.01	0.43
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.43
16:v:19:ILE:HG21	16:v:69:ILE:HD12	2.01	0.43
19:z:35:ARG:CD	19:z:35:ARG:H	2.31	0.43
28:A:411:LMG:C39	3:C:281:MET:HG3	2.49	0.43
19:z:1:MET:O	19:z:2:THR:C	2.60	0.43
30:C:522:DGD:O1A	30:C:522:DGD:HA41	2.18	0.43
1:a:296:ASN:HB3	3:c:401:LEU:HA	2.00	0.43
30:c:520:DGD:HE62	28:c:522:LMG:O3	2.19	0.43
17:y:19:ILE:HD13	17:y:20:ALA:CA	2.49	0.43
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.01	0.43
4:D:266:TRP:CD1	33:D:410:LHG:HC31	2.53	0.43
3:c:367:GLU:N	3:c:368:PRO:CD	2.82	0.43
11:l:2:GLU:N	11:l:3:PRO:HD3	2.34	0.43
25:D:406:BCR:H371	25:D:406:BCR:H24C	1.79	0.42
5:E:25:ILE:N	5:E:25:ILE:HD12	2.34	0.42
23:A:404:CLA:HBB1	23:A:404:CLA:HMB1	2.00	0.42
4:d:179:PHE:HA	4:d:182:LEU:HD22	2.00	0.42
28:d:409:LMG:C43	27:e:104:STE:C11	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:413:SQD:H192	29:A:413:SQD:H162	1.70	0.42
2:B:414:PRO:O	2:B:418:LYS:HG3	2.19	0.42
8:i:27:ASP:N	8:i:28:PRO:CD	2.81	0.42
1:A:214:MET:SD	24:A:406:PHO:CAD	3.07	0.42
25:C:515:BCR:H15C	25:C:515:BCR:H351	1.89	0.42
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.02	0.42
23:a:411:CLA:HBB1	23:a:411:CLA:HMB1	2.01	0.42
2:b:135:LEU:HB3	23:b:609:CLA:HBC2	2.01	0.42
23:b:612:CLA:C19	33:d:406:LHG:H223	2.47	0.42
3:c:38:GLY:HA3	23:c:511:CLA:HMD2	2.00	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.42
4:d:52:THR:O	4:d:66:SER:HA	2.19	0.42
29:A:413:SQD:H341	30:A:414:DGD:HAH2	2.00	0.42
19:Z:50:LEU:O	19:Z:54:VAL:HG23	2.20	0.42
23:c:512:CLA:H142	23:c:513:CLA:H142	2.01	0.42
5:e:20:TRP:CH2	27:e:101:STE:H152	2.50	0.42
18:x:3:ILE:N	18:x:3:ILE:HD12	2.34	0.42
1:A:183:MET:HA	23:A:404:CLA:HMD1	2.02	0.42
27:A:416:STE:H183	27:A:417:STE:H121	2.00	0.42
2:B:26:HIS:CE1	23:B:612:CLA:HMA2	2.55	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.37	0.42
33:D:410:LHG:H321	14:T:21:ILE:HD11	2.01	0.42
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.42
8:I:7:THR:O	8:I:11:VAL:HG23	2.20	0.42
27:J:101:STE:O1	27:J:101:STE:C4	2.68	0.42
25:b:617:BCR:HC8	25:b:617:BCR:C33	2.49	0.42
28:A:411:LMG:O10	28:A:411:LMG:C31	2.68	0.42
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.53	0.42
23:B:611:CLA:HMB3	23:B:611:CLA:HBB1	2.00	0.42
3:C:279:LEU:HD12	23:C:509:CLA:HED2	2.02	0.42
23:A:404:CLA:H201	33:D:410:LHG:H312	2.00	0.42
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.02	0.42
19:Z:55:GLY:HA2	19:Z:58:ASN:HB3	2.00	0.42
1:a:249:VAL:HG12	2:b:491:VAL:CG2	2.49	0.42
23:b:601:CLA:H43	7:h:45:ILE:HG22	2.01	0.42
1:A:63:ILE:HB	3:C:335:THR:HG21	2.01	0.42
23:C:508:CLA:H191	30:C:522:DGD:HA92	2.02	0.42
2:B:369:ILE:C	2:B:370:LEU:HD12	2.45	0.42
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	2.02	0.42
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.50	0.42
4:D:269:PHE:CD2	33:D:412:LHG:HC12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:272:LEU:HD23	4:D:272:LEU:O	2.20	0.42
13:O:54:GLU:O	13:O:63:ALA:CB	2.68	0.42
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.50	0.42
27:b:624:STE:H81	27:d:410:STE:H22	2.00	0.42
3:c:166:ILE:HG21	23:c:512:CLA:H202	2.02	0.42
4:d:99:GLY:HA3	27:x:102:STE:H41	2.02	0.42
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.02	0.42
2:B:26:HIS:O	2:B:30:VAL:HG23	2.20	0.41
25:b:616:BCR:H11C	25:b:616:BCR:H341	1.94	0.41
3:c:76:ILE:CD1	3:c:76:ILE:N	2.83	0.41
23:d:403:CLA:HBB1	23:d:403:CLA:CMB	2.50	0.41
16:v:2:GLU:HB2	36:v:312:HOH:O	2.20	0.41
3:C:148:GLY:O	3:C:156:LYS:NZ	2.50	0.41
4:D:24:ARG:NH2	18:X:35:ASP:OD2	2.53	0.41
4:D:272:LEU:C	4:D:272:LEU:CD2	2.93	0.41
11:L:14:ARG:HH22	29:b:620:SQD:H3	1.85	0.41
2:b:461:LEU:HD11	28:b:621:LMG:C25	2.50	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41
16:v:93:PRO:HA	16:v:101:PHE:CD2	2.55	0.41
27:A:416:STE:H183	27:A:417:STE:H141	2.00	0.41
2:B:67:ALA:HA	2:B:71:VAL:O	2.20	0.41
23:B:613:CLA:HMB1	23:B:613:CLA:HBB1	2.02	0.41
3:C:334:PRO:HA	13:O:153:THR:OG1	2.21	0.41
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.09	0.41
25:a:409:BCR:H20C	25:a:409:BCR:H361	1.92	0.41
2:b:137:LYS:HE3	36:h:207:HOH:O	2.21	0.41
23:b:613:CLA:H141	23:b:613:CLA:C17	2.50	0.41
13:o:149:PRO:HA	13:o:192:LEU:HD12	2.02	0.41
6:F:26:LEU:O	6:F:29:PRO:HD2	2.21	0.41
25:H:101:BCR:H11C	25:H:101:BCR:H341	1.93	0.41
3:c:190:ALA:O	3:c:191:PRO:C	2.62	0.41
23:c:513:CLA:H92	23:c:513:CLA:H51	2.03	0.41
19:z:34:ASP:O	19:z:35:ARG:C	2.64	0.41
23:B:602:CLA:H43	7:H:45:ILE:HG22	2.03	0.41
3:C:62:PHE:CD1	3:C:62:PHE:C	2.97	0.41
4:D:19:ASP:OD1	4:D:23:LYS:NZ	2.53	0.41
18:X:3:ILE:O	18:X:3:ILE:HG13	2.21	0.41
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.89	0.41
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.56	0.41
23:c:507:CLA:HAA2	23:c:507:CLA:HBD	2.03	0.41
33:d:406:LHG:H212	12:m:18:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:102:SQD:C44	29:f:102:SQD:O2	2.68	0.41
20:r:24:LEU:N	20:r:25:PRO:HD2	2.35	0.41
25:B:618:BCR:H20C	25:B:618:BCR:H361	1.90	0.41
25:B:618:BCR:H371	25:B:618:BCR:H24C	1.84	0.41
19:Z:31:GLN:CG	19:Z:32:ASP:H	2.34	0.41
20:R:6:LEU:HD11	20:R:10:LEU:HD13	2.03	0.41
3:c:128:GLY:HA3	23:c:513:CLA:C3C	2.51	0.41
13:o:110:MET:HE2	13:o:116:ILE:HD11	2.03	0.41
19:z:1:MET:O	19:z:4:LEU:N	2.46	0.41
4:D:32:TRP:CD1	28:D:408:LMG:H171	2.56	0.41
33:E:101:LHG:O10	27:E:103:STE:H92	2.21	0.41
25:T:101:BCR:H20C	25:T:101:BCR:H361	1.84	0.41
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.03	0.41
23:b:606:CLA:H62	23:b:606:CLA:H41	1.96	0.41
3:c:147:PHE:CD2	23:c:513:CLA:H3A	2.56	0.41
12:m:12:ALA:O	12:m:16:LEU:HG	2.21	0.41
16:v:95:LEU:HD11	16:v:112:LEU:HD11	2.02	0.41
17:y:41:VAL:C	17:y:43:ARG:H	2.29	0.41
24:A:406:PHO:HHD	24:A:406:PHO:HBC2	2.03	0.41
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.03	0.41
1:a:131:TRP:CD2	1:a:131:TRP:C	2.95	0.41
2:b:91:TRP:HE1	27:b:622:STE:H62	1.86	0.41
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.09	0.41
3:c:26:ARG:HD3	10:k:46:ARG:NH2	2.36	0.41
5:e:23:HIS:HA	5:e:26:THR:OG1	2.21	0.41
11:l:7:ARG:NH2	27:l:103:STE:H41	2.36	0.41
3:C:279:LEU:CD1	23:C:509:CLA:HED2	2.51	0.41
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.90	0.41
15:U:38:TYR:HB2	15:U:41:LEU:HD12	2.03	0.41
19:Z:31:GLN:CD	19:Z:32:ASP:H	2.29	0.41
2:b:67:ALA:HA	2:b:71:VAL:O	2.21	0.41
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.41
4:D:170:ALA:HB1	4:D:171:PRO:HD2	2.02	0.40
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.03	0.40
25:a:409:BCR:H24C	25:a:409:BCR:H371	1.83	0.40
2:b:121:GLU:OE2	7:h:12:ARG:NH1	2.46	0.40
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.56	0.40
2:b:414:PRO:N	2:b:415:PRO:CD	2.84	0.40
4:d:42:TYR:CZ	6:f:25:THR:HG23	2.55	0.40
23:d:403:CLA:H93	18:x:14:LEU:CD1	2.51	0.40
7:h:28:THR:HB	7:h:29:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:129:LYS:HD3	16:v:136:TYR:O	2.21	0.40
1:A:332:HIS:O	1:A:333:GLU:C	2.64	0.40
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.02	0.40
28:D:408:LMG:O2	28:D:408:LMG:C7	2.69	0.40
1:a:288:LEU:HG	3:c:432:VAL:HG22	2.03	0.40
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.51	0.40
5:e:63:ILE:HG23	5:e:64:PRO:HD2	2.03	0.40
14:t:11:ALA:HB3	25:t:101:BCR:H363	2.03	0.40
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.56	0.40
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.52	0.40
16:V:122:GLU:N	16:V:123:PRO:HD2	2.36	0.40
17:Y:42:ARG:O	17:Y:43:ARG:C	2.63	0.40
2:b:58:GLN:C	2:b:329:PRO:HB3	2.46	0.40
27:b:624:STE:H31	27:b:627:STE:H181	2.01	0.40
23:c:508:CLA:H191	30:c:520:DGD:C7A	2.51	0.40
25:c:514:BCR:H11C	25:c:514:BCR:H341	1.91	0.40
34:f:101:HEM:HMA1	20:r:23:ILE:CD1	2.51	0.40
23:h:101:CLA:H92	25:x:101:BCR:H402	2.03	0.40
24:D:402:PHO:NC	24:D:402:PHO:ND	2.68	0.40
33:E:101:LHG:HC41	27:E:103:STE:H121	2.04	0.40
30:H:102:DGD:HB21	30:H:102:DGD:HB51	2.00	0.40
28:b:623:LMG:O9	28:b:623:LMG:C9	2.68	0.40
27:b:624:STE:C6	27:b:627:STE:C17	2.95	0.40
3:c:203:THR:O	3:c:235:GLY:HA3	2.22	0.40
23:c:505:CLA:H193	28:c:524:LMG:H121	2.04	0.40
16:v:3:LEU:HD12	16:v:3:LEU:HA	1.94	0.40
25:x:101:BCR:C8	25:x:101:BCR:H331	2.51	0.40
1:A:210:LEU:HD23	1:A:214:MET:HG2	2.03	0.40
28:B:620:LMG:HC91	28:D:408:LMG:H152	2.03	0.40
28:D:408:LMG:O1	28:D:408:LMG:C10	2.69	0.40
2:b:167:TRP:NE1	2:b:267:LEU:HD11	2.35	0.40
2:b:168:VAL:CG2	2:b:179:GLN:HG3	2.52	0.40
23:b:604:CLA:H61	23:b:604:CLA:H41	1.92	0.40
3:c:109:PHE:N	3:c:110:PRO:CD	2.85	0.40
3:c:415:ASN:O	3:c:416:SER:OG	2.31	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	332/344 (96%)	328 (99%)	3 (1%)	1 (0%)	36	29
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	504/510 (99%)	493 (98%)	10 (2%)	1 (0%)	43	36
3	C	442/461 (96%)	432 (98%)	9 (2%)	1 (0%)	43	36
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	36
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	332 (98%)	8 (2%)	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%)	57 (90%)	6 (10%)	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%)	33 (97%)	1 (3%)	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%)	10 (4%)	2 (1%)	16	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	242/272 (89%)	233 (96%)	7 (3%)	2 (1%)	16 8
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%)	91 (96%)	4 (4%)	0	100 100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11 4
16	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18 10
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100 100
17	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2 0
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%)	36 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7 2
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	7 2
20	R	26/41 (63%)	26 (100%)	0	0	100 100
20	r	26/41 (63%)	25 (96%)	0	1 (4%)	2 0
All	All	5232/5700 (92%)	5089 (97%)	129 (2%)	14 (0%)	36 29

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	o	58	ASN
15	u	53	ALA
19	z	2	THR
17	Y	43	ARG
13	O	62	GLU
13	o	59	LYS
2	b	505	ARG
19	Z	31	GLN
20	r	25	PRO
13	O	133	VAL
1	A	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	269 (100%)	1 (0%)	84	87
1	a	269/280 (96%)	256 (95%)	13 (5%)	23	15
2	B	408/407 (100%)	400 (98%)	8 (2%)	48	46
2	b	403/407 (99%)	392 (97%)	11 (3%)	39	34
3	C	346/362 (96%)	341 (99%)	5 (1%)	59	59
3	c	354/362 (98%)	340 (96%)	14 (4%)	28	20
4	D	276/283 (98%)	273 (99%)	3 (1%)	65	67
4	d	277/283 (98%)	267 (96%)	10 (4%)	31	23
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	7
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	19
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	47
7	h	53/55 (96%)	49 (92%)	4 (8%)	12	6
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	8
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	29
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	19
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	4
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	26
10	k	30/37 (81%)	25 (83%)	5 (17%)	2	0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	31
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	23
12	m	28/32 (88%)	27 (96%)	1 (4%)	31	23
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	14
13	o	207/228 (91%)	200 (97%)	7 (3%)	32	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	T	26/28 (93%)	25 (96%)	1 (4%)	29 21
14	t	25/28 (89%)	25 (100%)	0	100 100
15	U	84/112 (75%)	80 (95%)	4 (5%)	23 15
15	u	84/112 (75%)	83 (99%)	1 (1%)	63 63
16	V	117/138 (85%)	111 (95%)	6 (5%)	21 13
16	v	117/138 (85%)	108 (92%)	9 (8%)	12 5
17	Y	19/37 (51%)	17 (90%)	2 (10%)	6 2
17	y	22/37 (60%)	19 (86%)	3 (14%)	3 1
18	X	31/34 (91%)	29 (94%)	2 (6%)	15 8
18	x	31/34 (91%)	26 (84%)	5 (16%)	2 1
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4 1
19	z	51/52 (98%)	45 (88%)	6 (12%)	5 2
20	R	22/33 (67%)	21 (96%)	1 (4%)	24 17
20	r	22/33 (67%)	18 (82%)	4 (18%)	2 0
All	All	4322/4654 (93%)	4157 (96%)	165 (4%)	29 21

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

Mol	Chain	Res	Type
1	A	205	VAL
2	B	76	SER
2	B	86	ILE
2	B	98	LEU
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	435	GLU
2	B	476	ARG
3	C	142	GLU
3	C	213	LEU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	43	LEU
4	D	259	ILE
4	D	345	VAL
5	E	14	ILE

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Mol	Chain	Res	Type
5	E	17	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
7	H	20	LYS
8	I	4	LEU
8	I	35	LYS
9	J	24	ILE
10	K	13	GLU
11	L	7	ARG
12	M	25	LEU
13	O	34	SER
13	O	40	ILE
13	O	62	GLU
13	O	78	LEU
13	O	86	LYS
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	189	ARG
13	O	214	THR
14	T	25	GLU
15	U	10	VAL
15	U	45	LEU
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	24	LYS
16	V	31	ARG
16	V	57	GLU
16	V	86	GLN
17	Y	41	VAL
17	Y	45	ASN
18	X	3	ILE
18	X	23	LEU
19	Z	2	THR
19	Z	15	LEU
19	Z	34	ASP
19	Z	35	ARG
19	Z	37	LYS
19	Z	46	LEU

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Mol	Chain	Res	Type
19	Z	50	LEU
20	R	6	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	230	THR
1	a	231	GLU
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	98	LEU
2	b	128	THR
2	b	137	LYS
2	b	149	LEU
2	b	179	GLN
2	b	236	THR
2	b	349	LYS
2	b	362	PHE
2	b	389	LYS
2	b	435	GLU
2	b	506	ARG
3	c	26	ARG
3	c	72	LEU
3	c	76	ILE
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	170	ILE
3	c	215	LYS
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	182	LEU

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Mol	Chain	Res	Type
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
4	d	329	MET
5	e	4	THR
5	e	65	LEU
5	e	83	LEU
7	h	3	ARG
7	h	6	TRP
7	h	7	LEU
7	h	63	LYS
8	i	6	ILE
9	j	7	ARG
9	j	21	VAL
10	k	10	LYS
10	k	24	VAL
10	k	27	VAL
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
13	o	39	ARG
13	o	49	THR
13	o	53	LYS
13	o	58	ASN
13	o	87	VAL
13	o	118	LEU
13	o	134	THR
15	u	15	GLU
16	v	18	THR
16	v	24	LYS
16	v	28	GLU
16	v	52	LEU
16	v	90	GLU
16	v	106	ASN

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Mol	Chain	Res	Type
16	v	107	LEU
16	v	110	LYS
16	v	129	LYS
17	y	19	ILE
17	y	23	THR
17	y	30	ILE
18	x	2	THR
18	x	14	LEU
18	x	15	LEU
18	x	31	ILE
18	x	38	GLN
19	z	4	LEU
19	z	20	VAL
19	z	29	SER
19	z	31	GLN
19	z	35	ARG
19	z	48	ILE
20	r	7	VAL
20	r	9	LEU
20	r	14	LEU
20	r	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	338	ASN
2	B	394	GLN
2	B	409	GLN
2	B	497	GLN
3	C	44	ASN
3	C	327	ASN
4	D	334	GLN
4	D	350	ASN
13	O	88	ASN
13	O	124	ASN
13	O	147	ASN
13	O	155	ASN
13	O	219	GLN
15	U	73	GLN
17	Y	45	ASN
18	X	38	GLN

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Mol	Chain	Res	Type
19	Z	6	GLN
20	R	22	ASN
1	a	19	ASN
1	a	165	GLN
1	a	234	ASN
2	b	179	GLN
2	b	338	GLN
2	b	409	GLN
3	c	201	ASN
3	c	378	ASN
4	d	350	ASN
5	e	74	GLN
5	e	82	GLN
6	f	44	GLN
7	h	59	ASN
13	o	36	GLN
13	o	61	GLN
13	o	155	ASN
13	o	196	GLN
16	v	34	GLN
16	v	106	ASN
18	x	33	GLN
19	z	6	GLN
19	z	58	ASN

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	1.27	1 (12%)	8,9,11	1.27	1 (12%)
12	FME	m	1	12	8,9,10	1.04	1 (12%)	8,9,11	0.93	0
8	FME	I	1	8	8,9,10	0.91	1 (12%)	8,9,11	1.42	1 (12%)
14	FME	T	1	14	8,9,10	0.91	0	8,9,11	1.35	1 (12%)
8	FME	i	1	8	8,9,10	1.01	0	8,9,11	1.34	1 (12%)
12	FME	M	1	12	8,9,10	0.86	0	8,9,11	0.99	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	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.90	1.42	1.46
12	m	1	FME	CA-N	-2.04	1.43	1.46
8	I	1	FME	CA-N	-2.01	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	CA-N-CN	-2.88	118.39	122.82
14	t	1	FME	CB-CA-N	2.60	115.25	110.52
8	i	1	FME	CA-N-CN	-2.47	119.02	122.82
14	T	1	FME	O1-CN-N	-2.07	119.96	125.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	O-C-CA-CB
14	T	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
12	M	1	FME	CA-CB-CG-SD
14	t	1	FME	CB-CG-SD-CE
14	t	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 212 ligands modelled in this entry, 6 are monoatomic - leaving 206 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	PL9	a	410	-	55,55,55	0.97	5 (9%)	68,69,69	1.59	12 (17%)
23	CLA	b	613	-	69,73,73	1.22	7 (10%)	82,113,113	1.55	10 (12%)
25	BCR	H	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.28	8 (14%)
27	STE	J	101	-	11,11,19	0.61	0	11,11,19	1.48	2 (18%)
25	BCR	d	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.11	3 (5%)
27	STE	T	102	-	15,15,19	0.53	0	14,14,19	0.55	0
28	LMG	C	524	-	48,48,55	1.03	4 (8%)	56,56,63	1.23	3 (5%)
28	LMG	A	411	-	48,48,55	1.05	3 (6%)	56,56,63	1.35	6 (10%)
24	PHO	A	406	-	58,69,69	1.89	10 (17%)	55,99,99	1.31	7 (12%)
25	BCR	x	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.32	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	STE	C	518	-	4,4,19	0.52	0	3,3,19	0.28	0
25	BCR	b	617	-	41,41,41	1.29	4 (9%)	56,56,56	1.16	8 (14%)
23	CLA	b	601	-	69,73,73	1.22	8 (11%)	82,113,113	1.47	10 (12%)
27	STE	A	410	-	8,8,19	0.41	0	7,7,19	0.72	0
27	STE	H	103	-	17,17,19	0.59	0	16,16,19	0.66	0
23	CLA	b	608	-	69,73,73	1.32	6 (8%)	82,113,113	1.43	11 (13%)
27	STE	Z	101	-	16,16,19	0.52	0	15,15,19	0.50	0
28	LMG	D	408	-	50,50,55	1.07	3 (6%)	58,58,63	1.28	4 (6%)
24	PHO	a	407	-	58,69,69	1.89	11 (18%)	55,99,99	1.47	8 (14%)
23	CLA	b	612	-	69,73,73	1.23	9 (13%)	82,113,113	1.20	10 (12%)
33	LHG	E	101	-	48,48,48	1.11	4 (8%)	51,54,54	1.14	2 (3%)
27	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.44	0
27	STE	m	102	-	14,14,19	0.61	0	13,13,19	0.59	0
34	HEM	f	101	6,5	50,50,50	1.47	7 (14%)	67,82,82	1.45	7 (10%)
23	CLA	C	506	-	69,73,73	1.56	7 (10%)	82,113,113	1.13	6 (7%)
25	BCR	K	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	7 (12%)
33	LHG	d	406	-	48,48,48	0.89	2 (4%)	51,54,54	1.38	7 (13%)
27	STE	A	417	-	10,10,19	0.42	0	9,9,19	0.84	0
25	BCR	T	101	-	41,41,41	1.33	6 (14%)	56,56,56	1.43	8 (14%)
27	STE	C	527	-	7,7,19	0.65	0	6,6,19	0.41	0
23	CLA	b	605	-	69,73,73	1.67	7 (10%)	82,113,113	1.39	7 (8%)
23	CLA	C	509	-	69,73,73	1.27	9 (13%)	82,113,113	1.34	9 (10%)
25	BCR	b	616	-	41,41,41	1.18	4 (9%)	56,56,56	1.35	8 (14%)
27	STE	D	414	-	8,8,19	0.40	0	7,7,19	0.99	0
27	STE	E	102	-	11,11,19	1.00	1 (9%)	11,11,19	0.94	0
23	CLA	c	512	-	69,73,73	1.24	7 (10%)	82,113,113	1.49	10 (12%)
29	SQD	F	102	-	34,36,54	1.65	6 (17%)	42,45,65	3.00	8 (19%)
23	CLA	b	606	36	69,73,73	1.10	5 (7%)	82,113,113	1.26	7 (8%)
23	CLA	c	509	-	69,73,73	1.17	7 (10%)	82,113,113	1.42	9 (10%)
27	STE	b	626	-	9,9,19	0.41	0	8,8,19	0.71	0
23	CLA	B	610	36	69,73,73	1.49	9 (13%)	82,113,113	1.37	7 (8%)
30	DGD	C	521	-	63,63,67	1.22	8 (12%)	77,77,81	1.51	12 (15%)
33	LHG	a	413	-	41,41,48	1.51	7 (17%)	44,47,54	1.35	4 (9%)
29	SQD	a	414	-	52,54,54	1.67	9 (17%)	62,65,65	1.67	7 (11%)
28	LMG	c	524	-	49,49,55	1.03	4 (8%)	57,57,63	1.31	6 (10%)
23	CLA	b	607	-	69,73,73	1.21	7 (10%)	82,113,113	1.23	8 (9%)
23	CLA	C	510	-	69,73,73	1.25	11 (15%)	82,113,113	1.52	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	STE	M	102	-	14,14,19	0.76	0	14,14,19	0.98	1 (7%)
23	CLA	D	405	-	69,73,73	1.53	10 (14%)	82,113,113	1.21	8 (9%)
27	STE	t	103	-	17,17,19	0.67	0	17,17,19	1.05	0
25	BCR	t	101	-	41,41,41	1.28	3 (7%)	56,56,56	1.30	6 (10%)
27	STE	d	411	-	11,11,19	0.84	0	11,11,19	0.88	0
25	BCR	C	514	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
32	BCT	a	404	21	3,3,3	1.16	0	2,3,3	3.44	2 (100%)
23	CLA	a	411	36	69,73,73	1.47	8 (11%)	82,113,113	1.28	7 (8%)
24	PHO	D	402	-	58,69,69	1.75	11 (18%)	55,99,99	1.43	6 (10%)
27	STE	e	101	-	8,8,19	0.58	0	7,7,19	0.61	0
28	LMG	M	101	-	51,51,55	1.04	4 (7%)	59,59,63	1.44	11 (18%)
23	CLA	B	605	-	69,73,73	1.12	6 (8%)	82,113,113	1.31	9 (10%)
28	LMG	c	522	-	46,46,55	1.21	5 (10%)	54,54,63	1.27	7 (12%)
23	CLA	c	505	-	69,73,73	1.18	8 (11%)	82,113,113	1.14	4 (4%)
27	STE	B	621	-	16,16,19	0.71	0	16,16,19	0.97	0
29	SQD	A	412	-	50,52,54	1.57	8 (16%)	60,63,65	1.99	14 (23%)
30	DGD	h	102	-	63,63,67	1.16	5 (7%)	77,77,81	1.45	13 (16%)
23	CLA	B	602	-	69,73,73	1.38	7 (10%)	82,113,113	1.21	7 (8%)
23	CLA	c	506	-	69,73,73	1.39	10 (14%)	82,113,113	1.23	7 (8%)
25	BCR	C	515	-	41,41,41	1.32	4 (9%)	56,56,56	1.34	7 (12%)
23	CLA	B	606	-	69,73,73	1.46	10 (14%)	82,113,113	1.53	8 (9%)
29	SQD	f	102	-	39,41,54	1.71	9 (23%)	49,52,65	1.68	8 (16%)
23	CLA	A	404	-	69,73,73	1.23	8 (11%)	82,113,113	1.12	4 (4%)
23	CLA	d	402	-	69,73,73	1.30	7 (10%)	82,113,113	1.41	12 (14%)
27	STE	D	413	-	19,19,19	0.71	0	19,19,19	1.30	2 (10%)
27	STE	e	104	-	12,12,19	0.64	0	12,12,19	1.25	2 (16%)
26	PL9	A	409	-	55,55,55	1.24	4 (7%)	68,69,69	1.62	13 (19%)
23	CLA	B	607	36	69,73,73	1.21	8 (11%)	82,113,113	1.43	5 (6%)
23	CLA	C	511	3	69,73,73	1.44	10 (14%)	82,113,113	1.26	9 (10%)
23	CLA	c	507	36	69,73,73	1.19	8 (11%)	82,113,113	1.26	9 (10%)
23	CLA	b	603	-	69,73,73	1.20	6 (8%)	82,113,113	1.44	9 (10%)
32	BCT	D	401	21	3,3,3	1.08	0	2,3,3	3.96	2 (100%)
29	SQD	l	101	-	52,54,54	1.55	10 (19%)	62,65,65	1.91	7 (11%)
27	STE	z	101	-	8,8,19	0.53	0	7,7,19	0.55	0
23	CLA	C	504	36	63,67,73	1.25	9 (14%)	74,105,113	1.25	9 (12%)
23	CLA	C	513	-	69,73,73	1.40	9 (13%)	82,113,113	1.44	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	612	-	69,73,73	1.13	6 (8%)	82,113,113	1.37	12 (14%)
23	CLA	B	613	-	69,73,73	1.51	8 (11%)	82,113,113	1.12	6 (7%)
27	STE	e	102	-	7,7,19	0.46	0	6,6,19	0.61	0
33	LHG	l	102	-	48,48,48	0.84	2 (4%)	51,54,54	1.24	4 (7%)
23	CLA	D	404	-	69,73,73	1.09	3 (4%)	82,113,113	1.22	9 (10%)
25	BCR	b	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	7 (12%)
23	CLA	C	502	-	69,73,73	1.19	6 (8%)	82,113,113	1.34	6 (7%)
28	LMG	c	523	-	48,48,55	1.04	2 (4%)	56,56,63	1.32	8 (14%)
23	CLA	B	614	-	69,73,73	1.23	4 (5%)	82,113,113	1.29	10 (12%)
23	CLA	c	508	-	68,72,73	1.45	8 (11%)	80,111,113	1.43	10 (12%)
23	CLA	b	604	-	69,73,73	1.22	8 (11%)	82,113,113	1.39	13 (15%)
27	STE	C	525	-	11,11,19	0.67	0	11,11,19	1.44	3 (27%)
27	STE	a	416	-	9,9,19	0.74	0	8,8,19	0.40	0
23	CLA	B	615	-	69,73,73	1.29	9 (13%)	82,113,113	1.13	6 (7%)
28	LMG	B	620	-	45,45,55	1.04	2 (4%)	53,53,63	1.37	4 (7%)
23	CLA	C	501	-	69,73,73	1.45	9 (13%)	82,113,113	1.38	8 (9%)
25	BCR	c	514	-	41,41,41	1.28	3 (7%)	56,56,56	1.29	6 (10%)
23	CLA	B	609	-	69,73,73	1.17	5 (7%)	82,113,113	1.27	6 (7%)
27	STE	A	415	-	7,7,19	0.45	0	6,6,19	0.58	0
27	STE	B	622	-	11,11,19	0.90	0	11,11,19	0.96	0
27	STE	i	101	-	11,11,19	0.86	0	11,11,19	1.03	0
23	CLA	B	603	-	69,73,73	1.23	8 (11%)	82,113,113	1.51	11 (13%)
23	CLA	a	406	36	69,73,73	1.24	10 (14%)	82,113,113	1.53	10 (12%)
27	STE	b	627	-	10,10,19	0.41	0	9,9,19	0.68	0
27	STE	C	516	-	13,13,19	0.77	0	13,13,19	0.87	0
27	STE	C	529	-	13,13,19	0.45	0	12,12,19	0.54	0
23	CLA	C	507	36	69,73,73	1.08	4 (5%)	82,113,113	1.42	11 (13%)
27	STE	j	102	-	15,15,19	0.58	0	14,14,19	0.55	0
31	OEX	a	418	36,1,3	0,15,15	-	-	-		
24	PHO	d	401	-	58,69,69	2.01	9 (15%)	55,99,99	1.59	11 (20%)
23	CLA	h	101	36	69,73,73	1.31	9 (13%)	82,113,113	1.53	10 (12%)
26	PL9	d	405	-	55,55,55	1.54	9 (16%)	68,69,69	1.57	12 (17%)
28	LMG	C	517	-	35,35,55	1.41	3 (8%)	43,43,63	1.72	8 (18%)
33	LHG	D	411	-	46,46,48	1.03	3 (6%)	49,52,54	1.29	4 (8%)
23	CLA	b	610	-	69,73,73	0.97	3 (4%)	82,113,113	1.33	10 (12%)
25	BCR	B	619	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	6 (10%)
27	STE	A	416	-	16,16,19	0.68	0	15,15,19	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	602	-	69,73,73	1.18	7 (10%)	82,113,113	1.43	13 (15%)
27	STE	x	102	-	19,19,19	0.91	1 (5%)	19,19,19	0.85	2 (10%)
28	LMG	a	415	-	55,55,55	1.45	8 (14%)	63,63,63	1.54	8 (12%)
27	STE	B	623	-	14,14,19	0.55	0	13,13,19	0.74	0
23	CLA	C	512	-	69,73,73	1.34	12 (17%)	82,113,113	1.30	13 (15%)
23	CLA	C	505	-	69,73,73	1.23	7 (10%)	82,113,113	1.22	5 (6%)
27	STE	b	625	-	15,15,19	0.86	0	15,15,19	1.13	2 (13%)
28	LMG	b	623	-	55,55,55	1.02	2 (3%)	63,63,63	1.53	10 (15%)
29	SQD	A	413	-	52,54,54	1.66	9 (17%)	62,65,65	1.84	12 (19%)
23	CLA	a	408	-	69,73,73	1.37	9 (13%)	82,113,113	1.36	9 (10%)
30	DGD	c	520	-	63,63,67	1.32	11 (17%)	77,77,81	1.54	16 (20%)
25	BCR	k	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.15	3 (5%)
33	LHG	L	101	-	48,48,48	0.98	1 (2%)	51,54,54	1.29	8 (15%)
23	CLA	C	503	-	69,73,73	1.34	9 (13%)	82,113,113	1.42	9 (10%)
25	BCR	D	406	-	41,41,41	1.24	2 (4%)	56,56,56	1.18	5 (8%)
23	CLA	B	604	-	69,73,73	1.21	5 (7%)	82,113,113	1.54	5 (6%)
27	STE	d	410	-	16,16,19	0.93	0	16,16,19	0.81	0
30	DGD	c	519	-	63,63,67	1.14	5 (7%)	77,77,81	1.45	11 (14%)
27	STE	d	412	-	9,9,19	0.51	0	8,8,19	0.60	0
30	DGD	C	523	-	63,63,67	0.95	4 (6%)	77,77,81	1.33	9 (11%)
35	HEC	V	201	16	46,50,50	1.88	8 (17%)	58,82,82	1.98	10 (17%)
33	LHG	D	412	-	48,48,48	1.02	2 (4%)	51,54,54	1.33	6 (11%)
29	SQD	b	620	-	47,49,54	1.57	8 (17%)	57,60,65	2.22	18 (31%)
27	STE	I	102	-	16,16,19	0.86	0	16,16,19	0.90	1 (6%)
23	CLA	b	611	-	69,73,73	1.51	9 (13%)	82,113,113	1.17	7 (8%)
27	STE	b	624	-	19,19,19	0.67	0	19,19,19	1.14	0
28	LMG	D	409	-	51,51,55	1.17	3 (5%)	59,59,63	1.35	5 (8%)
25	BCR	k	102	-	41,41,41	1.09	4 (9%)	56,56,56	1.15	4 (7%)
23	CLA	b	614	-	69,73,73	1.28	10 (14%)	82,113,113	1.34	9 (10%)
25	BCR	a	409	-	41,41,41	1.13	4 (9%)	56,56,56	1.17	5 (8%)
27	STE	C	526	-	15,15,19	0.60	0	14,14,19	0.47	0
28	LMG	b	621	-	51,51,55	1.01	4 (7%)	59,59,63	1.46	9 (15%)
29	SQD	a	412	-	52,54,54	1.43	7 (13%)	62,65,65	2.08	18 (29%)
33	LHG	d	408	-	38,38,48	0.99	2 (5%)	41,44,54	1.14	4 (9%)
23	CLA	c	503	-	69,73,73	1.13	6 (8%)	82,113,113	1.25	7 (8%)
23	CLA	c	511	3	69,73,73	1.27	7 (10%)	82,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	STE	E	104	-	19,19,19	0.82	1 (5%)	19,19,19	0.92	1 (5%)
23	CLA	b	615	-	64,68,73	1.25	8 (12%)	76,107,113	1.38	9 (11%)
27	STE	c	516	-	12,12,19	0.54	0	11,11,19	0.53	0
25	BCR	C	520	-	41,41,41	1.18	5 (12%)	56,56,56	1.15	5 (8%)
27	STE	b	622	-	19,19,19	0.78	1 (5%)	19,19,19	0.91	1 (5%)
23	CLA	c	510	-	69,73,73	1.34	5 (7%)	82,113,113	1.41	6 (7%)
35	HEC	v	201	16	46,50,50	1.92	6 (13%)	58,82,82	1.84	4 (6%)
23	CLA	A	405	36	69,73,73	1.10	6 (8%)	82,113,113	1.16	8 (9%)
25	BCR	B	617	-	41,41,41	1.13	3 (7%)	56,56,56	1.36	9 (16%)
23	CLA	a	405	-	69,73,73	1.22	9 (13%)	82,113,113	1.26	9 (10%)
23	CLA	c	513	-	69,73,73	1.43	11 (15%)	82,113,113	1.07	5 (6%)
27	STE	E	103	-	11,11,19	0.49	0	10,10,19	0.62	0
23	CLA	B	611	-	69,73,73	1.40	7 (10%)	82,113,113	1.56	9 (10%)
25	BCR	c	515	-	41,41,41	1.38	3 (7%)	56,56,56	1.39	9 (16%)
27	STE	i	102	-	5,5,19	0.51	0	4,4,19	0.43	0
30	DGD	A	414	-	67,67,67	1.33	10 (14%)	81,81,81	1.54	15 (18%)
30	DGD	c	521	-	63,63,67	0.92	4 (6%)	77,77,81	1.48	11 (14%)
23	CLA	D	403	36	69,73,73	1.28	10 (14%)	82,113,113	1.23	3 (3%)
27	STE	c	517	-	17,17,19	0.59	0	16,16,19	0.55	0
28	LMG	c	518	-	29,29,55	1.15	2 (6%)	31,31,63	1.10	2 (6%)
27	STE	I	101	-	14,14,19	0.54	0	13,13,19	0.55	0
23	CLA	B	608	-	69,73,73	1.04	5 (7%)	82,113,113	1.37	7 (8%)
28	LMG	d	409	-	44,44,55	1.11	4 (9%)	52,52,63	1.33	7 (13%)
26	PL9	D	407	-	55,55,55	1.57	7 (12%)	68,69,69	1.59	16 (23%)
27	STE	e	103	-	8,8,19	0.41	0	7,7,19	0.71	0
27	STE	l	103	-	17,17,19	0.37	0	16,16,19	0.70	0
28	LMG	b	619	-	22,22,55	1.03	2 (9%)	23,23,63	1.04	1 (4%)
27	STE	C	528	-	13,13,19	0.49	0	12,12,19	0.64	0
30	DGD	C	522	-	63,63,67	1.48	10 (15%)	77,77,81	1.27	7 (9%)
23	CLA	c	504	36	64,68,73	1.36	6 (9%)	76,107,113	1.27	9 (11%)
34	HEM	F	101	6,5	50,50,50	1.42	8 (16%)	67,82,82	1.31	9 (13%)
23	CLA	B	616	-	64,68,73	1.19	6 (9%)	76,107,113	1.41	6 (7%)
27	STE	a	417	-	11,11,19	0.79	0	11,11,19	1.16	2 (18%)
31	OEX	A	418	36,1,3	0,15,15	-	-	-		
23	CLA	c	502	-	69,73,73	1.07	6 (8%)	82,113,113	1.31	6 (7%)
23	CLA	B	601	36	69,73,73	1.43	7 (10%)	82,113,113	1.56	6 (7%)
27	STE	C	519	-	6,6,19	0.47	0	5,5,19	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	STE	j	101	-	11,11,19	0.81	0	11,11,19	0.94	0
33	LHG	D	410	-	48,48,48	0.97	2 (4%)	51,54,54	1.15	5 (9%)
25	BCR	B	618	-	41,41,41	1.21	2 (4%)	56,56,56	1.19	5 (8%)
23	CLA	b	609	36	69,73,73	1.24	8 (11%)	82,113,113	1.49	12 (14%)
23	CLA	d	403	-	69,73,73	1.30	10 (14%)	82,113,113	1.06	6 (7%)
27	STE	t	102	-	13,13,19	0.71	0	13,13,19	1.04	1 (7%)
30	DGD	H	102	-	63,63,67	1.29	8 (12%)	77,77,81	1.45	12 (15%)
33	LHG	d	407	-	48,48,48	0.92	2 (4%)	51,54,54	1.15	5 (9%)
23	CLA	A	407	-	58,62,73	1.61	5 (8%)	68,99,113	1.34	7 (10%)
23	CLA	C	508	-	69,73,73	1.41	7 (10%)	82,113,113	1.39	11 (13%)
25	BCR	A	408	-	41,41,41	1.14	4 (9%)	56,56,56	1.37	7 (12%)
23	CLA	c	501	-	69,73,73	1.13	6 (8%)	82,113,113	1.46	7 (8%)
27	STE	m	101	-	11,11,19	0.80	0	11,11,19	0.98	1 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	a	410	-	-	24/53/73/73	0/1/1/1
23	CLA	b	613	-	1/1/20/20	10/39/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	STE	J	101	-	-	3/9/9/17	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
27	STE	T	102	-	-	8/13/13/17	-
28	LMG	C	524	-	-	10/43/63/70	0/1/1/1
28	LMG	A	411	-	-	17/43/63/70	0/1/1/1
24	PHO	A	406	-	-	0/37/103/103	0/5/6/6
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
27	STE	C	518	-	-	1/2/2/17	-
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
23	CLA	b	601	-	-	4/39/115/115	-
27	STE	A	410	-	-	4/6/6/17	-
27	STE	H	103	-	-	8/15/15/17	-
23	CLA	b	608	-	1/1/20/20	3/39/115/115	-
27	STE	Z	101	-	-	9/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	D	408	-	-	18/45/65/70	0/1/1/1
24	PHO	a	407	-	-	2/37/103/103	0/5/6/6
23	CLA	b	612	-	1/1/20/20	4/39/115/115	-
33	LHG	E	101	-	-	28/53/53/53	-
27	STE	M	103	-	-	1/7/7/17	-
27	STE	m	102	-	-	6/12/12/17	-
34	HEM	f	101	6,5	-	4/14/54/54	-
23	CLA	C	506	-	1/1/20/20	8/39/115/115	-
25	BCR	K	101	-	-	6/29/63/63	0/2/2/2
33	LHG	d	406	-	-	18/53/53/53	-
27	STE	A	417	-	-	5/8/8/17	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
27	STE	C	527	-	-	4/5/5/17	-
23	CLA	b	605	-	1/1/20/20	5/39/115/115	-
23	CLA	C	509	-	1/1/20/20	10/39/115/115	-
25	BCR	b	616	-	-	4/29/63/63	0/2/2/2
27	STE	D	414	-	-	5/6/6/17	-
27	STE	E	102	-	-	5/9/9/17	-
23	CLA	c	512	-	1/1/20/20	16/39/115/115	-
29	SQD	F	102	-	-	12/28/48/69	0/1/1/1
23	CLA	b	606	36	1/1/20/20	10/39/115/115	-
23	CLA	c	509	-	1/1/20/20	10/39/115/115	-
27	STE	b	626	-	-	3/7/7/17	-
23	CLA	B	610	36	1/1/20/20	2/39/115/115	-
30	DGD	C	521	-	-	21/51/91/95	0/2/2/2
33	LHG	a	413	-	-	19/46/46/53	-
29	SQD	a	414	-	-	20/49/69/69	0/1/1/1
28	LMG	c	524	-	-	17/44/64/70	0/1/1/1
23	CLA	b	607	-	-	1/39/115/115	-
23	CLA	C	510	-	1/1/20/20	6/39/115/115	-
27	STE	M	102	-	-	9/12/12/17	-
23	CLA	D	405	-	-	12/39/115/115	-
27	STE	t	103	-	-	11/15/15/17	-
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
27	STE	d	411	-	-	1/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	514	-	-	8/29/63/63	0/2/2/2
23	CLA	a	411	36	-	2/39/115/115	-
24	PHO	D	402	-	-	0/37/103/103	0/5/6/6
27	STE	e	101	-	-	2/6/6/17	-
28	LMG	M	101	-	-	22/46/66/70	0/1/1/1
23	CLA	B	605	-	1/1/20/20	6/39/115/115	-
28	LMG	c	522	-	-	17/41/61/70	0/1/1/1
23	CLA	c	505	-	1/1/20/20	10/39/115/115	-
27	STE	B	621	-	-	7/14/14/17	-
29	SQD	A	412	-	-	19/47/67/69	0/1/1/1
30	DGD	h	102	-	-	18/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/20/20	8/39/115/115	-
23	CLA	c	506	-	1/1/20/20	14/39/115/115	-
25	BCR	C	515	-	-	2/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/20/20	9/39/115/115	-
29	SQD	f	102	-	-	13/36/56/69	0/1/1/1
23	CLA	A	404	-	1/1/20/20	3/39/115/115	-
23	CLA	d	402	-	1/1/20/20	7/39/115/115	-
27	STE	D	413	-	-	5/17/17/17	-
27	STE	e	104	-	-	5/10/10/17	-
26	PL9	A	409	-	-	16/53/73/73	0/1/1/1
23	CLA	B	607	36	1/1/20/20	3/39/115/115	-
23	CLA	c	507	36	1/1/20/20	7/39/115/115	-
23	CLA	C	511	3	-	2/39/115/115	-
23	CLA	b	603	-	1/1/20/20	11/39/115/115	-
29	SQD	l	101	-	-	23/49/69/69	0/1/1/1
27	STE	z	101	-	-	3/6/6/17	-
23	CLA	C	504	36	1/1/18/20	5/32/108/115	-
23	CLA	C	513	-	1/1/20/20	12/39/115/115	-
23	CLA	B	612	-	1/1/20/20	10/39/115/115	-
23	CLA	B	613	-	1/1/20/20	11/39/115/115	-
27	STE	e	102	-	-	3/5/5/17	-
33	LHG	l	102	-	-	17/53/53/53	-
23	CLA	D	404	-	1/1/20/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	618	-	-	2/29/63/63	0/2/2/2
23	CLA	C	502	-	-	4/39/115/115	-
28	LMG	c	523	-	-	21/43/63/70	0/1/1/1
23	CLA	B	614	-	1/1/20/20	10/39/115/115	-
23	CLA	c	508	-	-	6/38/114/115	-
23	CLA	b	604	-	1/1/20/20	4/39/115/115	-
27	STE	C	525	-	-	4/9/9/17	-
27	STE	a	416	-	-	4/7/7/17	-
23	CLA	B	615	-	1/1/20/20	10/39/115/115	-
28	LMG	B	620	-	-	13/40/60/70	0/1/1/1
23	CLA	C	501	-	1/1/20/20	4/39/115/115	-
25	BCR	c	514	-	-	7/29/63/63	0/2/2/2
23	CLA	B	609	-	-	3/39/115/115	-
27	STE	A	415	-	-	4/5/5/17	-
27	STE	B	622	-	-	5/9/9/17	-
27	STE	i	101	-	-	6/9/9/17	-
23	CLA	B	603	-	1/1/20/20	3/39/115/115	-
23	CLA	a	406	36	-	5/39/115/115	-
27	STE	b	627	-	-	6/8/8/17	-
27	STE	C	516	-	-	5/11/11/17	-
27	STE	C	529	-	-	6/11/11/17	-
23	CLA	C	507	36	1/1/20/20	7/39/115/115	-
27	STE	j	102	-	-	6/13/13/17	-
24	PHO	d	401	-	-	1/37/103/103	0/5/6/6
23	CLA	h	101	36	1/1/20/20	23/39/115/115	-
26	PL9	d	405	-	-	9/53/73/73	0/1/1/1
28	LMG	C	517	-	-	17/30/50/70	0/1/1/1
33	LHG	D	411	-	-	13/51/51/53	-
23	CLA	b	610	-	1/1/20/20	4/39/115/115	-
25	BCR	B	619	-	-	2/29/63/63	0/2/2/2
27	STE	A	416	-	-	9/14/14/17	-
23	CLA	b	602	-	1/1/20/20	12/39/115/115	-
27	STE	x	102	-	-	4/17/17/17	-
28	LMG	a	415	-	-	26/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	B	623	-	-	7/12/12/17	-
23	CLA	C	512	-	1/1/20/20	14/39/115/115	-
23	CLA	C	505	-	1/1/20/20	10/39/115/115	-
27	STE	b	625	-	-	6/13/13/17	-
28	LMG	b	623	-	-	28/50/70/70	0/1/1/1
29	SQD	A	413	-	-	16/49/69/69	0/1/1/1
23	CLA	a	408	-	1/1/20/20	15/39/115/115	-
30	DGD	c	520	-	-	19/51/91/95	0/2/2/2
25	BCR	k	101	-	-	10/29/63/63	0/2/2/2
33	LHG	L	101	-	-	12/53/53/53	-
23	CLA	C	503	-	-	2/39/115/115	-
25	BCR	D	406	-	-	4/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/20/20	8/39/115/115	-
27	STE	d	410	-	-	4/14/14/17	-
30	DGD	c	519	-	-	26/51/91/95	0/2/2/2
27	STE	d	412	-	-	3/7/7/17	-
30	DGD	C	523	-	-	13/51/91/95	0/2/2/2
35	HEC	V	201	16	-	6/14/54/54	-
33	LHG	D	412	-	-	14/53/53/53	-
29	SQD	b	620	-	-	17/44/64/69	0/1/1/1
27	STE	I	102	-	-	5/14/14/17	-
23	CLA	b	611	-	1/1/20/20	6/39/115/115	-
27	STE	b	624	-	-	7/17/17/17	-
28	LMG	D	409	-	-	16/46/66/70	0/1/1/1
25	BCR	k	102	-	-	1/29/63/63	0/2/2/2
23	CLA	b	614	-	1/1/20/20	5/39/115/115	-
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
27	STE	C	526	-	-	4/13/13/17	-
28	LMG	b	621	-	-	18/46/66/70	0/1/1/1
29	SQD	a	412	-	-	22/49/69/69	0/1/1/1
33	LHG	d	408	-	-	11/43/43/53	-
23	CLA	c	503	-	-	8/39/115/115	-
23	CLA	c	511	3	1/1/20/20	7/39/115/115	-
27	STE	E	104	-	-	13/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	615	-	1/1/19/20	9/33/109/115	-
27	STE	c	516	-	-	3/10/10/17	-
25	BCR	C	520	-	-	3/29/63/63	0/2/2/2
27	STE	b	622	-	-	8/17/17/17	-
23	CLA	c	510	-	1/1/20/20	10/39/115/115	-
35	HEC	v	201	16	-	6/14/54/54	-
23	CLA	A	405	36	-	1/39/115/115	-
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
23	CLA	a	405	-	1/1/20/20	4/39/115/115	-
23	CLA	c	513	-	1/1/20/20	18/39/115/115	-
27	STE	E	103	-	-	1/9/9/17	-
23	CLA	B	611	-	-	6/39/115/115	-
25	BCR	c	515	-	-	3/29/63/63	0/2/2/2
27	STE	i	102	-	-	3/3/3/17	-
30	DGD	A	414	-	-	22/55/95/95	0/2/2/2
30	DGD	c	521	-	-	17/51/91/95	0/2/2/2
23	CLA	D	403	36	-	3/39/115/115	-
27	STE	c	517	-	-	4/15/15/17	-
28	LMG	c	518	-	-	9/31/31/70	-
27	STE	I	101	-	-	5/12/12/17	-
23	CLA	B	608	-	-	1/39/115/115	-
28	LMG	d	409	-	-	13/39/59/70	0/1/1/1
26	PL9	D	407	-	-	4/53/73/73	0/1/1/1
27	STE	e	103	-	-	4/6/6/17	-
27	STE	l	103	-	-	9/15/15/17	-
28	LMG	b	619	-	-	8/21/21/70	-
27	STE	C	528	-	-	7/11/11/17	-
30	DGD	C	522	-	-	18/51/91/95	0/2/2/2
23	CLA	c	504	36	1/1/19/20	4/33/109/115	-
34	HEM	F	101	6,5	-	2/14/54/54	-
23	CLA	B	616	-	1/1/19/20	5/33/109/115	-
27	STE	a	417	-	-	4/9/9/17	-
23	CLA	c	502	-	-	2/39/115/115	-
23	CLA	B	601	36	1/1/20/20	14/39/115/115	-
27	STE	C	519	-	-	1/4/4/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	STE	j	101	-	-	6/9/9/17	-
33	LHG	D	410	-	-	21/53/53/53	-
25	BCR	B	618	-	-	1/29/63/63	0/2/2/2
23	CLA	b	609	36	1/1/20/20	6/39/115/115	-
23	CLA	d	403	-	-	7/39/115/115	-
27	STE	t	102	-	-	4/11/11/17	-
30	DGD	H	102	-	-	21/51/91/95	0/2/2/2
33	LHG	d	407	-	-	13/53/53/53	-
23	CLA	A	407	-	1/1/17/20	2/26/102/115	-
23	CLA	C	508	-	-	9/39/115/115	-
25	BCR	A	408	-	-	6/29/63/63	0/2/2/2
23	CLA	c	501	-	1/1/20/20	4/39/115/115	-
27	STE	m	101	-	-	4/9/9/17	-

All (906) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	401	PHO	C1B-C2B	8.60	1.49	1.39
24	a	407	PHO	C1B-C2B	8.57	1.48	1.39
24	A	406	PHO	C1B-C2B	8.56	1.48	1.39
23	A	407	CLA	MG-ND	-8.47	1.89	2.05
23	B	613	CLA	MG-ND	-8.39	1.89	2.05
23	b	605	CLA	MG-NA	8.31	2.26	2.06
24	d	401	PHO	C3B-C4B	7.72	1.49	1.41
24	D	402	PHO	C1B-C2B	7.33	1.47	1.39
23	B	610	CLA	MG-ND	-7.22	1.91	2.05
24	A	406	PHO	C3B-C4B	6.90	1.48	1.41
23	b	611	CLA	MG-ND	-6.66	1.92	2.05
24	a	407	PHO	C3B-C4B	6.59	1.48	1.41
23	C	506	CLA	MG-ND	-6.58	1.92	2.05
35	v	201	HEC	CAC-C3C	6.52	1.56	1.35
23	c	504	CLA	MG-ND	-6.46	1.93	2.05
35	V	201	HEC	CAC-C3C	6.45	1.56	1.35
23	C	506	CLA	MG-NB	6.44	2.18	2.05
23	B	606	CLA	MG-NA	6.43	2.21	2.06
23	B	611	CLA	MG-NA	6.41	2.21	2.06
23	D	405	CLA	MG-ND	-6.15	1.93	2.05
23	C	501	CLA	MG-NA	6.09	2.20	2.06
35	v	201	HEC	CAB-C3B	6.09	1.54	1.35
35	V	201	HEC	CAB-C3B	6.07	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	411	CLA	MG-NA	6.03	2.20	2.06
23	C	511	CLA	MG-NA	6.01	2.20	2.06
23	b	608	CLA	MG-NA	5.88	2.20	2.06
23	b	605	CLA	MG-NB	-5.83	1.94	2.05
24	D	402	PHO	C3B-C4B	5.76	1.47	1.41
23	c	510	CLA	MG-NA	5.72	2.19	2.06
23	C	503	CLA	MG-NA	5.68	2.19	2.06
23	B	601	CLA	MG-NA	5.61	2.19	2.06
23	c	506	CLA	MG-ND	-5.61	1.94	2.05
26	D	407	PL9	C7-C3	-5.50	1.44	1.51
23	a	408	CLA	MG-ND	-5.45	1.95	2.05
23	c	508	CLA	MG-NA	5.45	2.19	2.06
25	t	101	BCR	C30-C25	-5.36	1.46	1.53
28	C	517	LMG	O1-C1	5.35	1.49	1.40
26	d	405	PL9	C6-C1	-5.29	1.39	1.48
23	d	403	CLA	MG-ND	-5.24	1.95	2.05
25	c	515	BCR	C1-C6	-5.11	1.47	1.53
35	v	201	HEC	C3D-C2D	5.08	1.52	1.38
23	b	615	CLA	MG-ND	-5.02	1.95	2.05
23	C	513	CLA	MG-NA	4.94	2.18	2.06
25	C	515	BCR	C1-C6	-4.90	1.47	1.53
29	f	102	SQD	O48-C23	4.80	1.47	1.33
29	A	413	SQD	O48-C23	4.79	1.47	1.33
23	B	602	CLA	C1D-ND	4.79	1.44	1.37
23	C	508	CLA	MG-ND	4.79	2.15	2.05
29	l	101	SQD	O48-C23	4.79	1.47	1.33
23	B	604	CLA	MG-NC	4.78	2.17	2.06
23	c	513	CLA	MG-NA	4.73	2.17	2.06
23	B	602	CLA	MG-ND	-4.72	1.96	2.05
34	f	101	HEM	FE-NA	4.72	2.10	1.95
23	c	512	CLA	MG-NB	4.70	2.15	2.05
23	b	611	CLA	MG-NB	4.69	2.15	2.05
25	c	514	BCR	C1-C6	-4.64	1.47	1.53
25	x	101	BCR	C30-C25	-4.57	1.47	1.53
29	a	414	SQD	O48-C23	4.57	1.46	1.33
23	B	614	CLA	MG-NB	-4.54	1.96	2.05
23	d	402	CLA	MG-NA	4.52	2.17	2.06
25	B	618	BCR	C30-C25	-4.52	1.48	1.53
30	C	522	DGD	O5D-C6D	-4.50	1.35	1.43
23	D	405	CLA	MG-NB	-4.50	1.96	2.05
23	A	407	CLA	C1D-ND	4.48	1.43	1.37
23	C	502	CLA	MG-NA	4.47	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	405	PL9	C3-C4	-4.46	1.42	1.49
23	D	405	CLA	C1D-ND	4.45	1.43	1.37
29	F	102	SQD	O48-C23	4.42	1.46	1.33
23	c	511	CLA	MG-NA	4.41	2.16	2.06
23	b	601	CLA	MG-ND	-4.35	1.97	2.05
33	a	413	LHG	O8-C23	4.33	1.46	1.33
25	b	617	BCR	C30-C25	-4.33	1.48	1.53
23	a	408	CLA	MG-NA	4.30	2.16	2.06
25	d	404	BCR	C1-C6	-4.29	1.48	1.53
23	a	411	CLA	MG-NB	4.28	2.14	2.05
25	D	406	BCR	C1-C6	-4.27	1.48	1.53
23	C	508	CLA	MG-NA	4.24	2.16	2.06
25	K	101	BCR	C30-C25	-4.24	1.48	1.53
29	F	102	SQD	O5-C1	4.23	1.52	1.41
28	a	415	LMG	C4-C5	4.21	1.62	1.53
29	A	412	SQD	O48-C23	4.21	1.45	1.33
23	c	513	CLA	MG-NC	-4.18	1.96	2.06
23	B	609	CLA	MG-NA	4.16	2.16	2.06
23	c	508	CLA	C1D-ND	4.16	1.43	1.37
33	D	412	LHG	O7-C5	-4.14	1.36	1.46
25	T	101	BCR	C1-C6	-4.14	1.48	1.53
23	b	605	CLA	C1D-ND	4.13	1.43	1.37
23	C	511	CLA	MG-NB	-4.12	1.97	2.05
30	C	521	DGD	C4D-C3D	4.12	1.63	1.52
29	b	620	SQD	O48-C23	4.11	1.45	1.33
23	B	612	CLA	C4B-NB	4.11	1.43	1.37
29	a	414	SQD	O5-C1	4.10	1.52	1.41
23	B	610	CLA	MG-NA	4.09	2.16	2.06
23	C	509	CLA	MG-NB	-4.08	1.97	2.05
29	a	414	SQD	O47-C7	4.07	1.45	1.34
33	D	411	LHG	P-O6	4.06	1.75	1.59
24	d	401	PHO	CMC-C2C	-4.06	1.44	1.50
29	l	101	SQD	O47-C7	4.05	1.45	1.34
30	A	414	DGD	C3G-C2G	4.02	1.63	1.50
23	B	616	CLA	MG-NA	4.02	2.15	2.06
34	F	101	HEM	FE-NC	4.00	2.08	1.95
23	B	610	CLA	C1D-ND	3.99	1.43	1.37
23	c	508	CLA	MG-NB	3.99	2.13	2.05
23	C	512	CLA	MG-NA	3.98	2.15	2.06
29	A	412	SQD	O47-C45	-3.97	1.37	1.46
23	C	512	CLA	MG-NB	3.97	2.13	2.05
28	c	518	LMG	C7-C8	3.96	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	415	LMG	C4-C3	3.96	1.62	1.52
23	B	603	CLA	MG-ND	3.93	2.13	2.05
26	D	407	PL9	C3-C4	-3.93	1.43	1.49
23	B	604	CLA	MG-NA	3.93	2.15	2.06
23	b	603	CLA	MG-NA	3.93	2.15	2.06
28	D	408	LMG	C4-C5	3.92	1.61	1.53
23	b	606	CLA	MG-NB	-3.92	1.98	2.05
23	B	607	CLA	MG-NA	3.91	2.15	2.06
26	D	407	PL9	C7-C8	-3.91	1.44	1.50
24	d	401	PHO	C1D-C2D	3.89	1.43	1.39
25	b	618	BCR	C30-C25	-3.89	1.48	1.53
33	L	101	LHG	O7-C5	-3.86	1.37	1.46
26	A	409	PL9	C7-C3	-3.86	1.46	1.51
23	B	611	CLA	C1D-ND	3.86	1.42	1.37
23	b	607	CLA	MG-NA	3.85	2.15	2.06
29	a	412	SQD	O47-C45	-3.85	1.37	1.46
30	C	522	DGD	C1E-C2E	3.85	1.63	1.52
23	a	406	CLA	MG-NA	3.85	2.15	2.06
25	k	101	BCR	C30-C25	-3.84	1.48	1.53
30	H	102	DGD	C4D-C5D	3.84	1.61	1.53
29	A	413	SQD	O5-C1	3.84	1.51	1.41
23	C	501	CLA	C4B-NB	3.83	1.42	1.37
25	H	101	BCR	C30-C25	-3.81	1.48	1.53
23	D	403	CLA	C1D-ND	3.80	1.42	1.37
23	c	506	CLA	C1D-ND	3.79	1.42	1.37
23	A	405	CLA	MG-NB	-3.79	1.98	2.05
23	C	507	CLA	C1B-NB	-3.78	1.32	1.37
33	D	410	LHG	O7-C5	-3.77	1.37	1.46
23	B	601	CLA	C1D-ND	3.77	1.42	1.37
25	D	406	BCR	C30-C25	-3.77	1.49	1.53
33	E	101	LHG	P-O6	3.77	1.74	1.59
23	C	505	CLA	MG-NA	3.75	2.15	2.06
23	B	606	CLA	C1D-ND	3.75	1.42	1.37
23	C	513	CLA	MG-NB	-3.74	1.98	2.05
23	b	609	CLA	C1D-ND	3.73	1.42	1.37
23	C	509	CLA	C1D-ND	3.70	1.42	1.37
23	B	616	CLA	C1D-ND	3.70	1.42	1.37
24	D	402	PHO	C1D-C2D	3.70	1.43	1.39
23	b	609	CLA	MG-NB	-3.69	1.98	2.05
25	a	409	BCR	C1-C6	-3.69	1.49	1.53
23	D	404	CLA	MG-NA	3.69	2.15	2.06
29	b	620	SQD	O5-C1	3.69	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	C1D-ND	3.69	1.42	1.37
33	a	413	LHG	C24-C23	3.67	1.61	1.50
29	f	102	SQD	O47-C45	-3.66	1.38	1.46
23	a	405	CLA	MG-NB	3.65	2.13	2.05
30	c	520	DGD	C4D-C3D	3.64	1.61	1.52
23	b	612	CLA	C1D-ND	3.64	1.42	1.37
23	b	613	CLA	C1D-ND	3.63	1.42	1.37
33	a	413	LHG	P-O6	3.62	1.73	1.59
30	h	102	DGD	C4E-C5E	3.61	1.60	1.53
23	b	611	CLA	MG-NC	-3.61	1.97	2.06
29	f	102	SQD	O47-C7	3.61	1.44	1.34
23	c	513	CLA	MG-ND	-3.61	1.98	2.05
23	b	613	CLA	C4B-NB	3.60	1.42	1.37
23	B	601	CLA	MG-ND	-3.59	1.98	2.05
23	c	510	CLA	C1D-ND	3.58	1.42	1.37
30	h	102	DGD	O2D-C2D	-3.58	1.34	1.43
29	a	412	SQD	O48-C23	3.56	1.43	1.33
25	b	616	BCR	C30-C25	-3.56	1.49	1.53
23	h	101	CLA	C1D-ND	3.55	1.42	1.37
33	d	406	LHG	C24-C23	3.54	1.61	1.50
23	C	512	CLA	MG-ND	-3.53	1.98	2.05
23	C	508	CLA	C1D-ND	3.53	1.42	1.37
23	d	402	CLA	C4B-NB	3.53	1.42	1.37
35	V	201	HEC	C3D-C2D	3.53	1.48	1.38
24	A	406	PHO	C4D-ND	-3.53	1.33	1.38
23	C	504	CLA	C1D-ND	3.53	1.42	1.37
23	a	411	CLA	C1D-ND	3.49	1.42	1.37
23	C	502	CLA	C4B-NB	3.49	1.42	1.37
23	A	404	CLA	C1B-C2B	3.48	1.51	1.43
26	D	407	PL9	C6-C1	-3.48	1.42	1.48
29	b	620	SQD	O47-C7	3.47	1.44	1.34
23	C	501	CLA	MG-ND	-3.47	1.98	2.05
29	f	102	SQD	O5-C1	3.46	1.50	1.41
25	B	619	BCR	C30-C25	-3.46	1.49	1.53
23	B	614	CLA	C4B-NB	3.46	1.42	1.37
23	d	403	CLA	C4B-NB	3.45	1.42	1.37
23	c	504	CLA	C4B-NB	3.45	1.42	1.37
23	c	505	CLA	MG-NB	-3.44	1.99	2.05
23	d	402	CLA	MG-ND	-3.44	1.99	2.05
23	b	608	CLA	C1D-ND	3.44	1.42	1.37
23	C	510	CLA	C1D-ND	3.44	1.42	1.37
33	a	413	LHG	O8-C6	3.43	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	616	BCR	C1-C6	-3.43	1.49	1.53
23	B	601	CLA	C4B-NB	3.42	1.42	1.37
25	b	617	BCR	C1-C6	-3.42	1.49	1.53
25	B	617	BCR	C1-C6	-3.42	1.49	1.53
24	a	407	PHO	C4D-ND	-3.42	1.33	1.38
30	c	520	DGD	C4E-C5E	3.41	1.60	1.53
25	k	101	BCR	C1-C6	-3.41	1.49	1.53
29	A	413	SQD	O47-C7	3.41	1.43	1.34
30	A	414	DGD	C4D-C5D	3.40	1.60	1.53
23	b	603	CLA	C1D-ND	3.40	1.42	1.37
23	C	513	CLA	C1D-ND	3.40	1.42	1.37
30	c	519	DGD	C4D-C3D	3.38	1.61	1.52
23	c	501	CLA	C1D-ND	3.37	1.42	1.37
23	b	615	CLA	C1D-ND	3.36	1.42	1.37
23	D	405	CLA	MG-NA	3.36	2.14	2.06
28	M	101	LMG	C9-C8	3.36	1.61	1.50
26	d	405	PL9	C7-C8	-3.34	1.45	1.50
33	d	408	LHG	P-O6	3.34	1.72	1.59
23	B	611	CLA	C1B-C2B	3.32	1.50	1.43
25	c	515	BCR	C30-C25	-3.31	1.49	1.53
25	K	101	BCR	C1-C6	-3.31	1.49	1.53
23	C	513	CLA	MG-ND	3.31	2.12	2.05
25	c	514	BCR	C30-C25	-3.31	1.49	1.53
23	b	602	CLA	MG-NB	-3.30	1.99	2.05
29	A	413	SQD	C24-C23	3.30	1.60	1.50
23	b	603	CLA	C4B-NB	3.28	1.42	1.37
30	c	520	DGD	C6E-C5E	3.27	1.62	1.51
28	c	524	LMG	C4-C5	3.26	1.60	1.53
23	C	508	CLA	C3B-C4B	3.26	1.52	1.42
30	c	519	DGD	O3E-C3E	-3.25	1.34	1.43
25	A	408	BCR	C1-C6	-3.25	1.49	1.53
25	B	618	BCR	C1-C6	-3.24	1.49	1.53
28	b	619	LMG	C9-C8	3.24	1.58	1.50
23	h	101	CLA	C4B-NB	3.23	1.42	1.37
23	b	614	CLA	CMD-C2D	-3.22	1.44	1.50
23	a	411	CLA	MG-ND	-3.22	1.99	2.05
23	b	604	CLA	C1D-ND	3.21	1.42	1.37
23	h	101	CLA	C1B-C2B	3.21	1.50	1.43
24	d	401	PHO	C4D-CHA	3.21	1.44	1.39
23	B	615	CLA	C4B-NB	3.20	1.42	1.37
25	B	619	BCR	C1-C6	-3.20	1.49	1.53
23	C	510	CLA	CMC-C2C	-3.20	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	523	LMG	O1-C1	3.19	1.45	1.40
23	a	406	CLA	C1D-ND	3.19	1.42	1.37
30	c	519	DGD	O2E-C2E	-3.19	1.35	1.43
30	C	522	DGD	C6E-C5E	3.18	1.62	1.51
23	c	510	CLA	CMB-C2B	-3.18	1.44	1.50
28	a	415	LMG	C3-C2	3.18	1.60	1.52
23	b	605	CLA	MG-ND	3.18	2.12	2.05
25	T	101	BCR	C30-C25	-3.17	1.49	1.53
23	B	609	CLA	C1D-ND	3.17	1.42	1.37
29	l	101	SQD	O47-C45	-3.17	1.39	1.46
23	B	607	CLA	C1D-ND	3.16	1.42	1.37
25	C	520	BCR	C30-C25	-3.16	1.49	1.53
23	b	609	CLA	C1B-C2B	3.16	1.50	1.43
23	a	408	CLA	CMC-C2C	-3.15	1.44	1.50
25	C	514	BCR	C30-C25	-3.15	1.49	1.53
23	B	608	CLA	C1B-C2B	3.14	1.50	1.43
23	B	602	CLA	C4B-NB	3.14	1.42	1.37
23	b	614	CLA	MG-ND	-3.14	1.99	2.05
23	b	604	CLA	C1B-C2B	3.14	1.50	1.43
30	C	522	DGD	C4D-C3D	3.13	1.60	1.52
23	D	403	CLA	C4B-NB	3.13	1.42	1.37
28	D	409	LMG	C4-C5	3.13	1.59	1.53
23	c	509	CLA	C1B-C2B	3.13	1.50	1.43
23	b	614	CLA	C4B-NB	3.13	1.42	1.37
23	C	506	CLA	C1D-ND	3.12	1.42	1.37
23	B	605	CLA	C3B-C4B	3.11	1.51	1.42
23	B	615	CLA	C1B-C2B	3.11	1.50	1.43
23	b	612	CLA	MG-NB	-3.10	1.99	2.05
25	B	617	BCR	C30-C25	-3.10	1.49	1.53
29	A	412	SQD	O5-C1	3.10	1.49	1.41
23	b	614	CLA	MG-NB	3.09	2.11	2.05
24	A	406	PHO	CMB-C2B	-3.09	1.45	1.51
28	a	415	LMG	C7-C8	3.08	1.60	1.50
29	a	414	SQD	O47-C45	-3.08	1.39	1.46
23	c	501	CLA	MG-NA	3.08	2.13	2.06
23	b	604	CLA	MG-NA	3.08	2.13	2.06
23	c	508	CLA	C1B-C2B	3.08	1.50	1.43
28	B	620	LMG	C4-C3	3.07	1.60	1.52
23	b	608	CLA	MG-ND	-3.07	1.99	2.05
23	b	612	CLA	MG-ND	-3.07	1.99	2.05
23	B	615	CLA	MG-ND	-3.06	1.99	2.05
30	C	521	DGD	C4E-C3E	3.06	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	C1B-C2B	3.06	1.50	1.43
25	c	515	BCR	C33-C5	-3.04	1.46	1.50
28	C	524	LMG	C4-C3	3.04	1.60	1.52
23	C	508	CLA	CHC-C1C	3.03	1.44	1.38
28	c	522	LMG	C1-C2	3.03	1.61	1.52
29	a	412	SQD	O47-C7	3.03	1.42	1.34
29	F	102	SQD	O5-C5	3.02	1.51	1.44
23	c	507	CLA	C1B-C2B	3.01	1.50	1.43
23	c	513	CLA	C4B-NB	3.01	1.41	1.37
29	l	101	SQD	O5-C1	3.01	1.49	1.41
23	D	403	CLA	C3B-C4B	3.01	1.51	1.42
23	C	503	CLA	C1B-C2B	3.00	1.50	1.43
23	C	505	CLA	CHC-C1C	3.00	1.44	1.38
29	b	620	SQD	O47-C45	-3.00	1.39	1.46
25	C	514	BCR	C1-C6	-3.00	1.49	1.53
23	B	609	CLA	MG-NB	-3.00	1.99	2.05
30	C	522	DGD	O3D-C3D	-3.00	1.35	1.43
28	a	415	LMG	O1-C7	3.00	1.49	1.43
29	A	412	SQD	O6-C1	-2.99	1.35	1.40
23	C	502	CLA	C1B-C2B	2.99	1.50	1.43
23	B	615	CLA	MG-NA	2.99	2.13	2.06
28	C	524	LMG	O7-C8	-2.99	1.39	1.46
26	d	405	PL9	C26-C24	-2.99	1.45	1.51
33	a	413	LHG	C6-C5	2.99	1.60	1.50
28	d	409	LMG	C4-C5	2.99	1.59	1.53
25	A	408	BCR	C33-C5	-2.99	1.46	1.50
23	C	510	CLA	MG-NB	2.99	2.11	2.05
23	B	602	CLA	MG-NA	2.98	2.13	2.06
28	c	522	LMG	O1-C1	2.98	1.45	1.40
23	d	402	CLA	C1B-C2B	2.97	1.50	1.43
23	B	612	CLA	C1D-ND	2.97	1.41	1.37
23	B	605	CLA	MG-ND	-2.97	1.99	2.05
23	B	614	CLA	C1D-ND	2.97	1.41	1.37
24	A	406	PHO	CMD-C2D	-2.97	1.45	1.51
28	B	620	LMG	C4-C5	2.96	1.59	1.53
25	A	408	BCR	C30-C25	-2.96	1.50	1.53
23	c	511	CLA	C4B-NB	2.96	1.41	1.37
25	b	618	BCR	C1-C6	-2.96	1.50	1.53
23	c	511	CLA	C3B-C4B	2.96	1.51	1.42
23	c	501	CLA	C4B-NB	2.95	1.41	1.37
23	c	505	CLA	C4B-NB	2.95	1.41	1.37
23	C	510	CLA	C1B-C2B	2.95	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1B-C2B	2.95	1.50	1.43
30	c	520	DGD	O3D-C3D	-2.94	1.35	1.43
23	B	603	CLA	MG-NA	2.94	2.13	2.06
29	A	412	SQD	C24-C23	2.94	1.59	1.50
24	a	407	PHO	O2D-CGD	2.93	1.40	1.33
23	c	509	CLA	MG-ND	-2.93	2.00	2.05
23	B	612	CLA	MG-NA	2.93	2.13	2.06
24	a	407	PHO	C1D-C2D	2.93	1.42	1.39
23	b	611	CLA	CMC-C2C	-2.93	1.44	1.50
23	C	511	CLA	C1D-ND	2.93	1.41	1.37
29	A	413	SQD	O47-C45	-2.93	1.39	1.46
23	C	505	CLA	C1B-C2B	2.92	1.50	1.43
23	C	508	CLA	C1B-C2B	2.92	1.50	1.43
23	B	608	CLA	MG-NA	2.91	2.13	2.06
23	B	610	CLA	C4B-NB	2.91	1.41	1.37
23	c	509	CLA	C1D-ND	2.90	1.41	1.37
23	b	604	CLA	C3B-C4B	2.90	1.51	1.42
23	d	402	CLA	CMD-C2D	-2.90	1.44	1.50
29	a	412	SQD	O6-C1	-2.90	1.35	1.40
28	c	522	LMG	C7-C8	2.89	1.59	1.50
23	B	602	CLA	C1B-C2B	2.89	1.49	1.43
23	c	502	CLA	C1B-C2B	2.88	1.49	1.43
23	B	613	CLA	C1D-ND	2.88	1.41	1.37
23	B	613	CLA	MG-NA	2.88	2.13	2.06
29	a	414	SQD	C24-C23	2.87	1.59	1.50
30	A	414	DGD	C3E-C2E	2.87	1.59	1.52
30	c	521	DGD	C1D-C2D	2.86	1.60	1.52
26	d	405	PL9	C41-C39	-2.86	1.45	1.51
23	C	509	CLA	C4B-NB	2.86	1.41	1.37
23	C	505	CLA	C1D-ND	2.86	1.41	1.37
23	c	512	CLA	C1B-NB	-2.86	1.34	1.37
23	d	403	CLA	MG-NA	2.86	2.13	2.06
23	A	404	CLA	MG-NB	-2.85	2.00	2.05
23	C	505	CLA	MG-ND	-2.85	2.00	2.05
23	C	505	CLA	C4B-NB	2.85	1.41	1.37
23	A	407	CLA	MG-NB	-2.84	2.00	2.05
23	b	610	CLA	CMC-C2C	-2.84	1.44	1.50
23	B	612	CLA	C1B-C2B	2.83	1.49	1.43
23	a	406	CLA	C4B-NB	2.83	1.41	1.37
25	k	102	BCR	C30-C25	-2.83	1.50	1.53
23	a	408	CLA	C4B-NB	2.82	1.41	1.37
23	c	506	CLA	MG-NC	2.82	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	102	DGD	O5D-C1E	2.82	1.44	1.40
26	a	410	PL9	C53-C6	-2.81	1.45	1.50
23	b	610	CLA	CMD-C2D	-2.81	1.45	1.50
23	C	511	CLA	C1B-C2B	2.80	1.49	1.43
23	c	512	CLA	C1D-ND	2.80	1.41	1.37
23	b	602	CLA	CMC-C2C	-2.80	1.45	1.50
23	C	511	CLA	C3B-C4B	2.80	1.50	1.42
23	b	612	CLA	C4B-NB	2.80	1.41	1.37
29	f	102	SQD	C24-C23	2.79	1.58	1.50
23	C	501	CLA	C1B-C2B	2.79	1.49	1.43
33	l	102	LHG	O8-C6	-2.79	1.38	1.45
28	a	415	LMG	C9-C8	2.79	1.59	1.50
23	c	507	CLA	MG-NC	-2.79	1.99	2.06
30	C	521	DGD	C6D-C5D	2.78	1.59	1.51
23	C	513	CLA	C1B-C2B	2.78	1.49	1.43
23	b	607	CLA	CHC-C1C	2.78	1.44	1.38
23	a	405	CLA	CHC-C1C	2.77	1.44	1.38
23	B	615	CLA	C1D-ND	2.76	1.41	1.37
29	F	102	SQD	O6-C44	2.76	1.50	1.43
29	a	414	SQD	O7-S	2.76	1.52	1.45
23	b	614	CLA	C3B-C4B	2.76	1.50	1.42
30	A	414	DGD	O5D-C1E	2.76	1.44	1.40
23	b	601	CLA	C1D-ND	2.76	1.41	1.37
23	b	601	CLA	MG-NB	2.76	2.11	2.05
23	B	606	CLA	C4B-NB	2.75	1.41	1.37
23	C	512	CLA	C3B-C4B	2.75	1.50	1.42
29	b	620	SQD	C24-C23	2.75	1.58	1.50
28	D	408	LMG	C7-C8	2.75	1.59	1.50
23	B	614	CLA	MG-NA	2.74	2.12	2.06
23	C	504	CLA	C4B-NB	2.74	1.41	1.37
23	c	505	CLA	CHC-C1C	2.74	1.44	1.38
23	B	605	CLA	C1B-C2B	2.74	1.49	1.43
23	h	101	CLA	O2A-CGA	2.73	1.41	1.33
23	b	614	CLA	C1B-C2B	2.73	1.49	1.43
23	B	616	CLA	C1B-C2B	2.73	1.49	1.43
28	M	101	LMG	O3-C3	-2.72	1.36	1.43
23	c	511	CLA	CHC-C1C	2.72	1.43	1.38
28	a	415	LMG	C1-C2	2.72	1.60	1.52
23	b	601	CLA	CHC-C4B	-2.72	1.33	1.39
25	d	404	BCR	C30-C25	-2.72	1.50	1.53
23	A	404	CLA	C1D-ND	2.72	1.41	1.37
28	b	621	LMG	C1-C2	2.72	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	C1B-C2B	2.72	1.49	1.43
23	D	403	CLA	CHC-C1C	2.72	1.43	1.38
35	V	201	HEC	C3C-C2C	-2.72	1.32	1.41
23	C	512	CLA	CMD-C2D	-2.71	1.45	1.50
28	A	411	LMG	C1-C2	2.71	1.60	1.52
23	B	606	CLA	MG-NC	2.71	2.12	2.06
23	B	613	CLA	C1B-C2B	2.71	1.49	1.43
28	D	409	LMG	C7-C8	2.71	1.59	1.50
23	c	507	CLA	MG-NA	2.71	2.12	2.06
29	A	412	SQD	O47-C7	2.71	1.41	1.34
23	C	513	CLA	CHC-C4B	-2.71	1.33	1.39
23	h	101	CLA	C1D-C2D	2.70	1.50	1.45
23	c	503	CLA	C1B-C2B	2.70	1.49	1.43
23	b	606	CLA	MG-NA	2.70	2.12	2.06
34	f	101	HEM	CAB-C3B	2.70	1.54	1.47
30	c	520	DGD	C3E-C2E	2.70	1.59	1.52
23	d	403	CLA	C1D-ND	2.70	1.41	1.37
29	F	102	SQD	C24-C23	2.70	1.58	1.50
23	C	509	CLA	CMB-C2B	-2.69	1.45	1.50
23	a	408	CLA	C1D-ND	2.69	1.41	1.37
25	C	520	BCR	C1-C6	-2.69	1.50	1.53
34	f	101	HEM	C3B-C2B	-2.68	1.31	1.37
34	f	101	HEM	CAC-C3C	2.68	1.54	1.47
23	B	613	CLA	CMD-C2D	-2.67	1.45	1.50
25	x	101	BCR	C1-C6	-2.67	1.50	1.53
26	A	409	PL9	C30-C29	-2.67	1.44	1.50
24	a	407	PHO	C3B-C2B	-2.66	1.36	1.40
30	h	102	DGD	C1E-C2E	2.66	1.60	1.52
23	a	408	CLA	CMD-C2D	-2.66	1.45	1.50
23	c	501	CLA	MG-NB	-2.66	2.00	2.05
30	h	102	DGD	C4D-C3D	2.65	1.59	1.52
25	C	515	BCR	C30-C25	-2.65	1.50	1.53
23	b	602	CLA	C1D-ND	2.65	1.41	1.37
23	C	505	CLA	C1B-NB	-2.65	1.34	1.37
28	C	517	LMG	O1-C7	-2.65	1.39	1.43
23	C	503	CLA	CMD-C2D	-2.64	1.45	1.50
23	b	611	CLA	C1D-ND	2.64	1.41	1.37
30	A	414	DGD	C1E-C2E	2.64	1.60	1.52
28	D	408	LMG	O1-C1	2.64	1.44	1.40
23	c	506	CLA	MG-NB	2.64	2.11	2.05
24	D	402	PHO	CMB-C2B	-2.64	1.46	1.51
23	b	604	CLA	CHC-C4B	-2.64	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	l	101	SQD	C24-C23	2.63	1.58	1.50
23	c	504	CLA	CMD-C2D	-2.63	1.45	1.50
23	b	606	CLA	C1B-NB	-2.63	1.34	1.37
35	v	201	HEC	CMA-C3A	2.63	1.56	1.50
23	C	509	CLA	MG-ND	2.63	2.11	2.05
23	c	508	CLA	C3B-C4B	2.63	1.50	1.42
30	c	521	DGD	C6D-C5D	2.63	1.59	1.51
23	B	609	CLA	C1B-C2B	2.62	1.49	1.43
23	C	507	CLA	C1B-C2B	2.62	1.49	1.43
23	c	511	CLA	C1B-C2B	2.62	1.49	1.43
24	d	401	PHO	CAC-C3C	-2.62	1.47	1.51
23	C	506	CLA	C3B-C4B	2.62	1.50	1.42
30	C	522	DGD	O5D-C1E	2.62	1.44	1.40
25	a	409	BCR	C30-C25	-2.62	1.50	1.53
23	c	511	CLA	MG-ND	2.62	2.11	2.05
23	a	405	CLA	C1D-ND	2.62	1.41	1.37
23	c	510	CLA	MG-NC	-2.61	2.00	2.06
23	b	611	CLA	C1B-C2B	2.61	1.49	1.43
23	b	604	CLA	MG-NC	-2.61	2.00	2.06
26	A	409	PL9	C21-C19	2.61	1.56	1.51
23	c	505	CLA	MG-NC	2.61	2.12	2.06
23	C	511	CLA	C4B-NB	2.60	1.41	1.37
23	B	607	CLA	CMD-C2D	-2.59	1.45	1.50
23	B	613	CLA	C4B-NB	2.59	1.41	1.37
29	a	414	SQD	O5-C5	2.59	1.50	1.44
23	D	403	CLA	C1B-C2B	2.59	1.49	1.43
23	a	406	CLA	C1B-C2B	2.59	1.49	1.43
23	h	101	CLA	MG-NA	2.58	2.12	2.06
25	c	514	BCR	C33-C5	-2.58	1.46	1.50
24	D	402	PHO	C3B-C2B	-2.58	1.36	1.40
23	A	407	CLA	C4B-NB	2.58	1.41	1.37
23	B	602	CLA	CMB-C2B	-2.58	1.45	1.50
23	b	601	CLA	CAC-C3C	-2.57	1.44	1.51
23	C	504	CLA	C3B-C4B	2.57	1.50	1.42
23	B	605	CLA	CHC-C1C	2.57	1.43	1.38
28	C	524	LMG	C4-C5	2.57	1.58	1.53
23	c	502	CLA	C1D-ND	2.57	1.41	1.37
30	H	102	DGD	C6E-C5E	2.57	1.60	1.51
34	F	101	HEM	CMA-C3A	2.57	1.56	1.50
23	a	408	CLA	C1B-C2B	2.57	1.49	1.43
23	d	403	CLA	C1B-C2B	2.57	1.49	1.43
23	c	502	CLA	CMD-C2D	-2.56	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1D-ND	2.56	1.41	1.37
29	A	413	SQD	O5-C5	2.56	1.50	1.44
30	A	414	DGD	C4E-C5E	2.56	1.58	1.53
24	A	406	PHO	CAC-C3C	-2.56	1.47	1.51
23	C	501	CLA	CHC-C1C	2.56	1.43	1.38
30	H	102	DGD	O2D-C2D	-2.56	1.36	1.43
23	b	603	CLA	CHC-C1C	2.56	1.43	1.38
29	F	102	SQD	O9-S	2.56	1.52	1.45
23	a	411	CLA	CMB-C2B	-2.56	1.45	1.50
23	c	503	CLA	CMC-C2C	-2.55	1.45	1.50
23	a	406	CLA	CMD-C2D	-2.55	1.45	1.50
23	B	603	CLA	MG-NB	-2.54	2.00	2.05
35	v	201	HEC	C3B-C2B	-2.54	1.32	1.41
28	b	621	LMG	C4-C5	2.54	1.58	1.53
23	b	601	CLA	C1B-C2B	2.54	1.49	1.43
23	B	601	CLA	CMC-C2C	-2.54	1.45	1.50
23	D	405	CLA	CMB-C2B	-2.53	1.45	1.50
23	b	612	CLA	CMD-C2D	-2.53	1.45	1.50
26	d	405	PL9	C31-C29	-2.53	1.46	1.51
25	C	520	BCR	C33-C5	-2.53	1.46	1.50
28	C	517	LMG	C7-C8	2.53	1.58	1.50
23	a	411	CLA	C1B-NB	-2.53	1.34	1.37
26	d	405	PL9	C46-C44	-2.53	1.46	1.51
24	d	401	PHO	CMD-C2D	-2.53	1.46	1.51
23	a	406	CLA	CHC-C1C	2.52	1.43	1.38
23	a	408	CLA	CHC-C4B	-2.52	1.33	1.39
23	B	607	CLA	C1B-C2B	2.52	1.49	1.43
30	c	520	DGD	O3G-C1D	-2.51	1.36	1.40
25	B	617	BCR	C33-C5	-2.51	1.46	1.50
29	a	414	SQD	O9-S	2.51	1.52	1.45
23	b	602	CLA	MG-NA	2.51	2.12	2.06
23	c	513	CLA	C3B-C4B	2.51	1.50	1.42
25	T	101	BCR	C27-C26	-2.51	1.46	1.51
23	C	506	CLA	C4B-NB	2.51	1.41	1.37
28	c	522	LMG	C4-C3	2.51	1.58	1.52
33	E	101	LHG	O7-C5	-2.50	1.40	1.46
33	E	101	LHG	O8-C23	2.50	1.40	1.33
23	C	502	CLA	CHC-C1C	2.50	1.43	1.38
28	c	524	LMG	O6-C5	-2.49	1.38	1.44
29	A	412	SQD	O9-S	2.49	1.52	1.45
23	C	501	CLA	C3B-C4B	2.49	1.50	1.42
23	b	613	CLA	MG-NC	2.49	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	CMC-C2C	-2.49	1.46	1.50
23	b	609	CLA	C1B-NB	-2.49	1.34	1.37
29	A	413	SQD	O7-S	2.49	1.52	1.45
30	C	523	DGD	O2G-C2G	-2.49	1.40	1.46
23	C	509	CLA	O2D-CGD	2.49	1.39	1.33
25	k	102	BCR	C1-C6	-2.48	1.50	1.53
23	b	615	CLA	CMC-C2C	-2.48	1.45	1.50
23	B	606	CLA	CHC-C1C	2.48	1.43	1.38
23	c	501	CLA	C1B-C2B	2.48	1.49	1.43
25	T	101	BCR	C38-C26	-2.48	1.47	1.50
23	C	513	CLA	C3B-C4B	2.48	1.49	1.42
23	C	510	CLA	CMD-C2D	-2.48	1.45	1.50
33	d	407	LHG	O7-C5	-2.48	1.40	1.46
33	D	412	LHG	C24-C23	2.47	1.57	1.50
28	b	621	LMG	O6-C1	2.47	1.48	1.41
23	C	503	CLA	C4B-NB	2.46	1.41	1.37
23	B	611	CLA	CHC-C1C	2.46	1.43	1.38
23	C	501	CLA	CMC-C2C	-2.46	1.45	1.50
25	C	515	BCR	C33-C5	-2.46	1.47	1.50
23	B	607	CLA	MG-NB	-2.46	2.00	2.05
23	b	605	CLA	C4B-NB	2.46	1.41	1.37
23	d	403	CLA	CMD-C2D	-2.45	1.45	1.50
23	c	507	CLA	MG-ND	2.45	2.10	2.05
23	B	608	CLA	CMD-C2D	-2.45	1.45	1.50
30	A	414	DGD	O2G-C1B	2.45	1.41	1.34
23	c	507	CLA	CMC-C2C	-2.45	1.45	1.50
24	D	402	PHO	C4D-CHA	2.45	1.43	1.39
23	c	504	CLA	C1B-C2B	2.45	1.48	1.43
23	c	512	CLA	CMB-C2B	-2.45	1.45	1.50
23	b	615	CLA	C1B-C2B	2.44	1.48	1.43
23	B	603	CLA	C1D-ND	2.44	1.41	1.37
23	b	613	CLA	CHC-C1C	2.44	1.43	1.38
23	d	402	CLA	CMB-C2B	-2.44	1.45	1.50
26	a	410	PL9	C46-C44	2.44	1.56	1.51
23	b	607	CLA	C1D-ND	2.44	1.41	1.37
23	b	614	CLA	C1D-ND	2.44	1.41	1.37
23	B	607	CLA	C3B-C4B	2.43	1.49	1.42
28	b	621	LMG	C4-C3	2.43	1.58	1.52
23	c	513	CLA	CHC-C1C	2.43	1.43	1.38
23	A	405	CLA	CMD-C2D	-2.43	1.45	1.50
23	B	616	CLA	CMD-C2D	-2.43	1.45	1.50
23	D	405	CLA	CHC-C4B	-2.43	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	413	LHG	C4-C5	2.42	1.58	1.50
23	C	506	CLA	CHC-C1C	2.42	1.43	1.38
28	d	409	LMG	C7-C8	2.42	1.58	1.50
30	C	521	DGD	O5D-C1E	2.42	1.44	1.40
26	D	407	PL9	C53-C6	-2.42	1.45	1.50
23	C	507	CLA	CMD-C2D	-2.42	1.45	1.50
23	A	405	CLA	C1B-C2B	2.41	1.48	1.43
23	a	411	CLA	C1B-C2B	2.41	1.48	1.43
23	B	615	CLA	CMB-C2B	-2.41	1.45	1.50
28	A	411	LMG	C4-C3	2.41	1.58	1.52
29	b	620	SQD	O6-C44	2.41	1.48	1.43
23	A	404	CLA	MG-NC	2.41	2.12	2.06
35	v	201	HEC	CMD-C2D	2.41	1.55	1.50
26	D	407	PL9	C52-C5	-2.40	1.45	1.50
33	D	411	LHG	C3-C2	2.40	1.59	1.51
23	C	504	CLA	MG-ND	-2.40	2.01	2.05
23	C	511	CLA	CMB-C2B	-2.40	1.45	1.50
28	D	409	LMG	O3-C3	-2.40	1.37	1.43
23	c	513	CLA	CMC-C2C	-2.40	1.45	1.50
34	F	101	HEM	CAB-C3B	2.40	1.53	1.47
23	C	501	CLA	MG-NB	-2.39	2.01	2.05
23	D	404	CLA	C1D-ND	2.39	1.41	1.37
23	a	405	CLA	C4B-NB	2.39	1.41	1.37
23	C	504	CLA	C1B-NB	-2.39	1.34	1.37
24	d	401	PHO	CMB-C2B	-2.39	1.46	1.51
23	B	607	CLA	CMC-C2C	-2.39	1.45	1.50
30	C	522	DGD	C6D-C5D	2.39	1.58	1.51
23	D	403	CLA	CMD-C2D	-2.38	1.45	1.50
29	a	412	SQD	O5-C1	2.38	1.48	1.41
23	b	611	CLA	MG-NA	2.38	2.11	2.06
23	A	404	CLA	C4B-NB	2.38	1.41	1.37
23	D	404	CLA	CMD-C2D	-2.38	1.45	1.50
23	h	101	CLA	CHC-C1C	2.38	1.43	1.38
23	c	507	CLA	MG-NB	-2.38	2.01	2.05
33	d	406	LHG	O7-C5	-2.38	1.41	1.46
23	B	603	CLA	CMB-C2B	-2.38	1.45	1.50
23	B	610	CLA	CMB-C2B	-2.38	1.45	1.50
23	a	405	CLA	C3D-C4D	2.38	1.49	1.44
23	b	613	CLA	C3B-C4B	2.38	1.49	1.42
30	C	521	DGD	O1G-C1G	-2.37	1.39	1.45
23	b	612	CLA	MG-NA	2.37	2.11	2.06
23	A	405	CLA	C1D-ND	2.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C1B-C2B	2.37	1.48	1.43
23	a	406	CLA	C1B-NB	-2.36	1.34	1.37
23	B	606	CLA	C1B-C2B	2.36	1.48	1.43
30	h	102	DGD	C4E-C3E	2.36	1.58	1.52
26	D	407	PL9	C5-C4	-2.36	1.39	1.47
30	c	521	DGD	C2A-C1A	-2.35	1.43	1.50
24	D	402	PHO	CMD-C2D	-2.35	1.46	1.51
23	B	604	CLA	C1D-ND	2.35	1.40	1.37
23	C	507	CLA	C3B-C4B	2.35	1.49	1.42
23	c	504	CLA	C3B-C4B	2.35	1.49	1.42
23	C	504	CLA	O2D-CGD	2.35	1.39	1.33
24	D	402	PHO	C4D-ND	-2.35	1.35	1.38
30	A	414	DGD	O5D-C6D	-2.34	1.39	1.43
23	b	601	CLA	CMD-C2D	-2.34	1.46	1.50
23	b	615	CLA	C3B-C4B	2.34	1.49	1.42
23	b	609	CLA	CMB-C2B	-2.34	1.46	1.50
23	B	603	CLA	CMD-C2D	-2.34	1.46	1.50
24	A	406	PHO	CMC-C2C	-2.34	1.47	1.50
24	A	406	PHO	C1D-C2D	2.34	1.42	1.39
28	b	623	LMG	O8-C28	2.34	1.40	1.33
30	c	520	DGD	O5E-C6E	-2.33	1.32	1.42
30	c	519	DGD	C4D-C5D	2.33	1.58	1.53
23	b	604	CLA	MG-ND	2.33	2.10	2.05
23	b	614	CLA	CHC-C1C	2.33	1.43	1.38
23	c	503	CLA	C1D-ND	2.33	1.40	1.37
23	b	607	CLA	C1B-C2B	2.33	1.48	1.43
23	D	403	CLA	MG-NB	2.33	2.10	2.05
23	C	510	CLA	CHC-C1C	2.33	1.43	1.38
28	c	523	LMG	C4-C3	2.32	1.58	1.52
23	c	509	CLA	CMB-C2B	-2.32	1.46	1.50
25	T	101	BCR	C33-C5	-2.32	1.47	1.50
23	B	608	CLA	C3B-C4B	2.32	1.49	1.42
28	c	524	LMG	O7-C8	-2.32	1.41	1.46
23	c	503	CLA	C3B-C4B	2.32	1.49	1.42
23	C	510	CLA	CAA-C2A	-2.32	1.49	1.54
23	B	615	CLA	C1B-NB	-2.31	1.34	1.37
29	f	102	SQD	O6-C44	2.31	1.47	1.43
30	C	522	DGD	O3E-C3E	-2.31	1.37	1.43
23	B	605	CLA	MG-NA	2.31	2.11	2.06
23	a	405	CLA	C1B-C2B	2.31	1.48	1.43
29	a	412	SQD	O7-S	2.31	1.51	1.45
23	a	405	CLA	MG-ND	-2.31	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	101	HEM	C3B-C2B	-2.31	1.32	1.37
23	B	615	CLA	CHC-C4B	-2.31	1.34	1.39
23	b	604	CLA	MG-NB	-2.30	2.01	2.05
23	D	405	CLA	C1B-NB	-2.30	1.34	1.37
23	B	610	CLA	CMC-C2C	-2.30	1.46	1.50
23	C	504	CLA	MG-NB	2.30	2.10	2.05
23	C	503	CLA	C1D-ND	2.30	1.40	1.37
23	B	612	CLA	C3B-C4B	2.30	1.49	1.42
35	V	201	HEC	C3B-C2B	-2.30	1.33	1.41
23	b	607	CLA	MG-NC	-2.30	2.00	2.06
23	c	506	CLA	CHC-C1C	2.30	1.43	1.38
23	b	611	CLA	C3B-C4B	2.29	1.49	1.42
23	a	406	CLA	MG-NB	2.29	2.10	2.05
25	T	101	BCR	C4-C5	-2.29	1.46	1.51
23	D	405	CLA	C3D-C4D	2.29	1.49	1.44
23	B	604	CLA	C3B-C4B	2.29	1.49	1.42
24	A	406	PHO	C4D-CHA	2.29	1.43	1.39
28	d	409	LMG	O1-C7	-2.28	1.39	1.43
23	b	610	CLA	C1B-C2B	2.28	1.48	1.43
23	B	601	CLA	CMB-C2B	-2.28	1.46	1.50
23	c	502	CLA	CHC-C1C	2.28	1.43	1.38
23	C	503	CLA	MG-NB	2.28	2.10	2.05
25	a	409	BCR	C33-C5	-2.27	1.47	1.50
23	D	403	CLA	C1C-C2C	2.27	1.49	1.44
24	a	407	PHO	CAC-C3C	-2.27	1.47	1.51
30	A	414	DGD	C6E-C5E	2.27	1.59	1.51
23	B	603	CLA	C1B-C2B	2.27	1.48	1.43
23	c	505	CLA	C3B-C4B	2.27	1.49	1.42
23	b	607	CLA	CMB-C2B	-2.27	1.46	1.50
23	B	611	CLA	C3B-C4B	2.26	1.49	1.42
23	C	502	CLA	C1D-ND	2.26	1.40	1.37
29	A	413	SQD	C46-C45	2.26	1.57	1.50
23	c	506	CLA	C1B-NB	-2.26	1.34	1.37
23	d	403	CLA	CMC-C2C	-2.26	1.46	1.50
23	B	616	CLA	C3B-C4B	2.26	1.49	1.42
29	a	412	SQD	C24-C23	2.26	1.57	1.50
34	F	101	HEM	CMC-C2C	2.26	1.55	1.50
30	H	102	DGD	C1E-C2E	2.26	1.59	1.52
23	c	506	CLA	C4B-NB	2.25	1.40	1.37
30	C	523	DGD	O6E-C5E	2.25	1.49	1.44
23	c	507	CLA	C4B-NB	2.25	1.40	1.37
23	c	502	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	101	LHG	P-O3	2.24	1.68	1.59
28	M	101	LMG	O8-C28	2.24	1.39	1.33
23	C	510	CLA	C3D-C4D	2.24	1.49	1.44
23	B	610	CLA	CHC-C1C	2.24	1.43	1.38
35	V	201	HEC	CMB-C2B	2.24	1.55	1.50
24	D	402	PHO	C1D-ND	2.23	1.42	1.38
23	C	510	CLA	C3B-C4B	2.23	1.49	1.42
23	b	603	CLA	C3B-C4B	2.23	1.49	1.42
33	l	102	LHG	C24-C23	-2.23	1.44	1.50
23	B	610	CLA	C3B-C4B	2.23	1.49	1.42
23	A	404	CLA	C1D-C2D	2.23	1.49	1.45
23	b	606	CLA	CMD-C2D	-2.22	1.46	1.50
23	b	609	CLA	C4B-NB	2.22	1.40	1.37
28	c	518	LMG	O7-C10	2.22	1.40	1.34
23	D	405	CLA	C1B-C2B	2.22	1.48	1.43
23	A	404	CLA	C3B-C4B	2.22	1.49	1.42
23	A	405	CLA	C4B-NB	2.22	1.40	1.37
23	b	614	CLA	MG-NA	2.22	2.11	2.06
23	C	503	CLA	MG-ND	2.22	2.10	2.05
29	l	101	SQD	O7-S	2.22	1.51	1.45
30	H	102	DGD	O5E-C6E	-2.22	1.33	1.42
23	c	505	CLA	CMC-C2C	-2.21	1.46	1.50
23	b	609	CLA	CMD-C2D	-2.21	1.46	1.50
23	B	606	CLA	C3B-C4B	2.21	1.49	1.42
23	a	405	CLA	CMC-C2C	-2.21	1.46	1.50
24	a	407	PHO	C4D-CHA	2.21	1.42	1.39
23	b	613	CLA	CMC-C2C	-2.21	1.46	1.50
23	a	406	CLA	CMB-C2B	-2.21	1.46	1.50
28	M	101	LMG	O7-C10	2.20	1.40	1.34
23	c	503	CLA	CMD-C2D	-2.20	1.46	1.50
23	B	611	CLA	C4B-NB	2.20	1.40	1.37
23	b	608	CLA	C3D-C4D	2.20	1.49	1.44
23	b	603	CLA	C1B-C2B	2.20	1.48	1.43
28	C	524	LMG	O1-C1	2.20	1.43	1.40
33	d	407	LHG	O7-C7	2.20	1.40	1.34
33	d	408	LHG	C6-C5	2.20	1.57	1.50
23	c	505	CLA	O2D-CED	-2.19	1.40	1.45
34	F	101	HEM	CAC-C3C	2.19	1.53	1.47
30	H	102	DGD	C3E-C2E	2.19	1.58	1.52
27	b	622	STE	C2-C1	2.19	1.55	1.50
27	x	102	STE	C2-C1	2.19	1.55	1.50
29	b	620	SQD	O9-S	2.18	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C3B-C4B	2.18	1.49	1.42
23	C	513	CLA	CMC-C2C	-2.18	1.46	1.50
26	d	405	PL9	C53-C6	-2.18	1.46	1.50
23	c	513	CLA	CMB-C2B	-2.18	1.46	1.50
23	b	602	CLA	C4B-NB	2.18	1.40	1.37
23	B	602	CLA	C3B-C4B	2.18	1.49	1.42
25	k	102	BCR	C38-C26	-2.18	1.47	1.50
30	C	521	DGD	O3D-C3D	-2.18	1.37	1.43
23	c	508	CLA	O2D-CED	-2.18	1.40	1.45
26	d	405	PL9	C41-C42	-2.18	1.46	1.53
30	c	520	DGD	O4E-C4E	-2.17	1.37	1.43
23	b	612	CLA	CMB-C2B	-2.17	1.46	1.50
29	A	412	SQD	C8-C7	2.17	1.57	1.50
30	C	523	DGD	O5D-C1E	2.17	1.43	1.40
23	D	403	CLA	MG-NA	2.17	2.11	2.06
29	f	102	SQD	O9-S	2.17	1.51	1.45
23	C	512	CLA	C1D-ND	2.17	1.40	1.37
23	C	503	CLA	C3B-C4B	2.17	1.49	1.42
23	c	508	CLA	CMC-C2C	-2.17	1.46	1.50
23	c	509	CLA	O2D-CED	-2.17	1.40	1.45
23	b	613	CLA	C5-C3	-2.16	1.46	1.51
25	k	101	BCR	C33-C5	-2.16	1.47	1.50
30	C	522	DGD	O2D-C2D	-2.16	1.37	1.43
23	D	405	CLA	CMD-C2D	-2.16	1.46	1.50
23	c	510	CLA	CMC-C2C	-2.16	1.46	1.50
23	b	602	CLA	C1B-C2B	2.16	1.48	1.43
29	l	101	SQD	O9-S	2.16	1.51	1.45
23	b	612	CLA	C1B-C2B	2.16	1.48	1.43
23	d	403	CLA	C3B-C4B	2.16	1.49	1.42
29	A	413	SQD	O9-S	2.16	1.51	1.45
23	a	411	CLA	CMD-C2D	-2.16	1.46	1.50
30	H	102	DGD	C4E-C3E	2.15	1.57	1.52
23	c	504	CLA	C1D-ND	2.15	1.40	1.37
33	D	410	LHG	P-O3	2.15	1.67	1.59
26	a	410	PL9	C30-C29	-2.15	1.45	1.50
25	t	101	BCR	C33-C5	-2.15	1.47	1.50
23	a	405	CLA	C3B-C4B	2.15	1.49	1.42
23	C	511	CLA	CHC-C4B	-2.15	1.34	1.39
23	B	607	CLA	CMB-C2B	-2.15	1.46	1.50
23	B	605	CLA	C1D-ND	2.14	1.40	1.37
30	c	520	DGD	C4E-C3E	2.14	1.57	1.52
23	B	609	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C3B-C4B	2.14	1.49	1.42
24	a	407	PHO	CMC-C2C	-2.14	1.47	1.50
25	B	619	BCR	C27-C26	-2.13	1.47	1.51
34	F	101	HEM	C3D-C2D	-2.13	1.32	1.36
23	b	608	CLA	C3B-C4B	2.13	1.48	1.42
23	C	509	CLA	C1B-C2B	2.13	1.48	1.43
23	C	502	CLA	C3B-C4B	2.12	1.48	1.42
34	F	101	HEM	CHB-C4A	-2.12	1.34	1.39
23	C	512	CLA	C1A-CHA	-2.12	1.34	1.43
23	c	509	CLA	C3B-C4B	2.12	1.48	1.42
28	d	409	LMG	O6-C5	-2.12	1.39	1.44
23	C	510	CLA	O2A-CGA	2.12	1.39	1.33
23	c	503	CLA	C3D-C4D	2.12	1.49	1.44
23	B	612	CLA	CHC-C1C	2.12	1.42	1.38
33	D	411	LHG	C1-C2	2.12	1.59	1.51
23	B	608	CLA	C1D-C2D	2.12	1.49	1.45
23	C	512	CLA	C4B-NB	2.12	1.40	1.37
23	B	604	CLA	CMC-C2C	-2.12	1.46	1.50
23	b	615	CLA	CMD-C2D	-2.11	1.46	1.50
23	B	616	CLA	C4B-NB	2.11	1.40	1.37
23	c	506	CLA	C1B-C2B	2.11	1.48	1.43
29	b	620	SQD	C44-C45	2.11	1.57	1.50
23	c	512	CLA	C3D-C4D	2.11	1.48	1.44
23	d	402	CLA	C1D-ND	2.11	1.40	1.37
23	C	512	CLA	O2D-CED	-2.11	1.40	1.45
30	A	414	DGD	C4D-C3D	2.10	1.57	1.52
23	C	511	CLA	CMC-C2C	-2.10	1.46	1.50
26	a	410	PL9	C47-C48	2.10	1.56	1.50
23	D	403	CLA	MG-NC	2.10	2.11	2.06
23	C	513	CLA	C1D-C2D	2.10	1.49	1.45
33	a	413	LHG	P-O3	2.10	1.67	1.59
34	f	101	HEM	C2A-C3A	-2.10	1.33	1.38
23	A	404	CLA	CMD-C2D	-2.10	1.46	1.50
25	t	101	BCR	C4-C5	-2.10	1.47	1.51
23	C	512	CLA	CMB-C2B	-2.10	1.46	1.50
23	A	407	CLA	C1B-C2B	2.10	1.48	1.43
29	f	102	SQD	O7-S	2.09	1.51	1.45
24	A	406	PHO	C3B-C2B	-2.09	1.37	1.40
23	c	507	CLA	C1D-ND	2.09	1.40	1.37
30	C	523	DGD	C6D-C5D	2.08	1.57	1.51
23	C	509	CLA	C3B-C4B	2.08	1.48	1.42
30	C	522	DGD	C4E-C3E	2.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C1B-C2B	2.08	1.48	1.43
23	b	609	CLA	CHC-C4B	-2.08	1.34	1.39
25	C	520	BCR	C39-C30	-2.08	1.49	1.53
29	l	101	SQD	C44-C45	2.08	1.57	1.50
23	B	606	CLA	MG-ND	-2.08	2.01	2.05
25	b	617	BCR	C4-C5	-2.08	1.47	1.51
34	f	101	HEM	CMA-C3A	2.08	1.55	1.50
28	c	524	LMG	C3-C2	2.08	1.57	1.52
23	C	512	CLA	CHC-C1C	2.07	1.42	1.38
35	V	201	HEC	C3C-C4C	-2.07	1.42	1.46
23	h	101	CLA	C3B-C4B	2.07	1.48	1.42
28	b	619	LMG	O7-C10	2.07	1.40	1.34
29	l	101	SQD	C46-C45	2.07	1.57	1.50
28	a	415	LMG	O7-C10	2.07	1.40	1.34
23	B	606	CLA	C1B-NB	-2.07	1.35	1.37
29	l	101	SQD	C8-C7	2.07	1.56	1.50
23	c	508	CLA	CHC-C1C	2.07	1.42	1.38
25	C	520	BCR	C4-C5	-2.07	1.47	1.51
23	b	611	CLA	CMD-C2D	-2.07	1.46	1.50
23	b	607	CLA	C3B-C4B	2.07	1.48	1.42
23	c	501	CLA	CMD-C2D	-2.07	1.46	1.50
23	C	508	CLA	CMB-C2B	-2.07	1.46	1.50
30	c	519	DGD	C3E-C2E	2.06	1.57	1.52
23	B	606	CLA	CMB-C2B	-2.06	1.46	1.50
23	b	608	CLA	CMB-C2B	-2.06	1.46	1.50
23	a	406	CLA	C3B-C4B	2.06	1.48	1.42
23	b	605	CLA	CHC-C4B	-2.06	1.34	1.39
23	C	503	CLA	CHC-C1C	2.06	1.42	1.38
23	h	101	CLA	CMD-C2D	-2.06	1.46	1.50
24	a	407	PHO	C3D-C4D	2.06	1.44	1.41
23	b	614	CLA	CMB-C2B	-2.06	1.46	1.50
23	c	506	CLA	C3B-C4B	2.06	1.48	1.42
28	A	411	LMG	O1-C7	-2.06	1.40	1.43
23	b	615	CLA	MG-NA	2.05	2.11	2.06
23	c	506	CLA	CMD-C2D	-2.05	1.46	1.50
23	c	502	CLA	CMC-C2C	-2.05	1.46	1.50
23	C	509	CLA	C4C-C3C	2.05	1.48	1.45
23	c	509	CLA	C4B-NB	2.05	1.40	1.37
23	B	611	CLA	CMD-C2D	-2.05	1.46	1.50
23	c	513	CLA	CMD-C2D	-2.05	1.46	1.50
23	c	511	CLA	C1D-ND	2.05	1.40	1.37
28	b	623	LMG	C9-C8	2.04	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	414	SQD	C46-C45	2.04	1.57	1.50
35	V	201	HEC	C4B-NB	-2.04	1.35	1.39
26	A	409	PL9	C53-C6	-2.04	1.46	1.50
23	a	408	CLA	C1C-NC	-2.04	1.34	1.37
30	c	520	DGD	O5D-C1E	2.04	1.43	1.40
24	D	402	PHO	C3D-C4D	2.04	1.44	1.41
23	c	512	CLA	C3B-C4B	2.04	1.48	1.42
25	k	102	BCR	C33-C5	-2.04	1.47	1.50
25	A	408	BCR	C38-C26	-2.04	1.47	1.50
25	b	616	BCR	C33-C5	-2.03	1.47	1.50
23	b	606	CLA	CMC-C2C	-2.03	1.46	1.50
23	B	610	CLA	C1B-C2B	2.03	1.47	1.43
28	c	522	LMG	O2-C2	-2.03	1.37	1.43
23	b	605	CLA	C1B-C2B	2.03	1.47	1.43
29	f	102	SQD	C44-C45	2.03	1.57	1.50
23	b	601	CLA	C3B-C4B	2.03	1.48	1.42
27	E	102	STE	C2-C1	2.03	1.55	1.50
25	a	409	BCR	C38-C26	-2.03	1.47	1.50
27	E	104	STE	C2-C1	2.03	1.55	1.50
23	B	603	CLA	C3B-C4B	2.02	1.48	1.42
30	C	521	DGD	O4D-C4D	-2.02	1.37	1.43
25	b	617	BCR	C38-C26	-2.02	1.47	1.50
30	C	521	DGD	O2E-C2E	-2.02	1.38	1.43
23	C	504	CLA	CMD-C2D	-2.02	1.46	1.50
23	B	613	CLA	C3B-C4B	2.02	1.48	1.42
23	b	612	CLA	C1B-NB	-2.02	1.35	1.37
25	b	616	BCR	C4-C5	-2.02	1.47	1.51
23	d	403	CLA	CHC-C4B	-2.02	1.34	1.39
30	c	521	DGD	O2G-C2G	-2.02	1.41	1.46
23	B	613	CLA	MG-NC	2.02	2.11	2.06
24	d	401	PHO	CAA-C2A	-2.02	1.50	1.54
24	a	407	PHO	CMB-C2B	-2.01	1.47	1.51
23	c	505	CLA	CMB-C2B	-2.01	1.46	1.50
23	b	615	CLA	CMB-C2B	-2.01	1.46	1.50
23	C	510	CLA	C3C-C2C	2.01	1.41	1.36
23	C	511	CLA	MG-NC	2.01	2.11	2.06
23	d	403	CLA	CHC-C1C	2.01	1.42	1.38
25	C	515	BCR	C36-C18	-2.01	1.46	1.50
23	C	504	CLA	MG-NC	2.01	2.11	2.06
23	B	615	CLA	CMC-C2C	-2.00	1.46	1.50
26	a	410	PL9	C46-C47	2.00	1.60	1.53
34	f	101	HEM	C4A-NA	-2.00	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	520	DGD	O1G-C1A	2.00	1.39	1.33

All (1202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	102	SQD	O6-C1-C2	15.38	131.64	108.27
23	B	601	CLA	C4A-NA-C1A	10.12	111.30	106.68
23	B	604	CLA	C4A-NA-C1A	9.43	110.98	106.68
23	B	606	CLA	C4A-NA-C1A	9.16	110.86	106.68
23	B	607	CLA	C4A-NA-C1A	9.12	110.84	106.68
35	V	201	HEC	CBB-CAB-C3B	-9.08	109.28	127.43
29	b	620	SQD	O6-C1-C2	9.07	122.05	108.27
23	C	510	CLA	C4A-NA-C1A	8.44	110.53	106.68
35	v	201	HEC	CBB-CAB-C3B	-8.35	110.75	127.43
23	C	513	CLA	C4A-NA-C1A	8.05	110.35	106.68
29	l	101	SQD	O7-S-C6	7.89	118.53	106.76
23	a	406	CLA	C4A-NA-C1A	7.73	110.20	106.68
35	v	201	HEC	CBC-CAC-C3C	-7.60	112.24	127.43
23	b	613	CLA	C4A-NA-C1A	7.53	110.12	106.68
23	B	611	CLA	C4A-NA-C1A	7.48	110.09	106.68
23	c	510	CLA	C4A-NA-C1A	7.06	109.90	106.68
35	V	201	HEC	CBC-CAC-C3C	-7.00	113.44	127.43
29	a	412	SQD	C1-O5-C5	-6.92	100.20	113.72
23	c	511	CLA	C4A-NA-C1A	6.87	109.81	106.68
23	B	603	CLA	C4A-NA-C1A	6.84	109.80	106.68
29	F	102	SQD	C1-O5-C5	-6.82	100.41	113.72
23	b	603	CLA	C4A-NA-C1A	6.80	109.78	106.68
23	B	616	CLA	C4A-NA-C1A	6.79	109.78	106.68
23	c	502	CLA	C4A-NA-C1A	6.78	109.77	106.68
26	a	410	PL9	C7-C3-C4	6.64	122.38	116.91
23	h	101	CLA	C4A-NA-C1A	6.49	109.64	106.68
23	C	502	CLA	C4A-NA-C1A	6.44	109.62	106.68
23	a	411	CLA	C4A-NA-C1A	6.42	109.61	106.68
23	D	403	CLA	C4A-NA-C1A	6.39	109.59	106.68
23	C	501	CLA	C4A-NA-C1A	6.36	109.58	106.68
29	a	414	SQD	O7-S-C6	6.36	116.25	106.76
23	d	402	CLA	C4A-NA-C1A	6.35	109.58	106.68
23	c	509	CLA	C4A-NA-C1A	6.28	109.55	106.68
23	C	511	CLA	C4A-NA-C1A	6.10	109.46	106.68
23	B	610	CLA	C4A-NA-C1A	6.06	109.44	106.68
23	B	609	CLA	C4A-NA-C1A	6.00	109.42	106.68
23	c	508	CLA	C4A-NA-C1A	5.94	109.39	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C4A-NA-C1A	5.93	109.39	106.68
23	C	503	CLA	C4A-NA-C1A	5.89	109.37	106.68
24	a	407	PHO	C4D-CHA-CBD	-5.62	105.76	108.45
23	a	408	CLA	C4A-NA-C1A	5.61	109.24	106.68
29	a	412	SQD	O6-C1-C2	5.51	116.64	108.27
28	a	415	LMG	C1-C2-C3	-5.48	98.48	110.01
29	l	101	SQD	O6-C1-C2	5.46	116.57	108.27
23	c	501	CLA	C4A-NA-C1A	5.42	109.15	106.68
26	A	409	PL9	C7-C3-C4	5.41	121.36	116.91
23	c	501	CLA	O2D-CGD-O1D	-5.40	113.34	123.85
23	b	605	CLA	C4A-NA-C1A	5.30	109.10	106.68
26	d	405	PL9	C7-C3-C4	5.20	121.19	116.91
28	C	517	LMG	O1-C1-C2	-5.16	100.43	108.27
23	B	612	CLA	C4A-NA-C1A	5.14	109.03	106.68
29	f	102	SQD	O9-S-O7	-5.13	97.13	113.82
28	a	415	LMG	O1-C1-C2	5.10	116.02	108.27
29	A	412	SQD	O6-C44-C45	-5.09	98.43	110.82
29	A	413	SQD	O5-C5-C4	5.07	118.83	109.70
23	c	512	CLA	C1-C2-C3	-4.98	118.04	126.20
23	C	508	CLA	C4A-NA-C1A	4.96	108.94	106.68
28	B	620	LMG	C1-C2-C3	-4.92	99.65	110.01
29	A	413	SQD	O47-C7-C8	4.91	122.09	111.48
24	d	401	PHO	C4D-CHA-CBD	-4.90	106.11	108.45
23	B	608	CLA	C4A-NA-C1A	4.86	108.90	106.68
29	a	414	SQD	O9-S-O7	-4.84	98.09	113.82
23	b	601	CLA	C4A-NA-C1A	4.83	108.88	106.68
23	b	602	CLA	O2D-CGD-O1D	-4.80	114.51	123.85
29	l	101	SQD	O47-C7-C8	4.78	121.83	111.48
23	b	606	CLA	C4A-NA-C1A	4.76	108.85	106.68
30	C	521	DGD	O3G-C3G-C2G	-4.73	99.32	110.82
26	a	410	PL9	C7-C3-C2	-4.71	117.83	123.39
34	f	101	HEM	CBD-CAD-C3D	-4.71	99.51	112.53
29	A	412	SQD	O47-C7-C8	4.70	121.65	111.48
24	d	401	PHO	C2B-C1B-NB	-4.70	106.03	109.43
29	a	412	SQD	C3-C4-C5	4.70	118.75	110.23
23	C	505	CLA	C4A-NA-C1A	4.65	108.80	106.68
23	b	615	CLA	C4A-NA-C1A	4.65	108.80	106.68
23	C	501	CLA	O2D-CGD-O1D	-4.63	114.84	123.85
23	c	508	CLA	C3B-C4B-NB	-4.60	106.42	110.53
29	a	414	SQD	O47-C7-C8	4.56	121.34	111.48
32	D	401	BCT	O2-C-O1	4.56	131.33	119.68
29	A	412	SQD	C1-O5-C5	-4.55	104.84	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	l	101	SQD	O48-C23-C24	4.54	125.69	111.83
29	b	620	SQD	O5-C1-C2	-4.54	101.03	110.37
23	b	605	CLA	O2D-CGD-O1D	-4.54	115.01	123.85
23	b	614	CLA	C3B-C4B-NB	-4.51	106.50	110.53
23	C	512	CLA	C3B-C4B-NB	-4.51	106.51	110.53
23	b	615	CLA	O2D-CGD-O1D	-4.50	115.08	123.85
29	f	102	SQD	O7-S-C6	4.50	113.47	106.76
29	A	413	SQD	O48-C23-C24	4.46	125.45	111.83
23	A	407	CLA	O2D-CGD-O1D	-4.46	115.16	123.85
23	B	614	CLA	O2D-CGD-O1D	-4.45	115.19	123.85
29	A	412	SQD	O8-S-C6	4.42	114.50	105.97
23	D	404	CLA	C3B-C4B-NB	-4.38	106.62	110.53
29	a	412	SQD	C44-O6-C1	-4.37	104.42	113.80
23	b	614	CLA	C4A-NA-C1A	4.37	108.67	106.68
29	A	412	SQD	O5-C1-C2	-4.34	101.46	110.37
23	b	609	CLA	CAC-C3C-C4C	4.34	130.43	124.79
23	b	601	CLA	O2D-CGD-O1D	-4.32	115.44	123.85
23	B	605	CLA	C3B-C4B-NB	-4.31	106.69	110.53
23	h	101	CLA	O2D-CGD-O1D	-4.29	115.49	123.85
23	C	508	CLA	O2D-CGD-O1D	-4.29	115.51	123.85
28	b	623	LMG	O1-C1-C2	-4.28	101.77	108.27
23	B	613	CLA	C1-C2-C3	-4.28	119.18	126.20
23	C	503	CLA	C7-C6-C5	-4.28	101.86	113.26
23	b	608	CLA	O1D-CGD-CBD	4.28	132.95	124.52
23	c	505	CLA	C3B-C4B-NB	-4.26	106.72	110.53
28	C	517	LMG	O6-C5-C4	4.26	117.38	109.70
23	c	511	CLA	C3B-C4B-NB	-4.26	106.73	110.53
23	D	405	CLA	C4A-NA-C1A	4.24	108.61	106.68
23	h	101	CLA	O2D-CGD-CBD	4.23	118.62	111.23
23	B	611	CLA	O2D-CGD-O1D	-4.21	115.65	123.85
33	l	102	LHG	O4-P-O5	4.21	132.04	112.44
23	c	504	CLA	O2D-CGD-O1D	-4.21	115.65	123.85
33	D	411	LHG	O4-P-O5	4.20	131.99	112.44
33	a	413	LHG	O4-P-O5	4.20	131.97	112.44
30	c	519	DGD	O3G-C3G-C2G	-4.17	100.67	110.82
33	L	101	LHG	O4-P-O5	4.14	131.71	112.44
24	D	402	PHO	C2B-C1B-NB	-4.12	106.45	109.43
33	E	101	LHG	O4-P-O5	4.12	131.63	112.44
23	B	608	CLA	O2D-CGD-O1D	-4.11	115.84	123.85
23	b	609	CLA	C4A-NA-C1A	4.11	108.55	106.68
23	C	506	CLA	C4A-NA-C1A	4.10	108.55	106.68
23	C	509	CLA	C4A-NA-C1A	4.10	108.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	BCR	C27-C26-C25	4.08	128.22	122.70
33	d	406	LHG	O4-P-O5	4.08	131.41	112.44
23	c	501	CLA	O2D-CGD-CBD	4.06	118.33	111.23
26	d	405	PL9	C37-C38-C39	-4.06	118.33	127.62
23	c	509	CLA	O2A-CGA-O1A	-4.05	113.51	123.63
26	A	409	PL9	C7-C3-C2	-4.04	118.63	123.39
23	b	603	CLA	C3B-C4B-NB	-4.03	106.93	110.53
23	B	604	CLA	C3B-C4B-NB	-4.03	106.93	110.53
34	f	101	HEM	C3B-C2B-C1B	4.03	109.44	106.41
23	c	503	CLA	C4A-NA-C1A	4.02	108.51	106.68
29	b	620	SQD	O7-S-C6	4.01	112.75	106.76
24	A	406	PHO	O1D-CGD-CBD	4.01	130.81	124.72
32	a	404	BCT	O2-C-O1	4.00	129.91	119.68
34	F	101	HEM	CBD-CAD-C3D	-3.98	101.52	112.53
23	B	605	CLA	C4-C3-C5	3.97	122.12	115.23
23	c	509	CLA	CHB-C4A-NA	3.97	130.13	124.40
23	D	403	CLA	C3B-C4B-NB	-3.94	107.01	110.53
23	c	512	CLA	C3B-C4B-NB	-3.94	107.02	110.53
29	b	620	SQD	C3-C4-C5	3.92	117.35	110.23
23	c	512	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
29	A	412	SQD	C1-C2-C3	-3.90	101.81	110.01
30	C	522	DGD	O3G-C3G-C2G	-3.89	101.36	110.82
25	c	514	BCR	C33-C5-C6	-3.88	120.25	124.48
29	F	102	SQD	C44-O6-C1	3.86	120.28	113.68
25	b	616	BCR	C2-C1-C6	3.86	116.05	110.44
33	D	411	LHG	O8-C23-C24	3.86	123.59	111.83
29	a	412	SQD	O7-S-C6	3.86	112.51	106.76
29	A	413	SQD	C3-C4-C5	3.85	117.22	110.23
23	a	405	CLA	C3B-C4B-NB	-3.85	107.10	110.53
23	b	602	CLA	O2D-CGD-CBD	3.84	117.94	111.23
23	C	501	CLA	O2D-CGD-CBD	3.83	117.93	111.23
30	H	102	DGD	C1E-O6E-C5E	3.83	121.20	113.72
34	f	101	HEM	CHB-C1B-NB	3.82	129.10	124.37
23	c	507	CLA	C4A-NA-C1A	3.82	108.42	106.68
23	b	608	CLA	C4A-NA-C1A	3.82	108.42	106.68
34	f	101	HEM	CBA-CAA-C2A	-3.81	102.01	112.53
29	A	413	SQD	O9-S-O7	-3.81	101.45	113.82
29	f	102	SQD	O6-C1-C2	3.79	114.04	108.27
30	C	523	DGD	O3G-C3G-C2G	-3.77	101.65	110.82
23	b	613	CLA	C7-C6-C5	-3.77	103.23	113.26
33	d	406	LHG	O8-C23-C24	3.76	123.30	111.83
23	A	404	CLA	C4A-NA-C1A	3.75	108.39	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	CHB-C4A-NA	3.75	129.81	124.40
33	d	407	LHG	O4-P-O5	3.75	129.88	112.44
23	c	506	CLA	C4A-NA-C1A	3.74	108.39	106.68
24	d	401	PHO	C3B-C4B-NB	-3.72	105.04	107.46
23	B	610	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
23	B	614	CLA	O1D-CGD-CBD	3.71	131.83	124.52
23	b	609	CLA	O2D-CGD-O1D	-3.70	116.65	123.85
28	b	623	LMG	C1-O6-C5	-3.69	106.52	113.72
25	B	617	BCR	C2-C1-C6	3.68	115.79	110.44
29	b	620	SQD	O47-C7-C8	3.67	119.43	111.48
29	f	102	SQD	O9-S-C6	3.67	112.24	106.76
23	a	405	CLA	C4A-NA-C1A	3.67	108.35	106.68
33	D	412	LHG	O4-P-O5	3.67	129.50	112.44
28	a	415	LMG	O6-C1-C2	-3.66	102.84	110.37
30	c	519	DGD	O1G-C1A-O1A	-3.66	114.47	123.63
29	F	102	SQD	C1-C2-C3	-3.64	102.35	110.01
30	c	520	DGD	O3G-C3G-C2G	-3.64	101.97	110.82
23	B	616	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
23	b	601	CLA	O2D-CGD-CBD	3.62	117.55	111.23
29	A	412	SQD	O9-S-O7	-3.61	102.09	113.82
29	A	413	SQD	O7-S-C6	3.61	112.14	106.76
30	H	102	DGD	O3G-C3G-C2G	-3.60	102.06	110.82
23	h	101	CLA	CHB-C4A-NA	3.60	129.59	124.40
23	C	513	CLA	O2D-CGD-O1D	-3.59	116.85	123.85
25	T	101	BCR	C7-C8-C9	-3.59	120.92	126.23
23	b	607	CLA	C4A-NA-C1A	3.57	108.31	106.68
24	a	407	PHO	C2B-C1B-NB	-3.56	106.86	109.43
23	b	611	CLA	CAC-C3C-C4C	3.56	129.42	124.79
23	B	602	CLA	O2D-CGD-CBD	3.54	117.43	111.23
23	b	604	CLA	C4A-NA-C1A	3.54	108.29	106.68
23	c	508	CLA	O2D-CGD-O1D	-3.54	116.97	123.85
24	D	402	PHO	OBD-CAD-CBD	-3.54	120.64	125.82
33	D	412	LHG	O8-C23-O10	-3.53	114.79	123.63
25	T	101	BCR	C27-C26-C25	3.53	127.48	122.70
23	a	406	CLA	CHB-C4A-NA	3.53	129.50	124.40
25	c	515	BCR	C27-C26-C25	3.53	127.48	122.70
28	C	517	LMG	C6-C5-C4	-3.52	104.38	113.02
33	a	413	LHG	O8-C23-C24	3.51	122.55	111.83
23	B	602	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
23	a	408	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
23	b	609	CLA	C11-C12-C13	-3.50	104.33	115.97
33	d	408	LHG	O4-P-O5	3.50	128.71	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	612	CLA	C11-C12-C13	-3.49	104.35	115.97
25	C	515	BCR	C15-C16-C17	-3.49	116.38	123.52
25	C	515	BCR	C27-C26-C25	3.48	127.41	122.70
28	b	623	LMG	C8-O7-C10	3.48	126.12	117.80
23	B	601	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
23	C	504	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
23	b	607	CLA	C3B-C4B-NB	-3.46	107.44	110.53
26	A	409	PL9	C30-C29-C28	-3.46	114.74	123.63
23	b	609	CLA	C1-C2-C3	-3.46	120.53	126.20
30	A	414	DGD	C3G-O3G-C1D	3.45	121.19	113.80
23	d	402	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
23	C	501	CLA	C3B-C4B-NB	-3.44	107.46	110.53
28	D	409	LMG	O3-C3-C2	-3.44	102.26	110.38
30	A	414	DGD	C4E-C3E-C2E	-3.44	104.80	110.83
23	C	502	CLA	C3B-C4B-NB	-3.43	107.47	110.53
29	b	620	SQD	O8-S-C6	3.43	112.59	105.97
25	C	514	BCR	C11-C10-C9	-3.42	122.48	127.28
30	c	521	DGD	O3E-C3E-C2E	-3.42	102.31	110.38
23	A	404	CLA	CHB-C4A-NA	3.41	129.33	124.40
23	B	611	CLA	C1-C2-C3	-3.41	120.61	126.20
23	b	608	CLA	CMB-C2B-C1B	-3.41	120.23	125.42
23	b	610	CLA	O2D-CGD-CBD	3.39	117.16	111.23
23	a	408	CLA	O2D-CGD-CBD	3.39	117.16	111.23
25	b	618	BCR	C27-C26-C25	3.39	127.28	122.70
23	a	406	CLA	C3B-C4B-NB	-3.39	107.51	110.53
26	d	405	PL9	C7-C3-C2	-3.38	119.40	123.39
24	D	402	PHO	C4D-CHA-CBD	-3.38	106.83	108.45
23	B	610	CLA	C3B-C4B-NB	-3.38	107.52	110.53
23	b	610	CLA	C3B-C4B-NB	-3.38	107.52	110.53
23	B	614	CLA	C3B-C4B-NB	-3.37	107.52	110.53
26	d	405	PL9	C22-C23-C24	-3.37	119.92	127.62
26	D	407	PL9	C37-C38-C39	-3.36	119.92	127.62
28	b	623	LMG	O2-C2-C1	-3.35	102.08	110.08
23	A	407	CLA	O2D-CGD-CBD	3.35	117.09	111.23
23	b	610	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
30	A	414	DGD	O5D-C1E-C2E	3.33	113.33	108.27
23	c	513	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
29	b	620	SQD	O9-S-O7	-3.33	102.99	113.82
25	x	101	BCR	C38-C26-C25	-3.33	120.85	124.48
28	C	517	LMG	O7-C10-O9	-3.33	115.92	123.70
30	c	521	DGD	O3G-C3G-C2G	-3.33	102.73	110.82
23	B	611	CLA	O2D-CGD-CBD	3.33	117.04	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C7-C6-C5	-3.32	104.40	113.26
25	H	101	BCR	C38-C26-C25	-3.32	120.86	124.48
35	V	201	HEC	CHB-C4A-NA	3.32	128.07	124.45
26	D	407	PL9	C20-C19-C21	3.32	120.98	115.23
23	b	604	CLA	CHD-C1D-ND	-3.31	120.14	124.80
28	D	409	LMG	C3-C4-C5	-3.31	104.23	110.23
30	h	102	DGD	O6E-C5E-C4E	3.30	115.65	109.70
23	C	505	CLA	C3B-C4B-NB	-3.30	107.58	110.53
23	b	606	CLA	C4-C3-C5	3.29	120.95	115.23
24	A	406	PHO	O2D-CGD-O1D	-3.29	117.44	123.85
23	B	602	CLA	O2A-CGA-O1A	-3.29	115.39	123.63
28	D	408	LMG	O6-C1-O1	-3.28	102.30	110.04
26	D	407	PL9	C7-C3-C4	3.28	119.61	116.91
28	d	409	LMG	O6-C1-O1	-3.28	102.30	110.04
23	B	612	CLA	C3B-C4B-NB	-3.27	107.61	110.53
23	b	601	CLA	CHB-C4A-NA	3.27	129.12	124.40
32	D	401	BCT	O3-C-O1	-3.27	111.32	119.68
29	l	101	SQD	O9-S-O7	-3.26	103.20	113.82
33	D	410	LHG	O4-P-O5	3.26	127.61	112.44
23	C	503	CLA	C3B-C4B-NB	-3.26	107.62	110.53
25	C	520	BCR	C27-C26-C25	3.25	127.10	122.70
29	a	412	SQD	O8-S-C6	3.25	112.24	105.97
28	C	517	LMG	C7-O1-C1	3.25	120.75	113.80
23	b	613	CLA	C1-C2-C3	-3.24	120.89	126.20
23	a	406	CLA	O2D-CGD-CBD	3.24	116.89	111.23
29	F	102	SQD	O8-S-C6	3.24	112.22	105.97
25	x	101	BCR	C27-C26-C25	3.23	127.07	122.70
26	A	409	PL9	O1-C4-C3	-3.23	117.32	120.73
30	c	521	DGD	C3D-C4D-C5D	-3.22	104.40	110.23
25	B	619	BCR	C2-C1-C6	3.21	115.10	110.44
23	c	510	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
23	b	610	CLA	CHB-C4A-NA	3.21	129.03	124.40
28	c	524	LMG	O6-C1-O1	-3.21	102.46	110.04
28	D	409	LMG	O1-C1-C2	-3.20	103.41	108.27
23	b	613	CLA	O2A-CGA-O1A	-3.20	115.61	123.63
23	C	508	CLA	C3B-C4B-NB	-3.20	107.67	110.53
23	b	611	CLA	CHB-C4A-NA	3.19	129.01	124.40
35	V	201	HEC	CHD-C4C-NC	3.19	127.92	124.45
23	D	405	CLA	O2D-CGD-O1D	-3.18	117.65	123.85
25	B	617	BCR	C29-C30-C25	3.18	115.06	110.44
29	A	413	SQD	C44-O6-C1	3.17	120.59	113.80
23	d	402	CLA	C4-C3-C5	3.17	120.72	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	h	102	DGD	C1E-O6E-C5E	3.16	119.90	113.72
23	C	509	CLA	CHD-C1D-ND	-3.16	120.35	124.80
29	A	412	SQD	O9-S-C6	3.16	111.47	106.76
29	a	412	SQD	C1-C2-C3	-3.15	103.38	110.01
23	c	510	CLA	C3B-C4B-NB	-3.15	107.72	110.53
23	C	506	CLA	O1D-CGD-CBD	3.15	130.74	124.52
23	B	612	CLA	O2A-CGA-O1A	-3.15	115.75	123.63
23	B	613	CLA	CHA-C1A-NA	-3.15	119.27	126.39
30	c	521	DGD	O5D-C1E-C2E	3.14	113.05	108.27
30	C	521	DGD	O5D-C1E-C2E	-3.14	103.51	108.27
30	c	520	DGD	O6D-C1D-O3G	-3.13	102.65	110.04
23	c	504	CLA	C4A-NA-C1A	3.13	108.11	106.68
23	c	512	CLA	C4A-NA-C1A	3.13	108.11	106.68
23	b	613	CLA	CHB-C4A-NA	3.12	128.91	124.40
23	b	605	CLA	CHB-C1B-NB	3.12	128.73	124.05
25	k	102	BCR	C27-C26-C25	3.12	126.92	122.70
23	C	509	CLA	O2A-CGA-O1A	-3.11	115.84	123.63
23	b	601	CLA	CMB-C2B-C1B	-3.11	120.69	125.42
30	C	523	DGD	C8B-C7B-C6B	-3.10	98.69	114.37
25	c	515	BCR	C33-C5-C6	-3.10	121.10	124.48
34	F	101	HEM	CHB-C1B-NB	3.10	128.20	124.37
25	B	618	BCR	C29-C30-C25	3.10	114.94	110.44
23	h	101	CLA	CHD-C1D-ND	-3.09	120.45	124.80
30	h	102	DGD	O3E-C3E-C2E	-3.09	103.09	110.38
23	C	508	CLA	CHD-C1D-ND	-3.08	120.46	124.80
28	b	621	LMG	O3-C3-C2	-3.07	103.13	110.38
23	B	608	CLA	C3B-C4B-NB	-3.07	107.79	110.53
29	b	620	SQD	O2-C2-C1	3.07	117.38	110.08
23	A	405	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
23	C	507	CLA	O2A-CGA-O1A	-3.06	115.96	123.63
23	B	610	CLA	O2A-CGA-O1A	-3.05	115.99	123.63
23	B	606	CLA	C3B-C4B-NB	-3.05	107.81	110.53
23	a	405	CLA	C7-C6-C5	-3.05	105.14	113.26
29	A	412	SQD	O47-C7-O49	-3.05	116.58	123.70
24	D	402	PHO	CMB-C2B-C3B	3.05	130.77	124.68
33	L	101	LHG	C11-C10-C9	-3.05	98.97	114.37
23	C	512	CLA	C1-C2-C3	-3.04	121.21	126.20
25	K	101	BCR	C33-C5-C6	-3.04	121.17	124.48
23	c	502	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
29	A	412	SQD	C3-C4-C5	3.03	115.72	110.23
30	C	522	DGD	C1D-C2D-C3D	-3.03	103.65	110.01
25	K	101	BCR	C27-C26-C25	3.02	126.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	CHB-C4A-NA	3.02	128.76	124.40
25	k	101	BCR	C33-C5-C6	-3.02	121.19	124.48
23	b	613	CLA	C3B-C4B-NB	-3.02	107.83	110.53
30	C	521	DGD	C3G-C2G-C1G	-3.01	104.76	111.78
25	k	101	BCR	C27-C26-C25	3.01	126.77	122.70
23	a	405	CLA	CAC-C3C-C4C	3.01	128.70	124.79
23	b	612	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
26	A	409	PL9	O2-C1-C2	-3.00	115.01	121.83
23	a	411	CLA	CHB-C4A-NA	3.00	128.73	124.40
33	d	406	LHG	O8-C23-O10	-3.00	116.13	123.63
23	C	507	CLA	C3B-C4B-NB	-3.00	107.86	110.53
23	C	510	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
23	b	604	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
23	A	407	CLA	C1D-ND-C4D	-2.98	104.22	106.31
26	a	410	PL9	C22-C23-C24	-2.98	120.80	127.62
24	A	406	PHO	C2B-C1B-NB	-2.98	107.28	109.43
23	c	503	CLA	C3B-C4B-NB	-2.97	107.88	110.53
30	c	521	DGD	O6D-C1D-O3G	-2.97	103.03	110.04
30	H	102	DGD	C3D-C4D-C5D	-2.96	104.86	110.23
25	H	101	BCR	C2-C1-C6	2.96	114.75	110.44
23	b	612	CLA	C4A-NA-C1A	2.96	108.03	106.68
33	D	412	LHG	C11-C10-C9	-2.96	99.43	114.37
23	c	511	CLA	CHD-C1D-ND	-2.95	120.65	124.80
30	h	102	DGD	C3D-C4D-C5D	-2.95	104.89	110.23
23	a	405	CLA	O1D-CGD-CBD	2.95	130.33	124.52
26	a	410	PL9	C35-C34-C36	2.94	120.34	115.23
23	C	510	CLA	C7-C6-C5	-2.94	105.42	113.26
23	B	602	CLA	C4A-NA-C1A	2.94	108.02	106.68
29	a	412	SQD	C46-C45-C44	-2.94	104.93	111.78
30	H	102	DGD	O5D-C1E-C2E	2.93	112.73	108.27
23	b	604	CLA	C1-O2A-CGA	-2.93	109.56	116.65
23	C	507	CLA	CMB-C2B-C3B	2.93	133.44	126.55
23	C	506	CLA	C3B-C4B-NB	-2.93	107.92	110.53
29	A	412	SQD	O8-S-O7	-2.92	104.08	111.40
27	D	413	STE	O2-C1-C2	2.92	123.23	114.00
23	b	611	CLA	C11-C12-C13	-2.92	106.27	115.97
23	B	611	CLA	C3B-C4B-NB	-2.92	107.93	110.53
23	C	512	CLA	C4A-NA-C1A	2.91	108.01	106.68
28	c	524	LMG	C1-O6-C5	-2.91	108.04	113.72
29	b	620	SQD	C1-C2-C3	-2.90	103.90	110.01
23	b	605	CLA	O2D-CGD-CBD	2.90	116.30	111.23
25	a	409	BCR	C27-C26-C25	2.90	126.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	521	DGD	O6D-C1D-O3G	-2.90	103.19	110.04
25	D	406	BCR	C2-C1-C6	2.90	114.65	110.44
30	A	414	DGD	C3G-C2G-C1G	-2.90	105.03	111.78
23	B	608	CLA	O2D-CGD-CBD	2.90	116.30	111.23
30	A	414	DGD	O6E-C5E-C4E	2.90	114.92	109.70
24	d	401	PHO	C1-C2-C3	-2.89	121.45	126.20
26	D	407	PL9	C22-C23-C24	-2.89	121.01	127.62
25	c	514	BCR	C24-C23-C22	-2.89	121.97	126.23
23	c	507	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
23	A	405	CLA	CED-O2D-CGD	-2.88	109.38	115.92
23	B	616	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
23	C	506	CLA	CHB-C4A-NA	2.88	128.56	124.40
30	c	520	DGD	O3D-C3D-C4D	-2.88	103.59	110.38
26	D	407	PL9	C12-C13-C14	-2.88	121.04	127.62
30	c	521	DGD	O6E-C5E-C4E	2.88	114.88	109.70
33	d	406	LHG	C11-C10-C9	-2.87	99.84	114.37
23	a	408	CLA	CHB-C4A-NA	2.87	128.54	124.40
28	c	523	LMG	O6-C1-O1	-2.87	103.26	110.04
23	b	602	CLA	C4A-NA-C1A	2.87	107.99	106.68
30	c	520	DGD	O2G-C1B-O1B	-2.87	117.00	123.70
28	c	523	LMG	O1-C1-C2	-2.87	103.92	108.27
26	A	409	PL9	C40-C39-C41	2.86	120.20	115.23
25	K	101	BCR	C39-C30-C25	-2.86	105.75	110.24
23	B	605	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
30	C	521	DGD	CDB-CCB-CBB	-2.86	99.93	114.37
23	D	403	CLA	CHB-C4A-NA	2.85	128.52	124.40
23	A	405	CLA	C4A-NA-C1A	2.85	107.98	106.68
25	c	514	BCR	C15-C14-C13	-2.85	123.28	127.28
25	B	617	BCR	C11-C10-C9	-2.85	123.28	127.28
23	B	608	CLA	CHD-C1D-ND	-2.85	120.80	124.80
29	A	412	SQD	C46-C45-C44	-2.84	105.16	111.78
23	h	101	CLA	CBA-CAA-C2A	2.84	122.24	113.79
23	C	511	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
28	d	409	LMG	O1-C1-C2	-2.84	103.96	108.27
23	b	613	CLA	C4-C3-C5	2.83	120.15	115.23
28	d	409	LMG	C3-C4-C5	-2.83	105.10	110.23
29	a	412	SQD	O9-S-O7	-2.83	104.61	113.82
23	B	602	CLA	C1-C2-C3	-2.83	121.56	126.20
23	c	504	CLA	CHB-C4A-NA	2.83	128.48	124.40
30	C	523	DGD	O6D-C1D-O3G	-2.83	103.36	110.04
34	F	101	HEM	C4C-C3C-C2C	2.83	109.26	106.81
30	c	520	DGD	C1E-O6E-C5E	2.82	119.23	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	514	BCR	C2-C1-C6	2.82	114.54	110.44
23	C	509	CLA	CHB-C4A-NA	2.82	128.47	124.40
26	A	409	PL9	O2-C1-C6	2.82	124.96	120.48
23	B	601	CLA	C1-O2A-CGA	2.82	123.47	116.65
29	b	620	SQD	O48-C23-C24	2.81	120.41	111.83
23	C	503	CLA	CHD-C1D-ND	-2.81	120.85	124.80
23	b	615	CLA	CHB-C4A-NA	2.81	128.45	124.40
26	D	407	PL9	C42-C43-C44	-2.81	121.20	127.62
23	b	612	CLA	CHB-C4A-NA	2.80	128.44	124.40
23	b	614	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
23	B	603	CLA	C3B-C4B-NB	-2.80	108.03	110.53
30	c	520	DGD	C3G-O3G-C1D	2.79	119.78	113.80
28	b	623	LMG	O6-C5-C6	2.79	113.35	106.44
29	f	102	SQD	C1-O5-C5	-2.79	108.28	113.72
23	b	615	CLA	O1D-CGD-CBD	2.79	130.01	124.52
30	A	414	DGD	O3G-C3G-C2G	-2.79	104.04	110.82
29	A	413	SQD	O48-C23-O10	-2.79	116.66	123.63
26	D	407	PL9	C32-C33-C34	-2.78	121.25	127.62
23	h	101	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
28	A	411	LMG	C1-O6-C5	-2.78	108.28	113.72
23	B	603	CLA	CHD-C4C-NC	2.78	128.54	124.23
23	C	507	CLA	O2D-CGD-CBD	2.78	116.09	111.23
23	C	508	CLA	O2D-CGD-CBD	2.78	116.09	111.23
30	c	519	DGD	O3E-C3E-C2E	-2.78	103.83	110.38
34	F	101	HEM	CBA-CAA-C2A	-2.78	104.86	112.53
32	a	404	BCT	O3-C-O1	-2.77	112.58	119.68
23	C	509	CLA	C1-C2-C3	-2.77	121.66	126.20
28	C	517	LMG	O2-C2-C1	-2.77	103.48	110.08
25	b	616	BCR	C29-C30-C25	2.76	114.45	110.44
28	c	524	LMG	C40-C39-C38	-2.76	100.40	114.37
24	a	407	PHO	C3B-C4B-NB	-2.76	105.67	107.46
25	H	101	BCR	C29-C30-C25	2.75	114.44	110.44
23	c	513	CLA	CHB-C4A-NA	2.75	128.37	124.40
30	c	520	DGD	C1D-C2D-C3D	-2.75	104.22	110.01
23	B	606	CLA	C4-C3-C5	2.75	120.00	115.23
24	A	406	PHO	CMB-C2B-C3B	2.75	130.18	124.68
25	b	616	BCR	C15-C16-C17	-2.75	117.89	123.52
25	b	616	BCR	C27-C26-C25	2.75	126.42	122.70
25	B	618	BCR	C2-C1-C6	2.75	114.43	110.44
23	a	406	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
23	C	504	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
23	a	411	CLA	C3B-C4B-NB	-2.74	108.08	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	h	101	CLA	C3B-C4B-NB	-2.74	108.08	110.53
35	V	201	HEC	CMD-C2D-C1D	2.74	129.60	125.42
25	t	101	BCR	C2-C1-C6	2.74	114.42	110.44
23	a	408	CLA	CAC-C3C-C4C	2.74	128.36	124.79
25	C	514	BCR	C27-C26-C25	2.74	126.41	122.70
33	E	101	LHG	O8-C23-C24	2.74	120.19	111.83
30	h	102	DGD	O3G-C3G-C2G	-2.74	104.16	110.82
28	B	620	LMG	O8-C28-O10	-2.73	116.79	123.63
29	F	102	SQD	O9-S-C6	2.73	110.84	106.76
23	b	609	CLA	CAA-CBA-CGA	-2.73	105.44	113.21
25	A	408	BCR	C37-C22-C21	-2.73	118.39	122.82
28	d	409	LMG	O3-C3-C2	-2.73	103.94	110.38
29	a	412	SQD	O47-C7-C8	2.73	117.39	111.48
24	a	407	PHO	OBD-CAD-CBD	-2.73	121.82	125.82
23	b	609	CLA	O1D-CGD-CBD	2.73	129.89	124.52
28	A	411	LMG	O7-C10-O9	-2.72	117.34	123.70
25	b	618	BCR	C12-C13-C14	-2.72	114.73	119.01
26	D	407	PL9	C7-C3-C2	-2.72	120.18	123.39
33	D	412	LHG	O8-C23-C24	2.71	120.11	111.83
23	c	508	CLA	CHB-C4A-NA	2.71	128.32	124.40
30	A	414	DGD	O3G-C1D-C2D	-2.71	104.15	108.27
25	t	101	BCR	C7-C8-C9	-2.71	122.22	126.23
23	b	606	CLA	C3B-C4B-NB	-2.71	108.11	110.53
27	b	625	STE	O2-C1-O1	-2.71	116.36	123.33
23	b	615	CLA	C4-C3-C5	2.71	119.93	115.23
25	C	515	BCR	C38-C26-C27	-2.71	107.82	113.60
23	C	509	CLA	C3B-C4B-NB	-2.71	108.11	110.53
23	D	404	CLA	CED-O2D-CGD	2.71	122.05	115.92
33	d	408	LHG	O8-C23-O10	-2.70	116.87	123.63
33	D	410	LHG	C18-C17-C16	-2.70	100.71	114.37
23	A	407	CLA	C4A-NA-C1A	2.70	107.91	106.68
24	d	401	PHO	O1D-CGD-CBD	2.70	128.82	124.72
28	C	524	LMG	O1-C7-C8	-2.70	104.25	110.82
23	B	601	CLA	O2D-CGD-CBD	2.70	115.95	111.23
23	b	603	CLA	C6-C7-C8	-2.70	107.01	115.97
30	c	520	DGD	CDB-CCB-CBB	-2.69	100.77	114.37
23	c	506	CLA	C4-C3-C5	2.69	119.89	115.23
23	C	504	CLA	C3B-C4B-NB	-2.69	108.13	110.53
23	c	509	CLA	C1-O2A-CGA	-2.69	110.15	116.65
24	a	407	PHO	CMA-C3A-C4A	-2.69	108.82	114.61
30	C	523	DGD	C6B-C5B-C4B	-2.68	100.80	114.37
23	c	507	CLA	CHD-C1D-ND	-2.68	121.03	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	x	101	BCR	C2-C1-C6	2.68	114.33	110.44
25	D	406	BCR	C27-C26-C25	2.68	126.33	122.70
28	M	101	LMG	C1-C2-C3	-2.68	104.37	110.01
23	B	607	CLA	C1-C2-C3	-2.68	121.81	126.20
25	b	617	BCR	C27-C26-C25	2.67	126.32	122.70
23	c	513	CLA	C3B-C4B-NB	-2.67	108.14	110.53
23	C	510	CLA	CHD-C1D-ND	-2.67	121.05	124.80
25	b	616	BCR	C11-C10-C9	-2.66	123.54	127.28
23	C	501	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
23	b	612	CLA	C1-C2-C3	-2.66	121.84	126.20
23	B	612	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
27	b	625	STE	O2-C1-C2	2.65	122.39	114.00
25	T	101	BCR	C38-C26-C27	-2.65	107.94	113.60
25	B	617	BCR	C3-C4-C5	-2.65	109.33	114.06
25	b	616	BCR	C33-C5-C6	-2.65	121.59	124.48
23	b	606	CLA	C6-C7-C8	-2.65	107.15	115.97
23	C	507	CLA	CHB-C4A-NA	2.65	128.22	124.40
23	C	509	CLA	C2A-C3A-C4A	2.65	106.15	101.87
23	B	615	CLA	CHC-C4B-NB	2.65	128.02	124.05
23	c	506	CLA	C3B-C4B-NB	-2.64	108.17	110.53
23	C	503	CLA	O2A-C1-C2	-2.64	97.95	108.11
23	b	609	CLA	CAC-C3C-C2C	-2.64	122.71	127.56
28	b	623	LMG	O8-C28-O10	-2.64	117.03	123.63
23	C	506	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
23	B	613	CLA	C3B-C4B-NB	-2.64	108.18	110.53
28	M	101	LMG	C8-O7-C10	2.64	124.11	117.80
26	d	405	PL9	C35-C34-C36	2.63	119.80	115.23
23	b	610	CLA	C4A-NA-C1A	2.63	107.88	106.68
23	B	614	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
30	H	102	DGD	O6E-C5E-C4E	2.63	114.43	109.70
25	b	618	BCR	C38-C26-C25	-2.63	121.62	124.48
30	C	521	DGD	CBB-CAB-C9B	-2.63	101.09	114.37
23	b	607	CLA	O2D-CGD-CBD	2.63	115.82	111.23
23	b	613	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
23	C	505	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
23	c	511	CLA	CHD-C4C-NC	2.62	128.30	124.23
28	c	518	LMG	C9-C8-C7	-2.62	105.75	111.80
23	C	510	CLA	CHB-C4A-NA	2.62	128.18	124.40
25	C	515	BCR	C33-C5-C6	-2.62	121.63	124.48
23	b	602	CLA	C4-C3-C5	2.61	119.77	115.23
23	B	611	CLA	C7-C6-C5	-2.61	106.30	113.26
23	C	512	CLA	O2A-CGA-O1A	-2.61	117.10	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	f	102	SQD	O48-C23-C24	2.61	119.80	111.83
23	d	403	CLA	CHA-C1A-NA	-2.61	120.48	126.39
24	A	406	PHO	C1-C2-C3	-2.61	121.92	126.20
23	b	608	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
28	A	411	LMG	O7-C10-C11	2.61	117.12	111.48
28	b	621	LMG	O7-C10-O9	-2.61	117.61	123.70
23	b	603	CLA	CHB-C1B-NB	2.61	127.96	124.05
23	c	509	CLA	O1D-CGD-CBD	2.60	129.66	124.52
23	C	511	CLA	C4-C3-C5	2.60	119.75	115.23
30	C	521	DGD	C3D-C4D-C5D	-2.60	105.51	110.23
23	c	510	CLA	CHB-C4A-NA	2.60	128.16	124.40
30	A	414	DGD	C1E-O6E-C5E	2.60	118.80	113.72
23	c	507	CLA	C3B-C4B-NB	-2.60	108.21	110.53
33	d	408	LHG	O8-C23-C24	2.60	119.75	111.83
23	b	614	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
23	A	405	CLA	CHB-C4A-NA	2.60	128.15	124.40
23	B	610	CLA	O2D-CGD-CBD	2.60	115.77	111.23
23	C	512	CLA	CHA-C1A-NA	-2.59	120.52	126.39
23	c	507	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
23	B	615	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
25	t	101	BCR	C27-C26-C25	2.59	126.21	122.70
28	C	517	LMG	O1-C7-C8	-2.59	104.52	110.82
23	B	603	CLA	CHB-C4A-NA	2.59	128.14	124.40
30	c	520	DGD	O6E-C5E-C4E	2.59	114.36	109.70
23	b	604	CLA	C1-C2-C3	-2.59	121.95	126.20
28	b	619	LMG	C8-O7-C10	2.59	121.52	117.78
23	c	504	CLA	O2D-CGD-CBD	2.59	115.75	111.23
28	c	524	LMG	C38-C37-C36	-2.59	101.29	114.37
29	F	102	SQD	C3-C4-C5	2.59	114.92	110.23
30	c	521	DGD	CDB-CCB-CBB	-2.58	101.32	114.37
30	h	102	DGD	O1G-C1A-O1A	-2.58	117.18	123.63
23	b	609	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
23	c	502	CLA	C3B-C4B-NB	-2.58	108.23	110.53
23	C	507	CLA	CHD-C1D-ND	-2.58	121.18	124.80
23	C	502	CLA	O1D-CGD-CBD	2.58	129.60	124.52
23	c	502	CLA	C1-C2-C3	-2.57	121.98	126.20
23	b	607	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
26	A	409	PL9	C30-C29-C31	-2.57	110.76	115.23
25	T	101	BCR	C30-C25-C26	-2.57	119.12	122.64
23	b	601	CLA	CMB-C2B-C3B	2.57	132.59	126.55
23	b	604	CLA	CHD-C1D-C2D	2.57	130.82	125.49
23	C	510	CLA	O2D-CGD-CBD	2.56	115.71	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	405	PL9	C40-C39-C38	-2.56	117.04	123.63
23	C	507	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
23	C	503	CLA	C4D-CHA-C1A	2.56	124.30	121.24
30	c	520	DGD	O2D-C2D-C1D	-2.56	103.97	110.08
23	C	513	CLA	O2D-CGD-CBD	2.56	115.70	111.23
29	b	620	SQD	C1-O5-C5	-2.56	108.72	113.72
30	H	102	DGD	O5E-C6E-C5E	-2.56	102.62	111.33
27	C	525	STE	C3-C2-C1	-2.55	107.85	114.51
23	B	606	CLA	C1-C2-C3	-2.55	122.02	126.20
23	B	603	CLA	C5-C3-C2	-2.55	115.44	121.17
25	c	515	BCR	C2-C1-C6	2.55	114.14	110.44
29	a	412	SQD	O6-C44-C45	-2.55	104.62	110.82
23	c	505	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
23	b	608	CLA	C3B-C4B-NB	-2.54	108.26	110.53
23	c	504	CLA	C3B-C4B-NB	-2.54	108.26	110.53
33	a	413	LHG	C20-C19-C18	-2.54	101.51	114.37
28	d	409	LMG	O2-C2-C1	-2.54	104.02	110.08
30	C	521	DGD	O5D-C6D-C5D	-2.54	103.69	109.42
23	C	502	CLA	C4D-CHA-C1A	2.54	124.28	121.24
23	b	608	CLA	CMB-C2B-C3B	2.54	132.53	126.55
29	b	620	SQD	O5-C5-C4	2.54	114.28	109.70
23	B	604	CLA	CHB-C4A-NA	2.54	128.07	124.40
26	a	410	PL9	C27-C28-C29	-2.54	121.81	127.62
25	x	101	BCR	C35-C13-C14	-2.54	118.70	122.82
23	C	512	CLA	C6-C5-C3	-2.54	107.29	113.47
26	A	409	PL9	C20-C19-C21	2.54	119.63	115.23
33	L	101	LHG	O8-C23-O10	-2.54	117.28	123.63
23	D	405	CLA	CHC-C4B-NB	2.54	127.86	124.05
25	b	616	BCR	C8-C7-C6	-2.54	120.22	127.00
35	v	201	HEC	CMC-C2C-C1C	-2.54	121.56	125.42
30	c	519	DGD	CDB-CCB-CBB	-2.54	101.55	114.37
24	a	407	PHO	OBD-CAD-C3D	2.53	131.85	127.89
23	b	608	CLA	CHA-C1A-NA	-2.53	120.65	126.39
28	M	101	LMG	C1-O6-C5	-2.53	108.77	113.72
27	C	525	STE	C4-C3-C2	-2.53	103.82	113.13
29	A	413	SQD	O48-C46-C45	2.53	115.69	108.40
29	b	620	SQD	C46-C45-C44	-2.53	105.88	111.78
29	A	412	SQD	O5-C1-O6	2.53	116.02	110.04
23	c	511	CLA	CHB-C4A-NA	2.53	128.05	124.40
26	D	407	PL9	C30-C29-C31	-2.53	110.84	115.23
30	c	519	DGD	O6D-C1D-O3G	-2.53	104.07	110.04
33	l	102	LHG	C11-C10-C9	-2.53	101.59	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	401	PHO	C4B-NB-C1B	2.53	112.50	108.82
28	a	415	LMG	C38-C37-C36	-2.53	101.60	114.37
23	C	505	CLA	O1D-CGD-CBD	2.52	129.50	124.52
23	C	508	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
29	a	412	SQD	O48-C23-C24	2.52	119.53	111.83
28	B	620	LMG	O6-C1-O1	-2.52	104.08	110.04
30	c	519	DGD	O3G-C1D-C2D	-2.52	104.44	108.27
23	a	408	CLA	CHA-C1A-NA	-2.52	120.68	126.39
26	d	405	PL9	C42-C43-C44	-2.52	121.85	127.62
25	b	618	BCR	C2-C1-C6	2.52	114.10	110.44
28	b	621	LMG	C40-C39-C38	-2.52	101.63	114.37
23	C	512	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
23	b	604	CLA	C4D-CHA-C1A	2.52	124.25	121.24
23	C	501	CLA	CAC-C3C-C4C	2.51	128.06	124.79
25	t	101	BCR	C3-C4-C5	-2.51	109.57	114.06
23	c	507	CLA	C4-C3-C5	2.51	119.59	115.23
24	D	402	PHO	OBD-CAD-C3D	2.51	131.81	127.89
23	b	603	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
25	c	515	BCR	C15-C16-C17	-2.51	118.39	123.52
27	J	101	STE	O2-C1-C2	2.51	121.92	114.00
28	c	522	LMG	O8-C28-O10	-2.51	117.36	123.63
23	B	613	CLA	C4A-NA-C1A	2.51	107.82	106.68
23	B	610	CLA	CHB-C4A-NA	2.50	128.01	124.40
23	B	614	CLA	C1-C2-C3	-2.50	122.10	126.20
24	d	401	PHO	C3D-C4D-ND	2.50	110.91	107.71
25	k	102	BCR	C29-C30-C25	2.50	114.07	110.44
23	D	405	CLA	O2D-CGD-CBD	2.50	115.59	111.23
23	C	504	CLA	C4A-NA-C1A	2.50	107.82	106.68
23	c	508	CLA	CHD-C1D-ND	-2.50	121.29	124.80
28	M	101	LMG	C38-C37-C36	-2.49	101.76	114.37
29	F	102	SQD	C26-C25-C24	-2.49	103.96	113.13
28	c	522	LMG	O7-C10-O9	-2.49	117.88	123.70
33	l	102	LHG	C20-C19-C18	-2.49	101.77	114.37
33	d	406	LHG	C27-C26-C25	-2.49	101.78	114.37
23	b	601	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
30	A	414	DGD	O5E-C6E-C5E	-2.49	102.86	111.33
25	H	101	BCR	C27-C26-C25	2.49	126.07	122.70
28	c	523	LMG	O2-C2-C1	-2.49	104.15	110.08
24	a	407	PHO	O2A-CGA-O1A	-2.48	117.42	123.63
28	c	523	LMG	O8-C28-O10	-2.48	117.42	123.63
23	B	611	CLA	CHD-C1D-ND	-2.48	121.31	124.80
34	f	101	HEM	O2D-CGD-CBD	2.48	121.83	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	519	DGD	CBB-CAB-C9B	-2.48	101.84	114.37
26	D	407	PL9	C27-C28-C29	-2.48	121.95	127.62
30	c	521	DGD	C3G-C2G-C1G	-2.48	106.01	111.78
23	c	512	CLA	O1D-CGD-CBD	2.48	129.40	124.52
28	M	101	LMG	C40-C39-C38	-2.47	101.88	114.37
30	H	102	DGD	O1G-C1A-O1A	-2.47	117.45	123.63
23	b	609	CLA	CHC-C4B-NB	2.47	127.75	124.05
28	A	411	LMG	O8-C28-O10	-2.47	117.45	123.63
30	C	521	DGD	O3E-C3E-C2E	-2.47	104.56	110.38
27	C	525	STE	C6-C5-C4	-2.47	101.89	114.37
35	V	201	HEC	CBD-CAD-C3D	-2.47	105.71	112.53
23	B	615	CLA	O2D-CGD-CBD	2.47	115.54	111.23
23	B	614	CLA	C4-C3-C5	2.47	119.51	115.23
23	D	404	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	B	611	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	a	406	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
23	C	512	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	B	612	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
23	a	406	CLA	CHC-C1C-NC	2.46	128.01	124.31
23	c	509	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
23	h	101	CLA	CHD-C1D-C2D	2.45	130.58	125.49
23	c	509	CLA	O2A-CGA-CBA	2.45	119.30	111.83
25	H	101	BCR	C16-C15-C14	-2.45	118.51	123.52
23	b	605	CLA	CHB-C1B-C2B	-2.45	120.32	127.43
30	C	523	DGD	CBB-CAB-C9B	-2.45	102.00	114.37
24	D	402	PHO	C3B-C4B-NB	-2.45	105.87	107.46
23	c	503	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
28	d	409	LMG	O1-C7-C8	-2.44	104.87	110.82
28	c	522	LMG	O6-C1-O1	-2.44	104.27	110.04
23	b	614	CLA	O2D-CGD-CBD	2.44	115.50	111.23
23	C	509	CLA	CHD-C1D-C2D	2.44	130.57	125.49
25	a	409	BCR	C33-C5-C6	-2.44	121.82	124.48
28	M	101	LMG	O6-C1-O1	-2.44	104.27	110.04
30	h	102	DGD	C4D-C3D-C2D	-2.44	106.54	110.83
30	C	521	DGD	O2D-C2D-C1D	-2.44	104.26	110.08
30	C	522	DGD	O6D-C1D-O3G	-2.44	104.28	110.04
25	c	515	BCR	C32-C1-C6	-2.43	106.43	110.24
29	a	414	SQD	C9-C8-C7	-2.43	104.78	113.69
28	b	621	LMG	O6-C1-O1	-2.43	104.30	110.04
25	c	515	BCR	C7-C8-C9	-2.43	122.64	126.23
25	A	408	BCR	C2-C1-C6	2.43	113.97	110.44
26	D	407	PL9	C50-C49-C48	-2.43	115.36	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	l	101	SQD	O48-C23-O10	-2.43	117.55	123.63
25	b	617	BCR	C7-C8-C9	-2.42	122.65	126.23
34	F	101	HEM	C1D-C2D-C3D	2.42	109.53	106.98
27	J	101	STE	C6-C5-C4	-2.42	102.12	114.37
24	d	401	PHO	O2A-CGA-O1A	-2.42	117.57	123.63
23	b	603	CLA	O1D-CGD-CBD	2.42	129.29	124.52
26	D	407	PL9	C35-C34-C36	2.42	119.43	115.23
23	b	614	CLA	CHB-C1B-NB	2.42	127.68	124.05
30	h	102	DGD	O6D-C1D-O3G	-2.42	104.33	110.04
23	d	403	CLA	C3B-C4B-NB	-2.42	108.37	110.53
23	B	603	CLA	C7-C6-C5	-2.42	106.82	113.26
30	A	414	DGD	O2G-C2G-C3G	2.42	117.01	108.34
23	c	503	CLA	O1D-CGD-CBD	2.41	129.28	124.52
23	c	505	CLA	C11-C10-C8	-2.41	107.95	115.97
25	B	618	BCR	C27-C26-C25	2.41	125.96	122.70
23	C	513	CLA	C1-O2A-CGA	-2.41	110.82	116.65
23	b	601	CLA	CHC-C1C-C2C	-2.41	120.11	126.95
25	x	101	BCR	C35-C13-C12	2.41	121.76	118.09
23	b	601	CLA	CHC-C1C-NC	2.40	127.93	124.31
26	a	410	PL9	C32-C33-C34	-2.40	122.12	127.62
29	a	412	SQD	O3-C3-C2	-2.40	104.71	110.38
23	a	406	CLA	C2D-C1D-ND	-2.40	107.75	110.13
30	c	520	DGD	O5D-C1E-C2E	2.39	111.91	108.27
23	b	614	CLA	CHB-C4A-NA	2.39	127.85	124.40
23	B	612	CLA	C16-C15-C13	-2.39	108.03	115.97
23	b	602	CLA	CMB-C2B-C1B	-2.39	121.79	125.42
23	c	501	CLA	C2C-C1C-NC	2.39	112.49	109.98
23	C	513	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
28	c	523	LMG	O3-C3-C2	-2.39	104.75	110.38
23	B	614	CLA	CHC-C4B-NB	2.39	127.63	124.05
23	D	405	CLA	CHB-C1B-NB	2.39	127.63	124.05
23	B	609	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
23	a	408	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
23	C	513	CLA	CHD-C1D-ND	-2.39	121.45	124.80
23	B	612	CLA	CHB-C4A-NA	2.38	127.84	124.40
25	K	101	BCR	C30-C25-C26	-2.38	119.38	122.64
30	C	522	DGD	O5D-C6D-C5D	-2.38	104.05	109.42
23	B	607	CLA	C4-C3-C5	2.38	119.36	115.23
23	B	614	CLA	CHB-C4A-NA	2.38	127.83	124.40
28	b	621	LMG	O1-C1-C2	-2.38	104.66	108.27
26	A	409	PL9	C22-C23-C24	-2.38	122.18	127.62
23	b	605	CLA	C1C-C2C-C3C	-2.37	104.48	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	404	BCR	C33-C5-C6	-2.37	121.89	124.48
23	b	615	CLA	CMB-C2B-C3B	2.37	132.13	126.55
25	b	617	BCR	C15-C14-C13	-2.37	123.96	127.28
23	C	511	CLA	C1-C2-C3	-2.37	122.32	126.20
28	c	523	LMG	C9-C8-C7	-2.37	106.27	111.78
29	f	102	SQD	C46-C45-C44	-2.37	106.27	111.78
23	b	602	CLA	C3B-C4B-NB	-2.37	108.42	110.53
23	D	404	CLA	CAA-CBA-CGA	-2.37	106.49	113.21
26	d	405	PL9	C8-C7-C3	2.37	118.15	112.03
25	c	514	BCR	C2-C1-C6	2.36	113.87	110.44
25	D	406	BCR	C24-C23-C22	-2.36	122.74	126.23
23	c	504	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
23	h	101	CLA	CHD-C4C-NC	2.36	127.89	124.23
23	c	513	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
30	c	520	DGD	O2E-C2E-C1E	-2.36	104.45	110.08
23	b	614	CLA	C11-C12-C13	-2.36	108.12	115.97
23	b	602	CLA	CMA-C3A-C4A	2.36	118.12	111.77
25	C	514	BCR	C15-C16-C17	-2.36	118.69	123.52
23	d	402	CLA	C6-C5-C3	2.36	119.21	113.47
34	F	101	HEM	C2D-C1D-ND	-2.36	107.18	109.90
23	c	509	CLA	CHD-C1D-ND	-2.36	121.49	124.80
25	T	101	BCR	C3-C4-C5	-2.36	109.86	114.06
24	d	401	PHO	O2D-CGD-O1D	-2.35	119.27	123.85
24	A	406	PHO	CMA-C3A-C4A	-2.35	109.54	114.61
27	I	102	STE	O2-C1-C2	2.35	121.44	114.00
26	a	410	PL9	O2-C1-C2	-2.35	116.48	121.83
30	c	520	DGD	CBB-CAB-C9B	-2.35	102.48	114.37
30	c	521	DGD	CBB-CAB-C9B	-2.35	102.48	114.37
23	C	510	CLA	CHD-C4C-NC	2.35	127.87	124.23
24	d	401	PHO	CMB-C2B-C3B	2.35	129.37	124.68
25	B	618	BCR	C15-C16-C17	-2.35	118.72	123.52
23	b	604	CLA	CHA-C1A-NA	-2.35	121.08	126.39
24	d	401	PHO	CMA-C3A-C4A	-2.34	109.56	114.61
26	D	407	PL9	C11-C9-C8	-2.34	115.91	121.17
23	b	607	CLA	CHB-C4A-NA	2.34	127.78	124.40
23	B	616	CLA	O2D-CGD-CBD	2.34	115.32	111.23
30	c	520	DGD	C8B-C7B-C6B	-2.34	102.54	114.37
23	a	405	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
23	b	602	CLA	CHD-C1D-ND	-2.34	121.51	124.80
23	b	610	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
23	a	408	CLA	CMC-C2C-C1C	2.34	128.69	125.03
23	b	612	CLA	CHA-C1A-NA	-2.34	121.10	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	522	DGD	O2D-C2D-C1D	-2.34	104.51	110.08
23	b	608	CLA	CHB-C4A-NA	2.33	127.77	124.40
30	H	102	DGD	C8B-C7B-C6B	-2.33	102.57	114.37
23	b	606	CLA	CHB-C1B-NB	2.33	127.55	124.05
23	B	608	CLA	CHC-C4B-NB	2.33	127.55	124.05
23	B	606	CLA	CHA-C1A-NA	-2.33	121.11	126.39
23	b	604	CLA	C2C-C1C-NC	2.33	112.43	109.98
23	C	510	CLA	C11-C10-C8	-2.33	108.22	115.97
23	b	615	CLA	CAA-CBA-CGA	-2.33	106.59	113.21
23	c	506	CLA	CED-O2D-CGD	2.33	121.20	115.92
30	C	521	DGD	C4E-C3E-C2E	-2.32	106.75	110.83
23	c	501	CLA	CED-O2D-CGD	-2.32	110.64	115.92
25	x	101	BCR	C36-C18-C17	-2.32	119.05	122.82
23	c	501	CLA	CHD-C1D-ND	-2.32	121.54	124.80
23	B	612	CLA	CHD-C1D-ND	-2.32	121.54	124.80
23	C	504	CLA	C6-C7-C8	-2.32	108.26	115.97
25	B	617	BCR	C27-C26-C25	2.31	125.83	122.70
23	b	602	CLA	CMB-C2B-C3B	2.31	131.99	126.55
33	D	411	LHG	C11-C10-C9	-2.31	102.69	114.37
25	k	101	BCR	C38-C26-C25	-2.31	121.97	124.48
23	b	602	CLA	CHB-C1B-NB	2.31	127.51	124.05
30	h	102	DGD	O5E-C6E-C5E	-2.31	103.48	111.33
28	D	409	LMG	O2-C2-C1	-2.30	104.59	110.08
33	L	101	LHG	C18-C17-C16	-2.30	102.73	114.37
28	D	409	LMG	O6-C1-O1	-2.30	104.61	110.04
23	b	611	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
23	B	613	CLA	CHB-C4A-NA	2.30	127.72	124.40
28	C	524	LMG	O6-C1-O1	-2.30	104.62	110.04
23	b	613	CLA	CHD-C1D-ND	-2.29	121.57	124.80
25	B	619	BCR	C33-C5-C6	-2.29	121.98	124.48
23	b	604	CLA	C4-C3-C5	2.29	119.21	115.23
23	C	512	CLA	CMB-C2B-C3B	2.29	131.95	126.55
23	B	609	CLA	CAA-CBA-CGA	-2.29	106.69	113.21
26	d	405	PL9	C7-C8-C9	-2.29	122.88	126.83
28	C	524	LMG	O2-C2-C1	-2.29	104.62	110.08
26	a	410	PL9	O2-C1-C6	2.29	124.12	120.48
23	C	505	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
23	b	607	CLA	CHB-C1B-NB	2.29	127.48	124.05
23	d	402	CLA	CHA-C4D-ND	2.29	137.27	132.55
23	a	406	CLA	C1D-ND-C4D	2.29	107.92	106.31
28	M	101	LMG	O7-C10-O9	-2.29	118.36	123.70
23	b	607	CLA	CHA-C1A-NA	-2.28	121.22	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	515	BCR	C35-C13-C14	-2.28	119.11	122.82
23	B	612	CLA	O1D-CGD-CBD	2.28	129.02	124.52
23	D	404	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
23	a	411	CLA	O2D-CGD-CBD	2.28	115.22	111.23
23	B	615	CLA	C4A-NA-C1A	2.28	107.72	106.68
23	c	506	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	d	403	CLA	CAC-C3C-C4C	2.28	127.76	124.79
23	b	602	CLA	C5-C3-C2	-2.28	116.05	121.17
23	b	608	CLA	C16-C15-C13	-2.28	108.39	115.97
23	c	507	CLA	CHB-C4A-NA	2.28	127.69	124.40
23	b	611	CLA	CHA-C1A-NA	-2.28	121.23	126.39
23	b	611	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
25	b	617	BCR	C35-C13-C12	2.27	121.56	118.09
33	D	412	LHG	C18-C17-C16	-2.27	102.88	114.37
23	D	404	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
23	b	606	CLA	CED-O2D-CGD	2.27	121.07	115.92
23	B	603	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
23	b	601	CLA	C11-C10-C8	-2.27	108.42	115.97
23	D	405	CLA	CHA-C1A-NA	-2.27	121.25	126.39
29	A	413	SQD	O6-C44-C45	-2.27	105.30	110.82
33	d	408	LHG	C26-C25-C24	2.27	121.47	113.13
23	B	603	CLA	C6-C5-C3	2.27	118.99	113.47
26	a	410	PL9	C40-C39-C41	2.27	119.17	115.23
30	h	102	DGD	O6E-C5E-C6E	-2.27	100.82	106.44
25	D	406	BCR	C38-C26-C25	-2.27	122.01	124.48
23	B	601	CLA	CHB-C4A-NA	2.26	127.67	124.40
30	h	102	DGD	CBB-CAB-C9B	-2.26	102.92	114.37
23	d	403	CLA	C1-C2-C3	-2.26	122.49	126.20
30	c	519	DGD	O1G-C1A-C2A	-2.26	104.93	111.83
23	B	608	CLA	CHD-C4C-NC	2.26	127.74	124.23
23	d	402	CLA	O2D-CGD-CBD	2.26	115.18	111.23
30	h	102	DGD	O2D-C2D-C1D	-2.26	104.69	110.08
28	c	523	LMG	C6-C5-C4	-2.26	107.48	113.02
25	T	101	BCR	C23-C22-C21	-2.26	115.46	119.01
29	l	101	SQD	C1-O5-C5	-2.26	109.32	113.72
24	A	406	PHO	C3D-C4D-ND	2.25	110.59	107.71
26	d	405	PL9	C20-C19-C21	2.25	119.14	115.23
23	B	612	CLA	C3A-C2A-C1A	2.25	104.71	101.34
23	c	508	CLA	C7-C6-C5	-2.25	107.27	113.26
30	H	102	DGD	C1D-O6D-C5D	-2.25	109.33	113.72
23	b	612	CLA	C3B-C4B-NB	-2.25	108.52	110.53
29	A	412	SQD	C9-C8-C7	-2.25	105.46	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	617	BCR	C15-C16-C17	-2.25	118.92	123.52
29	f	102	SQD	O47-C7-C8	2.25	119.18	110.93
23	B	605	CLA	C1-C2-C3	-2.25	122.52	126.20
23	b	603	CLA	O2A-CGA-O1A	-2.24	118.01	123.63
23	c	512	CLA	CHD-C1D-ND	-2.24	121.64	124.80
29	a	414	SQD	O49-C7-C8	-2.24	115.01	123.78
23	c	510	CLA	O1D-CGD-CBD	2.24	128.94	124.52
23	C	504	CLA	O2D-CGD-CBD	2.24	115.15	111.23
23	c	505	CLA	C6-C7-C8	-2.24	108.52	115.97
23	a	405	CLA	CHB-C4A-NA	2.24	127.63	124.40
25	T	101	BCR	C4-C5-C6	2.24	125.73	122.70
23	b	614	CLA	CMB-C2B-C3B	2.24	131.82	126.55
25	A	408	BCR	C33-C5-C6	-2.24	122.04	124.48
27	e	104	STE	C3-C2-C1	-2.24	108.67	114.51
30	C	523	DGD	O6D-C5D-C6D	-2.24	102.26	106.69
30	C	522	DGD	CDB-CCB-CBB	-2.23	103.08	114.37
33	L	101	LHG	C15-C14-C13	-2.23	103.08	114.37
23	B	605	CLA	C16-C17-C18	-2.23	105.97	115.94
30	h	102	DGD	C7B-C6B-C5B	-2.23	103.09	114.37
29	a	412	SQD	O5-C1-O6	-2.23	104.77	110.04
25	c	514	BCR	C29-C30-C25	2.23	113.68	110.44
23	c	503	CLA	CHD-C1D-ND	-2.23	121.67	124.80
23	c	504	CLA	O1A-CGA-CBA	2.23	132.50	123.78
25	B	619	BCR	C29-C30-C25	2.23	113.67	110.44
27	D	413	STE	C12-C11-C10	-2.23	103.11	114.37
23	B	601	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
23	b	603	CLA	C11-C10-C8	-2.23	108.56	115.97
23	c	506	CLA	CHA-C1A-NA	-2.23	121.35	126.39
25	K	101	BCR	C23-C24-C25	-2.22	121.06	127.00
23	b	612	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
30	H	102	DGD	O6D-C1D-O3G	-2.22	104.80	110.04
28	b	621	LMG	O8-C28-O10	-2.22	118.07	123.63
23	C	512	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
28	c	518	LMG	C8-O7-C10	2.22	123.11	117.80
30	C	521	DGD	C3E-C4E-C5E	2.22	114.25	110.23
23	C	507	CLA	C1C-C2C-C3C	-2.22	104.65	106.98
23	b	604	CLA	CHB-C1B-NB	2.22	127.37	124.05
23	b	613	CLA	CMD-C2D-C1D	2.22	128.63	124.73
23	b	615	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
33	D	410	LHG	C20-C19-C18	-2.21	103.18	114.37
23	B	605	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
23	B	609	CLA	C2C-C1C-NC	2.21	112.31	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	612	CLA	CMC-C2C-C1C	-2.21	121.58	125.03
30	C	523	DGD	CDB-CCB-CBB	-2.21	103.19	114.37
23	B	612	CLA	CMB-C2B-C3B	2.20	131.73	126.55
23	B	611	CLA	C11-C12-C13	-2.20	108.64	115.97
35	V	201	HEC	CHD-C4C-C3C	-2.20	121.49	125.21
28	a	415	LMG	O8-C28-O10	-2.20	118.12	123.63
30	A	414	DGD	O1G-C1A-C2A	-2.20	105.13	111.83
25	x	101	BCR	C16-C15-C14	-2.20	119.02	123.52
26	D	407	PL9	C8-C7-C3	2.20	117.72	112.03
23	b	605	CLA	CHC-C4B-NB	2.20	127.35	124.05
23	B	604	CLA	C11-C10-C8	-2.20	108.66	115.97
28	c	523	LMG	O7-C10-O9	-2.20	118.57	123.70
23	B	603	CLA	C1D-ND-C4D	2.20	107.85	106.31
23	C	513	CLA	CHB-C4A-NA	2.20	127.57	124.40
25	C	515	BCR	C36-C18-C17	-2.19	119.26	122.82
23	b	612	CLA	C7-C6-C5	-2.19	107.41	113.26
26	A	409	PL9	C12-C13-C14	-2.19	122.60	127.62
28	b	623	LMG	C1-C2-C3	-2.19	105.40	110.01
25	T	101	BCR	C1-C6-C5	-2.19	119.64	122.64
25	C	520	BCR	C33-C5-C6	-2.19	122.09	124.48
23	b	609	CLA	CHA-C1A-NA	-2.19	121.43	126.39
23	B	610	CLA	CHA-C4D-ND	2.19	137.07	132.55
28	D	408	LMG	O7-C10-O9	-2.19	118.59	123.70
23	c	512	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
23	d	403	CLA	O2D-CGD-O1D	-2.18	119.59	123.85
35	v	201	HEC	C4D-ND-C1D	2.18	109.38	105.82
34	F	101	HEM	CHB-C1B-C2B	-2.18	120.74	126.95
25	b	618	BCR	C15-C16-C17	-2.18	119.05	123.52
23	C	503	CLA	C6-C7-C8	-2.18	108.71	115.97
28	b	623	LMG	C4-C3-C2	-2.18	107.00	110.83
25	H	101	BCR	C34-C9-C10	-2.18	119.29	122.82
30	C	523	DGD	CAB-C9B-C8B	-2.18	103.36	114.37
26	a	410	PL9	C7-C8-C9	-2.18	123.08	126.83
25	a	409	BCR	C8-C7-C6	-2.18	121.18	127.00
23	A	405	CLA	C2C-C1C-NC	2.18	112.27	109.98
23	a	411	CLA	C1-O2A-CGA	2.18	121.92	116.65
23	a	405	CLA	CHB-C1B-NB	2.17	127.31	124.05
23	B	604	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
25	C	515	BCR	C35-C13-C14	-2.17	119.30	122.82
23	B	609	CLA	CHC-C4B-NB	2.17	127.30	124.05
23	C	504	CLA	CHA-C1A-NA	-2.17	121.48	126.39
23	C	511	CLA	O2D-CGD-O1D	-2.17	119.63	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C17-C16-C15	-2.16	103.58	113.28
29	A	413	SQD	C11-C10-C9	-2.16	103.43	114.37
30	c	521	DGD	C7A-C6A-C5A	-2.16	103.43	114.37
23	b	610	CLA	CHD-C1D-C2D	2.16	129.99	125.49
26	d	405	PL9	C12-C13-C14	-2.16	122.67	127.62
30	A	414	DGD	CAB-C9B-C8B	-2.16	103.45	114.37
33	d	407	LHG	C20-C19-C18	-2.16	103.45	114.37
25	A	408	BCR	C38-C26-C27	-2.16	108.99	113.60
25	d	404	BCR	C29-C30-C25	2.16	113.57	110.44
25	d	404	BCR	C27-C26-C25	2.16	125.62	122.70
25	t	101	BCR	C1-C6-C5	-2.16	119.69	122.64
25	B	618	BCR	C15-C14-C13	-2.16	124.25	127.28
23	D	404	CLA	C4A-NA-C1A	2.16	107.66	106.68
23	c	508	CLA	C1-C2-C3	-2.16	122.67	126.20
25	D	406	BCR	C16-C15-C14	-2.16	119.11	123.52
25	H	101	BCR	C1-C6-C5	-2.15	119.69	122.64
25	a	409	BCR	C30-C25-C26	-2.15	119.69	122.64
25	b	617	BCR	C2-C1-C6	2.15	113.57	110.44
23	C	508	CLA	C7-C6-C5	-2.15	107.52	113.26
25	b	618	BCR	C16-C15-C14	-2.15	119.11	123.52
23	c	510	CLA	CHB-C1B-NB	2.15	127.28	124.05
25	b	617	BCR	C35-C13-C14	-2.15	119.33	122.82
23	c	511	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
23	d	403	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
33	d	407	LHG	C27-C26-C25	-2.15	103.51	114.37
23	b	602	CLA	O1A-CGA-CBA	2.15	132.18	123.78
33	D	410	LHG	O8-C23-C24	2.15	118.38	111.83
23	A	405	CLA	O2D-CGD-CBD	2.15	114.98	111.23
23	A	407	CLA	C2C-C1C-NC	2.15	112.23	109.98
23	C	512	CLA	CHA-C4D-ND	2.14	136.97	132.55
28	a	415	LMG	C1-O6-C5	-2.14	109.53	113.72
28	c	524	LMG	O5-C6-C5	-2.14	104.03	111.33
23	B	602	CLA	C6-C5-C3	-2.14	108.25	113.47
33	a	413	LHG	C18-C17-C16	-2.14	103.53	114.37
23	C	504	CLA	C4-C3-C5	2.14	118.95	115.23
23	B	609	CLA	C7-C6-C5	-2.14	107.55	113.26
25	a	409	BCR	C2-C1-C6	2.14	113.55	110.44
28	a	415	LMG	C9-C8-C7	-2.14	106.80	111.78
25	b	618	BCR	C7-C8-C9	-2.14	123.07	126.23
27	b	622	STE	O2-C1-C2	2.14	120.75	114.00
25	c	514	BCR	C15-C16-C17	-2.14	119.15	123.52
29	a	412	SQD	O4-C4-C5	-2.13	104.07	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	520	BCR	C11-C10-C9	-2.13	124.29	127.28
23	b	608	CLA	CHB-C1B-NB	2.13	127.25	124.05
30	c	519	DGD	O6E-C5E-C4E	2.13	113.54	109.70
28	c	522	LMG	C9-C8-C7	-2.13	106.82	111.78
23	A	405	CLA	CAC-C3C-C4C	2.13	127.56	124.79
28	b	621	LMG	C38-C37-C36	-2.13	103.61	114.37
28	D	408	LMG	C14-C13-C12	-2.13	103.61	114.37
23	d	402	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
23	c	508	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
28	b	623	LMG	O7-C10-O9	-2.13	118.73	123.70
25	b	617	BCR	C30-C25-C26	-2.13	119.73	122.64
23	C	503	CLA	CHD-C1D-C2D	2.13	129.91	125.49
27	M	102	STE	O2-C1-C2	2.12	120.71	114.00
25	B	619	BCR	C28-C27-C26	-2.12	110.27	114.06
23	B	616	CLA	C3B-C4B-NB	-2.12	108.64	110.53
23	B	606	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
23	a	406	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
23	c	501	CLA	CHD-C1D-C2D	2.12	129.90	125.49
23	c	503	CLA	C11-C12-C13	-2.12	108.91	115.97
25	B	617	BCR	C15-C14-C13	-2.12	124.30	127.28
25	K	101	BCR	C15-C16-C17	-2.12	119.18	123.52
23	c	504	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
29	a	412	SQD	C16-C15-C14	-2.12	103.66	114.37
30	H	102	DGD	CAB-C9B-C8B	-2.12	103.66	114.37
30	C	522	DGD	CBB-CAB-C9B	-2.12	103.66	114.37
23	D	404	CLA	CHA-C4D-ND	2.12	136.92	132.55
30	c	519	DGD	O2G-C1B-O1B	-2.12	118.76	123.70
29	a	414	SQD	C3-C4-C5	2.12	114.07	110.23
23	C	502	CLA	CHA-C1A-NA	-2.11	121.61	126.39
23	C	507	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
25	c	515	BCR	C1-C6-C5	-2.11	119.75	122.64
23	C	512	CLA	CHB-C1B-NB	2.11	127.22	124.05
30	H	102	DGD	O2G-C1B-O1B	-2.11	118.77	123.70
23	a	411	CLA	CHD-C1D-ND	-2.11	121.83	124.80
23	c	508	CLA	CHD-C1D-C2D	2.11	129.87	125.49
29	b	620	SQD	O47-C45-C46	2.11	115.91	108.34
26	d	405	PL9	C32-C33-C34	-2.11	122.80	127.62
26	A	409	PL9	C41-C39-C38	-2.11	116.44	121.17
23	c	507	CLA	CHC-C4B-NB	2.11	127.21	124.05
27	x	102	STE	O2-C1-O1	-2.10	117.92	123.33
23	d	402	CLA	C3B-C4B-NB	-2.10	108.65	110.53
26	a	410	PL9	C25-C24-C26	2.10	118.88	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	415	LMG	C22-C21-C20	-2.10	103.75	114.37
28	B	620	LMG	C8-O7-C10	2.10	122.82	117.80
23	C	508	CLA	CHB-C4A-NA	2.10	127.43	124.40
28	C	517	LMG	O3-C3-C2	-2.10	105.43	110.38
23	C	504	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
33	D	410	LHG	C27-C26-C25	-2.10	103.76	114.37
23	C	511	CLA	O1D-CGD-CBD	2.10	128.66	124.52
25	B	619	BCR	C3-C4-C5	-2.10	110.31	114.06
33	L	101	LHG	C29-C28-C27	-2.10	103.76	114.37
23	b	603	CLA	CMD-C2D-C3D	2.10	132.50	127.69
23	C	513	CLA	C3B-C4B-NB	-2.10	108.66	110.53
30	A	414	DGD	CDB-CCB-CBB	-2.10	103.77	114.37
23	B	603	CLA	C2D-C1D-ND	-2.09	108.05	110.13
23	c	512	CLA	C1D-ND-C4D	2.09	107.78	106.31
23	C	510	CLA	CHA-C1A-NA	-2.09	121.65	126.39
33	L	101	LHG	C13-C12-C11	-2.09	103.79	114.37
23	b	610	CLA	C2D-C1D-ND	-2.09	108.06	110.13
23	b	602	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
30	c	520	DGD	O3G-C1D-C2D	-2.09	105.10	108.27
23	a	408	CLA	C2A-C1A-CHA	2.09	127.49	123.87
29	a	414	SQD	O48-C23-C24	2.09	118.20	111.83
23	C	506	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
23	c	502	CLA	C4D-CHA-C1A	2.09	123.73	121.24
25	k	102	BCR	C2-C1-C6	2.09	113.47	110.44
28	c	522	LMG	C6-C5-C4	-2.09	107.90	113.02
27	t	102	STE	O2-C1-C2	2.09	120.59	114.00
28	D	408	LMG	O2-C2-C3	-2.08	105.47	110.38
25	x	101	BCR	C11-C10-C9	-2.08	124.36	127.28
27	a	417	STE	C3-C2-C1	-2.08	109.08	114.51
25	B	619	BCR	C15-C14-C13	-2.08	124.36	127.28
33	d	407	LHG	C18-C17-C16	-2.08	103.85	114.37
23	B	605	CLA	CHC-C4B-NB	2.08	127.17	124.05
23	d	402	CLA	CHB-C1B-NB	2.08	127.17	124.05
23	B	607	CLA	CHB-C1B-NB	2.08	127.17	124.05
28	b	623	LMG	C40-C39-C38	-2.08	103.86	114.37
29	a	412	SQD	O3-C3-C4	2.08	115.27	110.38
28	A	411	LMG	C9-C8-C7	-2.08	106.94	111.78
28	M	101	LMG	O2-C2-C1	-2.08	105.13	110.08
23	d	402	CLA	C4D-CHA-C1A	2.08	123.72	121.24
23	b	615	CLA	O2D-CGD-CBD	2.07	114.86	111.23
26	D	407	PL9	O2-C1-C6	2.07	123.78	120.48
30	c	520	DGD	C4D-C3D-C2D	2.07	114.47	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	404	CLA	O2D-CGD-CBD	2.07	114.85	111.23
23	A	407	CLA	CHA-C1A-NA	-2.07	121.70	126.39
33	d	406	LHG	C20-C19-C18	-2.07	103.90	114.37
28	d	409	LMG	O5-C6-C5	-2.07	104.29	111.33
23	c	508	CLA	O1D-CGD-CBD	2.07	128.60	124.52
29	a	412	SQD	O48-C23-O10	-2.07	118.45	123.63
23	B	603	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
23	C	507	CLA	CED-O2D-CGD	2.07	120.61	115.92
23	B	615	CLA	C5-C3-C2	-2.07	116.53	121.17
33	L	101	LHG	O7-C5-C4	-2.07	100.93	108.34
28	b	621	LMG	C9-C8-C7	-2.07	106.97	111.78
23	b	612	CLA	CMC-C2C-C3C	2.07	131.74	126.15
33	d	407	LHG	O8-C6-C5	-2.07	102.44	108.40
23	c	504	CLA	O1D-CGD-CBD	2.06	128.59	124.52
28	c	524	LMG	O7-C10-O9	-2.06	118.88	123.70
28	b	621	LMG	C1-C2-C3	-2.06	105.67	110.01
33	d	406	LHG	C18-C17-C16	-2.06	103.94	114.37
30	c	519	DGD	C4E-C3E-C2E	-2.06	107.21	110.83
23	B	614	CLA	CHB-C1B-NB	2.06	127.14	124.05
33	D	411	LHG	O8-C23-O10	-2.06	118.47	123.63
35	V	201	HEC	C1D-C2D-C3D	-2.06	104.46	106.82
28	M	101	LMG	C23-C22-C21	-2.06	103.96	114.37
33	l	102	LHG	C18-C17-C16	-2.06	103.96	114.37
24	a	407	PHO	CMD-C2D-C3D	2.06	128.79	124.68
23	c	506	CLA	CBC-CAC-C3C	-2.06	106.85	112.42
23	B	605	CLA	C16-C15-C13	-2.06	109.13	115.97
29	A	413	SQD	C13-C12-C11	-2.05	103.98	114.37
25	B	617	BCR	C33-C5-C6	-2.05	122.24	124.48
34	f	101	HEM	CAB-C3B-C2B	-2.05	121.76	128.43
28	M	101	LMG	O5-C6-C5	-2.05	104.35	111.33
23	b	604	CLA	CHD-C4C-C3C	-2.05	121.78	124.77
25	t	101	BCR	C1-C6-C7	2.05	121.21	115.65
25	C	514	BCR	C33-C5-C6	-2.05	122.25	124.48
28	c	522	LMG	C40-C39-C38	-2.05	104.01	114.37
23	C	511	CLA	C11-C10-C8	-2.05	109.16	115.97
23	C	509	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
25	B	617	BCR	C8-C7-C6	-2.05	121.53	127.00
23	A	407	CLA	C3D-C4D-ND	2.04	113.31	109.99
23	C	503	CLA	CHC-C4B-NB	2.04	127.12	124.05
25	c	515	BCR	C4-C5-C6	2.04	125.47	122.70
23	B	606	CLA	C2A-C1A-CHA	2.04	127.41	123.87
23	A	404	CLA	CHA-C1A-NA	-2.04	121.76	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	620	SQD	C20-C19-C18	-2.04	104.04	114.37
34	F	101	HEM	C3B-C4B-NB	2.04	110.94	109.47
23	b	608	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
30	c	521	DGD	CAB-C9B-C8B	-2.04	104.05	114.37
23	b	610	CLA	CHD-C1D-ND	-2.04	121.93	124.80
23	c	513	CLA	O2D-CGD-CBD	2.04	114.80	111.23
23	c	507	CLA	O1D-CGD-CBD	2.04	128.54	124.52
27	m	101	STE	O2-C1-C2	2.04	120.44	114.00
23	B	606	CLA	O1D-CGD-CBD	2.04	128.54	124.52
23	C	508	CLA	CHD-C1D-C2D	2.04	129.73	125.49
25	C	520	BCR	C38-C26-C27	-2.04	109.25	113.60
28	A	411	LMG	O6-C1-O1	-2.04	105.23	110.04
23	d	402	CLA	C2A-C1A-CHA	2.04	127.40	123.87
25	C	514	BCR	C24-C23-C22	-2.04	123.22	126.23
25	C	515	BCR	C2-C1-C6	2.04	113.40	110.44
23	b	607	CLA	CHD-C1D-ND	-2.04	121.94	124.80
30	C	523	DGD	O3E-C3E-C2E	-2.04	105.58	110.38
28	M	101	LMG	O1-C1-C2	-2.03	105.18	108.27
25	k	102	BCR	C38-C26-C25	-2.03	122.26	124.48
29	b	620	SQD	O48-C23-O10	-2.03	118.54	123.63
33	D	412	LHG	O3-P-O5	-2.03	100.88	108.94
23	B	613	CLA	CHA-C4D-ND	2.03	136.74	132.55
23	C	512	CLA	CMA-C3A-C2A	-2.03	106.12	113.98
25	A	408	BCR	C15-C16-C17	-2.03	119.36	123.52
23	C	510	CLA	C3B-C4B-NB	-2.03	108.72	110.53
23	C	508	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
25	C	520	BCR	C40-C30-C25	2.03	113.42	110.24
23	b	610	CLA	CMB-C2B-C3B	2.03	131.32	126.55
27	x	102	STE	O2-C1-C2	2.03	120.41	114.00
23	C	501	CLA	CHB-C1B-NB	2.03	127.09	124.05
23	b	604	CLA	CHC-C1C-C2C	-2.03	121.19	126.95
23	C	501	CLA	CHA-C1A-NA	-2.03	121.80	126.39
28	c	522	LMG	C38-C37-C36	-2.03	104.12	114.37
23	C	502	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
23	c	512	CLA	C4-C3-C5	2.03	118.75	115.23
25	K	101	BCR	C8-C7-C6	-2.03	121.59	127.00
23	B	607	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	A	405	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
35	V	201	HEC	CHB-C4A-C3A	-2.02	121.28	125.49
23	B	602	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
23	C	511	CLA	O1A-CGA-CBA	2.02	131.70	123.78
23	C	511	CLA	CHB-C4A-NA	2.02	127.32	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	H	101	BCR	C24-C23-C22	-2.02	123.24	126.23
23	a	411	CLA	C2A-C1A-CHA	2.02	127.38	123.87
25	A	408	BCR	C16-C15-C14	-2.02	119.38	123.52
25	b	617	BCR	C15-C16-C17	-2.02	119.38	123.52
35	V	201	HEC	CMC-C2C-C1C	-2.02	122.34	125.42
23	C	508	CLA	CMB-C2B-C3B	2.02	131.31	126.55
23	B	615	CLA	CHB-C4A-NA	2.02	127.32	124.40
23	b	611	CLA	CHD-C1D-ND	-2.02	121.96	124.80
29	b	620	SQD	O9-S-C6	2.02	109.78	106.76
23	B	605	CLA	CHA-C1A-NA	-2.02	121.81	126.39
27	e	104	STE	O2-C1-C2	2.02	120.38	114.00
23	c	502	CLA	CHB-C4A-NA	2.02	127.31	124.40
23	d	402	CLA	CHA-C1A-NA	-2.02	121.82	126.39
34	f	101	HEM	CMB-C2B-C3B	-2.02	123.54	128.43
30	A	414	DGD	O5D-C6D-C5D	-2.02	104.87	109.42
23	D	405	CLA	CHB-C4A-NA	2.02	127.31	124.40
23	a	405	CLA	CMB-C2B-C3B	2.02	131.29	126.55
23	b	606	CLA	C1-O2A-CGA	2.01	121.53	116.65
34	F	101	HEM	CHD-C4C-C3C	2.01	128.60	125.21
26	a	410	PL9	C50-C49-C48	-2.01	116.62	122.66
27	a	417	STE	C4-C3-C2	-2.01	105.74	113.13
25	b	616	BCR	C15-C14-C13	-2.01	124.46	127.28
30	A	414	DGD	C4A-C3A-C2A	-2.01	105.75	113.13
23	B	616	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	D	405	CLA	C4-C3-C5	2.01	118.71	115.23
27	E	104	STE	O2-C1-O1	-2.01	118.17	123.33
23	B	614	CLA	C4A-NA-C1A	2.01	107.59	106.68
23	c	509	CLA	C3B-C4B-NB	-2.01	108.74	110.53
26	D	407	PL9	O1-C4-C3	-2.00	118.62	120.73
26	A	409	PL9	C50-C49-C48	-2.00	116.65	122.66
29	b	620	SQD	C46-O48-C23	-2.00	109.80	117.12

All (52) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	610	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	404	CLA	ND
23	a	405	CLA	ND
23	a	408	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	c	501	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	513	CLA	ND
23	d	402	CLA	ND
23	h	101	CLA	ND

All (1685) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CBA-CGA-O2A-C1
23	B	601	CLA	O1A-CGA-O2A-C1
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	C4B-C3B-CAB-CBB
23	a	406	CLA	C4B-C3B-CAB-CBB
23	b	613	CLA	CAD-CBD-CGD-O1D
23	b	613	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	C4-C3-C5-C6
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C11-C10-C8-C9
23	c	512	CLA	C2B-C3B-CAB-CBB
23	c	512	CLA	C4B-C3B-CAB-CBB
23	h	101	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	CAD-CBD-CGD-O1D
23	h	101	CLA	CAD-CBD-CGD-O2D
23	h	101	CLA	CBD-CGD-O2D-CED
25	A	408	BCR	C20-C21-C22-C37
25	C	514	BCR	C10-C11-C12-C13
25	C	514	BCR	C16-C17-C18-C36
25	C	514	BCR	C20-C21-C22-C37
25	D	406	BCR	C23-C24-C25-C26
25	D	406	BCR	C23-C24-C25-C30
25	H	101	BCR	C7-C8-C9-C10
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C21-C22-C23-C24
25	K	101	BCR	C37-C22-C23-C24
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
25	k	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	k	101	BCR	C37-C22-C23-C24
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C27-C28-C29-C30
26	A	409	PL9	C27-C28-C29-C31
26	A	409	PL9	C37-C38-C39-C41
26	D	407	PL9	C32-C33-C34-C35
26	D	407	PL9	C32-C33-C34-C36
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C27-C28-C29-C31
26	a	410	PL9	C44-C46-C47-C48
26	d	405	PL9	C32-C33-C34-C35
26	d	405	PL9	C32-C33-C34-C36
28	A	411	LMG	O6-C1-O1-C7
28	A	411	LMG	O9-C10-O7-C8
28	A	411	LMG	C11-C10-O7-C8
28	C	517	LMG	C2-C1-O1-C7
28	C	517	LMG	O6-C1-O1-C7
28	D	408	LMG	O6-C1-O1-C7
28	D	408	LMG	C11-C10-O7-C8
28	b	619	LMG	O7-C8-C9-O8
28	b	619	LMG	C7-C8-O7-C10
28	b	623	LMG	O6-C1-O1-C7
28	c	524	LMG	O6-C1-O1-C7
29	A	413	SQD	O6-C44-C45-O47
29	A	413	SQD	O5-C5-C6-S
29	A	413	SQD	C5-C6-S-O7
29	A	413	SQD	C5-C6-S-O8
29	A	413	SQD	C5-C6-S-O9
29	a	412	SQD	C5-C6-S-O7
29	a	412	SQD	C5-C6-S-O8
29	a	412	SQD	C5-C6-S-O9
29	a	414	SQD	O6-C44-C45-O47
29	a	414	SQD	O5-C5-C6-S
29	a	414	SQD	C5-C6-S-O7
29	b	620	SQD	C46-C45-O47-C7
29	b	620	SQD	C8-C7-O47-C45
29	f	102	SQD	O5-C1-O6-C44
29	l	101	SQD	C2-C1-O6-C44
29	l	101	SQD	O5-C1-O6-C44
29	l	101	SQD	O6-C44-C45-O47
29	l	101	SQD	O49-C7-O47-C45
29	l	101	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
29	l	101	SQD	O5-C5-C6-S
30	A	414	DGD	C2B-C1B-O2G-C2G
30	A	414	DGD	O1B-C1B-O2G-C2G
33	D	410	LHG	O2-C2-C3-O3
33	D	410	LHG	C3-O3-P-O4
33	D	410	LHG	C3-O3-P-O5
33	D	410	LHG	C3-O3-P-O6
33	D	410	LHG	C4-O6-P-O4
33	E	101	LHG	C3-O3-P-O4
33	E	101	LHG	C3-O3-P-O5
33	E	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O3
33	a	413	LHG	O1-C1-C2-O2
33	a	413	LHG	O1-C1-C2-C3
33	a	413	LHG	C3-O3-P-O4
33	a	413	LHG	C3-O3-P-O5
33	a	413	LHG	C3-O3-P-O6
33	d	406	LHG	O1-C1-C2-C3
33	d	406	LHG	C3-O3-P-O4
33	d	406	LHG	C3-O3-P-O5
33	d	406	LHG	C4-O6-P-O5
33	d	407	LHG	C3-O3-P-O4
33	d	407	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	l	102	LHG	C4-O6-P-O3
33	l	102	LHG	C4-O6-P-O5
35	V	201	HEC	C2B-C3B-CAB-CBB
35	V	201	HEC	C4B-C3B-CAB-CBB
35	V	201	HEC	C2C-C3C-CAC-CBC
35	V	201	HEC	C4C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
35	v	201	HEC	C4B-C3B-CAB-CBB
35	v	201	HEC	C2C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
23	c	513	CLA	CBD-CGD-O2D-CED
28	B	620	LMG	O10-C28-O8-C9
26	A	409	PL9	C47-C48-C49-C51
26	a	410	PL9	C47-C48-C49-C50
29	f	102	SQD	O10-C23-O48-C46
29	l	101	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
23	h	101	CLA	O1D-CGD-O2D-CED
28	D	408	LMG	O9-C10-O7-C8
33	E	101	LHG	O9-C7-O7-C5
23	b	615	CLA	O1D-CGD-O2D-CED
28	B	620	LMG	C29-C28-O8-C9
29	f	102	SQD	C24-C23-O48-C46
29	l	101	SQD	C24-C23-O48-C46
23	B	612	CLA	CBD-CGD-O2D-CED
28	M	101	LMG	O10-C28-O8-C9
23	A	407	CLA	C4-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6
23	b	606	CLA	C2-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
26	A	409	PL9	C28-C29-C31-C32
26	a	410	PL9	C33-C34-C36-C37
23	b	601	CLA	C3-C5-C6-C7
23	h	101	CLA	C3-C5-C6-C7
28	C	517	LMG	C29-C28-O8-C9
29	F	102	SQD	C24-C23-O48-C46
29	F	102	SQD	O10-C23-O48-C46
29	b	620	SQD	O49-C7-O47-C45
27	A	417	STE	C13-C14-C15-C16
26	A	409	PL9	C47-C48-C49-C50
26	a	410	PL9	C47-C48-C49-C51
29	F	102	SQD	C44-C45-C46-O48
28	M	101	LMG	C29-C28-O8-C9
30	A	414	DGD	C4E-C5E-C6E-O5E
23	D	405	CLA	CBD-CGD-O2D-CED
30	A	414	DGD	O6E-C5E-C6E-O5E
29	A	413	SQD	C16-C17-C18-C19
23	c	513	CLA	O1D-CGD-O2D-CED
26	a	410	PL9	C35-C34-C36-C37
23	b	604	CLA	C2-C3-C5-C6
23	b	609	CLA	C2C-C3C-CAC-CBC
30	H	102	DGD	O6E-C5E-C6E-O5E
30	h	102	DGD	O6E-C5E-C6E-O5E
26	A	409	PL9	C24-C26-C27-C28
26	A	409	PL9	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C14-C16-C17-C18
26	a	410	PL9	C19-C21-C22-C23
26	a	410	PL9	C34-C36-C37-C38
29	F	102	SQD	O5-C1-O6-C44
29	b	620	SQD	O5-C1-O6-C44
23	c	512	CLA	CBA-CGA-O2A-C1
29	b	620	SQD	C24-C23-O48-C46
23	C	511	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
26	a	410	PL9	C27-C28-C29-C30
27	b	624	STE	C7-C8-C9-C10
27	i	101	STE	C6-C7-C8-C9
23	c	501	CLA	CBD-CGD-O2D-CED
28	d	409	LMG	C10-C11-C12-C13
33	D	410	LHG	C1-C2-C3-O3
33	a	413	LHG	C1-C2-C3-O3
23	B	616	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
28	c	518	LMG	C29-C28-O8-C9
30	A	414	DGD	C2A-C1A-O1G-C1G
27	d	412	STE	C10-C11-C12-C13
33	d	407	LHG	C28-C29-C30-C31
30	A	414	DGD	C1B-C2B-C3B-C4B
27	j	102	STE	C3-C4-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	b	602	CLA	C4-C3-C5-C6
23	A	407	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	b	602	CLA	C2-C3-C5-C6
23	b	613	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
23	C	508	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	C11-C12-C13-C14
23	C	507	CLA	C11-C10-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	C	512	CLA	C11-C10-C8-C9
23	b	605	CLA	C14-C13-C15-C16
23	c	508	CLA	C14-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C9
28	b	623	LMG	C2-C1-O1-C7
28	c	524	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
33	a	413	LHG	O2-C2-C3-O3
29	l	101	SQD	C29-C30-C31-C32
28	C	517	LMG	O10-C28-O8-C9
28	b	623	LMG	O10-C28-O8-C9
29	b	620	SQD	O10-C23-O48-C46
25	B	619	BCR	C37-C22-C23-C24
25	C	514	BCR	C11-C12-C13-C35
25	C	520	BCR	C7-C8-C9-C34
25	c	514	BCR	C7-C8-C9-C34
25	d	404	BCR	C37-C22-C23-C24
25	d	404	BCR	C21-C22-C23-C24
23	b	605	CLA	C2A-CAA-CBA-CGA
33	E	101	LHG	O10-C23-O8-C6
23	b	608	CLA	CBD-CGD-O2D-CED
33	E	101	LHG	C24-C23-O8-C6
23	h	101	CLA	C13-C15-C16-C17
23	c	506	CLA	C2-C1-O2A-CGA
29	a	414	SQD	C17-C18-C19-C20
23	B	601	CLA	C5-C6-C7-C8
23	c	512	CLA	C8-C10-C11-C12
23	c	513	CLA	C8-C10-C11-C12
33	d	406	LHG	O1-C1-C2-O2
23	b	610	CLA	C13-C15-C16-C17
23	B	601	CLA	C11-C12-C13-C15
23	b	613	CLA	C4-C3-C5-C6
28	d	409	LMG	C28-C29-C30-C31
33	a	413	LHG	C23-C24-C25-C26
26	A	409	PL9	C34-C36-C37-C38
26	a	410	PL9	C24-C26-C27-C28
33	a	413	LHG	C27-C28-C29-C30
27	A	416	STE	C14-C15-C16-C17
30	H	102	DGD	C4E-C5E-C6E-O5E
30	h	102	DGD	C4E-C5E-C6E-O5E
27	b	624	STE	C5-C6-C7-C8
29	A	412	SQD	C7-C8-C9-C10
30	c	521	DGD	C1A-C2A-C3A-C4A
23	A	405	CLA	C15-C16-C17-C18
23	B	603	CLA	C5-C6-C7-C8
23	C	505	CLA	C5-C6-C7-C8
23	b	601	CLA	C13-C15-C16-C17
23	b	605	CLA	C15-C16-C17-C18
23	b	606	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C10-C11-C12-C13
23	B	614	CLA	C15-C16-C17-C18
23	C	506	CLA	C15-C16-C17-C18
23	D	405	CLA	C5-C6-C7-C8
23	b	602	CLA	C8-C10-C11-C12
23	b	610	CLA	C15-C16-C17-C18
23	h	101	CLA	C10-C11-C12-C13
28	b	623	LMG	O6-C5-C6-O5
28	D	408	LMG	C10-C11-C12-C13
28	b	623	LMG	C28-C29-C30-C31
28	c	524	LMG	C28-C29-C30-C31
29	A	412	SQD	C23-C24-C25-C26
23	c	506	CLA	O1A-CGA-O2A-C1
23	d	402	CLA	C3-C5-C6-C7
33	D	412	LHG	C31-C32-C33-C34
23	B	601	CLA	C13-C15-C16-C17
23	B	608	CLA	C15-C16-C17-C18
23	C	506	CLA	C8-C10-C11-C12
23	a	408	CLA	C13-C15-C16-C17
23	c	503	CLA	C8-C10-C11-C12
23	c	506	CLA	C13-C15-C16-C17
23	c	507	CLA	C5-C6-C7-C8
23	c	512	CLA	O1A-CGA-O2A-C1
23	B	607	CLA	C13-C15-C16-C17
23	C	503	CLA	C5-C6-C7-C8
29	f	102	SQD	O49-C7-O47-C45
23	B	612	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	O1A-CGA-O2A-C1
28	a	415	LMG	C10-C11-C12-C13
28	a	415	LMG	C28-C29-C30-C31
27	i	101	STE	C3-C4-C5-C6
23	C	509	CLA	C10-C11-C12-C13
23	b	614	CLA	C5-C6-C7-C8
23	C	501	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
29	f	102	SQD	C8-C7-O47-C45
29	a	414	SQD	C30-C31-C32-C33
23	D	405	CLA	O1D-CGD-O2D-CED
29	a	412	SQD	C7-C8-C9-C10
30	H	102	DGD	C1A-C2A-C3A-C4A
27	B	622	STE	C5-C6-C7-C8
23	B	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C15-C16-C17-C18
23	b	610	CLA	C8-C10-C11-C12
28	b	619	LMG	C10-C11-C12-C13
23	B	606	CLA	C10-C11-C12-C13
23	B	611	CLA	C8-C10-C11-C12
23	b	603	CLA	C10-C11-C12-C13
23	B	611	CLA	C15-C16-C17-C18
23	b	614	CLA	C8-C10-C11-C12
23	c	503	CLA	C5-C6-C7-C8
23	c	506	CLA	C8-C10-C11-C12
23	b	615	CLA	C8-C10-C11-C12
27	E	102	STE	C1-C2-C3-C4
23	b	603	CLA	C4-C3-C5-C6
23	B	613	CLA	C8-C10-C11-C12
33	E	101	LHG	C8-C7-O7-C5
29	F	102	SQD	C2-C1-O6-C44
30	C	522	DGD	C2E-C1E-O5D-C6D
25	A	408	BCR	C35-C13-C14-C15
25	A	408	BCR	C16-C17-C18-C36
25	B	617	BCR	C11-C10-C9-C34
25	B	618	BCR	C16-C17-C18-C36
25	B	619	BCR	C11-C10-C9-C34
25	C	514	BCR	C11-C10-C9-C34
25	C	514	BCR	C35-C13-C14-C15
25	C	520	BCR	C11-C10-C9-C34
25	b	616	BCR	C11-C10-C9-C34
25	b	618	BCR	C35-C13-C14-C15
25	b	618	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	c	514	BCR	C20-C21-C22-C37
25	d	404	BCR	C11-C10-C9-C34
25	k	101	BCR	C35-C13-C14-C15
25	x	101	BCR	C16-C17-C18-C36
25	k	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C36-C18-C19-C20
28	a	415	LMG	O10-C28-O8-C9
30	c	521	DGD	O1A-C1A-O1G-C1G
23	B	606	CLA	C2A-CAA-CBA-CGA
23	h	101	CLA	C2A-CAA-CBA-CGA
33	D	411	LHG	O1-C1-C2-C3
23	C	509	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	A	415	STE	C15-C16-C17-C18
25	C	514	BCR	C16-C17-C18-C19
25	x	101	BCR	C11-C10-C9-C8
30	C	522	DGD	O6E-C1E-O5D-C6D
23	d	403	CLA	C8-C10-C11-C12
23	c	503	CLA	C15-C16-C17-C18
29	a	414	SQD	C34-C35-C36-C37
23	B	601	CLA	C16-C17-C18-C20
23	B	606	CLA	C16-C17-C18-C19
23	B	611	CLA	C16-C17-C18-C19
23	C	509	CLA	C16-C17-C18-C20
23	C	512	CLA	C16-C17-C18-C20
23	C	513	CLA	C16-C17-C18-C20
23	h	101	CLA	C16-C17-C18-C19
23	C	507	CLA	C10-C11-C12-C13
30	C	521	DGD	O6E-C5E-C6E-O5E
28	c	524	LMG	C17-C18-C19-C20
29	a	412	SQD	C13-C14-C15-C16
30	C	522	DGD	C3A-C4A-C5A-C6A
30	C	522	DGD	CCA-CDA-CEA-CFA
30	c	519	DGD	C2A-C3A-C4A-C5A
33	L	101	LHG	C17-C18-C19-C20
28	b	619	LMG	C14-C15-C16-C17
29	A	412	SQD	C12-C13-C14-C15
33	E	101	LHG	C33-C34-C35-C36
28	M	101	LMG	C28-C29-C30-C31
27	A	415	STE	C12-C13-C14-C15
27	B	623	STE	C10-C11-C12-C13
27	I	101	STE	C5-C6-C7-C8
27	c	517	STE	C12-C13-C14-C15
28	C	524	LMG	C30-C31-C32-C33
28	b	621	LMG	C31-C32-C33-C34
29	a	414	SQD	C9-C10-C11-C12
30	h	102	DGD	CCA-CDA-CEA-CFA
27	b	626	STE	C4-C5-C6-C7
27	c	517	STE	C9-C10-C11-C12
27	x	102	STE	C4-C5-C6-C7
28	A	411	LMG	C16-C17-C18-C19
28	B	620	LMG	C31-C32-C33-C34
28	D	408	LMG	C32-C33-C34-C35
29	A	413	SQD	C34-C35-C36-C37
30	H	102	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
30	h	102	DGD	CAA-CBA-CCA-CDA
33	d	407	LHG	C14-C15-C16-C17
27	t	102	STE	C11-C10-C9-C8
28	C	524	LMG	C17-C18-C19-C20
30	c	519	DGD	CBA-CCA-CDA-CEA
30	h	102	DGD	C6B-C7B-C8B-C9B
33	E	101	LHG	C11-C12-C13-C14
23	c	512	CLA	O1D-CGD-O2D-CED
23	c	505	CLA	C4B-C3B-CAB-CBB
33	d	406	LHG	C7-C8-C9-C10
27	b	622	STE	C4-C5-C6-C7
27	x	102	STE	C9-C10-C11-C12
33	l	102	LHG	C27-C28-C29-C30
23	B	601	CLA	C16-C17-C18-C19
23	B	611	CLA	C16-C17-C18-C20
23	C	512	CLA	C16-C17-C18-C19
23	C	513	CLA	C16-C17-C18-C19
23	a	408	CLA	C16-C17-C18-C19
23	b	612	CLA	C16-C17-C18-C20
23	c	513	CLA	C16-C17-C18-C19
23	c	513	CLA	C16-C17-C18-C20
27	E	104	STE	C12-C13-C14-C15
27	t	103	STE	C5-C6-C7-C8
29	A	412	SQD	C16-C17-C18-C19
23	C	513	CLA	C15-C16-C17-C18
28	D	409	LMG	C12-C13-C14-C15
29	a	412	SQD	C18-C19-C20-C21
27	C	526	STE	C4-C5-C6-C7
28	b	623	LMG	C15-C16-C17-C18
29	A	413	SQD	C27-C28-C29-C30
29	a	412	SQD	C31-C32-C33-C34
33	D	412	LHG	O2-C2-C3-O3
27	m	101	STE	C1-C2-C3-C4
27	B	621	STE	C4-C5-C6-C7
27	C	528	STE	C9-C10-C11-C12
27	E	104	STE	C13-C14-C15-C16
27	M	102	STE	C4-C5-C6-C7
28	D	408	LMG	C14-C15-C16-C17
28	M	101	LMG	C35-C36-C37-C38
29	a	414	SQD	C14-C15-C16-C17
29	b	620	SQD	C13-C14-C15-C16
29	l	101	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	A	414	DGD	CCA-CDA-CEA-CFA
33	l	102	LHG	C9-C10-C11-C12
23	c	511	CLA	O1D-CGD-O2D-CED
28	A	411	LMG	C36-C37-C38-C39
28	B	620	LMG	C32-C33-C34-C35
28	b	621	LMG	C29-C30-C31-C32
28	B	620	LMG	O6-C5-C6-O5
30	c	521	DGD	C3A-C4A-C5A-C6A
33	d	408	LHG	C30-C31-C32-C33
23	B	616	CLA	C5-C6-C7-C8
23	C	506	CLA	C13-C15-C16-C17
23	c	506	CLA	C5-C6-C7-C8
23	B	606	CLA	C16-C17-C18-C20
23	a	408	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
23	c	512	CLA	C16-C17-C18-C19
27	A	417	STE	C12-C13-C14-C15
29	A	413	SQD	C28-C29-C30-C31
30	A	414	DGD	C8B-C9B-CAB-CBB
30	c	519	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	CAB-CBB-CCB-CDB
27	M	102	STE	C5-C6-C7-C8
28	M	101	LMG	C15-C16-C17-C18
30	h	102	DGD	C2B-C3B-C4B-C5B
28	C	517	LMG	C7-C8-C9-O8
27	E	103	STE	C9-C10-C11-C12
27	b	627	STE	C9-C10-C11-C12
27	t	103	STE	C9-C10-C11-C12
28	d	409	LMG	C33-C34-C35-C36
33	l	102	LHG	C14-C15-C16-C17
23	C	509	CLA	C3-C5-C6-C7
29	a	414	SQD	C23-C24-C25-C26
23	C	511	CLA	O1D-CGD-O2D-CED
30	C	523	DGD	C8A-C9A-CAA-CBA
30	C	523	DGD	CBA-CCA-CDA-CEA
30	c	521	DGD	CCB-CDB-CEB-CFB
27	C	529	STE	C10-C11-C12-C13
27	T	102	STE	C4-C5-C6-C7
27	l	103	STE	C5-C6-C7-C8
29	A	413	SQD	C14-C15-C16-C17
33	l	102	LHG	C13-C14-C15-C16
28	C	517	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	C	521	DGD	CCA-CDA-CEA-CFA
33	d	408	LHG	C31-C32-C33-C34
27	b	624	STE	C11-C12-C13-C14
27	b	627	STE	C14-C15-C16-C17
27	d	410	STE	C5-C6-C7-C8
27	e	104	STE	C5-C6-C7-C8
23	c	506	CLA	C16-C17-C18-C20
23	C	512	CLA	C2B-C3B-CAB-CBB
23	a	406	CLA	C2B-C3B-CAB-CBB
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
27	C	529	STE	C12-C13-C14-C15
27	j	102	STE	C4-C5-C6-C7
33	d	406	LHG	C27-C28-C29-C30
28	C	524	LMG	C32-C33-C34-C35
30	c	521	DGD	C4A-C5A-C6A-C7A
33	d	406	LHG	C29-C30-C31-C32
29	a	414	SQD	C32-C33-C34-C35
30	c	519	DGD	C2B-C3B-C4B-C5B
33	E	101	LHG	C30-C31-C32-C33
27	j	101	STE	C1-C2-C3-C4
29	l	101	SQD	C23-C24-C25-C26
27	A	416	STE	C2-C3-C4-C5
27	E	104	STE	C4-C5-C6-C7
27	e	104	STE	C3-C4-C5-C6
28	B	620	LMG	C29-C30-C31-C32
28	D	409	LMG	C14-C15-C16-C17
28	c	524	LMG	C34-C35-C36-C37
29	l	101	SQD	C33-C34-C35-C36
28	c	518	LMG	O10-C28-O8-C9
27	E	104	STE	C3-C4-C5-C6
27	l	103	STE	C6-C7-C8-C9
29	A	412	SQD	C27-C28-C29-C30
30	c	521	DGD	C4B-C5B-C6B-C7B
25	c	514	BCR	C18-C19-C20-C21
23	b	602	CLA	C13-C15-C16-C17
26	a	410	PL9	C23-C24-C26-C27
27	D	414	STE	C14-C15-C16-C17
28	B	620	LMG	C14-C15-C16-C17
30	c	519	DGD	C4B-C5B-C6B-C7B
30	c	520	DGD	CAB-CBB-CCB-CDB
23	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	c	519	DGD	C2A-C1A-O1G-C1G
23	a	408	CLA	C11-C12-C13-C14
27	b	624	STE	C3-C4-C5-C6
27	e	101	STE	C12-C13-C14-C15
30	A	414	DGD	C4B-C5B-C6B-C7B
30	A	414	DGD	C6B-C7B-C8B-C9B
23	c	505	CLA	C15-C16-C17-C18
28	b	623	LMG	C31-C32-C33-C34
33	d	408	LHG	C28-C29-C30-C31
25	d	404	BCR	C22-C23-C24-C25
27	C	527	STE	C12-C13-C14-C15
27	C	529	STE	C14-C15-C16-C17
27	b	624	STE	C12-C13-C14-C15
28	b	623	LMG	C12-C13-C14-C15
29	f	102	SQD	C25-C26-C27-C28
33	D	411	LHG	C29-C30-C31-C32
28	c	523	LMG	C38-C39-C40-C41
30	c	520	DGD	C1B-C2B-C3B-C4B
30	c	520	DGD	O6E-C5E-C6E-O5E
28	a	415	LMG	C18-C19-C20-C21
28	b	623	LMG	C19-C20-C21-C22
33	D	412	LHG	C27-C28-C29-C30
27	A	410	STE	C2-C3-C4-C5
27	B	621	STE	C7-C8-C9-C10
27	B	623	STE	C3-C4-C5-C6
27	D	413	STE	C7-C8-C9-C10
27	b	622	STE	C10-C11-C12-C13
27	j	101	STE	C2-C3-C4-C5
30	C	523	DGD	C3A-C4A-C5A-C6A
27	b	624	STE	C15-C16-C17-C18
23	D	405	CLA	C16-C17-C18-C20
28	b	621	LMG	C11-C10-O7-C8
28	d	409	LMG	O6-C5-C6-O5
28	M	101	LMG	O9-C10-O7-C8
28	b	623	LMG	O9-C10-O7-C8
28	c	523	LMG	O9-C10-O7-C8
28	b	623	LMG	C33-C34-C35-C36
27	e	102	STE	C11-C12-C13-C14
29	b	620	SQD	C30-C31-C32-C33
25	C	515	BCR	C11-C12-C13-C35
27	A	416	STE	C5-C6-C7-C8
27	B	623	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
27	J	101	STE	C2-C3-C4-C5
30	h	102	DGD	C7A-C8A-C9A-CAA
29	A	412	SQD	C26-C27-C28-C29
30	C	522	DGD	C8A-C9A-CAA-CBA
25	x	101	BCR	C11-C12-C13-C14
27	A	416	STE	C11-C10-C9-C8
27	t	103	STE	C6-C7-C8-C9
28	D	409	LMG	C18-C19-C20-C21
30	c	519	DGD	C3A-C4A-C5A-C6A
23	B	602	CLA	C16-C17-C18-C19
23	B	602	CLA	C16-C17-C18-C20
23	c	506	CLA	C16-C17-C18-C19
27	t	103	STE	C11-C12-C13-C14
30	c	521	DGD	C6B-C7B-C8B-C9B
33	E	101	LHG	C28-C29-C30-C31
33	E	101	LHG	C29-C30-C31-C32
27	m	101	STE	C6-C7-C8-C9
27	b	622	STE	C3-C4-C5-C6
27	x	102	STE	C5-C6-C7-C8
30	c	519	DGD	C5B-C6B-C7B-C8B
33	L	101	LHG	C27-C28-C29-C30
28	B	620	LMG	C15-C16-C17-C18
28	M	101	LMG	C39-C40-C41-C42
33	D	410	LHG	C30-C31-C32-C33
30	C	522	DGD	C6B-C7B-C8B-C9B
33	d	406	LHG	C10-C11-C12-C13
27	H	103	STE	C6-C7-C8-C9
28	M	101	LMG	C33-C34-C35-C36
33	d	407	LHG	C18-C19-C20-C21
26	a	410	PL9	C29-C31-C32-C33
23	C	505	CLA	C10-C11-C12-C13
23	b	612	CLA	C10-C11-C12-C13
23	b	606	CLA	C16-C17-C18-C19
28	D	408	LMG	C16-C17-C18-C19
29	A	412	SQD	C10-C11-C12-C13
33	l	102	LHG	C32-C33-C34-C35
28	D	409	LMG	O6-C5-C6-O5
28	M	101	LMG	C16-C17-C18-C19
30	C	522	DGD	C7B-C8B-C9B-CAB
27	i	101	STE	C1-C2-C3-C4
28	c	524	LMG	C10-C11-C12-C13
23	C	507	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	O1D-CGD-O2D-CED
29	a	412	SQD	C15-C16-C17-C18
23	C	512	CLA	C3-C5-C6-C7
28	a	415	LMG	O7-C8-C9-O8
28	c	523	LMG	O7-C8-C9-O8
30	C	522	DGD	C6A-C7A-C8A-C9A
27	b	625	STE	C2-C3-C4-C5
28	D	408	LMG	C13-C14-C15-C16
28	c	523	LMG	C30-C31-C32-C33
30	C	522	DGD	C5A-C6A-C7A-C8A
30	h	102	DGD	C8B-C9B-CAB-CBB
23	c	509	CLA	C13-C15-C16-C17
28	C	517	LMG	O6-C5-C6-O5
27	C	516	STE	C5-C6-C7-C8
28	a	415	LMG	C11-C12-C13-C14
28	b	621	LMG	C14-C15-C16-C17
28	c	524	LMG	C31-C32-C33-C34
29	b	620	SQD	C10-C11-C12-C13
33	d	408	LHG	C27-C28-C29-C30
28	M	101	LMG	C30-C31-C32-C33
28	c	523	LMG	C31-C32-C33-C34
28	D	409	LMG	C16-C17-C18-C19
28	b	623	LMG	C39-C40-C41-C42
27	B	623	STE	C5-C6-C7-C8
33	D	412	LHG	C1-C2-C3-O3
23	B	607	CLA	C15-C16-C17-C18
27	E	104	STE	C9-C10-C11-C12
27	H	103	STE	C13-C14-C15-C16
27	I	102	STE	C7-C8-C9-C10
29	f	102	SQD	C29-C30-C31-C32
28	c	523	LMG	O6-C5-C6-O5
27	A	416	STE	C7-C8-C9-C10
27	t	103	STE	C4-C5-C6-C7
30	c	521	DGD	C8A-C9A-CAA-CBA
27	a	417	STE	C3-C4-C5-C6
27	d	412	STE	C12-C13-C14-C15
27	j	101	STE	C6-C7-C8-C9
33	a	413	LHG	C24-C25-C26-C27
28	a	415	LMG	C13-C14-C15-C16
30	C	521	DGD	C4B-C5B-C6B-C7B
23	b	603	CLA	C16-C17-C18-C19
23	c	509	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C24-C25-C26-C27
23	C	508	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C13-C15-C16-C17
27	b	627	STE	C13-C14-C15-C16
29	l	101	SQD	C25-C26-C27-C28
27	C	528	STE	C12-C13-C14-C15
28	D	409	LMG	C30-C31-C32-C33
33	L	101	LHG	O6-C4-C5-C6
28	b	619	LMG	O9-C10-O7-C8
23	C	508	CLA	C12-C13-C15-C16
23	a	405	CLA	C12-C13-C15-C16
23	a	408	CLA	C6-C7-C8-C10
23	b	603	CLA	C11-C12-C13-C15
23	b	605	CLA	C6-C7-C8-C10
23	b	605	CLA	C12-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C15
23	c	505	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	d	403	CLA	C12-C13-C15-C16
28	A	411	LMG	C13-C14-C15-C16
28	D	409	LMG	C35-C36-C37-C38
29	A	412	SQD	C32-C33-C34-C35
29	F	102	SQD	C29-C30-C31-C32
30	C	523	DGD	CAB-CBB-CCB-CDB
23	c	511	CLA	C16-C17-C18-C19
23	B	605	CLA	C8-C10-C11-C12
28	a	415	LMG	O6-C5-C6-O5
27	a	416	STE	C4-C5-C6-C7
28	c	523	LMG	C16-C17-C18-C19
23	B	612	CLA	C10-C11-C12-C13
27	e	103	STE	C11-C12-C13-C14
29	a	414	SQD	C33-C34-C35-C36
23	b	606	CLA	C8-C10-C11-C12
28	c	523	LMG	C11-C10-O7-C8
23	B	604	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	D	405	CLA	C11-C10-C8-C9
23	a	408	CLA	C6-C7-C8-C9
23	b	602	CLA	C11-C10-C8-C9
23	b	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C11-C12-C13-C14
23	c	513	CLA	C14-C13-C15-C16
23	d	403	CLA	C14-C13-C15-C16
28	M	101	LMG	C34-C35-C36-C37
28	b	621	LMG	C16-C17-C18-C19
29	A	412	SQD	C11-C10-C9-C8
33	D	410	LHG	C11-C10-C9-C8
33	E	101	LHG	C23-C24-C25-C26
28	b	623	LMG	C29-C28-O8-C9
23	C	505	CLA	C15-C16-C17-C18
26	a	410	PL9	C22-C23-C24-C25
27	c	516	STE	C7-C8-C9-C10
27	E	104	STE	C11-C10-C9-C8
33	L	101	LHG	O9-C7-O7-C5
30	c	520	DGD	C2E-C1E-O5D-C6D
27	Z	101	STE	C10-C11-C12-C13
27	e	102	STE	C14-C15-C16-C17
29	a	414	SQD	C31-C32-C33-C34
29	f	102	SQD	C34-C35-C36-C37
27	B	621	STE	C1-C2-C3-C4
28	C	517	LMG	O1-C7-C8-C9
28	a	415	LMG	C7-C8-C9-O8
28	b	623	LMG	O1-C7-C8-C9
28	c	523	LMG	C7-C8-C9-O8
29	a	412	SQD	C44-C45-C46-O48
29	a	414	SQD	O6-C44-C45-C46
29	l	101	SQD	O6-C44-C45-C46
30	A	414	DGD	C1G-C2G-C3G-O3G
33	a	413	LHG	C4-C5-C6-O8
27	m	101	STE	C2-C3-C4-C5
28	b	623	LMG	C29-C30-C31-C32
30	h	102	DGD	CBA-CCA-CDA-CEA
30	c	519	DGD	O6D-C5D-C6D-O5D
30	c	519	DGD	O6E-C5E-C6E-O5E
33	a	413	LHG	C11-C12-C13-C14
23	b	603	CLA	C15-C16-C17-C18
27	E	104	STE	C10-C11-C12-C13
27	e	104	STE	C4-C5-C6-C7
29	a	414	SQD	C11-C10-C9-C8
30	C	521	DGD	C4A-C5A-C6A-C7A
23	D	405	CLA	C16-C17-C18-C19
23	c	511	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	m	102	STE	C11-C10-C9-C8
30	A	414	DGD	C9B-CAB-CBB-CCB
27	B	621	STE	C10-C11-C12-C13
27	C	529	STE	C7-C8-C9-C10
27	b	622	STE	C7-C8-C9-C10
28	D	409	LMG	C31-C32-C33-C34
33	D	412	LHG	C25-C26-C27-C28
25	K	101	BCR	C20-C21-C22-C37
23	B	606	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	c	508	CLA	C8-C10-C11-C12
30	A	414	DGD	C4A-C5A-C6A-C7A
33	d	408	LHG	C25-C26-C27-C28
23	C	513	CLA	O1A-CGA-O2A-C1
28	M	101	LMG	C17-C18-C19-C20
33	l	102	LHG	C29-C30-C31-C32
26	D	407	PL9	C45-C44-C46-C47
23	C	504	CLA	C2-C3-C5-C6
27	d	410	STE	C2-C3-C4-C5
28	M	101	LMG	C38-C39-C40-C41
28	A	411	LMG	C33-C34-C35-C36
29	a	414	SQD	C15-C16-C17-C18
29	l	101	SQD	C9-C10-C11-C12
23	B	605	CLA	C16-C17-C18-C19
27	C	526	STE	C5-C6-C7-C8
30	A	414	DGD	O1A-C1A-O1G-C1G
23	B	616	CLA	C10-C11-C12-C13
23	b	614	CLA	C13-C15-C16-C17
23	b	615	CLA	C10-C11-C12-C13
23	c	513	CLA	C5-C6-C7-C8
33	D	410	LHG	C32-C33-C34-C35
23	c	507	CLA	C8-C10-C11-C12
28	b	621	LMG	C28-C29-C30-C31
28	B	620	LMG	C30-C31-C32-C33
29	l	101	SQD	C11-C12-C13-C14
30	c	520	DGD	C7B-C8B-C9B-CAB
27	e	102	STE	C15-C16-C17-C18
23	C	512	CLA	O2A-C1-C2-C3
28	D	408	LMG	C7-C8-O7-C10
28	b	623	LMG	C9-C8-O7-C10
33	d	406	LHG	C32-C33-C34-C35
23	b	610	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	C	524	LMG	C18-C19-C20-C21
33	E	101	LHG	C17-C18-C19-C20
23	b	603	CLA	C16-C17-C18-C20
27	D	414	STE	C13-C14-C15-C16
28	c	523	LMG	C41-C42-C43-C44
30	C	523	DGD	C9A-CAA-CBA-CCA
30	H	102	DGD	CBA-CCA-CDA-CEA
27	A	410	STE	C4-C5-C6-C7
25	x	101	BCR	C16-C17-C18-C19
28	d	409	LMG	C30-C31-C32-C33
30	H	102	DGD	C3B-C4B-C5B-C6B
23	b	609	CLA	C4C-C3C-CAC-CBC
29	a	412	SQD	C28-C29-C30-C31
30	c	520	DGD	C5A-C6A-C7A-C8A
27	e	104	STE	C6-C7-C8-C9
27	m	102	STE	C14-C15-C16-C17
28	a	415	LMG	C30-C31-C32-C33
28	c	523	LMG	C35-C36-C37-C38
30	C	523	DGD	C5A-C6A-C7A-C8A
26	d	405	PL9	C15-C14-C16-C17
26	a	410	PL9	C18-C19-C21-C22
27	D	414	STE	C10-C11-C12-C13
27	H	103	STE	C2-C3-C4-C5
27	b	627	STE	C11-C12-C13-C14
27	d	412	STE	C11-C12-C13-C14
27	l	103	STE	C11-C10-C9-C8
28	c	522	LMG	C16-C17-C18-C19
29	A	412	SQD	C11-C12-C13-C14
30	H	102	DGD	CCA-CDA-CEA-CFA
27	t	103	STE	C10-C11-C12-C13
28	b	621	LMG	C19-C20-C21-C22
28	b	623	LMG	C23-C24-C25-C26
29	b	620	SQD	C26-C27-C28-C29
30	c	519	DGD	C5A-C6A-C7A-C8A
30	c	519	DGD	C7A-C8A-C9A-CAA
33	a	413	LHG	C11-C10-C9-C8
33	l	102	LHG	C17-C18-C19-C20
27	A	416	STE	C10-C11-C12-C13
27	C	528	STE	C7-C8-C9-C10
28	c	522	LMG	C31-C32-C33-C34
29	F	102	SQD	C32-C33-C34-C35
30	C	521	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
28	A	411	LMG	O1-C7-C8-O7
29	a	412	SQD	O47-C45-C46-O48
30	A	414	DGD	O2G-C2G-C3G-O3G
33	E	101	LHG	O7-C5-C6-O8
27	a	416	STE	C1-C2-C3-C4
30	C	521	DGD	CDA-CEA-CFA-CGA
27	l	103	STE	C3-C4-C5-C6
28	B	620	LMG	C33-C34-C35-C36
28	C	517	LMG	C17-C18-C19-C20
30	H	102	DGD	O2G-C1B-C2B-C3B
33	D	412	LHG	C23-C24-C25-C26
28	b	623	LMG	C30-C31-C32-C33
30	C	521	DGD	C5B-C6B-C7B-C8B
33	d	406	LHG	C28-C29-C30-C31
23	C	506	CLA	C3-C5-C6-C7
27	C	528	STE	C10-C11-C12-C13
27	b	622	STE	C15-C16-C17-C18
27	B	622	STE	C2-C3-C4-C5
27	C	527	STE	C15-C16-C17-C18
27	m	102	STE	C4-C5-C6-C7
30	c	520	DGD	C9A-CAA-CBA-CCA
33	L	101	LHG	C31-C32-C33-C34
23	a	408	CLA	CBA-CGA-O2A-C1
27	A	415	STE	C11-C12-C13-C14
27	j	101	STE	C4-C5-C6-C7
27	c	516	STE	C2-C3-C4-C5
27	i	102	STE	C7-C8-C9-C10
29	b	620	SQD	C11-C10-C9-C8
26	d	405	PL9	C45-C44-C46-C47
23	c	513	CLA	CBA-CGA-O2A-C1
27	B	621	STE	C2-C3-C4-C5
27	a	417	STE	C2-C3-C4-C5
28	B	620	LMG	C13-C14-C15-C16
28	D	409	LMG	C39-C40-C41-C42
33	d	406	LHG	C30-C31-C32-C33
28	c	522	LMG	O9-C10-O7-C8
28	c	524	LMG	O9-C10-O7-C8
33	d	408	LHG	O1-C1-C2-O2
23	B	612	CLA	C14-C13-C15-C16
23	D	404	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C11-C12-C13-C14
23	h	101	CLA	C6-C7-C8-C9
27	J	101	STE	C6-C7-C8-C9
27	d	410	STE	C6-C7-C8-C9
28	b	623	LMG	C40-C41-C42-C43
23	C	509	CLA	C13-C15-C16-C17
23	B	606	CLA	C4B-C3B-CAB-CBB
23	B	615	CLA	C4B-C3B-CAB-CBB
27	I	101	STE	C9-C10-C11-C12
27	I	102	STE	C4-C5-C6-C7
28	c	522	LMG	C17-C18-C19-C20
28	c	522	LMG	C10-C11-C12-C13
27	b	622	STE	C9-C10-C11-C12
30	C	521	DGD	C8B-C9B-CAB-CBB
33	E	101	LHG	C14-C15-C16-C17
23	b	613	CLA	C8-C10-C11-C12
27	B	621	STE	C12-C13-C14-C15
23	B	613	CLA	C16-C17-C18-C20
27	A	416	STE	C11-C12-C13-C14
28	M	101	LMG	C13-C14-C15-C16
29	f	102	SQD	C2-C1-O6-C44
23	c	505	CLA	C13-C15-C16-C17
27	A	417	STE	C9-C10-C11-C12
29	a	414	SQD	C25-C26-C27-C28
30	H	102	DGD	C7A-C8A-C9A-CAA
33	d	407	LHG	C12-C13-C14-C15
23	B	615	CLA	C3-C5-C6-C7
33	E	101	LHG	O6-C4-C5-C6
33	l	102	LHG	O6-C4-C5-C6
28	c	523	LMG	C15-C16-C17-C18
23	c	501	CLA	O1D-CGD-O2D-CED
28	M	101	LMG	C20-C21-C22-C23
23	B	604	CLA	C12-C13-C15-C16
23	B	612	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	D	405	CLA	C11-C10-C8-C7
23	b	602	CLA	C11-C10-C8-C7
23	b	606	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C12-C13-C15
23	c	513	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	d	402	CLA	C6-C7-C8-C10
23	C	513	CLA	C10-C11-C12-C13
30	A	414	DGD	O6D-C5D-C6D-O5D
27	l	103	STE	C15-C16-C17-C18
29	a	412	SQD	C23-C24-C25-C26
27	l	103	STE	C1-C2-C3-C4
27	T	102	STE	C6-C7-C8-C9
23	C	513	CLA	C8-C10-C11-C12
23	d	403	CLA	C16-C17-C18-C20
27	A	416	STE	C12-C13-C14-C15
28	c	518	LMG	C31-C32-C33-C34
27	E	102	STE	C7-C8-C9-C10
23	C	505	CLA	C4-C3-C5-C6
23	C	510	CLA	C4-C3-C5-C6
23	c	509	CLA	C4-C3-C5-C6
26	A	409	PL9	C15-C14-C16-C17
28	b	619	LMG	C7-C8-C9-O8
30	c	520	DGD	O6E-C1E-O5D-C6D
28	d	409	LMG	C35-C36-C37-C38
23	D	405	CLA	C10-C11-C12-C13
30	c	519	DGD	C4D-C5D-C6D-O5D
27	J	101	STE	C5-C6-C7-C8
27	x	102	STE	C10-C11-C12-C13
28	D	408	LMG	C31-C32-C33-C34
25	C	514	BCR	C15-C16-C17-C18
30	H	102	DGD	CDB-CEB-CFB-CGB
27	T	102	STE	C10-C11-C12-C13
30	c	521	DGD	CBA-CCA-CDA-CEA
33	D	410	LHG	C13-C14-C15-C16
33	D	412	LHG	C17-C18-C19-C20
28	c	522	LMG	C4-C5-C6-O5
29	A	413	SQD	C26-C27-C28-C29
27	e	104	STE	C11-C10-C9-C8
29	a	412	SQD	C11-C12-C13-C14
27	b	626	STE	C1-C2-C3-C4
28	c	523	LMG	C29-C28-O8-C9
33	E	101	LHG	C4-C5-C6-O8
28	D	408	LMG	C39-C40-C41-C42
23	d	403	CLA	C16-C17-C18-C19
23	a	408	CLA	C5-C6-C7-C8
28	c	522	LMG	C39-C40-C41-C42
30	H	102	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C11-C10-C9-C8
27	M	102	STE	C6-C7-C8-C9
28	c	523	LMG	C29-C30-C31-C32
29	b	620	SQD	C17-C18-C19-C20
33	l	102	LHG	C16-C17-C18-C19
28	c	522	LMG	C28-C29-C30-C31
28	d	409	LMG	C37-C38-C39-C40
23	C	505	CLA	C2-C3-C5-C6
23	C	510	CLA	C2-C3-C5-C6
28	b	623	LMG	C37-C38-C39-C40
33	d	406	LHG	C17-C18-C19-C20
27	D	413	STE	C3-C4-C5-C6
28	a	415	LMG	C22-C23-C24-C25
30	H	102	DGD	C4A-C5A-C6A-C7A
30	c	521	DGD	CAB-CBB-CCB-CDB
23	c	503	CLA	C16-C17-C18-C19
33	a	413	LHG	O6-C4-C5-O7
25	c	514	BCR	C1-C6-C7-C8
30	C	521	DGD	CBA-CCA-CDA-CEA
29	b	620	SQD	C7-C8-C9-C10
27	Z	101	STE	C11-C12-C13-C14
28	d	409	LMG	C38-C39-C40-C41
23	C	508	CLA	C10-C11-C12-C13
23	b	611	CLA	C10-C11-C12-C13
33	d	407	LHG	C19-C20-C21-C22
29	a	412	SQD	C16-C17-C18-C19
30	c	519	DGD	C8A-C9A-CAA-CBA
27	E	102	STE	C6-C7-C8-C9
28	C	517	LMG	O1-C7-C8-O7
28	b	623	LMG	O1-C7-C8-O7
27	t	103	STE	C2-C3-C4-C5
28	b	623	LMG	C32-C33-C34-C35
28	c	524	LMG	C29-C30-C31-C32
29	a	412	SQD	C27-C28-C29-C30
27	M	102	STE	C10-C11-C12-C13
27	D	414	STE	C15-C16-C17-C18
23	B	609	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
27	Z	101	STE	C9-C10-C11-C12
28	a	415	LMG	C35-C36-C37-C38
25	d	404	BCR	C18-C19-C20-C21
23	c	509	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C2-C3-C5-C6
28	C	517	LMG	C16-C17-C18-C19
28	d	409	LMG	C34-C35-C36-C37
23	h	101	CLA	C16-C17-C18-C20
27	B	623	STE	C11-C10-C9-C8
27	T	102	STE	C13-C14-C15-C16
27	c	517	STE	C3-C4-C5-C6
29	f	102	SQD	C24-C25-C26-C27
30	c	521	DGD	C9B-CAB-CBB-CCB
27	E	104	STE	C1-C2-C3-C4
33	a	413	LHG	C7-C8-C9-C10
27	b	627	STE	C10-C11-C12-C13
27	t	103	STE	C12-C13-C14-C15
33	E	101	LHG	C16-C17-C18-C19
27	B	622	STE	C7-C8-C9-C10
23	B	601	CLA	C11-C12-C13-C14
23	B	605	CLA	C6-C7-C8-C9
23	C	505	CLA	C14-C13-C15-C16
30	h	102	DGD	CCB-CDB-CEB-CFB
23	c	509	CLA	CAA-CBA-CGA-O2A
29	A	412	SQD	C9-C10-C11-C12
23	c	507	CLA	O1D-CGD-O2D-CED
27	C	516	STE	C7-C8-C9-C10
28	D	408	LMG	C34-C35-C36-C37
30	c	521	DGD	C5B-C6B-C7B-C8B
27	a	416	STE	C7-C8-C9-C10
27	Z	101	STE	C6-C7-C8-C9
27	b	622	STE	C14-C15-C16-C17
29	F	102	SQD	C34-C35-C36-C37
28	D	408	LMG	C2-C1-O1-C7
28	b	621	LMG	C22-C23-C24-C25
26	a	410	PL9	C9-C11-C12-C13
28	c	522	LMG	C37-C38-C39-C40
28	c	524	LMG	C14-C15-C16-C17
28	c	524	LMG	C38-C39-C40-C41
30	C	522	DGD	C9A-CAA-CBA-CCA
28	b	623	LMG	C4-C5-C6-O5
28	c	524	LMG	C37-C38-C39-C40
30	h	102	DGD	C3B-C4B-C5B-C6B
33	D	411	LHG	C11-C12-C13-C14
30	c	521	DGD	C2A-C1A-O1G-C1G
28	A	411	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
29	a	414	SQD	C29-C30-C31-C32
26	D	407	PL9	C43-C44-C46-C47
23	b	612	CLA	C16-C17-C18-C19
30	c	519	DGD	C6B-C7B-C8B-C9B
23	B	602	CLA	C15-C16-C17-C18
28	b	621	LMG	O9-C10-O7-C8
29	A	412	SQD	C25-C26-C27-C28
30	C	522	DGD	C9B-CAB-CBB-CCB
25	B	617	BCR	C20-C21-C22-C37
25	D	406	BCR	C20-C21-C22-C37
25	K	101	BCR	C16-C17-C18-C36
25	b	616	BCR	C20-C21-C22-C37
25	k	101	BCR	C16-C17-C18-C36
25	t	101	BCR	C20-C21-C22-C37
30	C	523	DGD	O1A-C1A-O1G-C1G
23	c	504	CLA	C5-C6-C7-C8
33	L	101	LHG	C13-C14-C15-C16
30	A	414	DGD	CAB-CBB-CCB-CDB
23	B	604	CLA	C11-C12-C13-C15
23	B	614	CLA	C11-C12-C13-C15
23	B	615	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C10-C8-C7
23	c	513	CLA	C11-C10-C8-C7
23	h	101	CLA	C6-C7-C8-C10
27	D	413	STE	C9-C10-C11-C12
27	Z	101	STE	C13-C14-C15-C16
27	t	102	STE	C4-C5-C6-C7
27	A	410	STE	C1-C2-C3-C4
27	C	528	STE	C5-C6-C7-C8
28	d	409	LMG	C15-C16-C17-C18
28	c	522	LMG	C12-C13-C14-C15
28	c	524	LMG	C19-C20-C21-C22
33	E	101	LHG	C34-C35-C36-C37
27	z	101	STE	C5-C6-C7-C8
23	a	408	CLA	O1A-CGA-O2A-C1
28	C	524	LMG	O10-C28-O8-C9
28	b	621	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	a	415	LMG	C8-C7-O1-C1
29	a	414	SQD	C5-C6-S-O8
30	C	522	DGD	C2G-C3G-O3G-C1D
30	C	522	DGD	C5D-C6D-O5D-C1E
30	c	520	DGD	C2G-C3G-O3G-C1D
30	c	520	DGD	C5D-C6D-O5D-C1E
23	B	612	CLA	C13-C15-C16-C17
29	a	412	SQD	C8-C7-O47-C45
28	B	620	LMG	O9-C10-O7-C8
27	m	102	STE	C9-C10-C11-C12
23	c	513	CLA	O1A-CGA-O2A-C1
23	B	609	CLA	C2-C3-C5-C6
30	C	522	DGD	CDB-CEB-CFB-CGB
28	M	101	LMG	C19-C20-C21-C22
30	C	521	DGD	C5A-C6A-C7A-C8A
27	E	104	STE	C15-C16-C17-C18
27	m	101	STE	C7-C8-C9-C10
33	l	102	LHG	C19-C20-C21-C22
28	a	415	LMG	C20-C21-C22-C23
28	b	623	LMG	C16-C17-C18-C19
28	c	518	LMG	C16-C17-C18-C19
23	C	513	CLA	O2A-C1-C2-C3
29	l	101	SQD	C46-C45-O47-C7
27	M	102	STE	C7-C8-C9-C10
30	C	523	DGD	C3B-C4B-C5B-C6B
23	B	615	CLA	C16-C17-C18-C19
27	C	528	STE	C11-C10-C9-C8
23	D	405	CLA	C15-C16-C17-C18
27	m	102	STE	C6-C7-C8-C9
30	c	519	DGD	C9B-CAB-CBB-CCB
28	M	101	LMG	C7-C8-C9-O8
29	A	413	SQD	O6-C44-C45-C46
23	B	612	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
27	i	101	STE	C5-C6-C7-C8
23	C	506	CLA	C4-C3-C5-C6
27	A	410	STE	C3-C4-C5-C6
29	f	102	SQD	C32-C33-C34-C35
33	D	412	LHG	C11-C12-C13-C14
29	A	413	SQD	C24-C25-C26-C27
29	f	102	SQD	C28-C29-C30-C31
28	M	101	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C12-C13-C14
23	b	612	CLA	C6-C7-C8-C9
23	b	615	CLA	C6-C7-C8-C9
23	h	101	CLA	C11-C10-C8-C9
23	B	613	CLA	C16-C17-C18-C19
28	A	411	LMG	C11-C12-C13-C14
27	t	103	STE	C7-C8-C9-C10
28	D	409	LMG	C20-C21-C22-C23
23	a	408	CLA	C10-C11-C12-C13
27	t	102	STE	C6-C7-C8-C9
28	C	524	LMG	C37-C38-C39-C40
33	D	411	LHG	C26-C27-C28-C29
30	h	102	DGD	C3A-C4A-C5A-C6A
23	b	602	CLA	C5-C6-C7-C8
23	B	616	CLA	C2-C1-O2A-CGA
23	B	610	CLA	C16-C17-C18-C19
23	B	612	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	c	512	CLA	C5-C6-C7-C8
27	l	103	STE	C11-C12-C13-C14
33	D	412	LHG	C28-C29-C30-C31
33	d	407	LHG	C30-C31-C32-C33
23	C	504	CLA	C4-C3-C5-C6
23	c	512	CLA	C4-C3-C5-C6
27	A	416	STE	C4-C5-C6-C7
33	D	410	LHG	C29-C30-C31-C32
33	E	101	LHG	C15-C16-C17-C18
27	d	410	STE	C4-C5-C6-C7
33	D	411	LHG	C34-C35-C36-C37
23	a	405	CLA	C16-C17-C18-C20
23	c	503	CLA	C16-C17-C18-C20
23	c	505	CLA	C16-C17-C18-C20
23	c	510	CLA	C8-C10-C11-C12
30	C	521	DGD	C6A-C7A-C8A-C9A
23	C	501	CLA	O1D-CGD-O2D-CED
27	b	626	STE	C3-C4-C5-C6
30	H	102	DGD	C8B-C9B-CAB-CBB
27	H	103	STE	C5-C6-C7-C8
33	D	411	LHG	C15-C16-C17-C18
23	C	508	CLA	O1D-CGD-O2D-CED
33	E	101	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	l	102	LHG	C26-C27-C28-C29
33	L	101	LHG	O10-C23-O8-C6
25	A	408	BCR	C37-C22-C23-C24
25	c	515	BCR	C11-C12-C13-C35
30	A	414	DGD	C4D-C5D-C6D-O5D
23	B	601	CLA	C4B-C3B-CAB-CBB
23	c	512	CLA	C13-C15-C16-C17
28	D	409	LMG	C33-C34-C35-C36
26	a	410	PL9	C32-C33-C34-C36
33	D	410	LHG	C17-C18-C19-C20
30	H	102	DGD	CAB-CBB-CCB-CDB
30	C	521	DGD	C2B-C3B-C4B-C5B
29	a	412	SQD	O49-C7-O47-C45
27	e	101	STE	C13-C14-C15-C16
23	B	613	CLA	C11-C12-C13-C15
23	B	613	CLA	C12-C13-C15-C16
23	C	509	CLA	C12-C13-C15-C16
23	D	405	CLA	C12-C13-C15-C16
23	a	406	CLA	C11-C10-C8-C7
23	c	508	CLA	C12-C13-C15-C16
23	c	512	CLA	C6-C7-C8-C10
33	D	412	LHG	C33-C34-C35-C36
33	E	101	LHG	C10-C11-C12-C13
23	B	614	CLA	C16-C17-C18-C20
23	a	405	CLA	C16-C17-C18-C19
27	j	102	STE	C13-C14-C15-C16
23	c	509	CLA	C8-C10-C11-C12
28	b	623	LMG	C17-C18-C19-C20
28	c	522	LMG	C30-C31-C32-C33
30	c	520	DGD	CCA-CDA-CEA-CFA
27	b	624	STE	C9-C10-C11-C12
33	D	410	LHG	C25-C26-C27-C28
27	m	102	STE	C13-C14-C15-C16
29	a	412	SQD	C12-C13-C14-C15
24	d	401	PHO	C2C-C3C-CAC-CBC
29	F	102	SQD	C25-C26-C27-C28
23	B	614	CLA	C16-C17-C18-C19
28	b	621	LMG	C18-C19-C20-C21
30	c	520	DGD	CCB-CDB-CEB-CFB
27	H	103	STE	C7-C8-C9-C10
27	C	518	STE	C3-C4-C5-C6
33	E	101	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	O6-C4-C5-O7
33	l	102	LHG	O6-C4-C5-O7
28	a	415	LMG	C11-C10-O7-C8
23	B	615	CLA	C14-C13-C15-C16
23	C	503	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	C	512	CLA	C11-C12-C13-C14
23	C	513	CLA	C11-C10-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	a	405	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	615	CLA	C11-C10-C8-C9
23	c	513	CLA	C11-C10-C8-C9
23	d	402	CLA	C6-C7-C8-C9
28	C	517	LMG	C11-C12-C13-C14
30	H	102	DGD	C5A-C6A-C7A-C8A
28	b	619	LMG	C1-C2-C3-C4
27	a	417	STE	C6-C7-C8-C9
30	c	521	DGD	C3B-C4B-C5B-C6B
30	C	521	DGD	C7B-C8B-C9B-CAB
33	d	406	LHG	C15-C16-C17-C18
23	b	613	CLA	C13-C15-C16-C17
28	M	101	LMG	C22-C23-C24-C25
28	C	517	LMG	O7-C8-C9-O8
33	a	413	LHG	O7-C5-C6-O8
27	i	101	STE	C7-C8-C9-C10
23	B	605	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C20
29	l	101	SQD	C44-C45-C46-O48
27	d	411	STE	C3-C4-C5-C6
33	d	408	LHG	C29-C30-C31-C32
23	c	512	CLA	C2-C3-C5-C6
29	A	412	SQD	C33-C34-C35-C36
23	B	601	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
29	b	620	SQD	C12-C13-C14-C15
27	M	103	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
27	l	103	STE	C10-C11-C12-C13
27	b	625	STE	C9-C10-C11-C12
28	c	518	LMG	C29-C30-C31-C32
33	D	410	LHG	C33-C34-C35-C36
33	D	412	LHG	C24-C25-C26-C27
33	l	102	LHG	C35-C36-C37-C38
27	T	102	STE	C12-C13-C14-C15
27	c	517	STE	C5-C6-C7-C8
27	I	101	STE	C6-C7-C8-C9
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
33	D	410	LHG	C4-O6-P-O3
33	E	101	LHG	C3-O3-P-O6
33	L	101	LHG	C4-O6-P-O5
33	d	406	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O5
23	B	607	CLA	C3-C5-C6-C7
30	C	522	DGD	C4A-C5A-C6A-C7A
26	a	410	PL9	C45-C44-C46-C47
23	c	505	CLA	C2B-C3B-CAB-CBB
27	e	103	STE	C10-C11-C12-C13
23	b	603	CLA	C2-C3-C5-C6
30	h	102	DGD	CBB-CCB-CDB-CEB
33	D	411	LHG	C2-C3-O3-P
33	d	408	LHG	C2-C3-O3-P
30	H	102	DGD	C7B-C8B-C9B-CAB
23	B	609	CLA	C13-C15-C16-C17
23	b	613	CLA	C16-C17-C18-C19
30	c	519	DGD	CDB-CEB-CFB-CGB
28	c	518	LMG	C30-C31-C32-C33
26	a	410	PL9	C4-C3-C7-C8
33	a	413	LHG	C19-C20-C21-C22
29	b	620	SQD	C11-C12-C13-C14
28	A	411	LMG	O6-C5-C6-O5
28	A	411	LMG	C9-C8-O7-C10
28	a	415	LMG	C7-C8-O7-C10
28	c	524	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
29	A	413	SQD	C11-C12-C13-C14
29	F	102	SQD	C33-C34-C35-C36
30	h	102	DGD	O2G-C1B-C2B-C3B
23	d	403	CLA	C10-C11-C12-C13
23	C	506	CLA	C2-C3-C5-C6
28	c	523	LMG	C10-C11-C12-C13
29	b	620	SQD	C27-C28-C29-C30
23	B	610	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C19
29	A	412	SQD	C14-C15-C16-C17
30	C	521	DGD	O6D-C5D-C6D-O5D
29	l	101	SQD	C13-C14-C15-C16
23	C	509	CLA	C14-C13-C15-C16
23	D	405	CLA	C11-C12-C13-C14
23	h	101	CLA	C11-C12-C13-C14
23	B	602	CLA	C11-C12-C13-C15
23	B	606	CLA	C6-C7-C8-C10
23	b	601	CLA	C6-C7-C8-C10
30	H	102	DGD	C3A-C4A-C5A-C6A
28	a	415	LMG	C12-C13-C14-C15
33	d	407	LHG	C34-C35-C36-C37
27	C	525	STE	C4-C5-C6-C7
27	E	104	STE	C5-C6-C7-C8
27	T	102	STE	C7-C8-C9-C10
27	i	102	STE	C9-C10-C11-C12
30	C	523	DGD	CDB-CEB-CFB-CGB
26	a	410	PL9	C20-C19-C21-C22
28	c	522	LMG	C29-C28-O8-C9
27	j	102	STE	C5-C6-C7-C8
28	b	619	LMG	C12-C13-C14-C15
29	l	101	SQD	O47-C45-C46-O48
30	c	519	DGD	C4A-C5A-C6A-C7A
27	B	621	STE	C11-C12-C13-C14
28	A	411	LMG	O1-C7-C8-C9
33	d	406	LHG	C33-C34-C35-C36
25	B	617	BCR	C7-C8-C9-C34
28	c	522	LMG	C34-C35-C36-C37
23	D	403	CLA	C16-C17-C18-C19
30	C	523	DGD	O6D-C5D-C6D-O5D
27	Z	101	STE	C4-C5-C6-C7
28	A	411	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
28	c	523	LMG	C14-C15-C16-C17
28	b	623	LMG	C8-C7-O1-C1
27	E	102	STE	C4-C5-C6-C7
33	D	412	LHG	C16-C17-C18-C19
28	D	409	LMG	C15-C16-C17-C18
28	a	415	LMG	C40-C41-C42-C43
30	C	522	DGD	CAB-CBB-CCB-CDB
23	C	508	CLA	C11-C10-C8-C9
23	a	406	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	b	606	CLA	C6-C7-C8-C9
28	a	415	LMG	C29-C28-O8-C9
30	c	521	DGD	O6D-C5D-C6D-O5D
23	C	502	CLA	C16-C17-C18-C20
28	b	621	LMG	C32-C33-C34-C35
23	A	404	CLA	C2C-C3C-CAC-CBC
23	h	101	CLA	C5-C6-C7-C8
23	c	508	CLA	C15-C16-C17-C18
33	d	406	LHG	C25-C26-C27-C28
27	E	102	STE	C2-C3-C4-C5
28	a	415	LMG	C14-C15-C16-C17
28	b	621	LMG	C37-C38-C39-C40
23	B	613	CLA	C11-C10-C8-C7
23	C	505	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C12-C13-C15
23	B	601	CLA	C10-C11-C12-C13
28	D	409	LMG	C22-C23-C24-C25
33	D	411	LHG	C25-C26-C27-C28
27	H	103	STE	C11-C12-C13-C14
28	c	523	LMG	C39-C40-C41-C42
30	c	520	DGD	C8B-C9B-CAB-CBB
30	c	520	DGD	CAA-CBA-CCA-CDA
23	c	504	CLA	C10-C11-C12-C13
29	A	412	SQD	C30-C31-C32-C33
27	z	101	STE	C6-C7-C8-C9
27	C	528	STE	C13-C14-C15-C16
23	a	411	CLA	C2C-C3C-CAC-CBC
27	b	622	STE	C11-C10-C9-C8
25	c	515	BCR	C11-C10-C9-C34
27	C	525	STE	C7-C8-C9-C10
23	C	505	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C13-C15-C16-C17
23	c	513	CLA	C15-C16-C17-C18
28	a	415	LMG	C15-C16-C17-C18
23	b	615	CLA	C2-C1-O2A-CGA
27	C	527	STE	C13-C14-C15-C16
23	b	607	CLA	C13-C15-C16-C17
28	C	517	LMG	C12-C13-C14-C15
29	F	102	SQD	C24-C25-C26-C27
28	D	409	LMG	C13-C14-C15-C16
25	c	515	BCR	C7-C8-C9-C10
23	c	513	CLA	C4-C3-C5-C6
30	C	521	DGD	C4D-C5D-C6D-O5D
27	a	416	STE	C2-C3-C4-C5
23	c	503	CLA	C10-C11-C12-C13
28	d	409	LMG	C39-C40-C41-C42
30	h	102	DGD	O1B-C1B-C2B-C3B
23	b	611	CLA	C3-C5-C6-C7
23	c	510	CLA	C11-C12-C13-C14
23	c	511	CLA	C14-C13-C15-C16
33	D	410	LHG	O1-C1-C2-C3
28	a	415	LMG	C24-C25-C26-C27
27	i	101	STE	C2-C3-C4-C5
27	b	625	STE	C7-C8-C9-C10
27	I	101	STE	C12-C13-C14-C15
28	c	523	LMG	C42-C43-C44-C45
28	C	517	LMG	C7-C8-O7-C10
23	b	603	CLA	C3-C5-C6-C7
30	H	102	DGD	CDA-CEA-CFA-CGA
27	Z	101	STE	C5-C6-C7-C8
29	a	414	SQD	C7-C8-C9-C10
27	H	103	STE	C11-C10-C9-C8
30	C	523	DGD	C7B-C8B-C9B-CAB
26	d	405	PL9	C43-C44-C46-C47
33	D	412	LHG	O1-C1-C2-O2
27	E	104	STE	O1-C1-C2-C3
28	b	621	LMG	C39-C40-C41-C42
23	c	509	CLA	CAA-CBA-CGA-O1A
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
25	k	101	BCR	C11-C10-C9-C8
27	b	625	STE	O1-C1-C2-C3
27	e	103	STE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	T	102	STE	C5-C6-C7-C8
23	B	601	CLA	C2B-C3B-CAB-CBB
23	b	609	CLA	C2B-C3B-CAB-CBB
25	H	101	BCR	C23-C24-C25-C30
25	b	616	BCR	C1-C6-C7-C8
25	c	514	BCR	C5-C6-C7-C8
25	k	101	BCR	C23-C24-C25-C30
25	k	102	BCR	C1-C6-C7-C8
27	C	516	STE	C1-C2-C3-C4
27	I	102	STE	O1-C1-C2-C3
33	E	101	LHG	C2-C3-O3-P
23	b	613	CLA	C3-C5-C6-C7
27	M	102	STE	O2-C1-C2-C3
34	F	101	HEM	CAD-CBD-CGD-O1D
23	h	101	CLA	C4-C3-C5-C6
27	c	516	STE	C6-C7-C8-C9
29	f	102	SQD	C33-C34-C35-C36
33	a	413	LHG	O6-C4-C5-C6
33	a	413	LHG	C12-C13-C14-C15
23	b	609	CLA	C13-C15-C16-C17
23	C	509	CLA	C11-C10-C8-C7
23	b	611	CLA	C11-C10-C8-C7
23	h	101	CLA	C11-C12-C13-C15
27	C	526	STE	C11-C10-C9-C8
23	B	603	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
29	A	413	SQD	C23-C24-C25-C26
27	b	625	STE	O2-C1-C2-C3
30	H	102	DGD	CCB-CDB-CEB-CFB
26	A	409	PL9	C4-C3-C7-C8
23	b	604	CLA	C10-C11-C12-C13
28	D	408	LMG	C17-C18-C19-C20
30	C	522	DGD	C4B-C5B-C6B-C7B
30	H	102	DGD	C6B-C7B-C8B-C9B
30	c	520	DGD	C4A-C5A-C6A-C7A
28	c	518	LMG	O8-C28-C29-C30
27	Z	101	STE	C2-C3-C4-C5
28	B	620	LMG	C34-C35-C36-C37
25	D	406	BCR	C37-C22-C23-C24
27	D	414	STE	C11-C12-C13-C14
23	a	408	CLA	C4-C3-C5-C6
23	B	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C5-C6-C7-C8
23	c	513	CLA	C2-C3-C5-C6
26	A	409	PL9	C13-C14-C16-C17
26	A	409	PL9	C18-C19-C21-C22
26	a	410	PL9	C43-C44-C46-C47
26	d	405	PL9	C13-C14-C16-C17
23	c	506	CLA	C15-C16-C17-C18
35	v	201	HEC	CAD-CBD-CGD-O2D
29	b	620	SQD	C29-C30-C31-C32
23	B	604	CLA	C11-C10-C8-C9
23	b	611	CLA	C11-C10-C8-C9
28	a	415	LMG	C34-C35-C36-C37
23	C	512	CLA	C8-C10-C11-C12
23	B	603	CLA	C15-C16-C17-C18
27	M	102	STE	O1-C1-C2-C3
27	M	102	STE	C9-C10-C11-C12
23	b	613	CLA	C16-C17-C18-C20
34	F	101	HEM	CAD-CBD-CGD-O2D
30	C	521	DGD	C7A-C8A-C9A-CAA
28	D	408	LMG	C30-C31-C32-C33
33	D	411	LHG	C32-C33-C34-C35
35	V	201	HEC	CAD-CBD-CGD-O2D
27	C	526	STE	C6-C7-C8-C9
35	V	201	HEC	CAD-CBD-CGD-O1D
28	A	411	LMG	C17-C18-C19-C20
23	b	609	CLA	C4B-C3B-CAB-CBB
23	h	101	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C5-C6-C7-C8
35	v	201	HEC	CAD-CBD-CGD-O1D
27	I	102	STE	O2-C1-C2-C3
33	d	408	LHG	C35-C36-C37-C38
24	a	407	PHO	CHA-CBD-CGD-O1D
25	C	515	BCR	C20-C21-C22-C37
25	a	409	BCR	C35-C13-C14-C15
25	x	101	BCR	C11-C10-C9-C34
30	C	523	DGD	CCA-CDA-CEA-CFA
23	A	404	CLA	C4C-C3C-CAC-CBC
27	t	103	STE	O2-C1-C2-C3
23	h	101	CLA	C2-C3-C5-C6
23	C	510	CLA	C15-C16-C17-C18
23	C	512	CLA	C10-C11-C12-C13
28	a	415	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	b	602	CLA	C12-C13-C15-C16
23	d	402	CLA	C11-C12-C13-C15
27	Z	101	STE	C3-C4-C5-C6
27	C	519	STE	C2-C3-C4-C5
27	A	417	STE	C11-C12-C13-C14
27	C	525	STE	C6-C7-C8-C9
27	e	103	STE	C14-C15-C16-C17
28	c	524	LMG	C40-C41-C42-C43
30	h	102	DGD	C5B-C6B-C7B-C8B
30	c	520	DGD	CBA-CCA-CDA-CEA
23	D	405	CLA	C14-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	508	CLA	C11-C10-C8-C9
27	b	625	STE	C6-C7-C8-C9
27	C	529	STE	C11-C12-C13-C14
28	b	621	LMG	C8-C7-O1-C1
29	a	412	SQD	C45-C44-O6-C1
27	M	102	STE	C3-C4-C5-C6
23	b	609	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	C2-C1-O2A-CGA
30	c	519	DGD	CDA-CEA-CFA-CGA
30	A	414	DGD	C3B-C4B-C5B-C6B
27	E	104	STE	O2-C1-C2-C3
33	D	412	LHG	O1-C1-C2-C3
24	a	407	PHO	O2A-C1-C2-C3
30	c	520	DGD	CDA-CEA-CFA-CGA
28	A	411	LMG	C37-C38-C39-C40
30	A	414	DGD	C9A-CAA-CBA-CCA
30	H	102	DGD	C5B-C6B-C7B-C8B
27	j	101	STE	C5-C6-C7-C8
27	t	103	STE	O1-C1-C2-C3
27	t	102	STE	C2-C3-C4-C5
29	A	412	SQD	C15-C16-C17-C18
29	a	414	SQD	C35-C36-C37-C38
30	C	523	DGD	C6A-C7A-C8A-C9A
33	E	101	LHG	C27-C28-C29-C30
28	c	522	LMG	O1-C7-C8-C9
30	h	102	DGD	C1G-C2G-C3G-O3G
26	A	409	PL9	C37-C38-C39-C40
33	D	410	LHG	C34-C35-C36-C37
28	b	623	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C2A-CAA-CBA-CGA
27	D	413	STE	C11-C10-C9-C8
27	a	417	STE	C4-C5-C6-C7
29	l	101	SQD	C11-C10-C9-C8
33	d	407	LHG	C15-C16-C17-C18
27	I	102	STE	C6-C7-C8-C9
28	M	101	LMG	C12-C13-C14-C15
27	C	516	STE	O2-C1-C2-C3
28	c	522	LMG	O6-C5-C6-O5
27	A	415	STE	C13-C14-C15-C16
28	C	517	LMG	C15-C16-C17-C18
33	l	102	LHG	C11-C12-C13-C14
23	b	602	CLA	C6-C7-C8-C9
27	z	101	STE	C2-C3-C4-C5
27	j	102	STE	C1-C2-C3-C4
26	A	409	PL9	C42-C43-C44-C45
28	d	409	LMG	O7-C10-C11-C12
33	D	411	LHG	O8-C23-C24-C25
27	l	103	STE	C4-C5-C6-C7
27	A	417	STE	C11-C10-C9-C8
23	B	604	CLA	C11-C10-C8-C7
23	B	611	CLA	C6-C7-C8-C10
23	a	408	CLA	C11-C10-C8-C7
23	b	602	CLA	C6-C7-C8-C10
23	c	501	CLA	C11-C12-C13-C15
23	d	403	CLA	C11-C12-C13-C15
27	C	529	STE	C5-C6-C7-C8
23	B	606	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C2B-C3B-CAB-CBB
25	A	408	BCR	C23-C24-C25-C26
25	A	408	BCR	C23-C24-C25-C30
25	b	616	BCR	C5-C6-C7-C8
25	x	101	BCR	C23-C24-C25-C26
25	x	101	BCR	C23-C24-C25-C30
33	D	410	LHG	O9-C7-O7-C5
28	c	523	LMG	C34-C35-C36-C37
23	d	402	CLA	C2-C1-O2A-CGA
29	F	102	SQD	C26-C27-C28-C29
28	C	524	LMG	C12-C13-C14-C15
27	C	527	STE	C11-C12-C13-C14
23	h	101	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	C	524	LMG	C10-C11-C12-C13
23	b	613	CLA	C10-C11-C12-C13
28	C	517	LMG	C11-C10-O7-C8
29	a	412	SQD	C10-C11-C12-C13
28	b	621	LMG	C12-C13-C14-C15
23	B	604	CLA	C2C-C3C-CAC-CBC
28	c	523	LMG	C33-C34-C35-C36
29	A	412	SQD	O47-C7-C8-C9
27	B	623	STE	C9-C10-C11-C12
27	j	101	STE	C3-C4-C5-C6
30	c	519	DGD	C3B-C4B-C5B-C6B
23	B	604	CLA	C10-C11-C12-C13
33	D	410	LHG	C16-C17-C18-C19
23	B	613	CLA	CAA-CBA-CGA-O2A
33	D	410	LHG	O1-C1-C2-O2
23	B	611	CLA	C6-C7-C8-C9
23	C	505	CLA	C6-C7-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
27	B	623	STE	C4-C5-C6-C7
33	l	102	LHG	C15-C16-C17-C18
27	B	622	STE	C1-C2-C3-C4
23	c	510	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	O7-C10-C11-C12
29	l	101	SQD	O48-C23-C24-C25
23	B	602	CLA	C1A-C2A-CAA-CBA
33	D	411	LHG	C10-C11-C12-C13
23	a	411	CLA	C4C-C3C-CAC-CBC
28	c	518	LMG	C10-C11-C12-C13
26	a	410	PL9	C30-C29-C31-C32
26	d	405	PL9	C40-C39-C41-C42
30	c	519	DGD	O6E-C1E-O5D-C6D
34	f	101	HEM	CAD-CBD-CGD-O2D
25	C	520	BCR	C17-C18-C19-C20
28	D	408	LMG	C11-C12-C13-C14
26	d	405	PL9	C47-C48-C49-C50
34	f	101	HEM	CAA-CBA-CGA-O2A
34	f	101	HEM	CAD-CBD-CGD-O1D
23	B	614	CLA	C2A-CAA-CBA-CGA
28	c	522	LMG	C29-C30-C31-C32
29	a	412	SQD	C24-C25-C26-C27
28	C	524	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	j	102	STE	C2-C3-C4-C5
27	E	104	STE	C14-C15-C16-C17
26	d	405	PL9	C11-C12-C13-C14
27	b	627	STE	C15-C16-C17-C18
23	A	404	CLA	C2-C1-O2A-CGA
23	D	404	CLA	C2-C1-O2A-CGA
23	B	601	CLA	C11-C10-C8-C7
23	B	615	CLA	C6-C7-C8-C10
23	C	512	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16
23	a	406	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C12-C13-C15
23	c	512	CLA	C11-C12-C13-C15
23	b	602	CLA	C15-C16-C17-C18
30	c	519	DGD	C6A-C7A-C8A-C9A
23	b	608	CLA	C16-C17-C18-C19
23	c	505	CLA	C16-C17-C18-C19
29	A	412	SQD	C35-C36-C37-C38
28	a	415	LMG	C9-C8-O7-C10
23	C	508	CLA	C13-C15-C16-C17
30	c	520	DGD	C3A-C4A-C5A-C6A
28	b	621	LMG	O8-C28-C29-C30
30	c	521	DGD	C2A-C3A-C4A-C5A
25	T	101	BCR	C13-C14-C15-C16
23	C	501	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C16-C17-C18-C19
33	D	410	LHG	C15-C16-C17-C18
23	a	408	CLA	C8-C10-C11-C12
23	B	602	CLA	C3A-C2A-CAA-CBA
30	C	521	DGD	O1B-C1B-C2B-C3B
28	c	523	LMG	C36-C37-C38-C39
27	C	516	STE	O1-C1-C2-C3
28	c	518	LMG	O10-C28-C29-C30
30	c	520	DGD	O1B-C1B-C2B-C3B
28	c	522	LMG	O6-C1-O1-C7
27	T	102	STE	C11-C12-C13-C14
33	D	411	LHG	C17-C18-C19-C20
23	B	612	CLA	C11-C10-C8-C9
23	B	613	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C12-C13-C14
23	b	602	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	C11-C10-C8-C9
27	I	101	STE	C11-C10-C9-C8
27	H	103	STE	C9-C10-C11-C12
27	D	413	STE	C10-C11-C12-C13
28	d	409	LMG	C29-C30-C31-C32
30	A	414	DGD	CDB-CEB-CFB-CGB
29	l	101	SQD	O10-C23-C24-C25
23	B	612	CLA	CAA-CBA-CGA-O2A
30	c	519	DGD	O1A-C1A-C2A-C3A
33	D	411	LHG	O10-C23-C24-C25
30	c	521	DGD	C9A-CAA-CBA-CCA
30	C	521	DGD	C1B-C2B-C3B-C4B
28	C	524	LMG	C34-C35-C36-C37
28	D	409	LMG	C17-C18-C19-C20
30	c	519	DGD	O2G-C1B-C2B-C3B
25	c	514	BCR	C11-C12-C13-C14
23	B	615	CLA	C13-C15-C16-C17
30	c	519	DGD	C7B-C8B-C9B-CAB
33	d	406	LHG	C24-C25-C26-C27
28	M	101	LMG	C8-C7-O1-C1
30	C	521	DGD	C5D-C6D-O5D-C1E
30	c	519	DGD	C5D-C6D-O5D-C1E
30	C	521	DGD	O1B-C1B-O2G-C2G
28	c	524	LMG	O1-C7-C8-O7
27	i	102	STE	C11-C10-C9-C8
29	A	412	SQD	O49-C7-C8-C9
28	A	411	LMG	C7-C8-C9-O8
27	C	525	STE	O2-C1-C2-C3
23	c	510	CLA	CAA-CBA-CGA-O1A
26	a	410	PL9	C21-C22-C23-C24
28	a	415	LMG	C19-C20-C21-C22
23	b	611	CLA	CAA-CBA-CGA-O2A
23	a	408	CLA	C2-C3-C5-C6
23	C	504	CLA	C11-C12-C13-C14
23	C	501	CLA	CAD-CBD-CGD-O2D
28	c	524	LMG	O8-C28-C29-C30
34	f	101	HEM	CAA-CBA-CGA-O1A
33	d	408	LHG	O10-C23-C24-C25
28	M	101	LMG	C10-C11-C12-C13
23	h	101	CLA	O1A-CGA-O2A-C1
30	C	522	DGD	O6D-C5D-C6D-O5D
23	C	509	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	B	622	STE	O2-C1-C2-C3
23	B	613	CLA	CAA-CBA-CGA-O1A
29	A	413	SQD	C19-C20-C21-C22
23	b	611	CLA	CAA-CBA-CGA-O1A
28	b	621	LMG	O10-C28-C29-C30
28	D	408	LMG	C28-C29-C30-C31
28	D	408	LMG	O8-C28-C29-C30
29	a	412	SQD	C9-C10-C11-C12
33	L	101	LHG	O9-C7-C8-C9
30	C	521	DGD	C3B-C4B-C5B-C6B
30	A	414	DGD	CFA-CGA-CHA-CIA
28	b	623	LMG	C22-C23-C24-C25

There are no ring outliers.

129 monomers are involved in 272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	a	410	PL9	2	0
23	b	613	CLA	3	0
25	H	101	BCR	3	0
27	J	101	STE	2	0
25	d	404	BCR	2	0
28	A	411	LMG	2	0
24	A	406	PHO	3	0
25	x	101	BCR	3	0
25	b	617	BCR	4	0
23	b	601	CLA	1	0
28	D	408	LMG	5	0
24	a	407	PHO	1	0
23	b	612	CLA	5	0
33	E	101	LHG	4	0
34	f	101	HEM	7	0
23	C	506	CLA	2	0
25	K	101	BCR	3	0
33	d	406	LHG	7	0
27	A	417	STE	9	0
25	T	101	BCR	4	0
23	b	605	CLA	1	0
23	C	509	CLA	4	0
25	b	616	BCR	1	0
27	D	414	STE	2	0
23	c	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	F	102	SQD	2	0
23	b	606	CLA	1	0
23	c	509	CLA	1	0
30	C	521	DGD	2	0
33	a	413	LHG	1	0
29	a	414	SQD	6	0
28	c	524	LMG	1	0
23	C	510	CLA	1	0
25	t	101	BCR	4	0
25	C	514	BCR	2	0
23	a	411	CLA	1	0
24	D	402	PHO	1	0
27	e	101	STE	4	0
23	B	605	CLA	2	0
28	c	522	LMG	1	0
23	c	505	CLA	1	0
23	B	602	CLA	2	0
23	c	506	CLA	1	0
25	C	515	BCR	1	0
23	B	606	CLA	1	0
29	f	102	SQD	2	0
23	A	404	CLA	3	0
27	e	104	STE	3	0
23	C	511	CLA	2	0
23	c	507	CLA	2	0
23	b	603	CLA	1	0
23	C	504	CLA	3	0
23	C	513	CLA	2	0
23	B	612	CLA	3	0
23	B	613	CLA	2	0
33	l	102	LHG	1	0
23	D	404	CLA	1	0
25	b	618	BCR	1	0
23	C	502	CLA	1	0
28	c	523	LMG	1	0
23	c	508	CLA	3	0
23	b	604	CLA	4	0
28	B	620	LMG	1	0
25	c	514	BCR	6	0
27	A	415	STE	1	0
27	B	622	STE	1	0
27	i	101	STE	3	0

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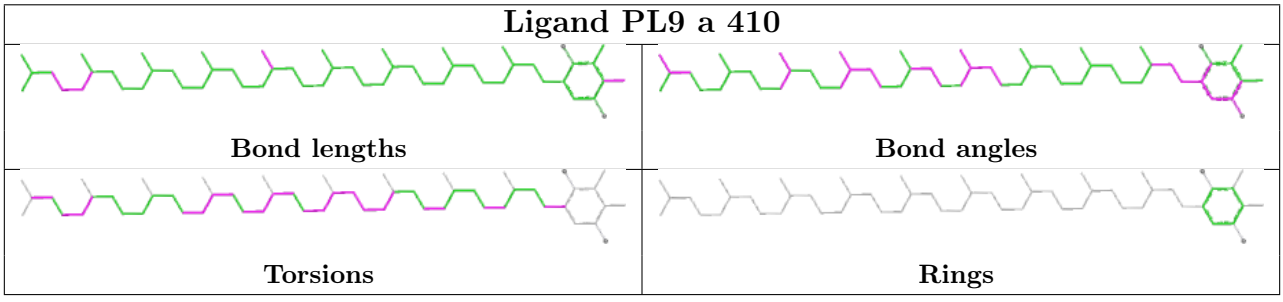
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	627	STE	7	0
23	C	507	CLA	3	0
27	j	102	STE	4	0
24	d	401	PHO	1	0
23	h	101	CLA	2	0
28	C	517	LMG	3	0
25	B	619	BCR	2	0
27	A	416	STE	8	0
27	x	102	STE	1	0
28	a	415	LMG	1	0
23	C	512	CLA	2	0
23	C	505	CLA	1	0
28	b	623	LMG	2	0
29	A	413	SQD	12	0
30	c	520	DGD	3	0
25	k	101	BCR	1	0
25	D	406	BCR	6	0
23	B	604	CLA	1	0
27	d	410	STE	2	0
30	c	519	DGD	1	0
27	d	412	STE	2	0
33	D	412	LHG	1	0
29	b	620	SQD	1	0
27	b	624	STE	13	0
23	b	614	CLA	2	0
25	a	409	BCR	3	0
27	C	526	STE	2	0
28	b	621	LMG	2	0
29	a	412	SQD	4	0
23	c	503	CLA	2	0
23	c	511	CLA	2	0
27	E	104	STE	1	0
23	b	615	CLA	1	0
27	c	516	STE	1	0
25	C	520	BCR	1	0
27	b	622	STE	1	0
23	c	510	CLA	1	0
35	v	201	HEC	3	0
23	a	405	CLA	1	0
23	c	513	CLA	6	0
27	E	103	STE	5	0
23	B	611	CLA	1	0

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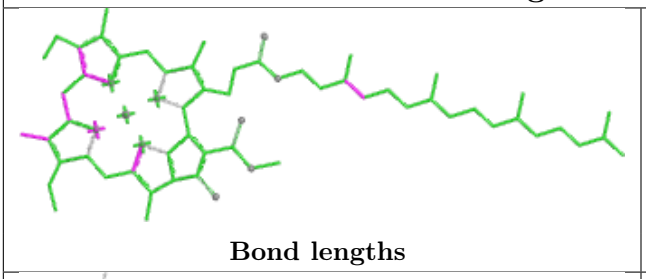
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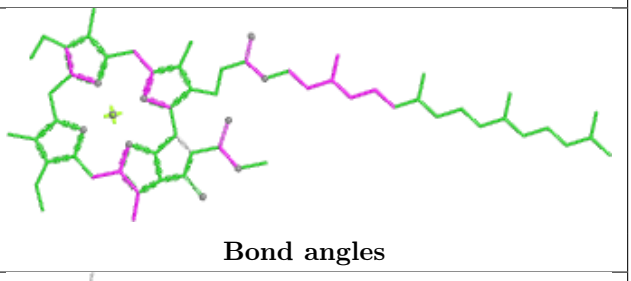
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	515	BCR	1	0
30	A	414	DGD	7	0
23	D	403	CLA	3	0
27	I	101	STE	2	0
28	d	409	LMG	1	0
27	l	103	STE	3	0
28	b	619	LMG	10	0
27	C	528	STE	3	0
30	C	522	DGD	3	0
23	c	504	CLA	1	0
34	F	101	HEM	2	0
23	B	616	CLA	1	0
23	B	601	CLA	2	0
33	D	410	LHG	3	0
25	B	618	BCR	6	0
23	b	609	CLA	1	0
23	d	403	CLA	3	0
30	H	102	DGD	1	0
23	C	508	CLA	4	0
23	c	501	CLA	2	0

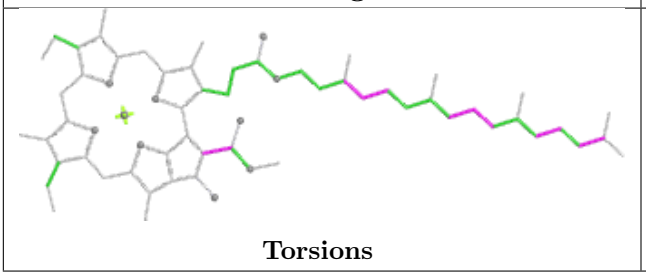
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

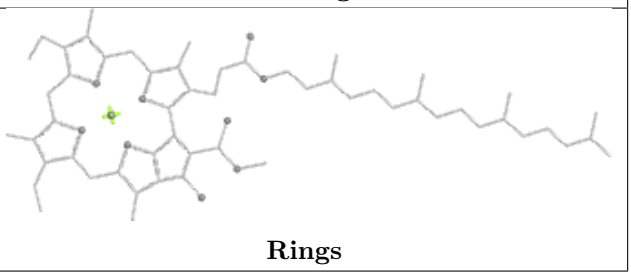


Ligand CLA b 613

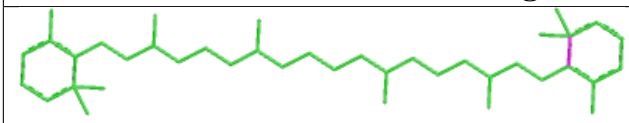

Bond lengths

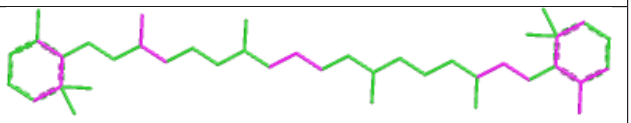

Bond angles

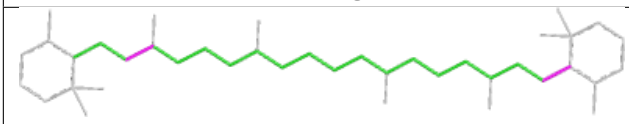

Torsions

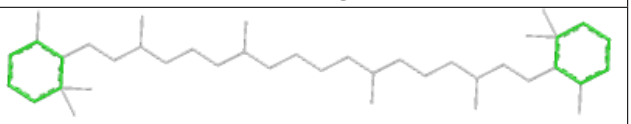

Rings

Ligand BCR H 101

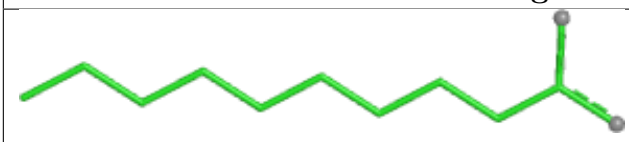

Bond lengths

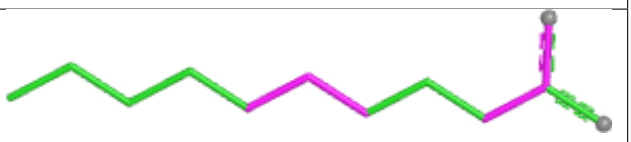

Bond angles

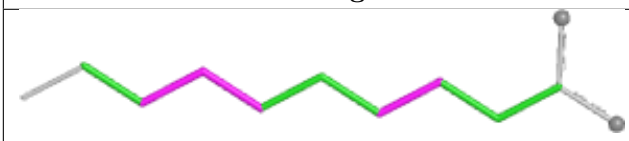

Torsions

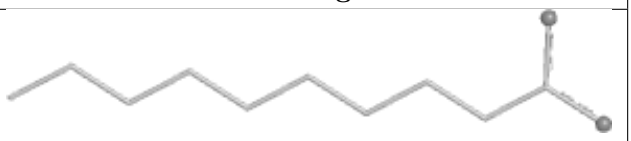

Rings

Ligand STE J 101

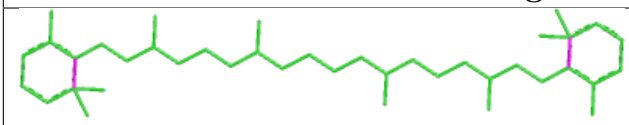

Bond lengths

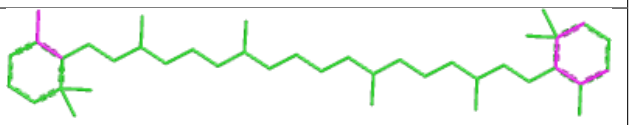

Bond angles

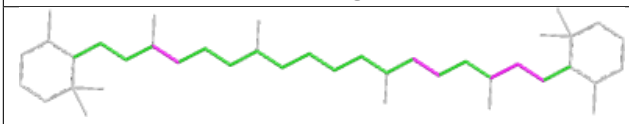

Torsions

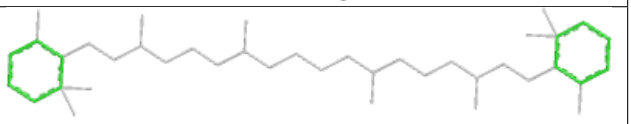

Rings

Ligand BCR d 404

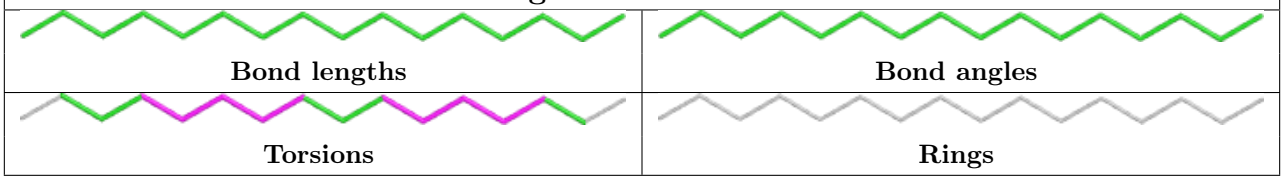

Bond lengths


Bond angles

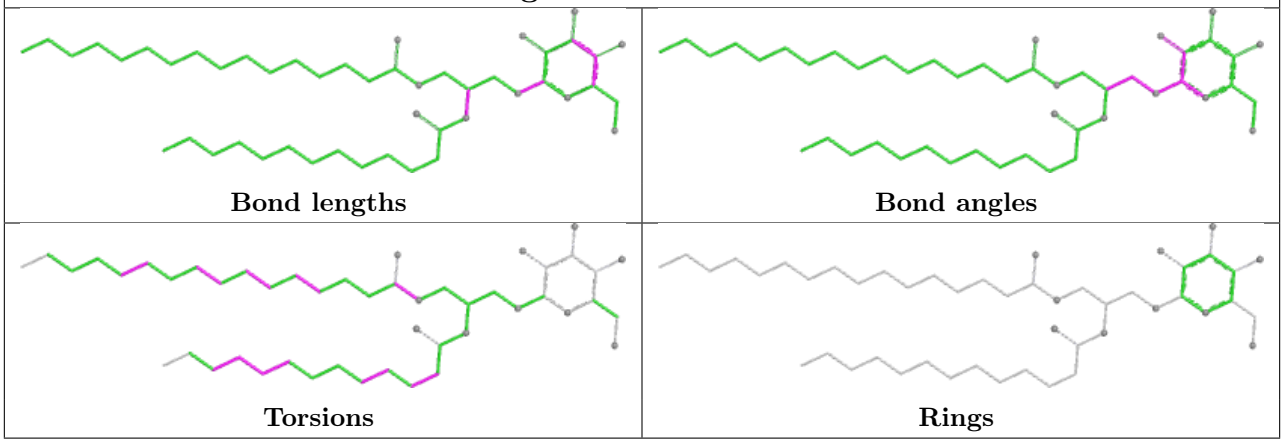

Torsions


Rings

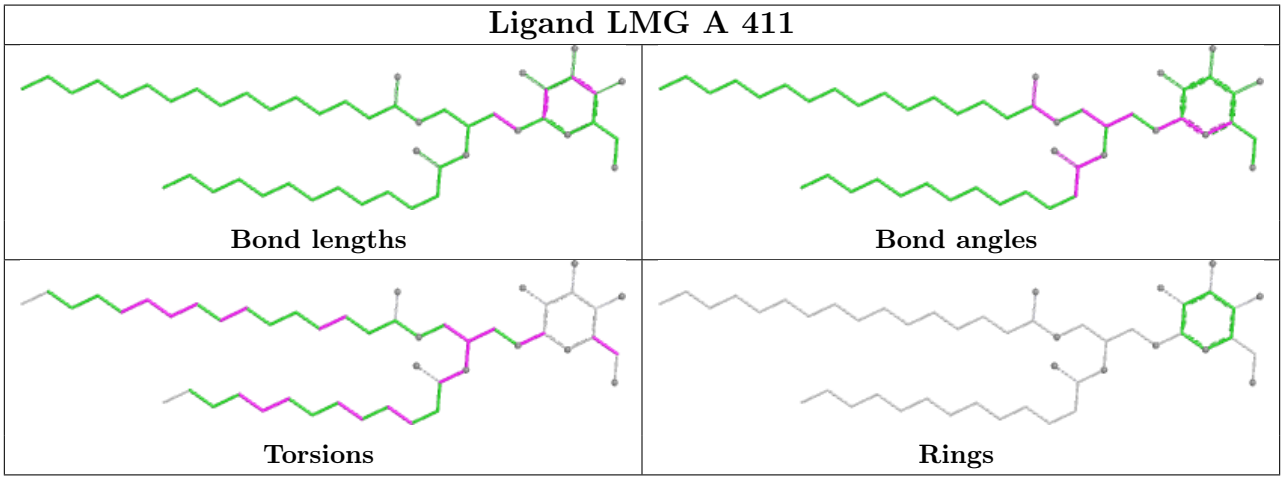
Ligand STE T 102



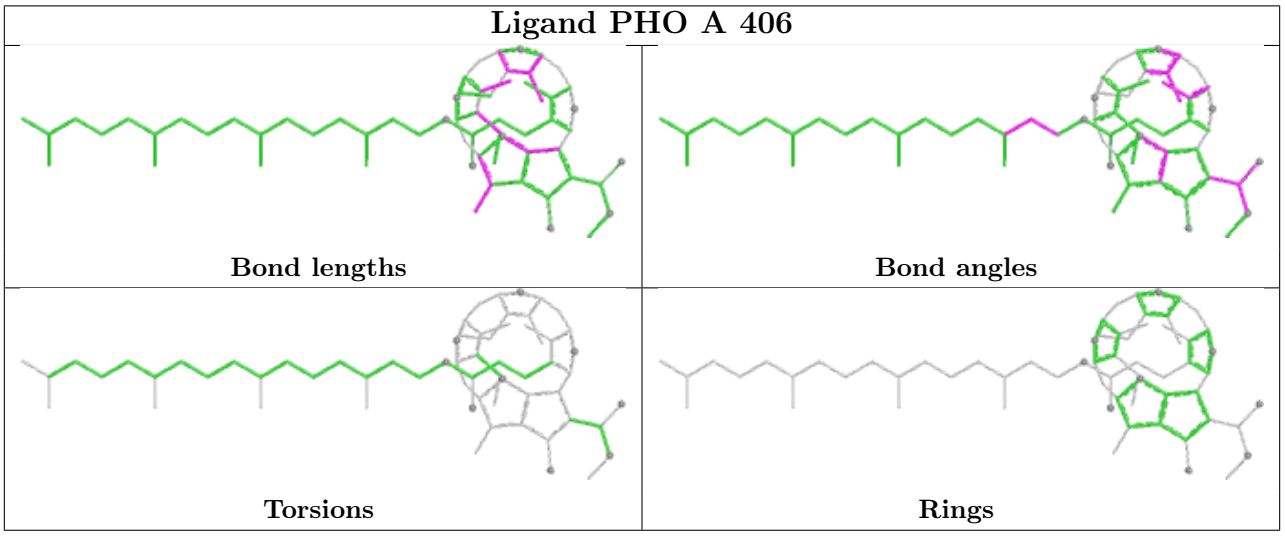
Ligand LMG C 524



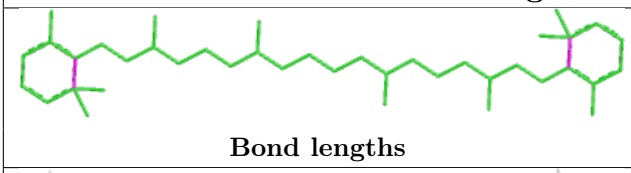
Ligand LMG A 411

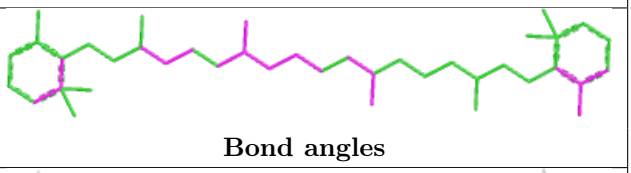


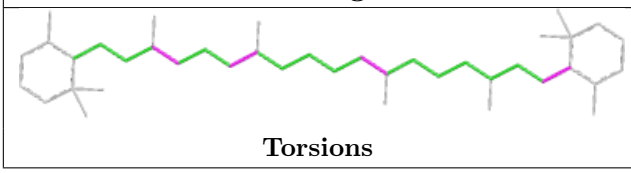
Ligand PHO A 406

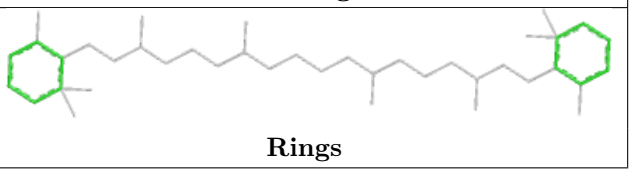


Ligand BCR x 101


Bond lengths


Bond angles

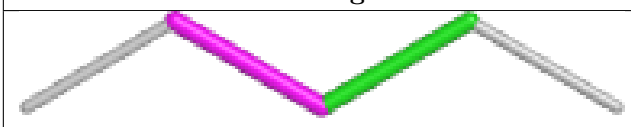

Torsions


Rings

Ligand STE C 518


Bond lengths

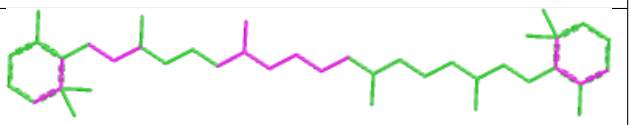

Bond angles

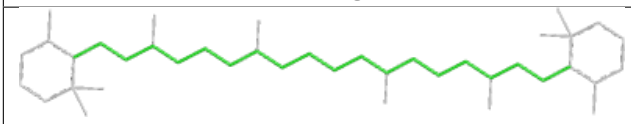

Torsions

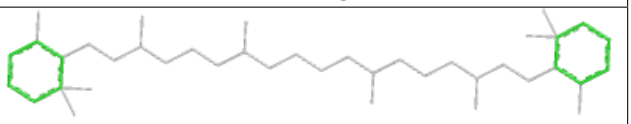

Rings

Ligand BCR b 617

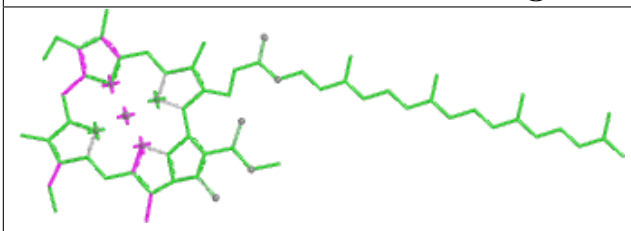

Bond lengths

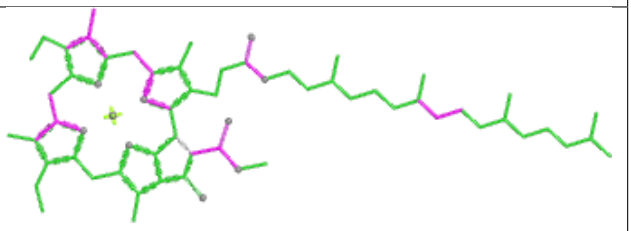

Bond angles

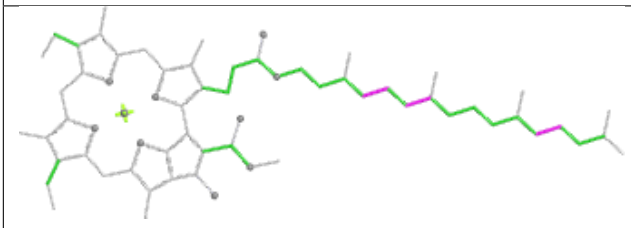

Torsions

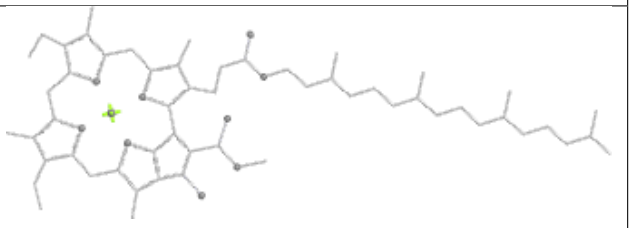

Rings

Ligand CLA b 601

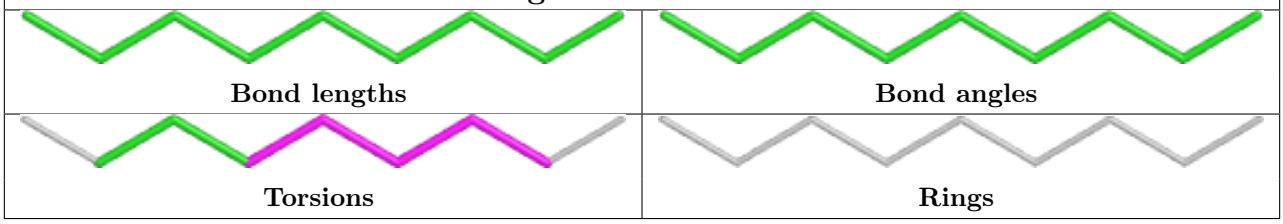

Bond lengths


Bond angles

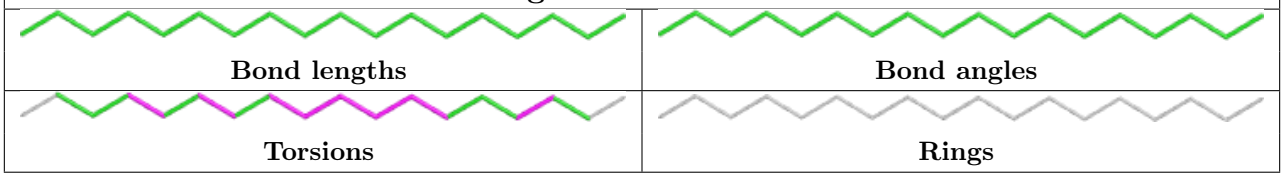

Torsions


Rings

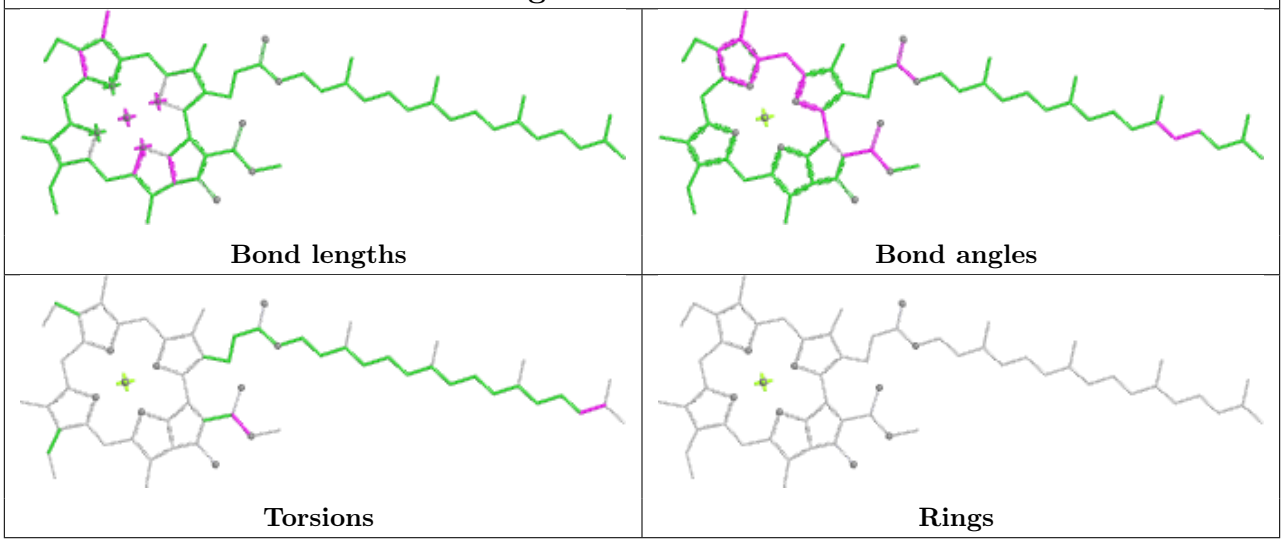
Ligand STE A 410



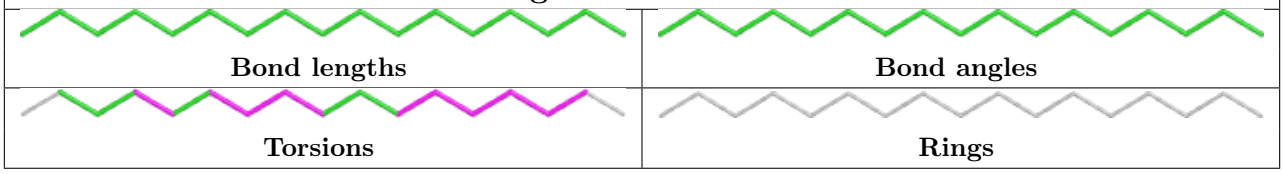
Ligand STE H 103



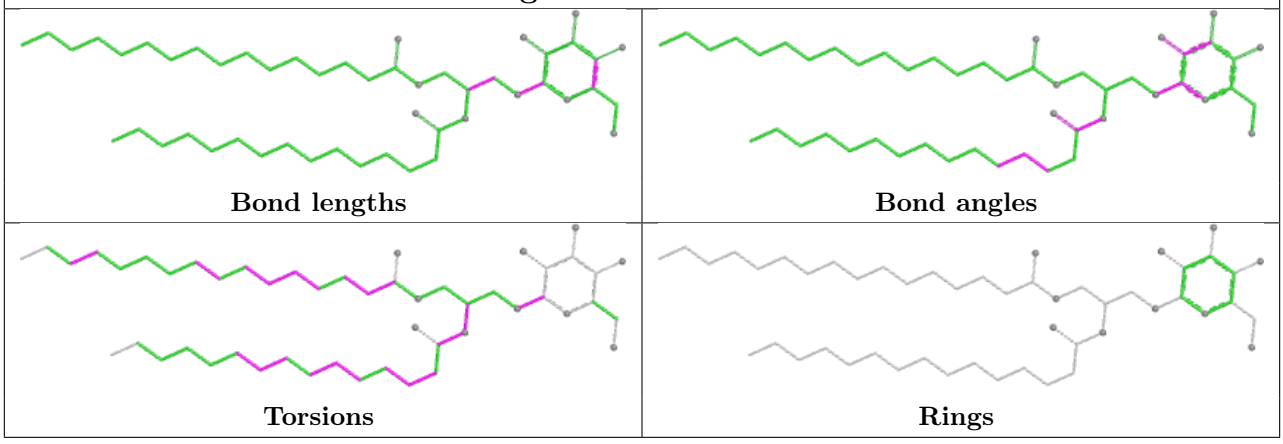
Ligand CLA b 608



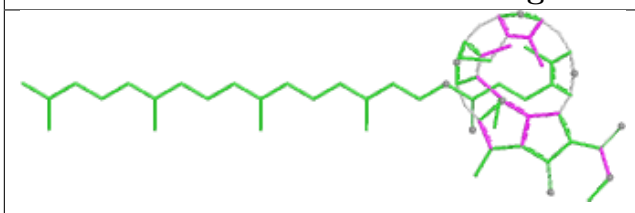
Ligand STE Z 101



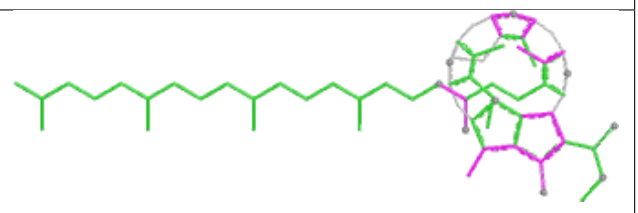
Ligand LMG D 408



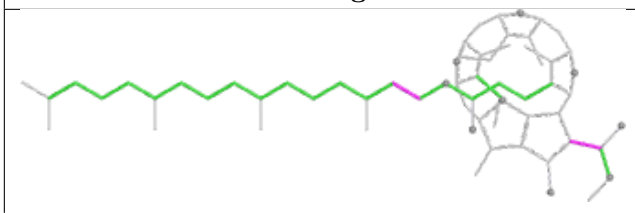
Ligand PHO a 407



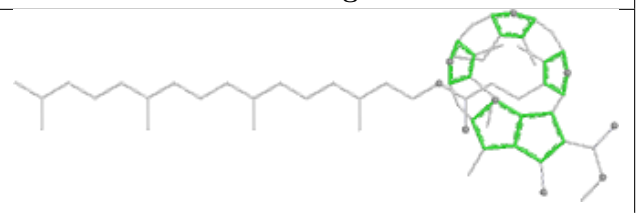
Bond lengths



Bond angles

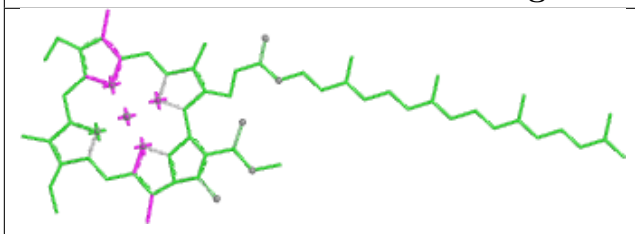


Torsions

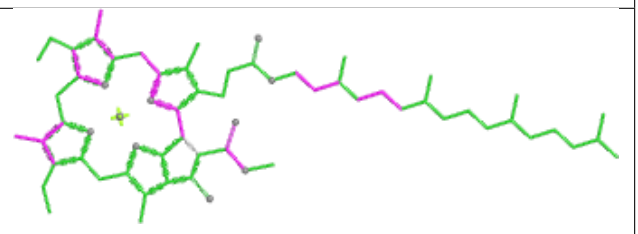


Rings

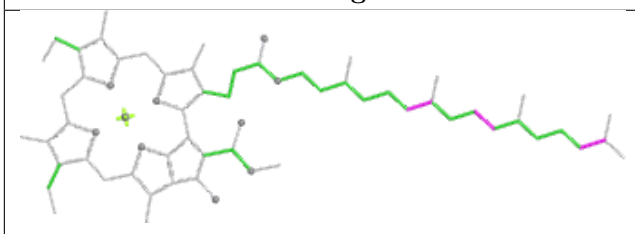
Ligand CLA b 612



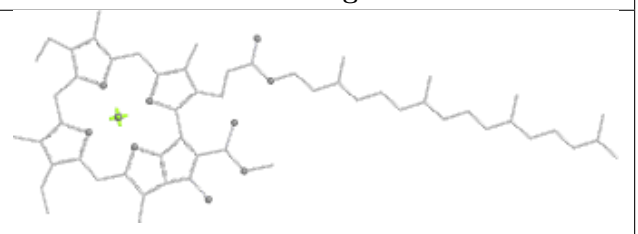
Bond lengths



Bond angles

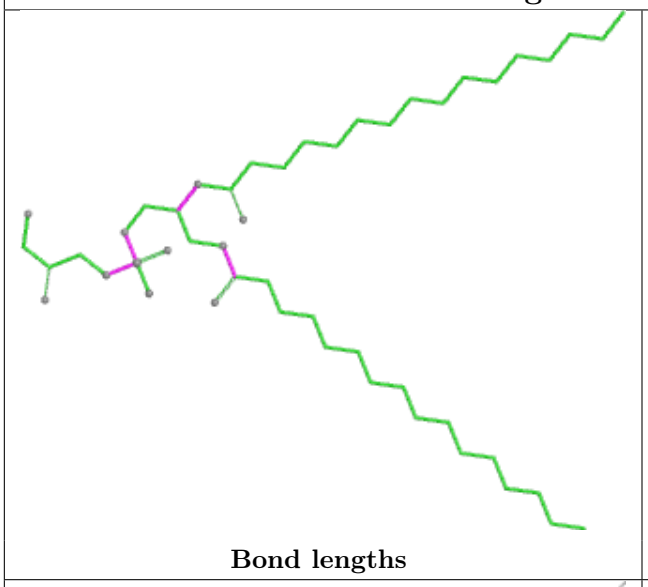


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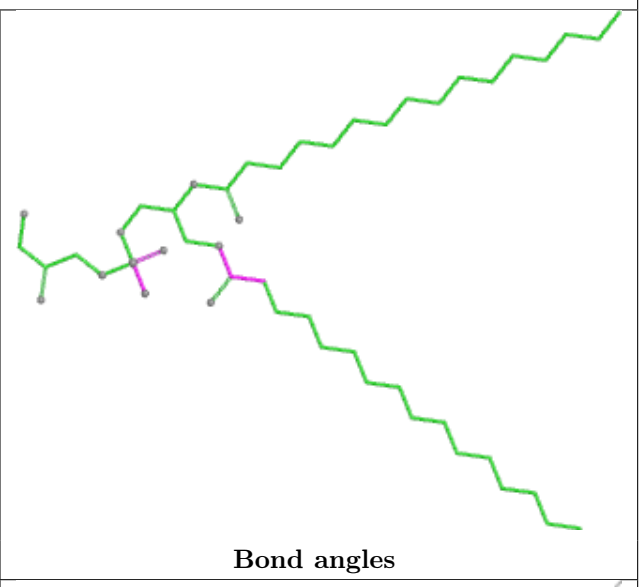


Rings

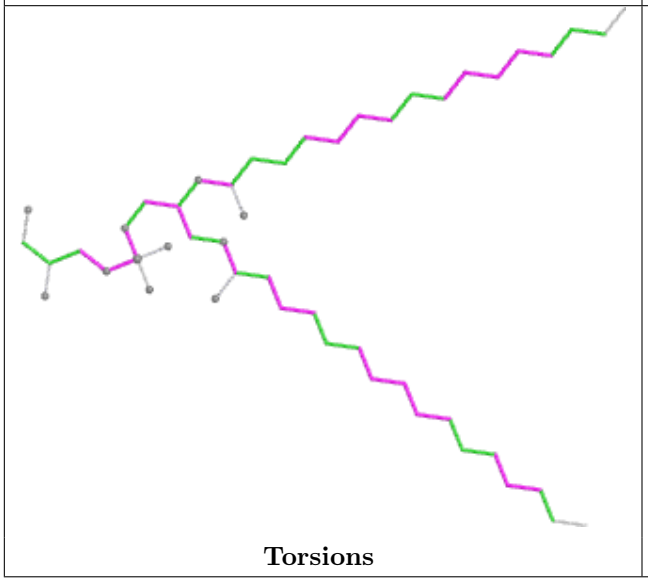
Ligand LHG E 101



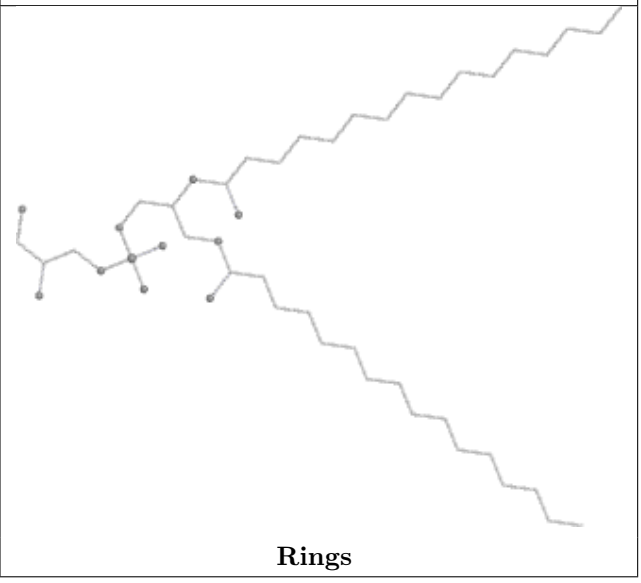
Bond lengths



Bond angles



Torsions



Rings

Ligand STE M 103



Bond lengths



Bond angles

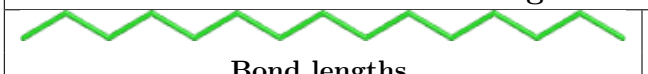


Torsions

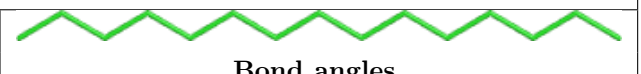


Rings

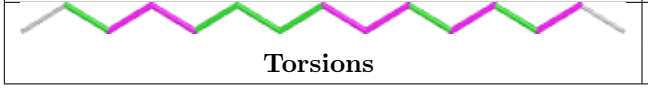
Ligand STE m 102



Bond lengths



Bond angles

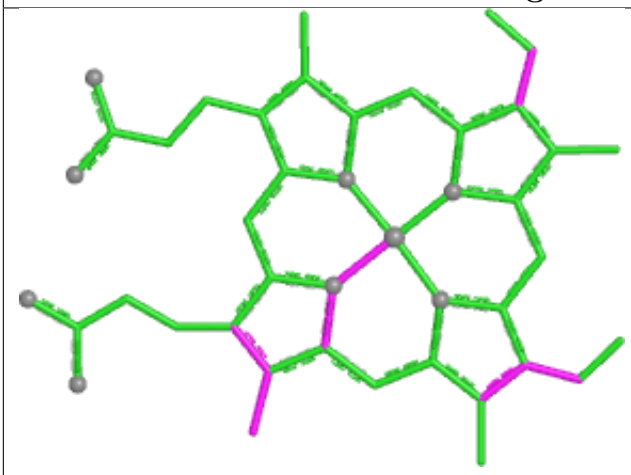


Torsions

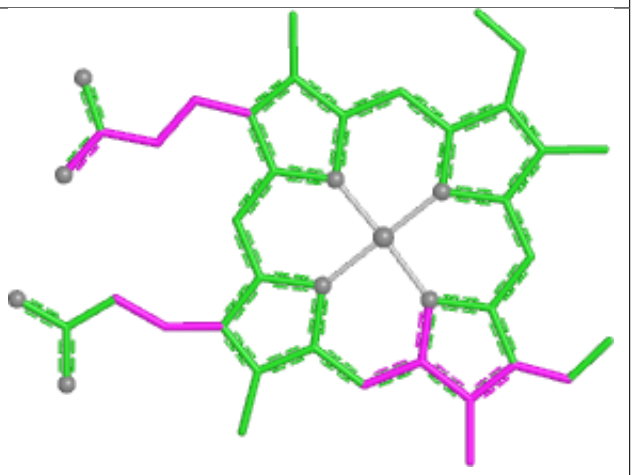


Rings

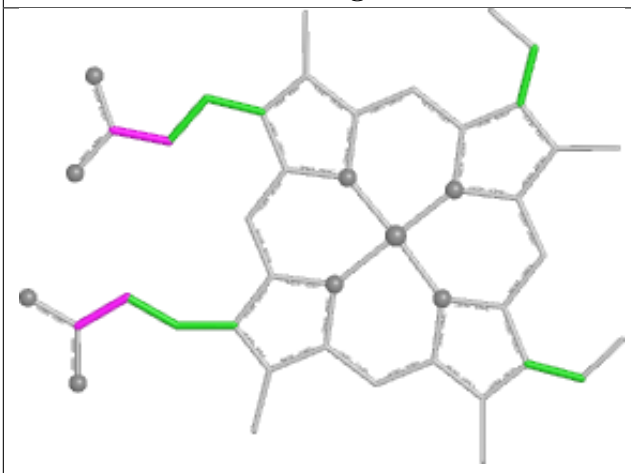
Ligand HEM f 101



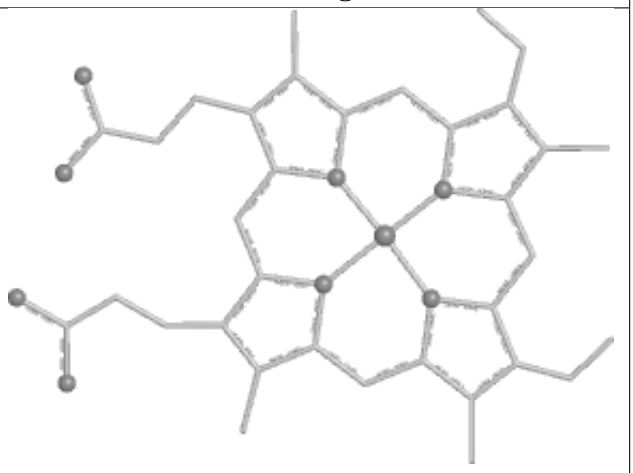
Bond lengths



Bond angles

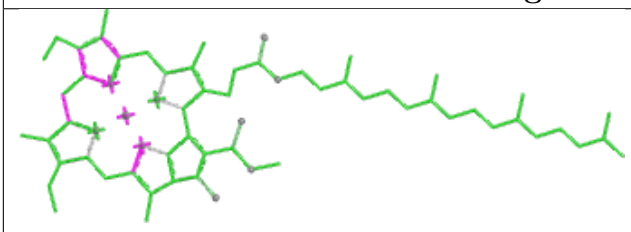


Torsions

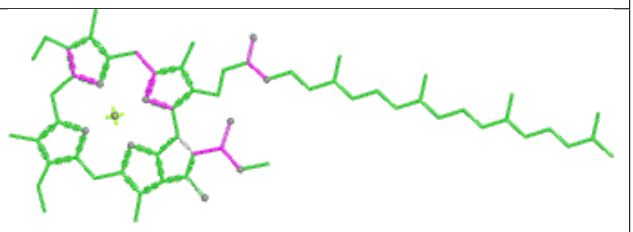


Rings

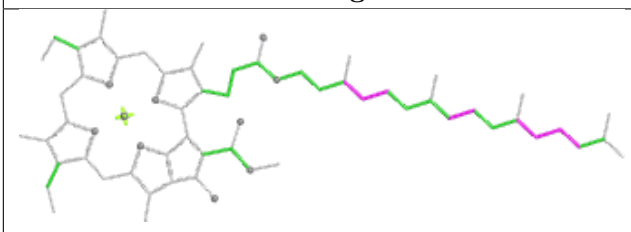
Ligand CLA C 506



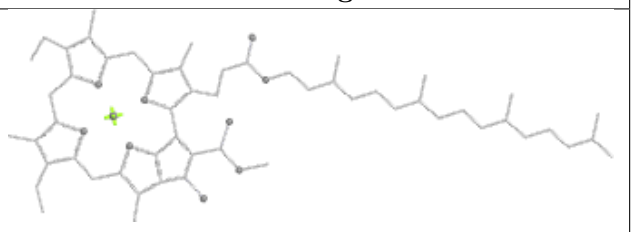
Bond lengths



Bond angles

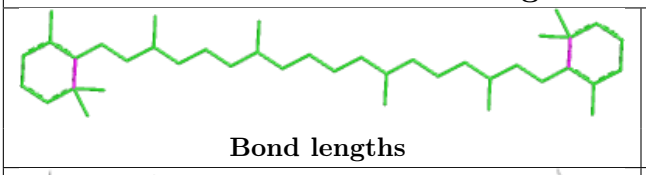


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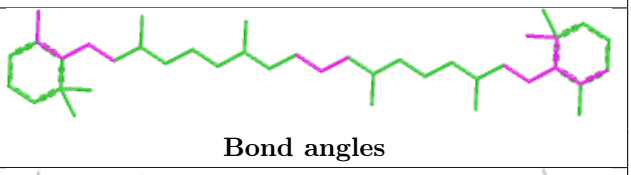


Rings

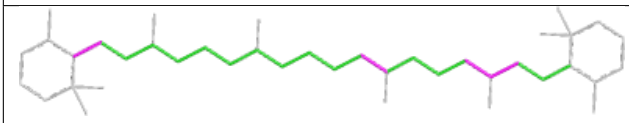
Ligand BCR K 101



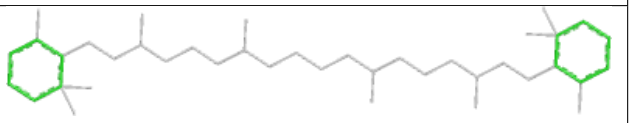
Bond lengths



Bond angles

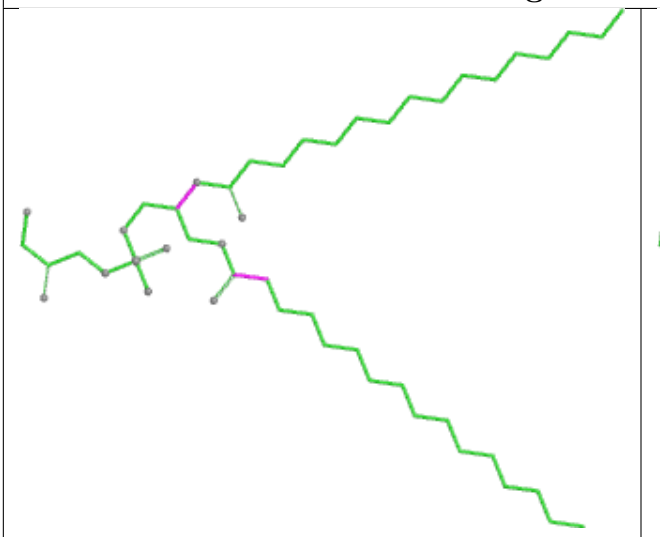


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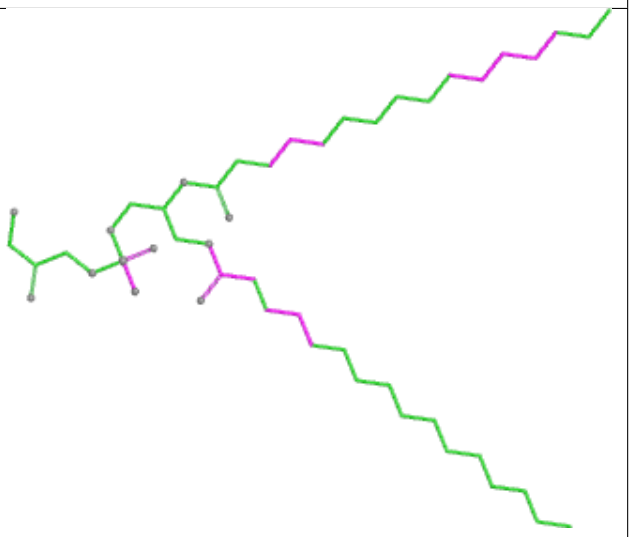


Rings

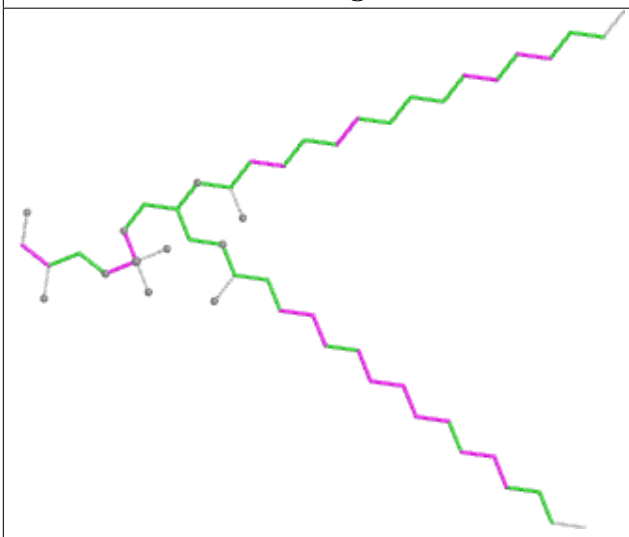
Ligand LHG d 406



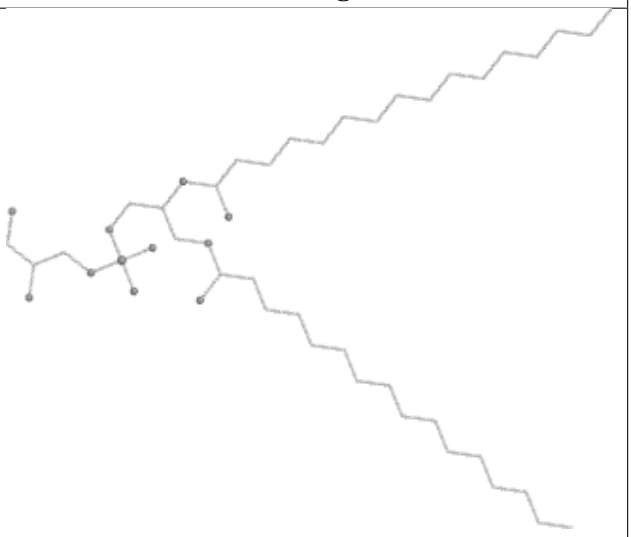
Bond lengths



Bond angles

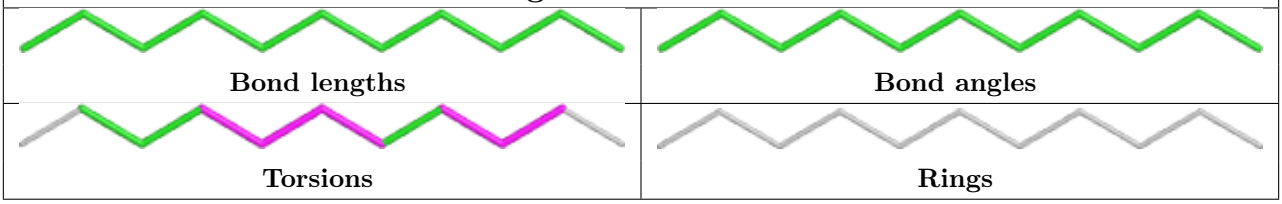


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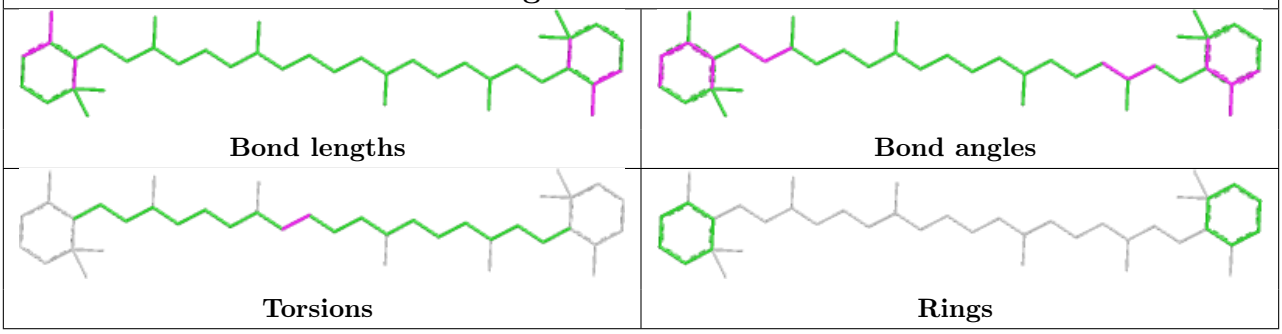


Rings

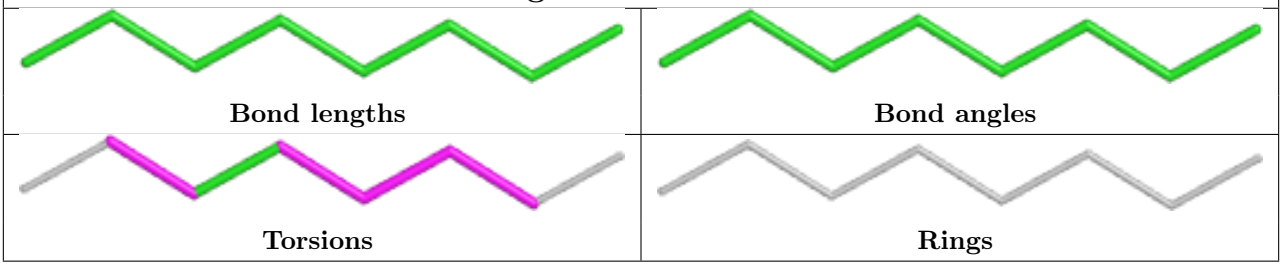
Ligand STE A 417



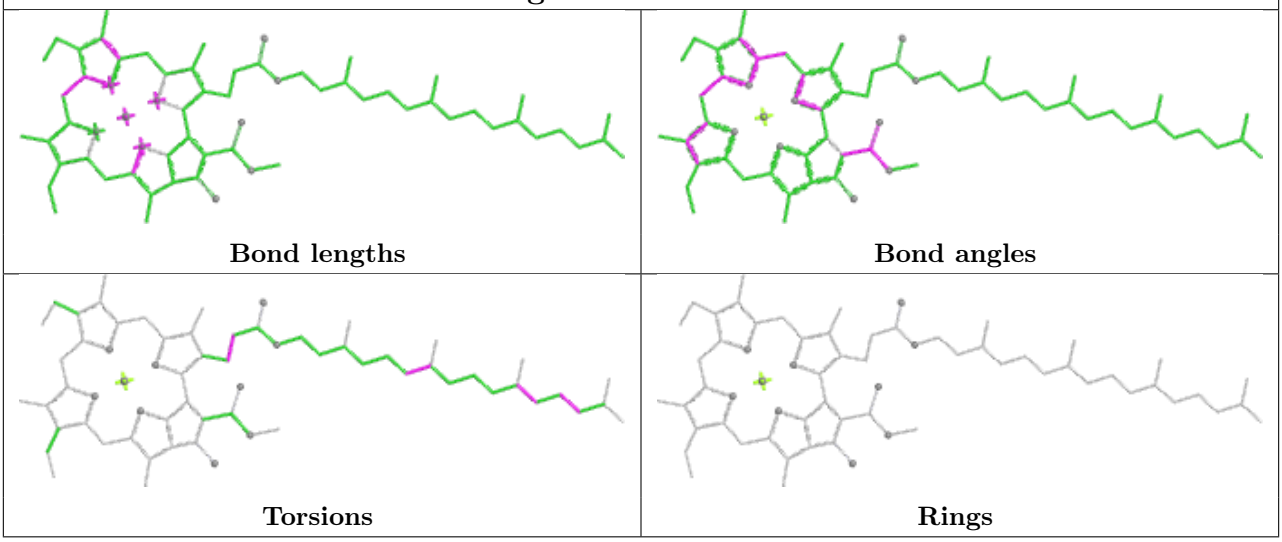
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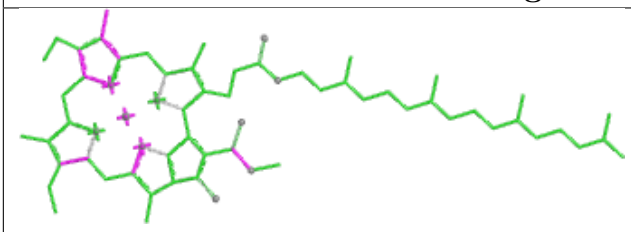
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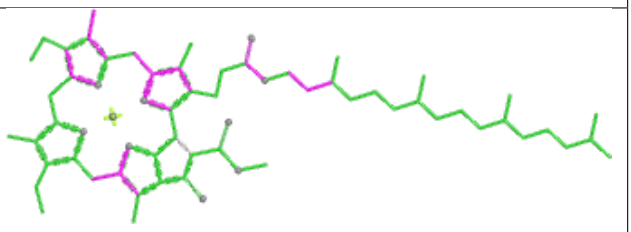


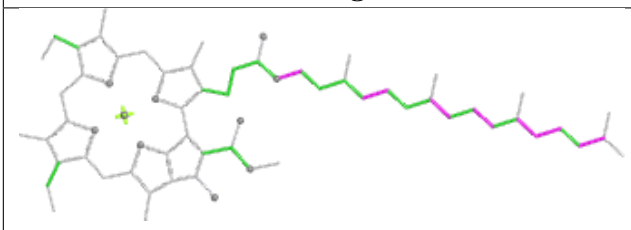
Ligand CLA b 605

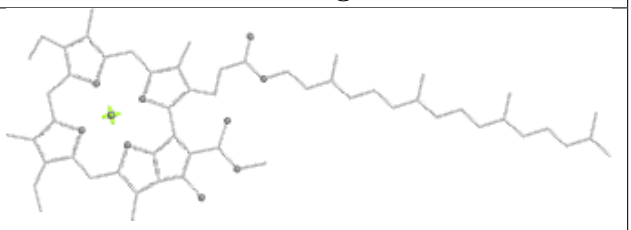


Ligand CLA C 509


Bond lengths

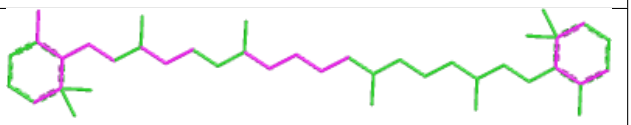

Bond angles

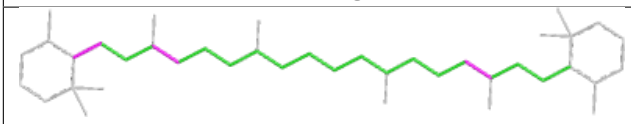

Torsions

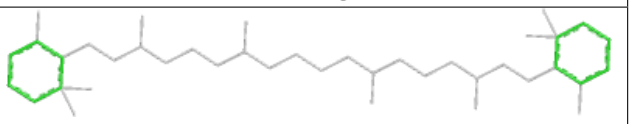

Rings

Ligand BCR b 616


Bond lengths


Bond angles


Torsions


Rings

Ligand STE D 414

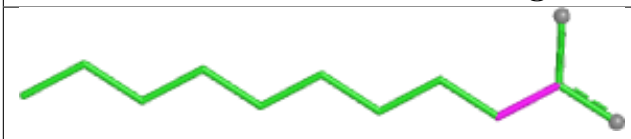

Bond lengths

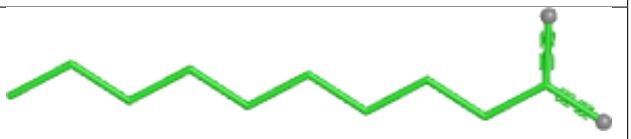

Bond angles

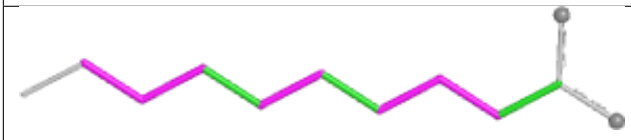

Torsions

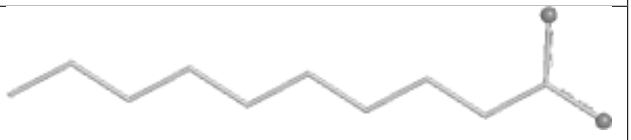

Rings

Ligand STE E 102

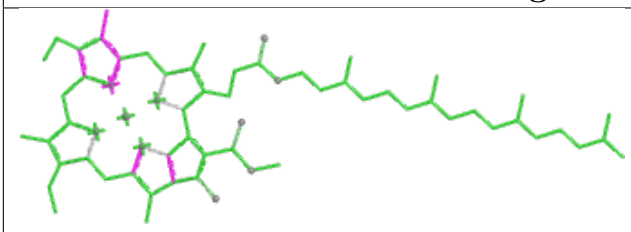

Bond lengths


Bond angles

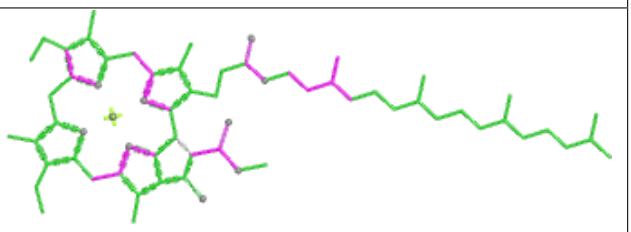

Torsions


Rings

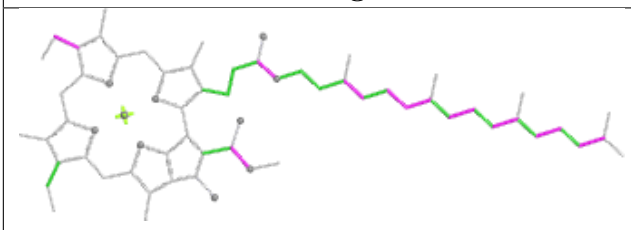
Ligand CLA c 512



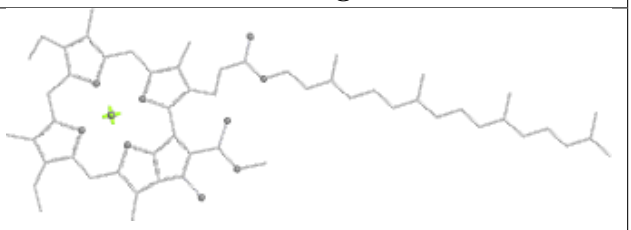
Bond lengths



Bond angles

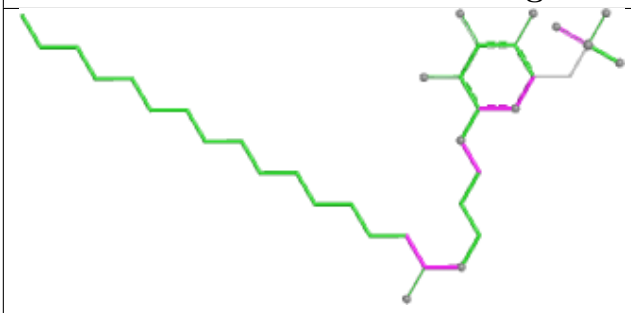


Torsions

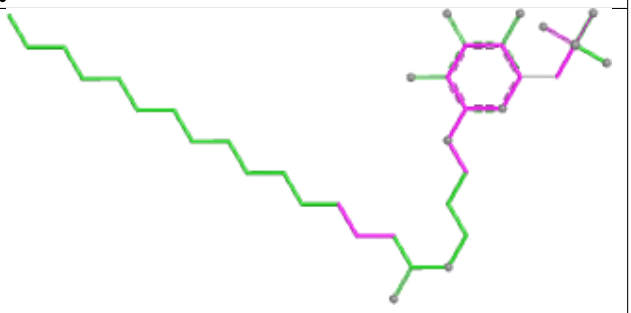


Rings

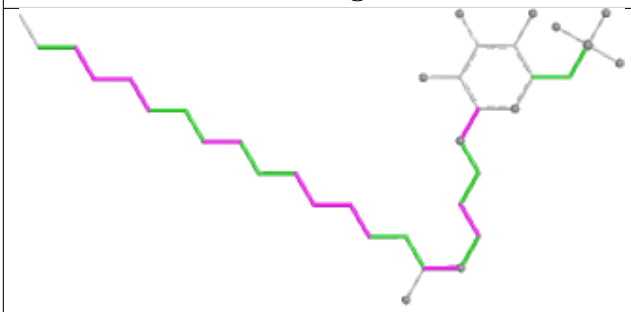
Ligand SQD F 102



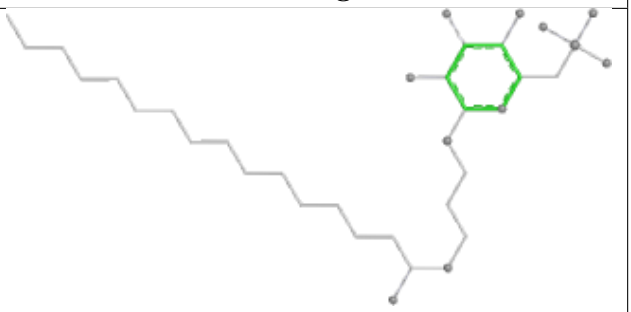
Bond lengths



Bond angles

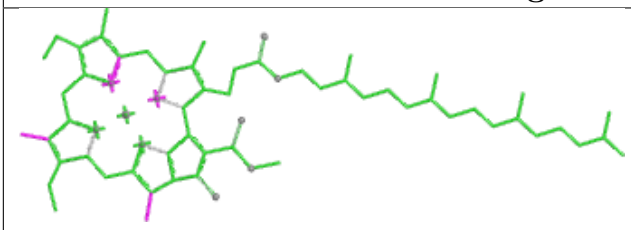


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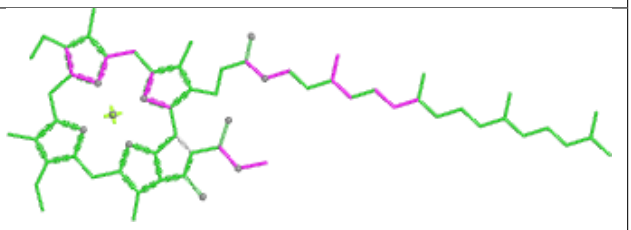


Rings

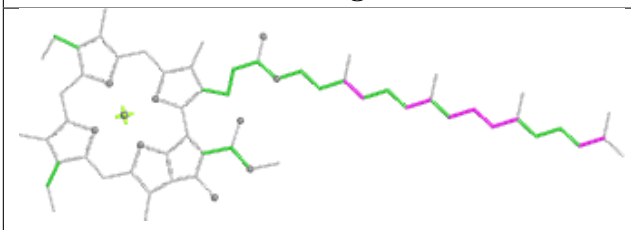
Ligand CLA b 606



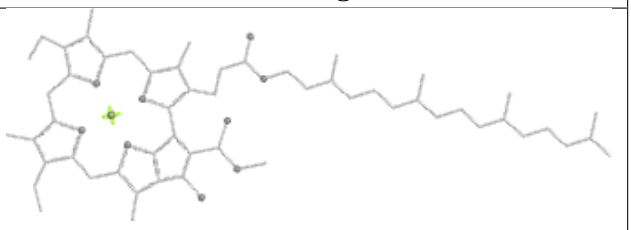
Bond lengths



Bond angles

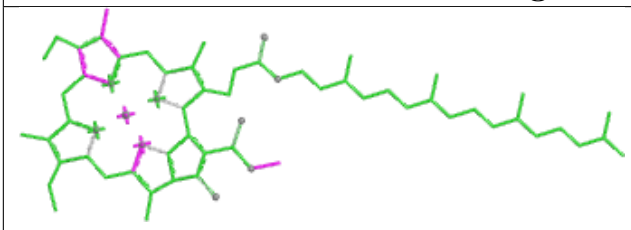


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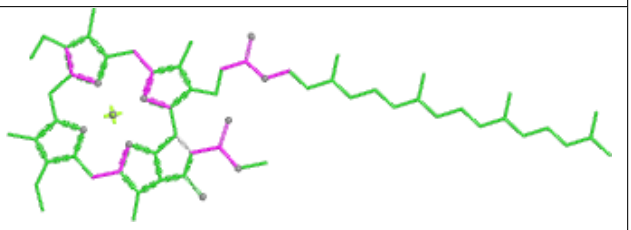


Rings

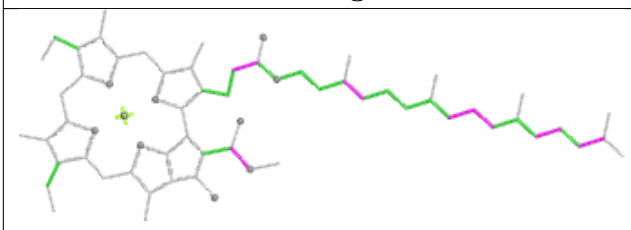
Ligand CLA c 509



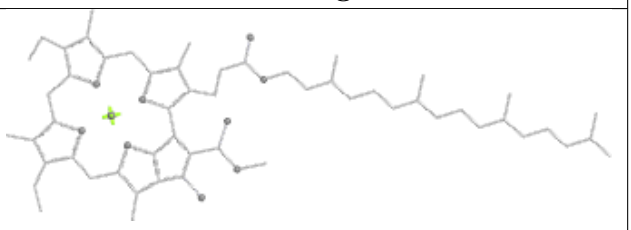
Bond lengths



Bond angles



Torsions



Rings

Ligand STE b 626



Bond lengths



Bond angles

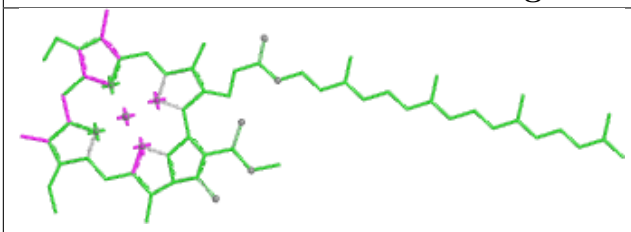


Torsions

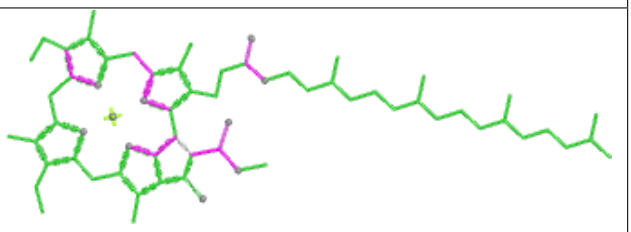


Rings

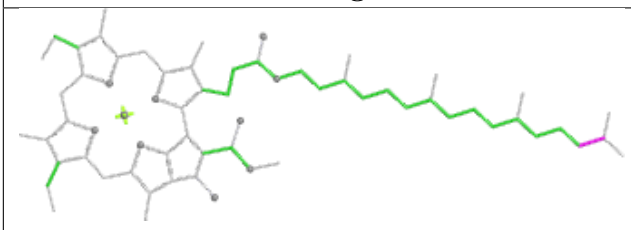
Ligand CLA B 610



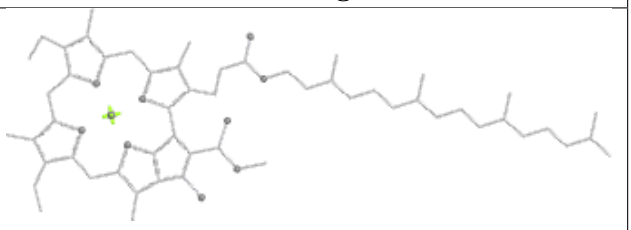
Bond lengths



Bond angles

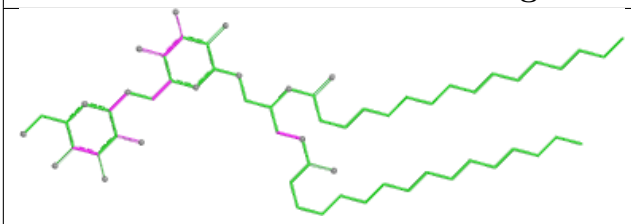


Torsions

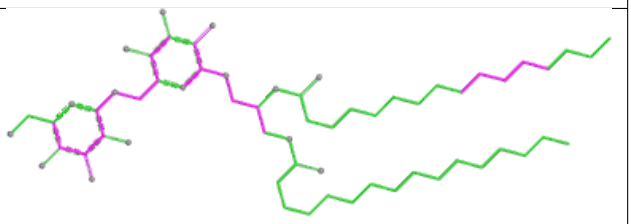


Rings

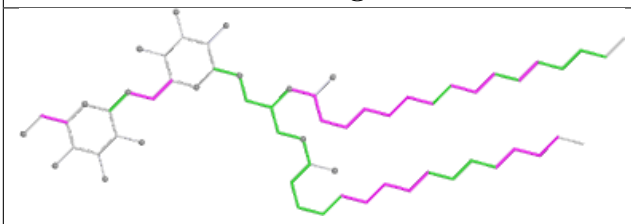
Ligand DGD C 521



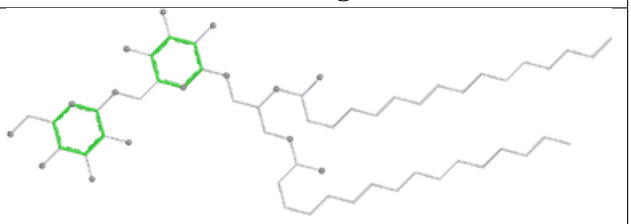
Bond lengths



Bond angles

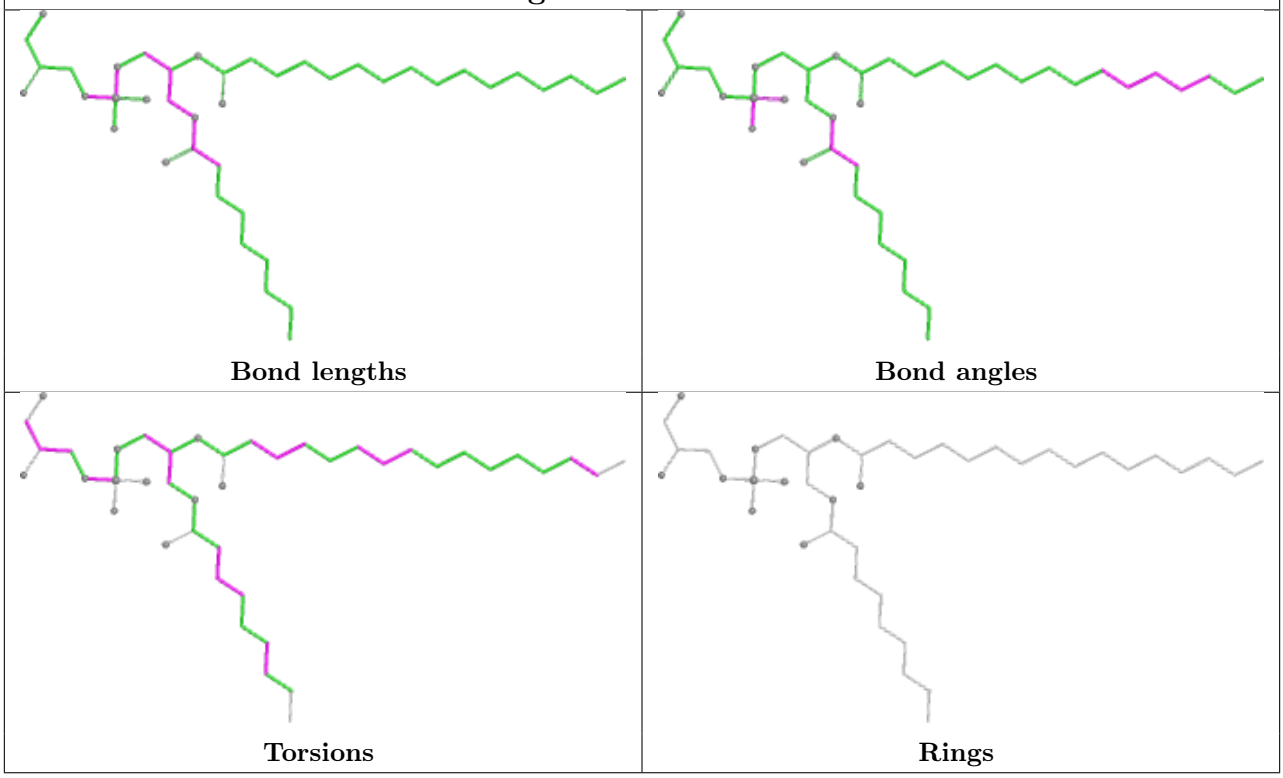


Torsions

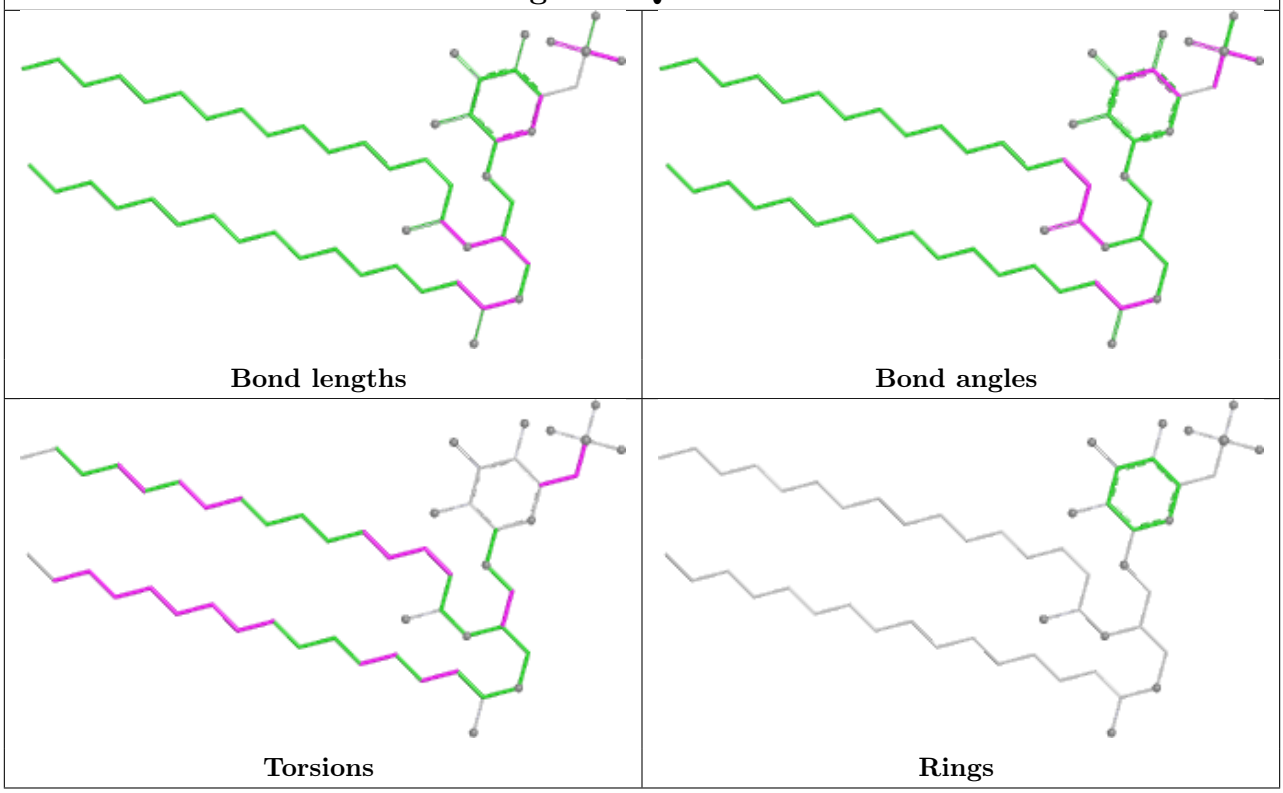


Rings

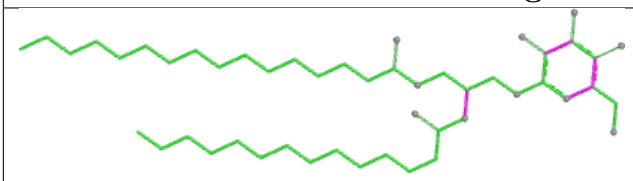
Ligand LHG a 413



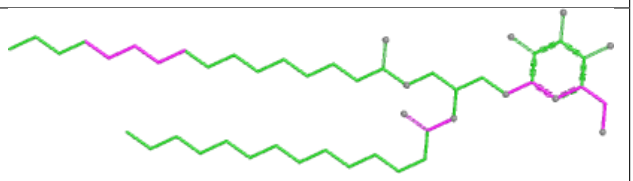
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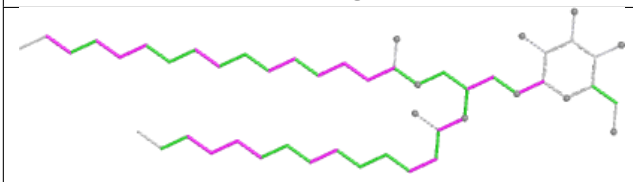
Ligand LMG c 524



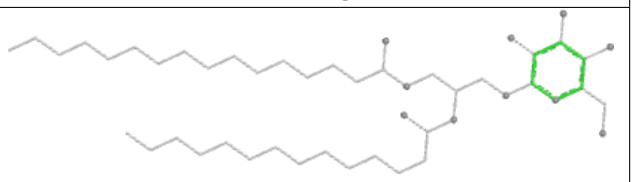
Bond lengths



Bond angles

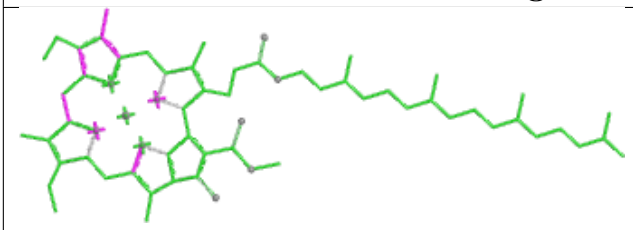


Torsions

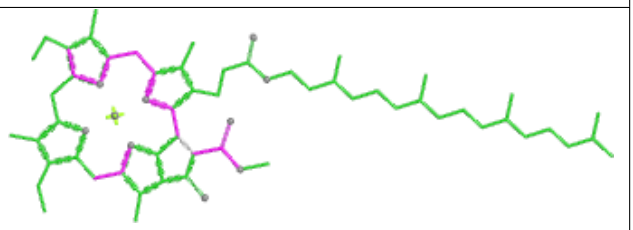


Rings

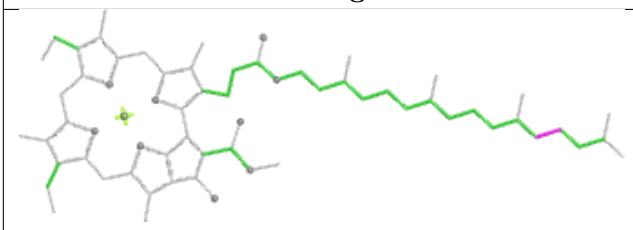
Ligand CLA b 607



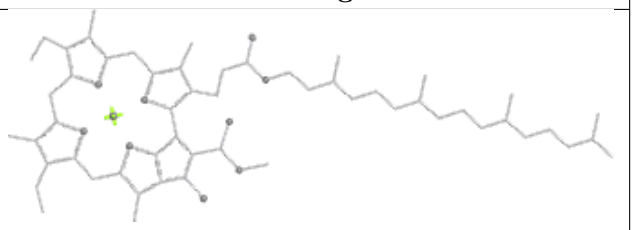
Bond lengths



Bond angles

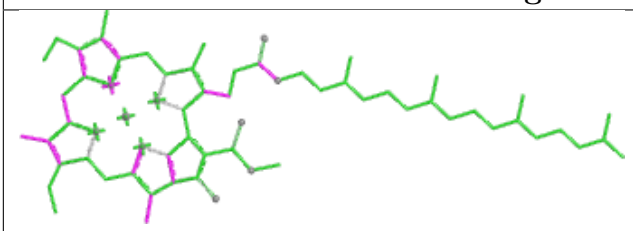


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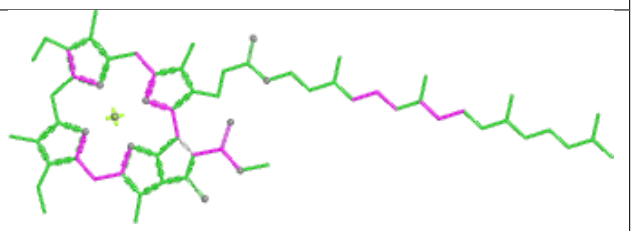


Rings

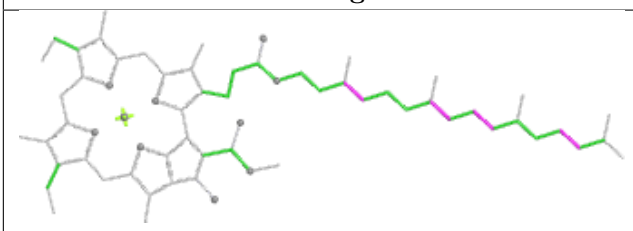
Ligand CLA C 510



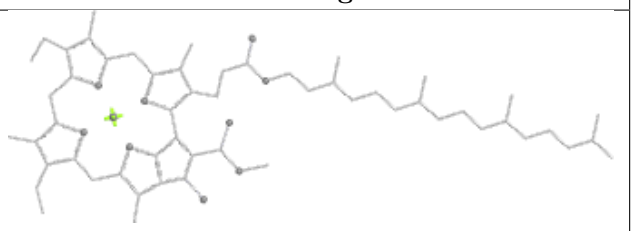
Bond lengths



Bond angles

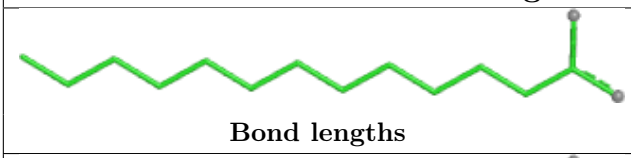


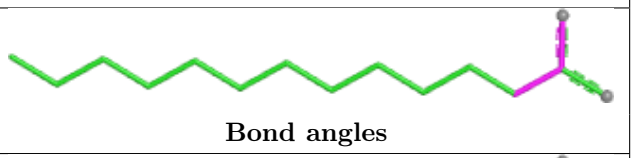
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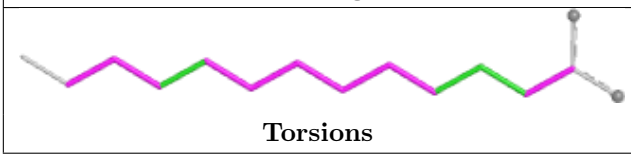


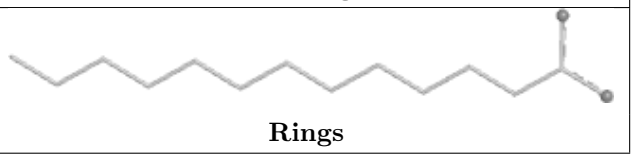
Rings

Ligand STE M 102

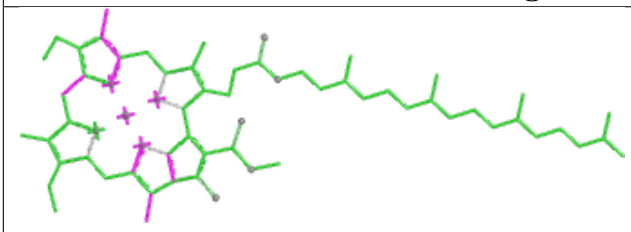

Bond lengths

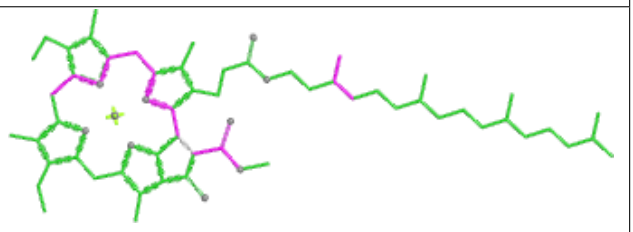

Bond angles

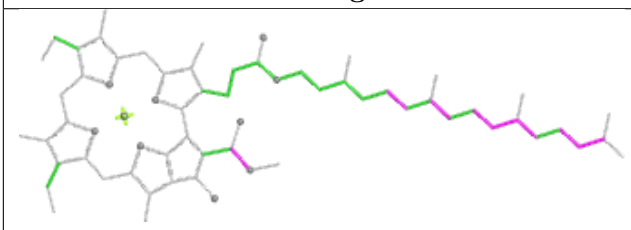

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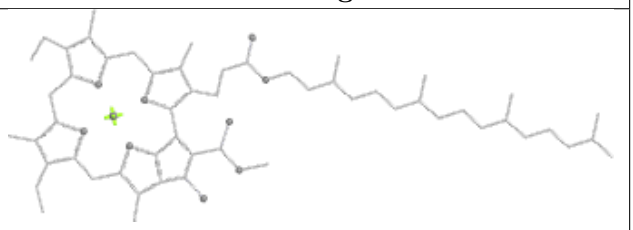

Rings

Ligand CLA D 405


Bond lengths


Bond angles

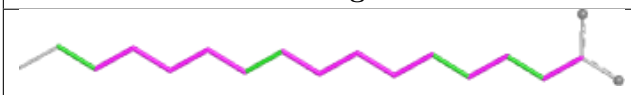

Torsions

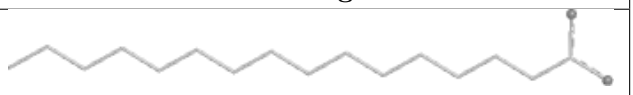

Rings

Ligand STE t 103

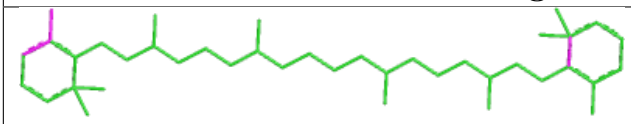

Bond lengths

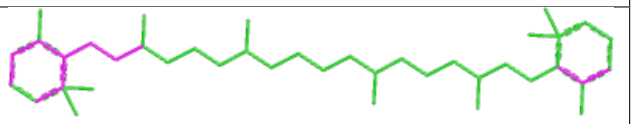

Bond angles

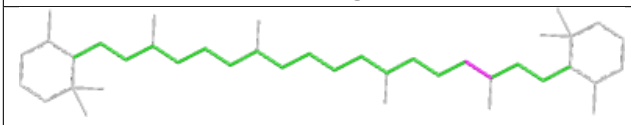

Torsions

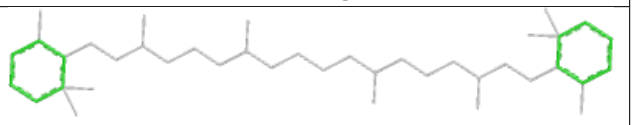

Rings

Ligand BCR t 101

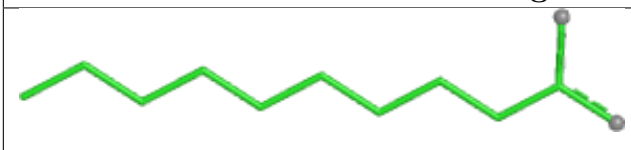

Bond lengths


Bond angles

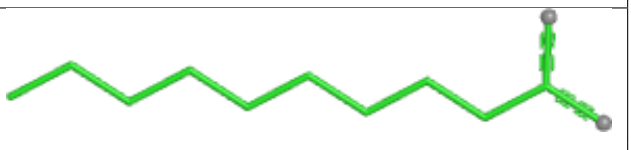

Torsions


Rings

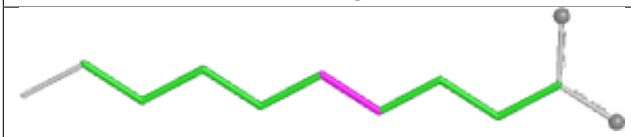
Ligand STE d 411



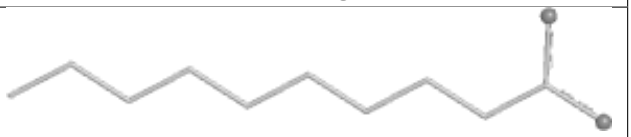
Bond lengths



Bond angles

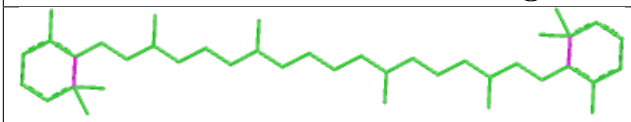


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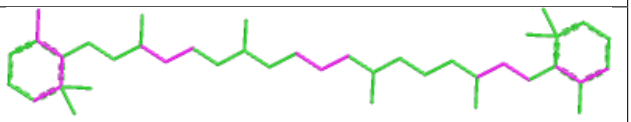


Rings

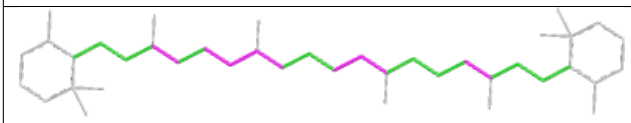
Ligand BCR C 514



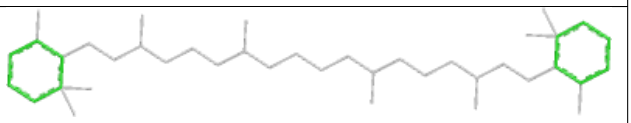
Bond lengths



Bond angles

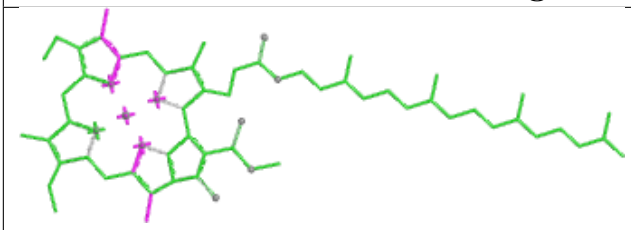


Torsions

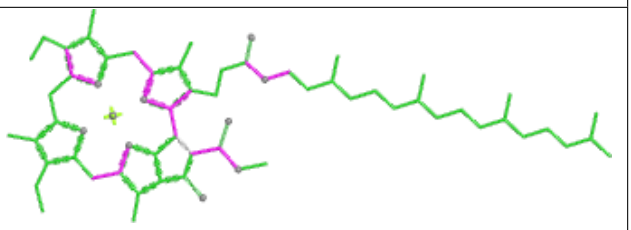


Rings

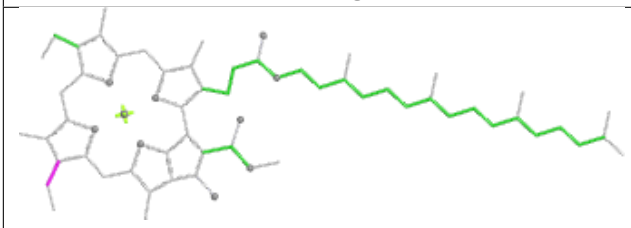
Ligand CLA a 411



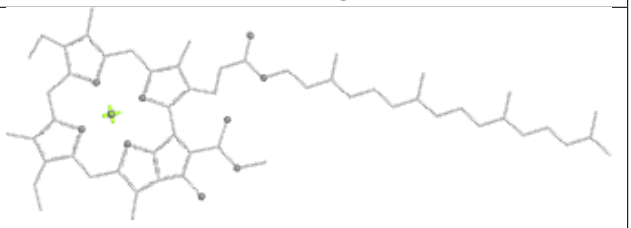
Bond lengths



Bond angles

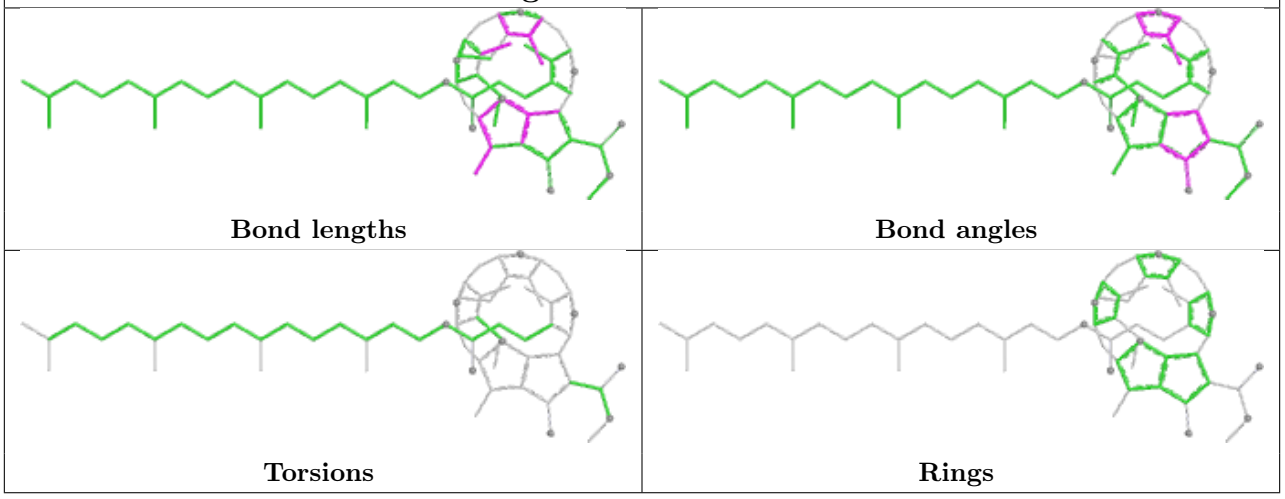


Torsions

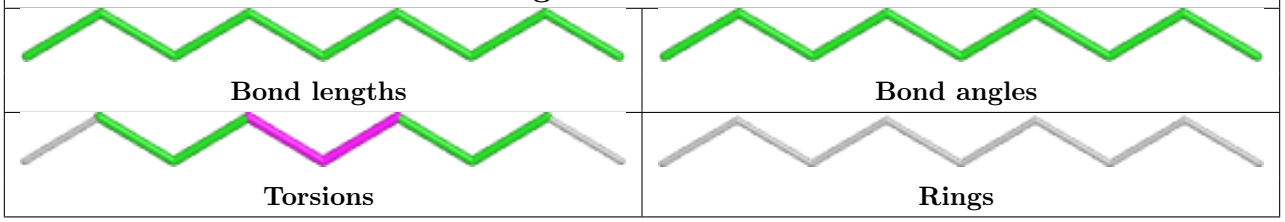


Rings

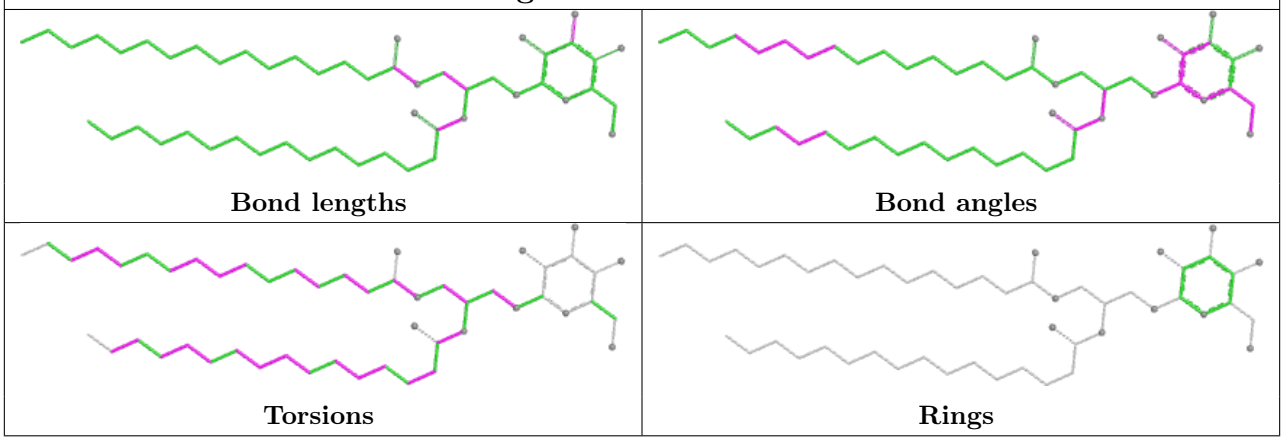
Ligand PHO D 402



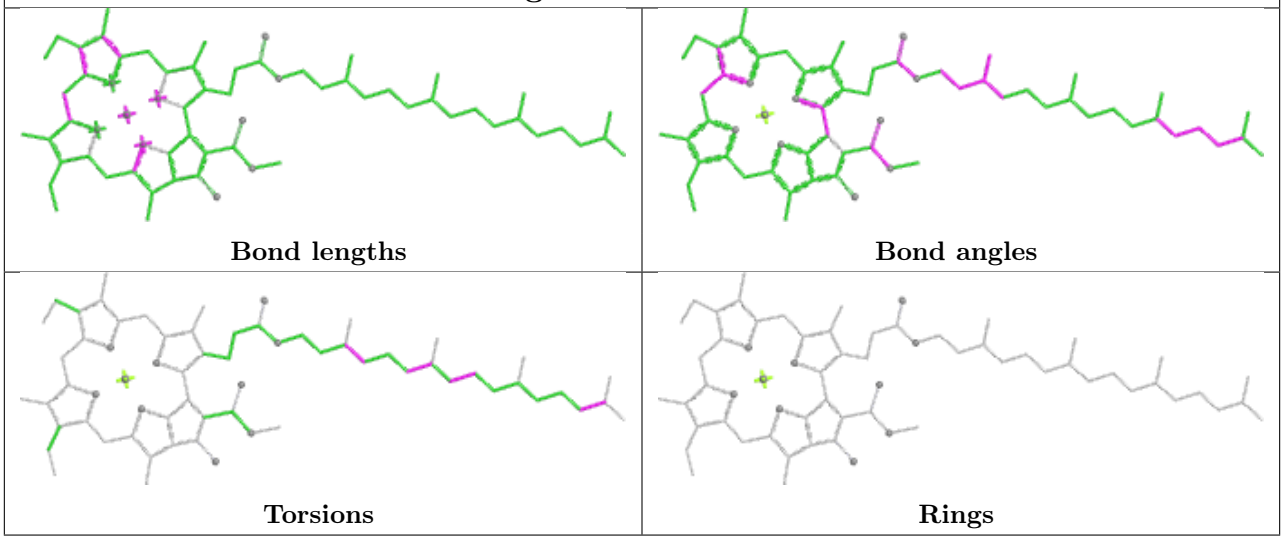
Ligand STE e 101



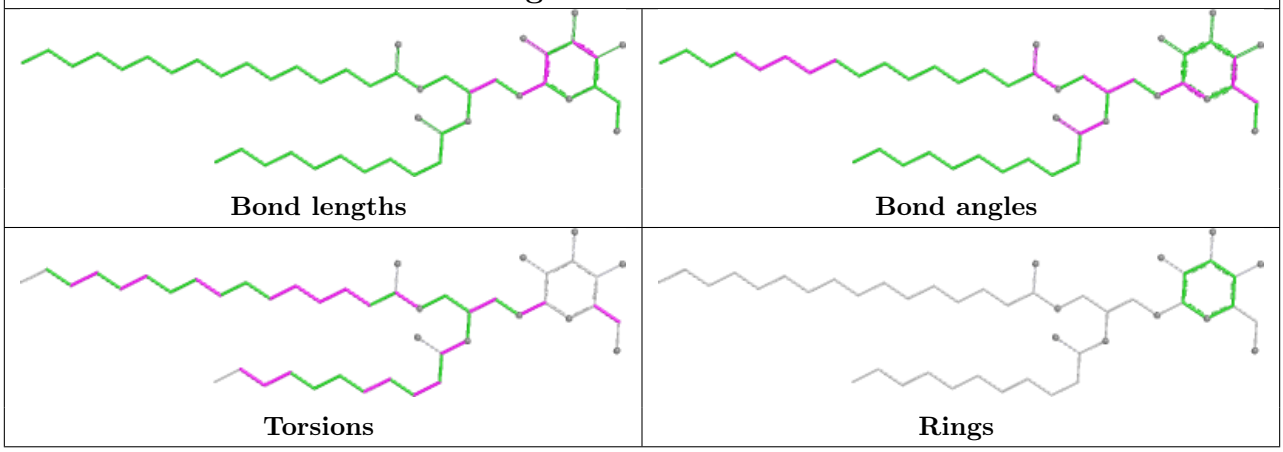
Ligand LMG M 101



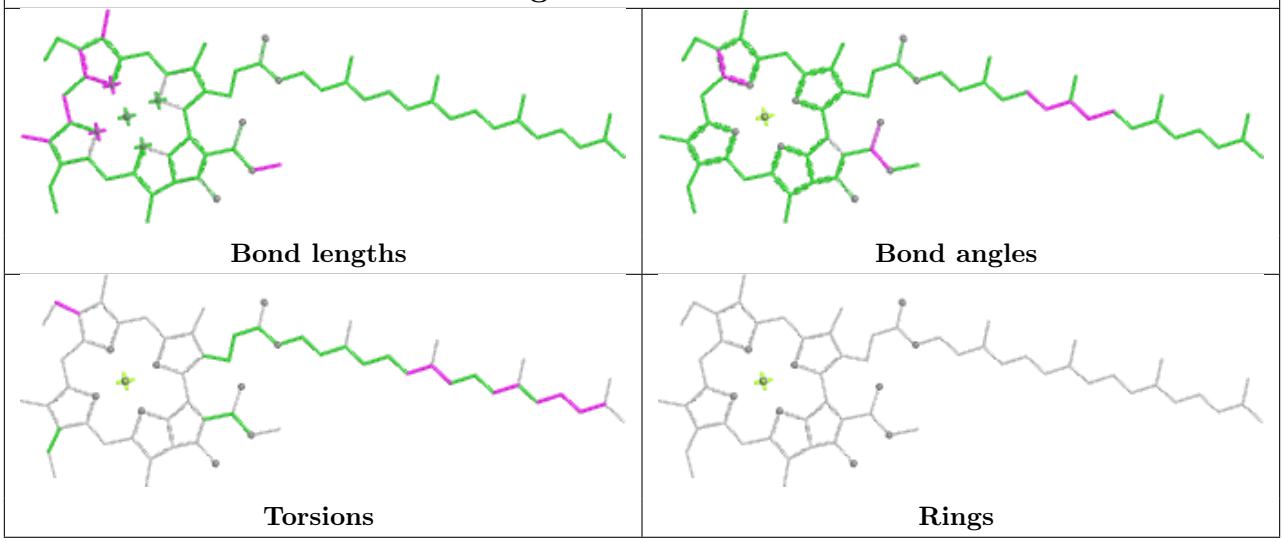
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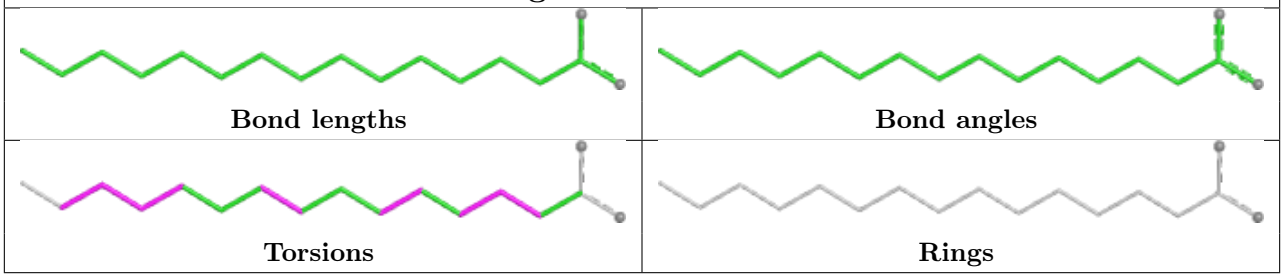
Ligand LMG c 522



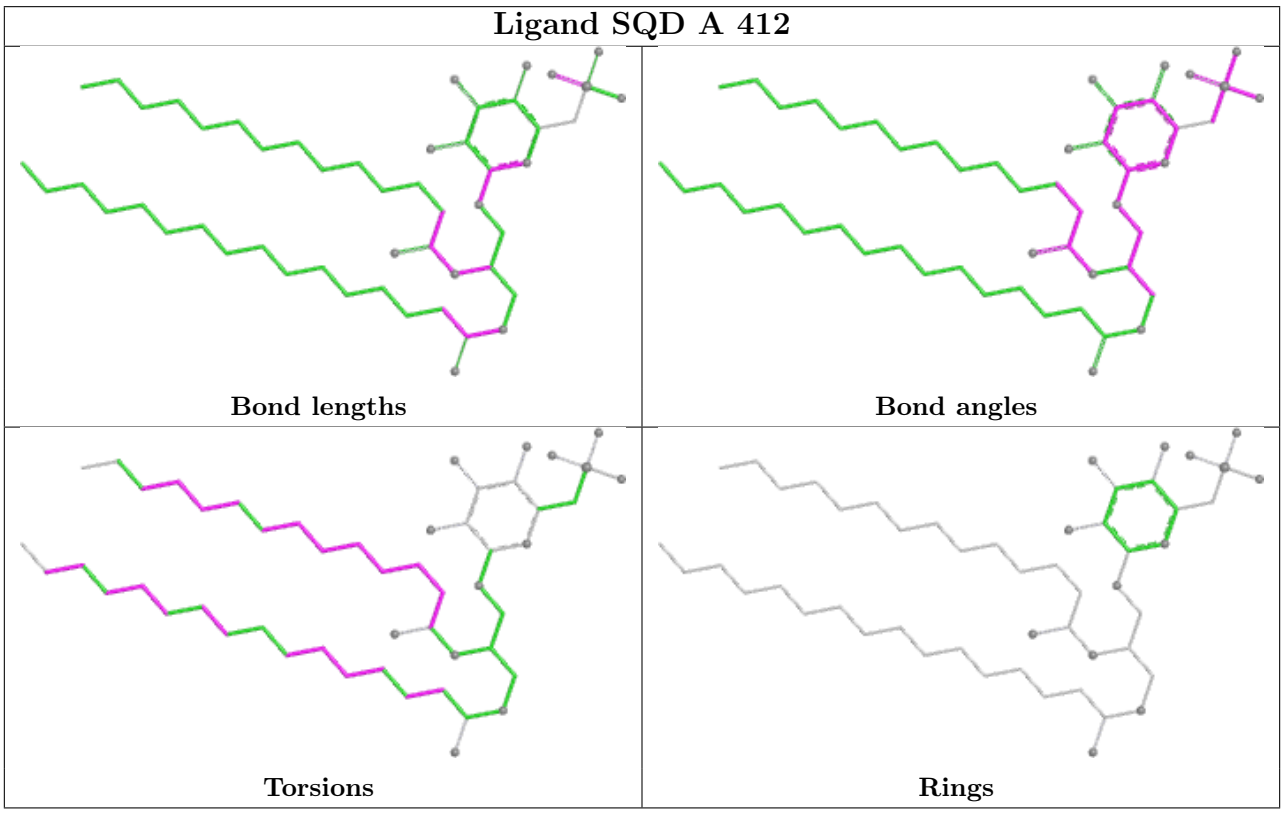
Ligand CLA c 505



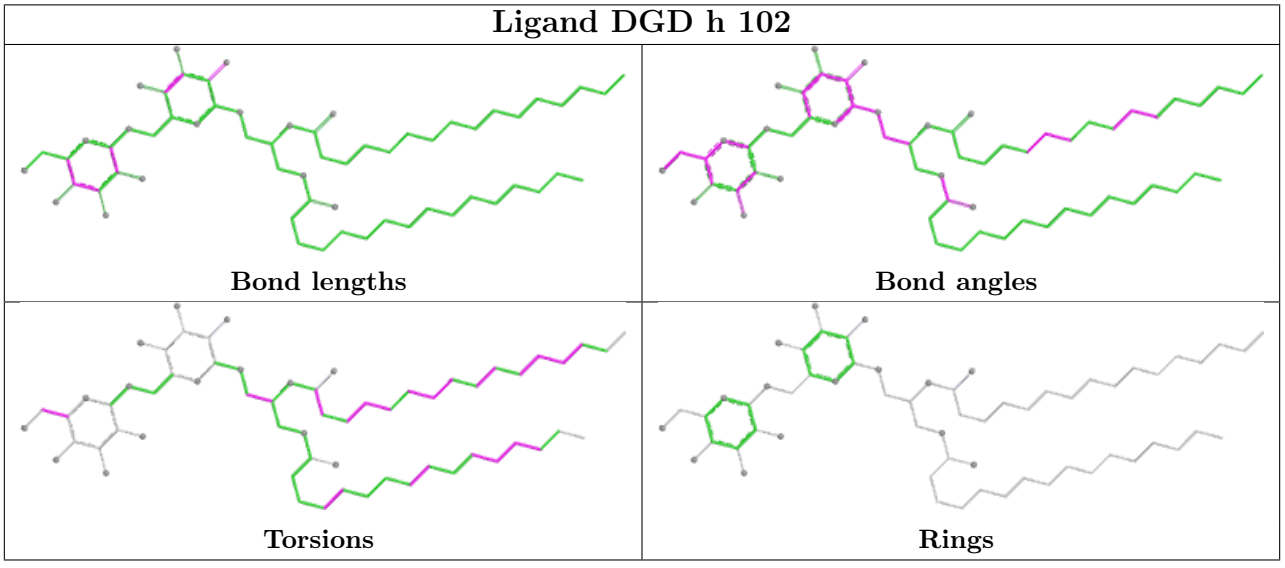
Ligand STE B 621



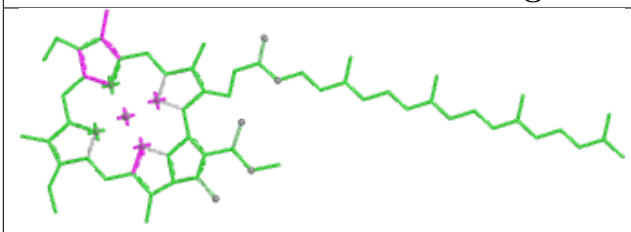
Ligand SQD A 412



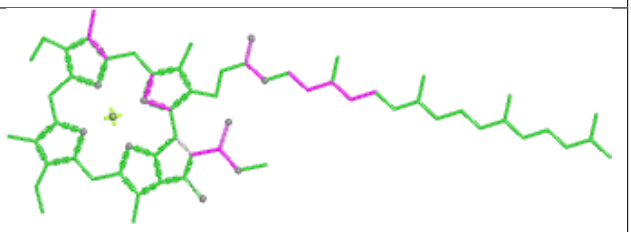
Ligand DGD h 102



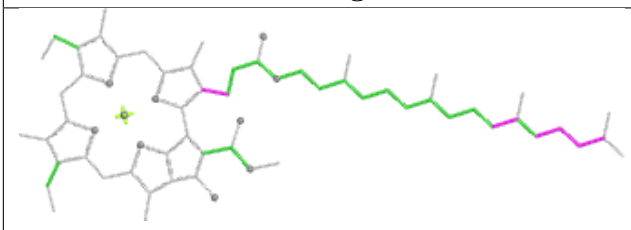
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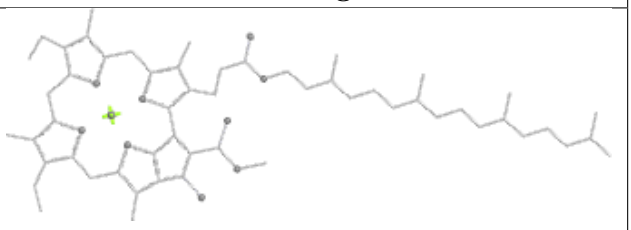
Bond lengths



Bond angles

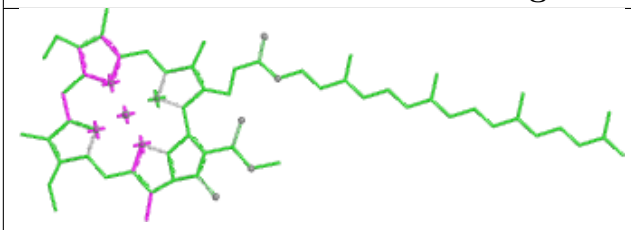


Torsions

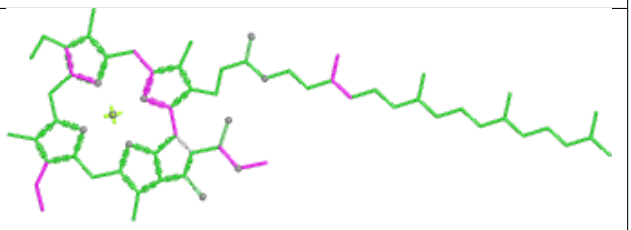


Rings

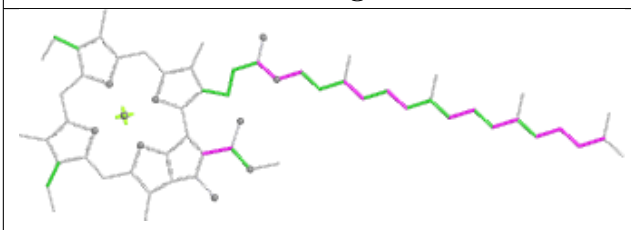
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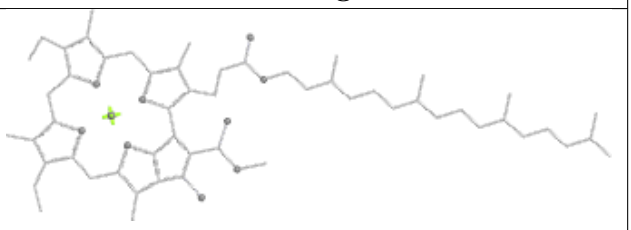
Bond lengths



Bond angles



Torsions

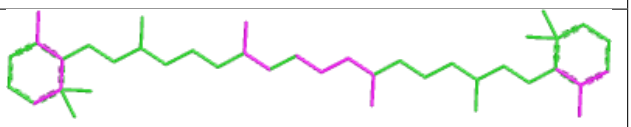


Rings

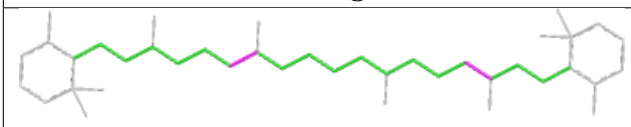
Ligand BCR C 515



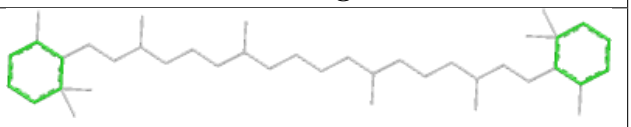
Bond lengths



Bond angles

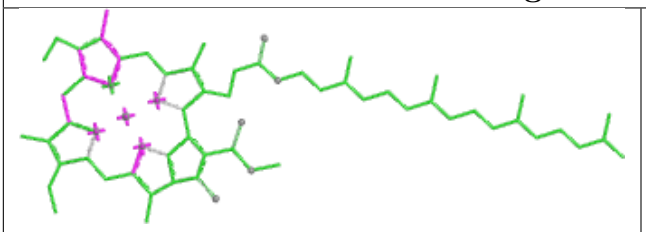


Torsions

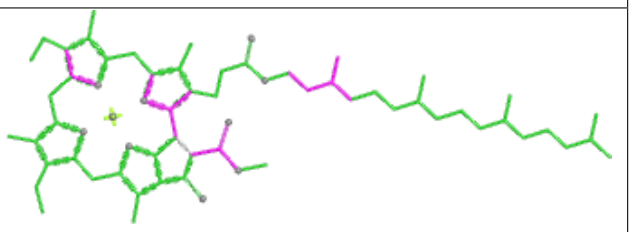


Rings

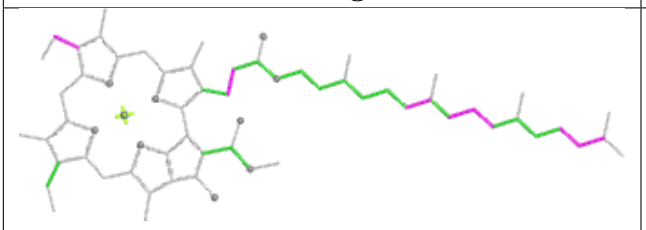
Ligand CLA B 606



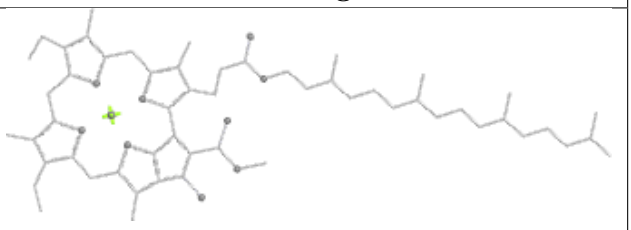
Bond lengths



Bond angles

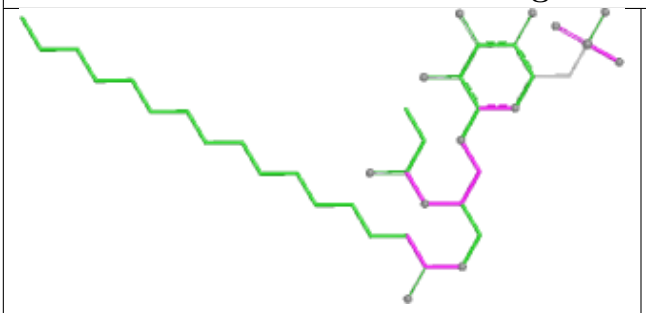


Torsions

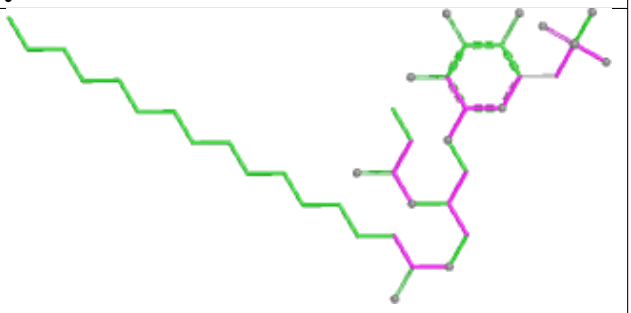


Rings

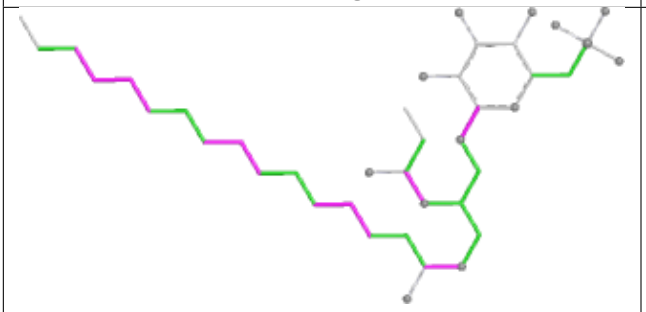
Ligand SQD f 102



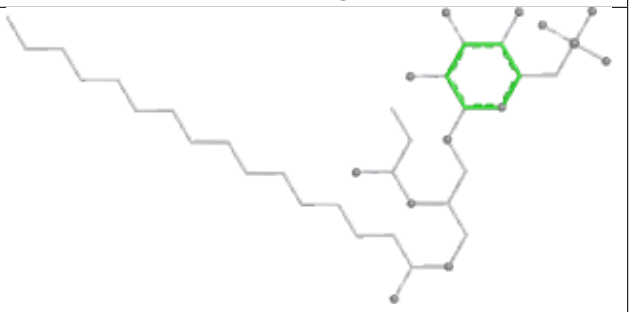
Bond lengths



Bond angles

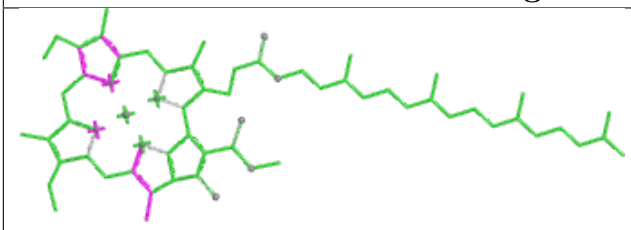


Torsions

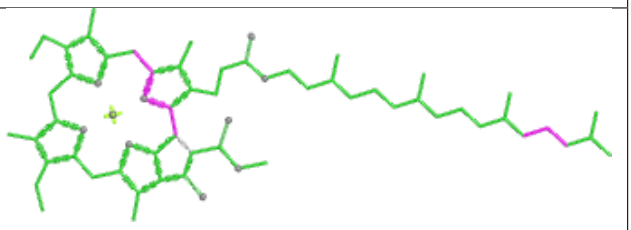


Rings

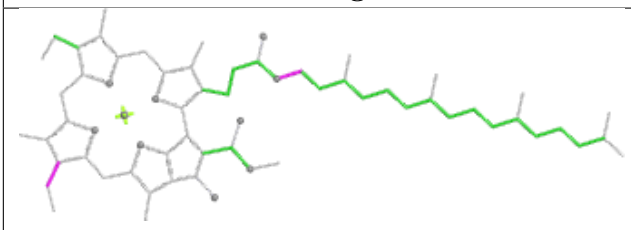
Ligand CLA A 404



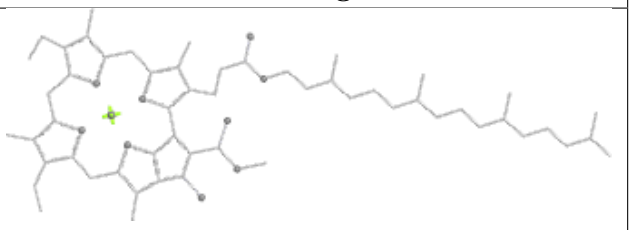
Bond lengths



Bond angles

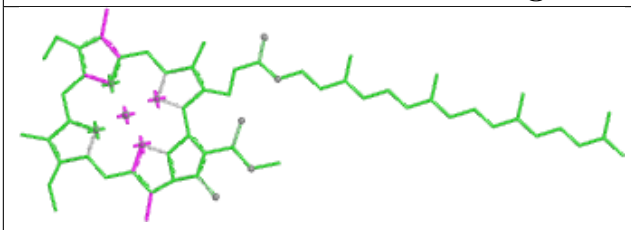


Torsions

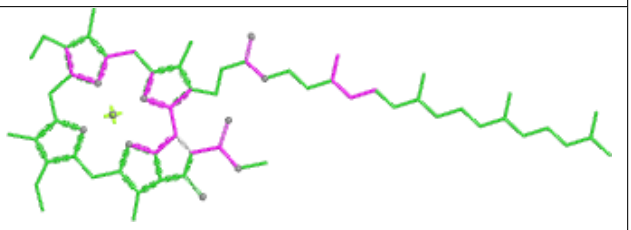


Rings

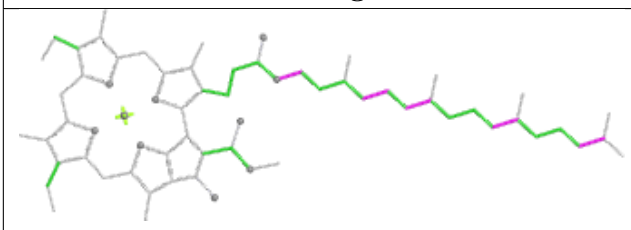
Ligand CLA d 402



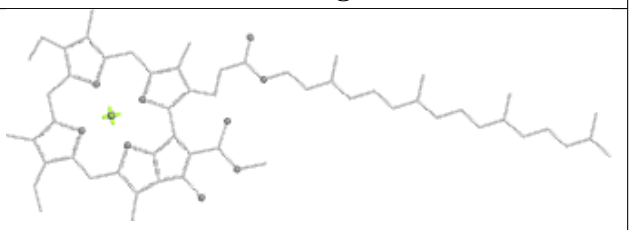
Bond lengths



Bond angles



Torsions

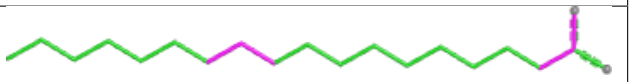


Rings

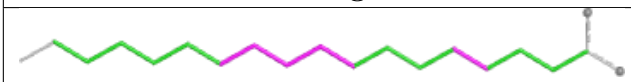
Ligand STE D 413



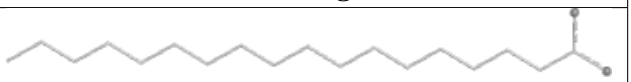
Bond lengths



Bond angles

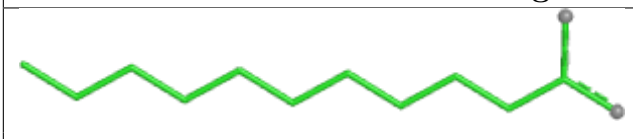


Torsions

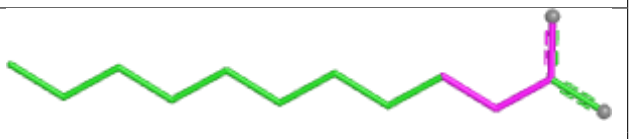


Rings

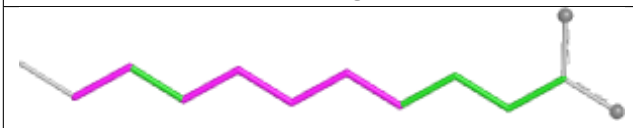
Ligand STE e 104



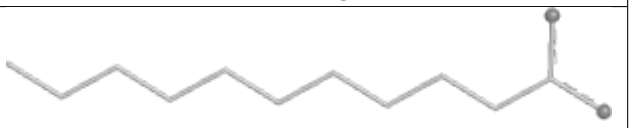
Bond lengths



Bond angles

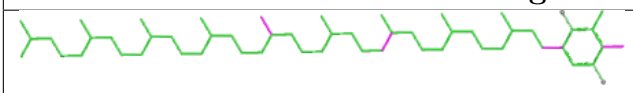


Torsions



Rings

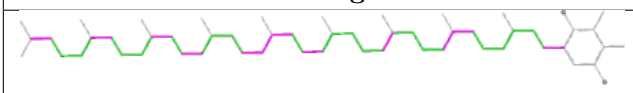
Ligand PL9 A 409



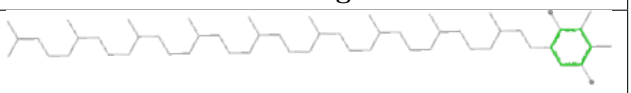
Bond lengths



Bond angles

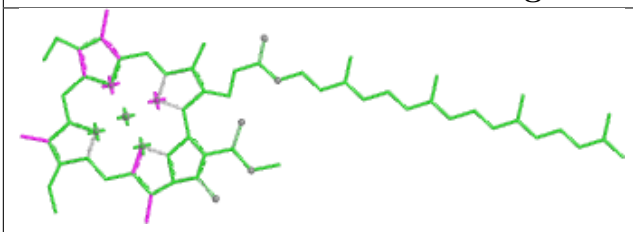


Torsions

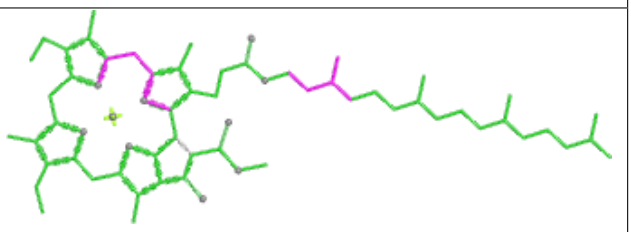


Rings

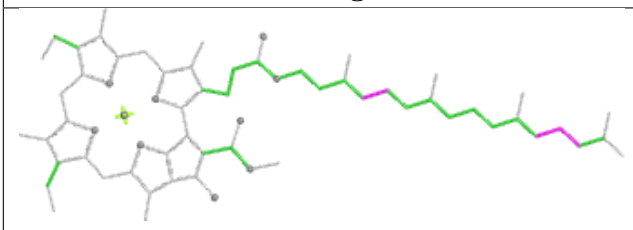
Ligand CLA B 607



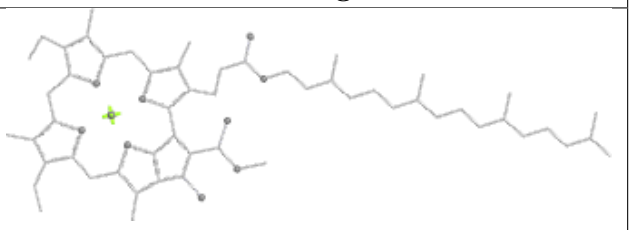
Bond lengths



Bond angles

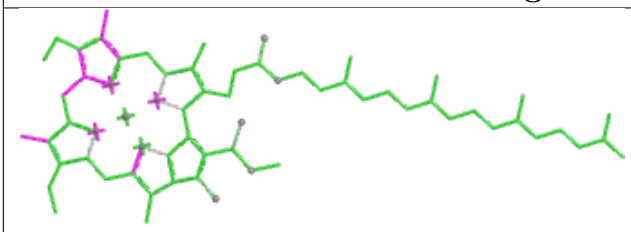


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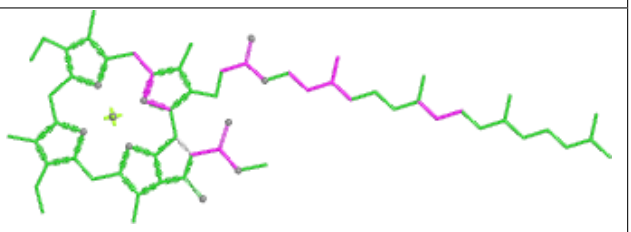


Rings

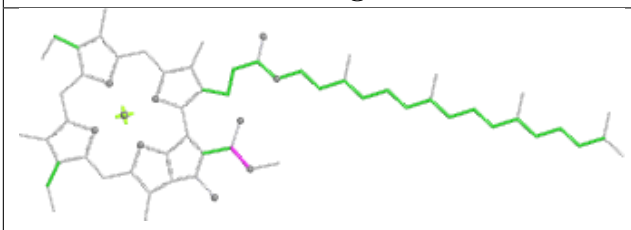
Ligand CLA C 511



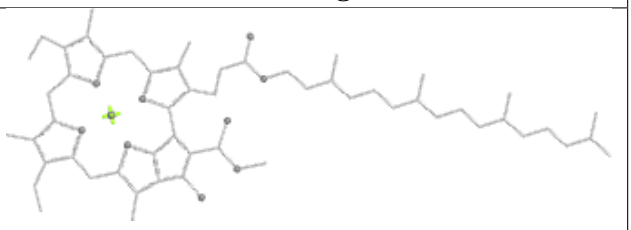
Bond lengths



Bond angles

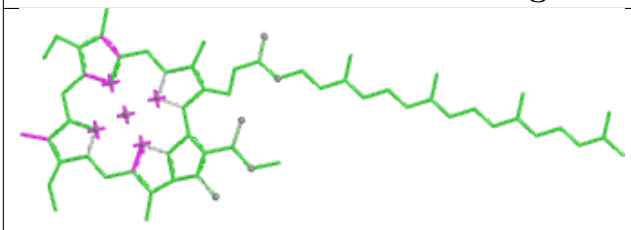


Torsions

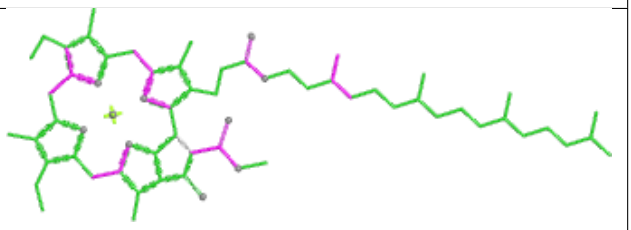


Rings

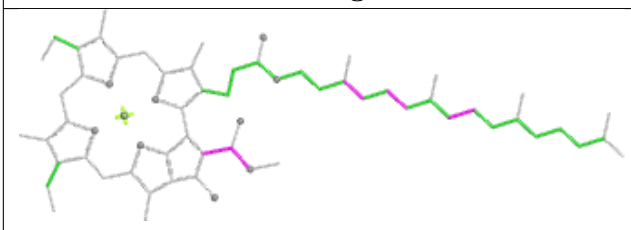
Ligand CLA c 507



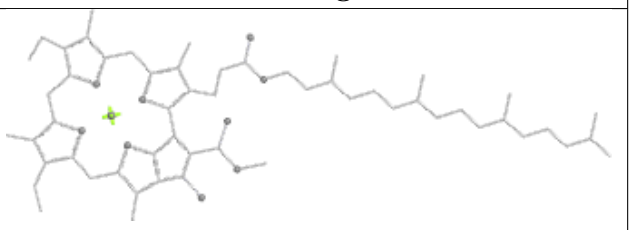
Bond lengths



Bond angles

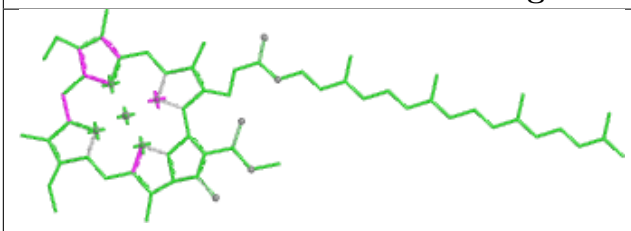


Torsions

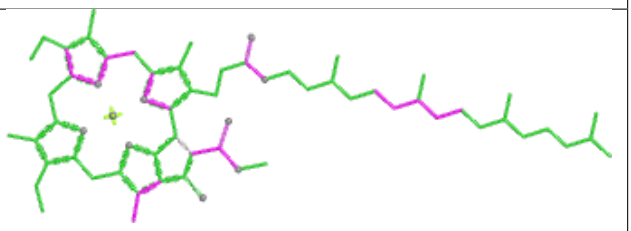


Rings

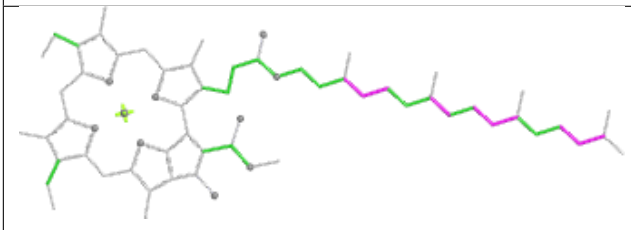
Ligand CLA b 603



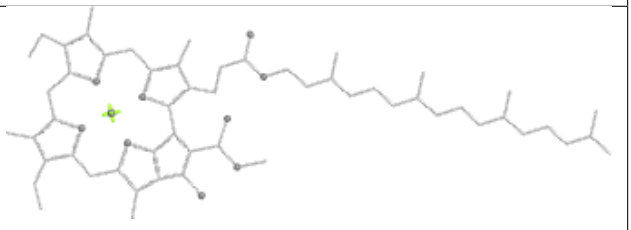
Bond lengths



Bond angles

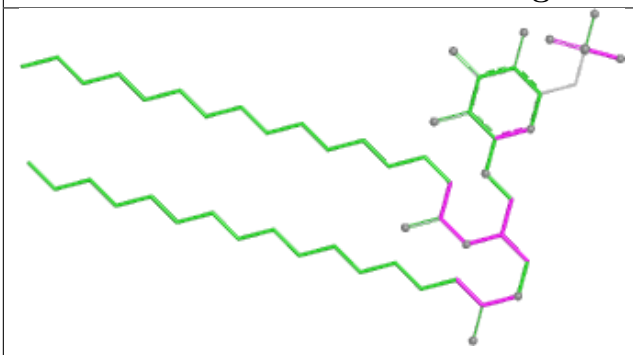


Torsions

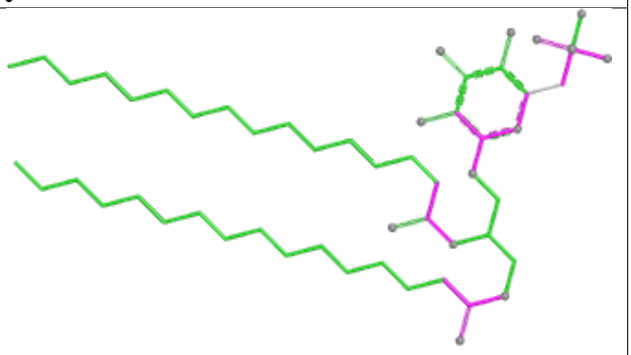


Rings

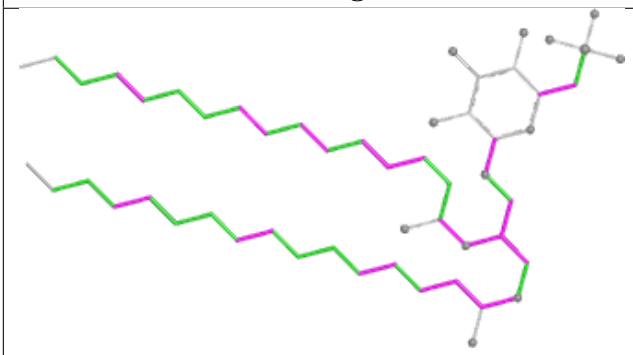
Ligand SQD l 101



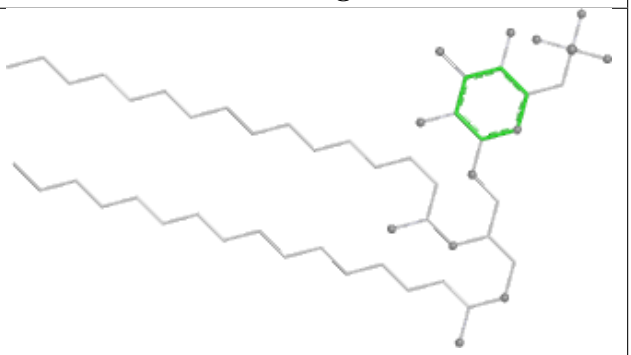
Bond lengths



Bond angles

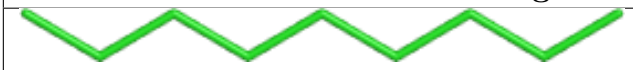


Torsions

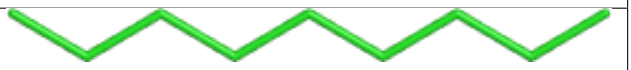


Rings

Ligand STE z 101



Bond lengths



Bond angles

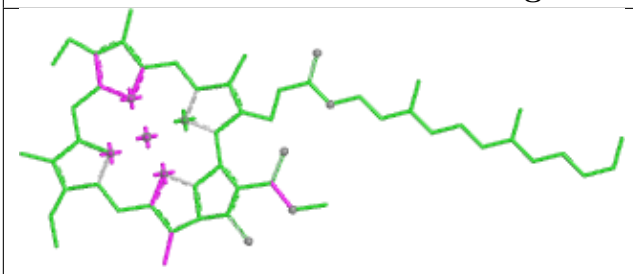


Torsions

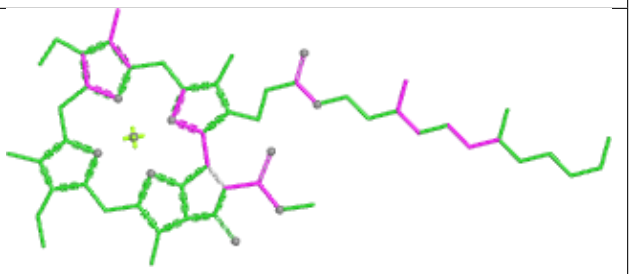


Rings

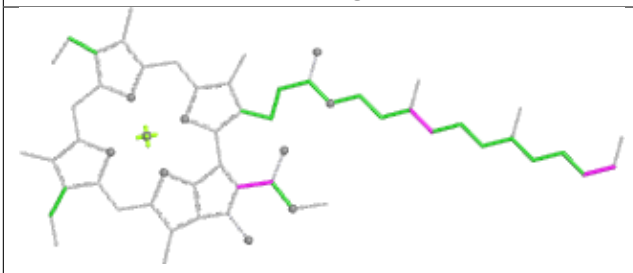
Ligand CLA C 504



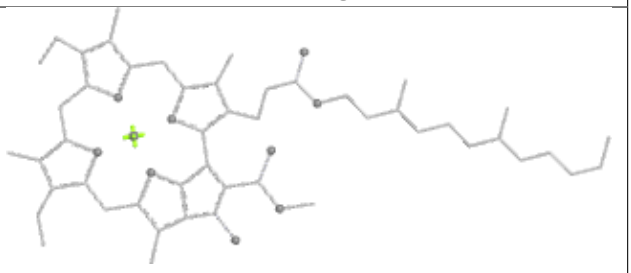
Bond lengths



Bond angles

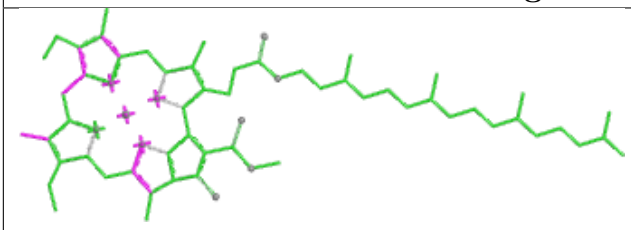


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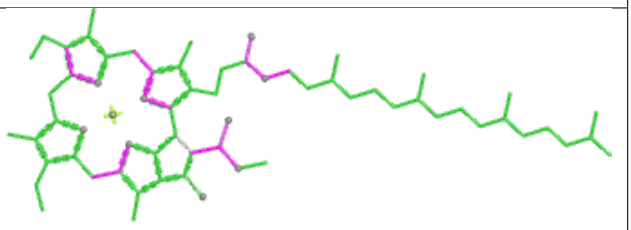


Rings

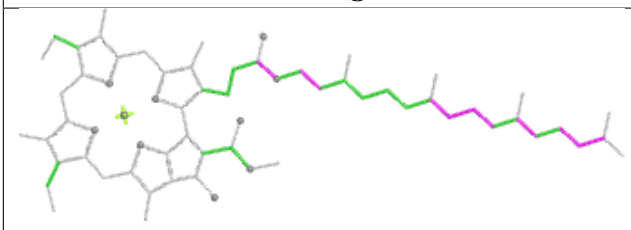
Ligand CLA C 513



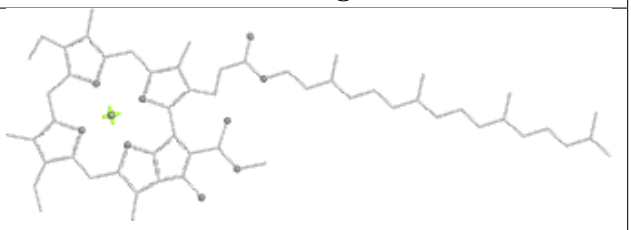
Bond lengths



Bond angles

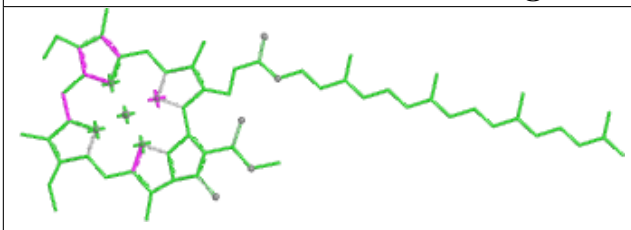


Torsions

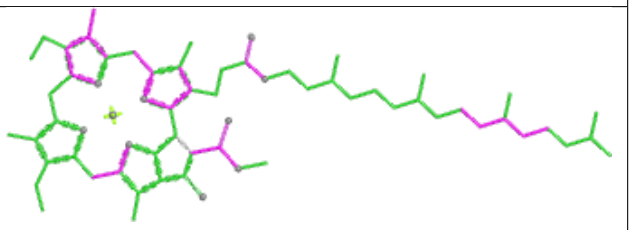


Rings

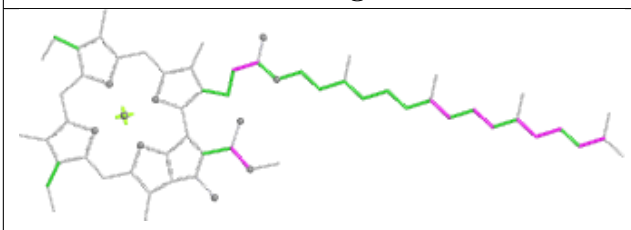
Ligand CLA B 612



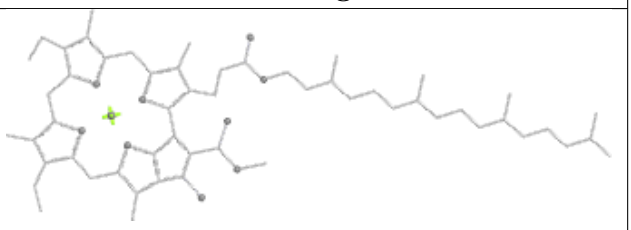
Bond lengths



Bond angles

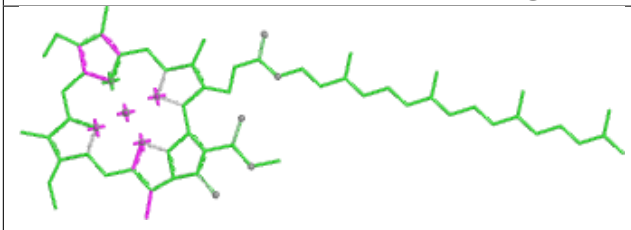


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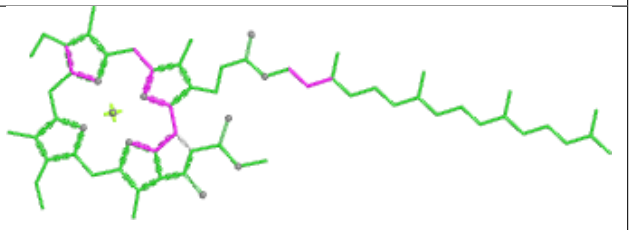


Rings

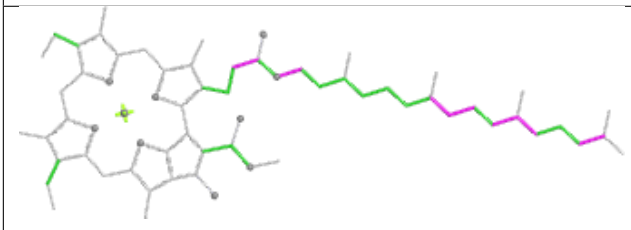
Ligand CLA B 613



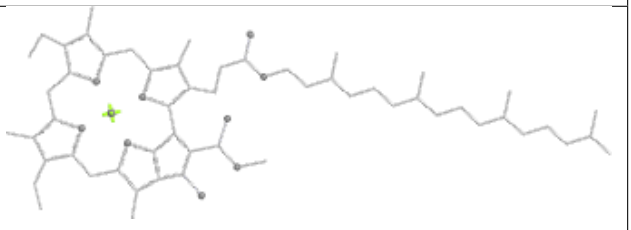
Bond lengths



Bond angles

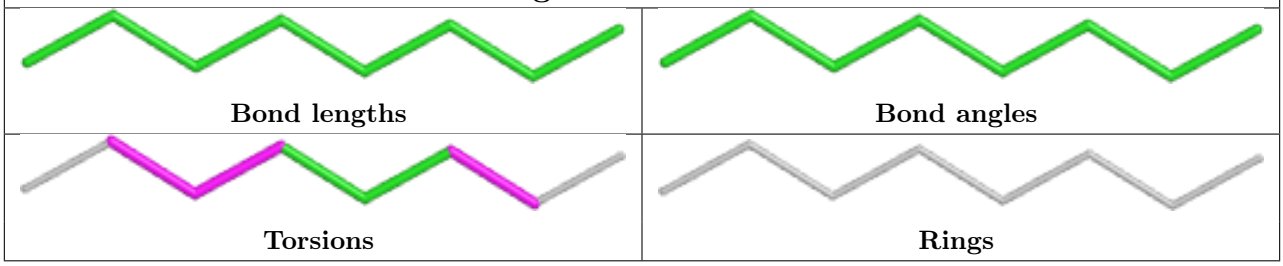


Torsions

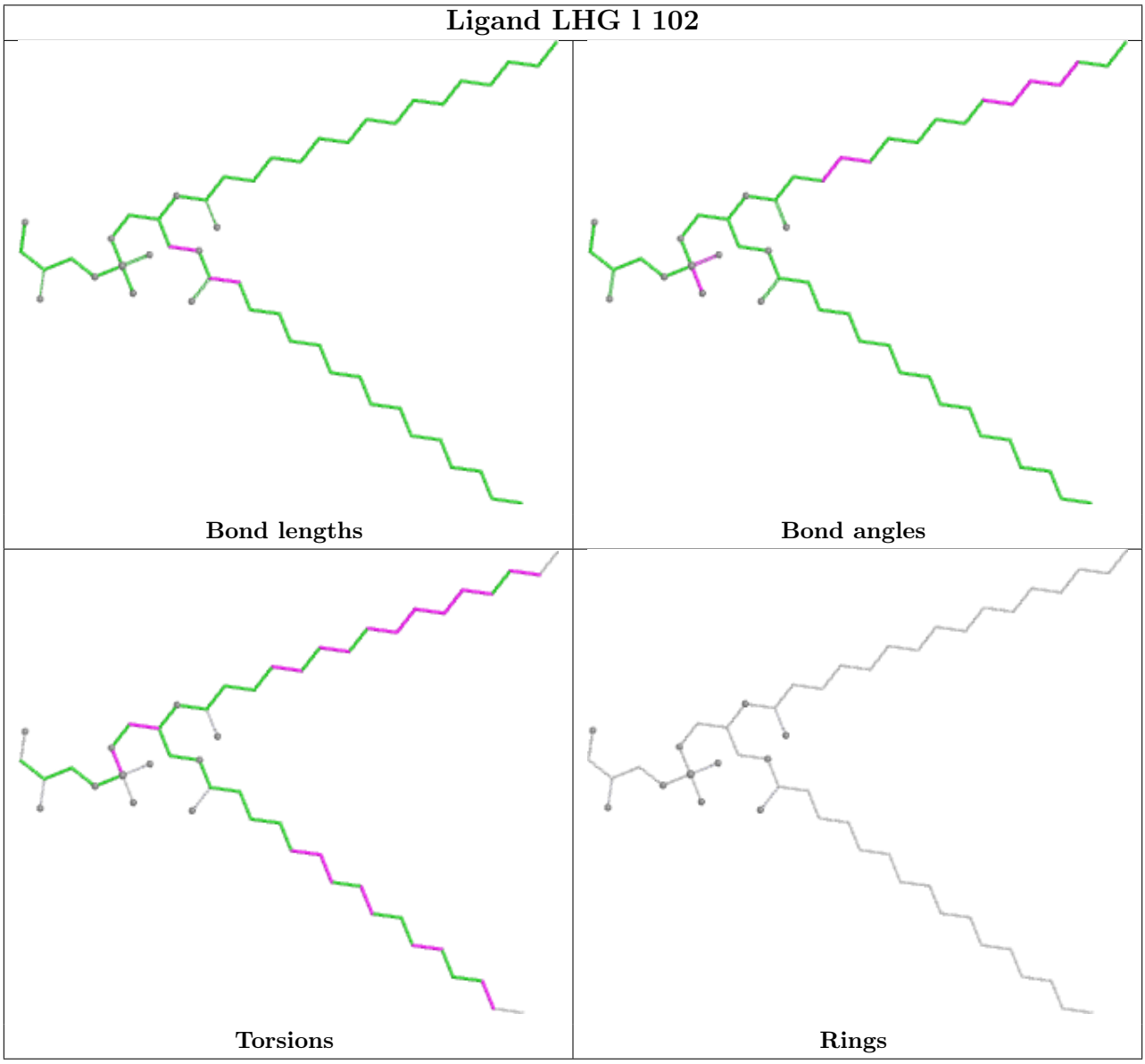


Rings

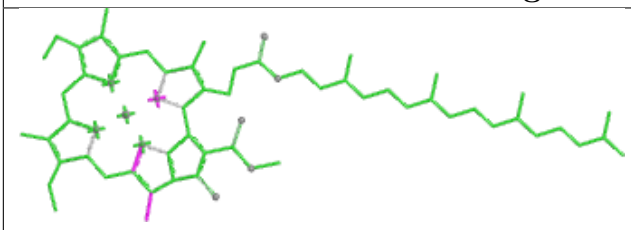
Ligand STE e 102



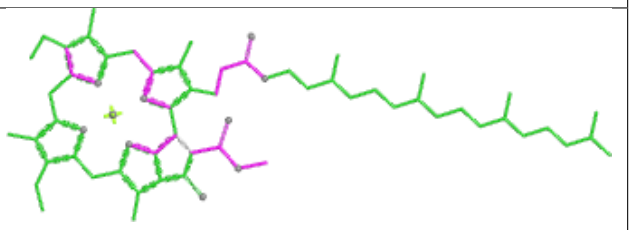
Ligand LHG l 102



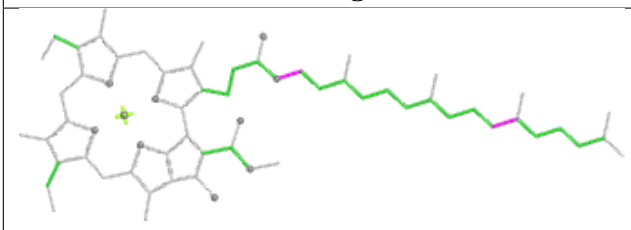
Ligand CLA D 404



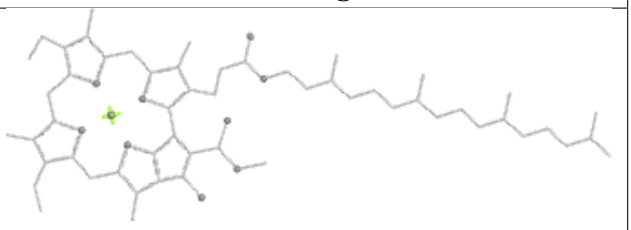
Bond lengths



Bond angles

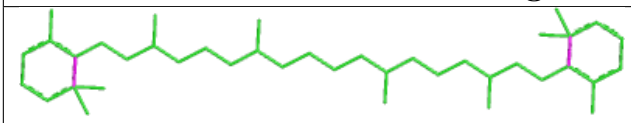


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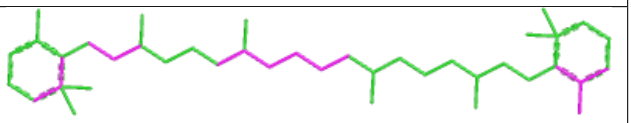


Rings

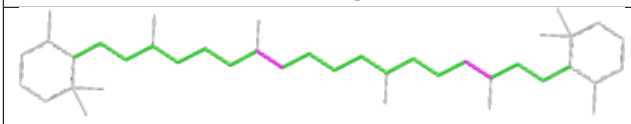
Ligand BCR b 618



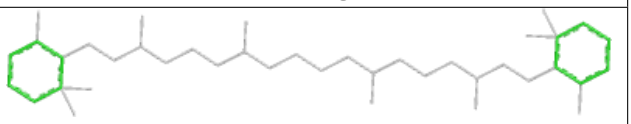
Bond lengths



Bond angles

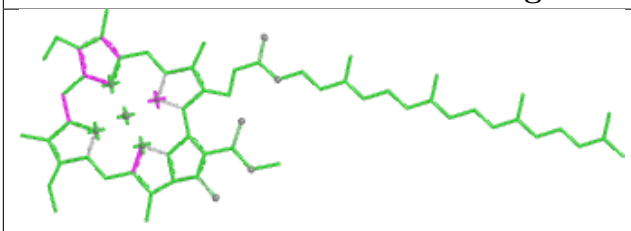


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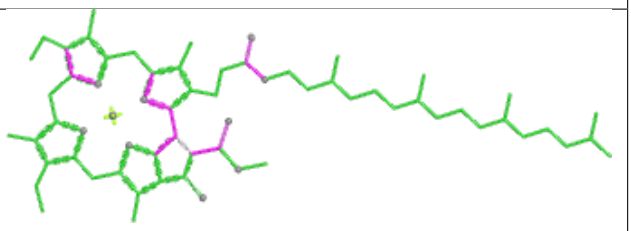


Rings

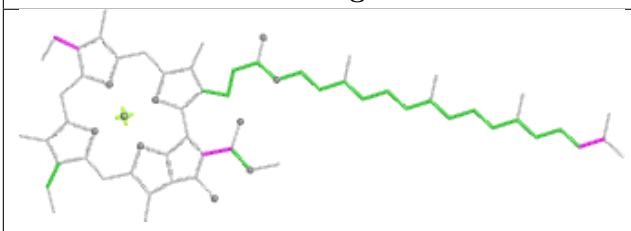
Ligand CLA C 502



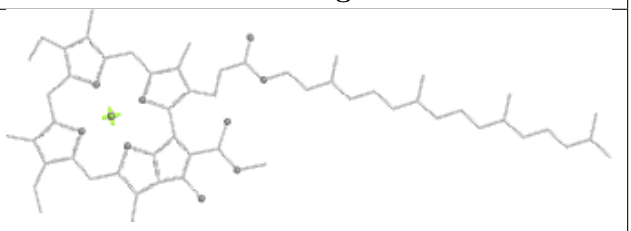
Bond lengths



Bond angles

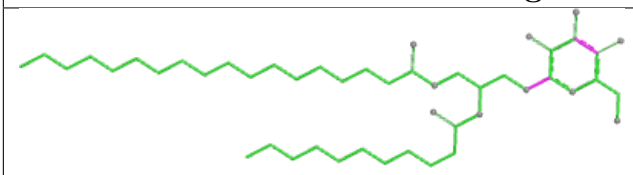


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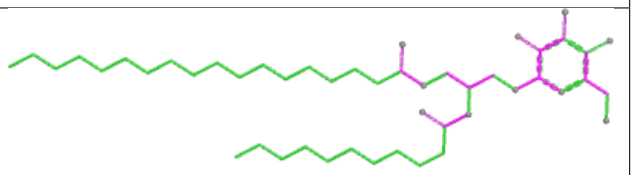


Rings

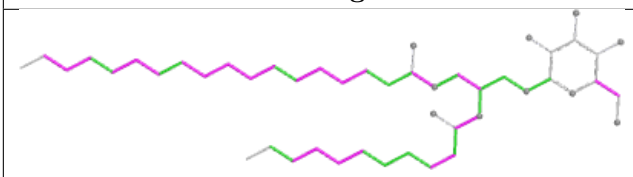
Ligand LMG c 523



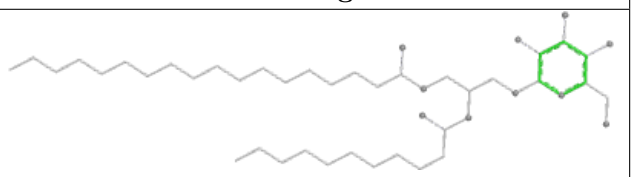
Bond lengths



Bond angles

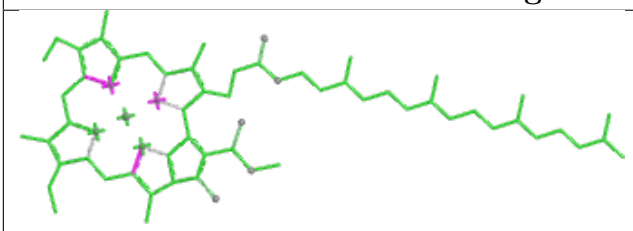


Torsions

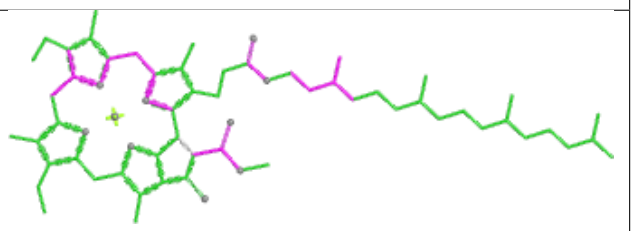


Rings

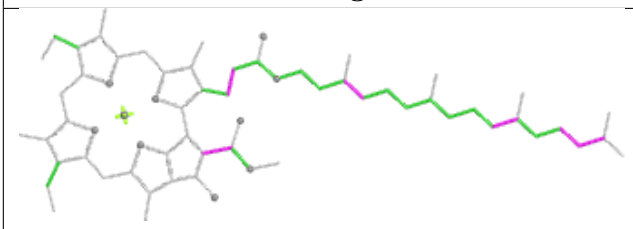
Ligand CLA B 614



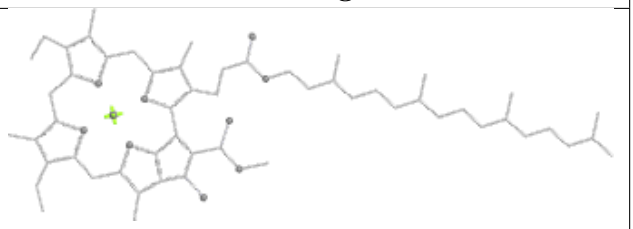
Bond lengths



Bond angles

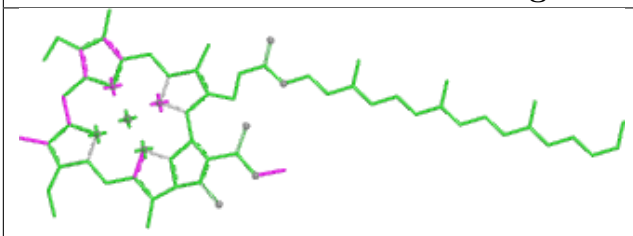


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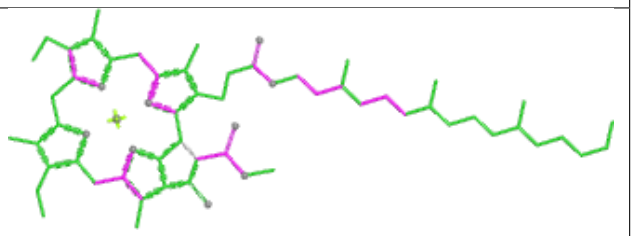


Rings

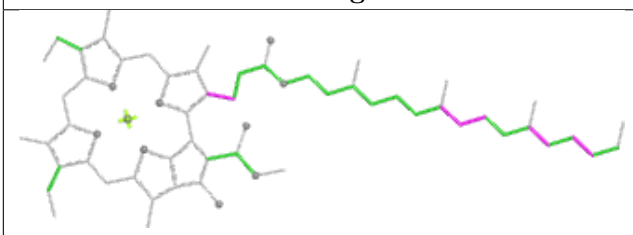
Ligand CLA c 508



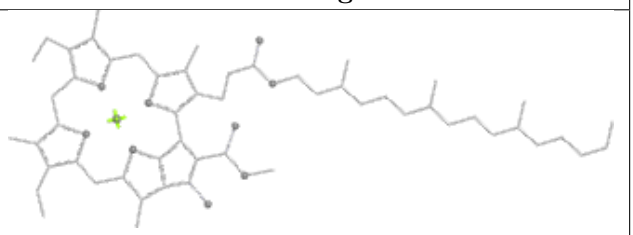
Bond lengths



Bond angles

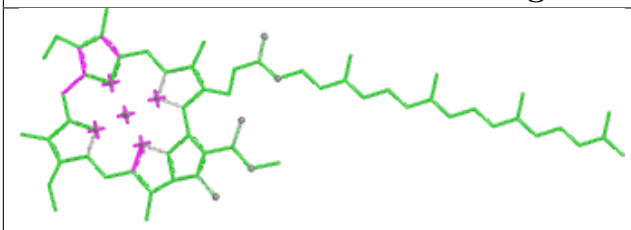


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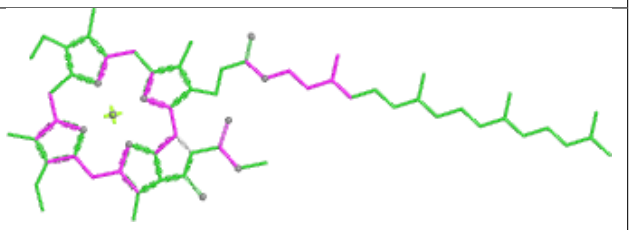


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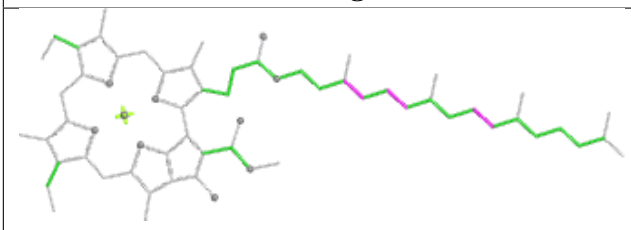
Ligand CLA b 604



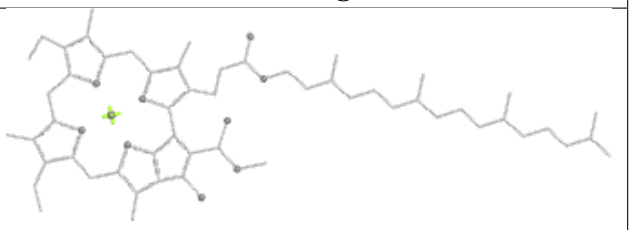
Bond lengths



Bond angles

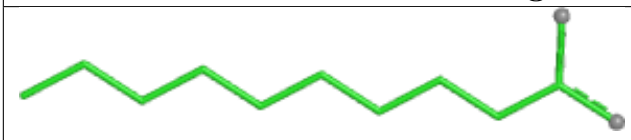


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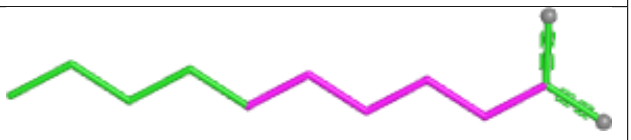


Rings

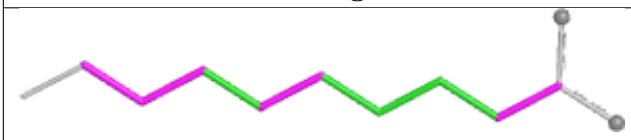
Ligand STE C 525



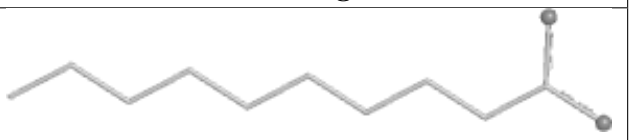
Bond lengths



Bond angles



Torsions

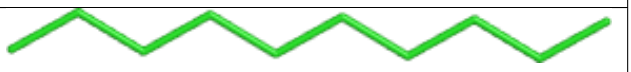


Rings

Ligand STE a 416



Bond lengths



Bond angles

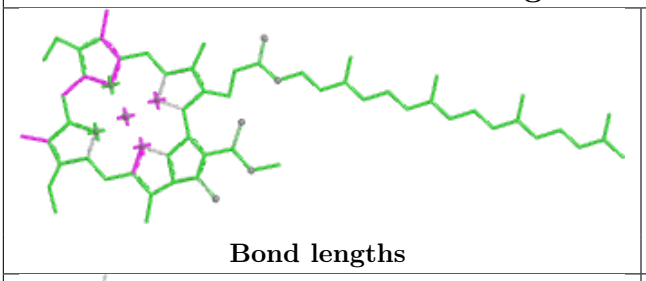


Torsions

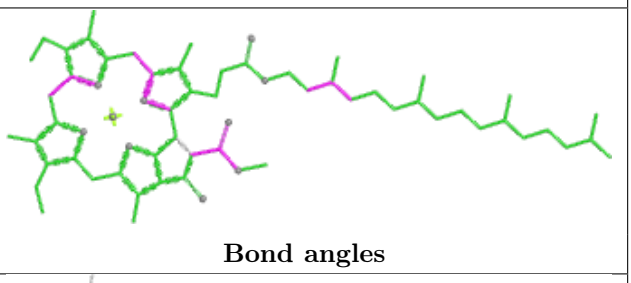


Rings

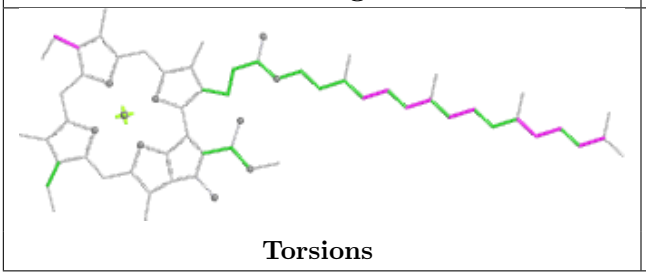
Ligand CLA B 615



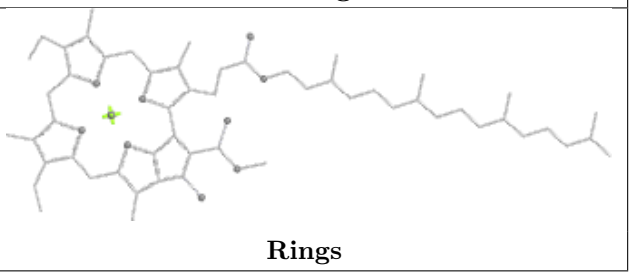
Bond lengths



Bond angles

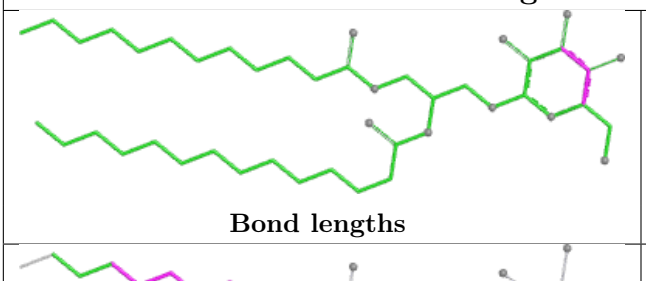


Torsions

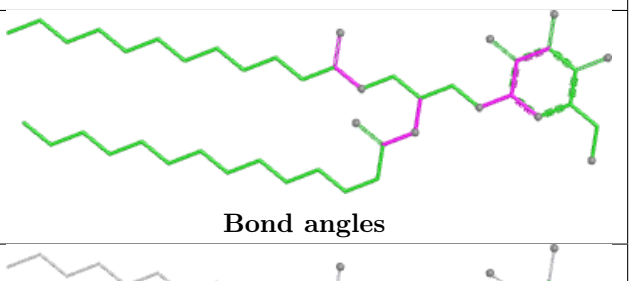


Rings

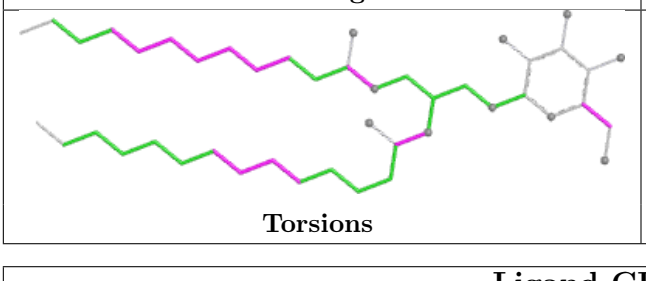
Ligand LMG B 620



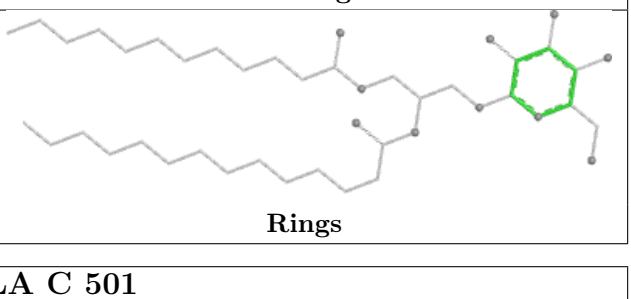
Bond lengths



Bond angles

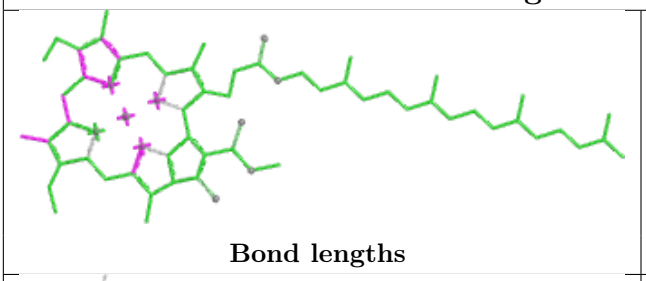


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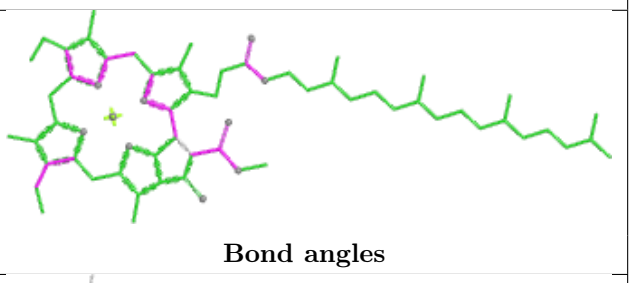


Rings

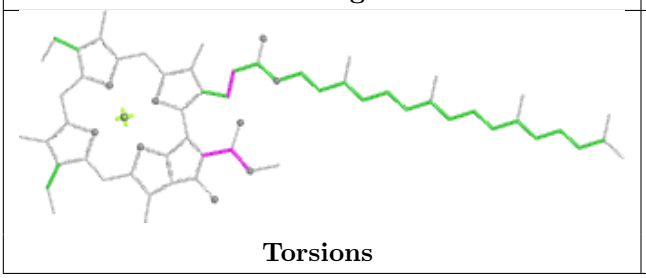
Ligand CLA C 501



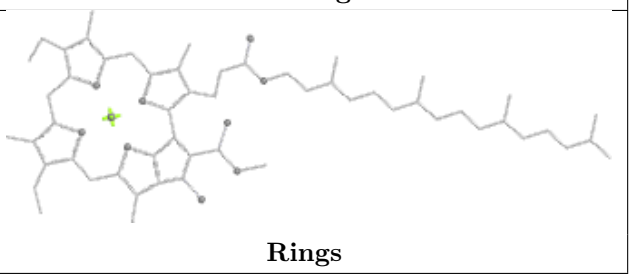
Bond lengths



Bond angles

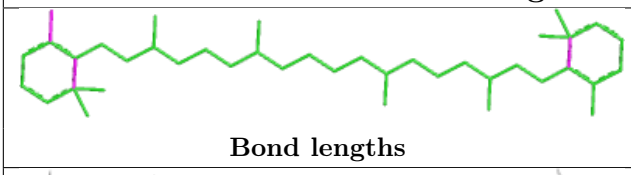


Torsions

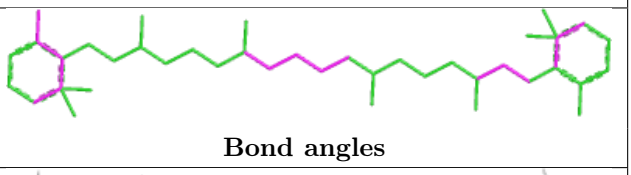


Rings

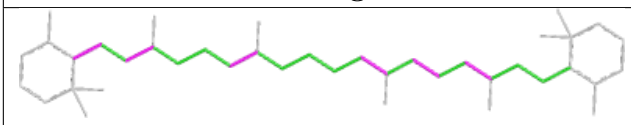
Ligand BCR c 514



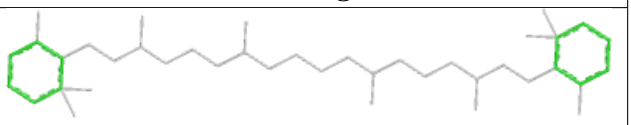
Bond lengths



Bond angles

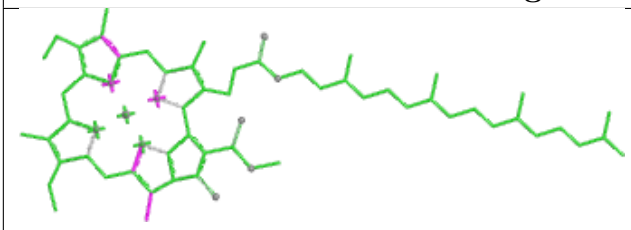


Torsions

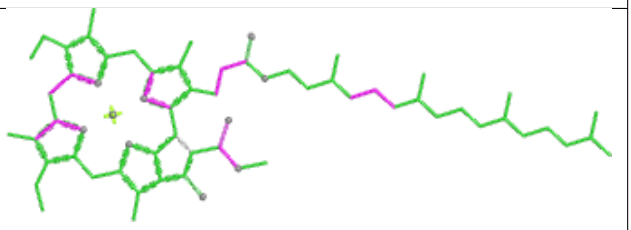


Rings

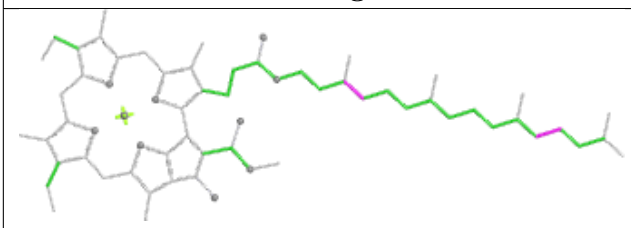
Ligand CLA B 609



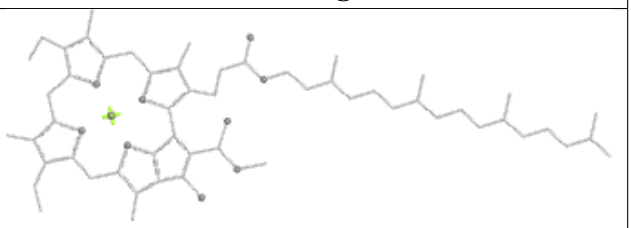
Bond lengths



Bond angles

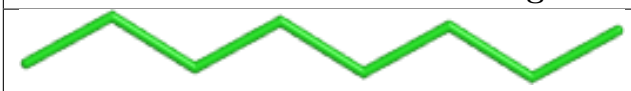


Torsions



Rings

Ligand STE A 415



Bond lengths



Bond angles

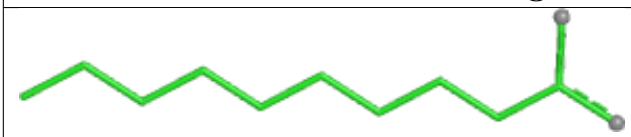


Torsions

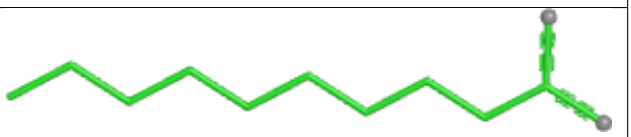


Rings

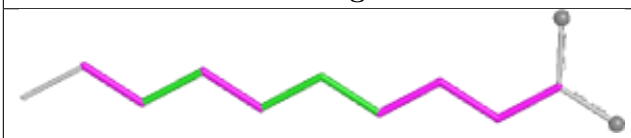
Ligand STE B 622



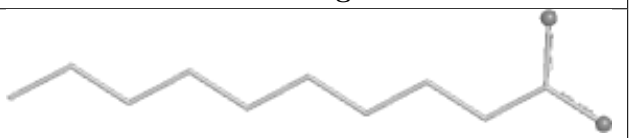
Bond lengths



Bond angles

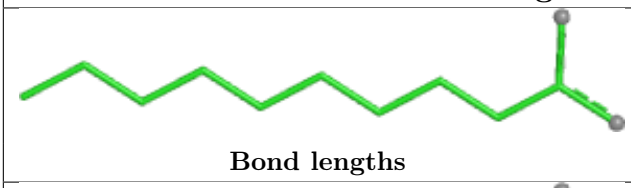


Torsions

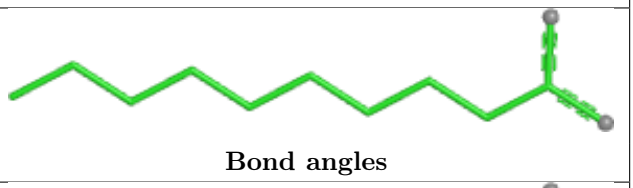


Rings

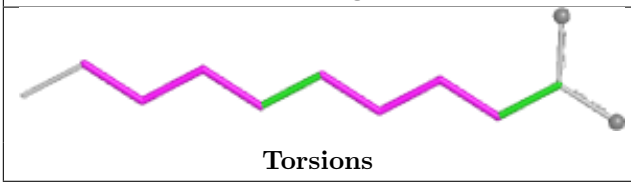
Ligand STE i 101



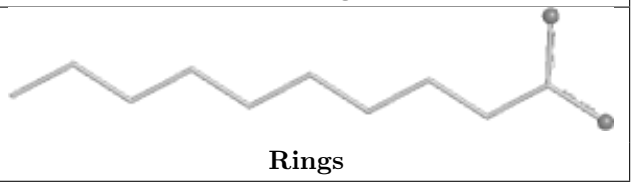
Bond lengths



Bond angles

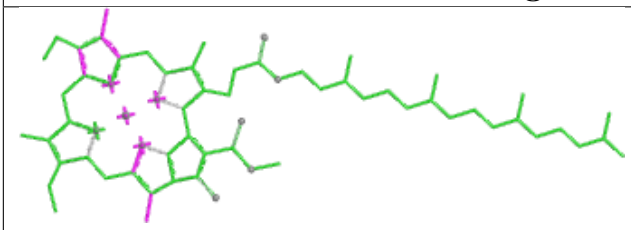


Torsions

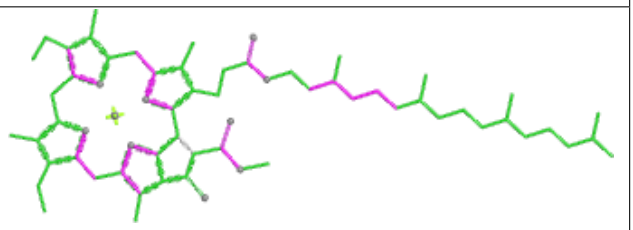


Rings

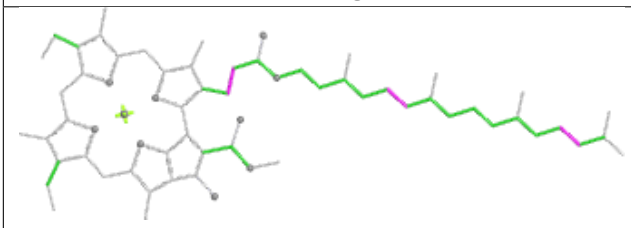
Ligand CLA B 603



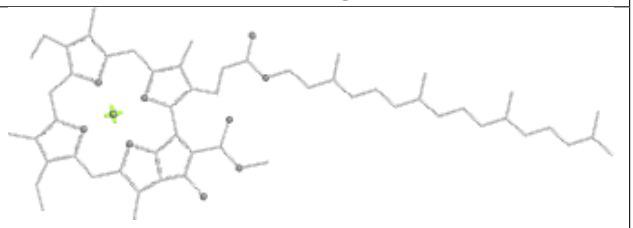
Bond lengths



Bond angles

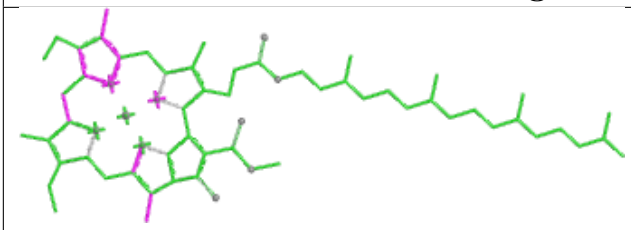


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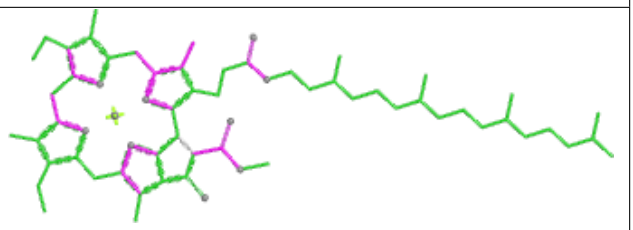


Rings

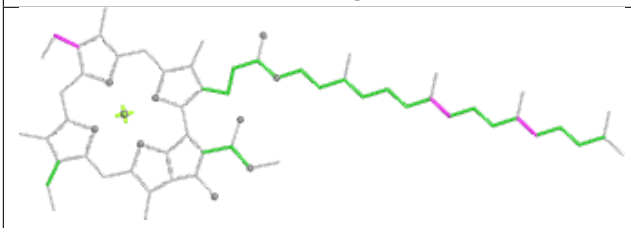
Ligand CLA a 406



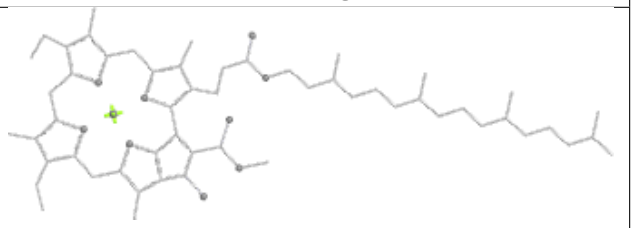
Bond lengths



Bond angles



Torsions



Rings

Ligand STE b 627

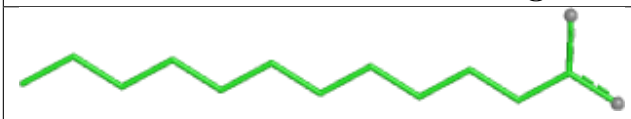

Bond lengths

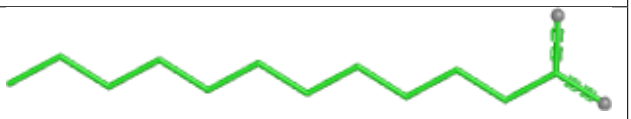

Bond angles

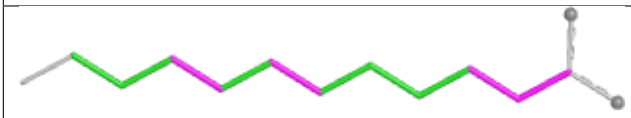

Torsions

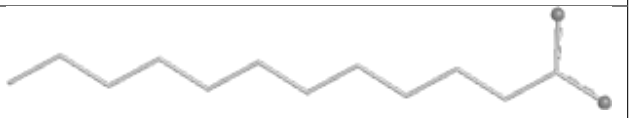

Rings

Ligand STE C 516


Bond lengths

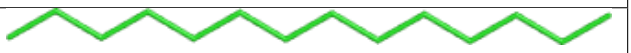

Bond angles


Torsions

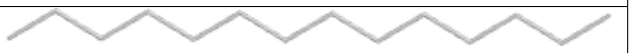

Rings

Ligand STE C 529

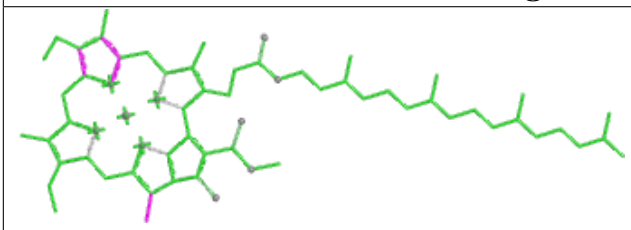

Bond lengths

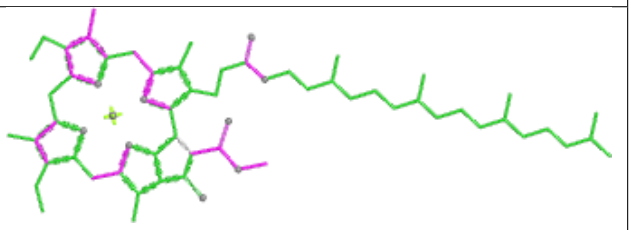

Bond angles

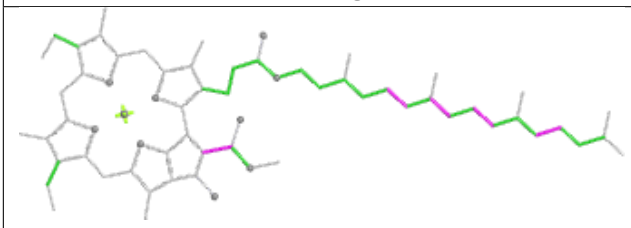

Torsions

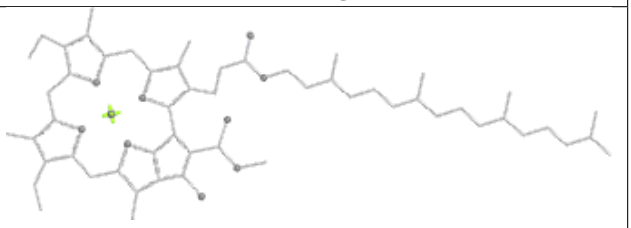

Rings

Ligand CLA C 507


Bond lengths


Bond angles

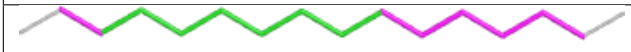

Torsions


Rings

Ligand STE j 102

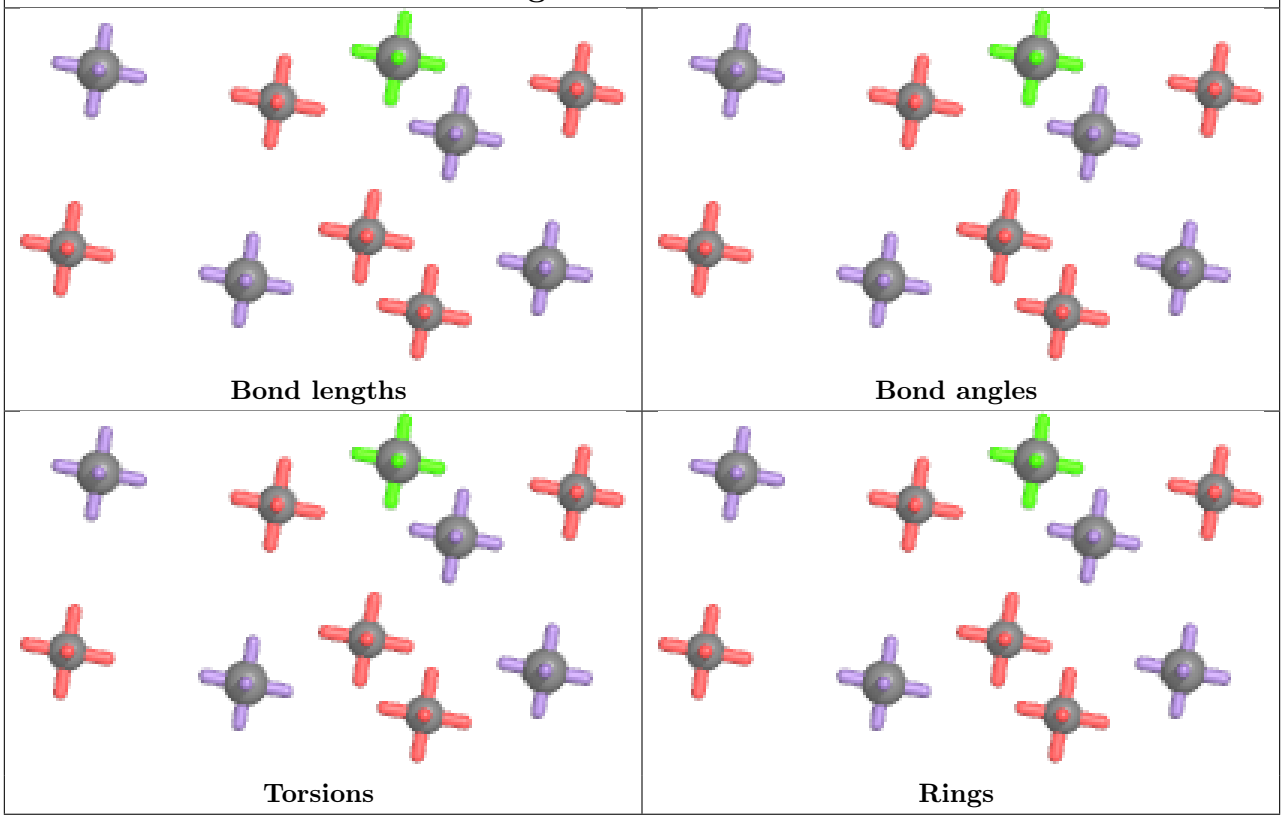

Bond lengths


Bond angles

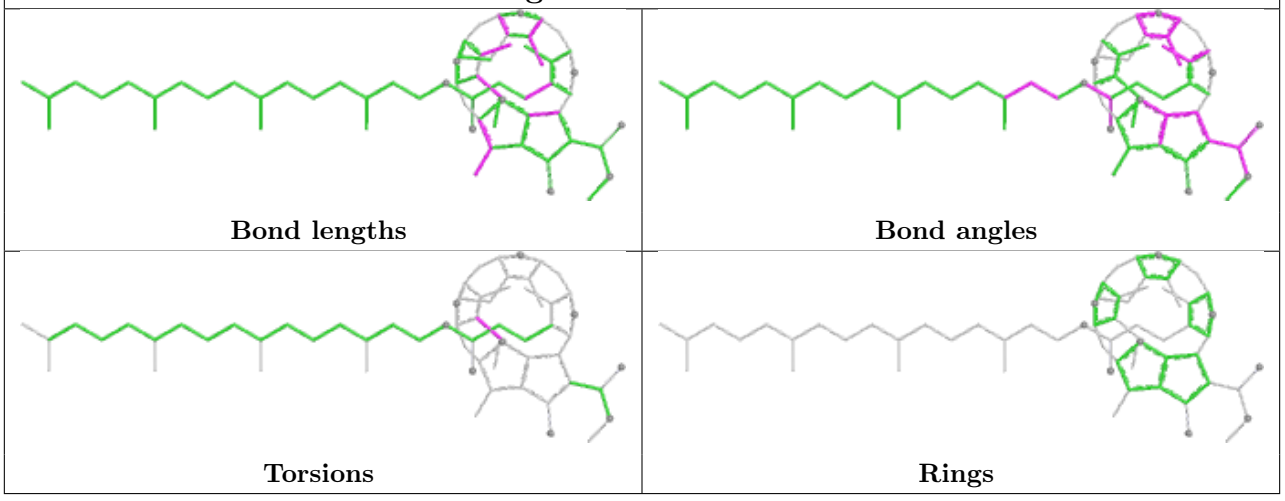

Torsions


Rings

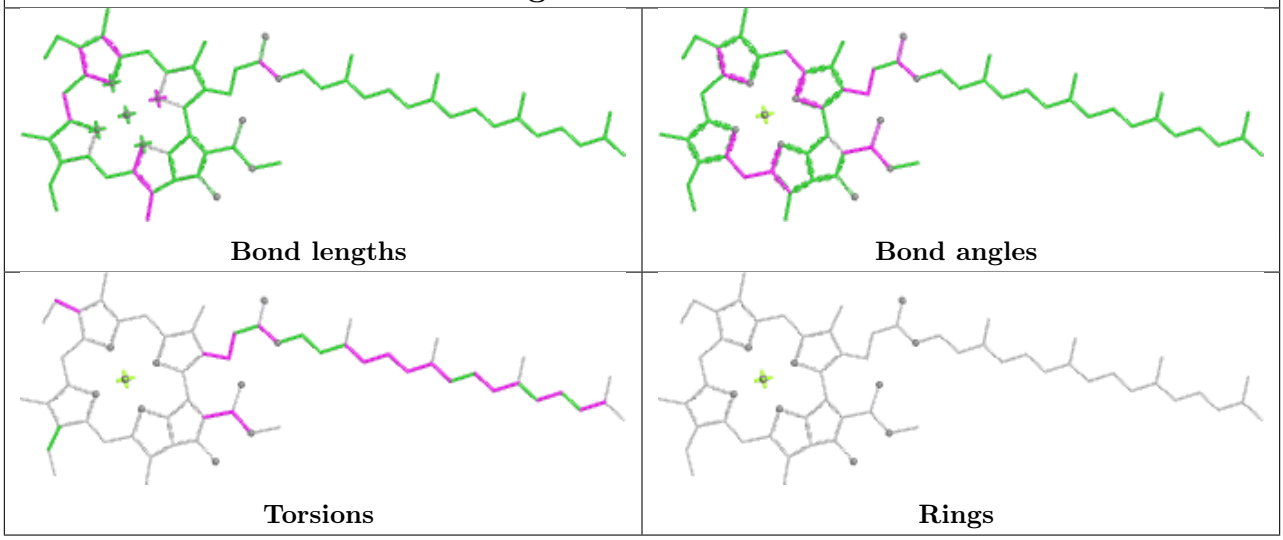
Ligand OEX a 418



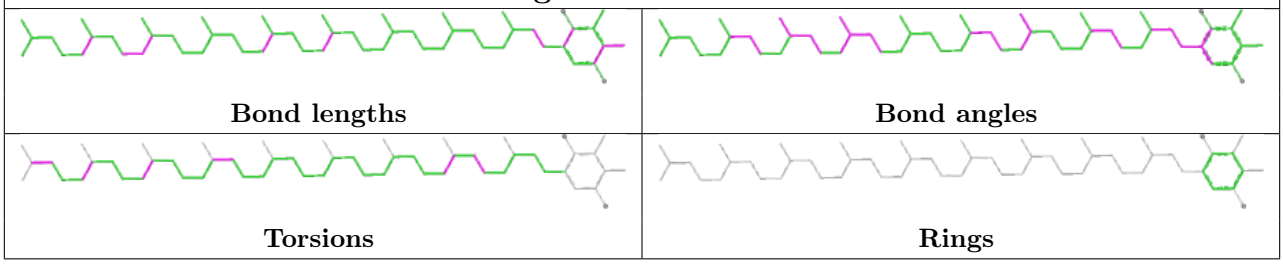
Ligand PHO d 401



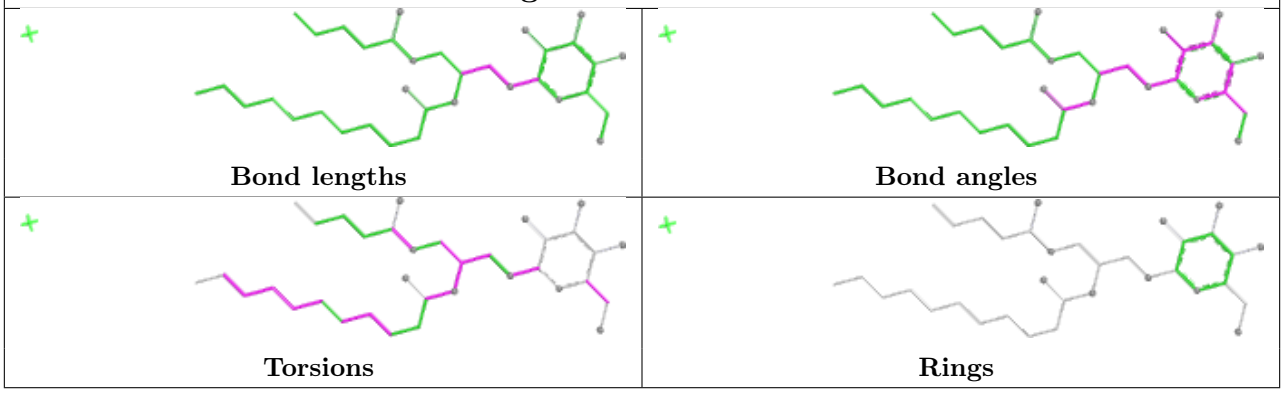
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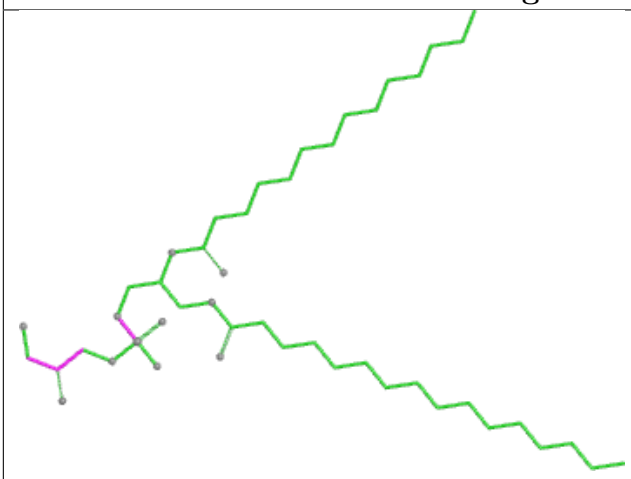
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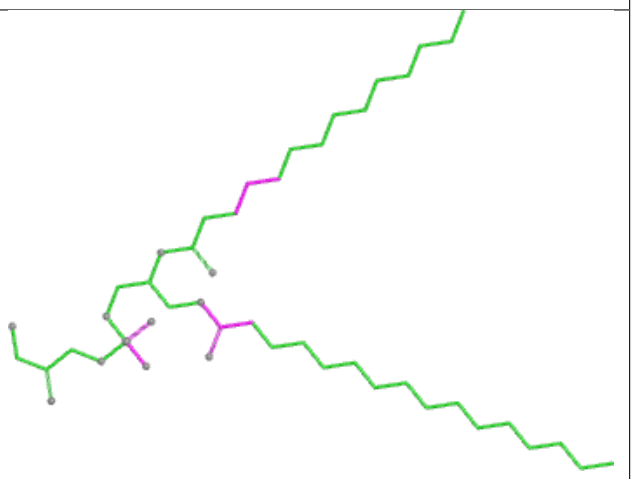
Ligand LMG C 517



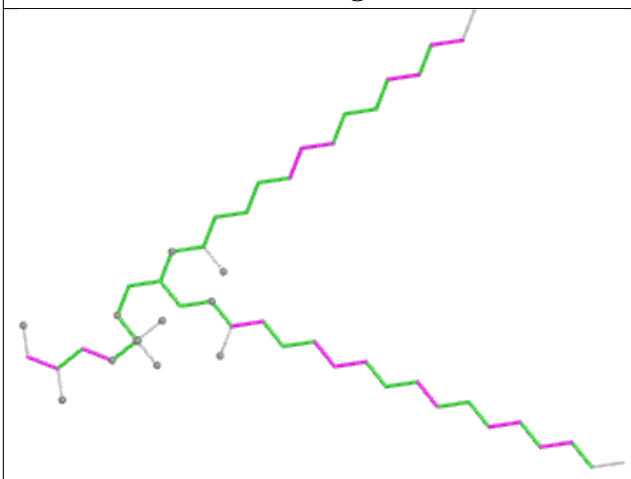
Ligand LHG D 411



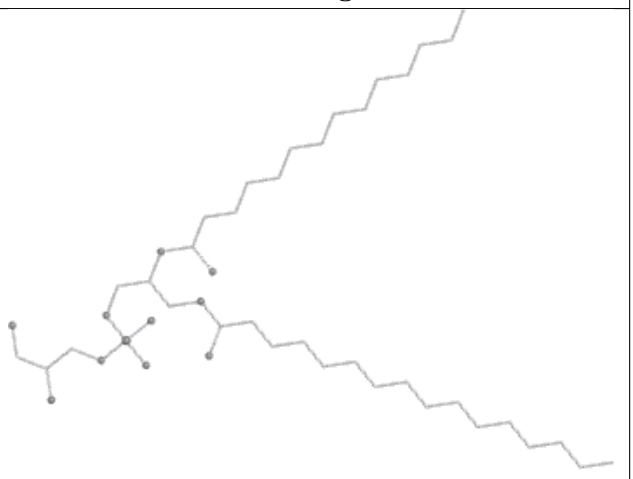
Bond lengths



Bond angles

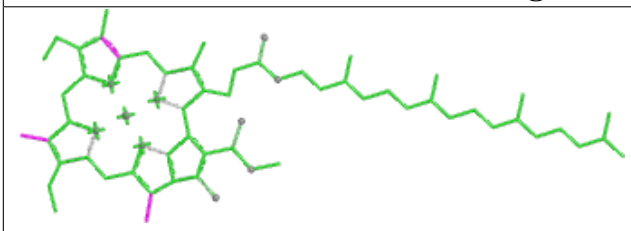


Torsions

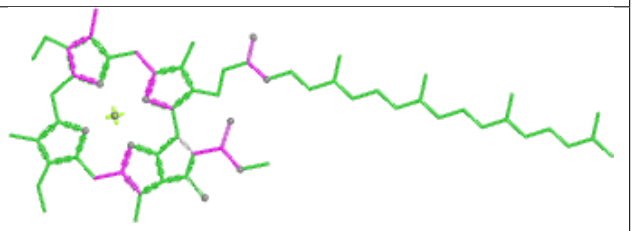


Rings

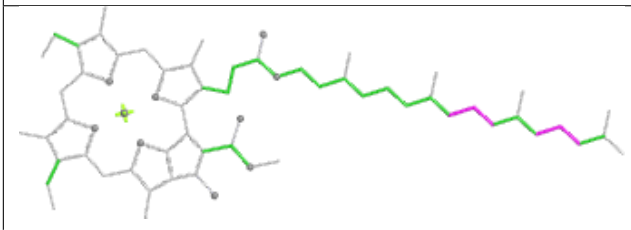
Ligand CLA b 610



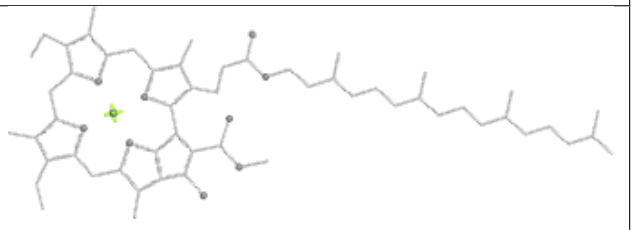
Bond lengths



Bond angles

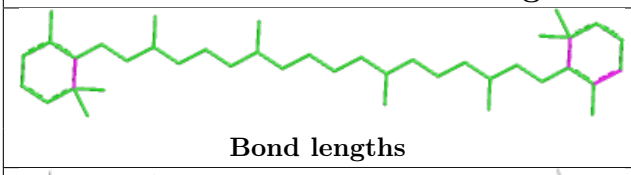


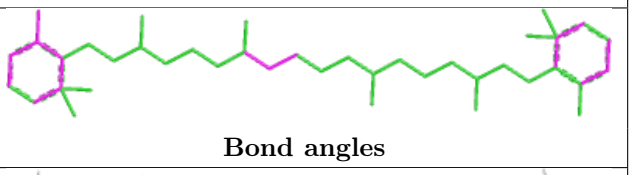
Torsions

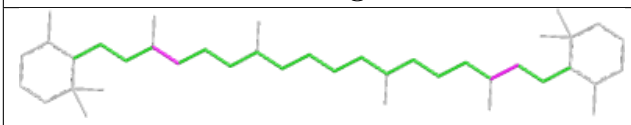


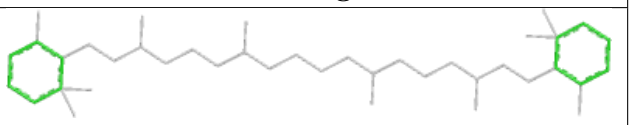
Rings

Ligand BCR B 619


Bond lengths


Bond angles


Torsions


Rings

Ligand STE A 416

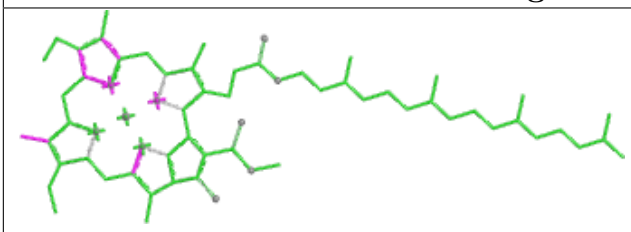

Bond lengths

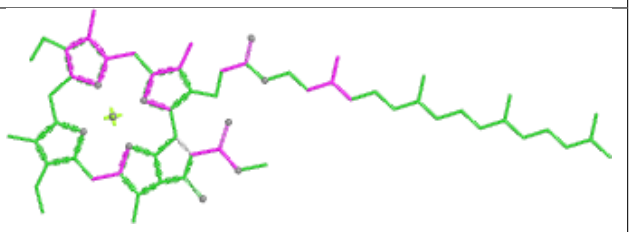

Bond angles

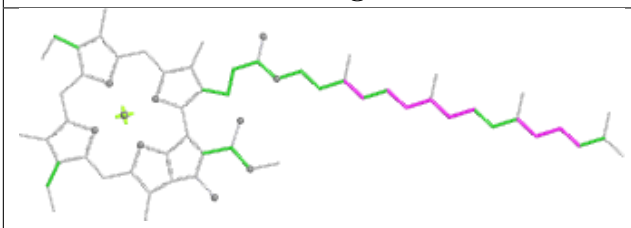

Torsions

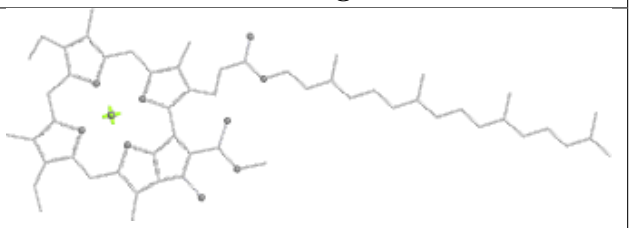

Rings

Ligand CLA b 602


Bond lengths


Bond angles

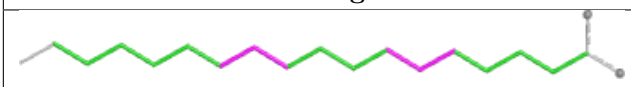

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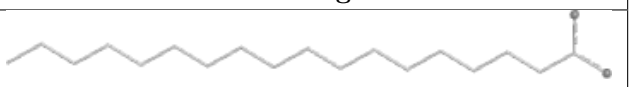

Rings

Ligand STE x 102

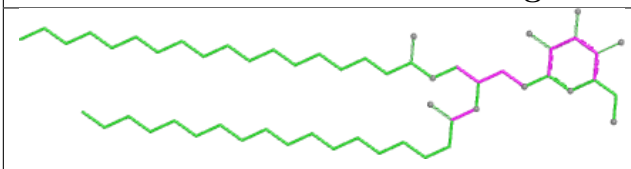

Bond lengths


Bond angles

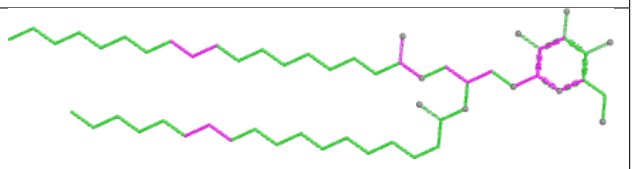

Torsions


Rings

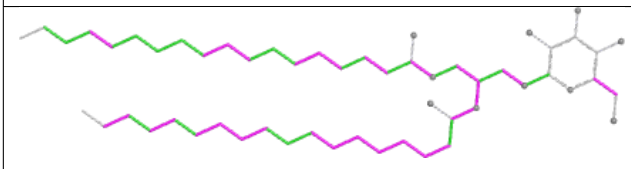
Ligand LMG a 415



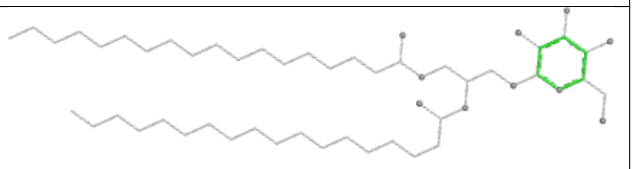
Bond lengths



Bond angles



Torsions



Rings

Ligand STE B 623



Bond lengths



Bond angles

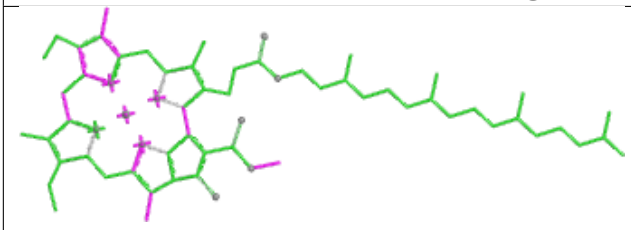


Torsions

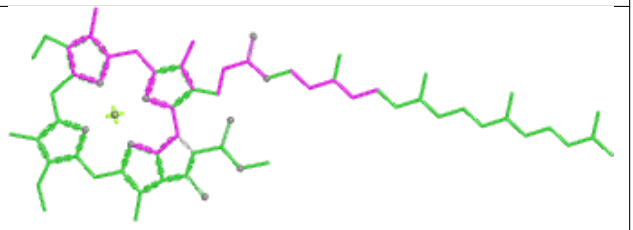


Rings

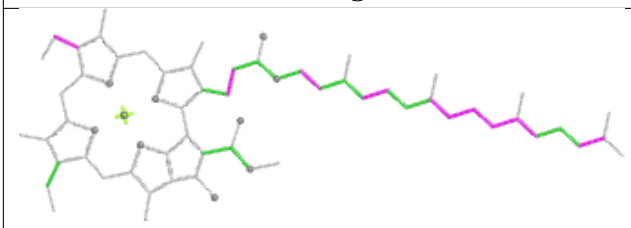
Ligand CLA C 512



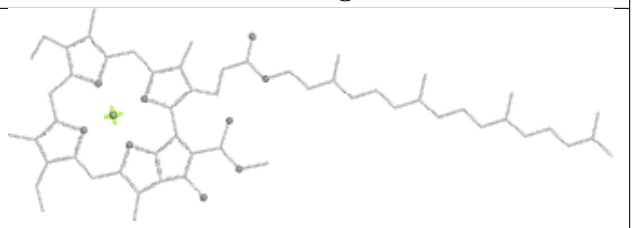
Bond lengths



Bond angles

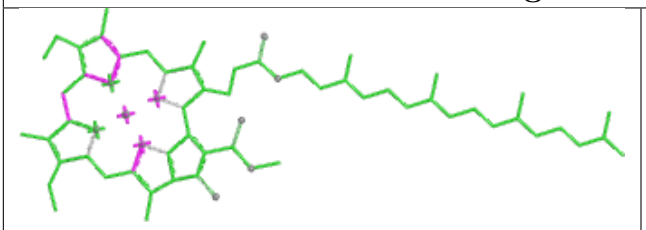


Torsions

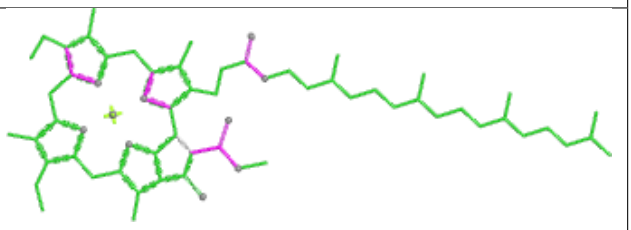


Rings

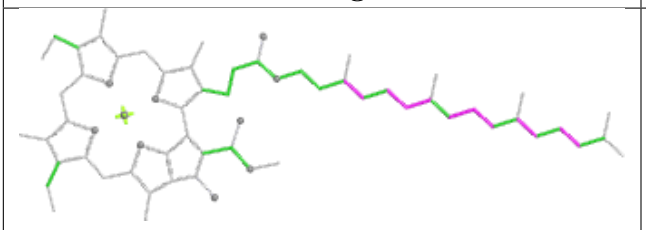
Ligand CLA C 505



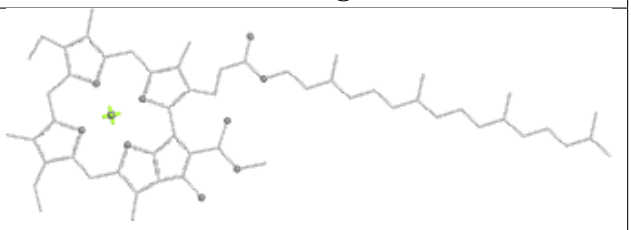
Bond lengths



Bond angles

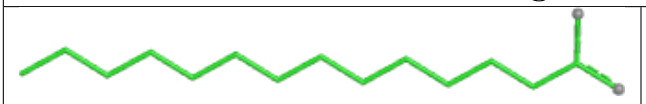


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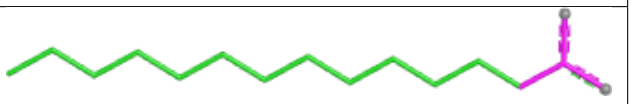


Rings

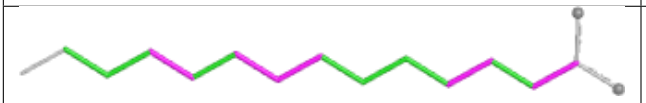
Ligand STE b 625



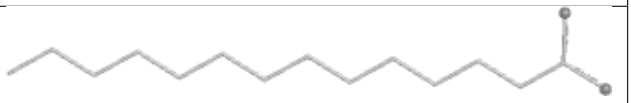
Bond lengths



Bond angles

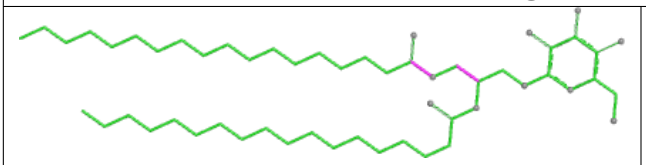


Torsions

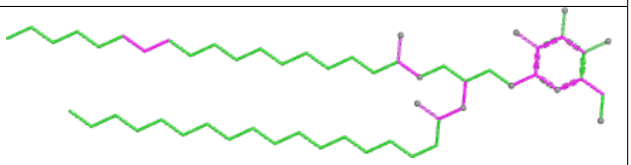


Rings

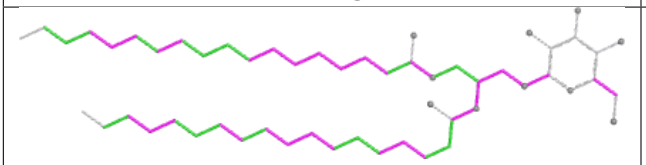
Ligand LMG b 623



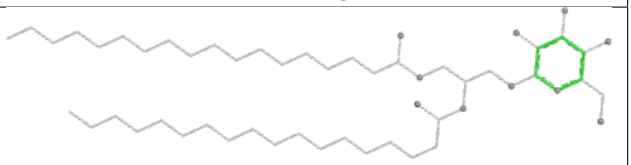
Bond lengths



Bond angles

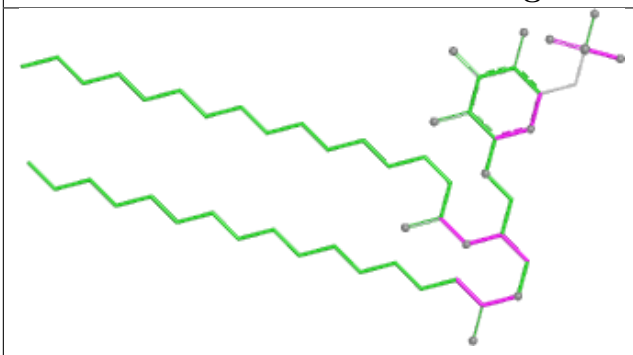


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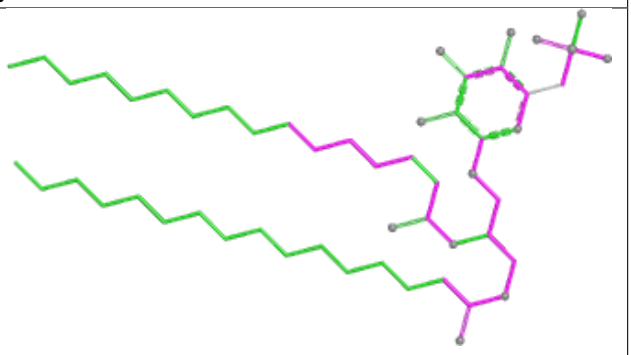


Rings

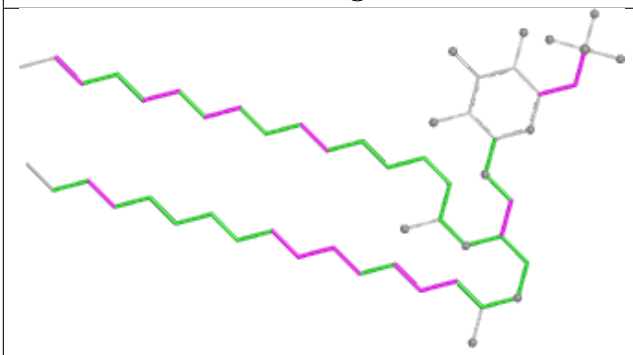
Ligand SQD A 413



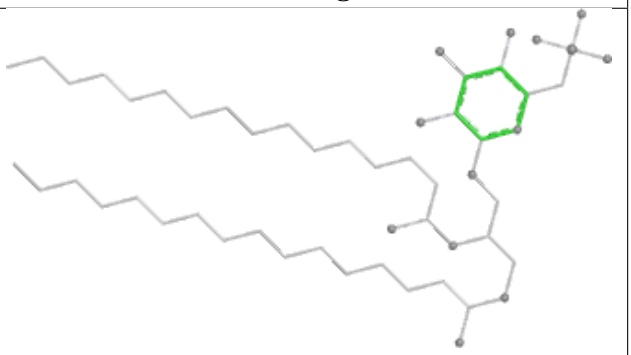
Bond lengths



Bond angles

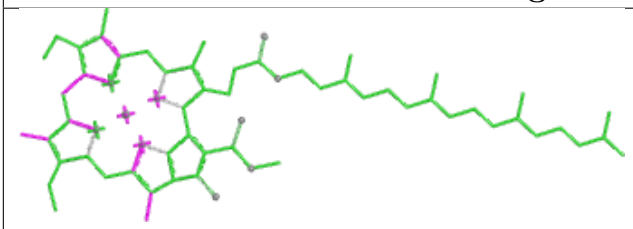


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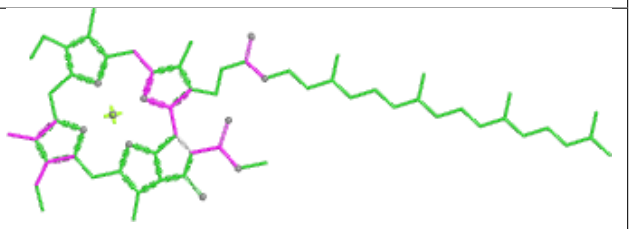


Rings

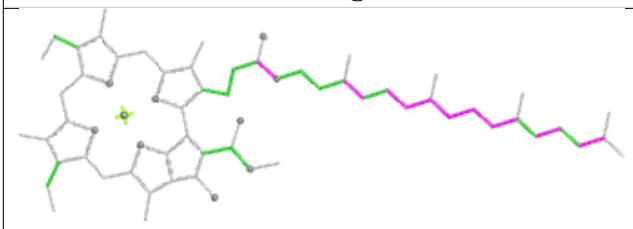
Ligand CLA a 408



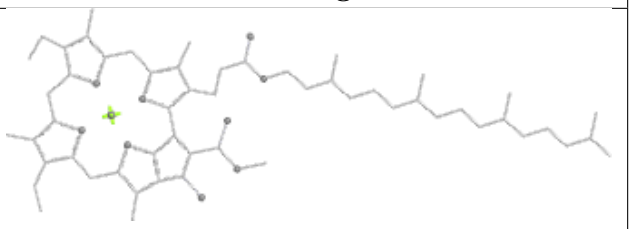
Bond lengths



Bond angles

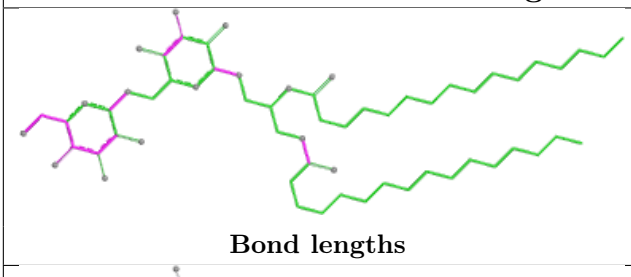


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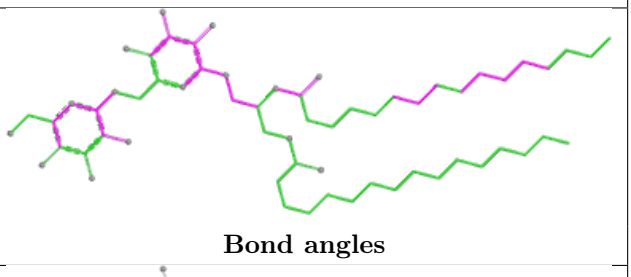


Rings

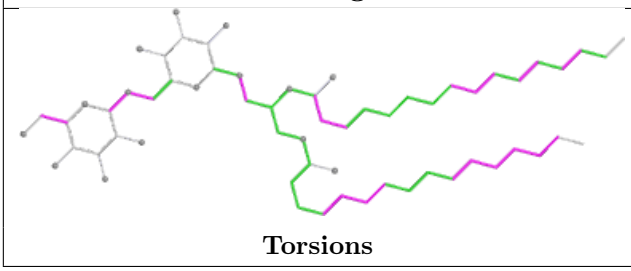
Ligand DGD c 520



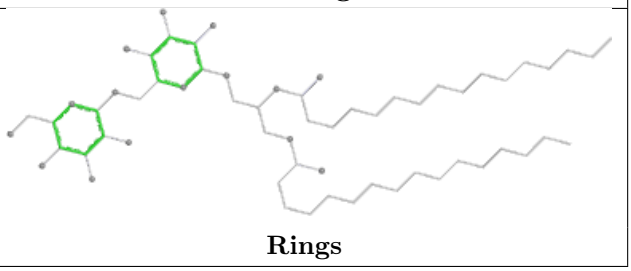
Bond lengths



Bond angles

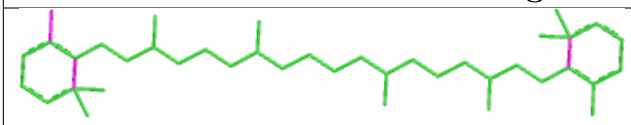


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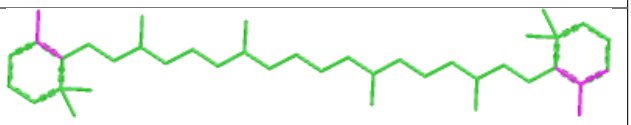


Rings

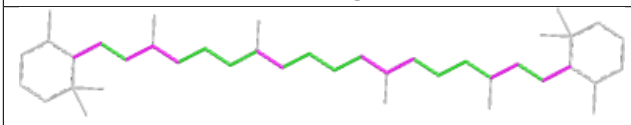
Ligand BCR k 101



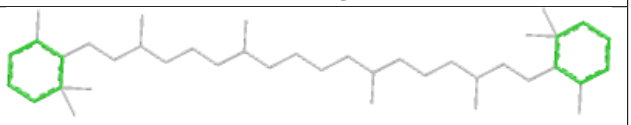
Bond lengths



Bond angles

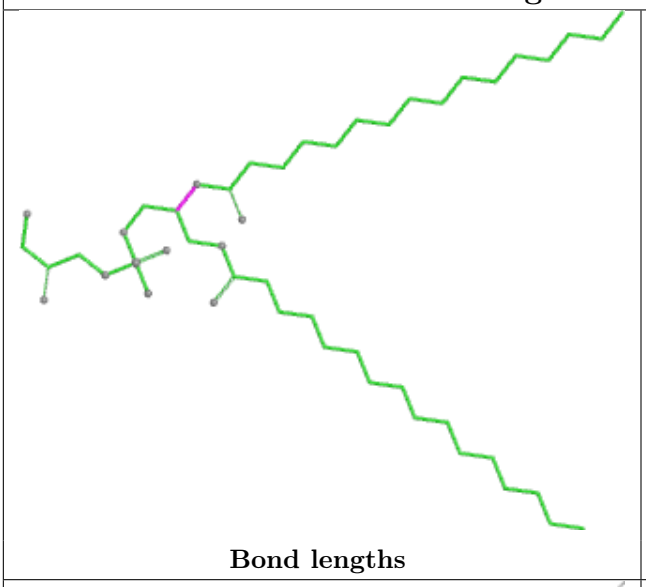


Torsions

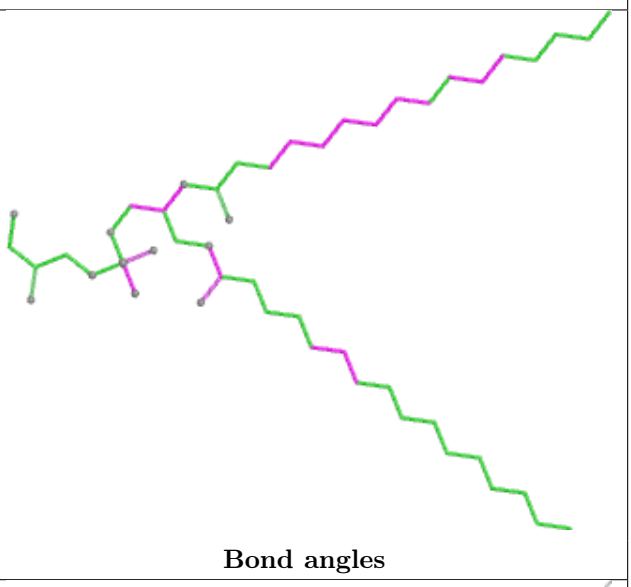


Rings

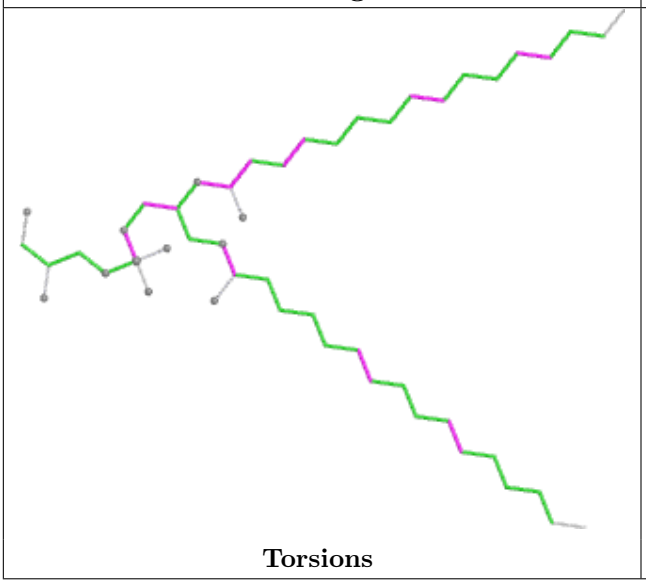
Ligand LHG L 101



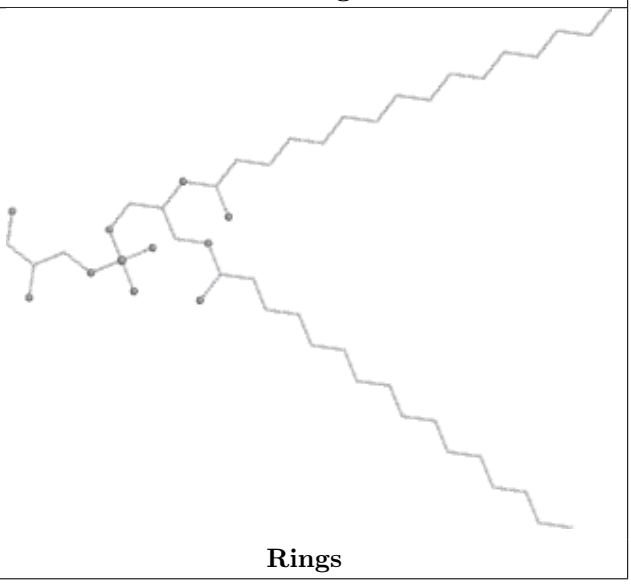
Bond lengths



Bond angles

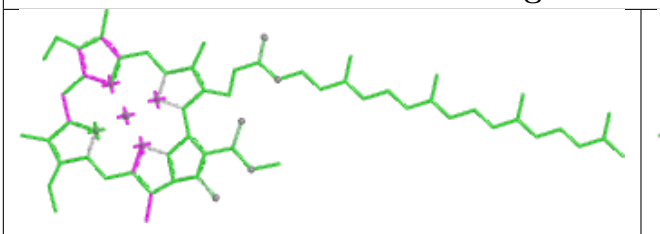


Torsions

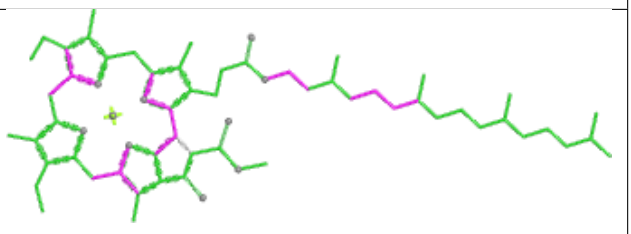


Rings

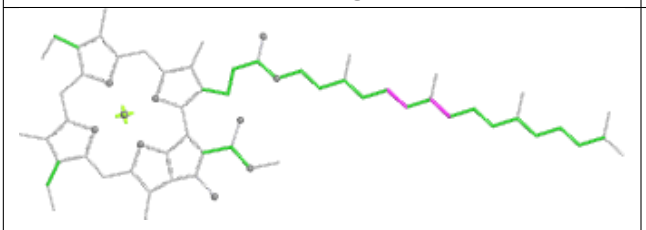
Ligand CLA C 503



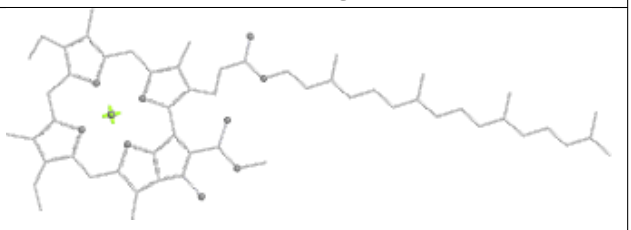
Bond lengths



Bond angles

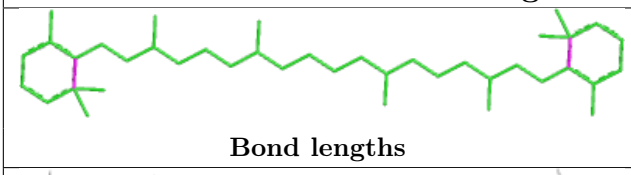


Torsions

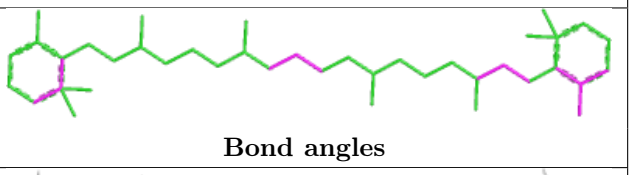


Rings

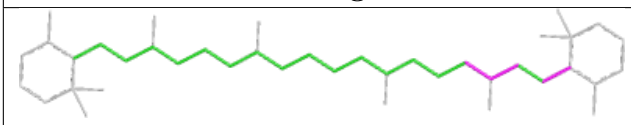
Ligand BCR D 406



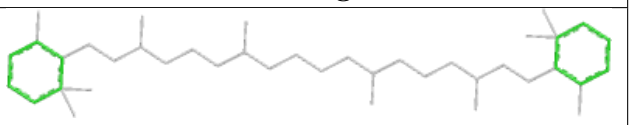
Bond lengths



Bond angles

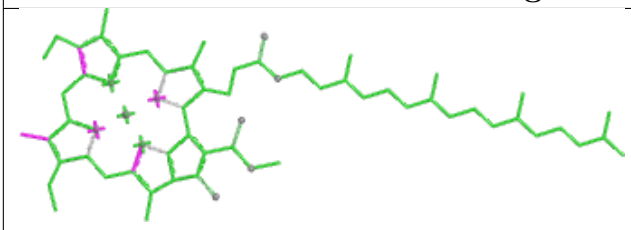


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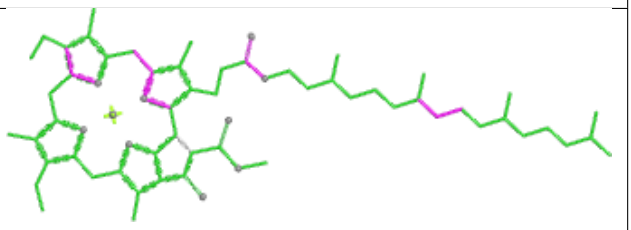


Rings

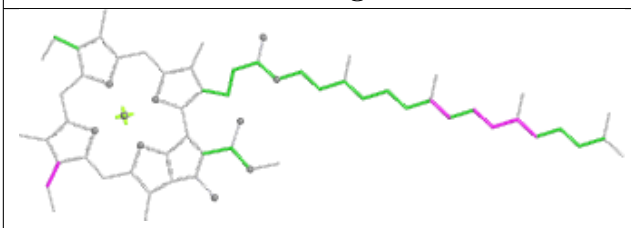
Ligand CLA B 604



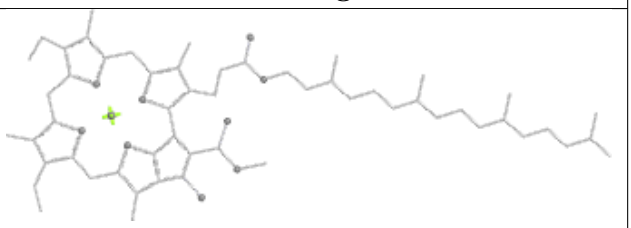
Bond lengths



Bond angles

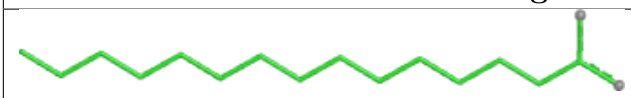


Torsions

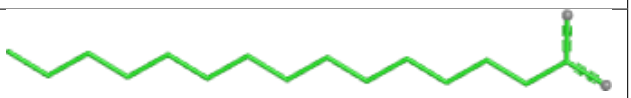


Rings

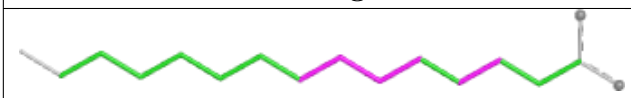
Ligand STE d 410



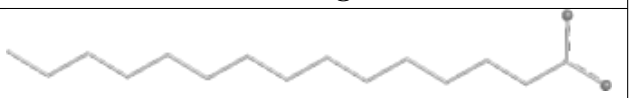
Bond lengths



Bond angles

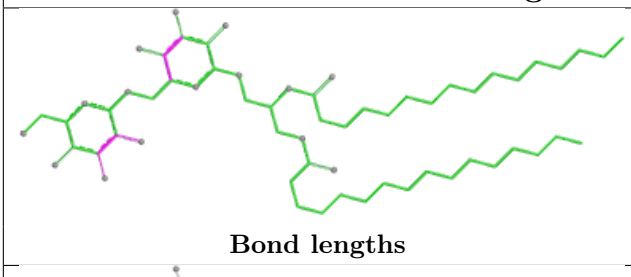


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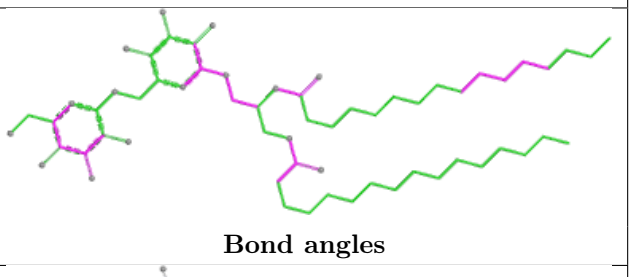


Rings

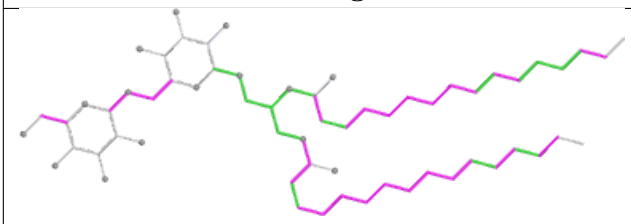
Ligand DGD c 519



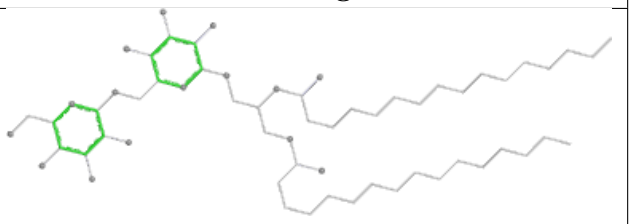
Bond lengths



Bond angles



Torsions



Rings

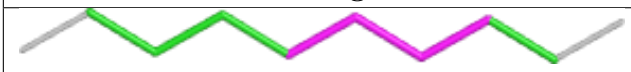
Ligand STE d 412



Bond lengths



Bond angles

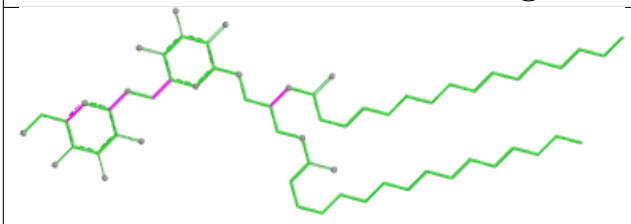


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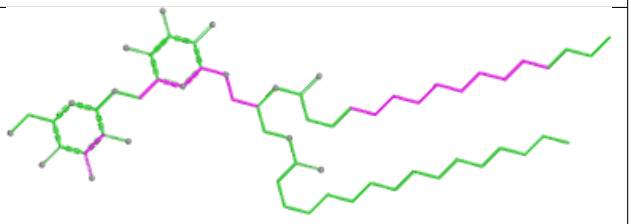


Rings

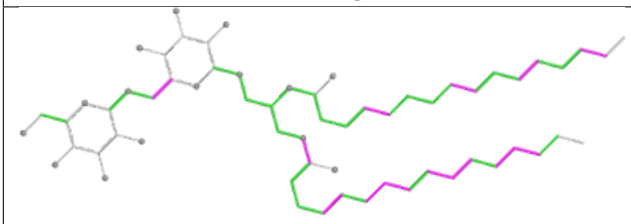
Ligand DGD C 523



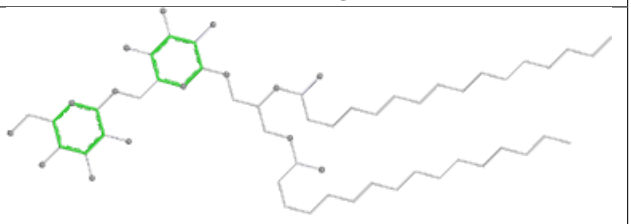
Bond lengths



Bond angles

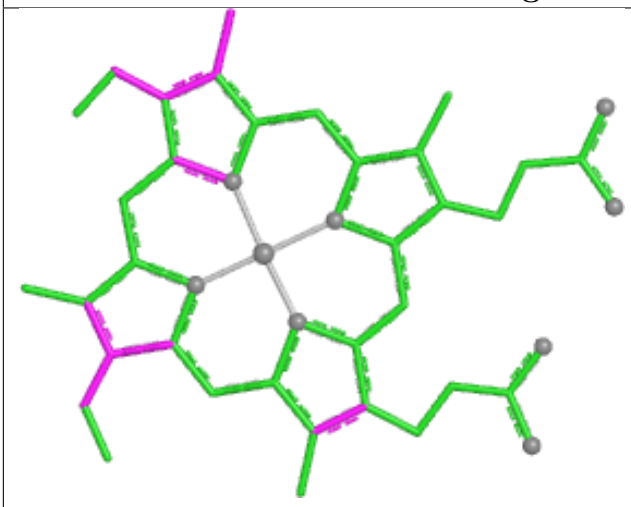


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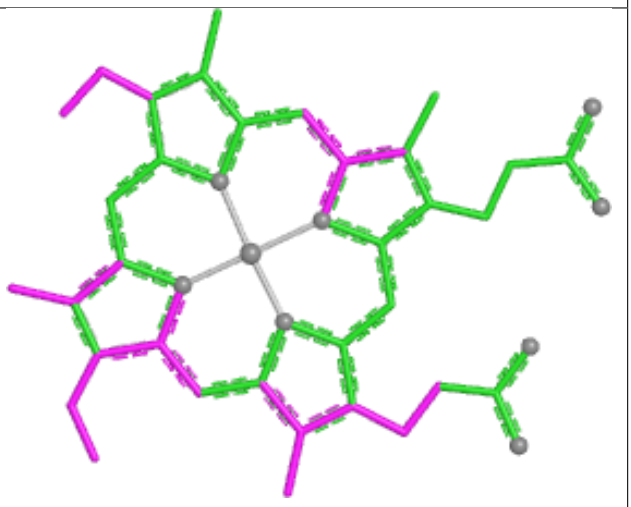


Rings

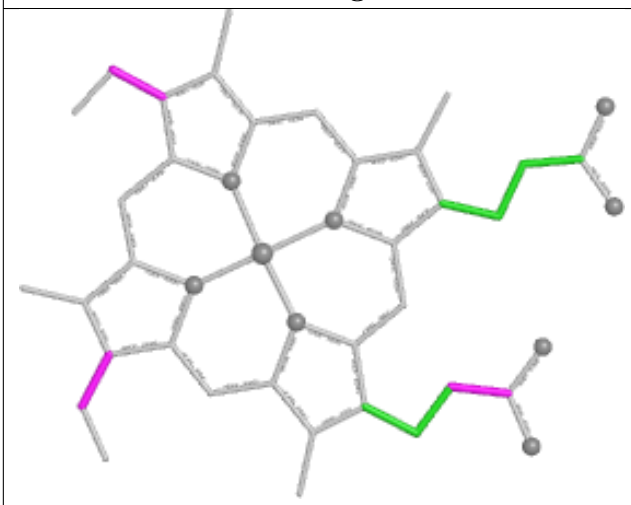
Ligand HEC V 201



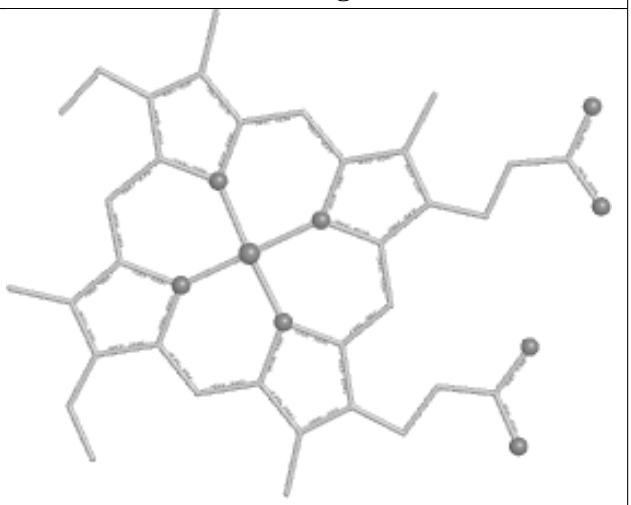
Bond lengths



Bond angles

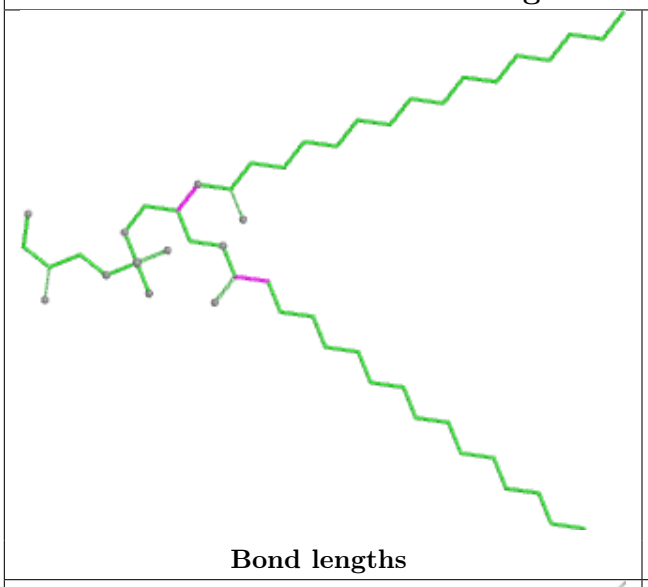


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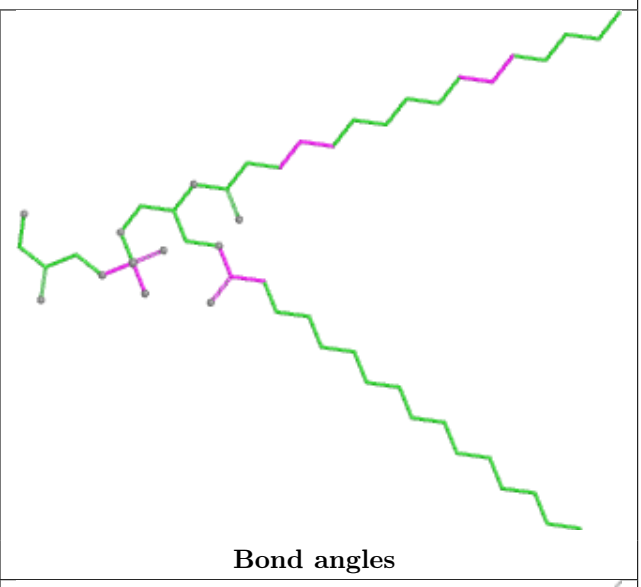


Rings

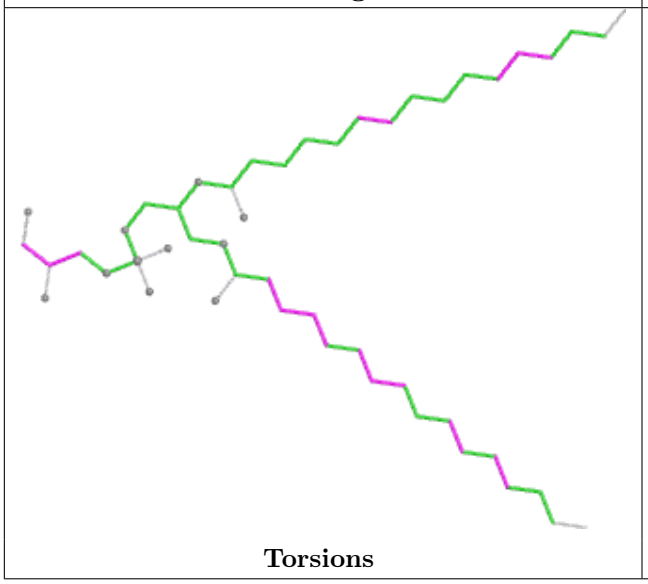
Ligand LHG D 412



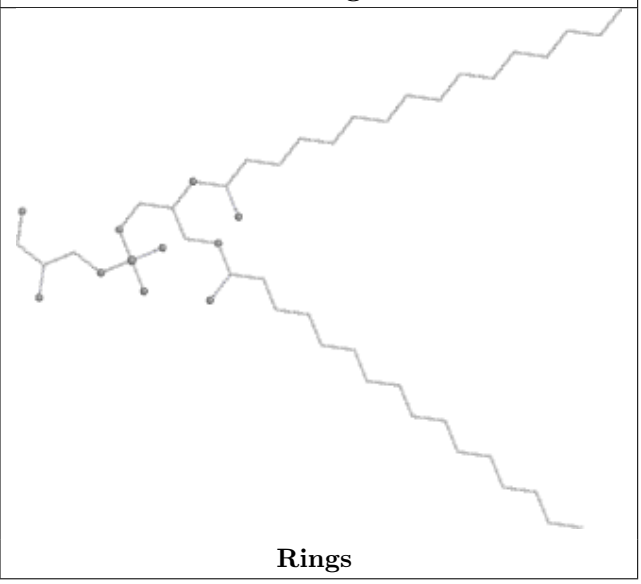
Bond lengths



Bond angles

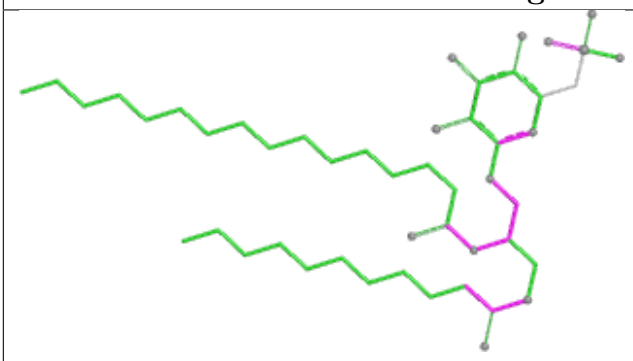


Torsions

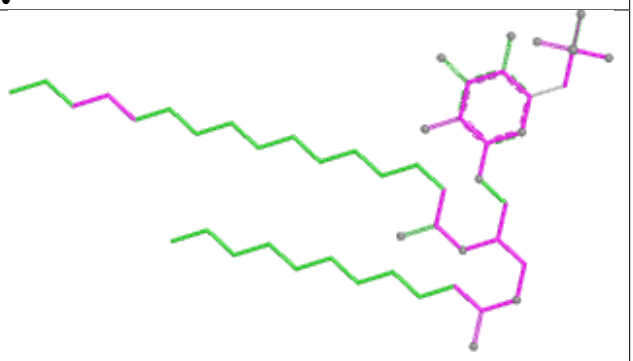


Rings

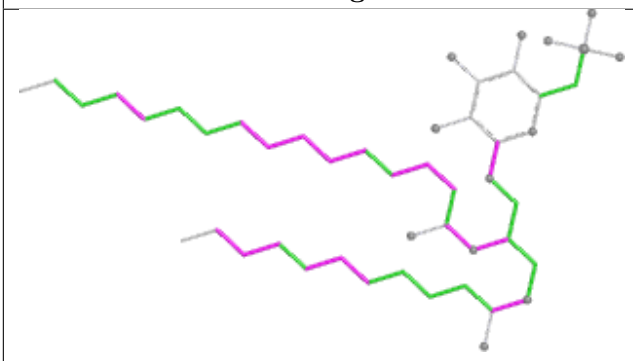
Ligand SQD b 620



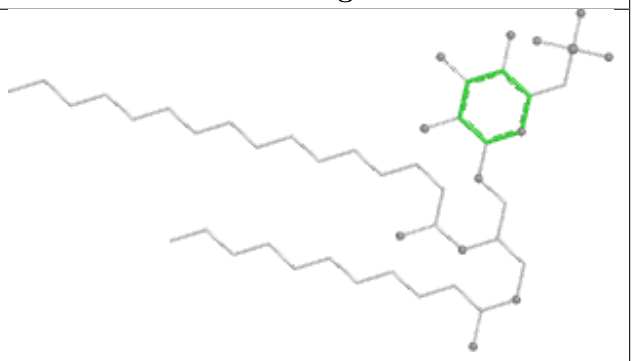
Bond lengths



Bond angles

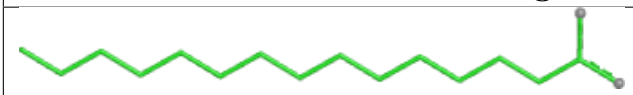


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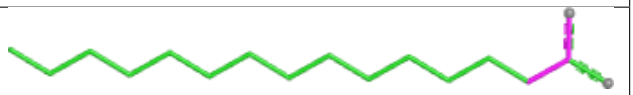


Rings

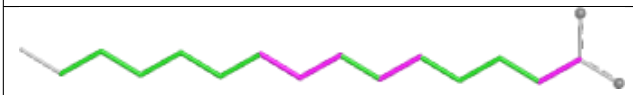
Ligand STE I 102



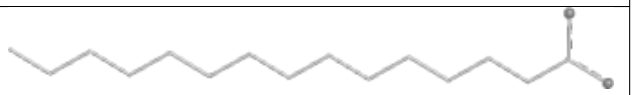
Bond lengths



Bond angles

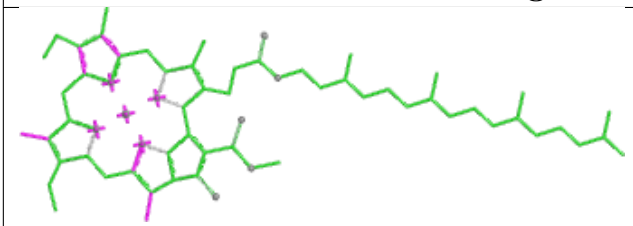


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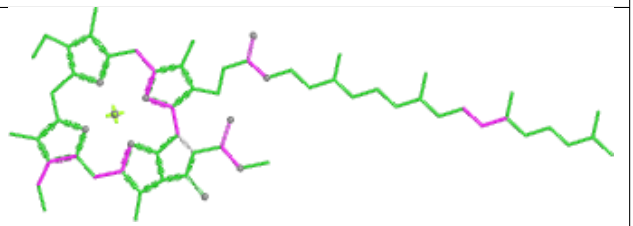


Rings

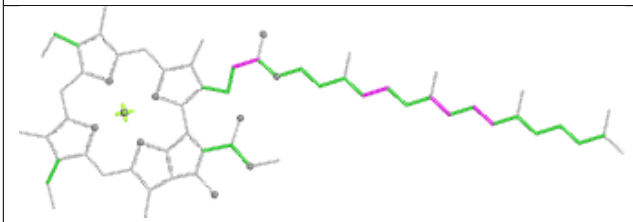
Ligand CLA b 611



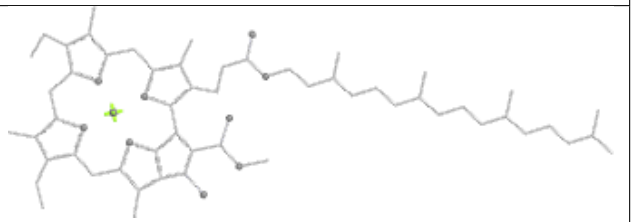
Bond lengths



Bond angles

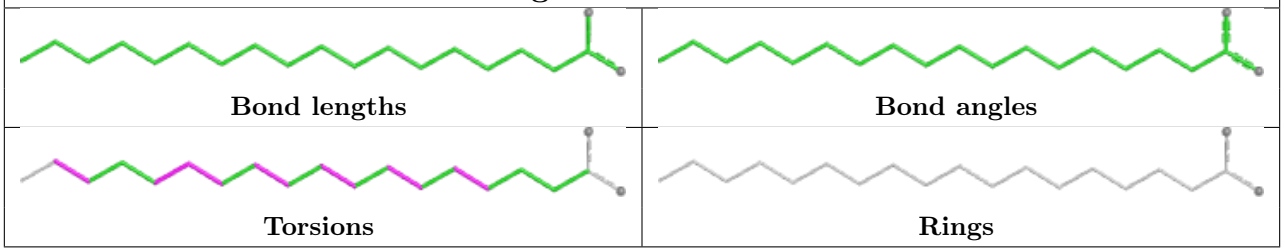


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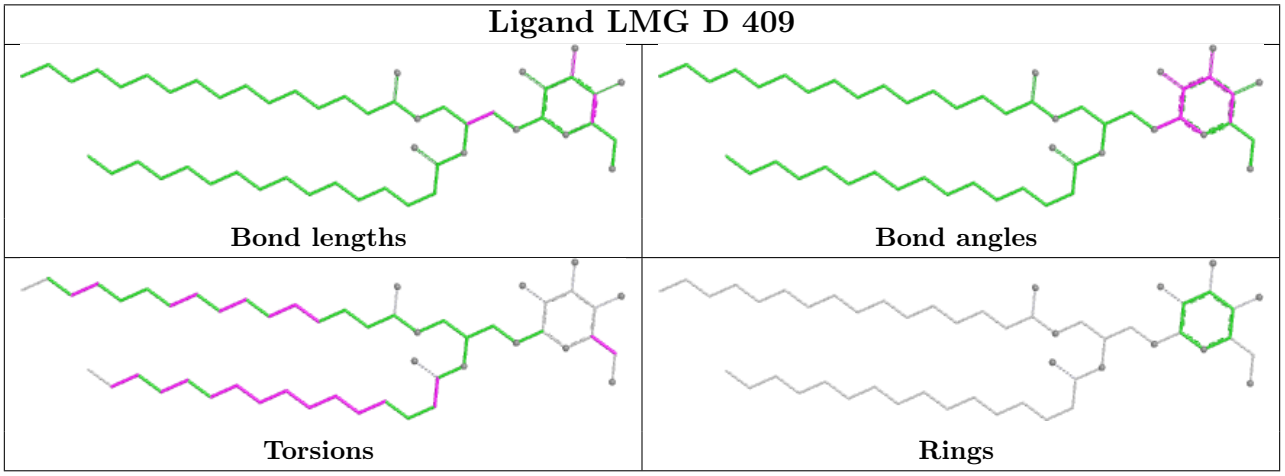


Rings

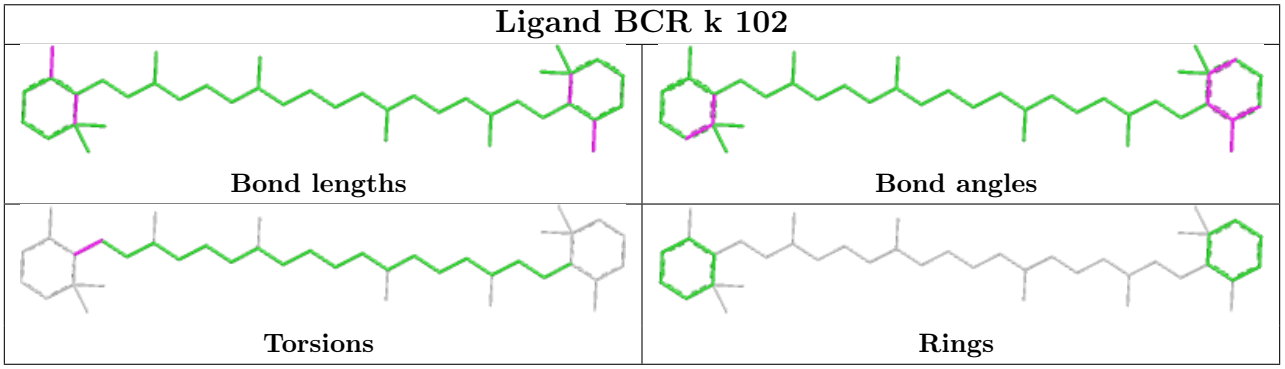
Ligand STE b 624



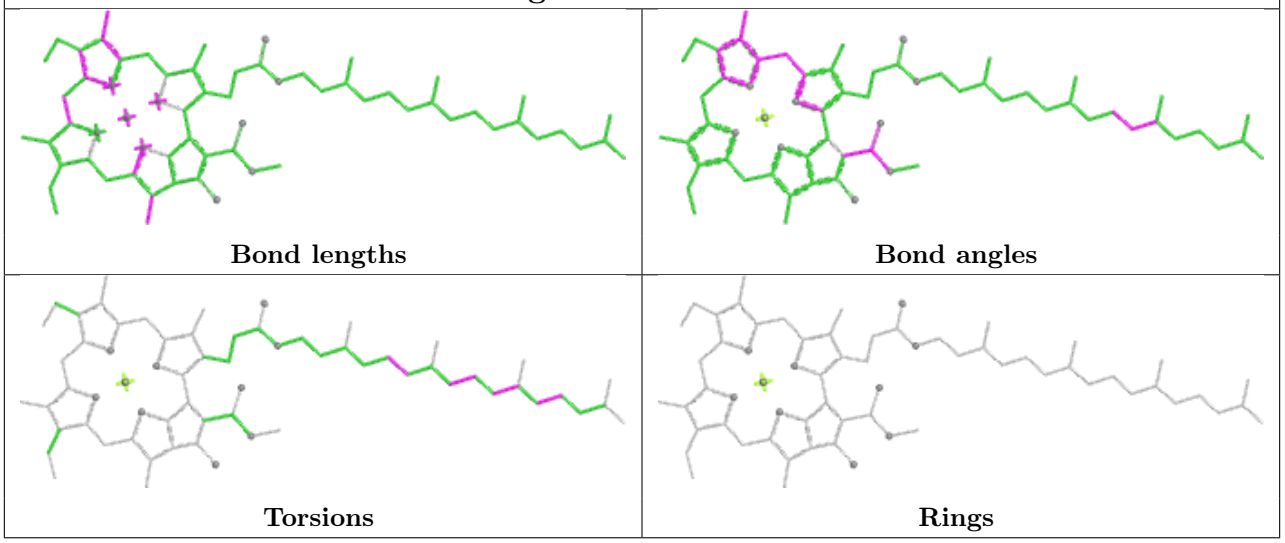
Ligand LMG D 409



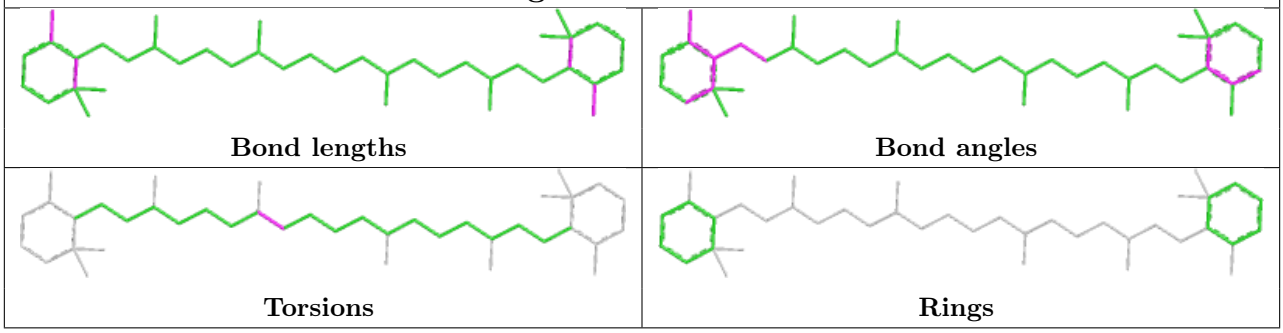
Ligand BCR k 102



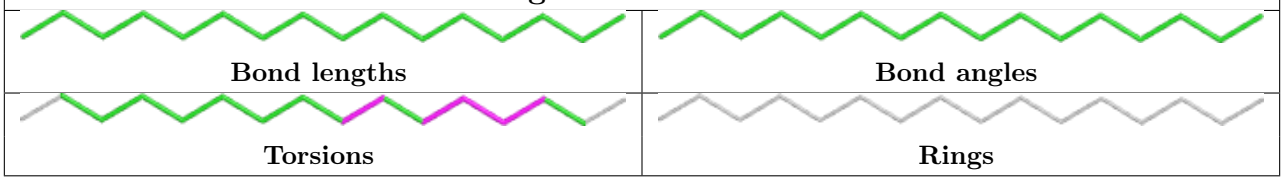
Ligand CLA b 614



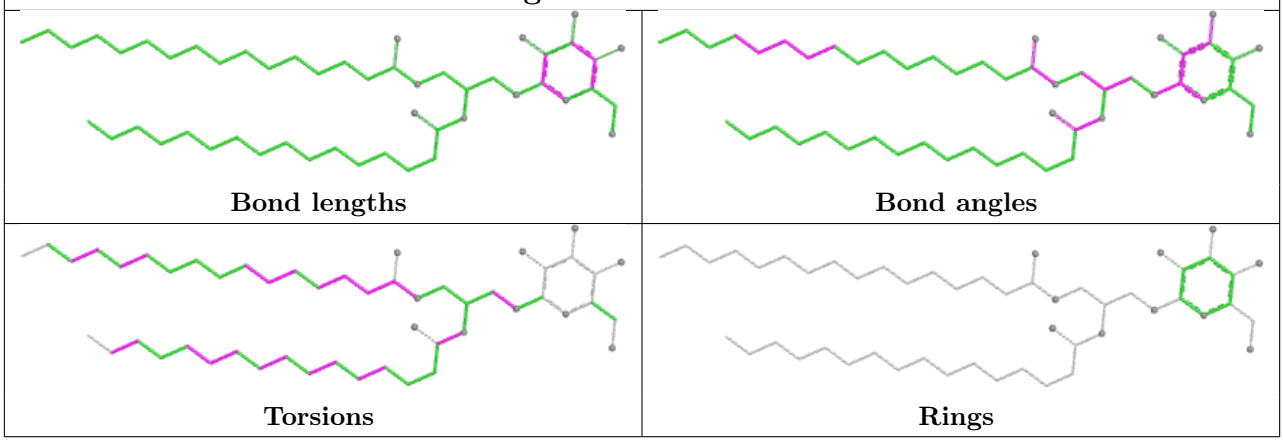
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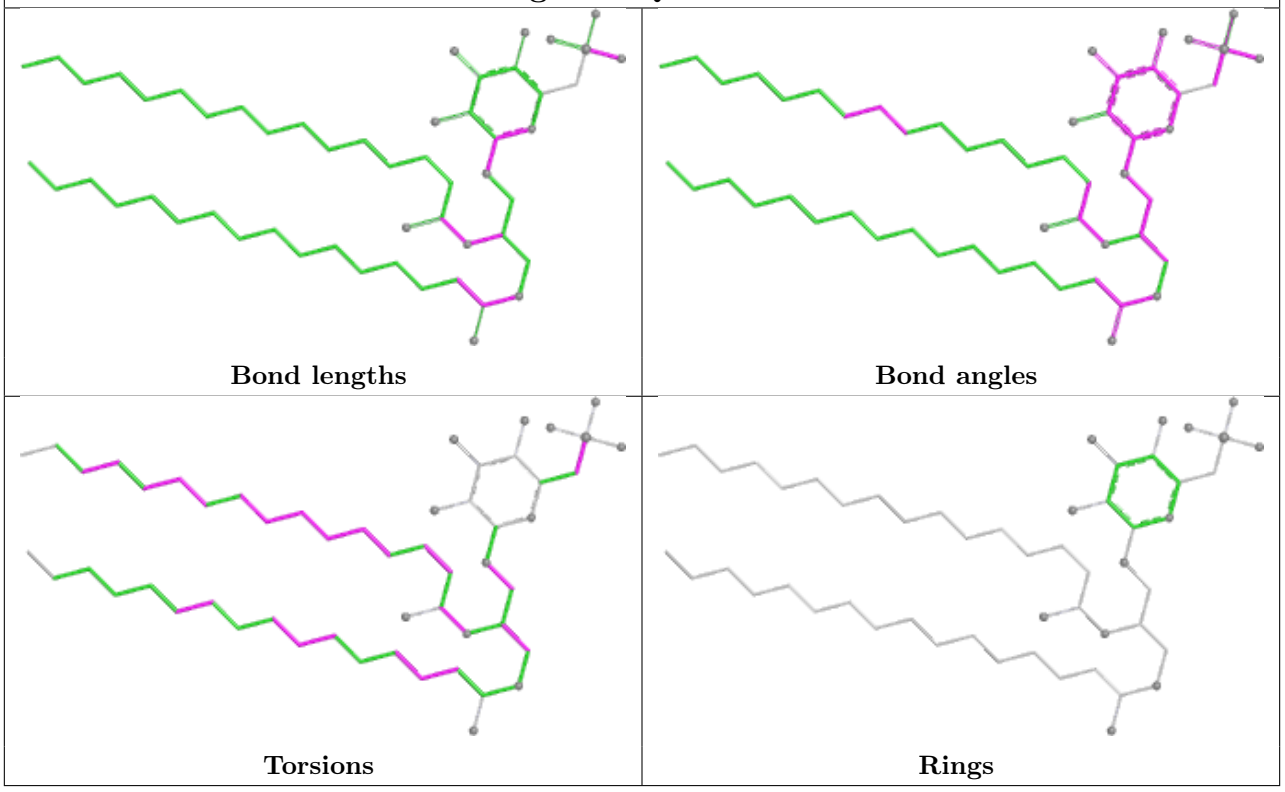
Ligand STE C 526



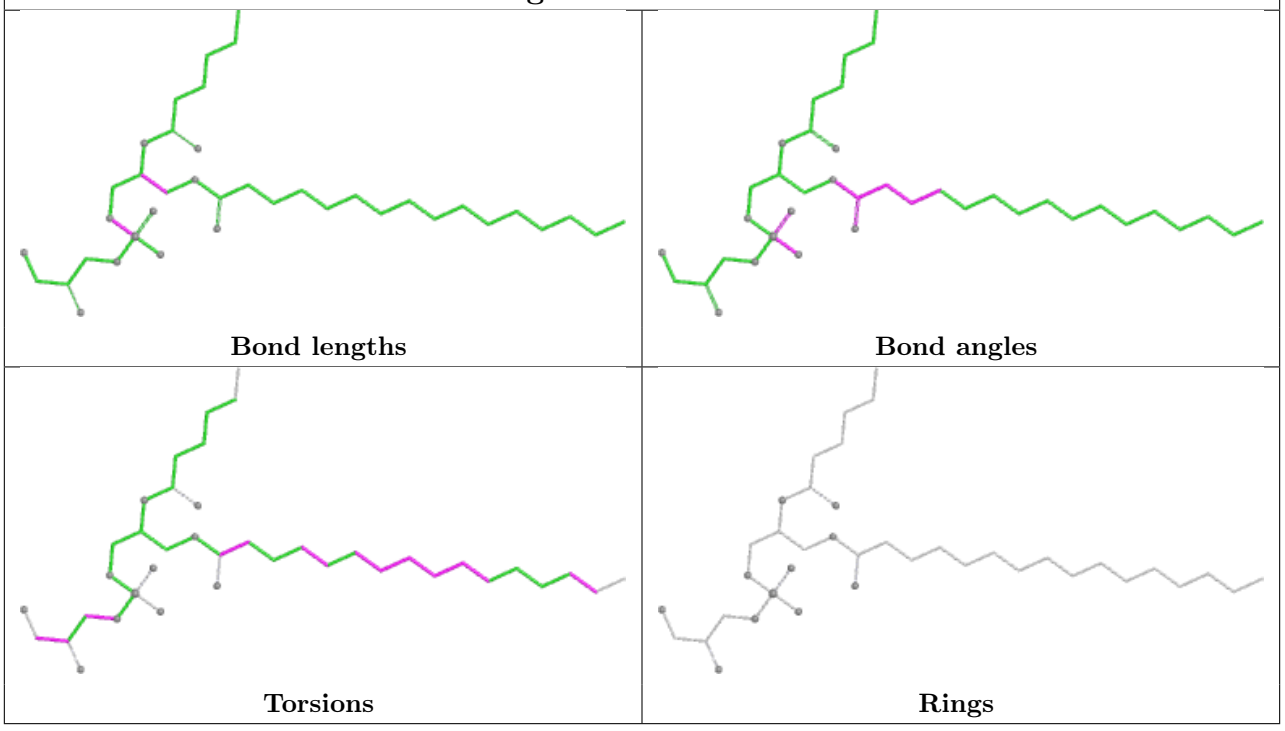
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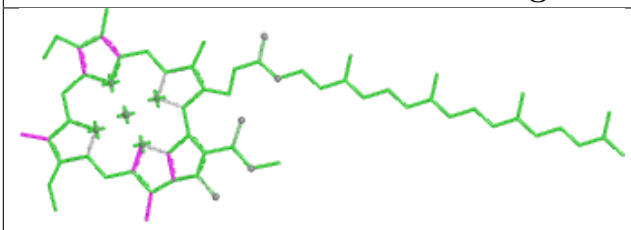
Ligand SQD a 412



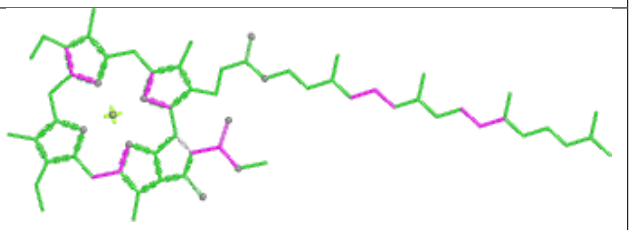
Ligand LHG d 408



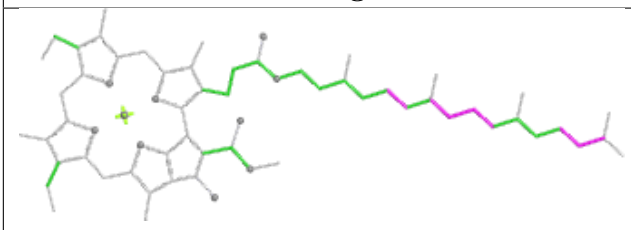
Ligand CLA c 503



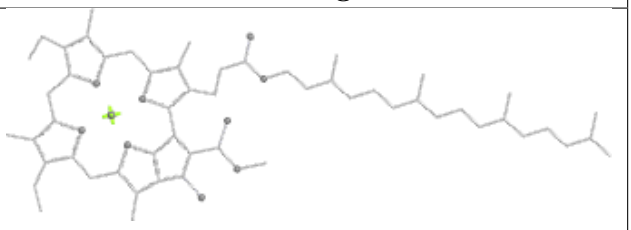
Bond lengths



Bond angles

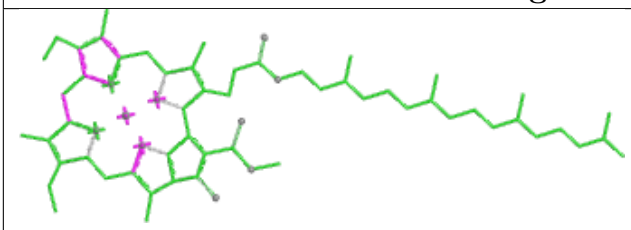


Torsions

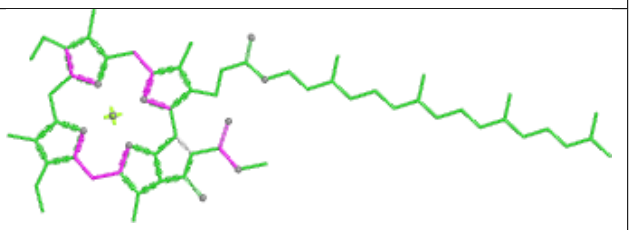


Rings

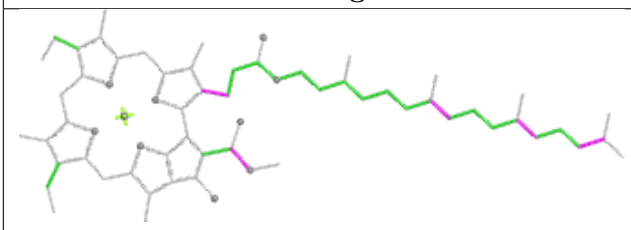
Ligand CLA c 511



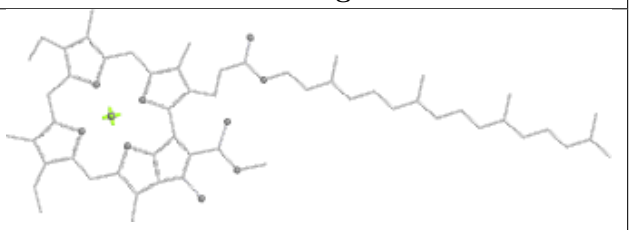
Bond lengths



Bond angles



Torsions



Rings

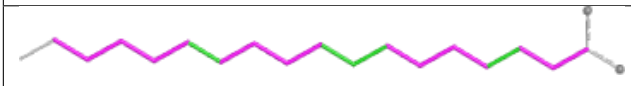
Ligand STE E 104



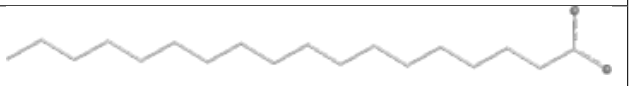
Bond lengths



Bond angles

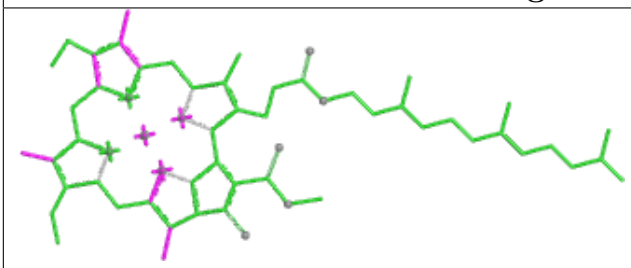


Torsions

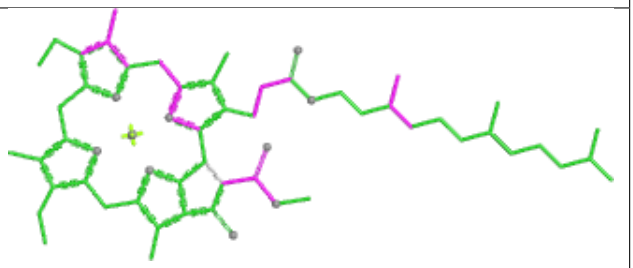


Rings

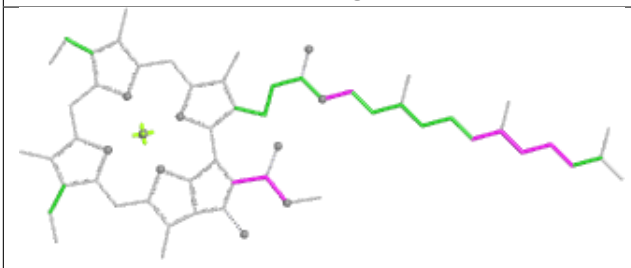
Ligand CLA b 615



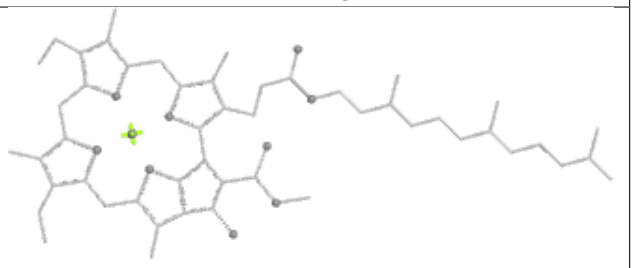
Bond lengths



Bond angles

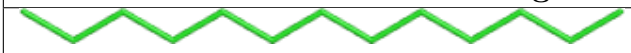


Torsions

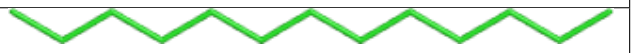


Rings

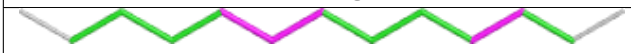
Ligand STE c 516



Bond lengths



Bond angles



Torsions



Rings

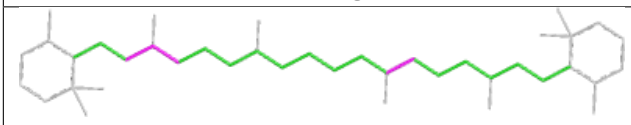
Ligand BCR C 520



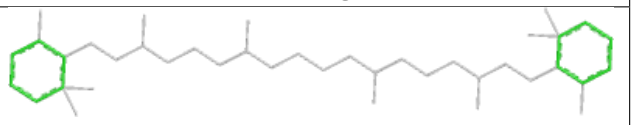
Bond lengths



Bond angles

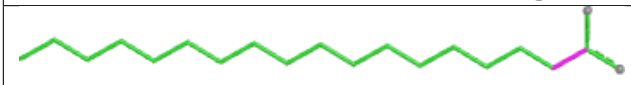


Torsions

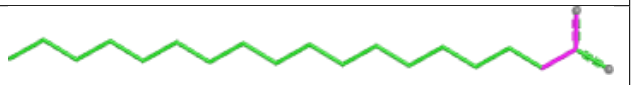


Rings

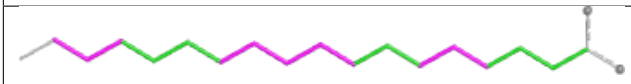
Ligand STE b 622



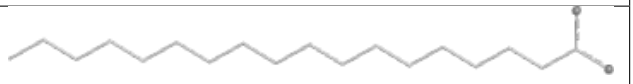
Bond lengths



Bond angles

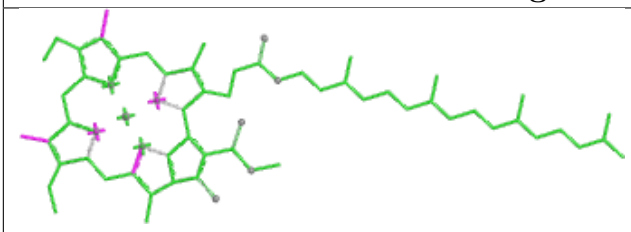


Torsions

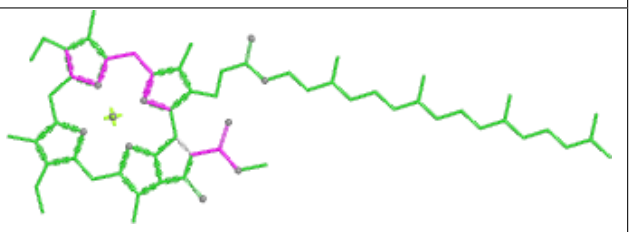


Rings

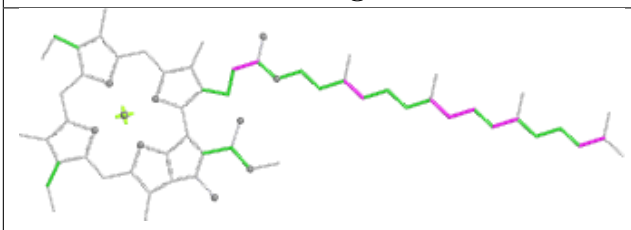
Ligand CLA c 510



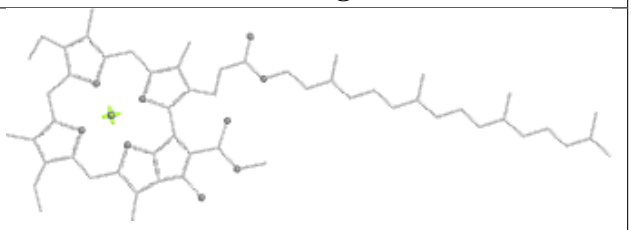
Bond lengths



Bond angles

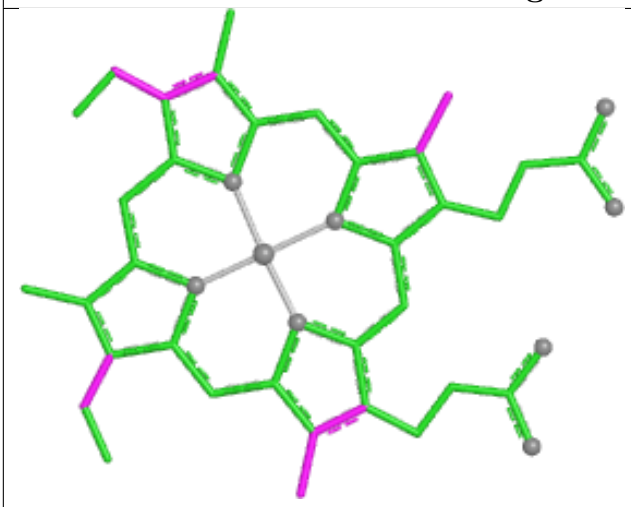


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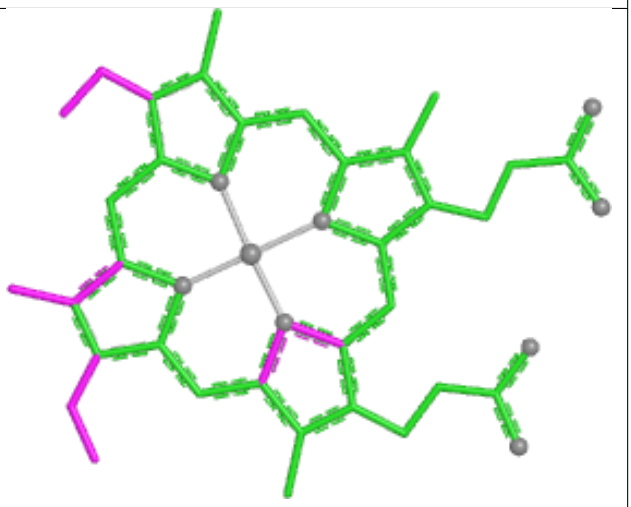


Rings

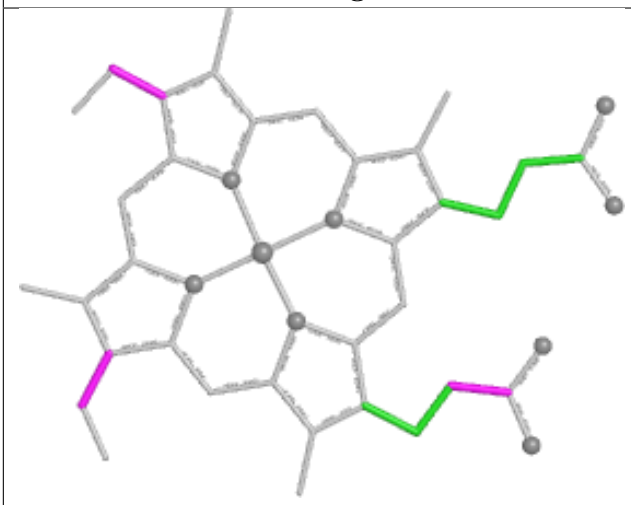
Ligand HEC v 201



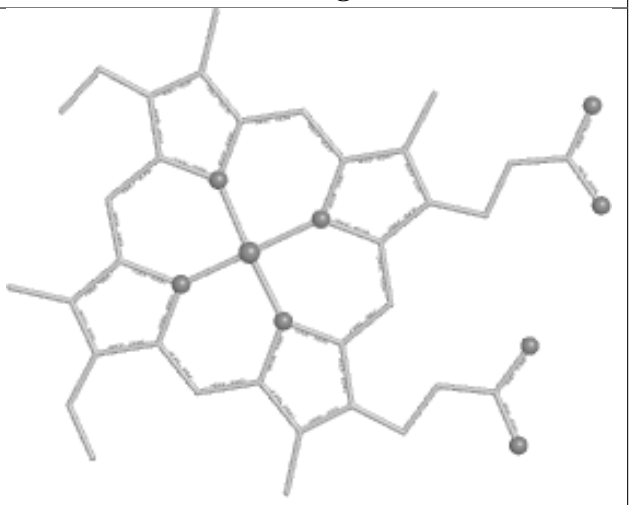
Bond lengths



Bond angles

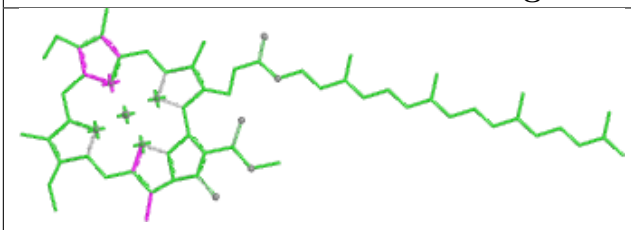


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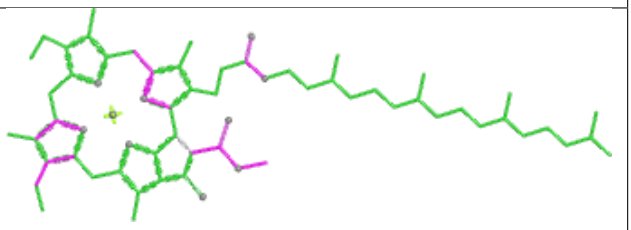


Rings

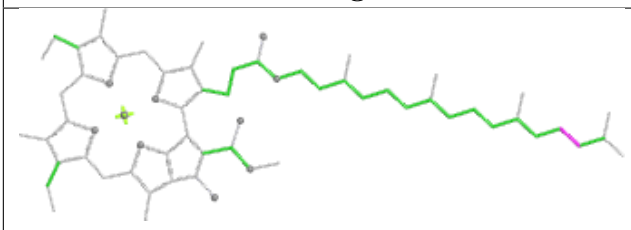
Ligand CLA A 405



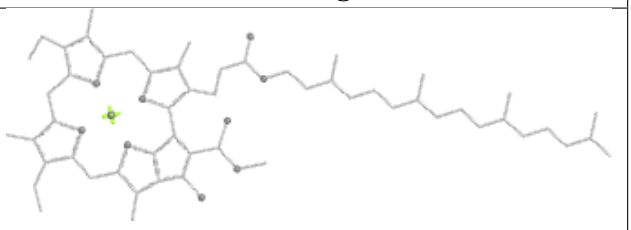
Bond lengths



Bond angles

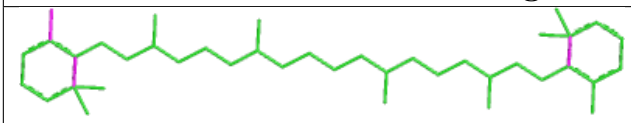


Torsions

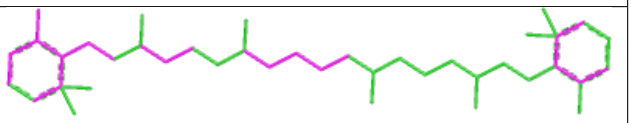


Rings

Ligand BCR B 617



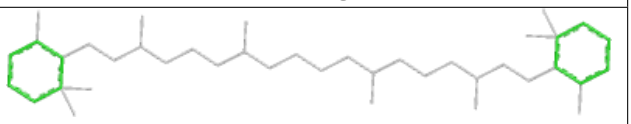
Bond lengths



Bond angles

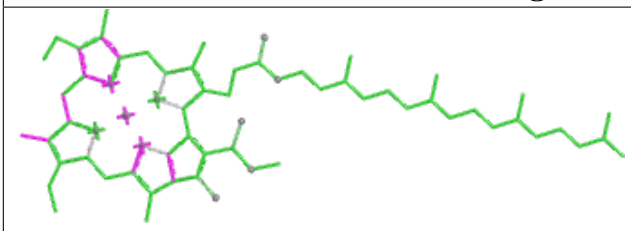


Torsions

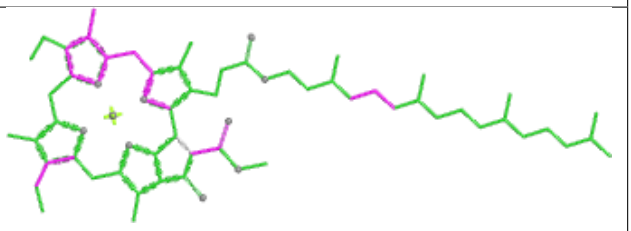


Rings

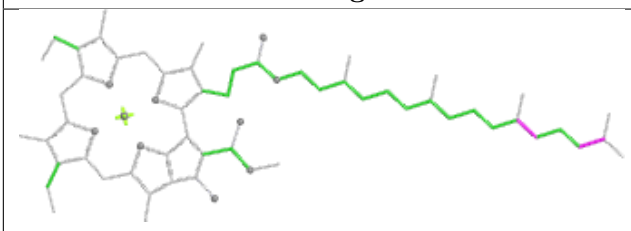
Ligand CLA a 405



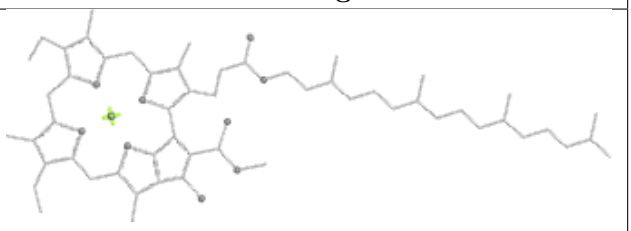
Bond lengths



Bond angles

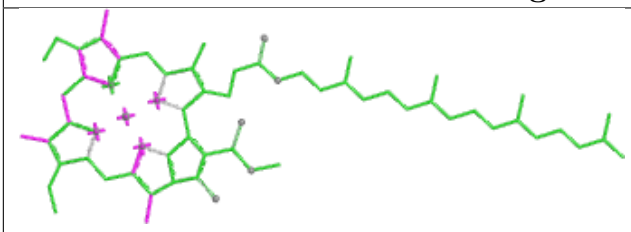


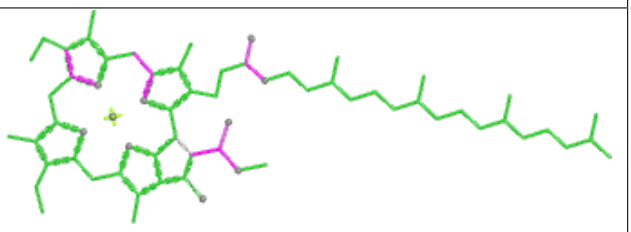
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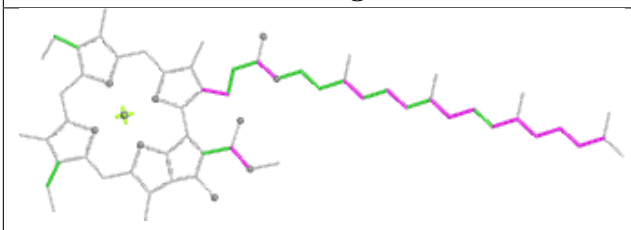


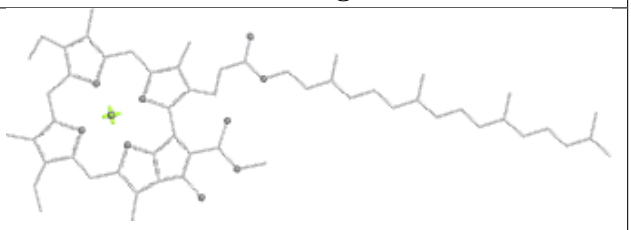
Rings

Ligand CLA c 513


Bond lengths


Bond angles

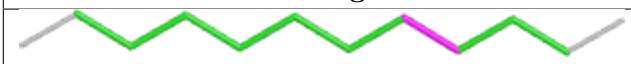

Torsions


Rings

Ligand STE E 103

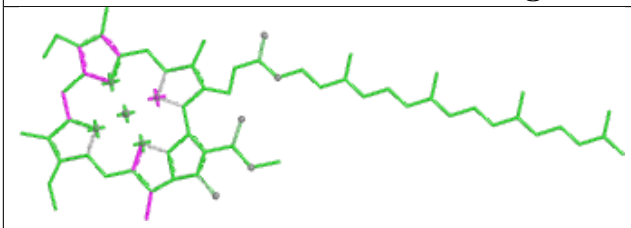

Bond lengths

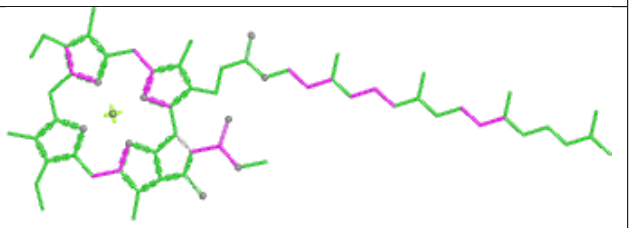

Bond angles

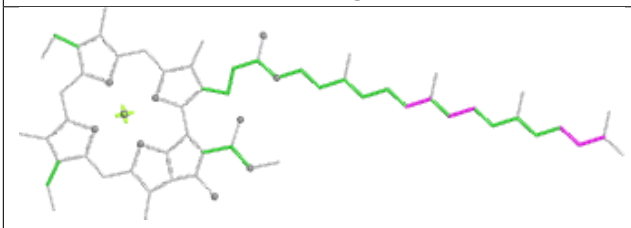

Torsions

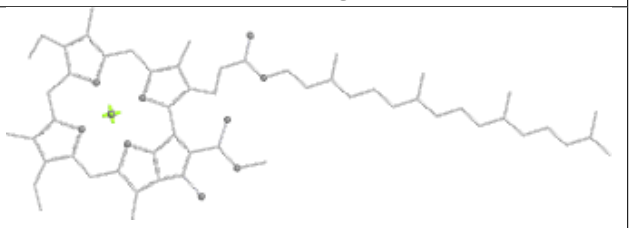

Rings

Ligand CLA B 611


Bond lengths

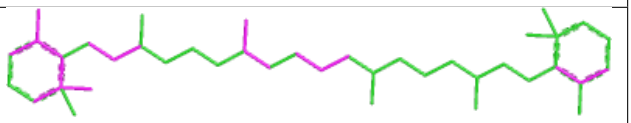

Bond angles

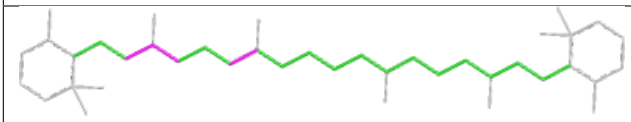

Torsions

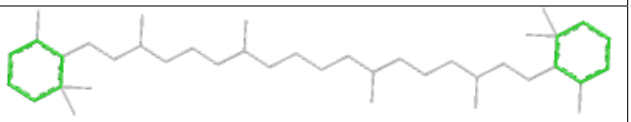

Rings

Ligand BCR c 515

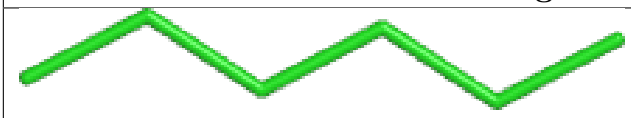

Bond lengths

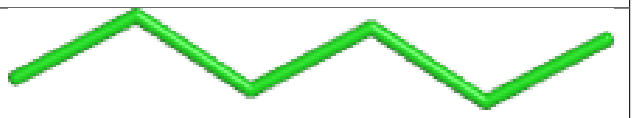

Bond angles

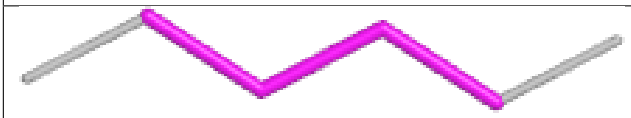

Torsions


Rings

Ligand STE i 102

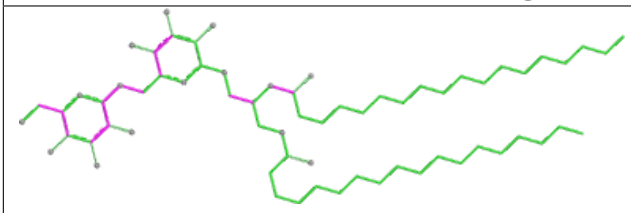

Bond lengths

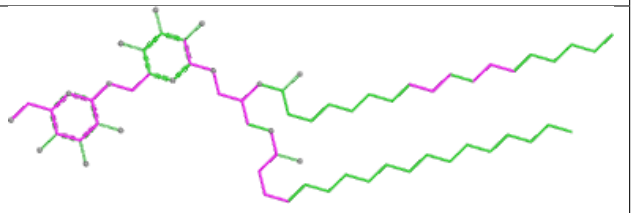

Bond angles

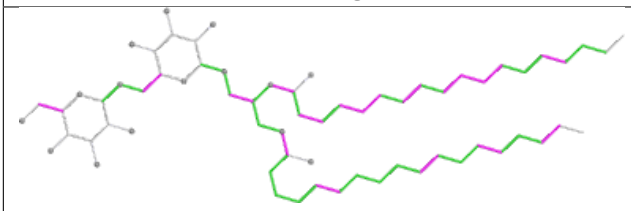

Torsions

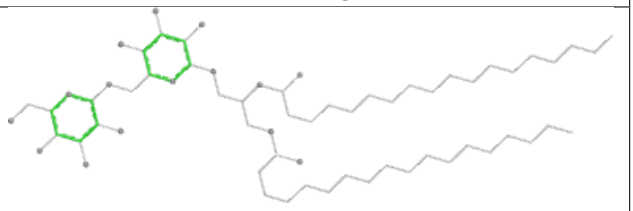

Rings

Ligand DGD A 414

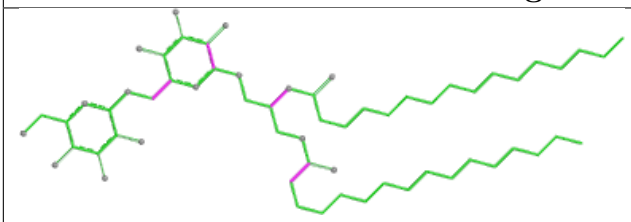

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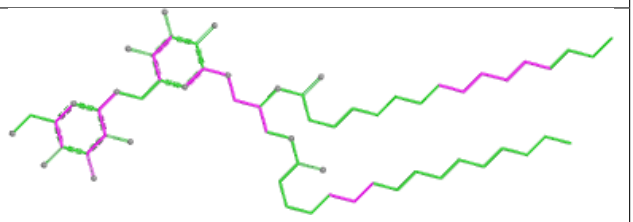

Bond angles

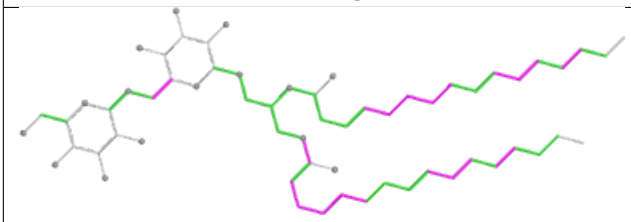

Torsions

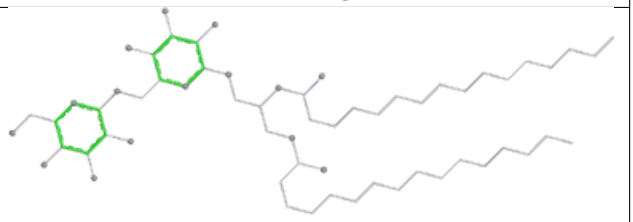

Rings

Ligand DGD c 521

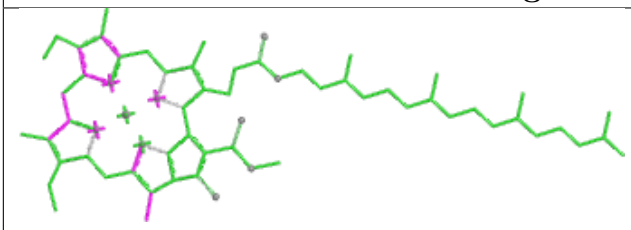

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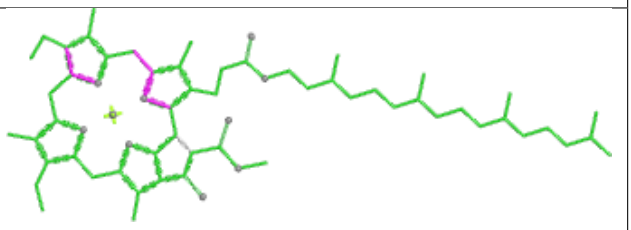

Bond angles

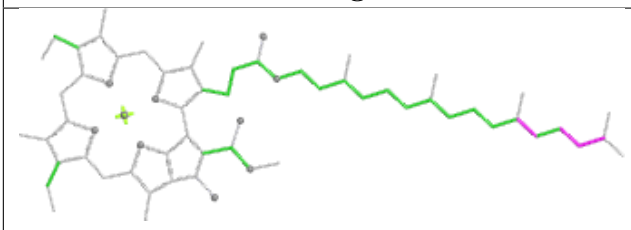

Torsions

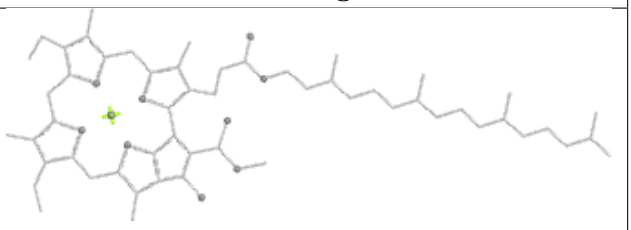

Rings

Ligand CLA D 403


Bond lengths

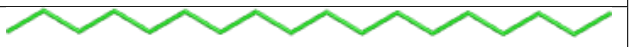

Bond angles


Torsions


Rings

Ligand STE c 517

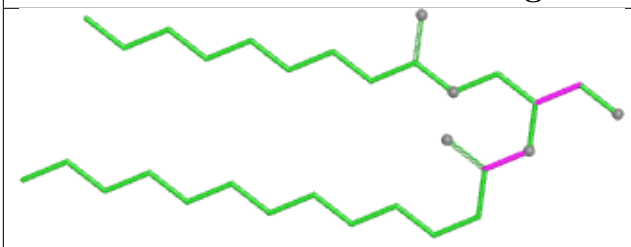

Bond lengths

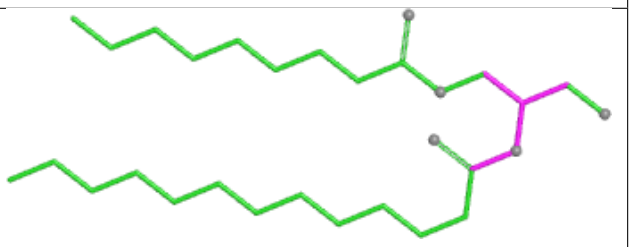

Bond angles

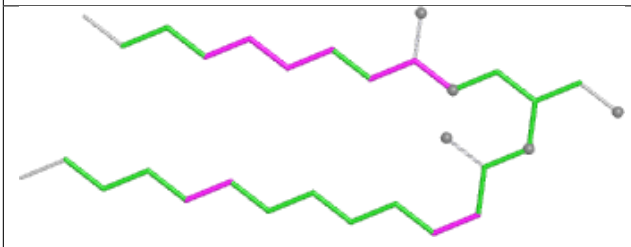

Torsions

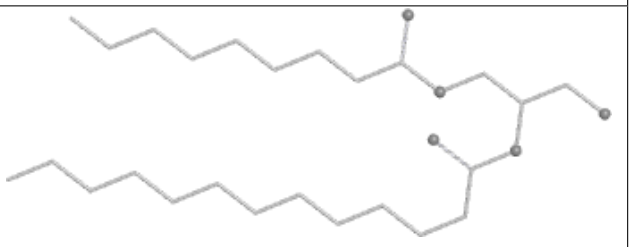

Rings

Ligand LMG c 518


Bond lengths


Bond angles


Torsions


Rings

Ligand STE I 101

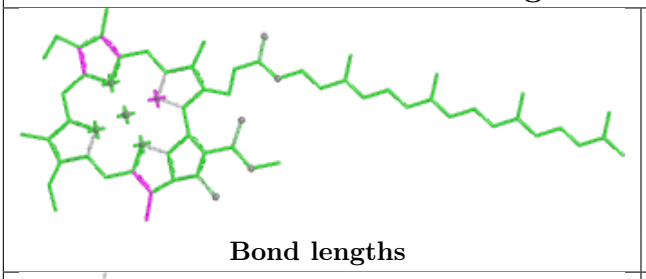

Bond lengths

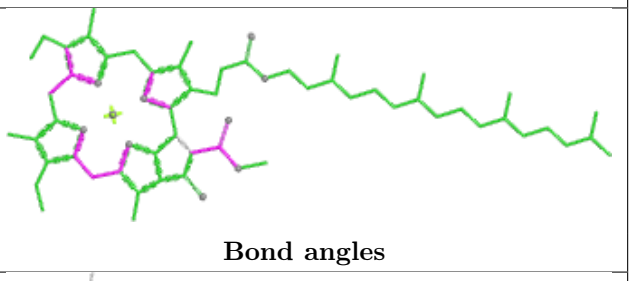

Bond angles

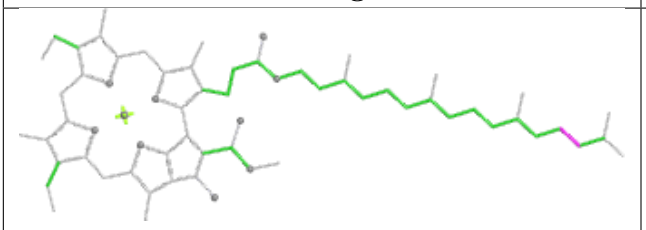

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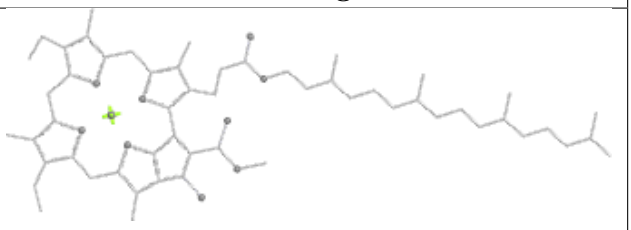

Rings

Ligand CLA B 608

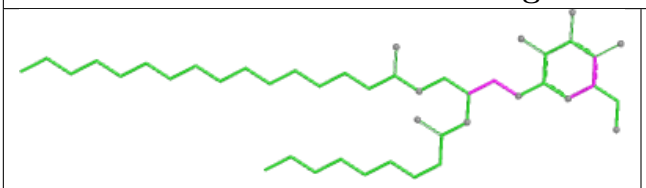

Bond lengths

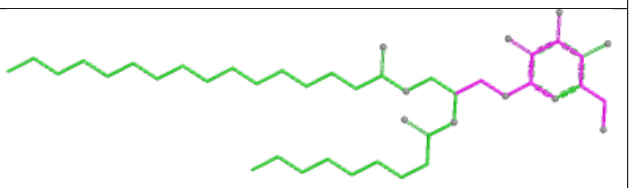

Bond angles

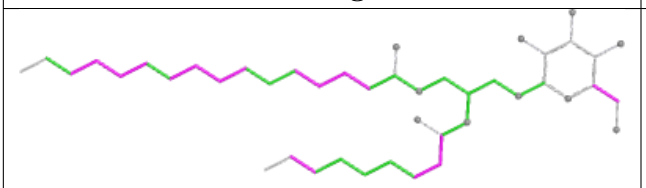

Torsions

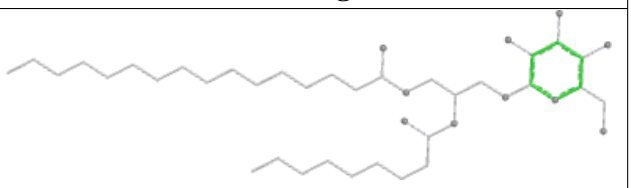

Rings

Ligand LMG d 409


Bond lengths

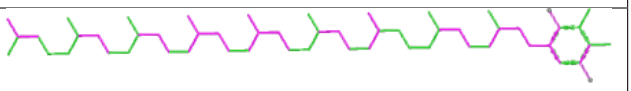

Bond angles

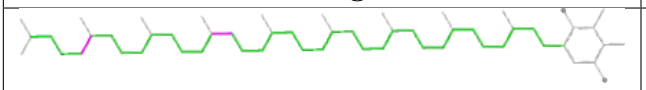

Torsions

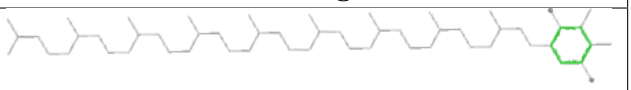

Rings

Ligand PL9 D 407


Bond lengths


Bond angles


Torsions


Rings

Ligand STE e 103

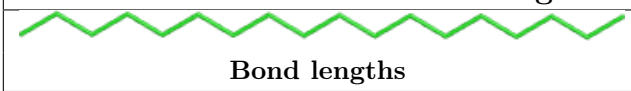

Bond lengths

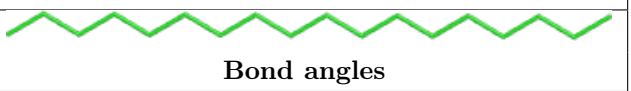

Bond angles

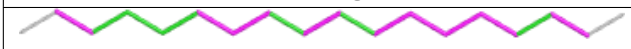

Torsions

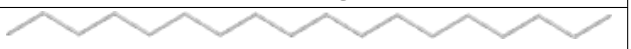

Rings

Ligand STE l 103

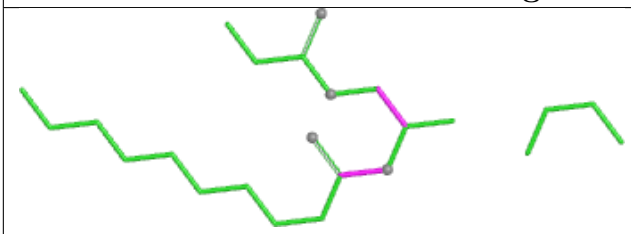

Bond lengths

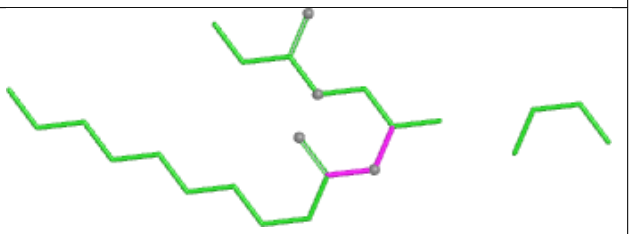

Bond angles

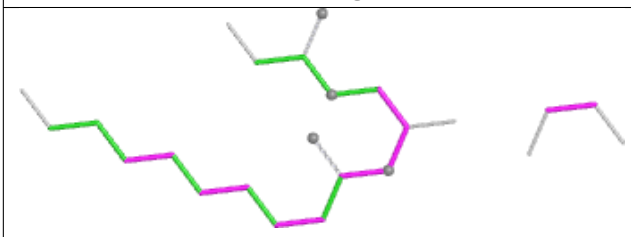

Torsions

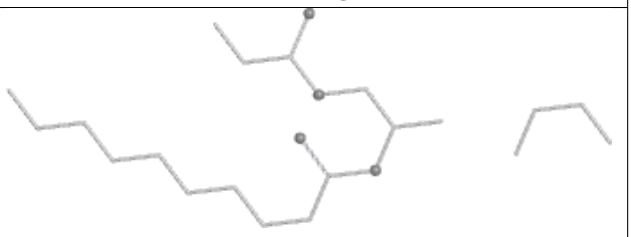

Rings

Ligand LMG b 619


Bond lengths

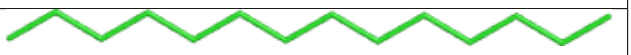

Bond angles


Torsions

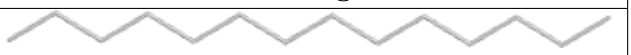

Rings

Ligand STE C 528

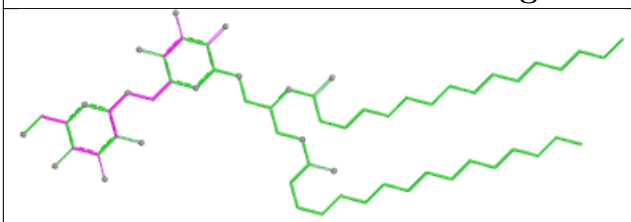

Bond lengths

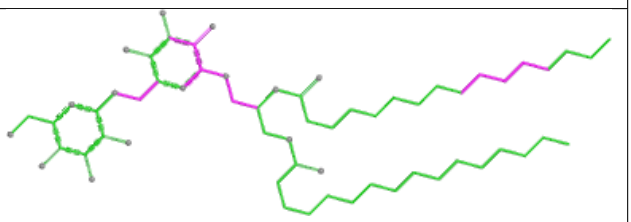

Bond angles

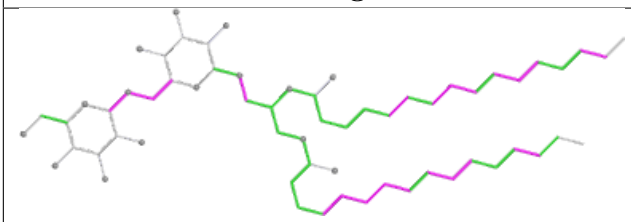

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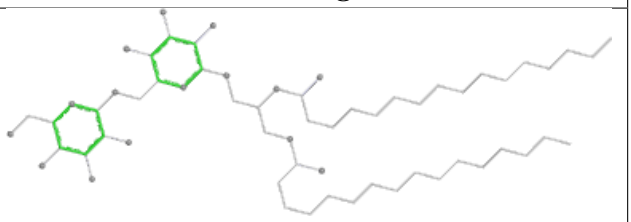

Rings

Ligand DGD C 522

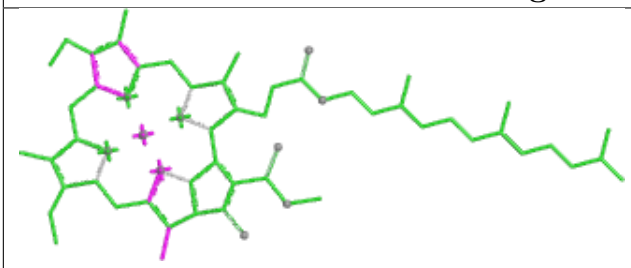

Bond lengths


Bond angles

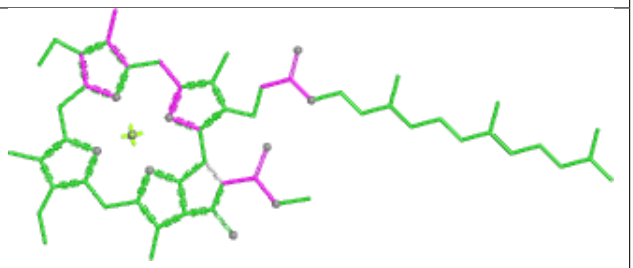

Torsions


Rings

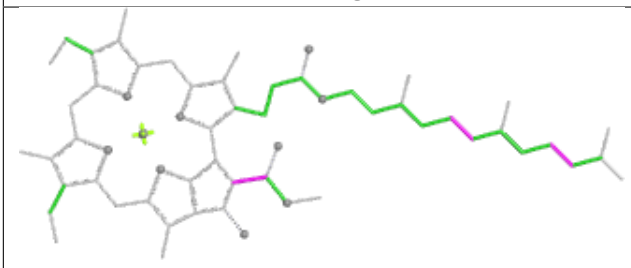
Ligand CLA c 504



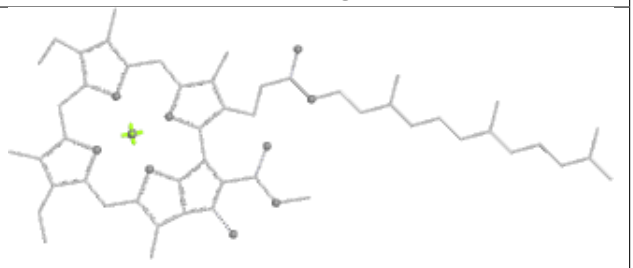
Bond lengths



Bond angles

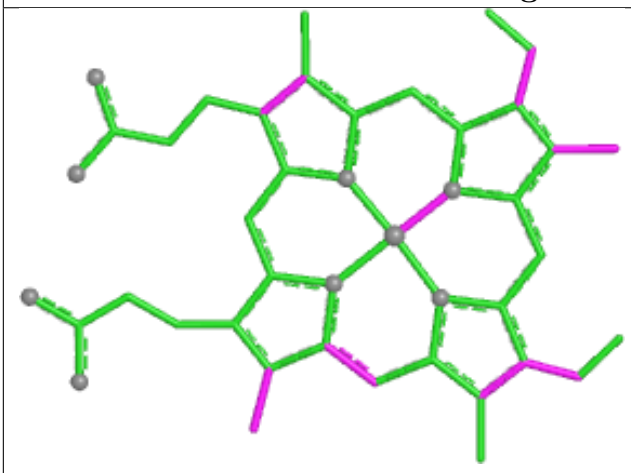


Torsions

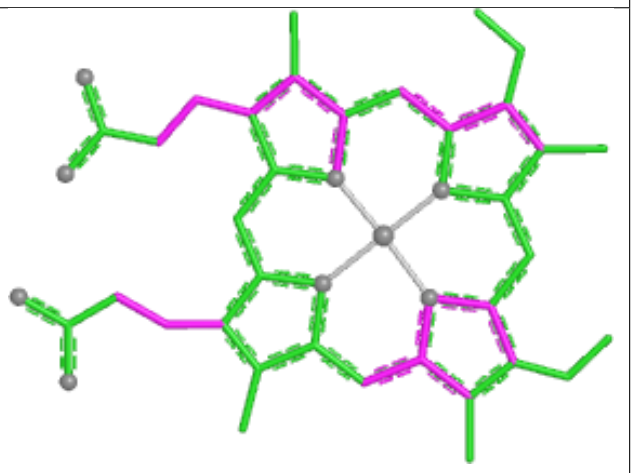


Rings

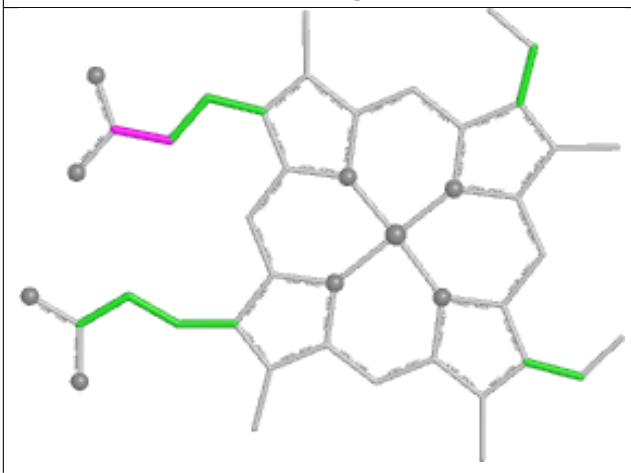
Ligand HEM F 101



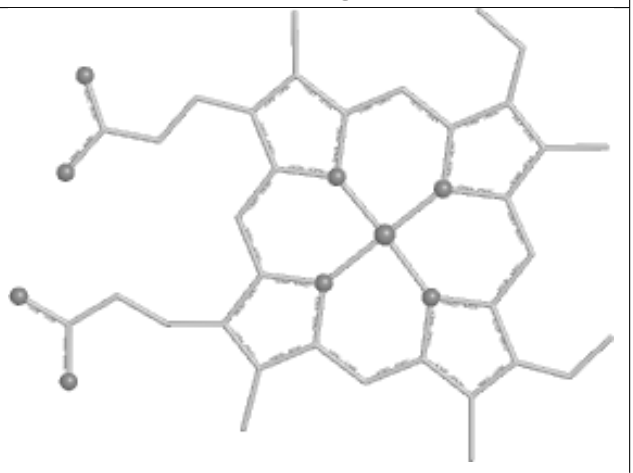
Bond lengths



Bond angles

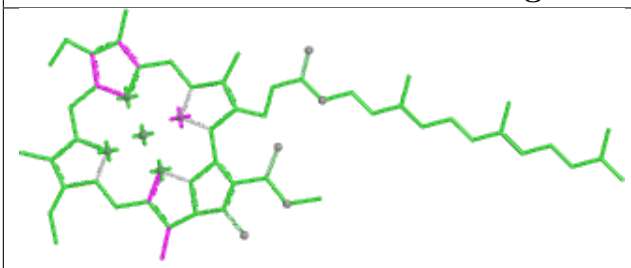


Torsions

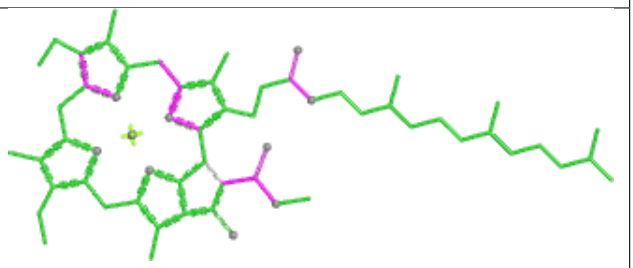


Rings

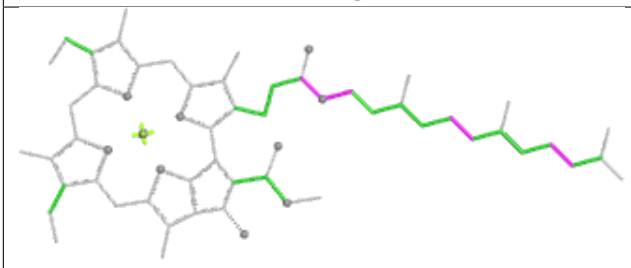
Ligand CLA B 616



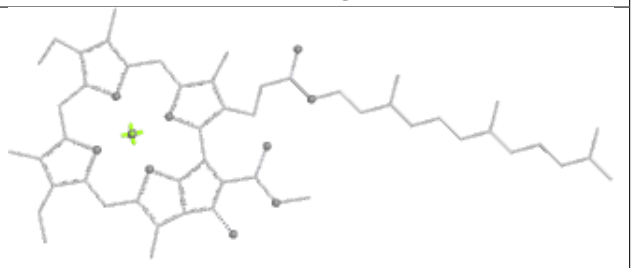
Bond lengths



Bond angles

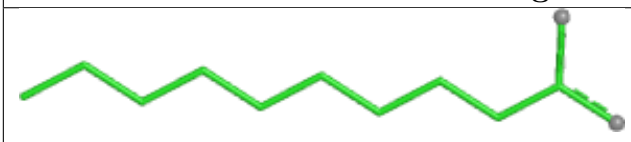


Torsions

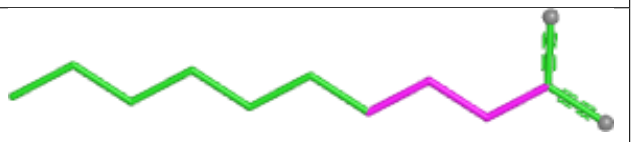


Rings

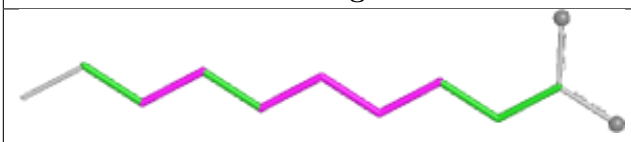
Ligand STE a 417



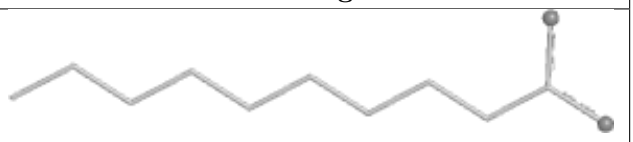
Bond lengths



Bond angles

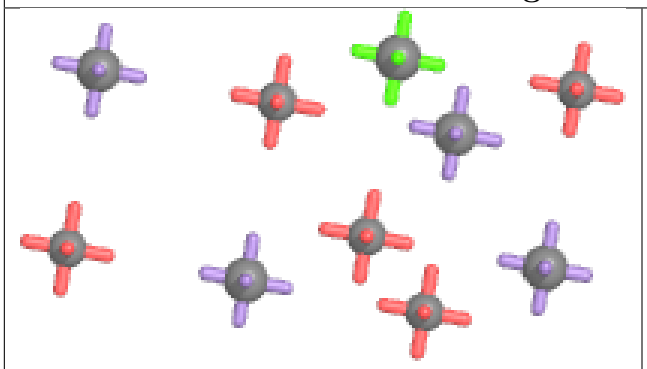


Torsions

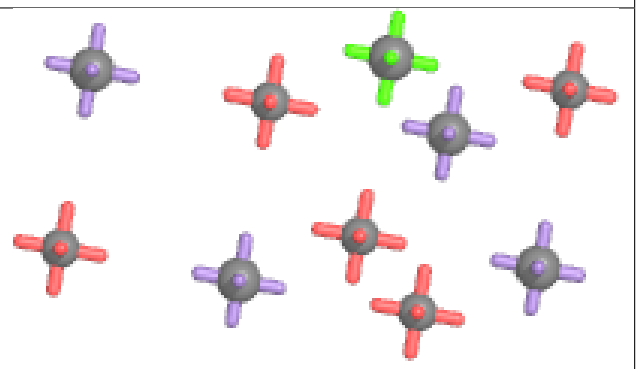


Rings

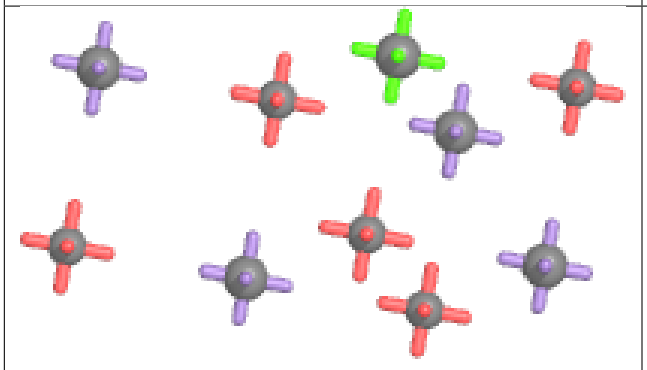
Ligand OEX A 418



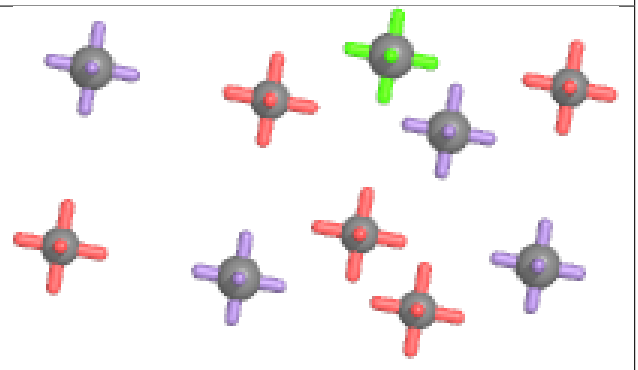
Bond lengths



Bond angles

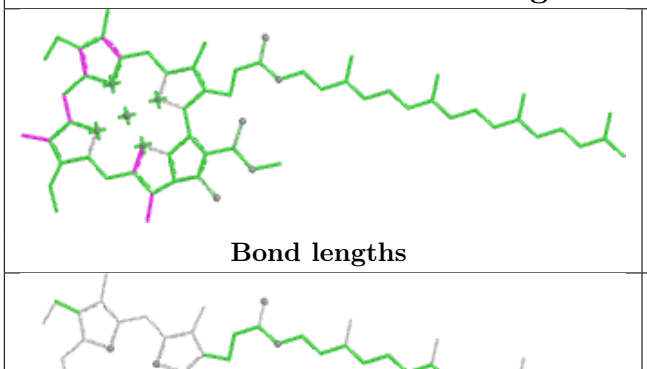


Torsions

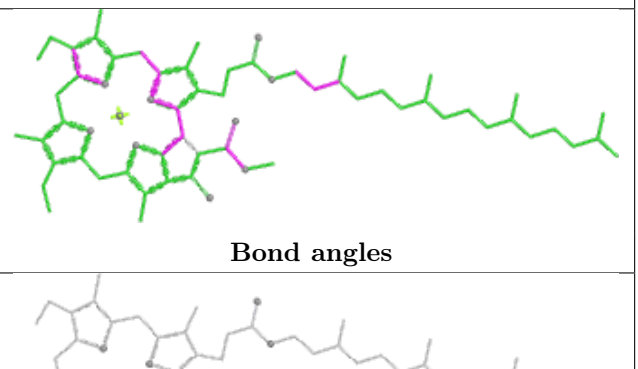


Rings

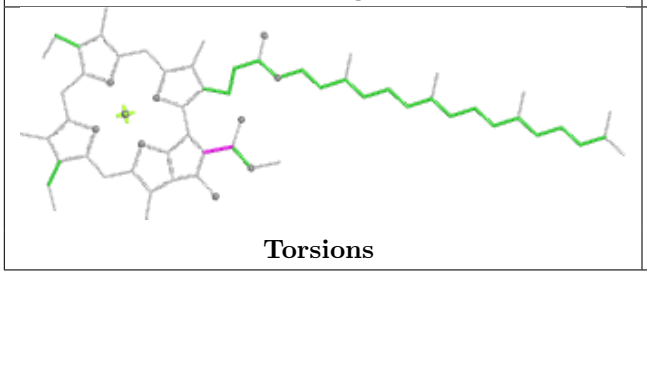
Ligand CLA c 502



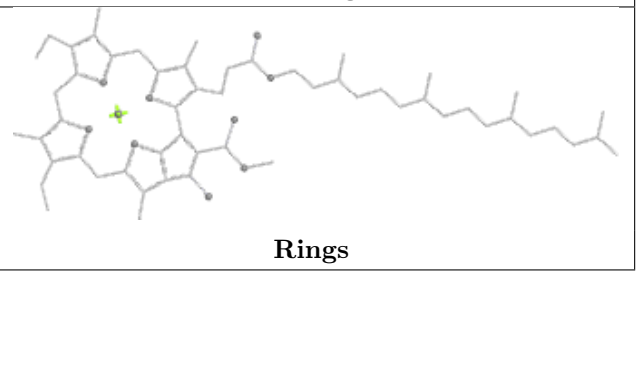
Bond lengths



Bond angles

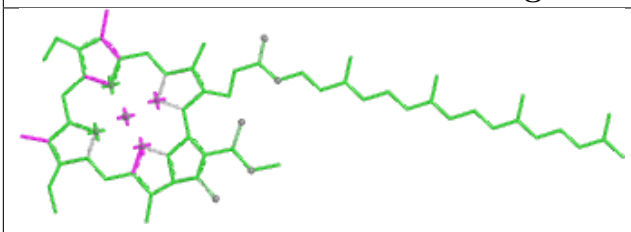


Torsions

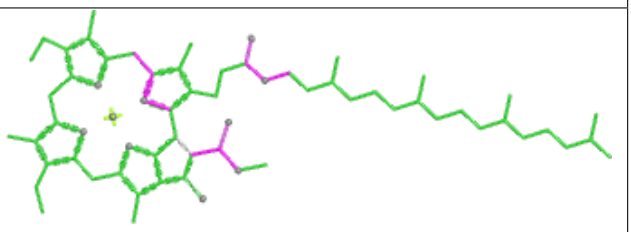


Rings

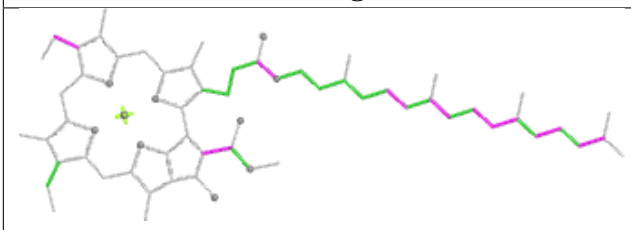
Ligand CLA B 601



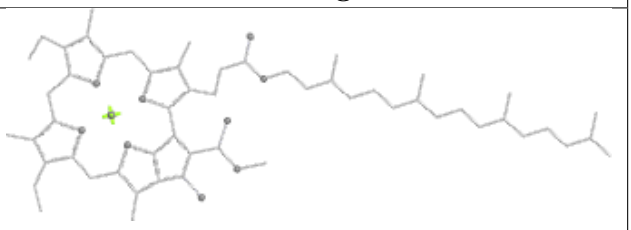
Bond lengths



Bond angles



Torsions



Rings

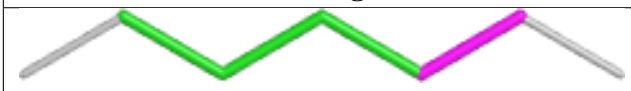
Ligand STE C 519



Bond lengths



Bond angles

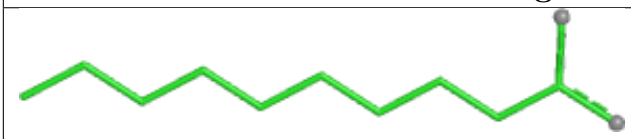


Torsions

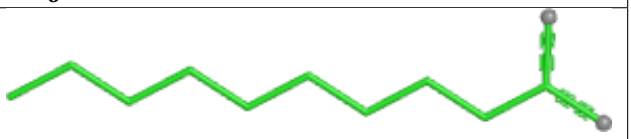


Rings

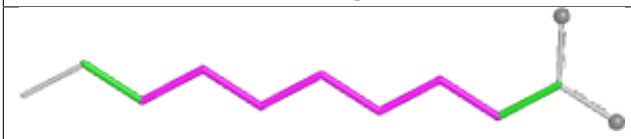
Ligand STE j 101



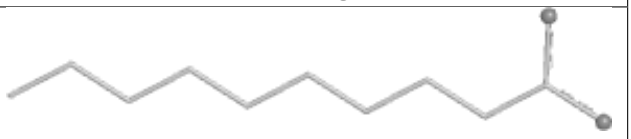
Bond lengths



Bond angles

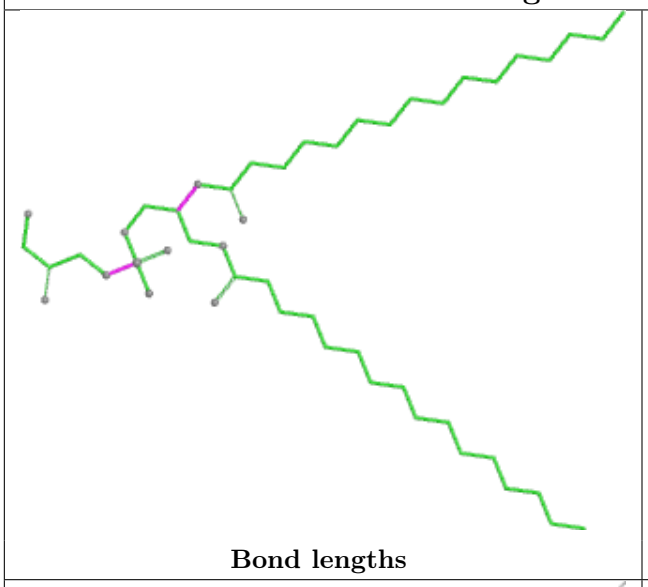


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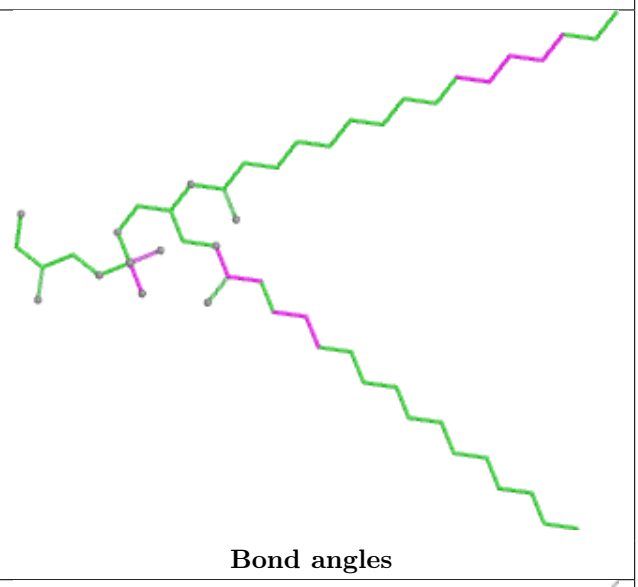


Rings

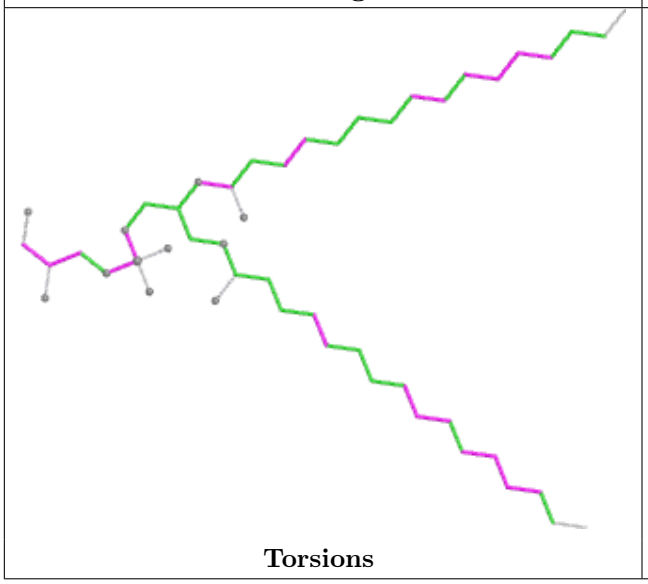
Ligand LHG D 410



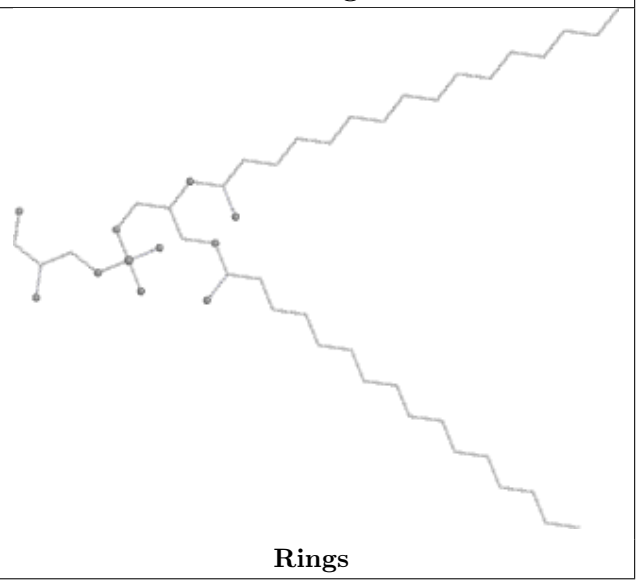
Bond lengths



Bond angles



Torsions

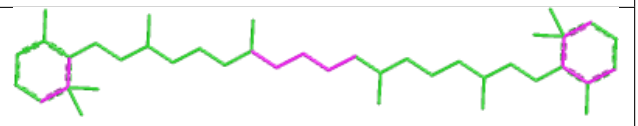


Rings

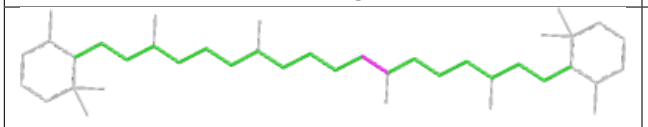
Ligand BCR B 618



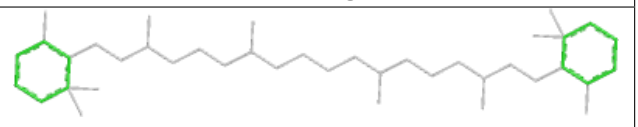
Bond lengths



Bond angles

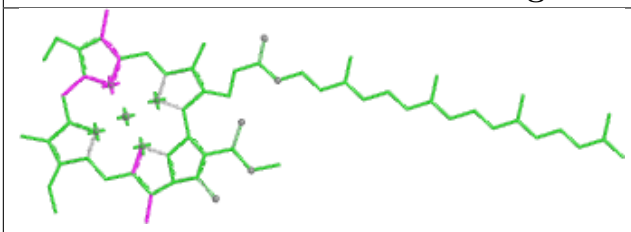


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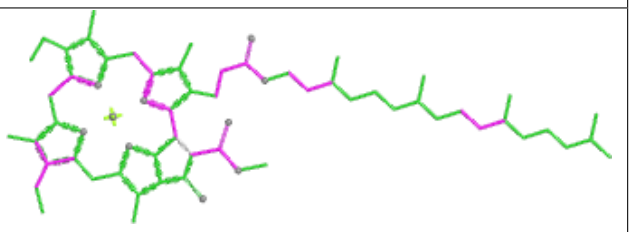


Rings

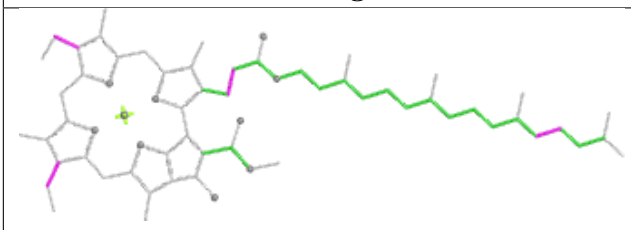
Ligand CLA b 609



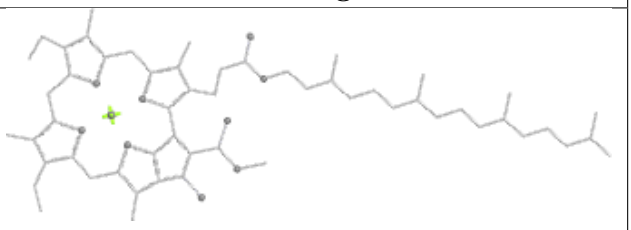
Bond lengths



Bond angles

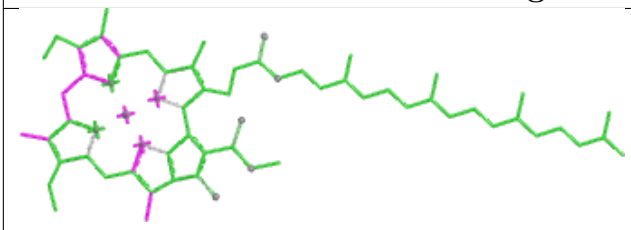


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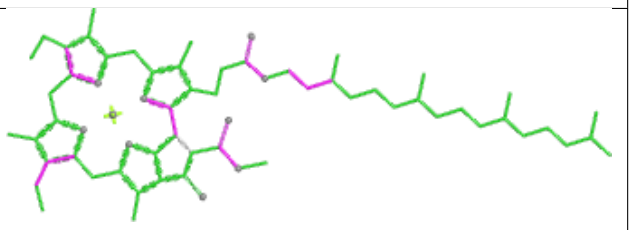


Rings

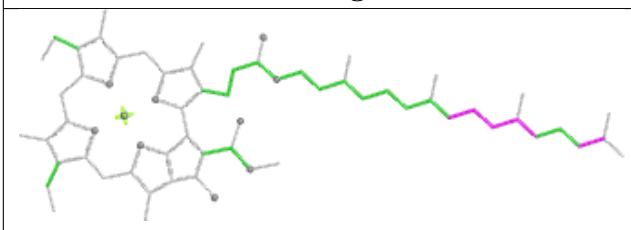
Ligand CLA d 403



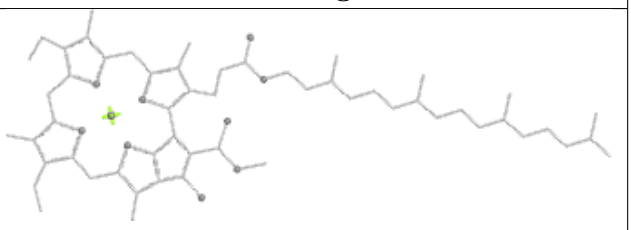
Bond lengths



Bond angles

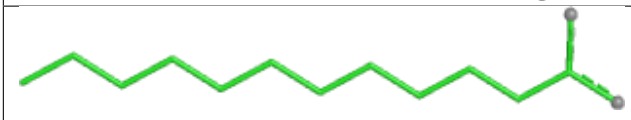


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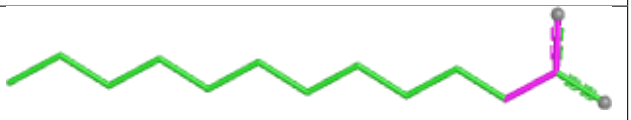


Rings

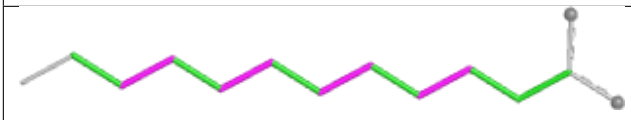
Ligand STE t 102



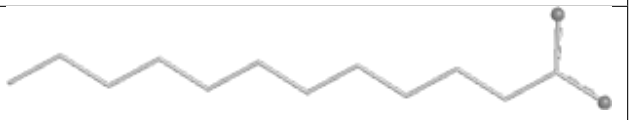
Bond lengths



Bond angles

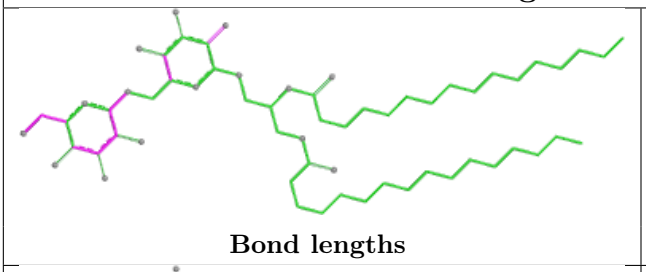


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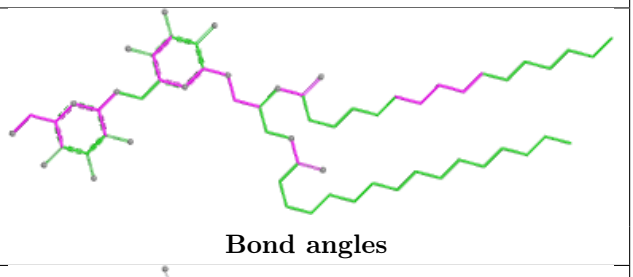


Rings

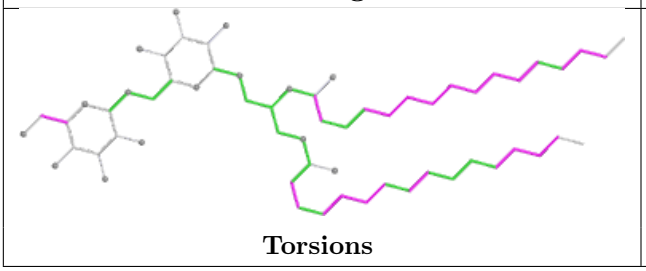
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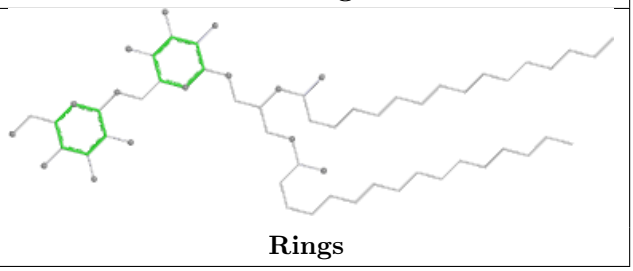
Bond lengths



Bond angles

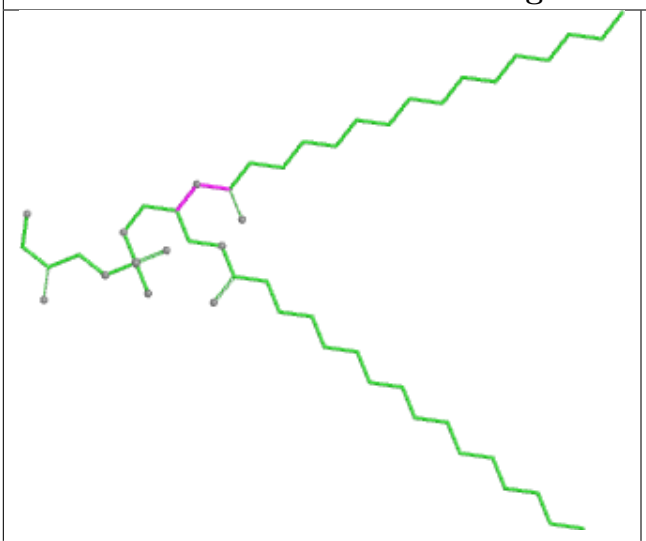


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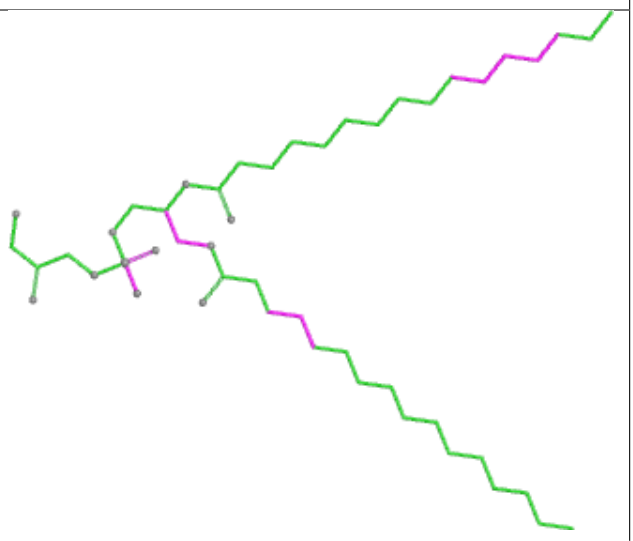


Rings

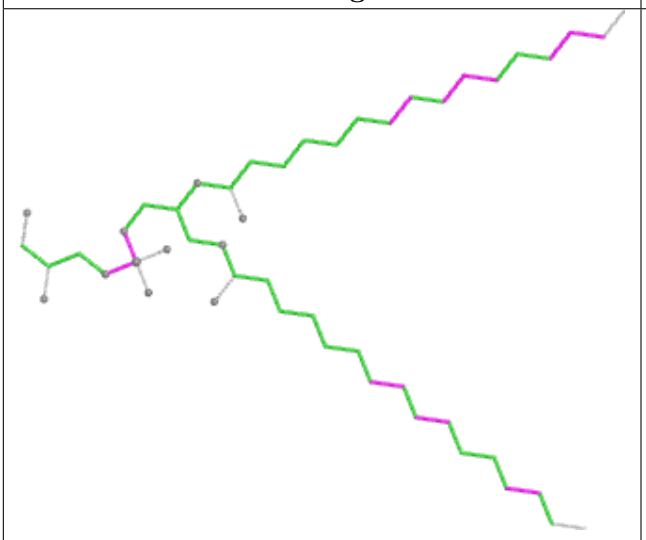
Ligand LHG d 407



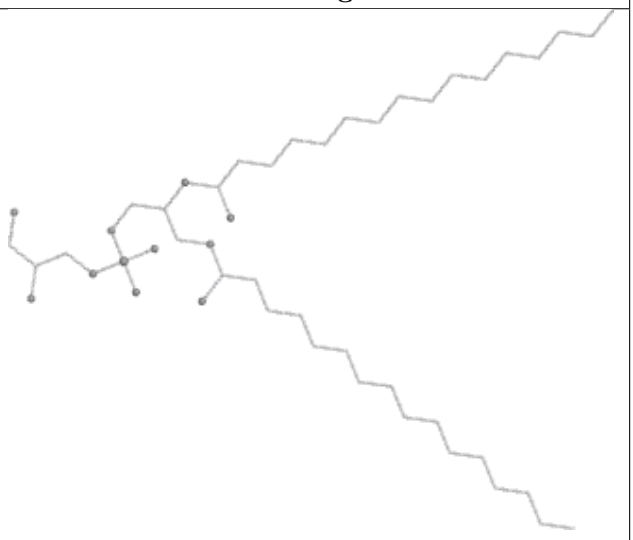
Bond lengths



Bond angles

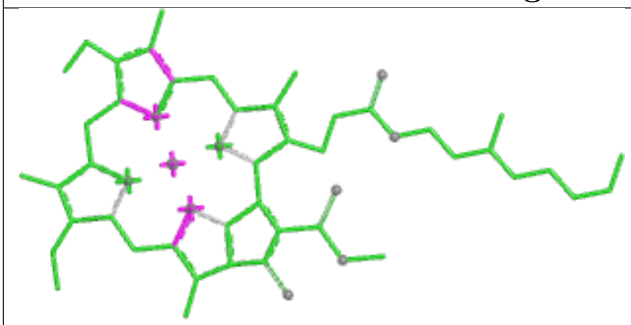


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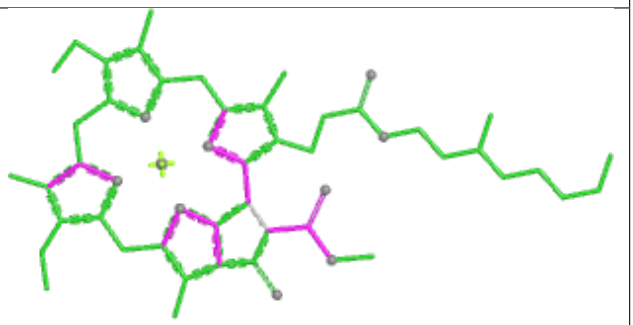


Rings

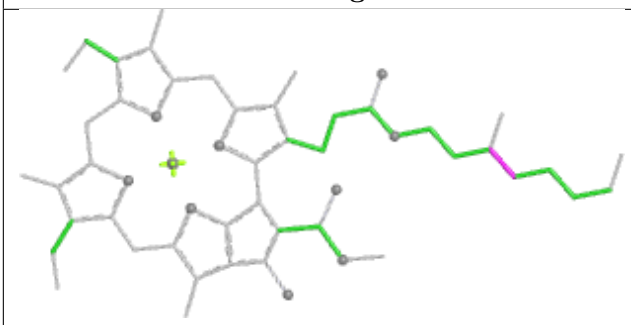
Ligand CLA A 407



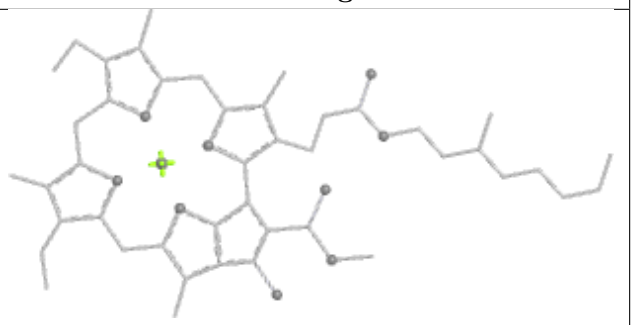
Bond lengths



Bond angles

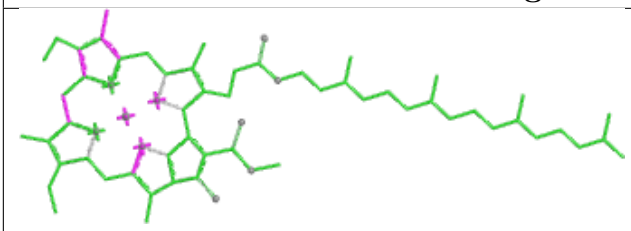


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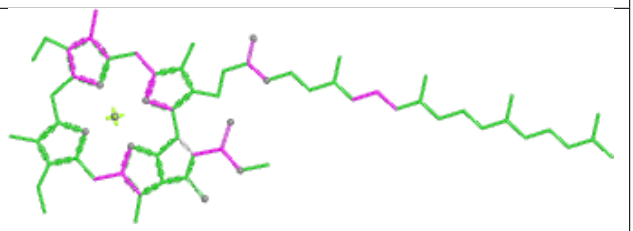


Rings

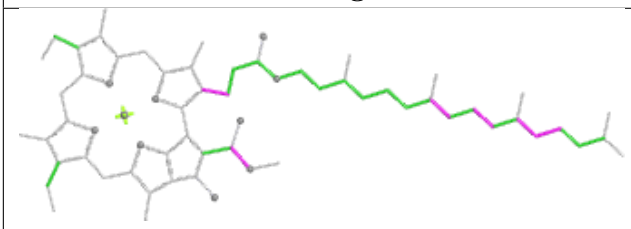
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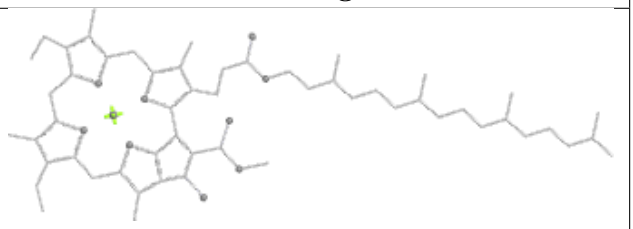
Bond lengths



Bond angles

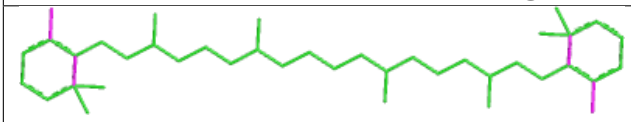


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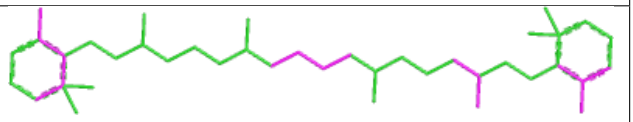


Rings

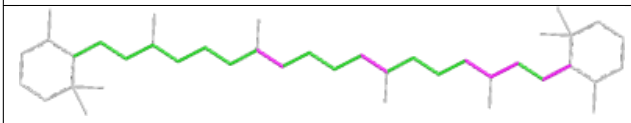
Ligand BCR A 408



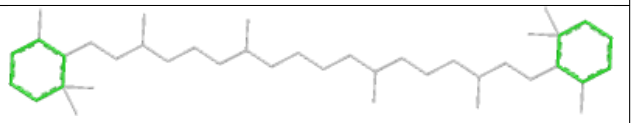
Bond lengths



Bond angles

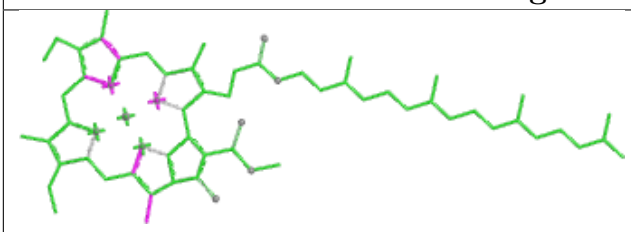


Torsions

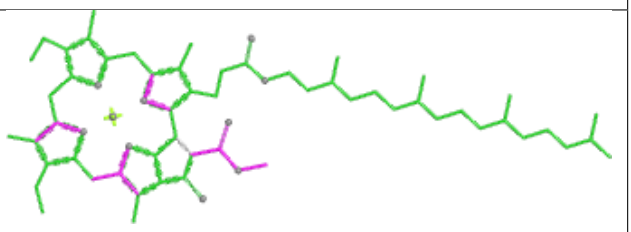


Rings

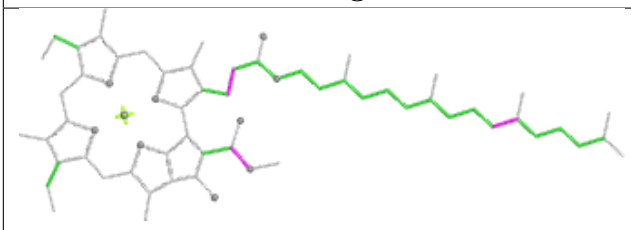
Ligand CLA c 501



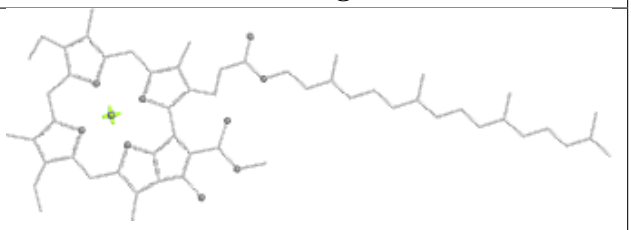
Bond lengths



Bond angles

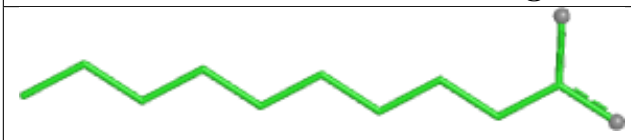


Torsions

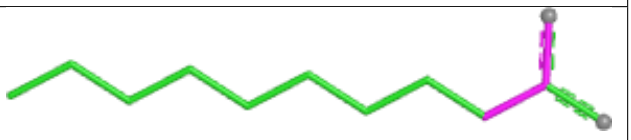


Rings

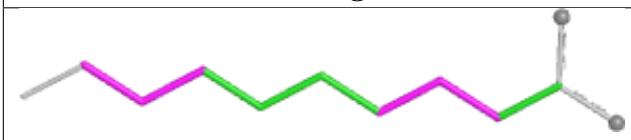
Ligand STE m 101



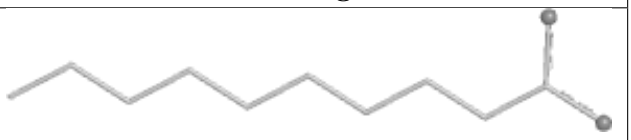
Bond lengths



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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.61	0 100 100	21, 27, 48, 85	0
1	a	334/344 (97%)	-0.53	2 (0%) 85 87	20, 30, 57, 85	0
2	B	505/510 (99%)	-0.46	0 100 100	15, 32, 62, 99	4 (0%)
2	b	505/510 (99%)	-0.32	5 (0%) 79 82	25, 36, 73, 115	1 (0%)
3	C	442/461 (95%)	-0.45	0 100 100	15, 35, 53, 83	1 (0%)
3	c	451/461 (97%)	-0.34	2 (0%) 88 90	18, 39, 63, 99	2 (0%)
4	D	341/352 (96%)	-0.62	0 100 100	19, 29, 47, 85	0
4	d	341/352 (96%)	-0.47	0 100 100	23, 33, 57, 80	1 (0%)
5	E	82/84 (97%)	0.08	1 (1%) 76 79	28, 51, 69, 82	1 (1%)
5	e	82/84 (97%)	0.18	1 (1%) 76 79	37, 60, 78, 94	0
6	F	34/45 (75%)	-0.14	0 100 100	35, 42, 67, 90	0
6	f	34/45 (75%)	0.03	0 100 100	40, 50, 83, 102	0
7	H	65/66 (98%)	-0.25	3 (4%) 37 40	29, 41, 63, 83	0
7	h	63/66 (95%)	-0.03	3 (4%) 35 38	39, 50, 71, 78	0
8	I	35/38 (92%)	-0.44	0 100 100	28, 39, 71, 86	0
8	i	35/38 (92%)	-0.22	0 100 100	32, 40, 80, 86	0
9	J	36/40 (90%)	-0.15	0 100 100	32, 49, 75, 97	0
9	j	36/40 (90%)	-0.03	0 100 100	37, 52, 91, 94	0
10	K	37/46 (80%)	-0.14	0 100 100	40, 50, 76, 78	0
10	k	37/46 (80%)	-0.03	0 100 100	46, 56, 72, 78	0
11	L	37/37 (100%)	-0.57	0 100 100	22, 30, 68, 75	0
11	l	36/37 (97%)	-0.62	0 100 100	24, 30, 78, 83	0
12	M	32/36 (88%)	-0.42	0 100 100	27, 33, 58, 72	0
12	m	31/36 (86%)	-0.49	0 100 100	26, 34, 50, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.28	1 (0%) 88 90	23, 41, 86, 128	1 (0%)
13	o	244/272 (89%)	-0.32	1 (0%) 88 90	23, 40, 81, 130	0
14	T	29/32 (90%)	-0.54	2 (6%) 23 24	24, 30, 62, 80	0
14	t	29/32 (90%)	-0.45	2 (6%) 23 24	25, 30, 86, 96	0
15	U	97/134 (72%)	-0.22	0 100 100	28, 43, 69, 89	0
15	u	97/134 (72%)	-0.33	1 (1%) 79 82	27, 40, 56, 85	0
16	V	137/163 (84%)	-0.42	0 100 100	28, 39, 58, 77	0
16	v	137/163 (84%)	-0.18	0 100 100	31, 47, 70, 91	0
17	Y	27/46 (58%)	0.96	3 (11%) 10 11	53, 77, 91, 106	0
17	y	30/46 (65%)	0.55	0 100 100	60, 74, 95, 99	0
18	X	38/41 (92%)	-0.12	1 (2%) 57 61	37, 50, 79, 87	0
18	x	39/41 (95%)	0.10	1 (2%) 57 61	50, 60, 89, 100	0
19	Z	62/62 (100%)	0.67	4 (6%) 25 26	54, 70, 112, 124	0
19	z	62/62 (100%)	0.58	1 (1%) 70 74	54, 73, 107, 124	0
20	R	28/41 (68%)	0.70	1 (3%) 46 49	63, 74, 92, 102	0
20	r	28/41 (68%)	1.49	9 (32%) 1 1	77, 104, 114, 124	0
All	All	5293/5700 (92%)	-0.33	44 (0%) 82 85	15, 37, 75, 130	11 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	h	64	ALA	4.2
14	t	30	THR	4.1
3	c	23	ALA	3.5
7	H	41	PHE	3.5
13	o	58	ASN	3.5
19	z	33	TRP	3.3
18	x	40	SER	3.0
2	b	499	VAL	3.0
17	Y	20	ALA	2.9
1	a	11	ALA	2.9
17	Y	22	LEU	2.9
2	b	495	PHE	2.9
7	h	41	PHE	2.7
20	r	27	ALA	2.7
7	H	65	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
20	r	14	LEU	2.7
1	a	248	ILE	2.6
19	Z	62	VAL	2.6
14	T	29	ILE	2.6
20	r	20	VAL	2.5
20	R	7	VAL	2.4
19	Z	3	ILE	2.4
20	r	28	VAL	2.4
17	Y	25	ILE	2.3
20	r	29	LYS	2.3
13	O	60	ARG	2.3
3	c	24	THR	2.2
15	u	53	ALA	2.2
5	E	79	PHE	2.2
5	e	79	PHE	2.2
7	h	6	TRP	2.2
19	Z	41	PHE	2.2
20	r	3	TRP	2.2
18	X	2	THR	2.2
7	H	66	GLY	2.2
2	b	491	VAL	2.1
20	r	19	ALA	2.1
19	Z	33	TRP	2.1
20	r	10	LEU	2.1
20	r	12	VAL	2.0
14	t	29	ILE	2.0
2	b	84	THR	2.0
14	T	30	THR	2.0
2	b	502	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.96	0.07	37,48,62,65	0
12	FME	M	1	10/11	0.96	0.09	39,50,77,85	0
14	FME	T	1	10/11	0.96	0.08	27,45,62,62	0
14	FME	t	1	10/11	0.96	0.07	23,40,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.98	0.05	41,49,59,64	0
12	FME	m	1	10/11	0.98	0.05	31,44,69,83	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	STE	i	102	6/20	0.63	0.22	66,89,108,108	0
27	STE	i	101	12/20	0.68	0.18	58,75,94,95	0
27	STE	c	517	18/20	0.68	0.17	50,81,102,102	0
27	STE	C	527	8/20	0.69	0.24	38,55,61,70	0
27	STE	C	529	14/20	0.70	0.15	53,78,105,109	0
27	STE	I	102	17/20	0.73	0.15	56,72,86,87	0
27	STE	H	103	18/20	0.73	0.18	47,73,92,93	0
28	LMG	b	619	24/55	0.73	0.24	40,54,75,79	0
27	STE	A	417	11/20	0.74	0.21	45,56,73,77	0
27	STE	C	528	14/20	0.75	0.23	43,61,87,92	0
27	STE	j	102	16/20	0.76	0.20	42,60,69,70	0
27	STE	e	101	9/20	0.77	0.25	44,50,58,62	0
27	STE	B	623	15/20	0.77	0.20	38,62,88,89	0
27	STE	I	101	15/20	0.77	0.17	36,58,84,88	0
27	STE	E	102	12/20	0.77	0.18	50,74,88,91	0
27	STE	E	104	20/20	0.77	0.14	52,67,80,82	0
27	STE	d	411	12/20	0.78	0.13	46,73,99,104	0
27	STE	E	103	12/20	0.78	0.18	49,57,79,82	0
27	STE	A	416	17/20	0.78	0.15	51,74,94,96	0
28	LMG	D	408	50/55	0.79	0.15	35,67,111,123	0
33	LHG	a	413	42/49	0.79	0.15	61,86,110,123	0
27	STE	d	412	10/20	0.80	0.21	43,55,70,73	0
27	STE	a	417	12/20	0.80	0.14	47,66,71,71	0
27	STE	C	516	14/20	0.80	0.15	54,70,89,93	0
28	LMG	c	518	30/55	0.80	0.13	37,70,100,110	0
27	STE	a	416	10/20	0.80	0.14	43,64,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	STE	T	102	16/20	0.81	0.18	38,61,99,102	0
27	STE	b	626	10/20	0.81	0.14	46,58,66,69	0
27	STE	C	518	5/20	0.81	0.14	47,56,67,67	0
28	LMG	C	517	36/55	0.81	0.14	36,65,90,102	0
27	STE	c	516	13/20	0.82	0.13	47,75,84,88	0
27	STE	d	410	17/20	0.82	0.13	35,56,72,74	0
33	LHG	E	101	49/49	0.82	0.14	43,80,110,116	0
28	LMG	a	415	55/55	0.82	0.14	37,64,89,93	0
27	STE	m	102	15/20	0.83	0.15	41,58,87,92	0
27	STE	A	410	9/20	0.83	0.20	46,52,60,64	0
27	STE	B	622	12/20	0.84	0.13	49,66,81,85	0
27	STE	b	625	16/20	0.84	0.15	49,62,85,92	0
28	LMG	b	623	55/55	0.84	0.15	48,77,98,104	0
26	PL9	a	410	55/55	0.84	0.14	41,63,83,95	0
28	LMG	c	523	48/55	0.84	0.14	46,78,112,122	0
27	STE	Z	101	17/20	0.84	0.16	48,69,95,100	0
26	PL9	A	409	55/55	0.84	0.15	37,66,87,103	0
27	STE	C	519	7/20	0.85	0.17	45,47,51,52	0
27	STE	z	101	9/20	0.85	0.16	49,64,75,76	0
29	SQD	A	413	54/54	0.85	0.14	39,60,97,100	0
30	DGD	A	414	66/66	0.85	0.12	43,68,103,107	0
28	LMG	B	620	45/55	0.85	0.13	38,60,103,130	0
27	STE	C	526	16/20	0.85	0.12	36,56,73,74	0
29	SQD	a	414	54/54	0.86	0.14	36,53,87,104	0
27	STE	t	103	18/20	0.87	0.11	46,61,76,78	0
27	STE	b	624	20/20	0.87	0.14	36,54,73,77	0
27	STE	j	101	12/20	0.87	0.10	45,57,63,64	0
27	STE	e	104	13/20	0.87	0.17	61,66,79,81	0
23	CLA	h	101	65/65	0.87	0.12	39,64,95,103	0
28	LMG	C	524	48/55	0.88	0.12	35,69,87,101	0
27	STE	b	622	20/20	0.88	0.10	38,59,75,77	0
27	STE	e	102	8/20	0.88	0.22	48,58,60,67	0
27	STE	x	102	20/20	0.89	0.11	36,55,74,82	0
29	SQD	f	102	41/54	0.89	0.13	50,83,102,112	0
27	STE	C	525	12/20	0.89	0.11	37,50,60,60	0
27	STE	t	102	14/20	0.89	0.10	35,51,61,61	0
27	STE	m	101	12/20	0.89	0.12	44,57,75,75	0
28	LMG	c	522	46/55	0.90	0.11	40,67,84,89	0
27	STE	D	414	9/20	0.90	0.15	39,45,58,58	0
28	LMG	c	524	49/55	0.90	0.10	35,59,92,115	0
27	STE	e	103	9/20	0.90	0.16	46,49,56,57	0
27	STE	b	627	11/20	0.90	0.17	45,52,54,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	LMG	A	411	48/55	0.90	0.10	38,58,77,95	0
29	SQD	l	101	54/54	0.90	0.10	38,62,90,105	0
28	LMG	b	621	51/55	0.90	0.10	38,55,78,90	0
27	STE	J	101	12/20	0.90	0.11	48,62,68,73	0
27	STE	B	621	17/20	0.90	0.10	35,53,70,73	0
28	LMG	M	101	51/55	0.91	0.09	32,51,74,81	0
27	STE	M	103	10/20	0.91	0.11	32,47,57,65	0
32	BCT	a	404	4/4	0.91	0.11	30,30,45,54	0
29	SQD	b	620	49/54	0.91	0.09	38,58,89,103	0
25	BCR	C	514	40/40	0.91	0.11	41,56,69,74	0
27	STE	l	103	18/20	0.92	0.10	35,49,87,89	0
27	STE	M	102	15/20	0.92	0.10	38,47,60,75	0
25	BCR	K	101	40/40	0.92	0.09	33,51,69,76	0
25	BCR	d	404	40/40	0.92	0.09	32,48,86,93	0
25	BCR	k	101	40/40	0.92	0.08	40,56,69,72	0
23	CLA	c	513	65/65	0.93	0.09	41,66,99,112	0
23	CLA	B	601	65/65	0.93	0.09	30,63,91,105	0
27	STE	A	415	8/20	0.93	0.12	41,49,54,55	0
25	BCR	x	101	40/40	0.93	0.08	34,51,70,71	0
29	SQD	A	412	52/54	0.93	0.10	32,62,92,102	0
25	BCR	c	514	40/40	0.93	0.08	43,59,73,73	0
29	SQD	F	102	36/54	0.93	0.09	43,70,88,99	0
29	SQD	a	412	54/54	0.93	0.09	38,68,90,94	0
25	BCR	D	406	40/40	0.94	0.09	24,42,77,89	0
25	BCR	H	101	40/40	0.94	0.07	29,43,58,61	0
30	DGD	C	522	62/66	0.94	0.09	28,52,100,111	0
30	DGD	H	102	62/66	0.94	0.08	26,45,61,64	0
30	DGD	c	520	62/66	0.94	0.08	29,52,91,99	0
30	DGD	h	102	62/66	0.94	0.09	24,49,60,71	0
23	CLA	c	512	65/65	0.94	0.08	37,56,96,103	0
23	CLA	C	513	65/65	0.94	0.09	38,62,92,99	0
27	STE	D	413	20/20	0.94	0.08	30,47,73,81	0
33	LHG	d	406	49/49	0.94	0.10	33,52,73,84	0
23	CLA	C	510	65/65	0.95	0.07	25,40,61,63	0
25	BCR	k	102	40/40	0.95	0.08	35,49,64,69	0
25	BCR	C	515	40/40	0.95	0.07	24,38,49,58	0
25	BCR	C	520	40/40	0.95	0.09	30,48,65,70	0
23	CLA	C	512	65/65	0.95	0.08	34,52,95,108	0
23	CLA	C	503	65/65	0.95	0.06	25,39,51,54	0
25	BCR	A	408	40/40	0.95	0.06	21,34,45,48	0
25	BCR	b	616	40/40	0.95	0.06	26,38,49,52	0
28	LMG	d	409	44/55	0.95	0.09	29,51,86,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	BCT	D	401	4/4	0.95	0.11	26,28,34,40	0
25	BCR	b	618	40/40	0.95	0.06	26,42,59,63	0
25	BCR	B	618	40/40	0.95	0.07	21,37,53,54	0
28	LMG	D	409	51/55	0.95	0.10	24,54,83,89	0
25	BCR	B	619	40/40	0.95	0.07	20,39,59,65	0
25	BCR	T	101	40/40	0.96	0.06	22,36,49,50	0
25	BCR	a	409	40/40	0.96	0.05	20,33,44,45	0
23	CLA	c	506	65/65	0.96	0.08	28,45,91,97	0
25	BCR	b	617	40/40	0.96	0.06	24,37,54,55	0
23	CLA	c	508	64/65	0.96	0.08	26,41,95,111	0
23	CLA	c	509	65/65	0.96	0.07	27,43,67,72	0
25	BCR	c	515	40/40	0.96	0.07	28,42,57,65	0
23	CLA	c	511	65/65	0.96	0.07	35,49,69,71	0
23	CLA	C	509	65/65	0.96	0.07	22,41,62,69	0
23	CLA	C	502	65/65	0.96	0.06	23,37,56,61	0
25	BCR	t	101	40/40	0.96	0.06	22,36,53,53	0
23	CLA	d	403	65/65	0.96	0.08	26,46,89,98	0
23	CLA	C	511	65/65	0.96	0.07	28,46,65,71	0
24	PHO	a	407	64/64	0.96	0.06	17,28,39,40	0
26	PL9	d	405	55/55	0.96	0.06	20,33,45,50	0
24	PHO	d	401	64/64	0.96	0.06	24,35,48,48	0
23	CLA	B	606	65/65	0.96	0.07	21,32,69,72	0
25	BCR	B	617	40/40	0.96	0.06	23,34,54,56	0
30	DGD	C	523	62/66	0.96	0.08	25,48,79,87	0
23	CLA	C	505	65/65	0.96	0.08	21,36,71,85	0
23	CLA	b	601	65/65	0.96	0.07	24,40,60,66	0
30	DGD	c	521	62/66	0.96	0.08	24,53,88,94	0
23	CLA	b	605	65/65	0.96	0.07	21,36,74,84	0
23	CLA	b	608	65/65	0.96	0.07	24,42,62,67	0
23	CLA	b	609	65/65	0.96	0.07	23,36,48,51	0
33	LHG	D	411	47/49	0.96	0.09	23,48,78,94	0
33	LHG	D	412	49/49	0.96	0.09	27,44,73,79	0
23	CLA	b	614	65/65	0.96	0.07	24,38,61,64	0
23	CLA	b	615	60/65	0.96	0.08	25,38,95,99	0
23	CLA	c	503	65/65	0.96	0.06	29,42,52,60	0
33	LHG	d	408	39/49	0.96	0.08	30,43,74,86	0
33	LHG	l	102	49/49	0.96	0.07	25,43,59,71	0
23	CLA	c	510	65/65	0.97	0.06	26,45,63,67	0
23	CLA	C	506	65/65	0.97	0.07	20,38,96,105	0
23	CLA	C	507	65/65	0.97	0.06	21,37,63,67	0
23	CLA	C	508	65/65	0.97	0.07	23,38,101,106	0
23	CLA	d	402	65/65	0.97	0.06	17,31,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	A	404	65/65	0.97	0.06	12,26,48,57	0
23	CLA	B	607	65/65	0.97	0.07	16,31,62,64	0
24	PHO	A	406	64/64	0.97	0.05	21,31,41,48	0
24	PHO	D	402	64/64	0.97	0.05	16,26,35,39	0
23	CLA	B	608	65/65	0.97	0.05	18,34,52,61	0
23	CLA	B	609	65/65	0.97	0.06	23,34,58,62	0
23	CLA	B	610	65/65	0.97	0.06	19,30,42,46	0
23	CLA	D	403	65/65	0.97	0.05	16,26,50,58	0
23	CLA	D	404	65/65	0.97	0.06	16,27,57,62	0
23	CLA	D	405	65/65	0.97	0.07	21,40,105,116	0
23	CLA	a	405	65/65	0.97	0.06	16,28,49,59	0
23	CLA	a	406	65/65	0.97	0.07	22,35,95,100	0
23	CLA	a	408	65/65	0.97	0.07	18,34,79,90	0
23	CLA	a	411	65/65	0.97	0.06	17,27,49,53	0
23	CLA	B	611	65/65	0.97	0.05	17,29,51,54	0
23	CLA	b	602	65/65	0.97	0.06	21,33,69,82	0
23	CLA	b	603	65/65	0.97	0.07	17,32,81,98	0
23	CLA	b	604	65/65	0.97	0.06	19,32,51,55	0
23	CLA	B	612	65/65	0.97	0.06	18,29,47,51	0
23	CLA	b	606	65/65	0.97	0.07	17,34,67,70	0
23	CLA	b	607	65/65	0.97	0.07	22,40,58,68	0
23	CLA	B	614	65/65	0.97	0.08	19,32,82,94	0
23	CLA	B	615	65/65	0.97	0.06	22,34,62,70	0
23	CLA	b	610	65/65	0.97	0.05	20,30,53,58	0
30	DGD	C	521	62/66	0.97	0.07	18,43,81,98	0
23	CLA	b	611	65/65	0.97	0.06	18,33,49,64	0
23	CLA	b	612	65/65	0.97	0.07	16,31,72,80	0
23	CLA	b	613	65/65	0.97	0.06	22,36,74,85	0
30	DGD	c	519	62/66	0.97	0.07	18,42,79,86	0
23	CLA	B	616	60/65	0.97	0.08	20,34,98,116	0
23	CLA	C	501	65/65	0.97	0.06	19,33,49,58	0
26	PL9	D	407	55/55	0.97	0.05	18,31,46,50	0
23	CLA	c	501	65/65	0.97	0.06	26,36,50,57	0
23	CLA	c	502	65/65	0.97	0.06	26,39,59,63	0
33	LHG	D	410	49/49	0.97	0.06	18,41,53,62	0
23	CLA	B	602	65/65	0.97	0.06	20,33,56,62	0
23	CLA	c	504	60/65	0.97	0.07	27,44,81,84	0
23	CLA	c	505	65/65	0.97	0.07	24,38,69,81	0
33	LHG	L	101	49/49	0.97	0.06	22,42,59,69	0
23	CLA	B	604	65/65	0.97	0.06	18,28,70,78	0
23	CLA	c	507	65/65	0.97	0.06	25,41,56,72	0
33	LHG	d	407	49/49	0.97	0.07	27,42,56,63	0

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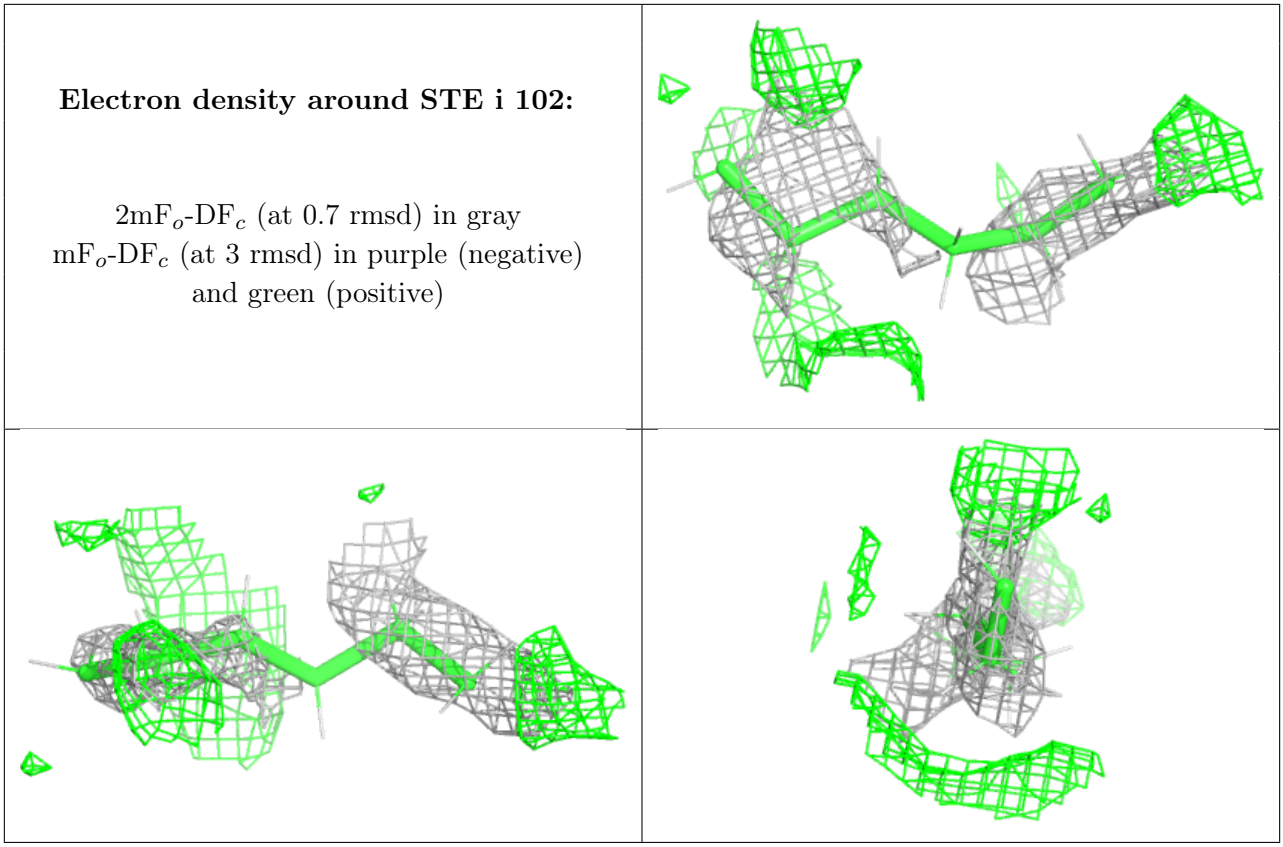
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	504	59/65	0.97	0.06	25,37,81,86	0
23	CLA	B	605	65/65	0.97	0.06	17,30,50,54	0
34	HEM	f	101	43/43	0.97	0.07	41,55,76,78	0
22	CL	A	403	1/1	0.98	0.04	24,24,24,24	0
23	CLA	A	405	65/65	0.98	0.07	18,31,97,104	0
23	CLA	B	603	65/65	0.98	0.06	19,30,61,69	0
23	CLA	A	407	54/65	0.98	0.05	16,30,63,69	0
34	HEM	F	101	43/43	0.98	0.07	28,45,59,61	0
23	CLA	B	613	65/65	0.98	0.06	18,30,69,75	0
35	HEC	v	201	43/43	0.98	0.05	23,33,40,43	0
22	CL	a	403	1/1	0.99	0.07	24,24,24,24	0
21	FE2	a	401	1/1	0.99	0.02	29,29,29,29	0
22	CL	A	402	1/1	0.99	0.03	25,25,25,25	0
21	FE2	A	401	1/1	0.99	0.01	23,23,23,23	0
31	OEX	A	418	10/10	0.99	0.04	22,23,26,27	0
31	OEX	a	418	10/10	0.99	0.03	22,23,27,30	0
35	HEC	V	201	43/43	0.99	0.05	21,29,38,42	0
22	CL	a	402	1/1	0.99	0.03	25,25,25,25	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.

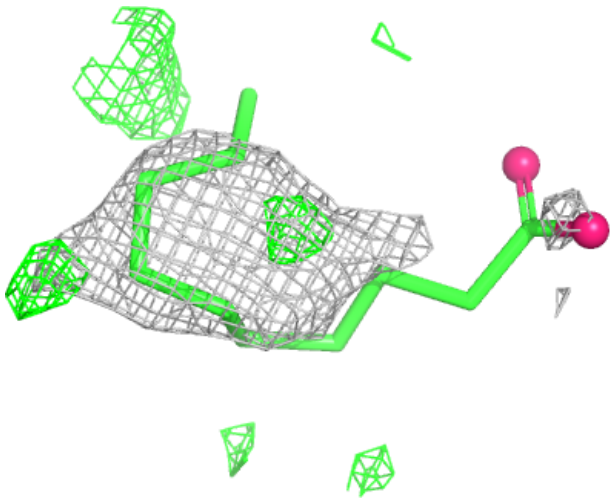
Electron density around STE i 102:

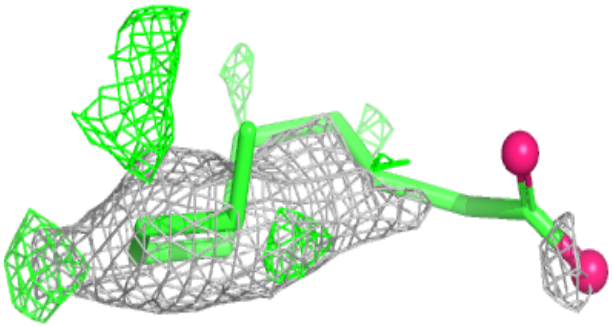
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

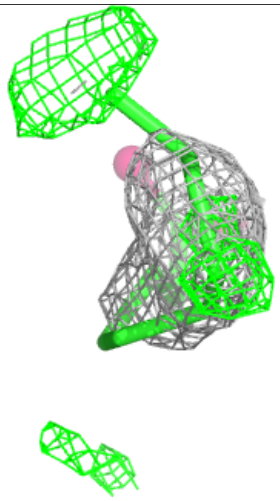


Electron density around STE i 101:

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

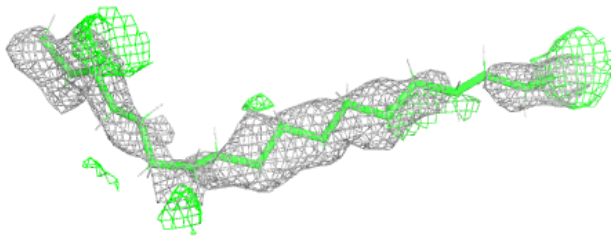


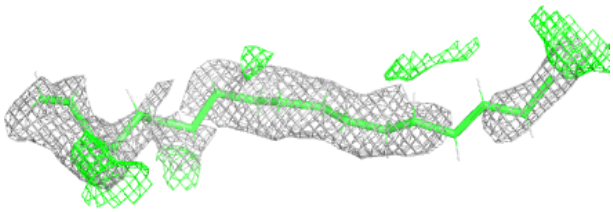


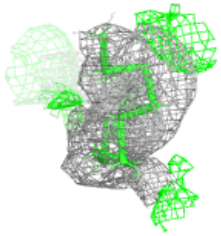


Electron density around STE c 517:

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

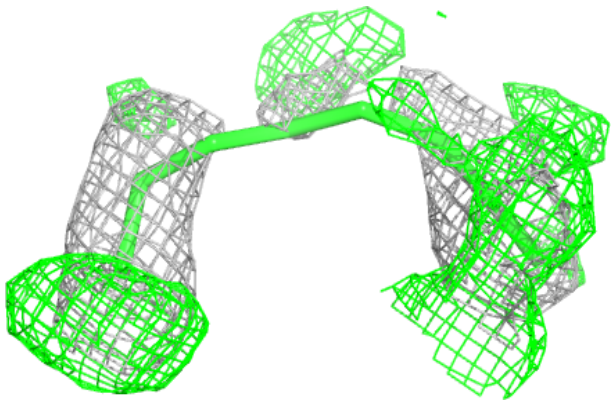


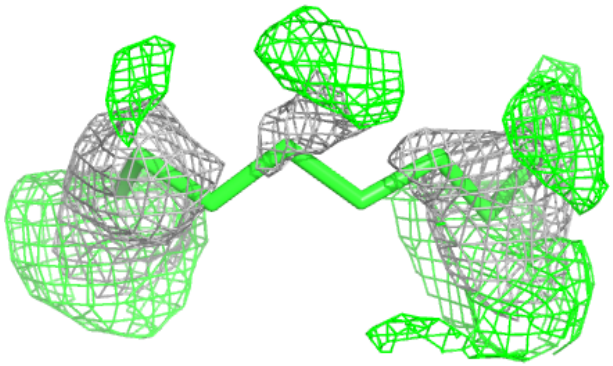


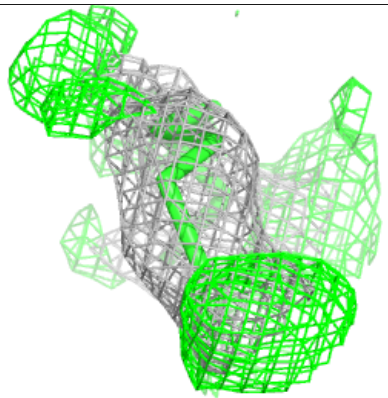


Electron density around STE C 527:

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

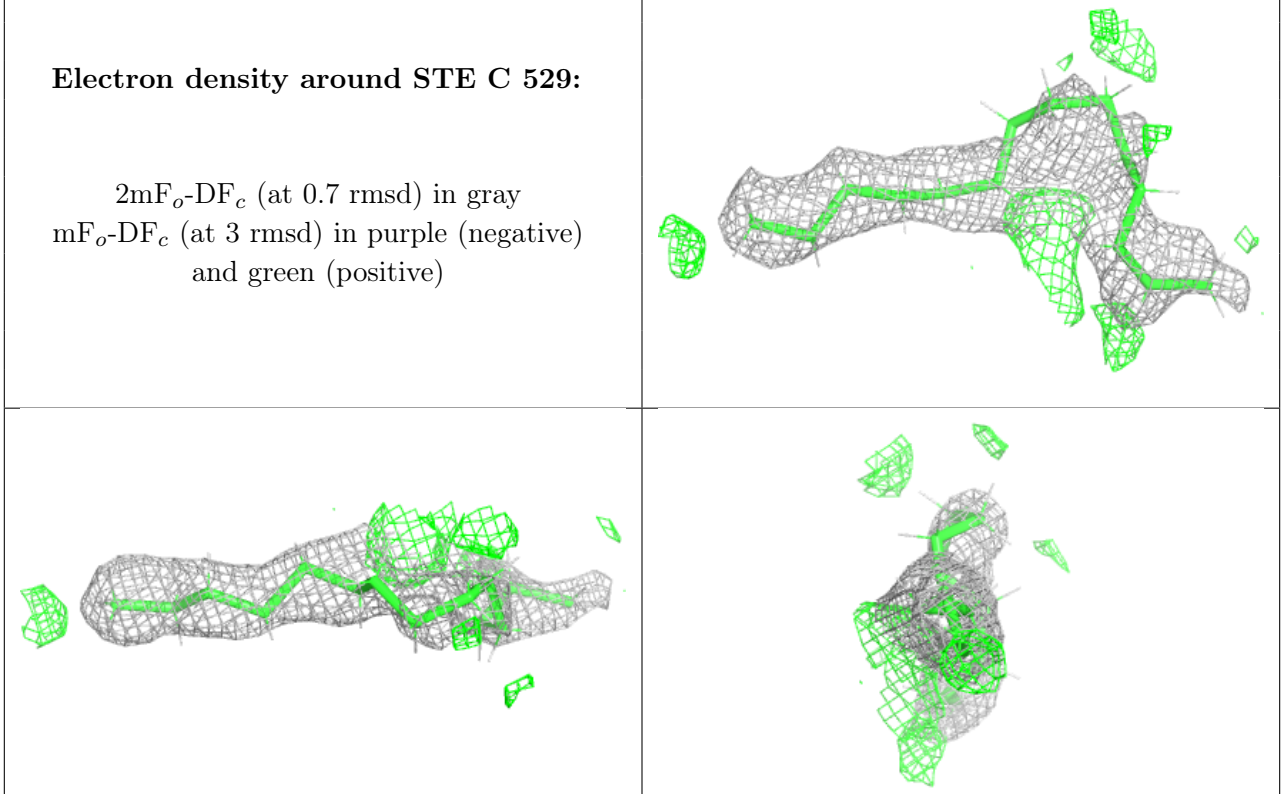






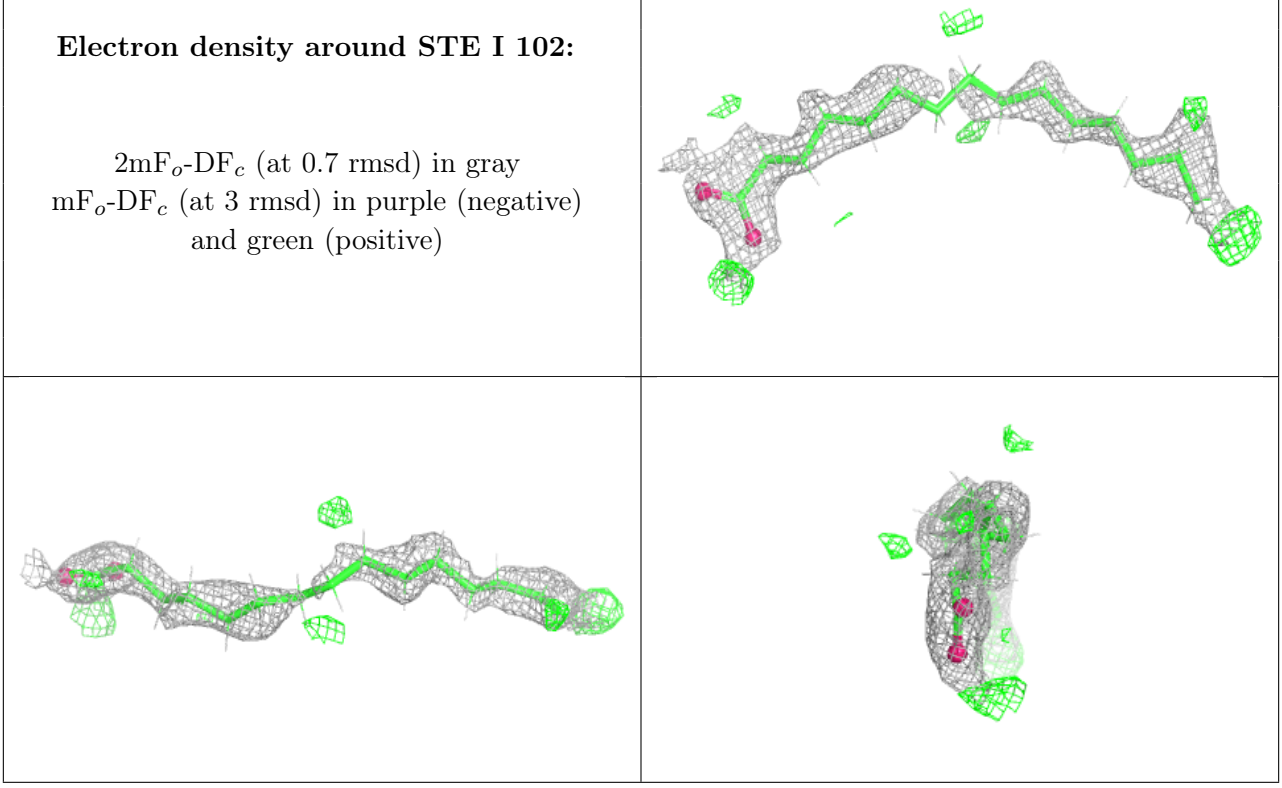
Electron density around STE C 529:

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



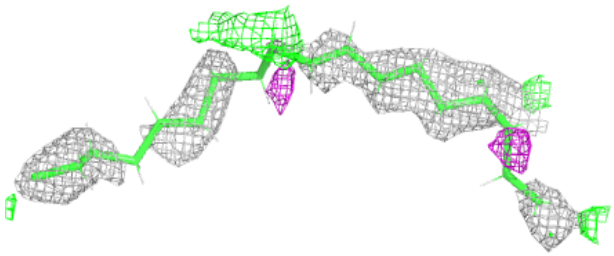
Electron density around STE I 102:

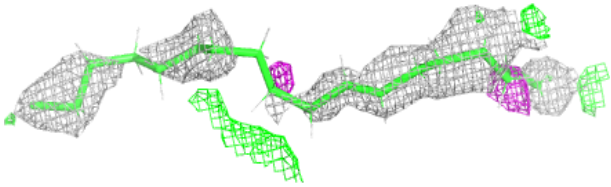
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

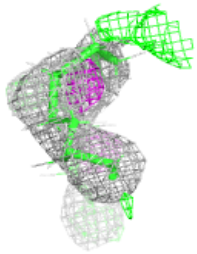


Electron density around STE H 103:

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

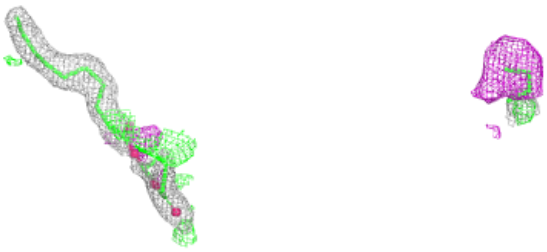




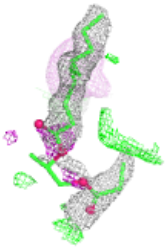


Electron density around LMG b 619:

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

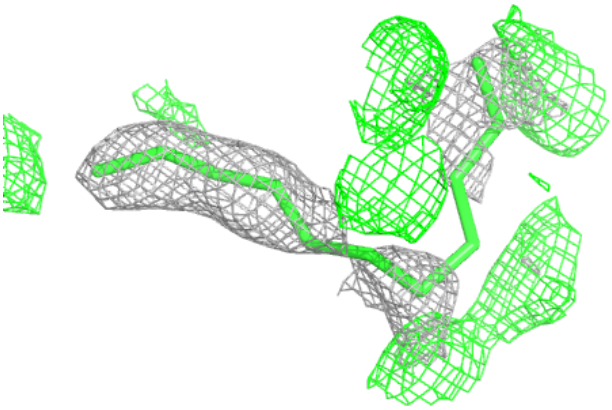


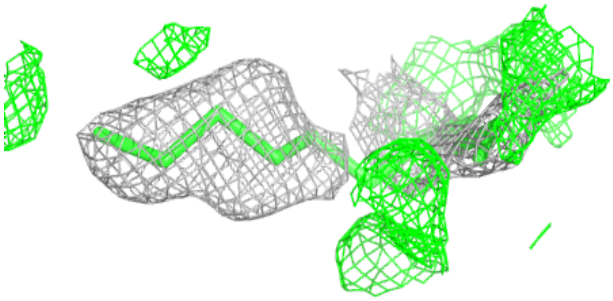


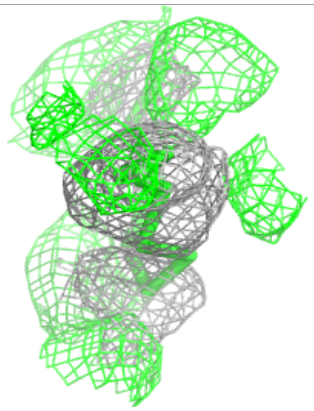


Electron density around STE A 417:

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

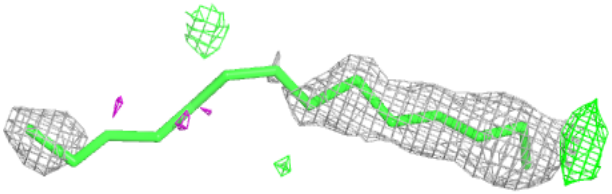


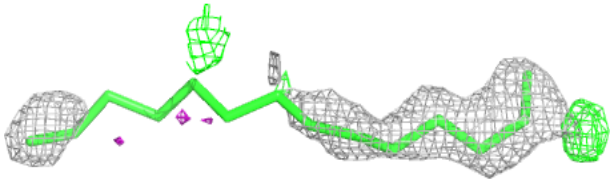


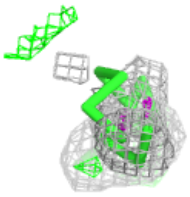


Electron density around STE C 528:

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

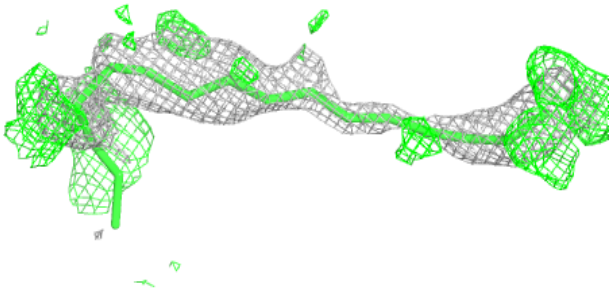


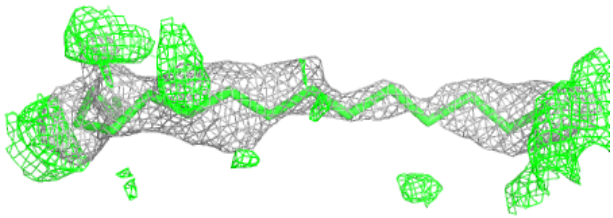


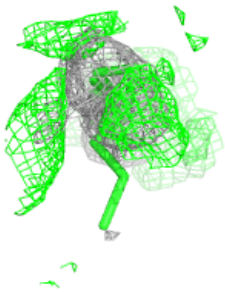


Electron density around STE j 102:

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

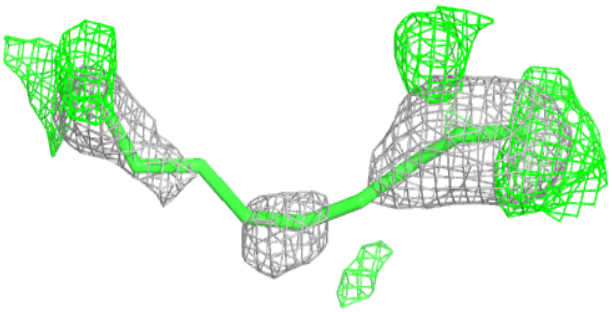


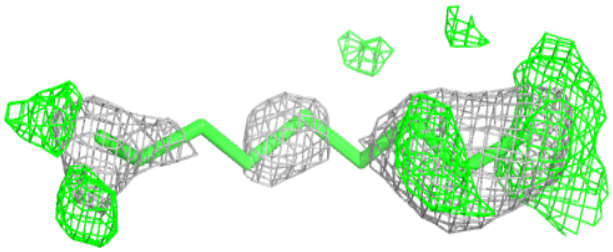


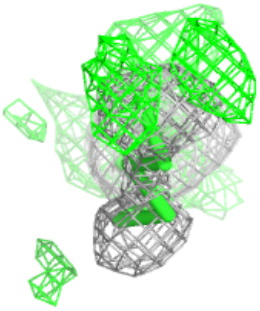


Electron density around STE e 101:

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

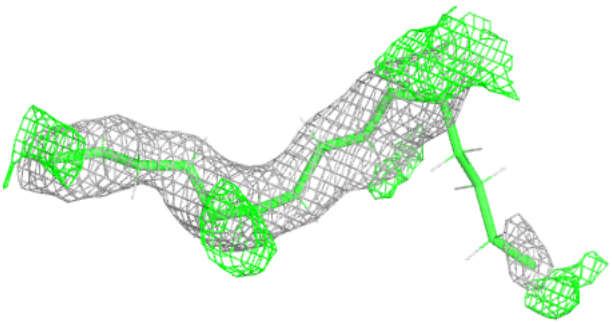


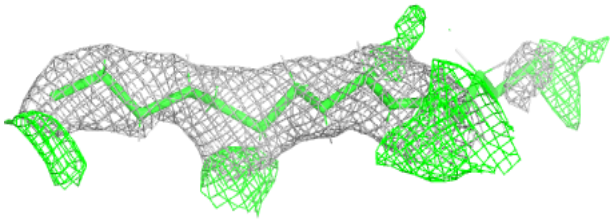


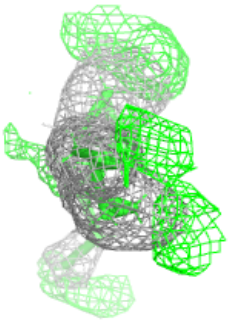


Electron density around STE B 623:

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

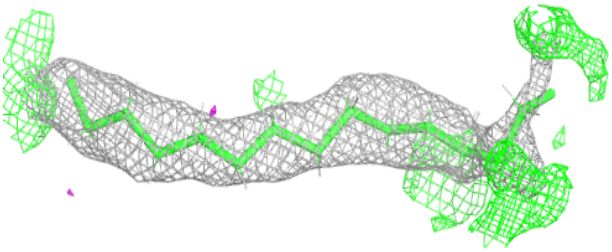


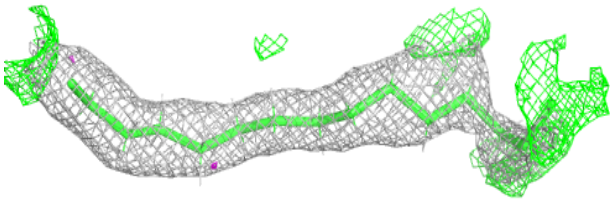


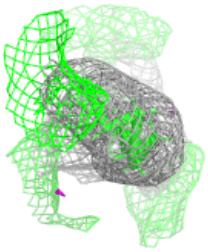


Electron density around STE I 101:

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

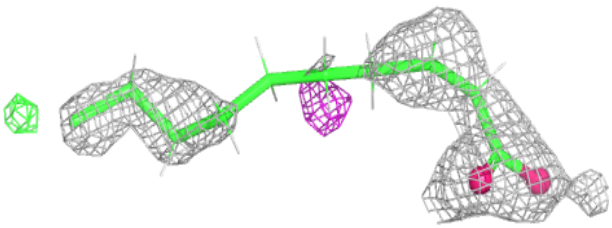


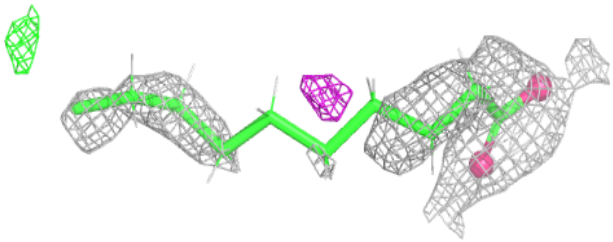


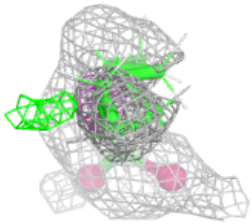


Electron density around STE E 102:

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

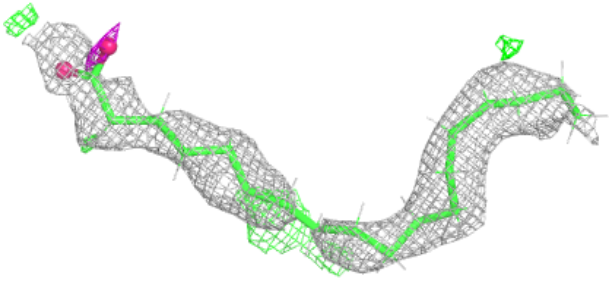


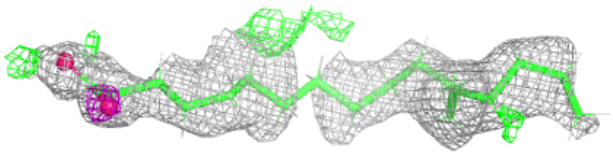


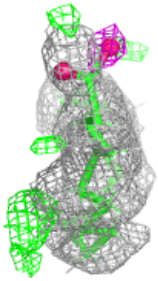


Electron density around STE E 104:

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

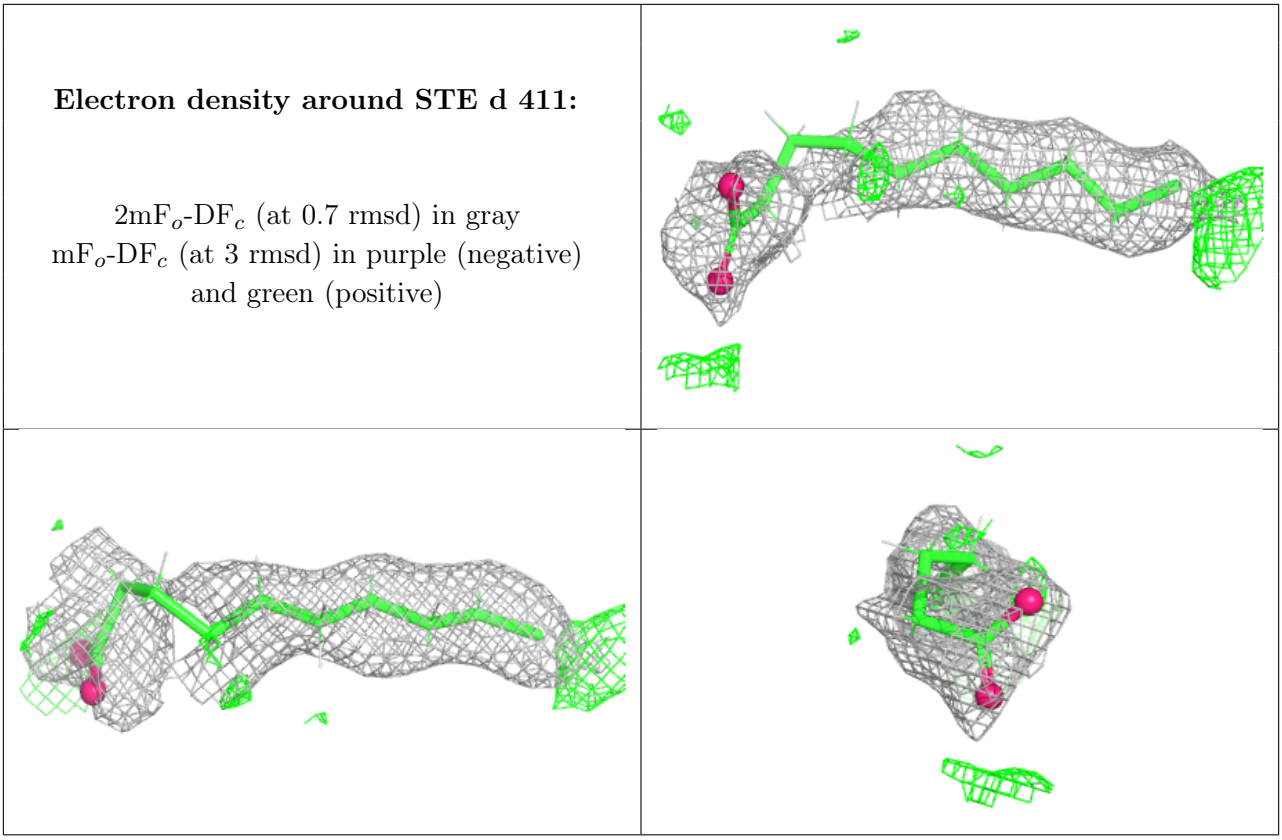






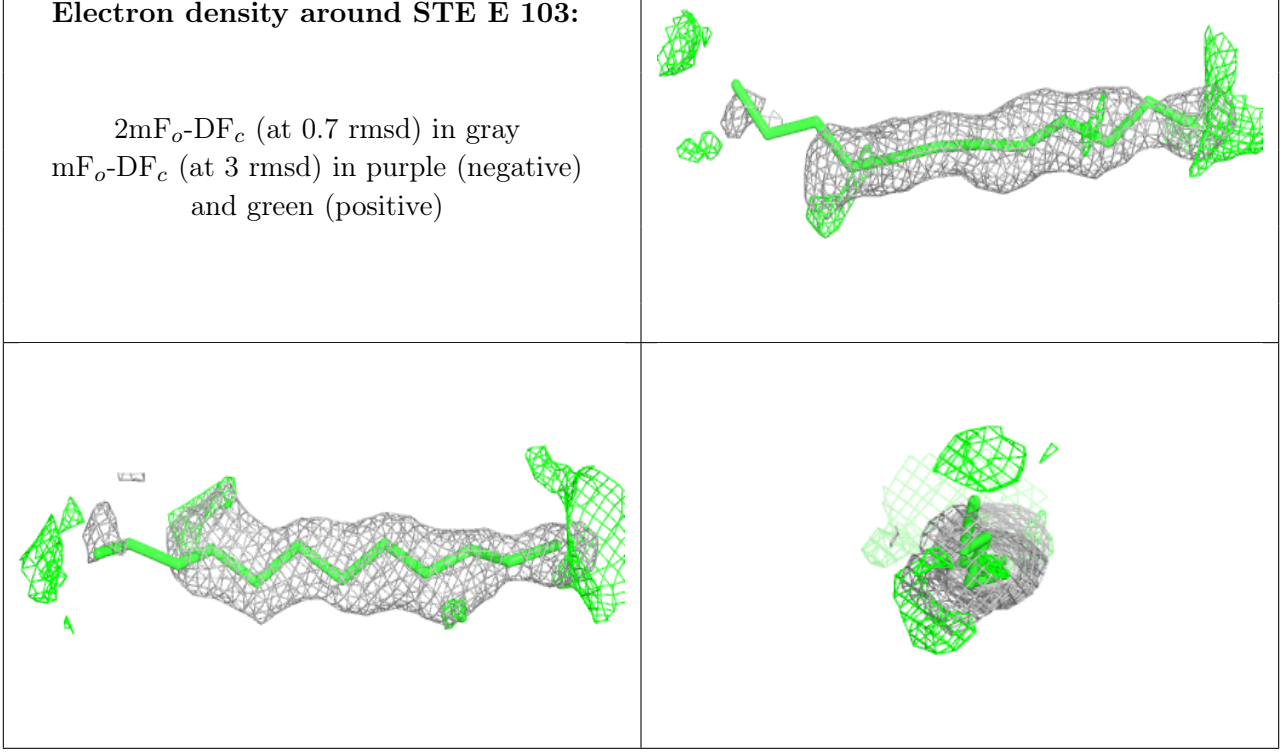
Electron density around STE d 411:

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



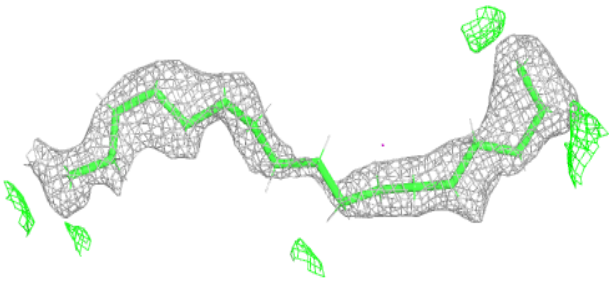
Electron density around STE E 103:

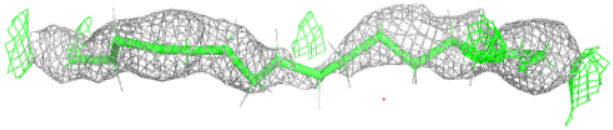
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

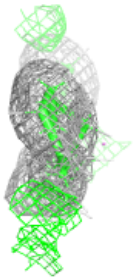


Electron density around STE A 416:

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

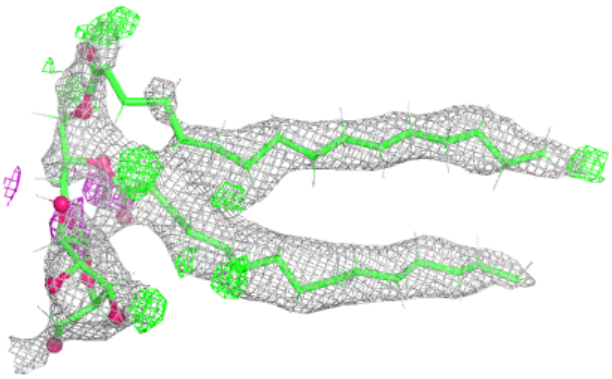


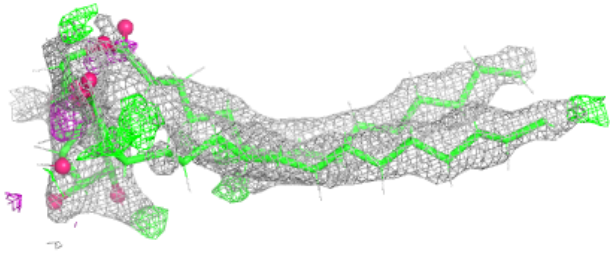


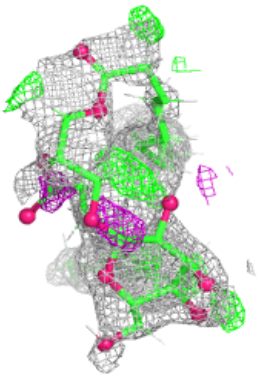


Electron density around LMG D 408:

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

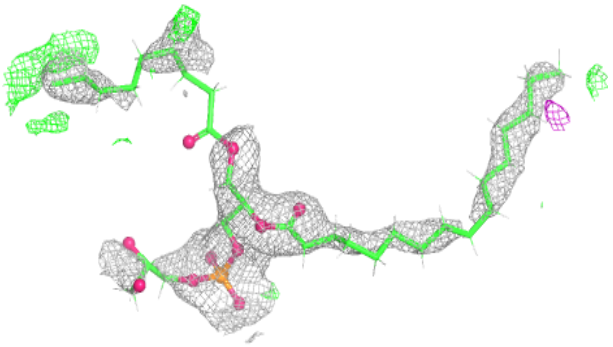


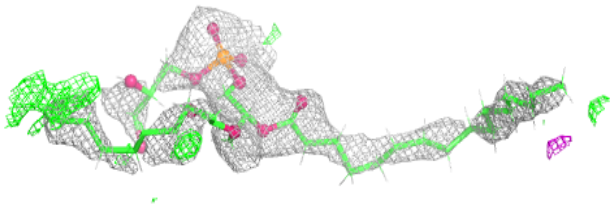


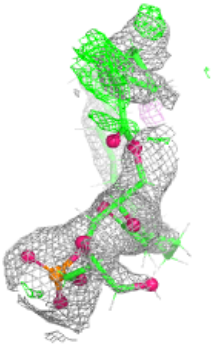


Electron density around LHG a 413:

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

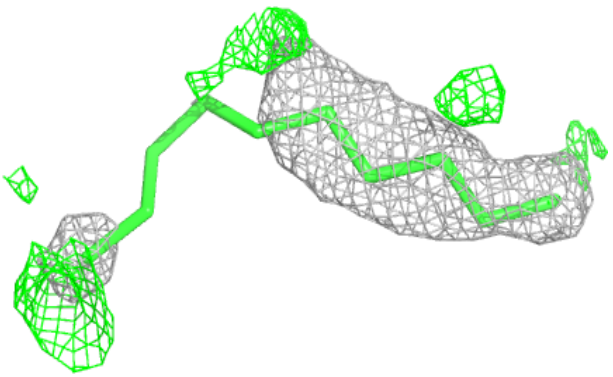


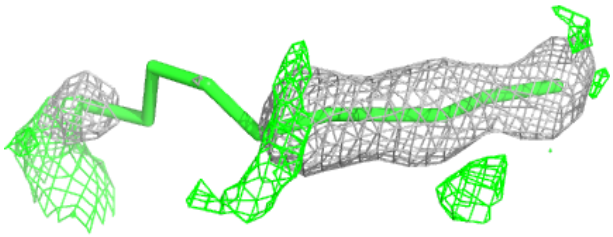


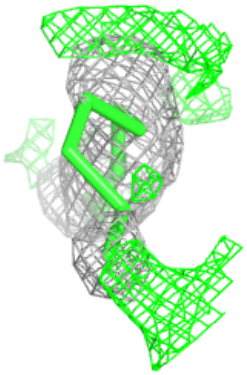


Electron density around STE d 412:

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

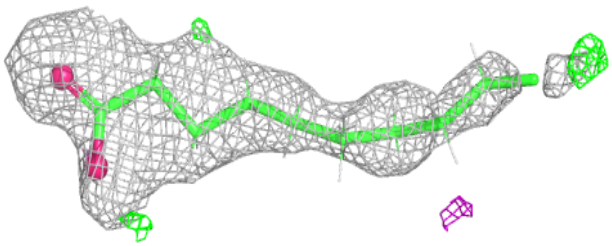


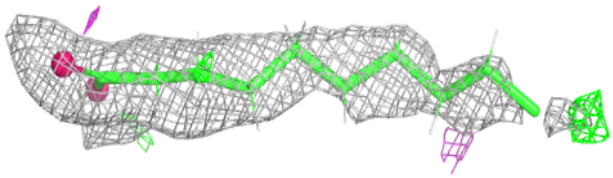


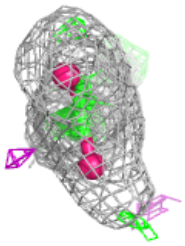


Electron density around STE a 417:

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

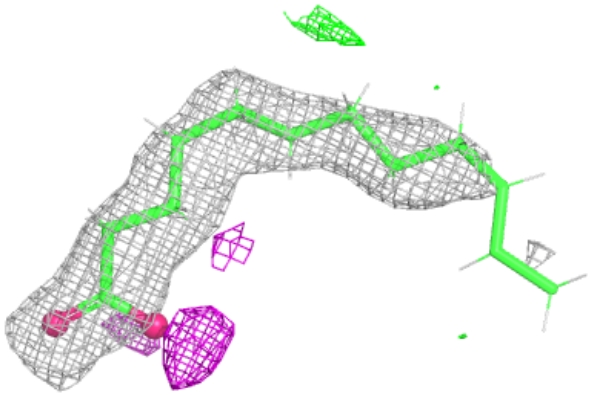


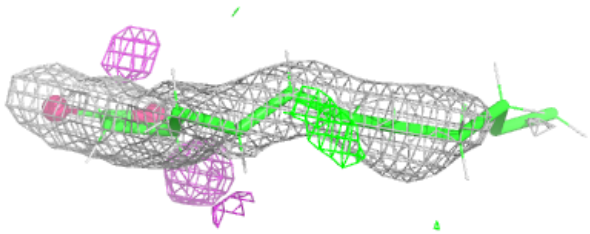


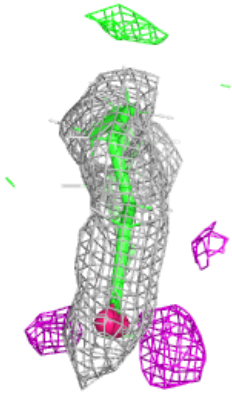


Electron density around STE C 516:

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

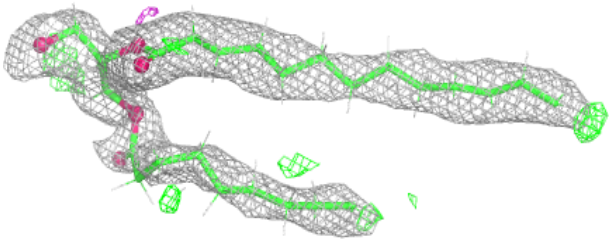


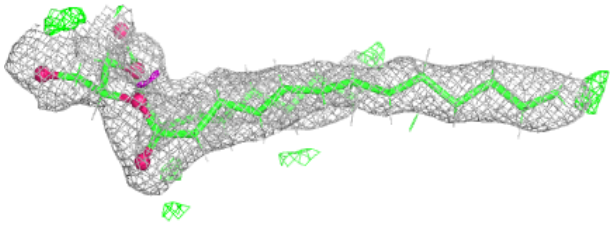


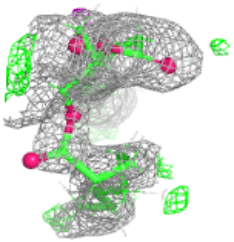


Electron density around LMG c 518:

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

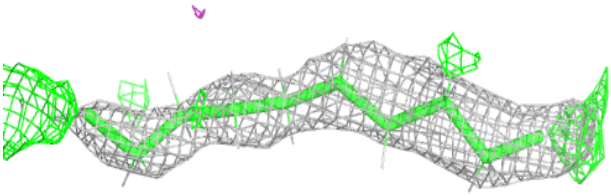


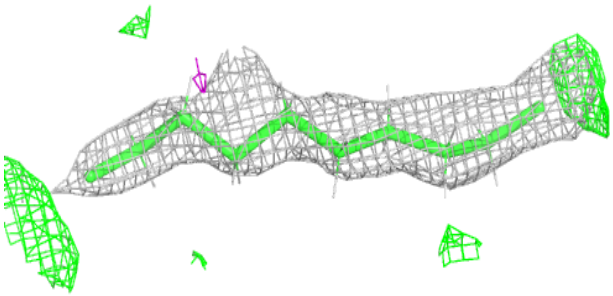


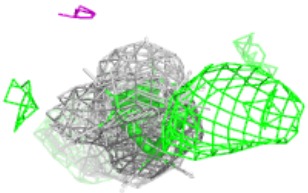


Electron density around STE a 416:

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

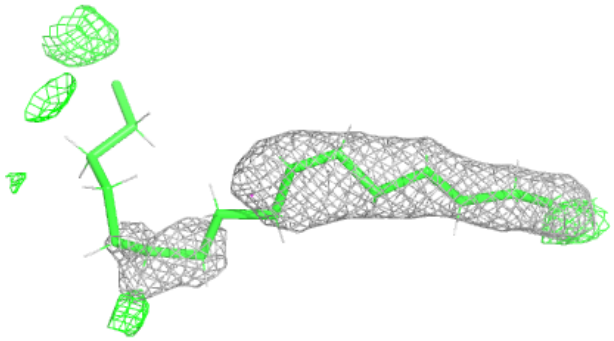


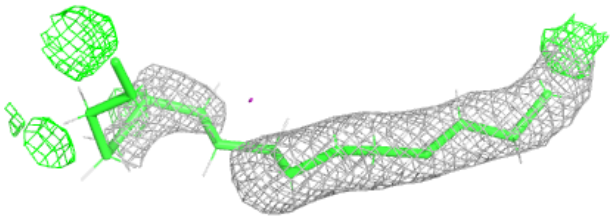


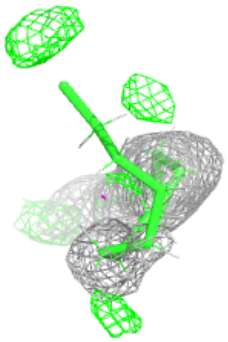


Electron density around STE T 102:

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

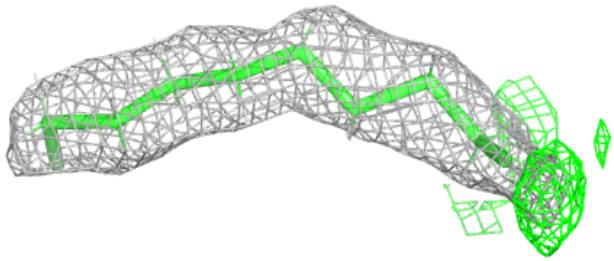


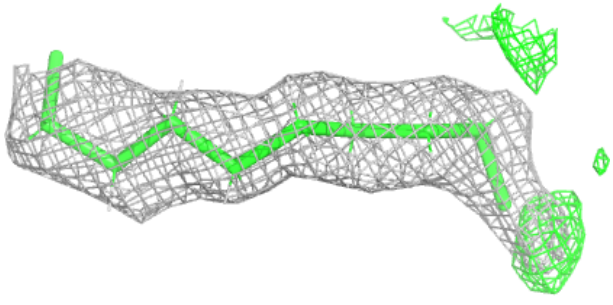


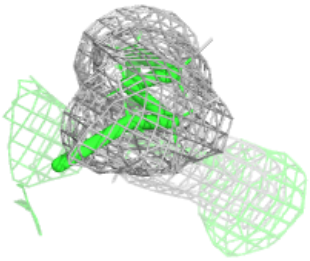


Electron density around STE b 626:

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

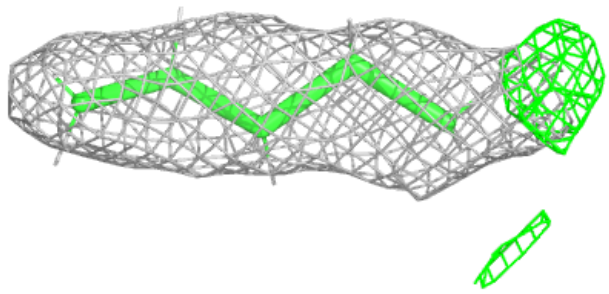


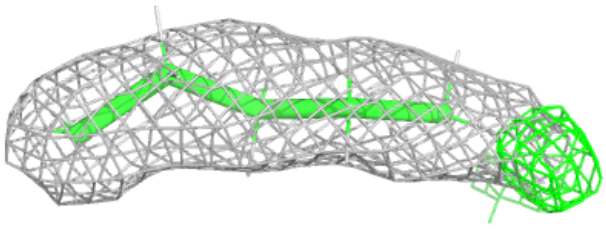


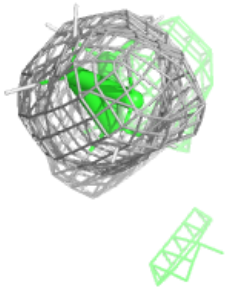


Electron density around STE C 518:

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

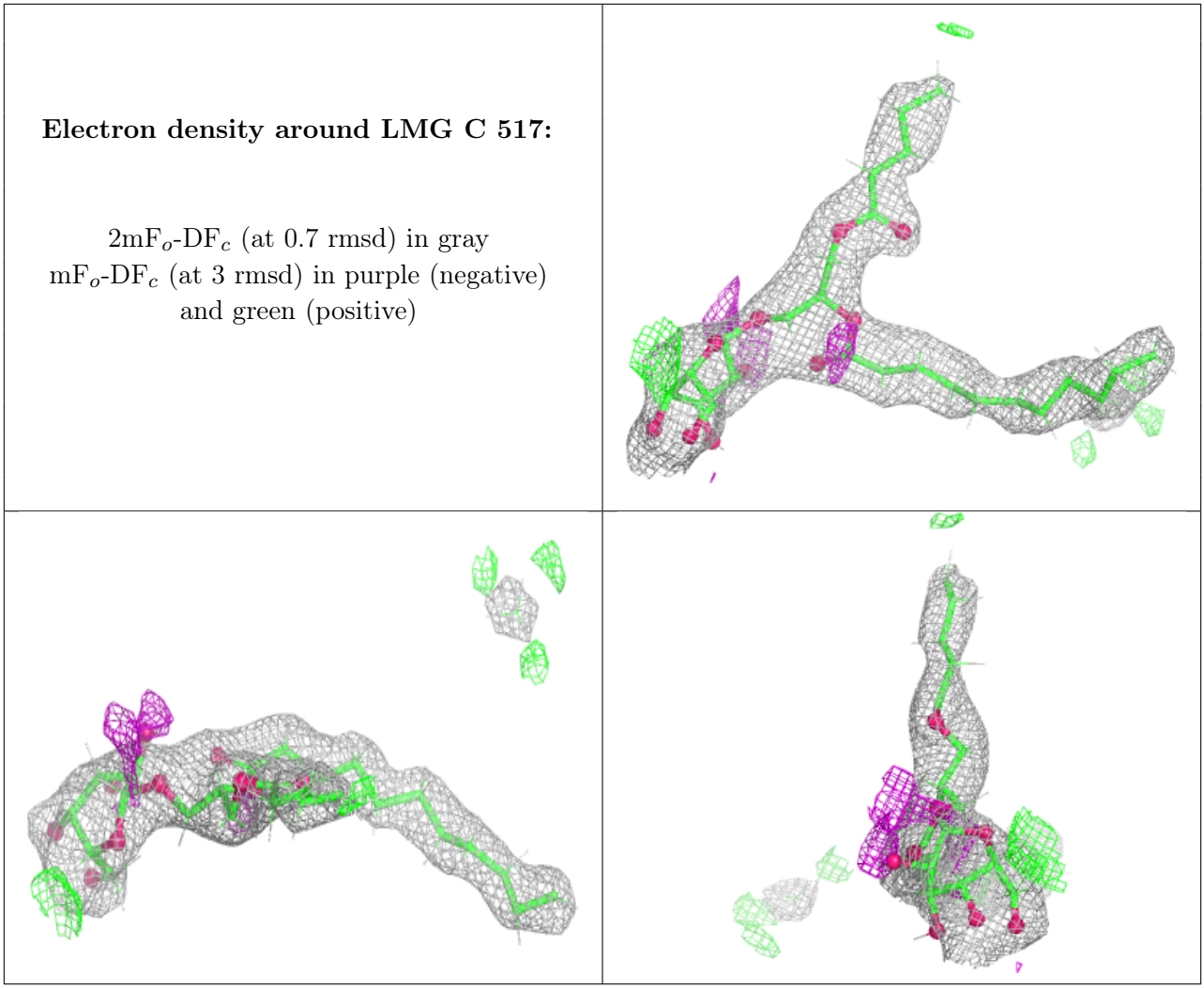






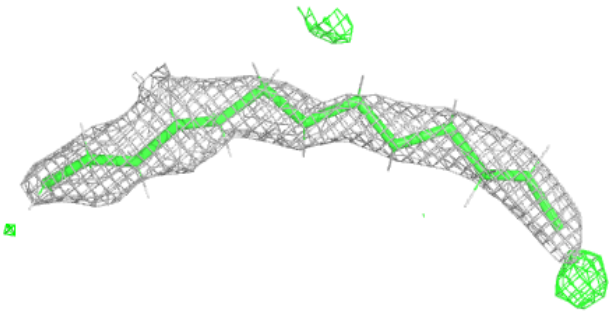
Electron density around LMG C 517:

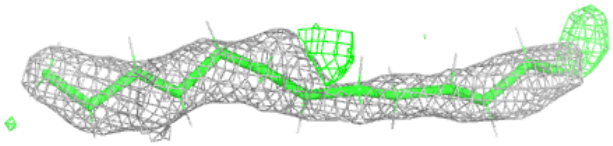
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

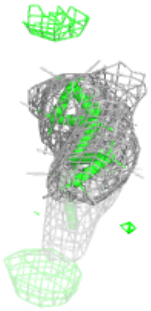


Electron density around STE c 516:

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

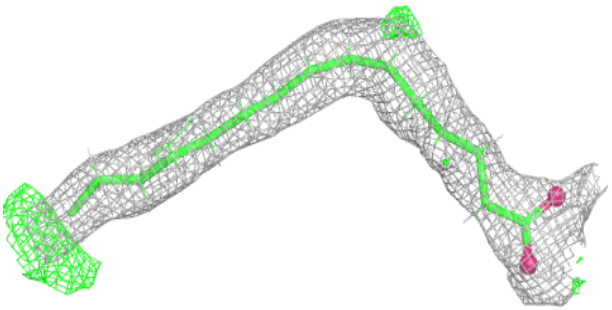


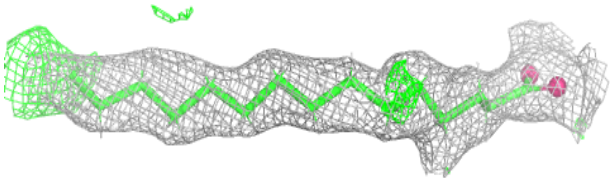


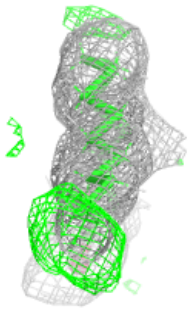


Electron density around STE d 410:

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

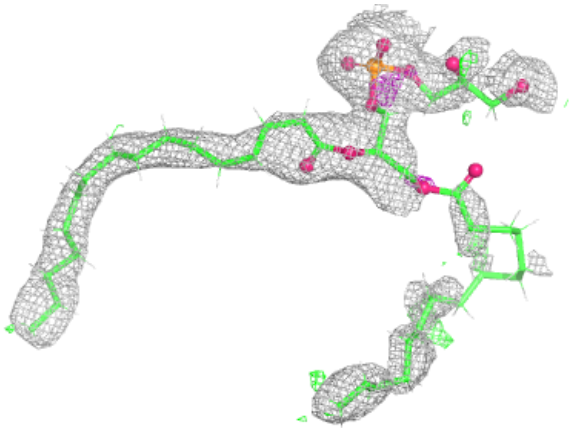


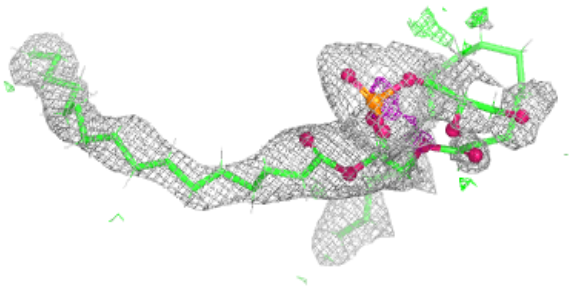


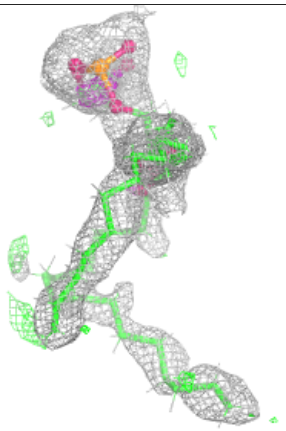


Electron density around LHG E 101:

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

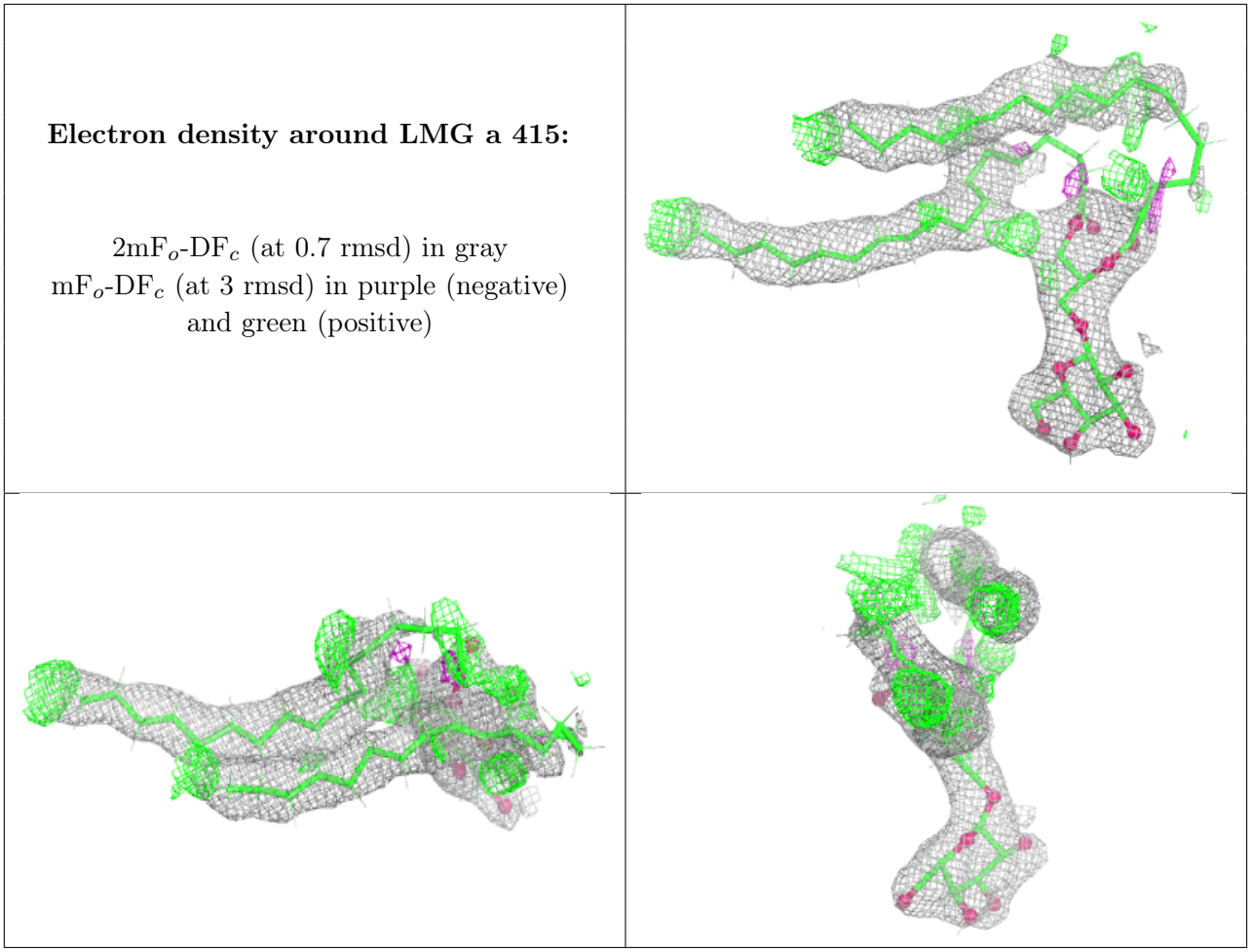






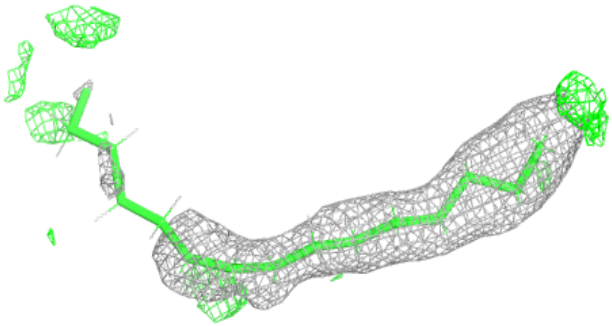
Electron density around LMG a 415:

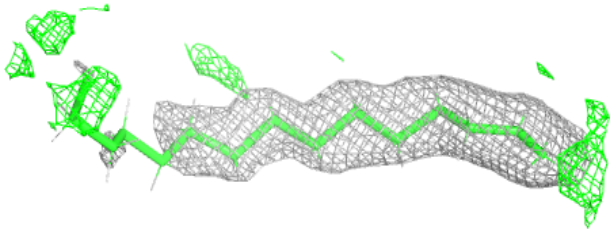
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

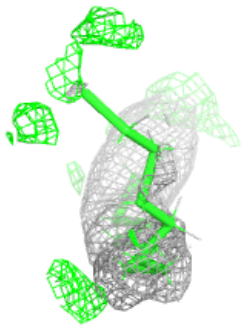


Electron density around STE m 102:

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

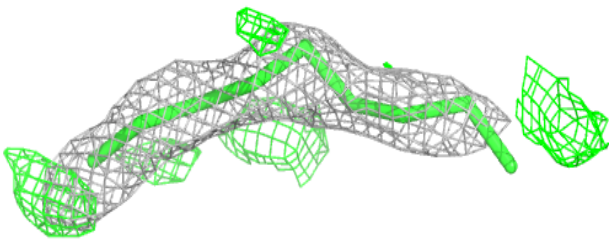


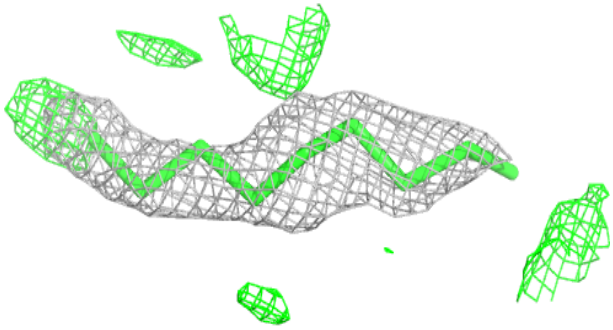


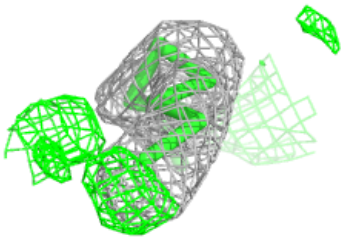


Electron density around STE A 410:

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

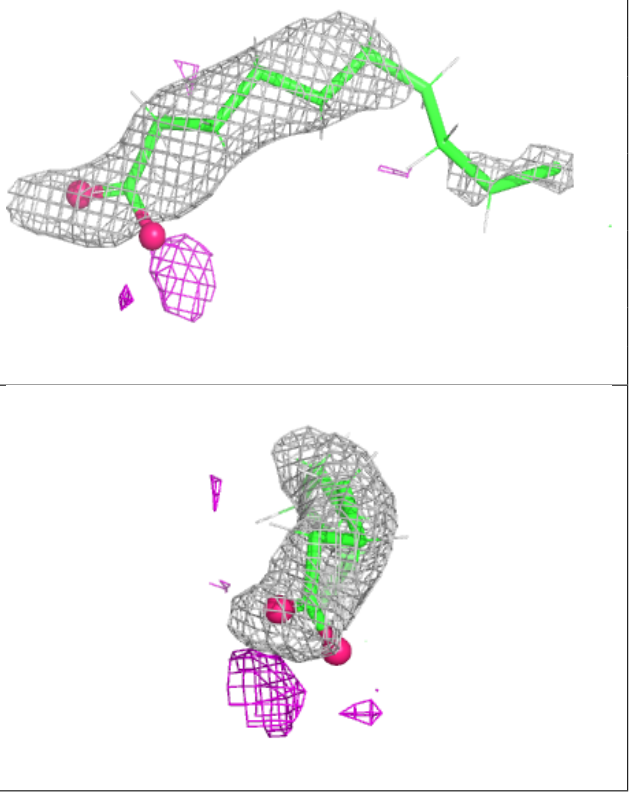






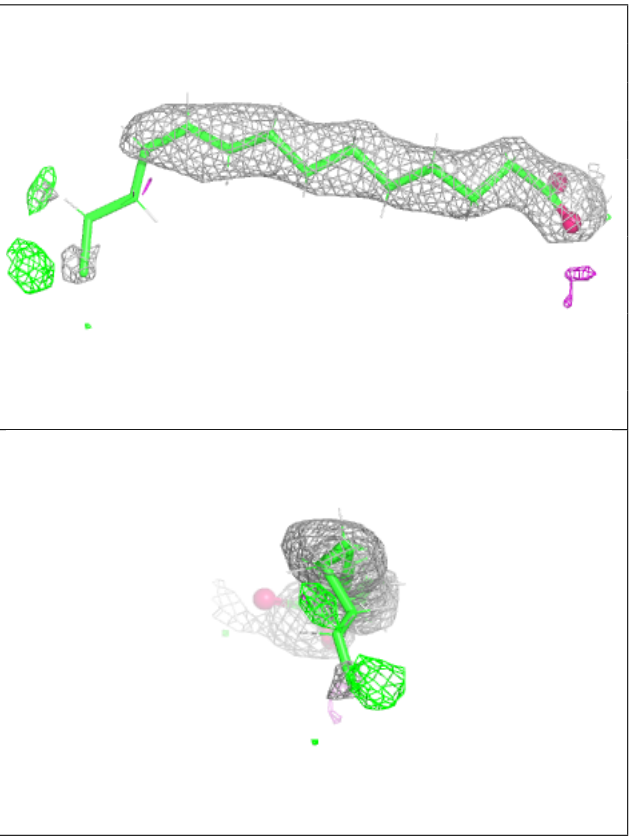
Electron density around STE B 622:

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



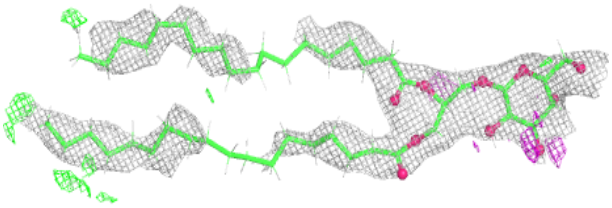
Electron density around STE b 625:

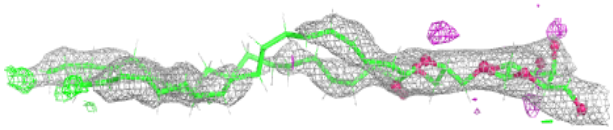
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

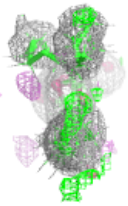


Electron density around LMG b 623:

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

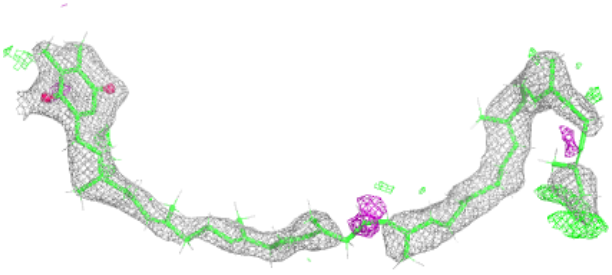


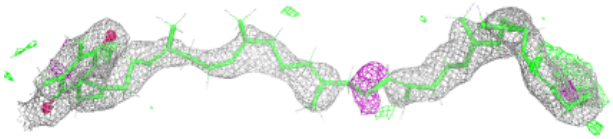


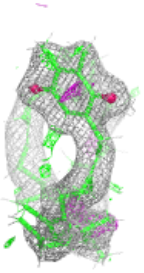


Electron density around PL9 a 410:

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

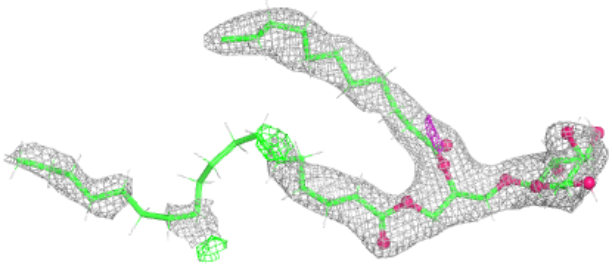


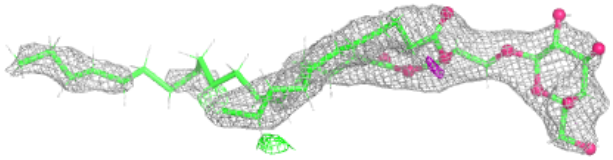


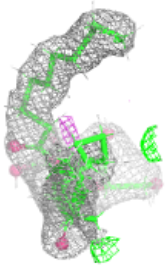


Electron density around LMG c 523:

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

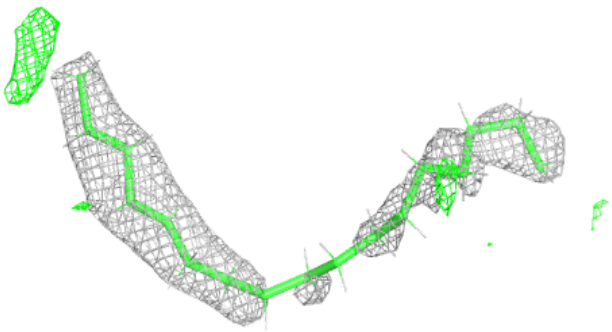


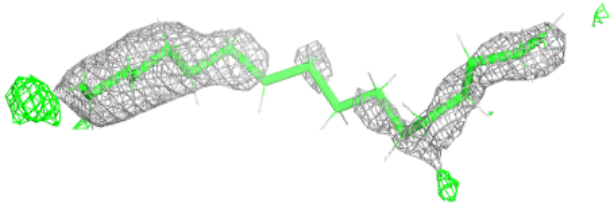


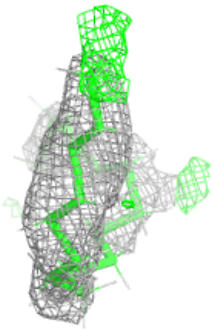


Electron density around STE Z 101:

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

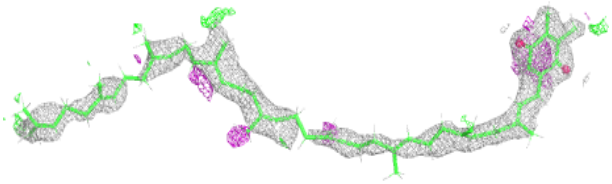


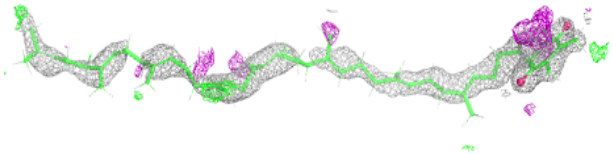


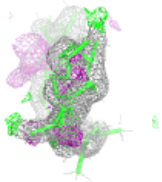


Electron density around PL9 A 409:

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

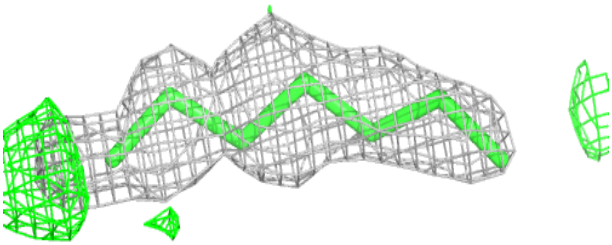


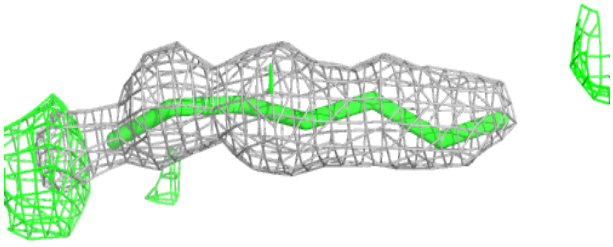


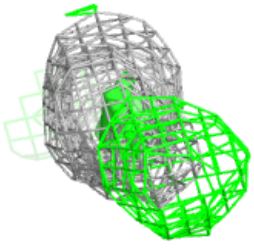


Electron density around STE C 519:

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

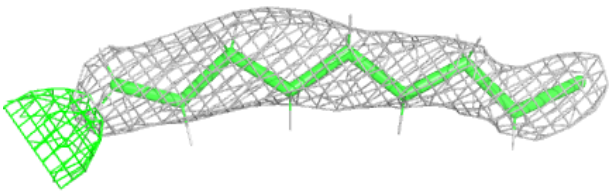


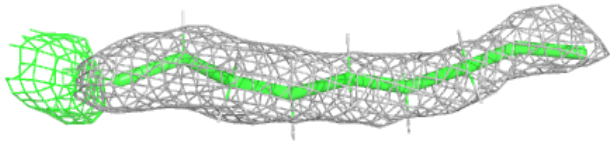


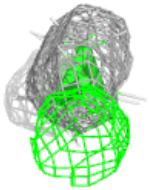


Electron density around STE z 101:

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

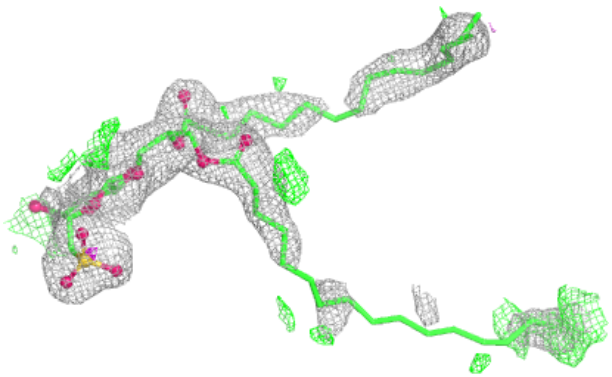


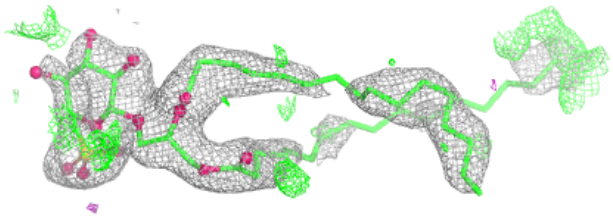


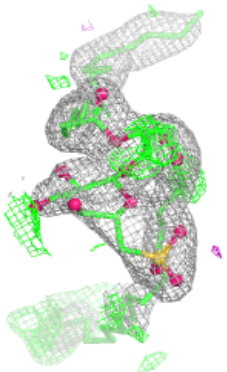


Electron density around SQD A 413:

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

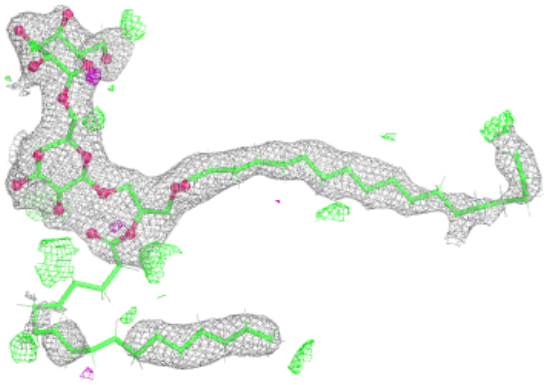


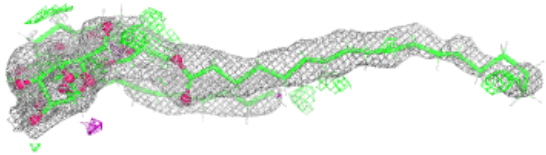




Electron density around DGD A 414:

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

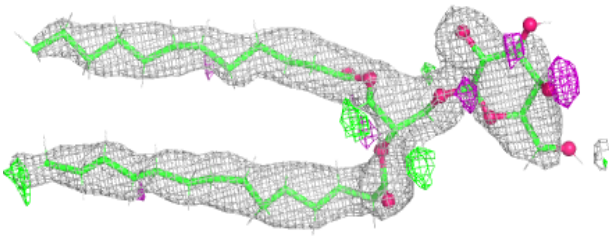


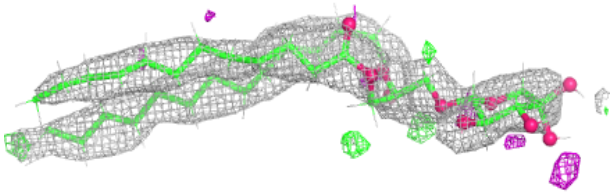


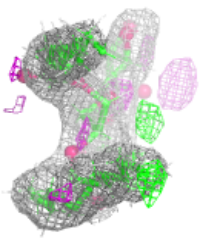


Electron density around LMG B 620:

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

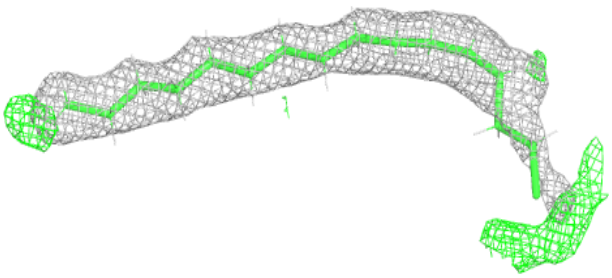


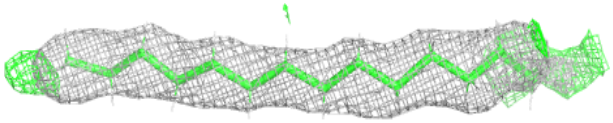


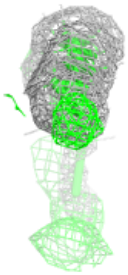


Electron density around STE C 526:

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

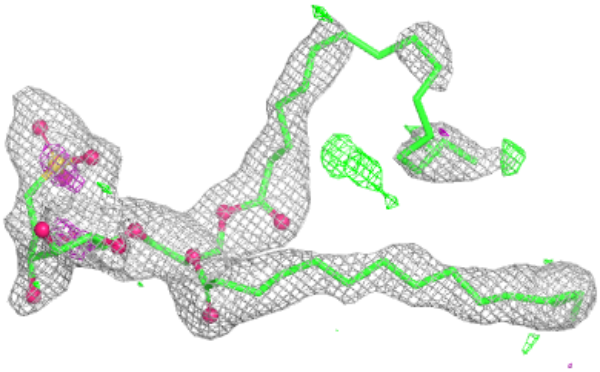


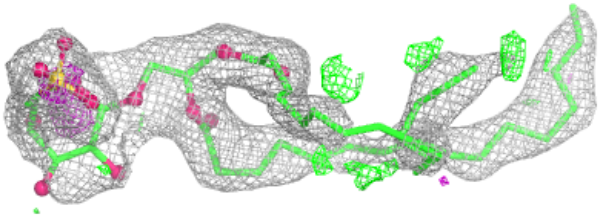


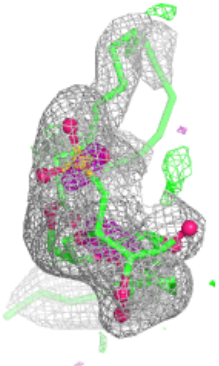


Electron density around SQD a 414:

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

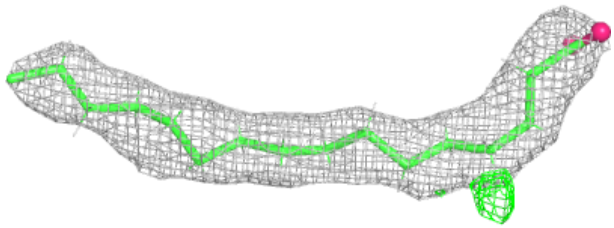


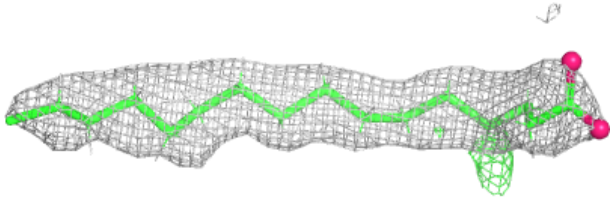


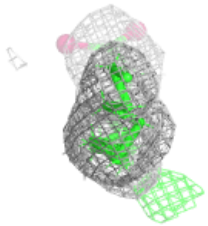


Electron density around STE t 103:

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

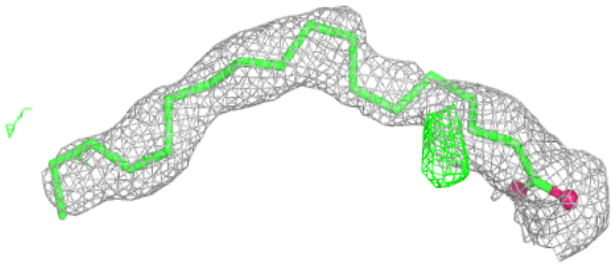


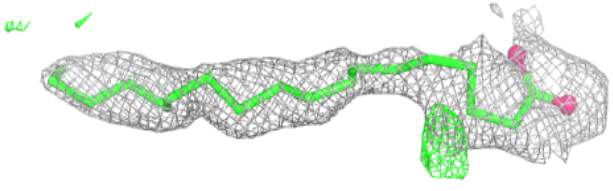


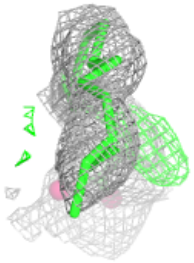


Electron density around STE b 624:

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

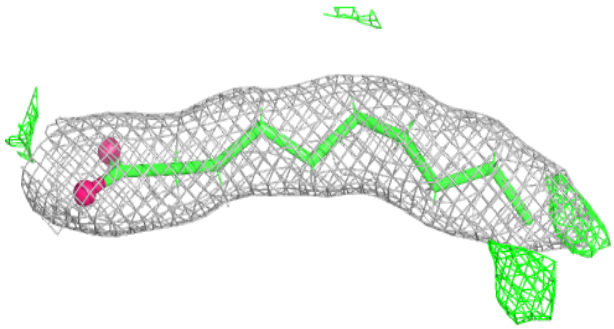


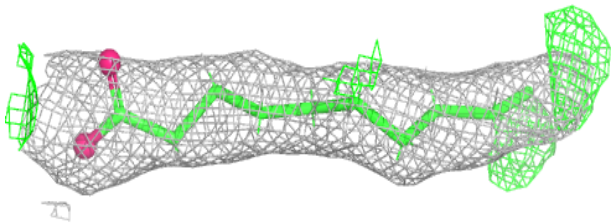


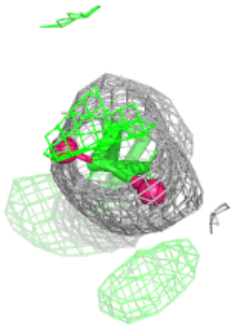


Electron density around STE j 101:

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

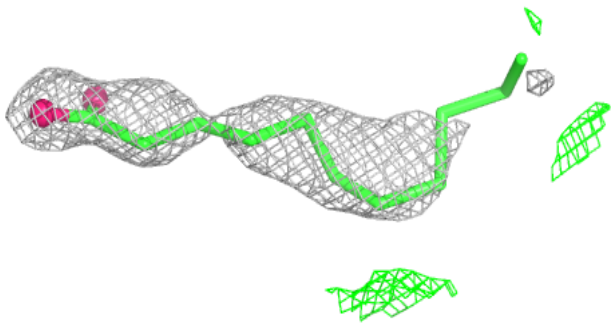


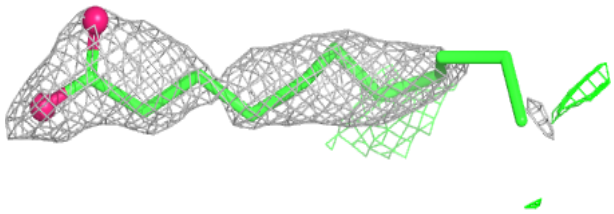


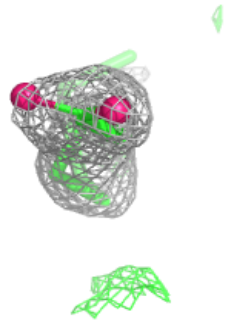


Electron density around STE e 104:

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

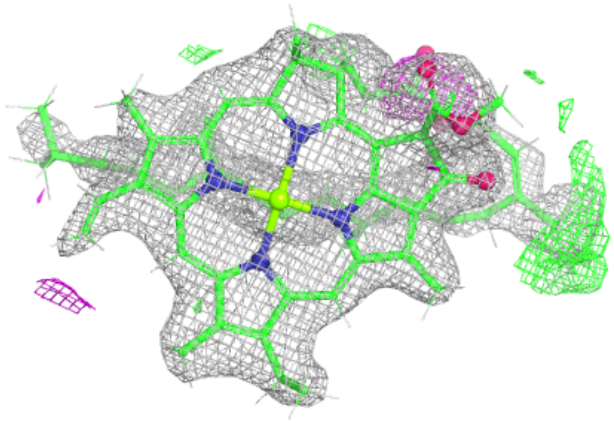


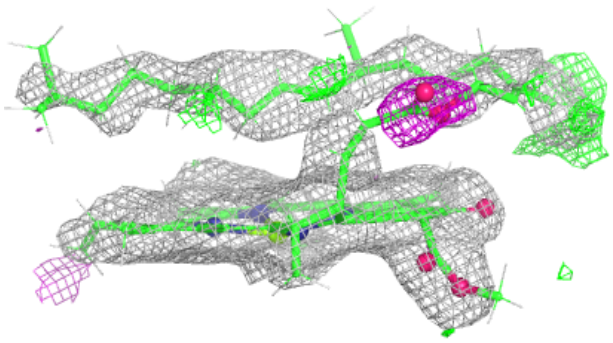




Electron density around CLA h 101:

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

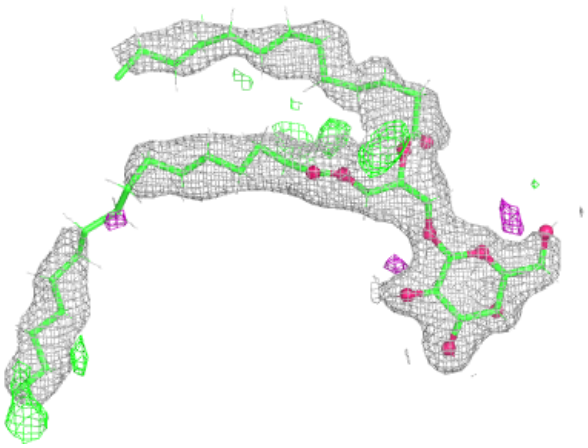


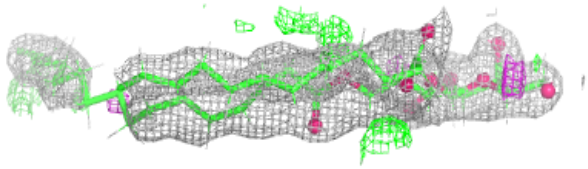


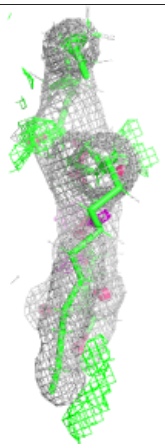


Electron density around LMG C 524:

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

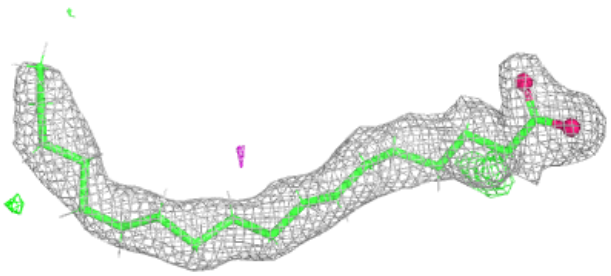


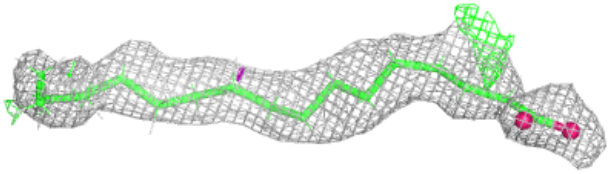


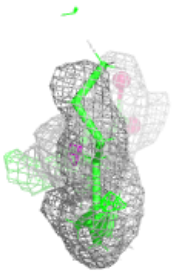


Electron density around STE b 622:

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

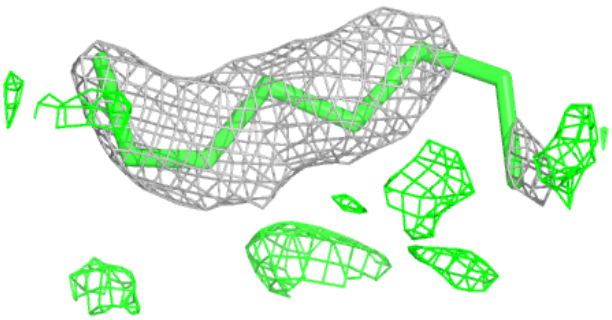


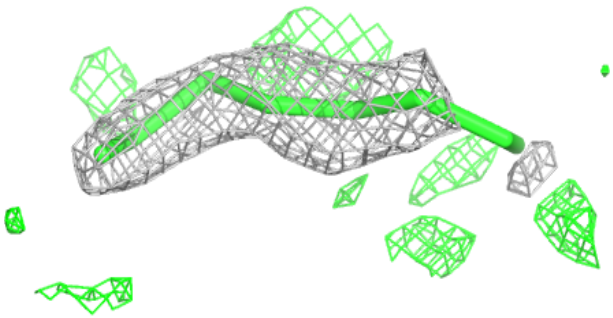


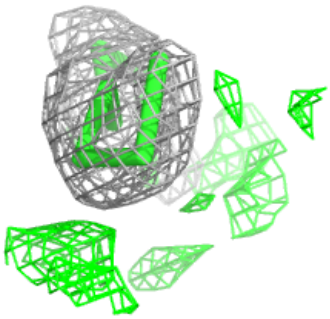


Electron density around STE e 102:

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

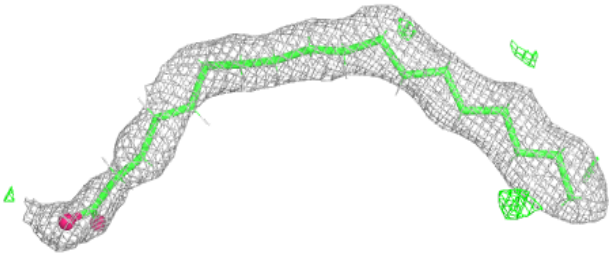


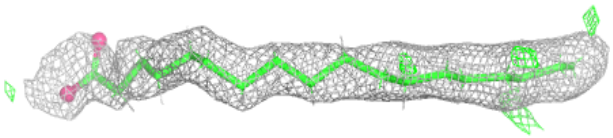


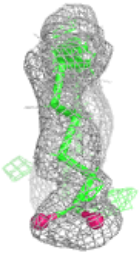


Electron density around STE x 102:

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

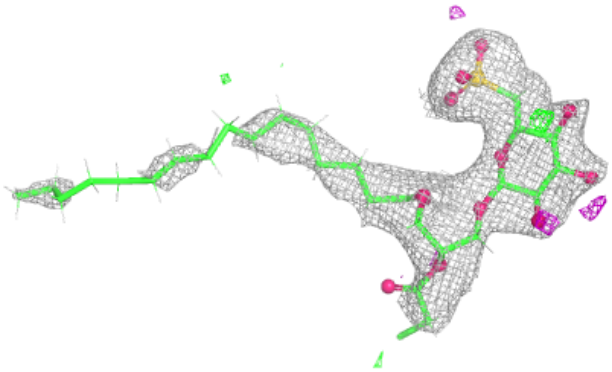


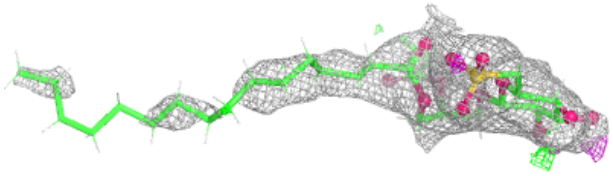


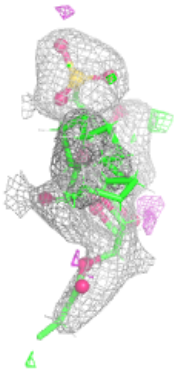


Electron density around SQD f 102:

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

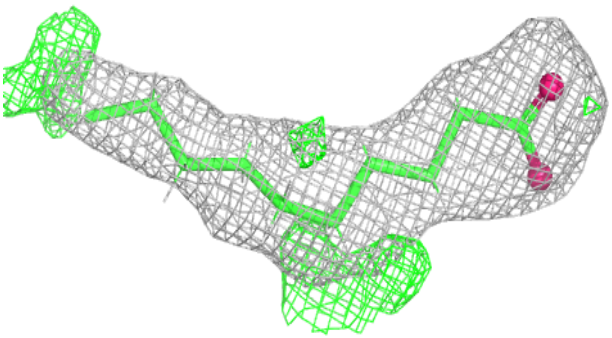


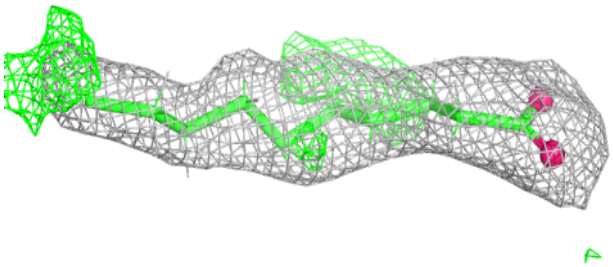


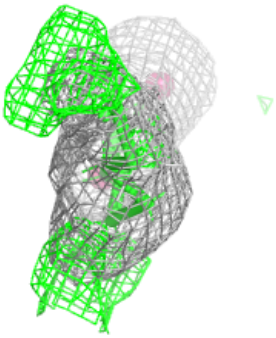


Electron density around STE C 525:

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

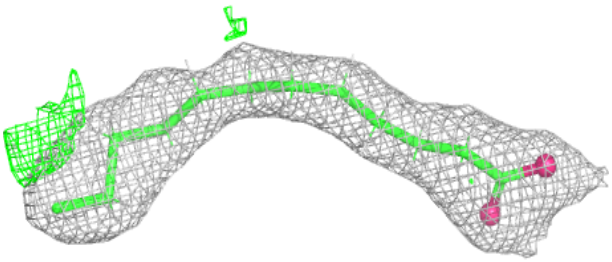


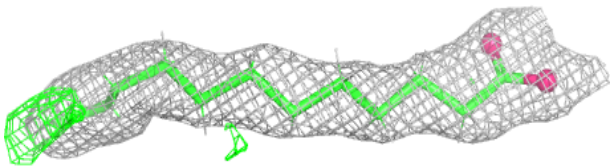


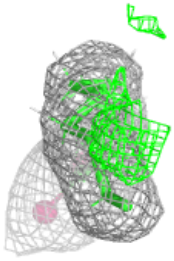


Electron density around STE t 102:

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

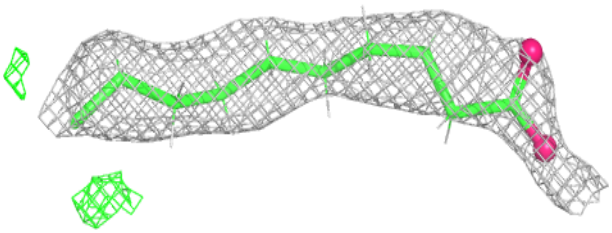


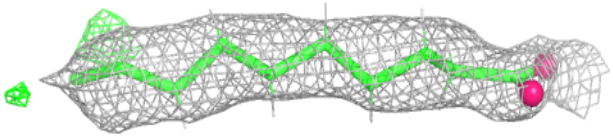


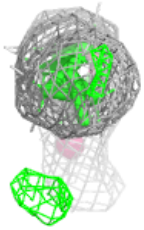


Electron density around STE m 101:

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

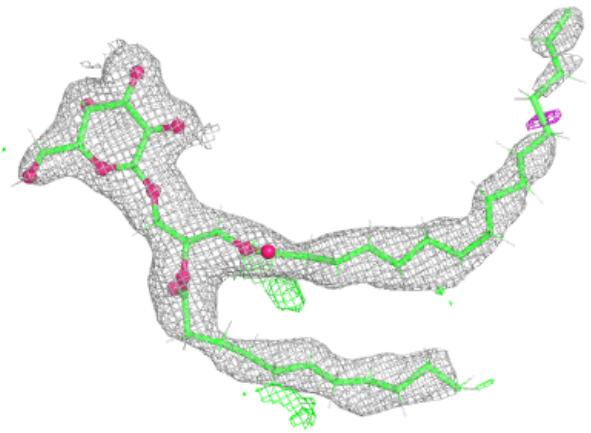


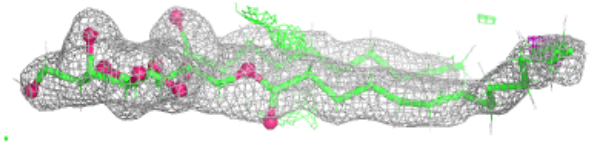


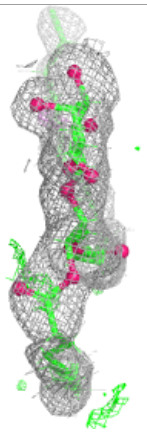


Electron density around LMG c 522:

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

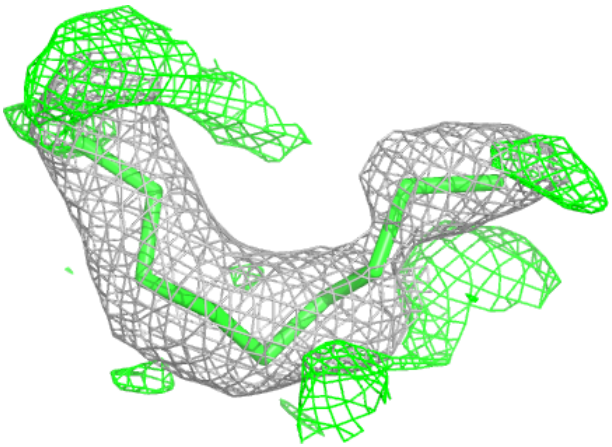


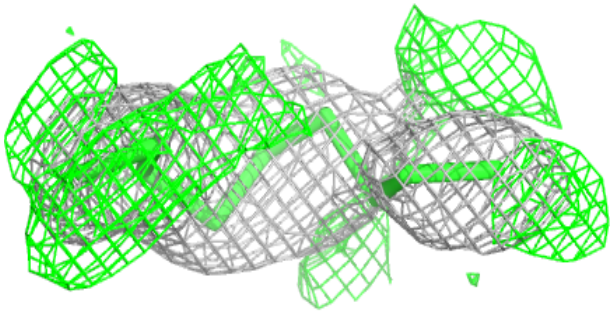


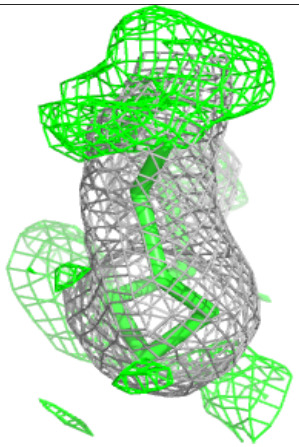


Electron density around STE D 414:

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

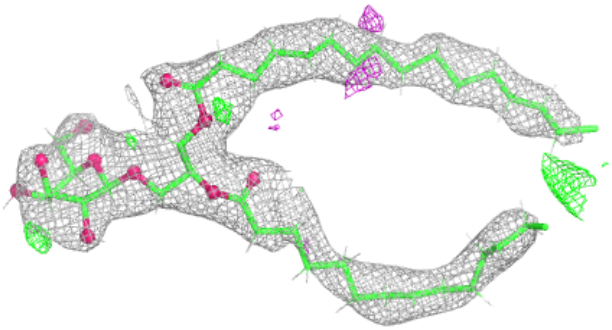


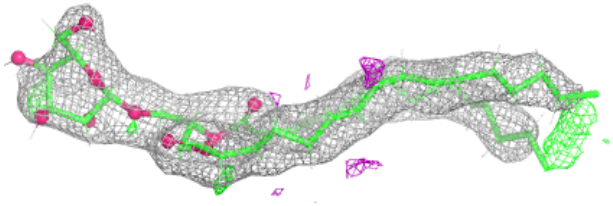


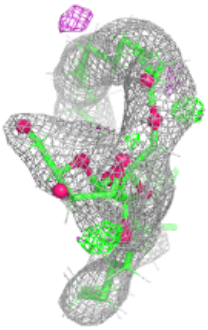


Electron density around LMG c 524:

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

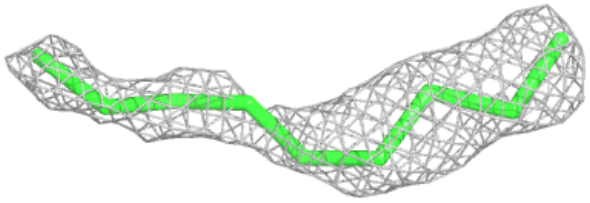


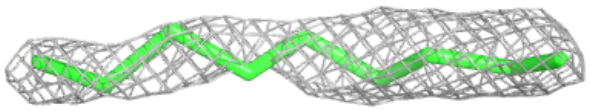


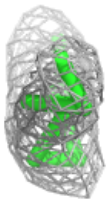


Electron density around STE e 103:

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

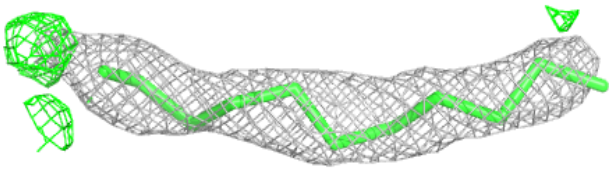


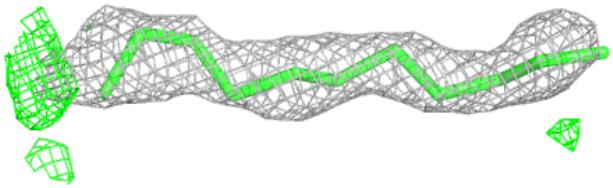


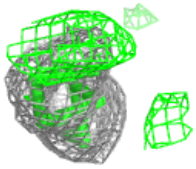


Electron density around STE b 627:

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

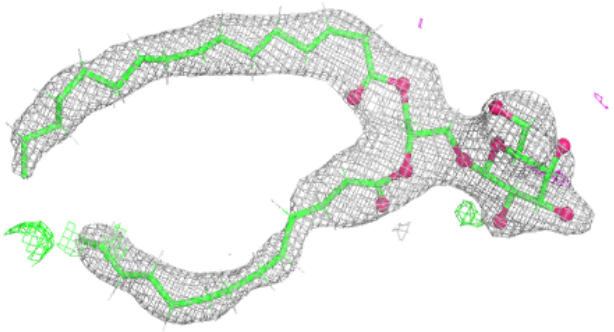


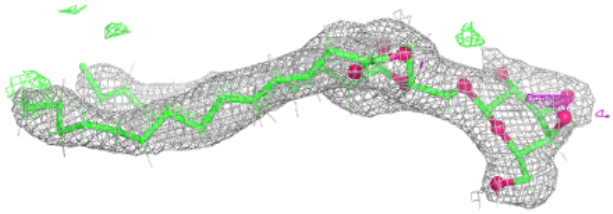


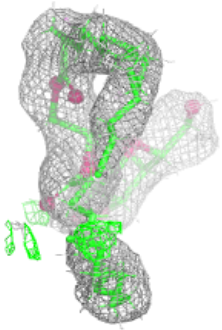


Electron density around LMG A 411:

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

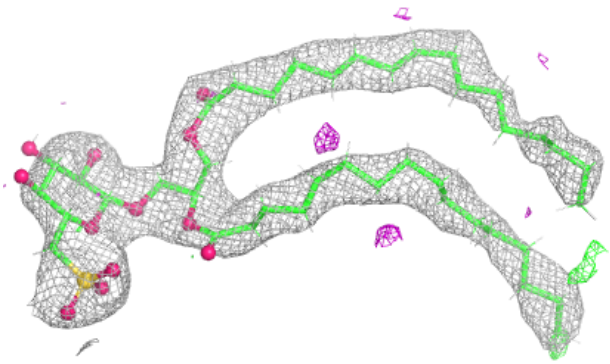


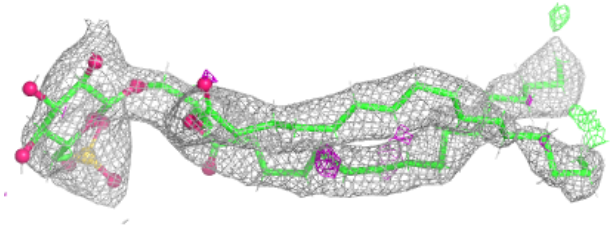


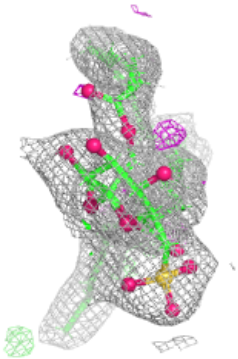


Electron density around SQD l 101:

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

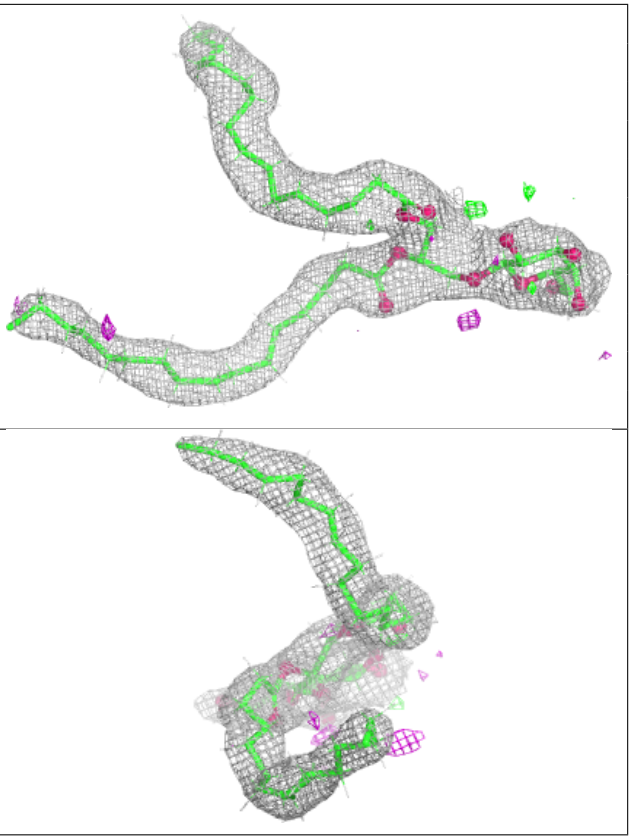






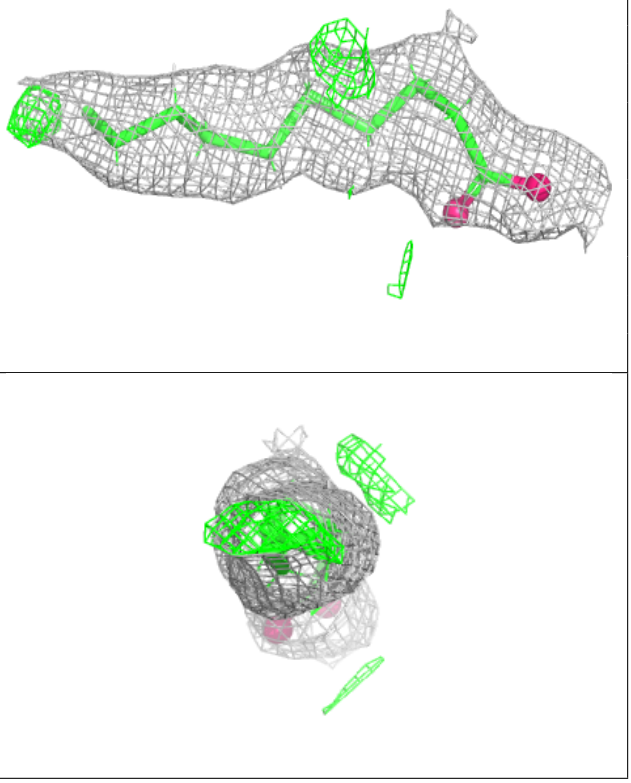
Electron density around LMG b 621:

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



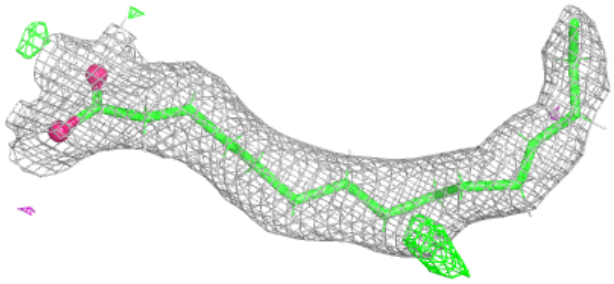
Electron density around STE J 101:

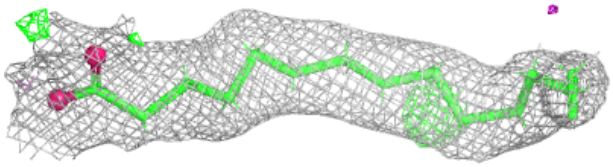
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

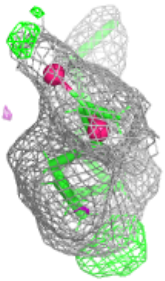


Electron density around STE B 621:

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

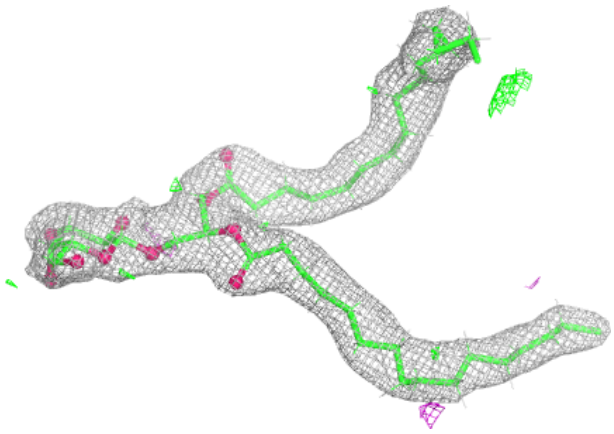


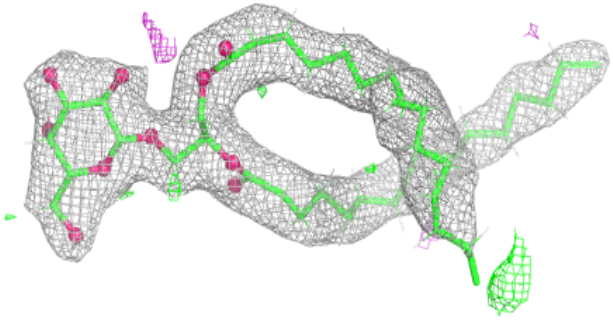


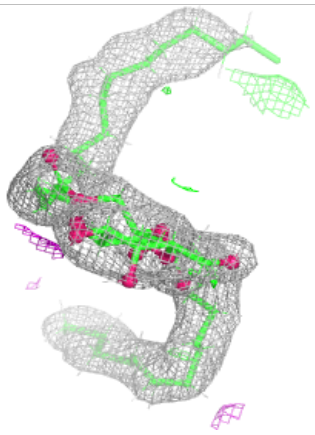


Electron density around LMG M 101:

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

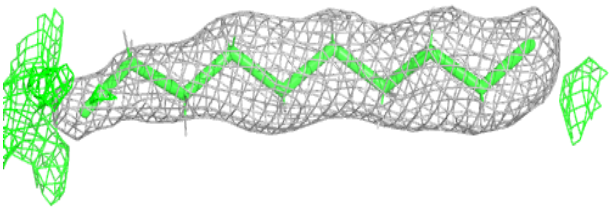


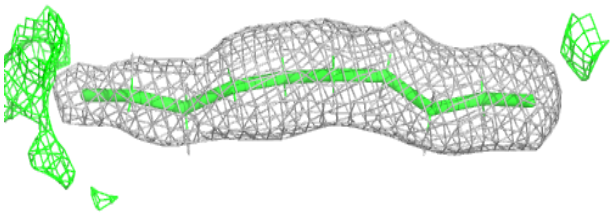


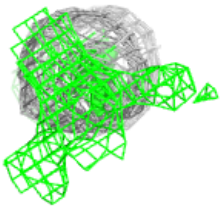


Electron density around STE M 103:

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

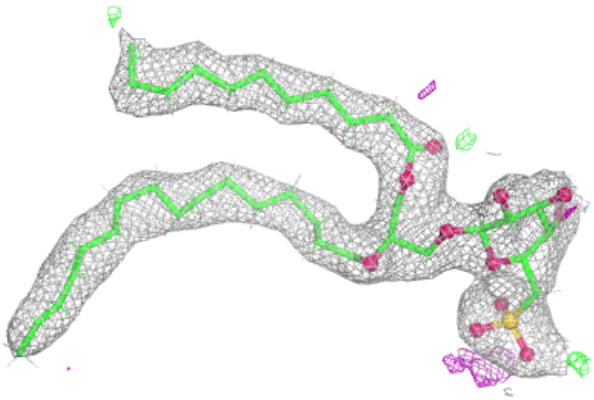


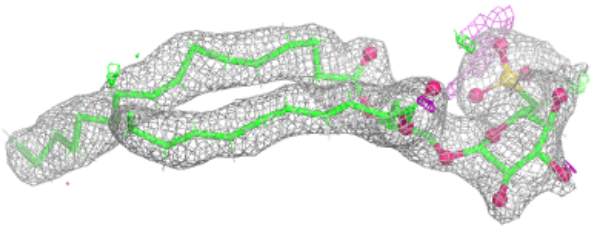


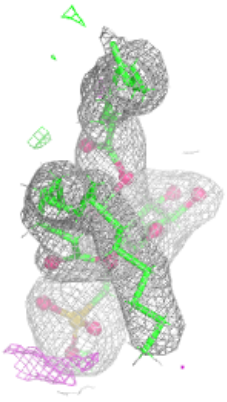


Electron density around SQD b 620:

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

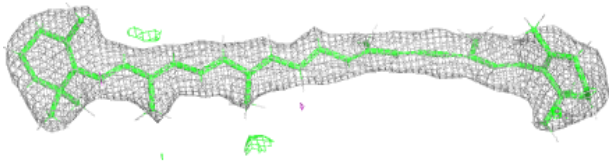


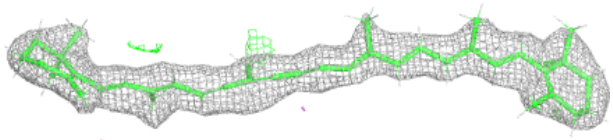


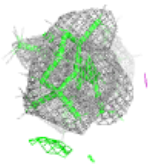


Electron density around BCR C 514:

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

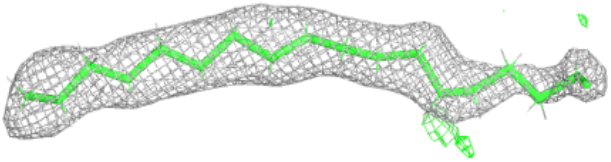


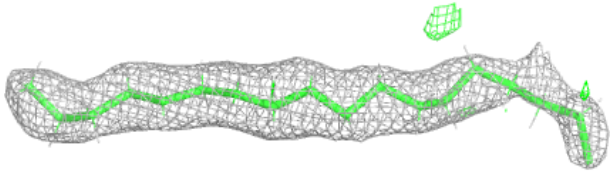


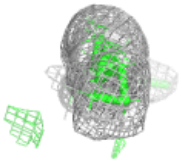


Electron density around STE l 103:

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

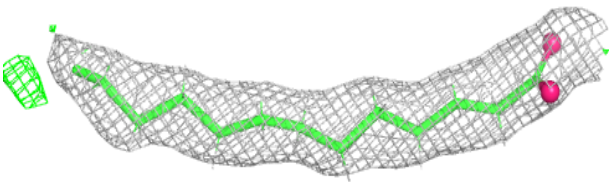


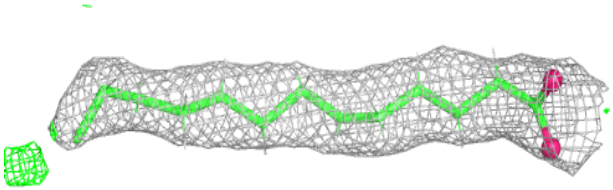


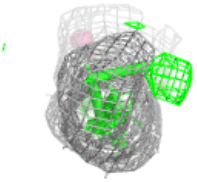


Electron density around STE M 102:

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

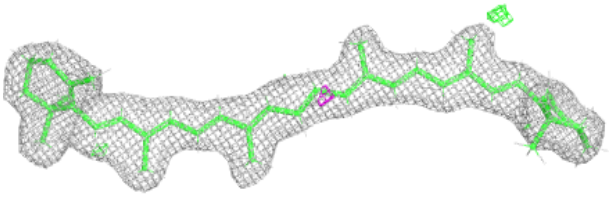


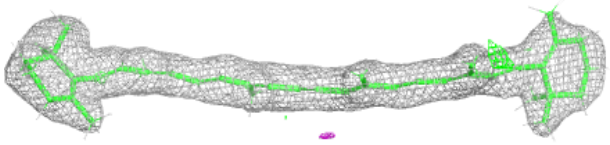


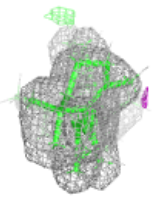


Electron density around BCR K 101:

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

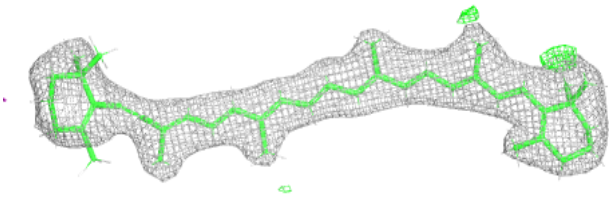


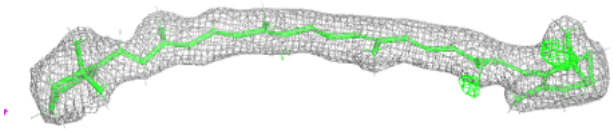


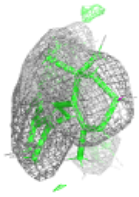


Electron density around BCR d 404:

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

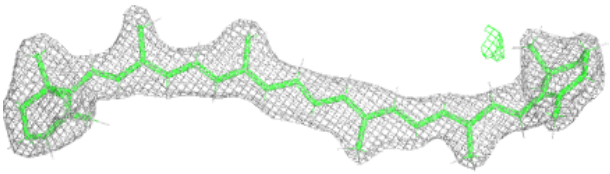


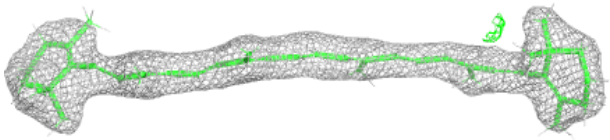


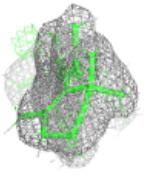


Electron density around BCR k 101:

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

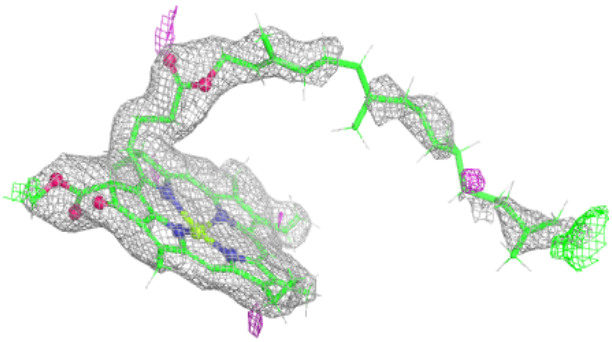


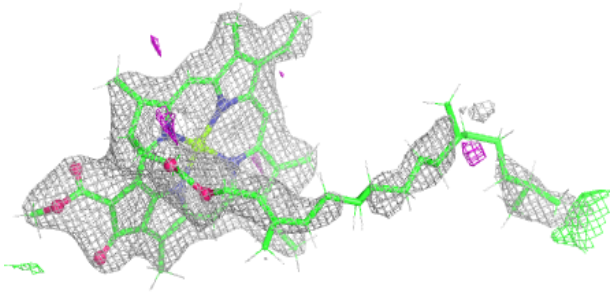


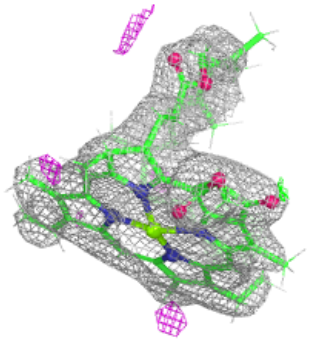


Electron density around CLA c 513:

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

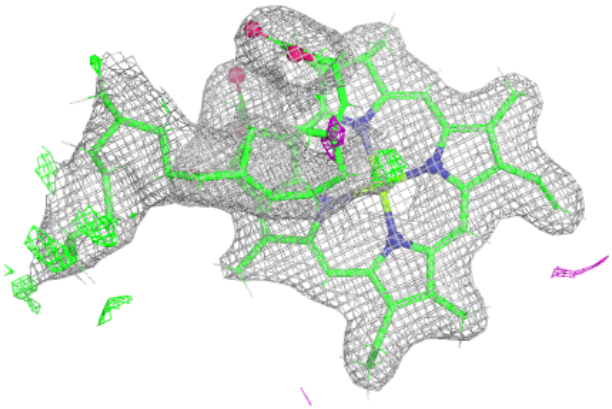


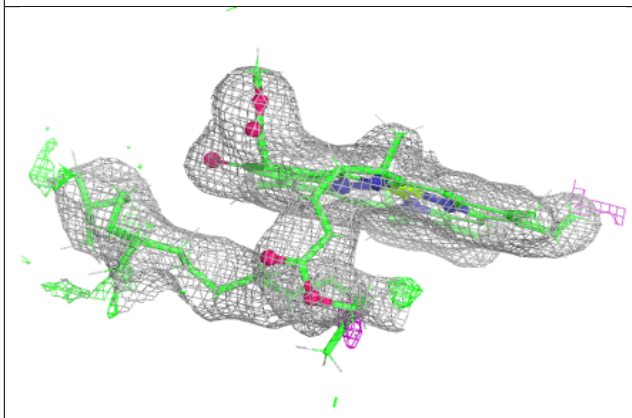


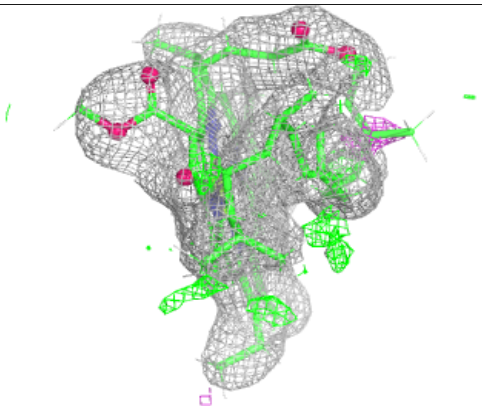


Electron density around CLA B 601:

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

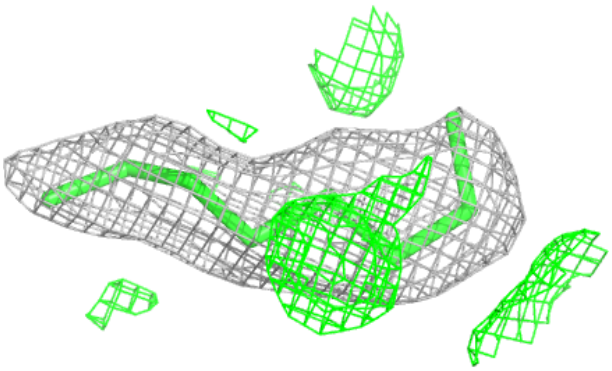


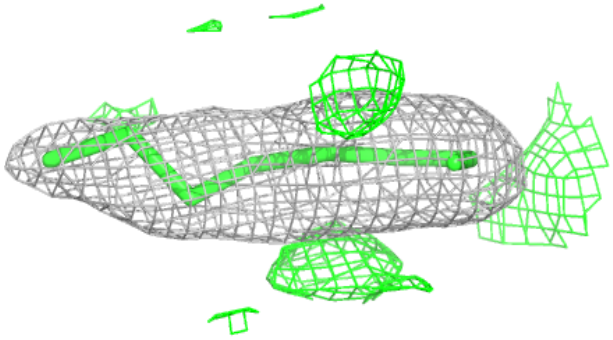


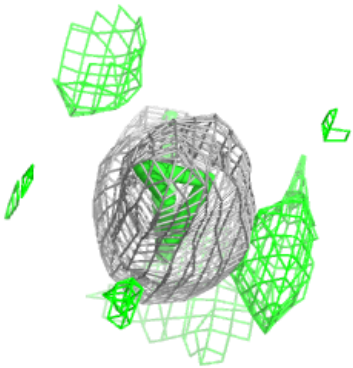


Electron density around STE A 415:

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

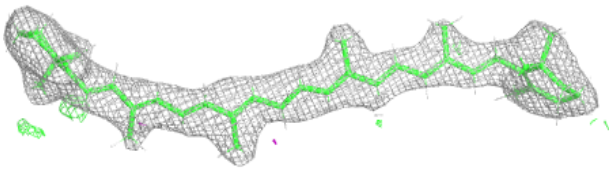


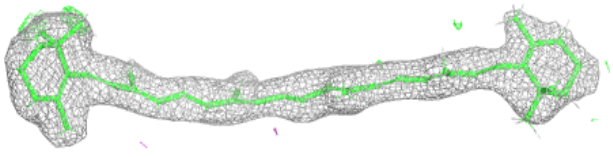


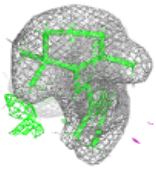


Electron density around BCR x 101:

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

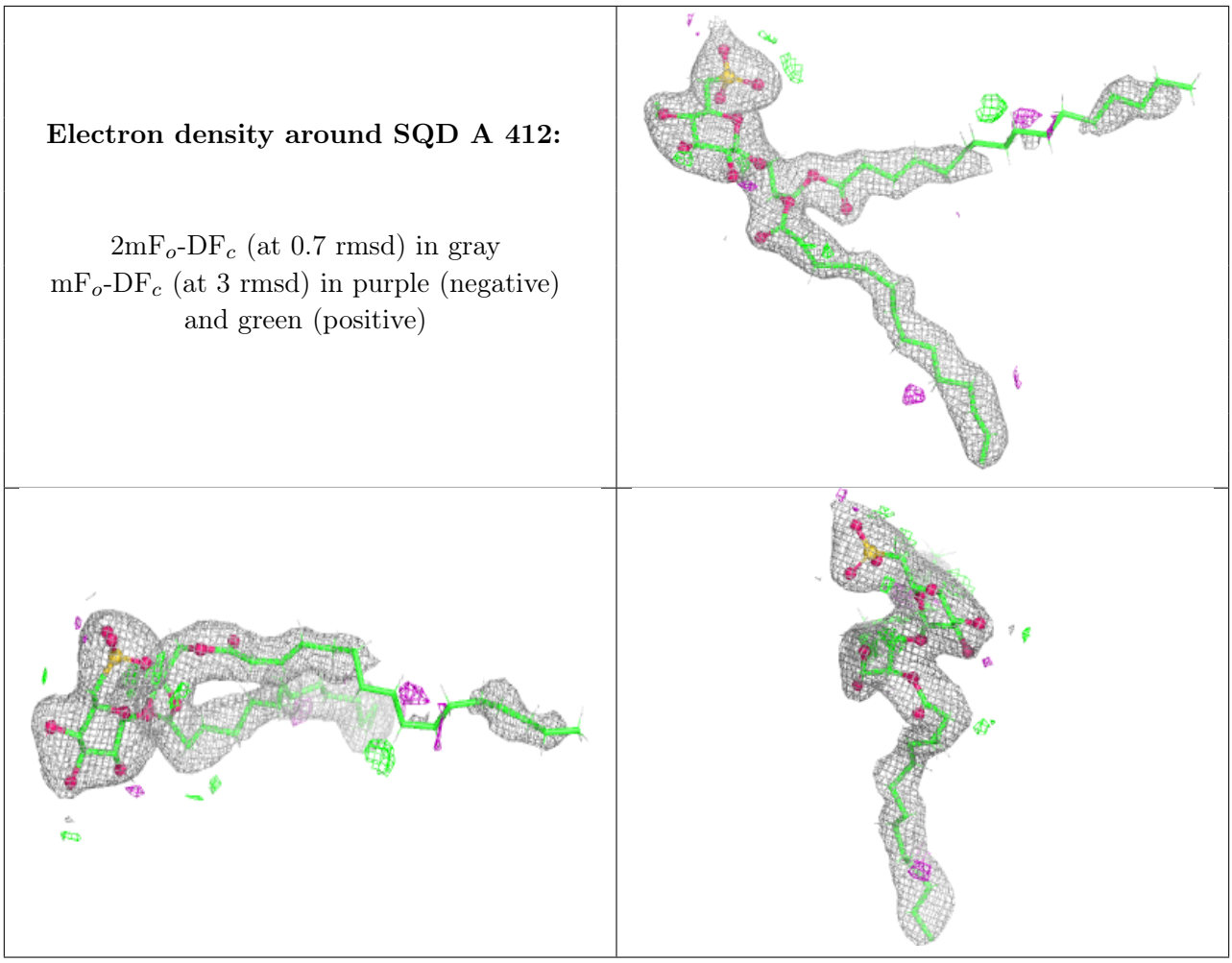






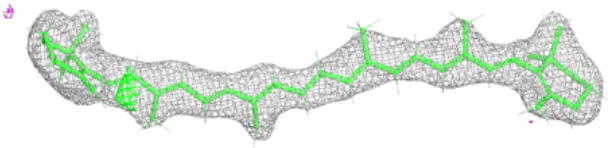
Electron density around SQD A 412:

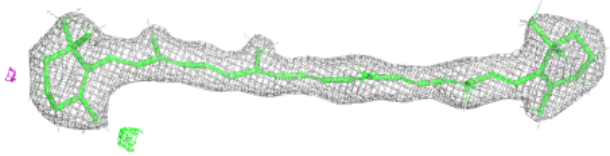
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

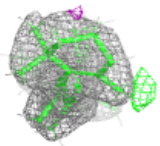


Electron density around BCR c 514:

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

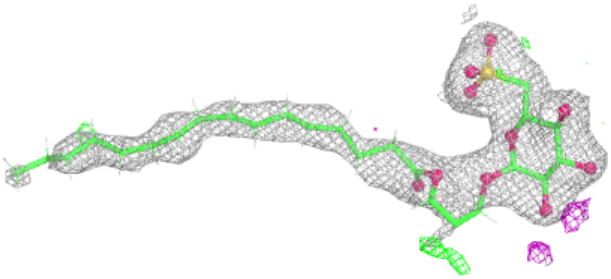


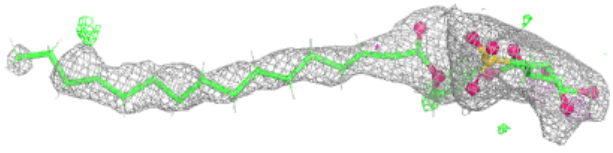


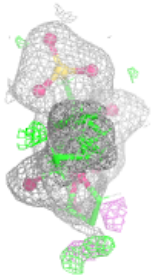


Electron density around SQD F 102:

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

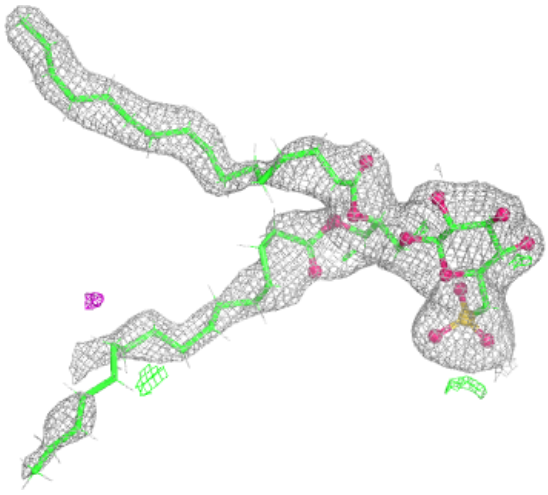


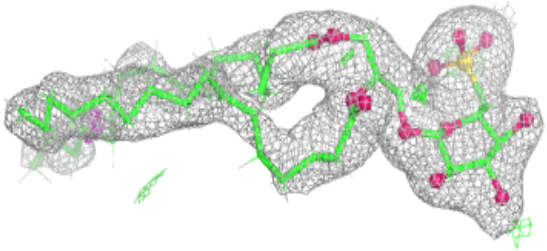


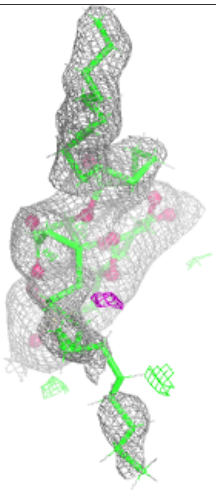


Electron density around SQD a 412:

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

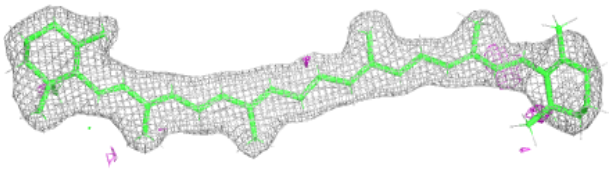


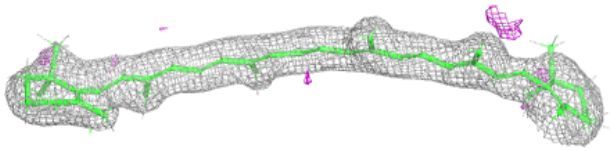


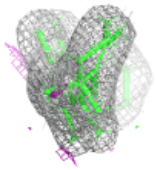


Electron density around BCR D 406:

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

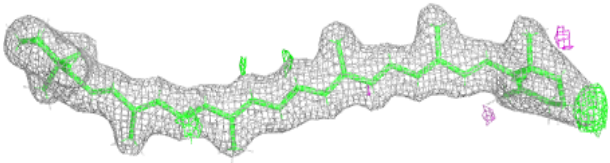


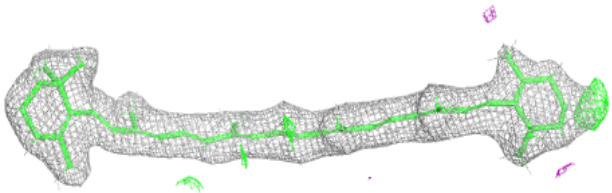


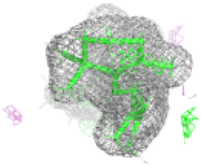


Electron density around BCR H 101:

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

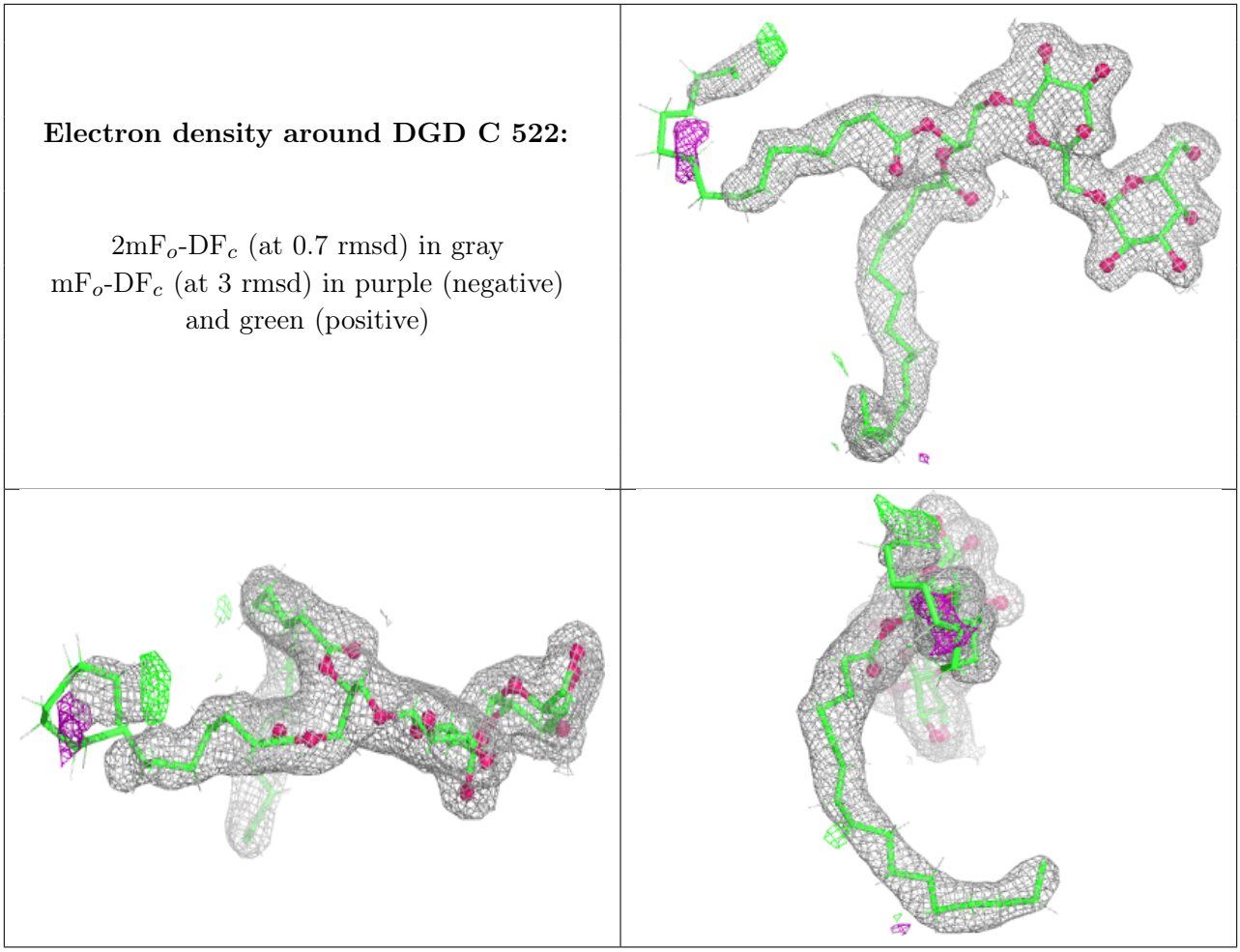






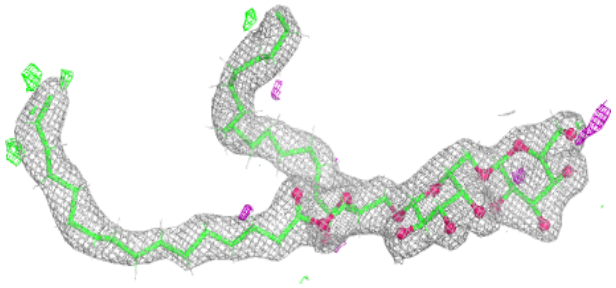
Electron density around DGD C 522:

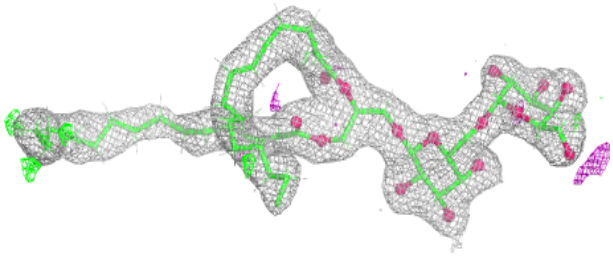
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 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)

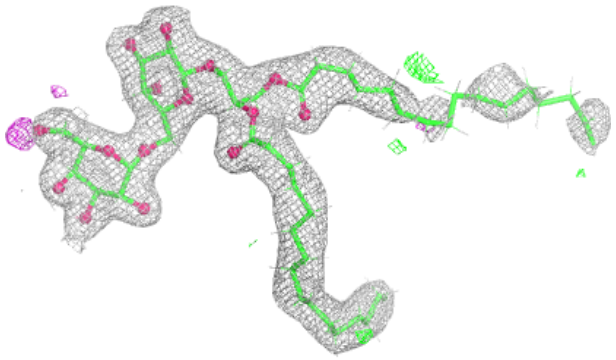


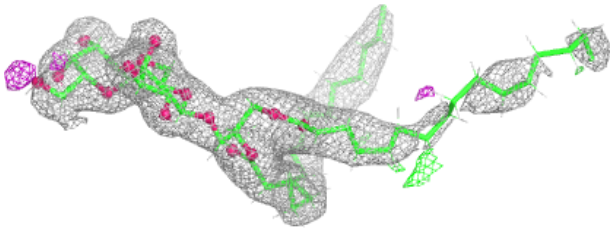


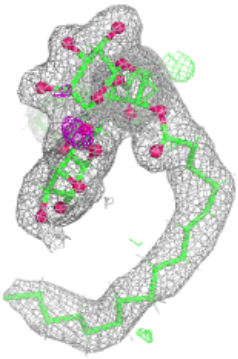


Electron density around DGD c 520:

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

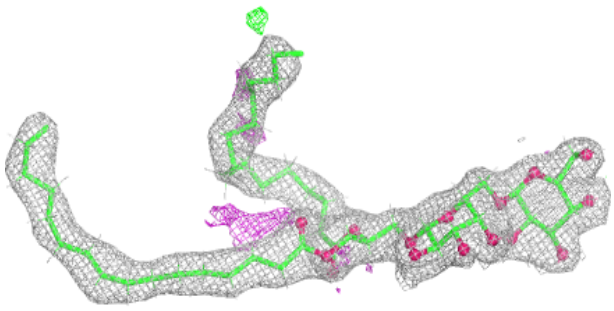


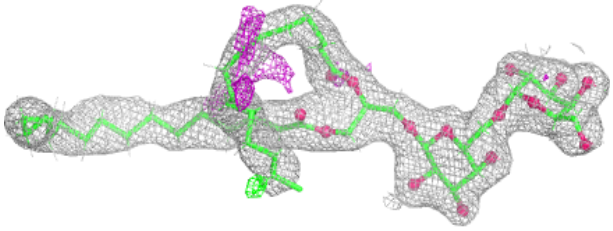


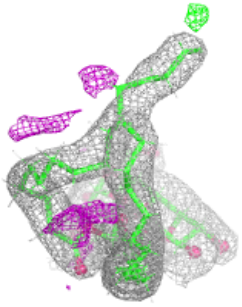


Electron density around DGD h 102:

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

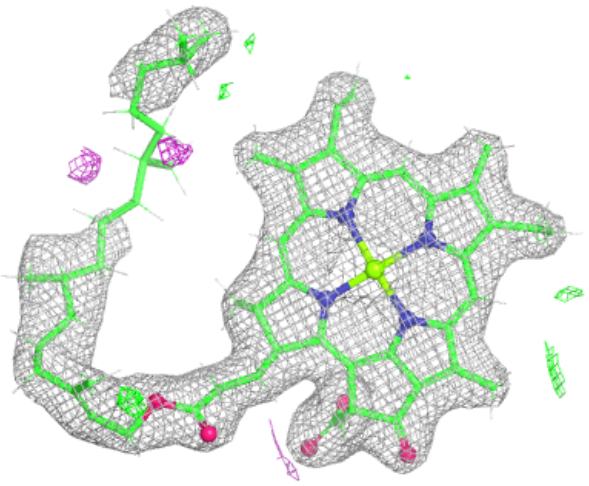


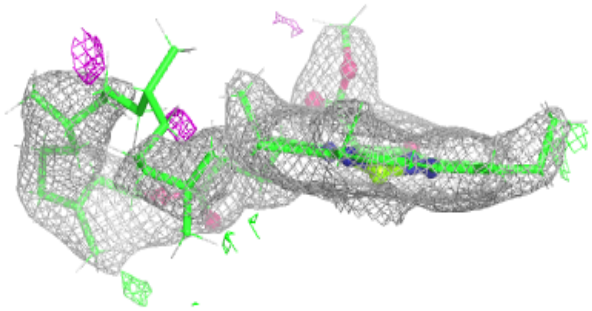


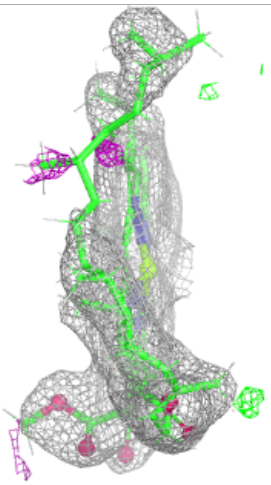


Electron density around CLA c 512:

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

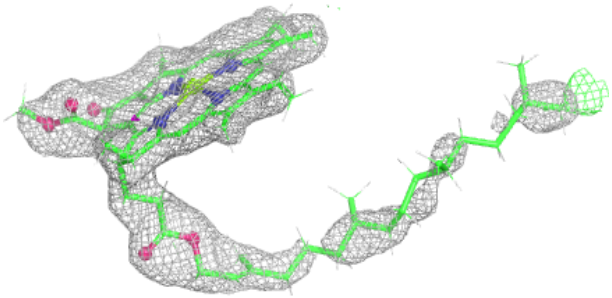


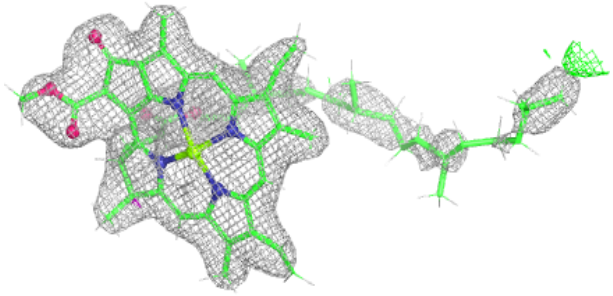


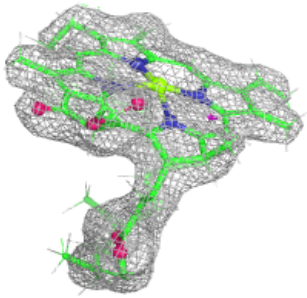


Electron density around CLA C 513:

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

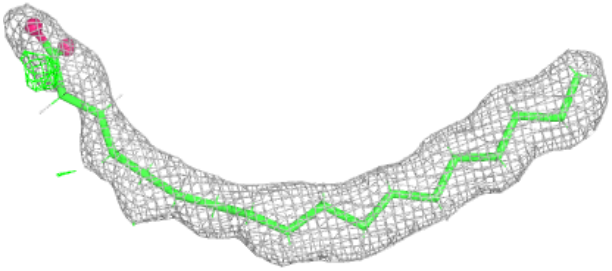


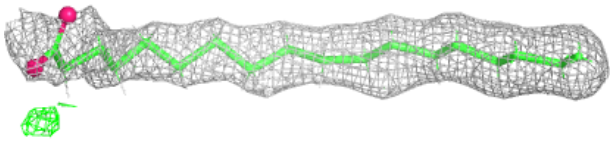


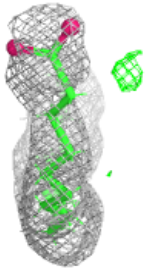


Electron density around STE D 413:

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

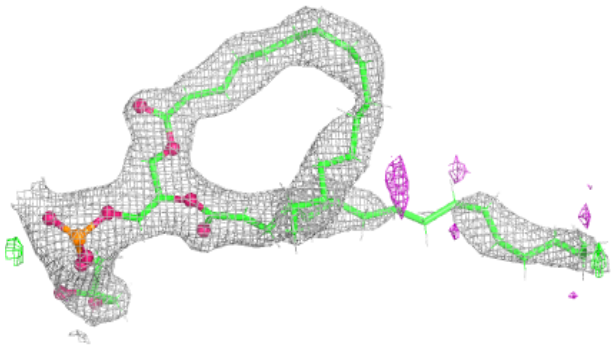


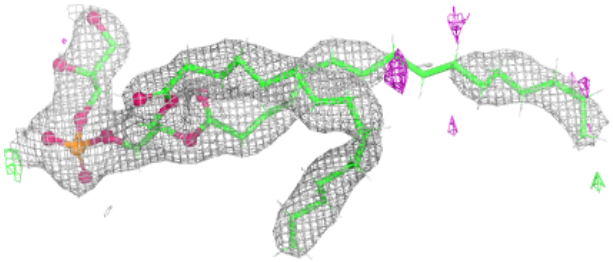


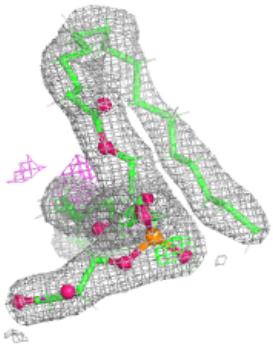


Electron density around LHG d 406:

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

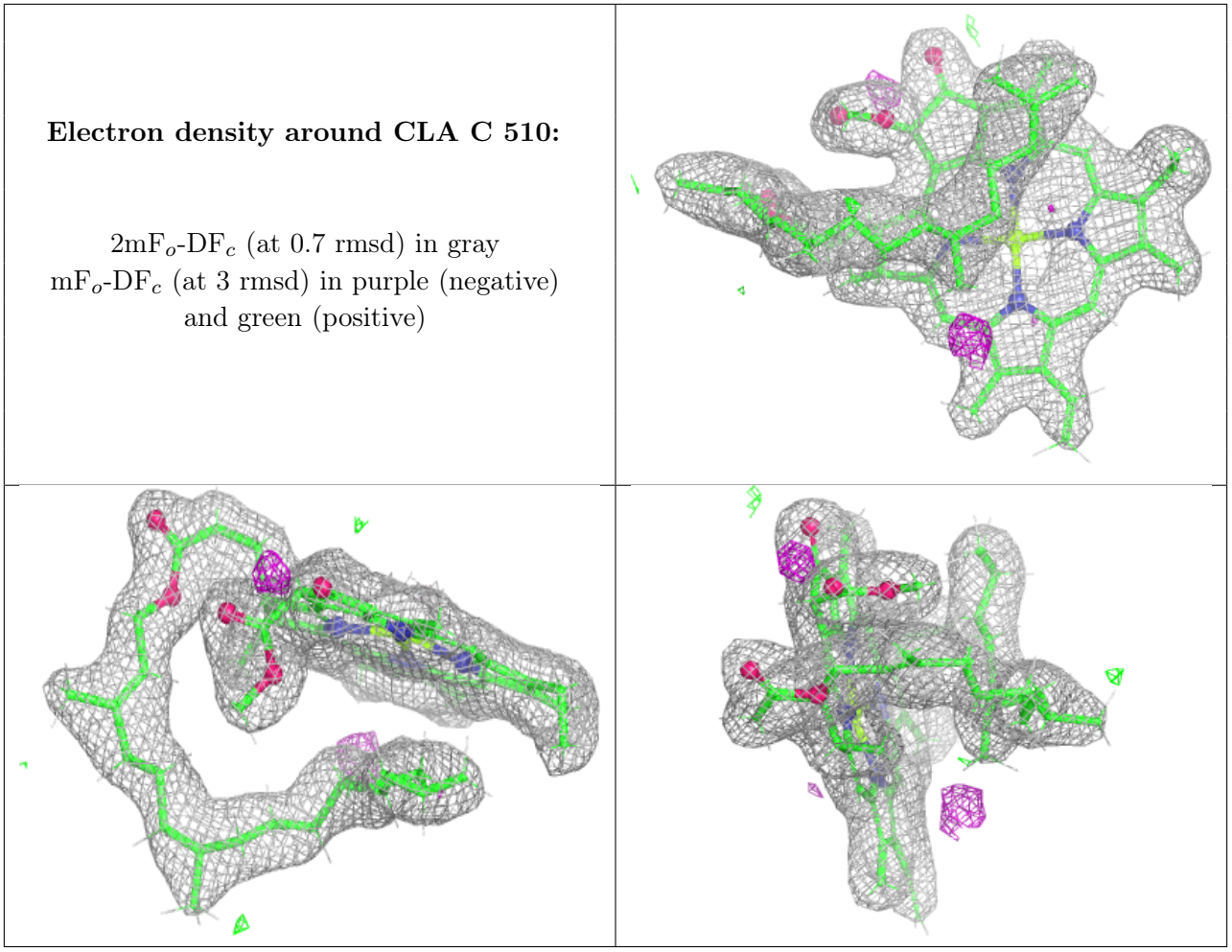






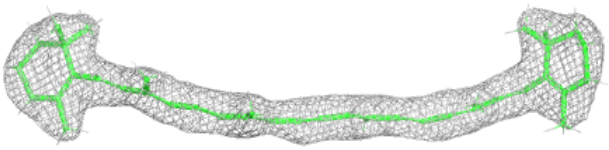
Electron density around CLA C 510:

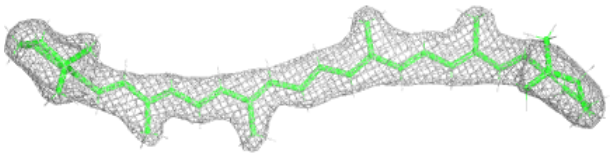
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

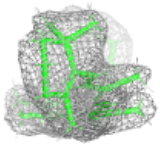


Electron density around BCR k 102:

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

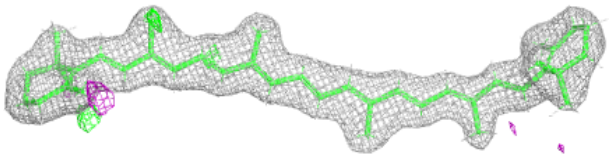


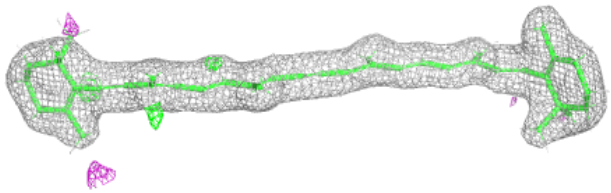


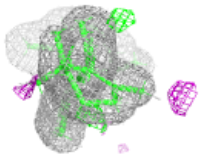


Electron density around BCR C 515:

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

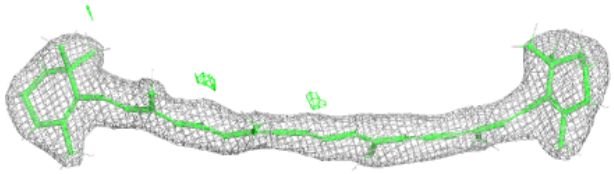


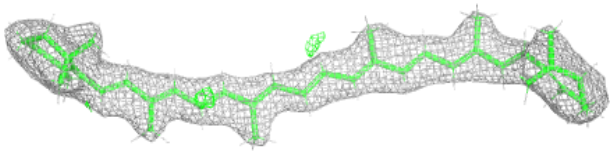


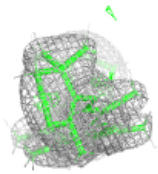


Electron density around BCR C 520:

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

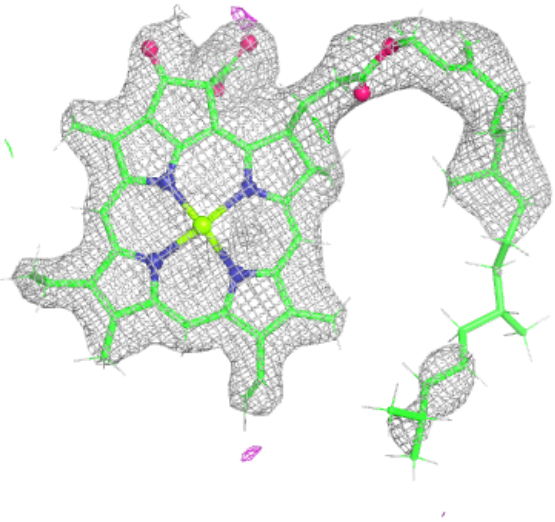


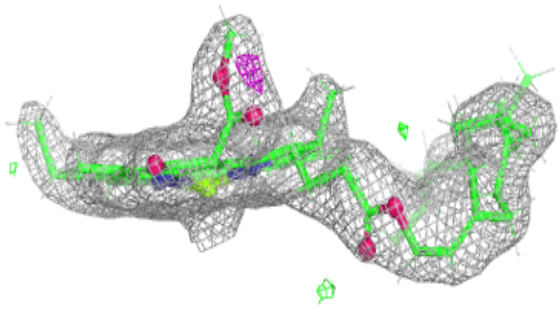


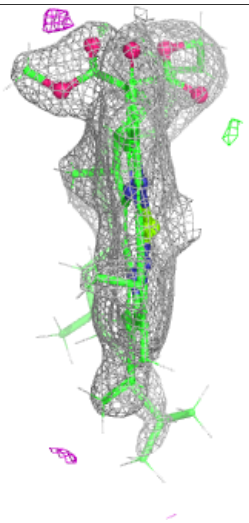


Electron density around CLA C 512:

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

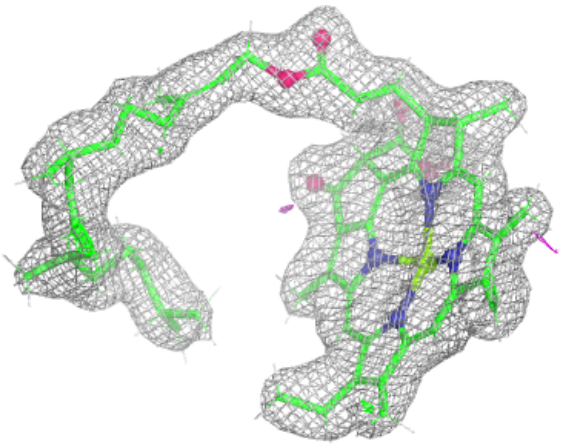


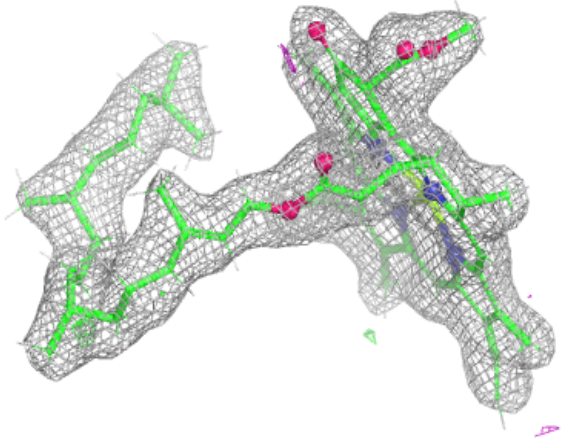


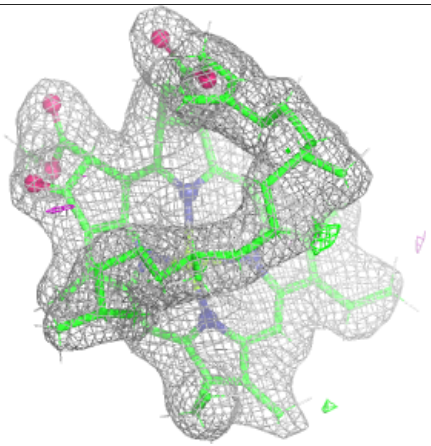


Electron density around CLA C 503:

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

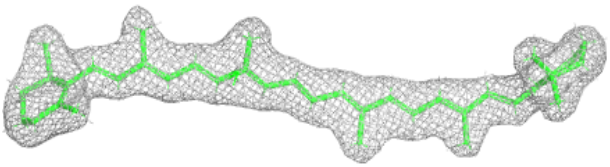


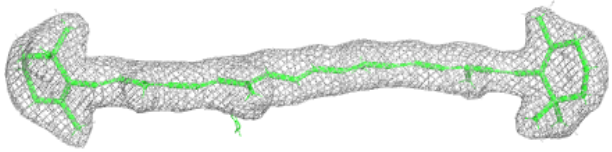


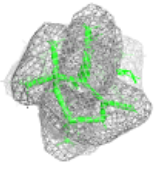


Electron density around BCR A 408:

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

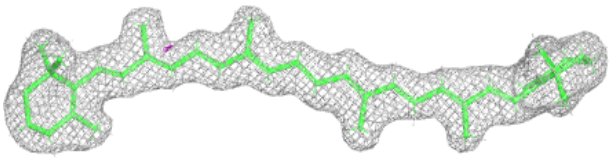


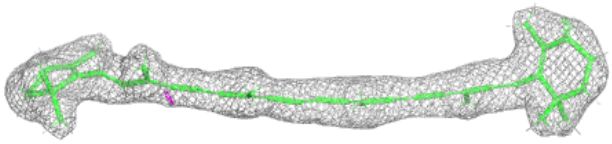


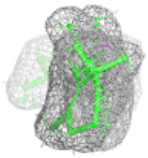


Electron density around BCR b 616:

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

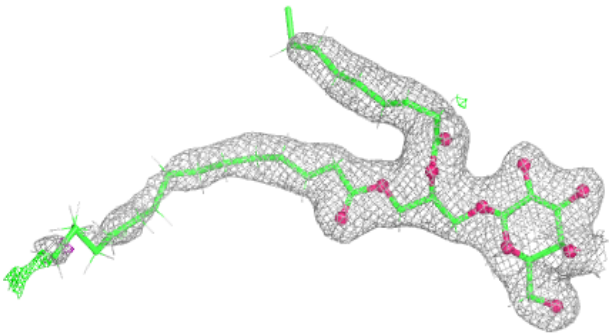


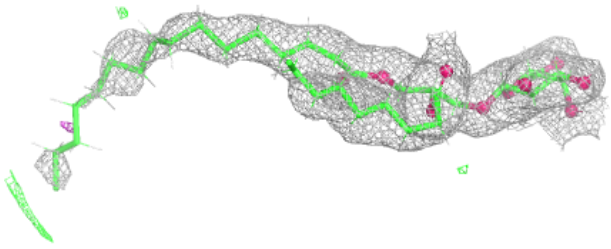


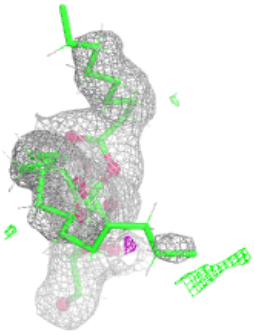


Electron density around LMG d 409:

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

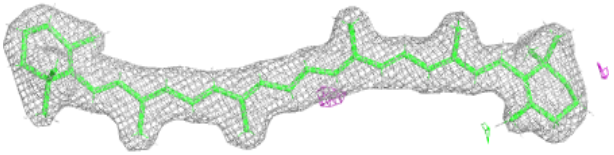


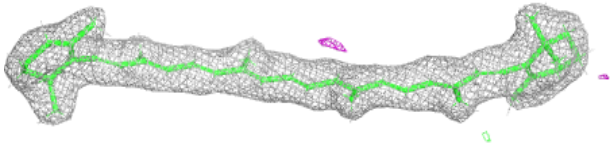


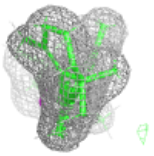


Electron density around BCR b 618:

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

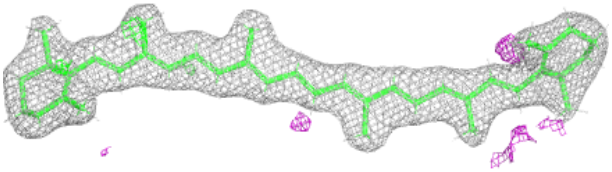


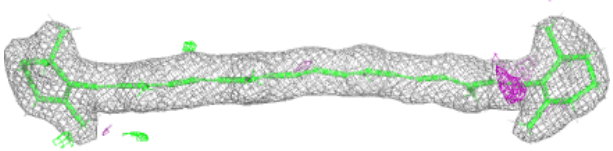


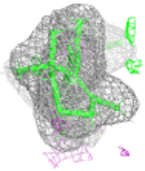


Electron density around BCR B 618:

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

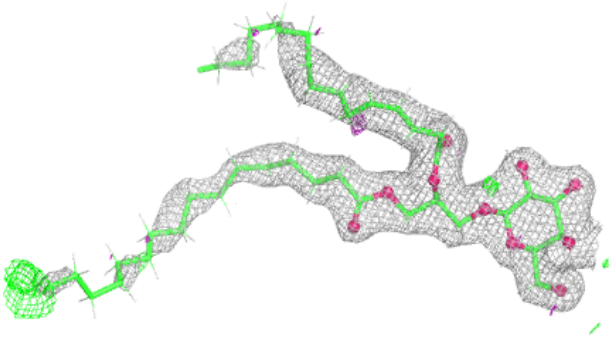


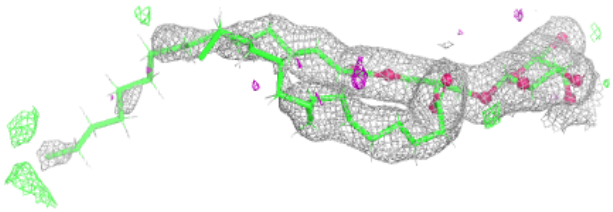


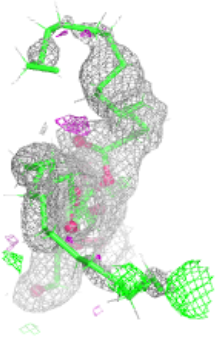


Electron density around LMG D 409:

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

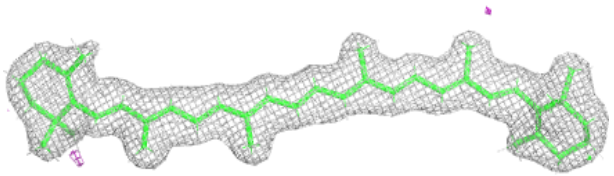


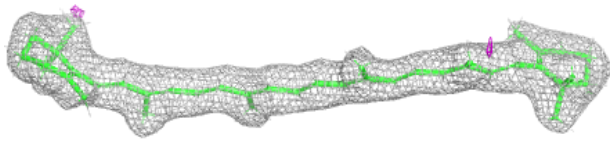


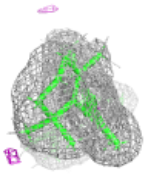


Electron density around BCR B 619:

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

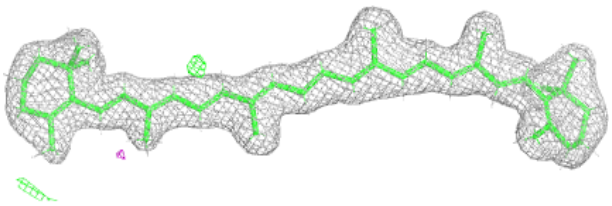


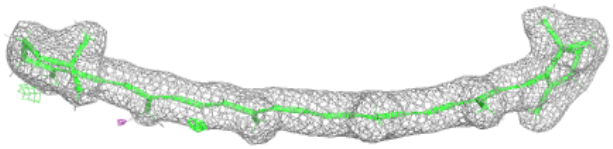


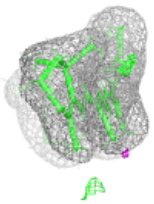


Electron density around BCR T 101:

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

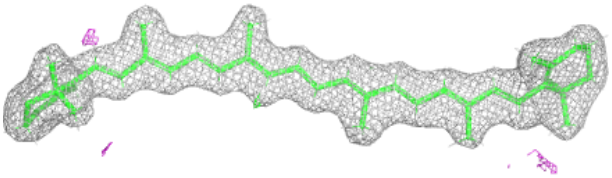


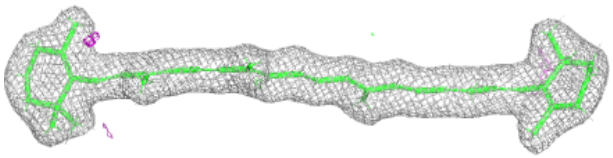


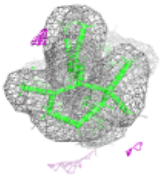


Electron density around BCR a 409:

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

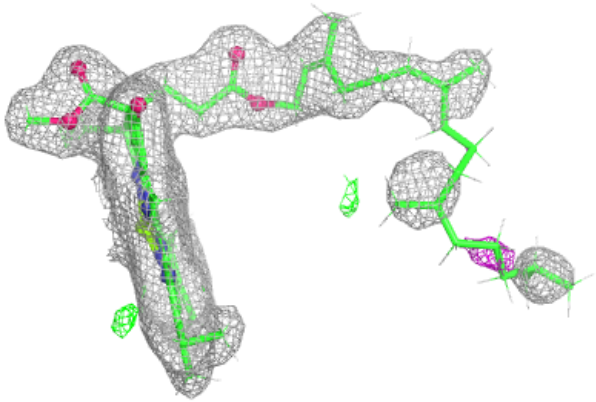


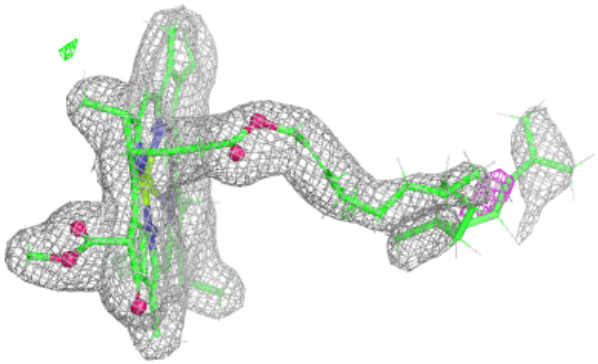


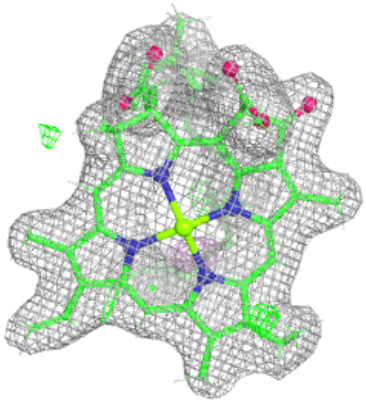


Electron density around CLA c 506:

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

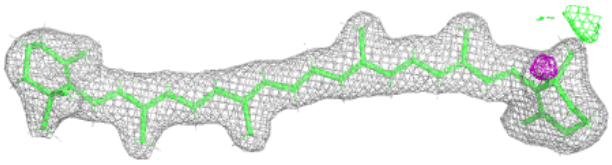


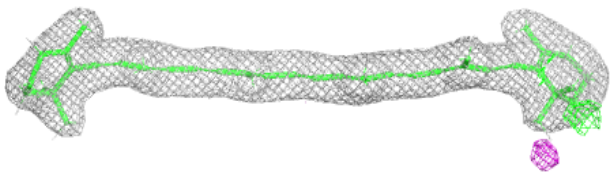


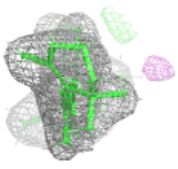


Electron density around BCR b 617:

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

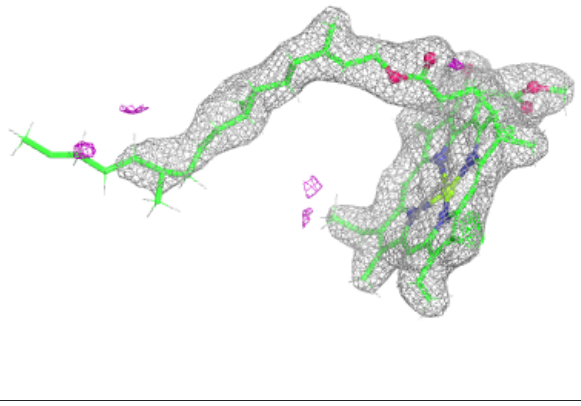


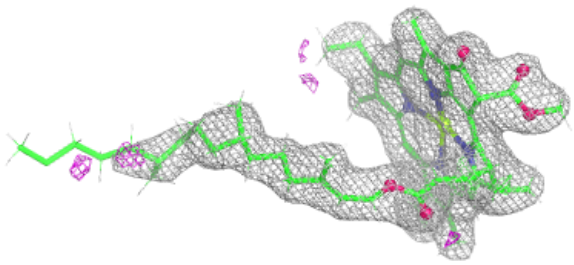


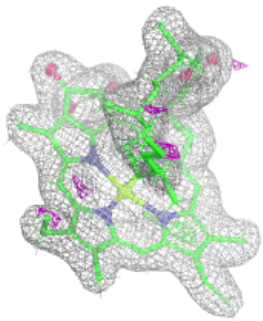


Electron density around CLA c 508:

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

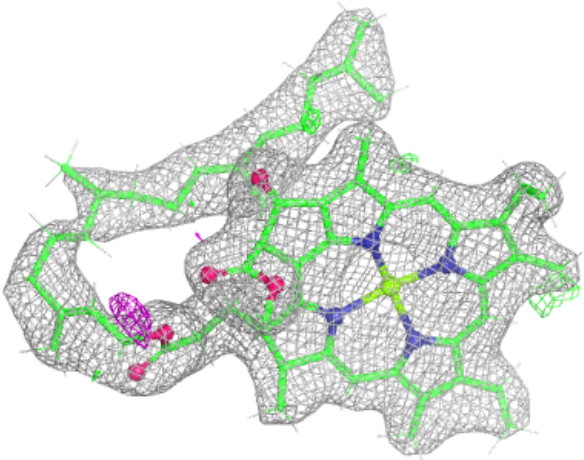


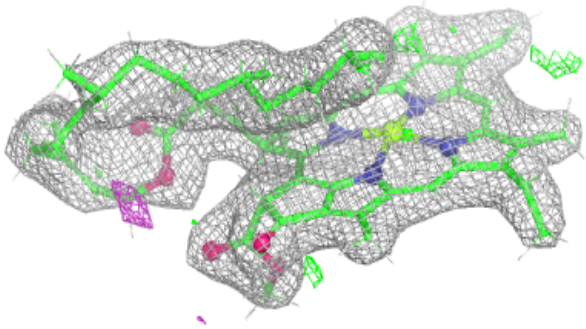


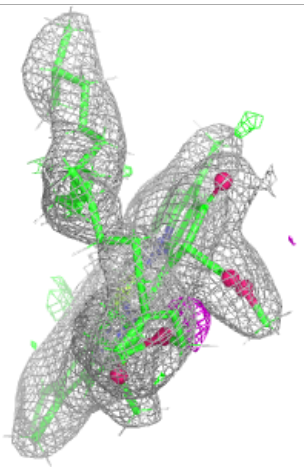


Electron density around CLA c 509:

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

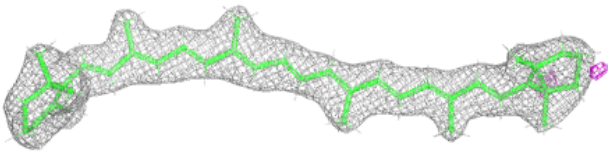


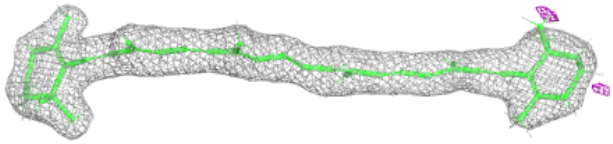


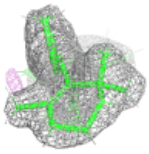


Electron density around BCR c 515:

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

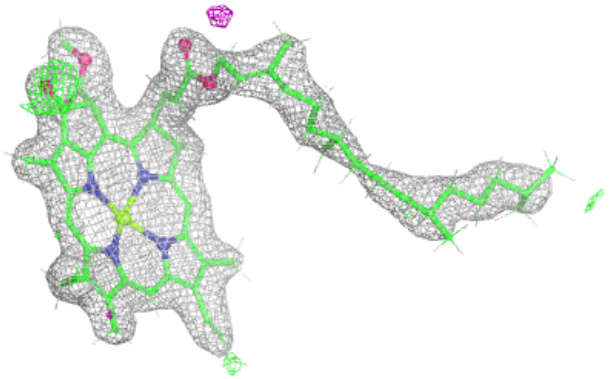


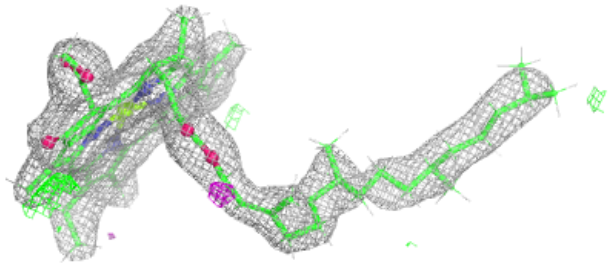


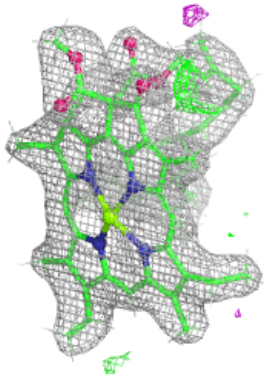


Electron density around CLA c 511:

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

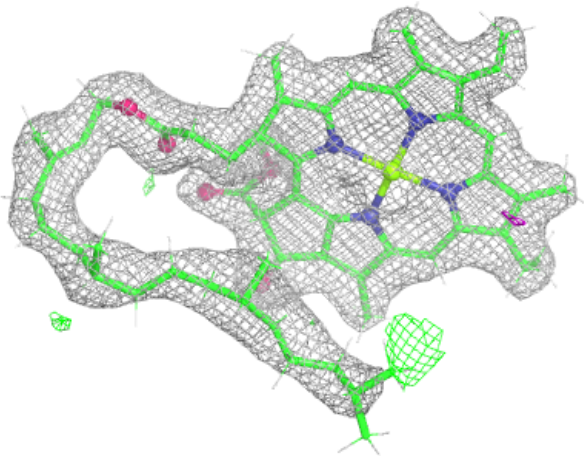


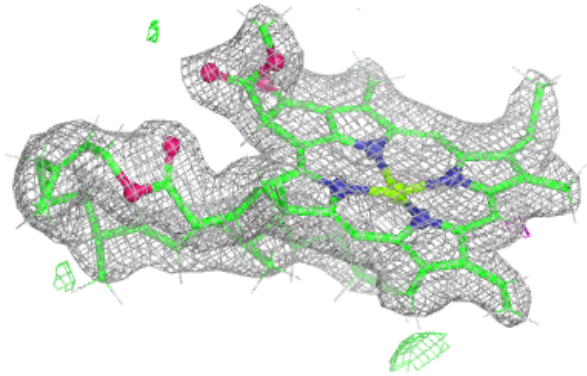


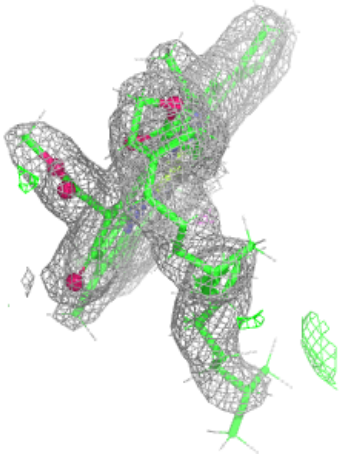


Electron density around CLA C 509:

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

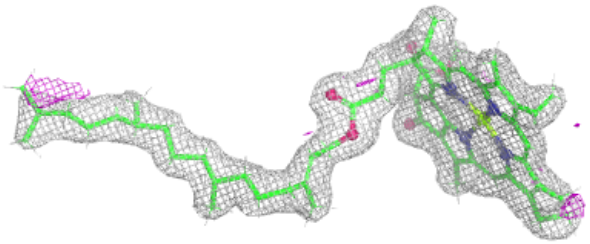


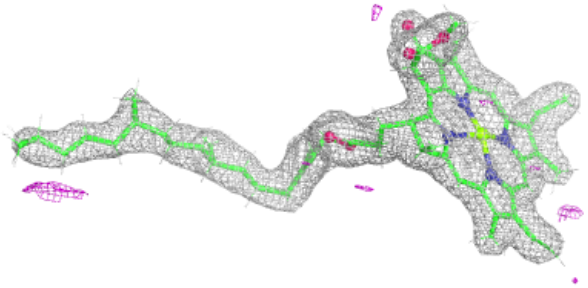


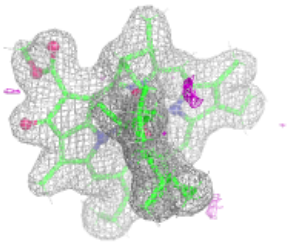


Electron density around CLA C 502:

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

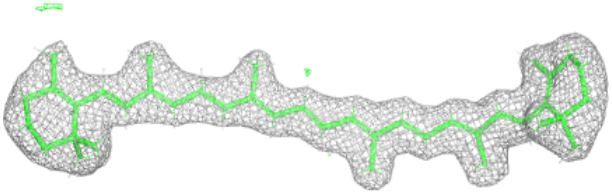


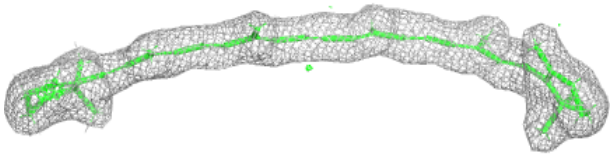


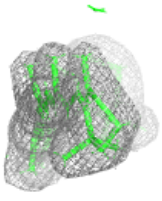


Electron density around BCR t 101:

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

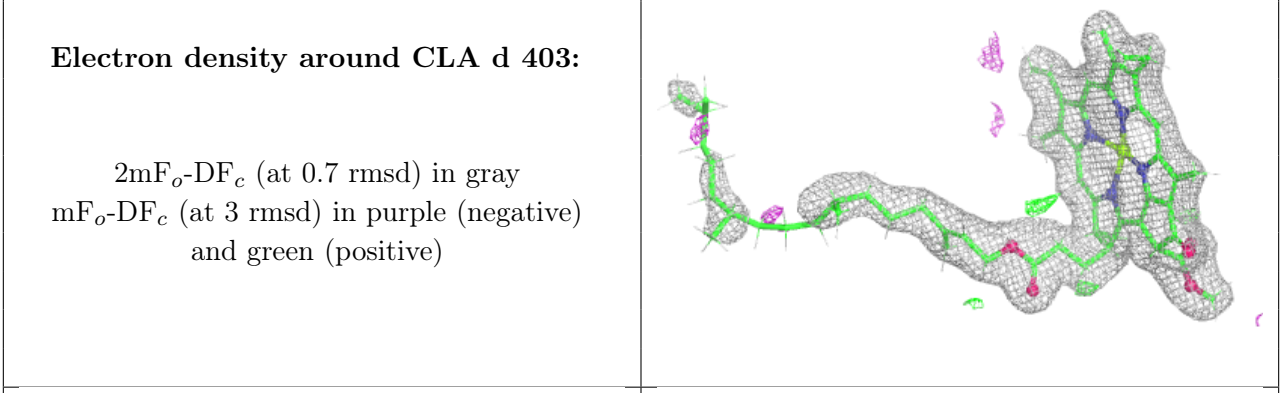






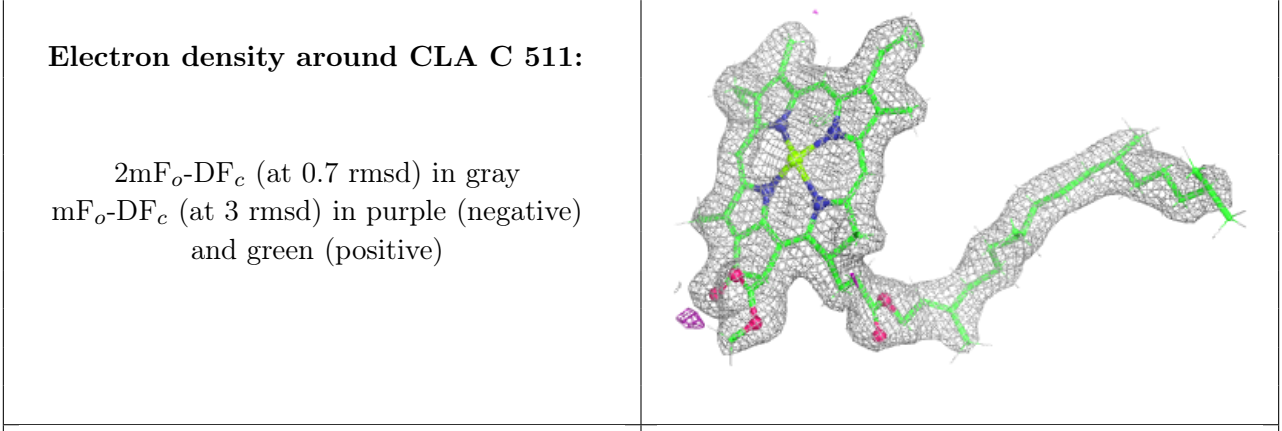
Electron density around CLA d 403:

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



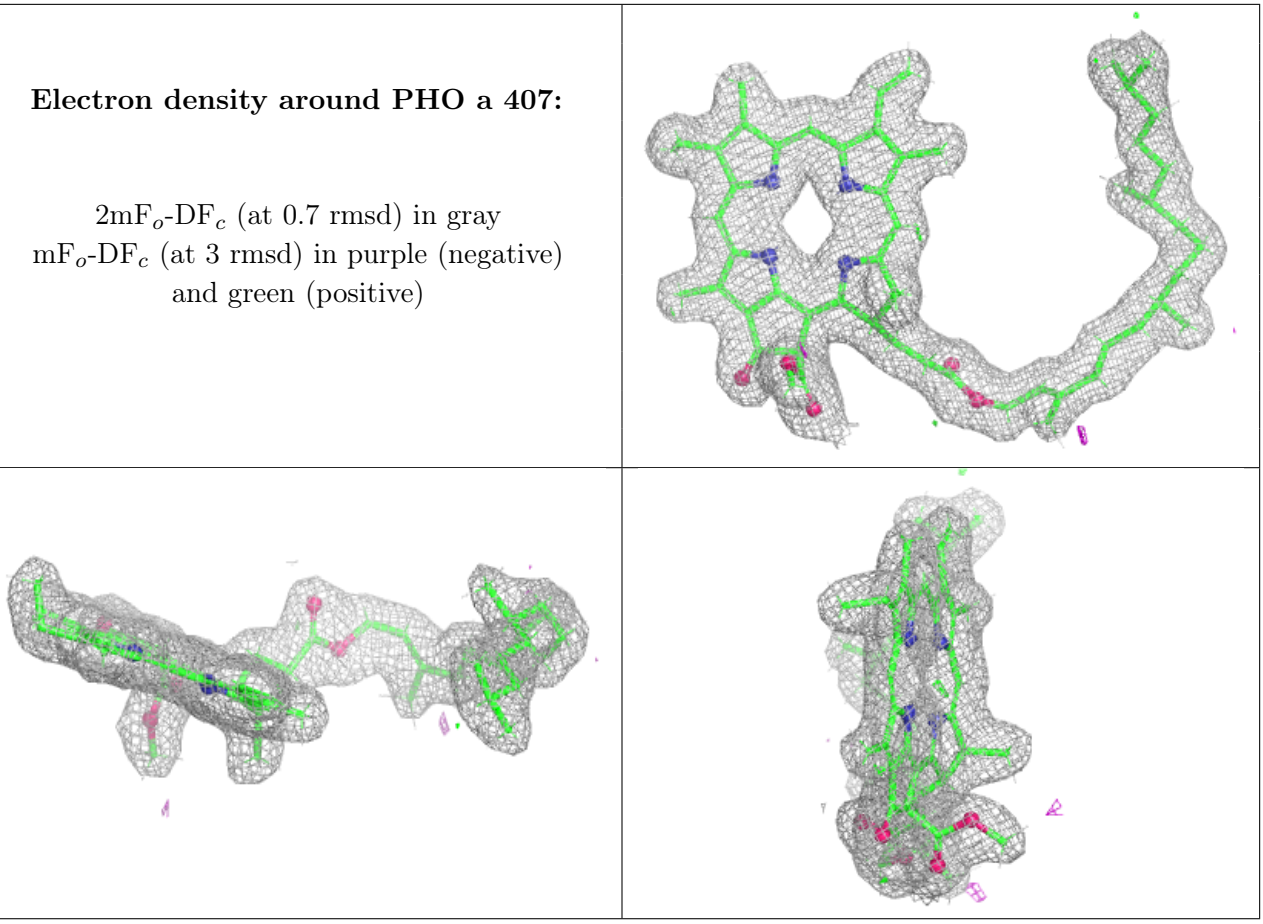
Electron density around CLA C 511:

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



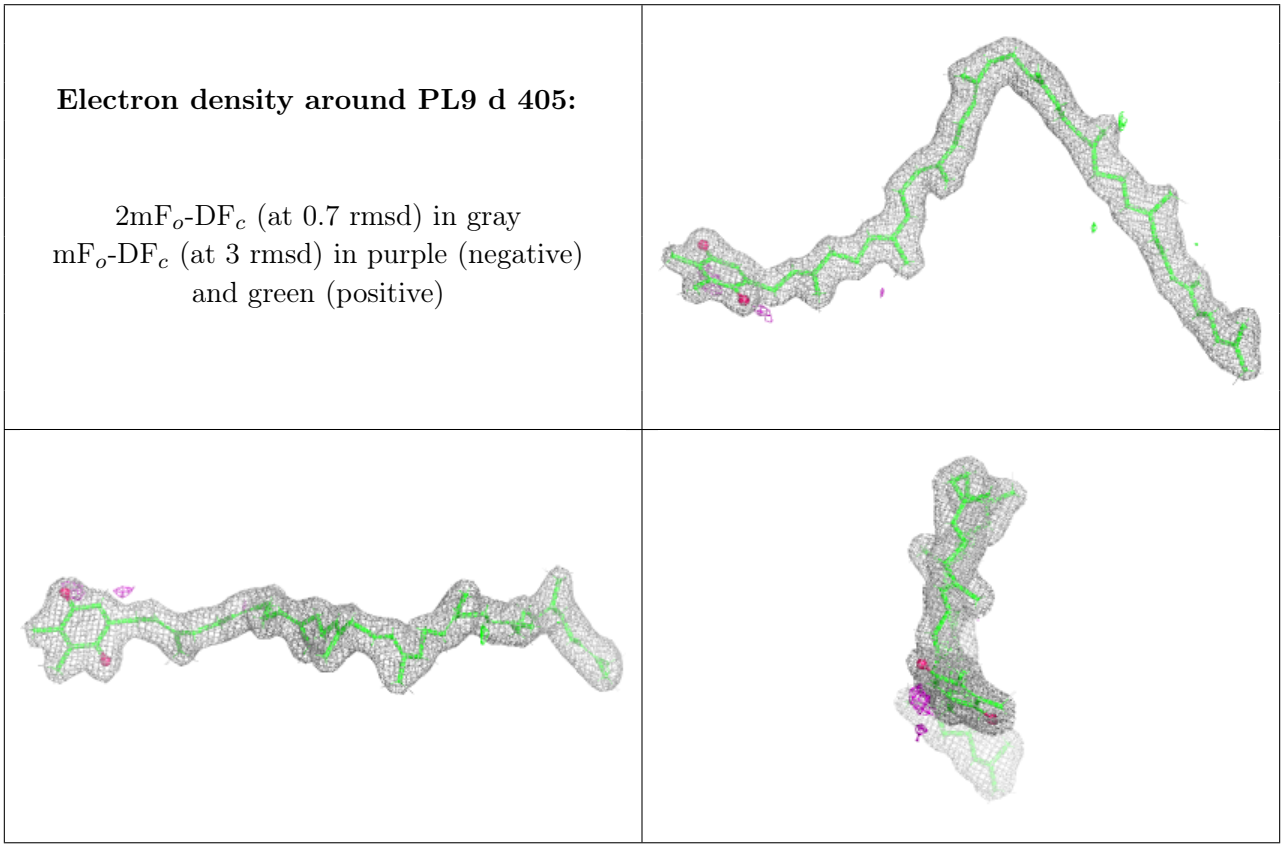
Electron density around PHO a 407:

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



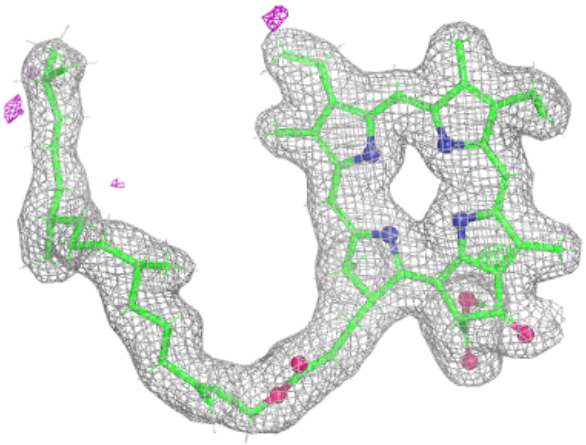
Electron density around PL9 d 405:

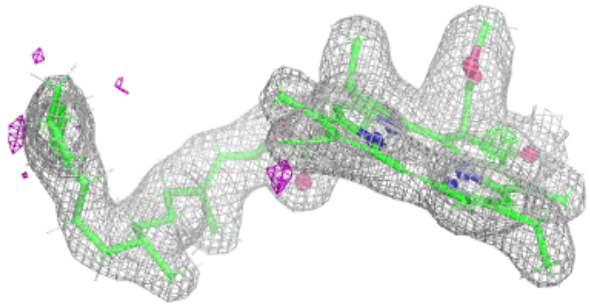
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

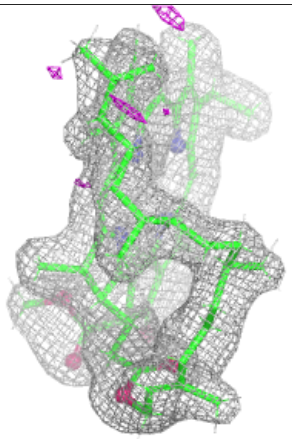


Electron density around PHO d 401:

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

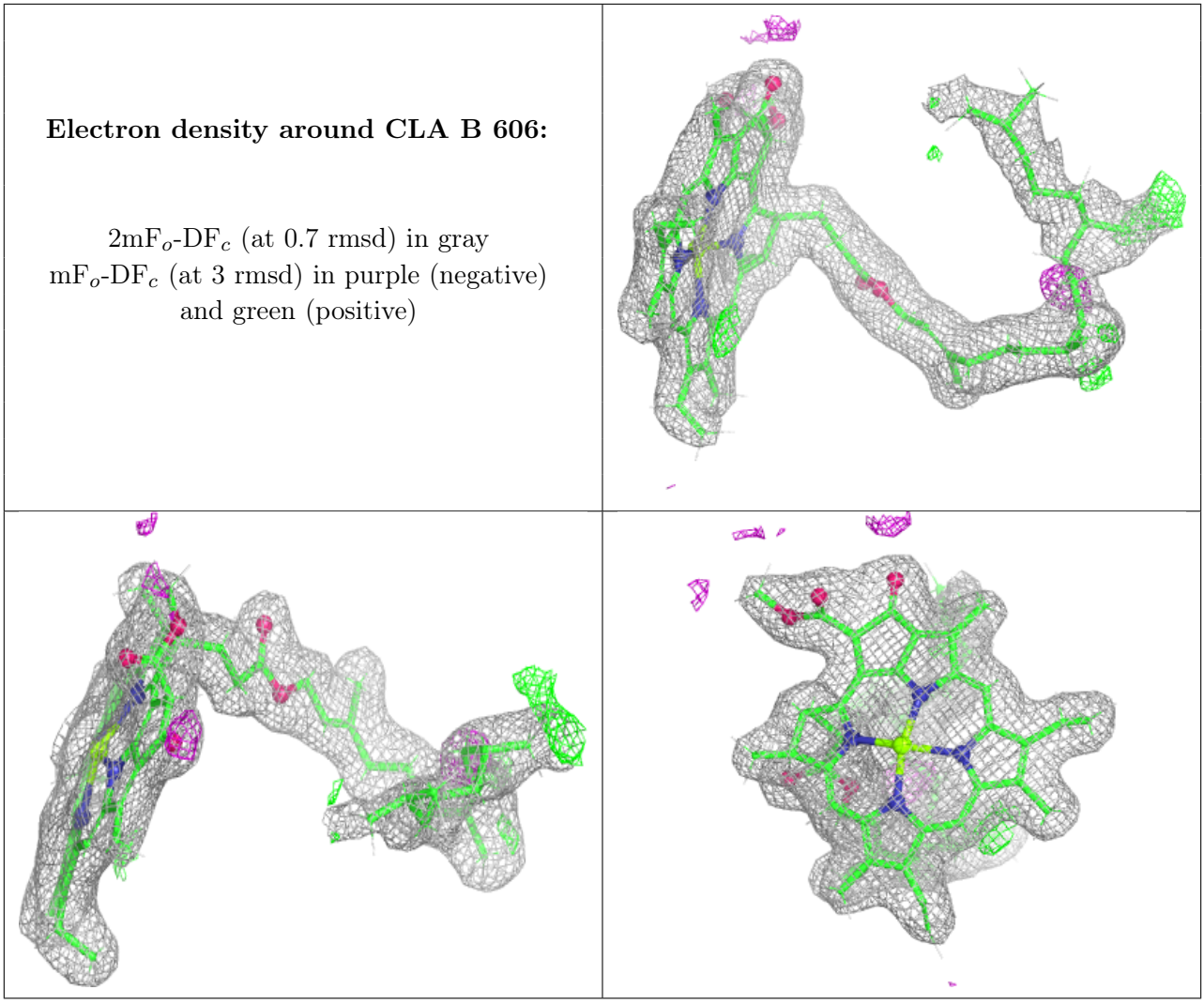






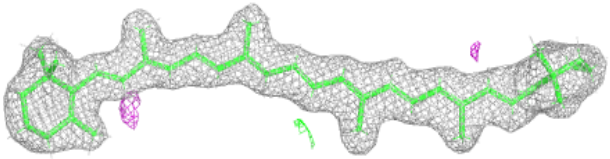
Electron density around CLA B 606:

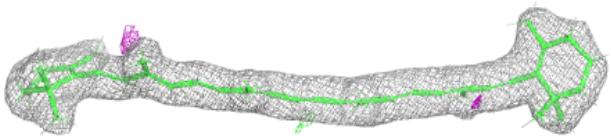
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

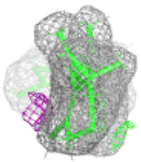


Electron density around BCR B 617:

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

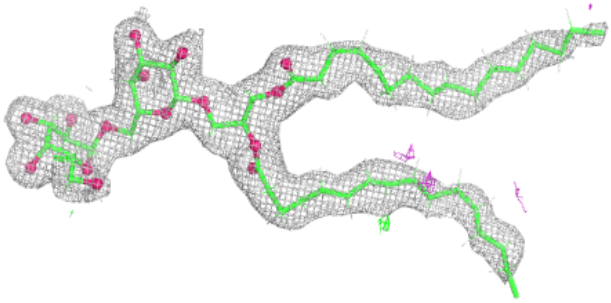


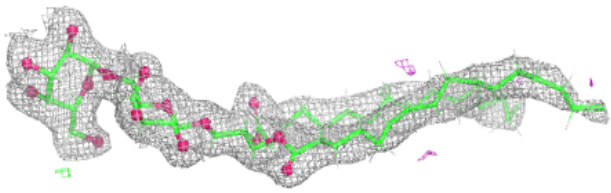


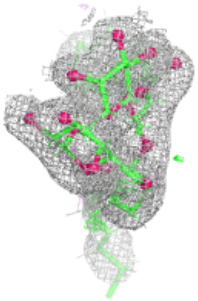


Electron density around DGD C 523:

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

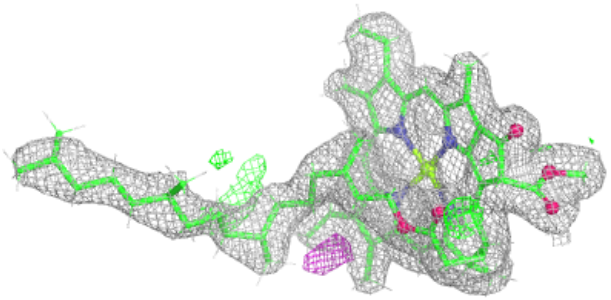


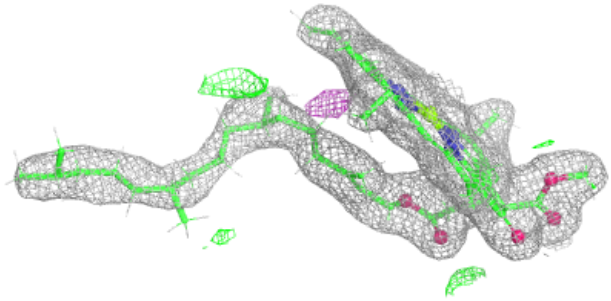


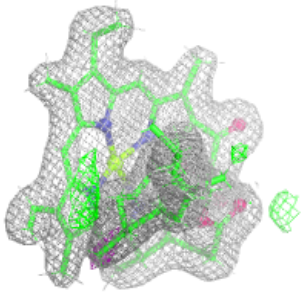


Electron density around CLA C 505:

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

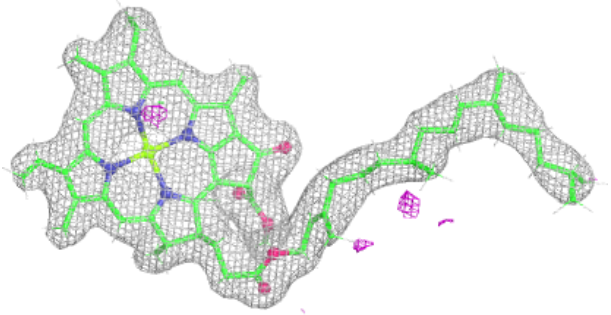


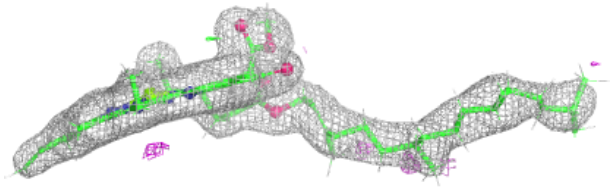


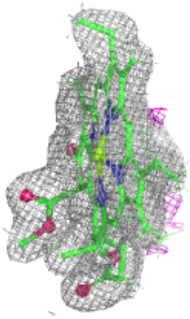


Electron density around CLA b 601:

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

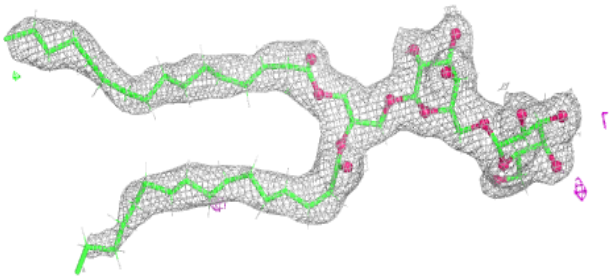


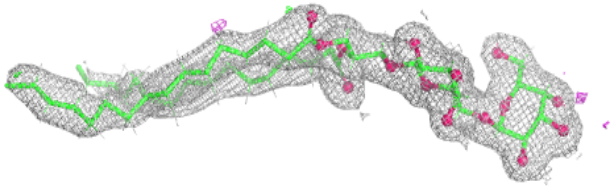


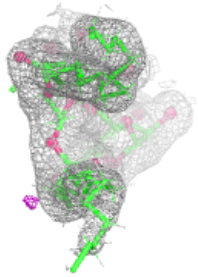


Electron density around DGD c 521:

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

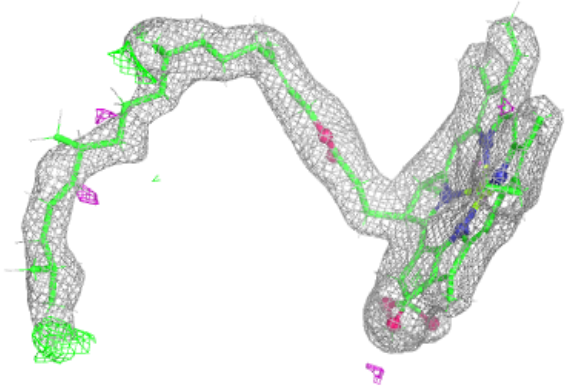


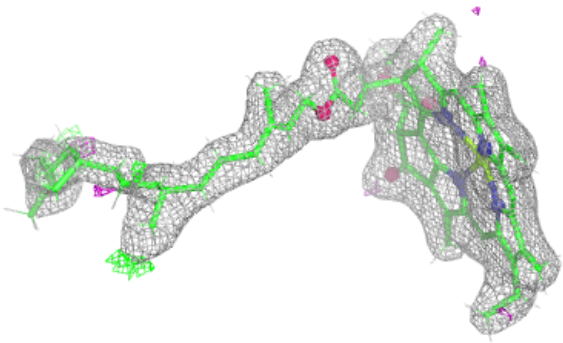


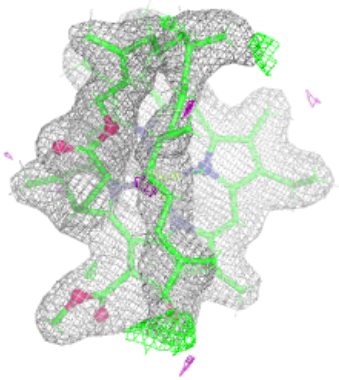


Electron density around CLA b 605:

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

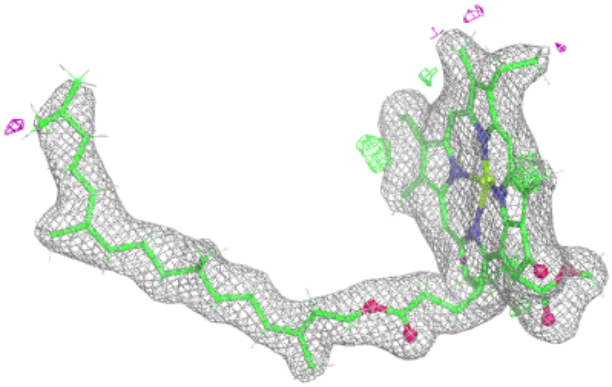


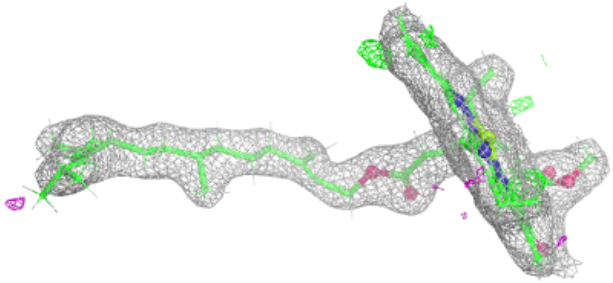


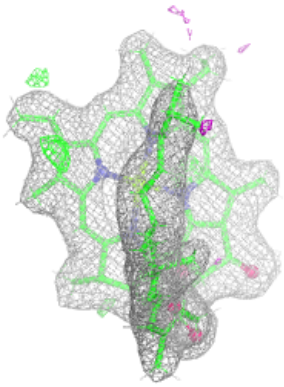


Electron density around CLA b 608:

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

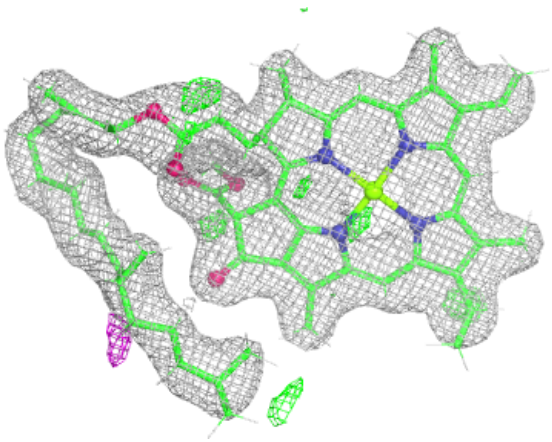


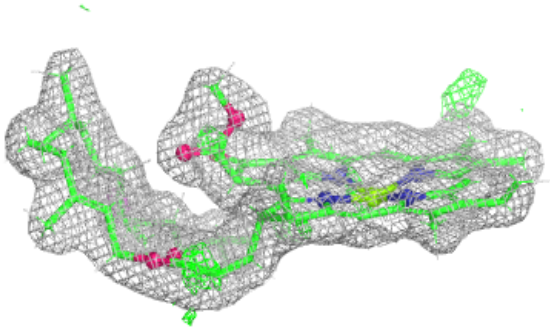


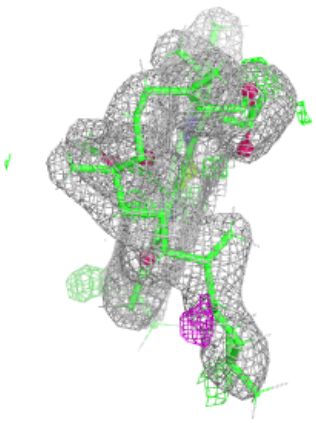


Electron density around CLA b 609:

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

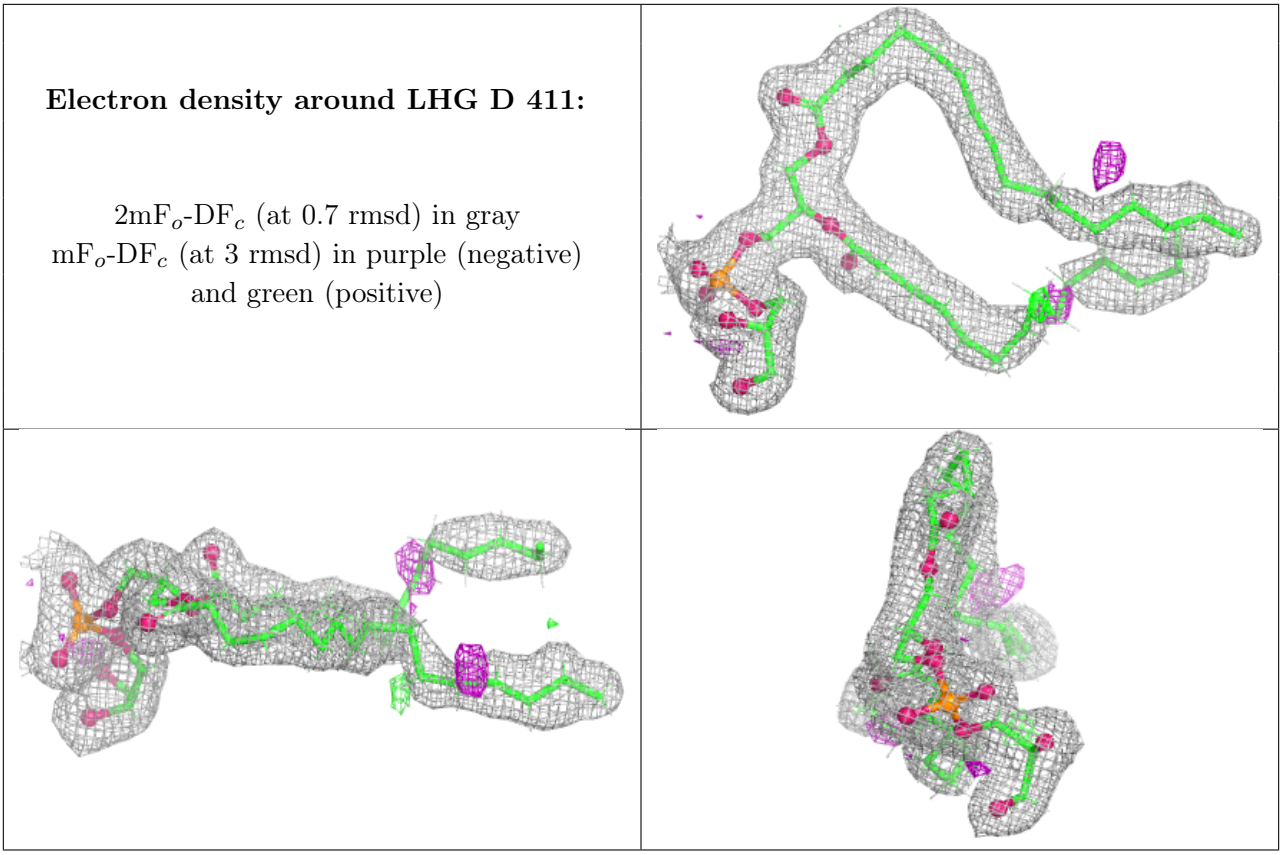






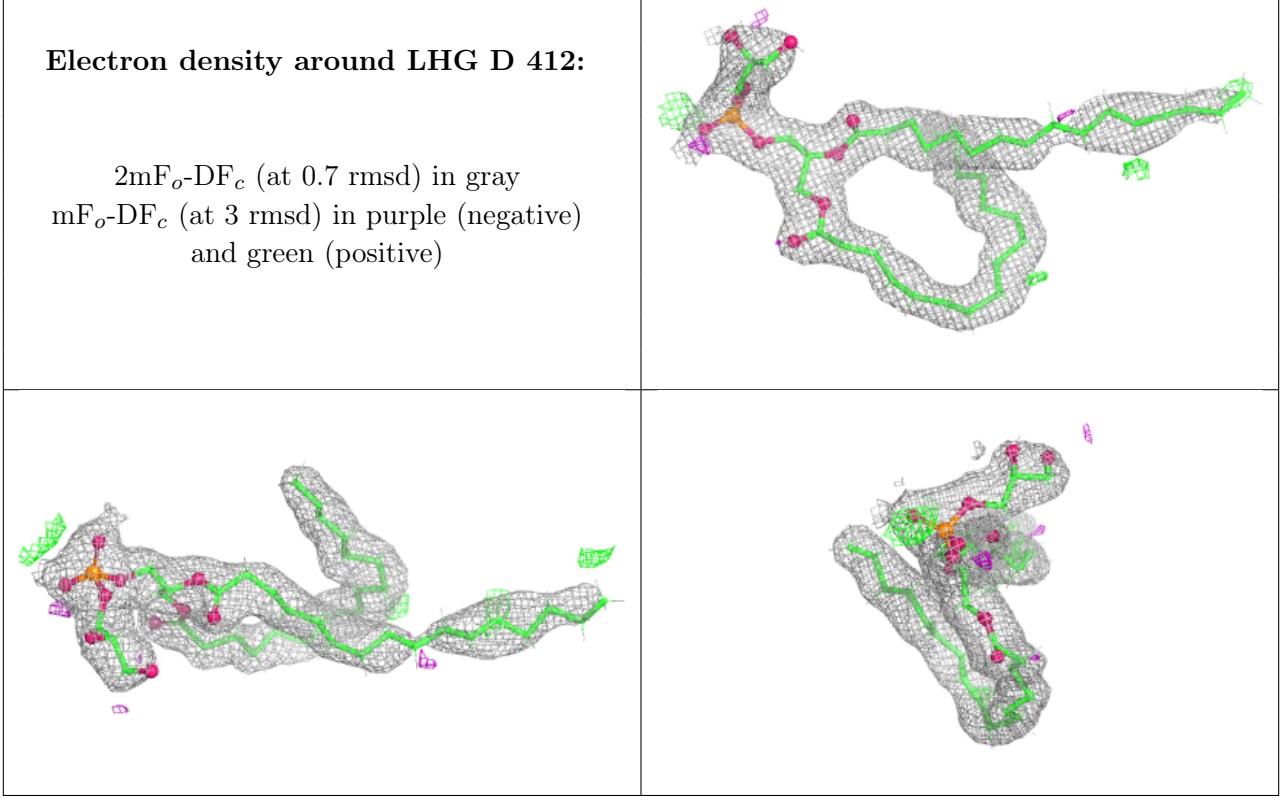
Electron density around LHG D 411:

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



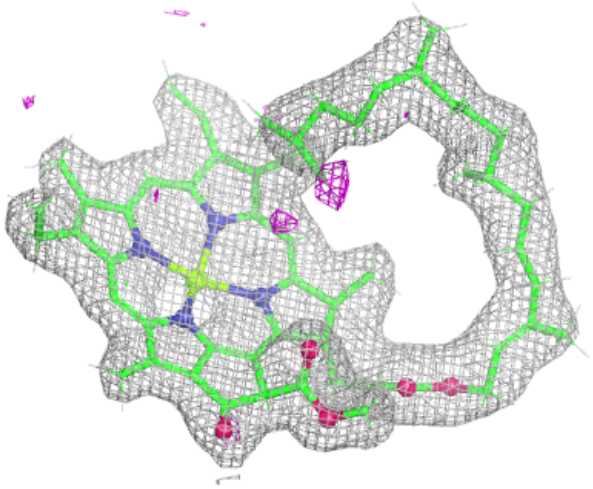
Electron density around LHG D 412:

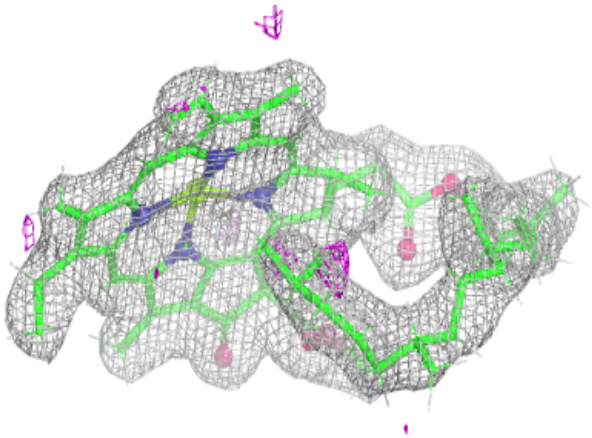
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

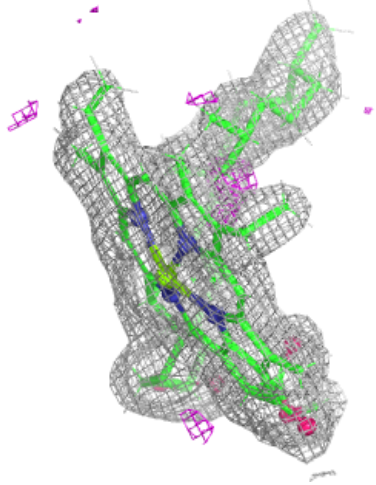


Electron density around CLA b 614:

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

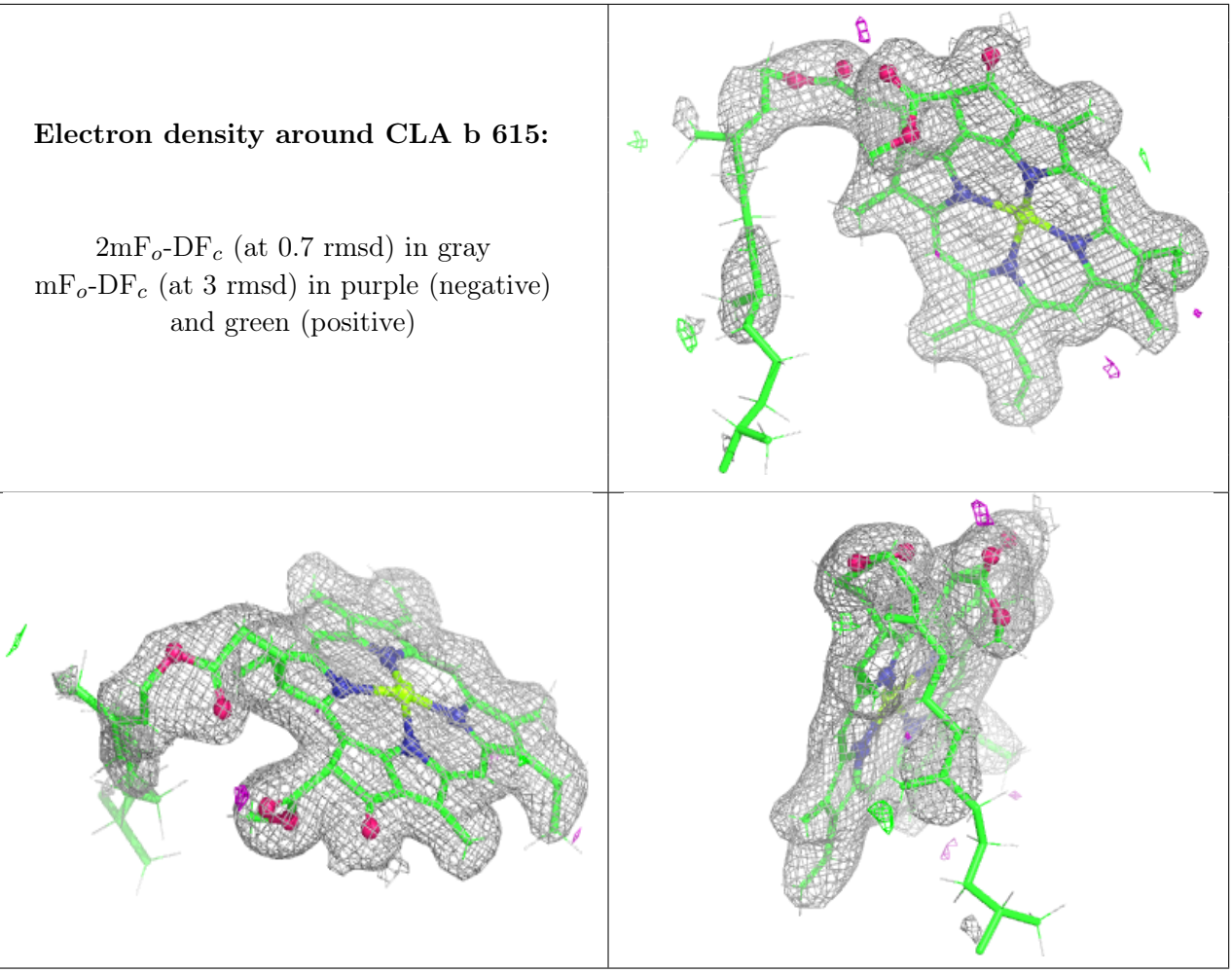






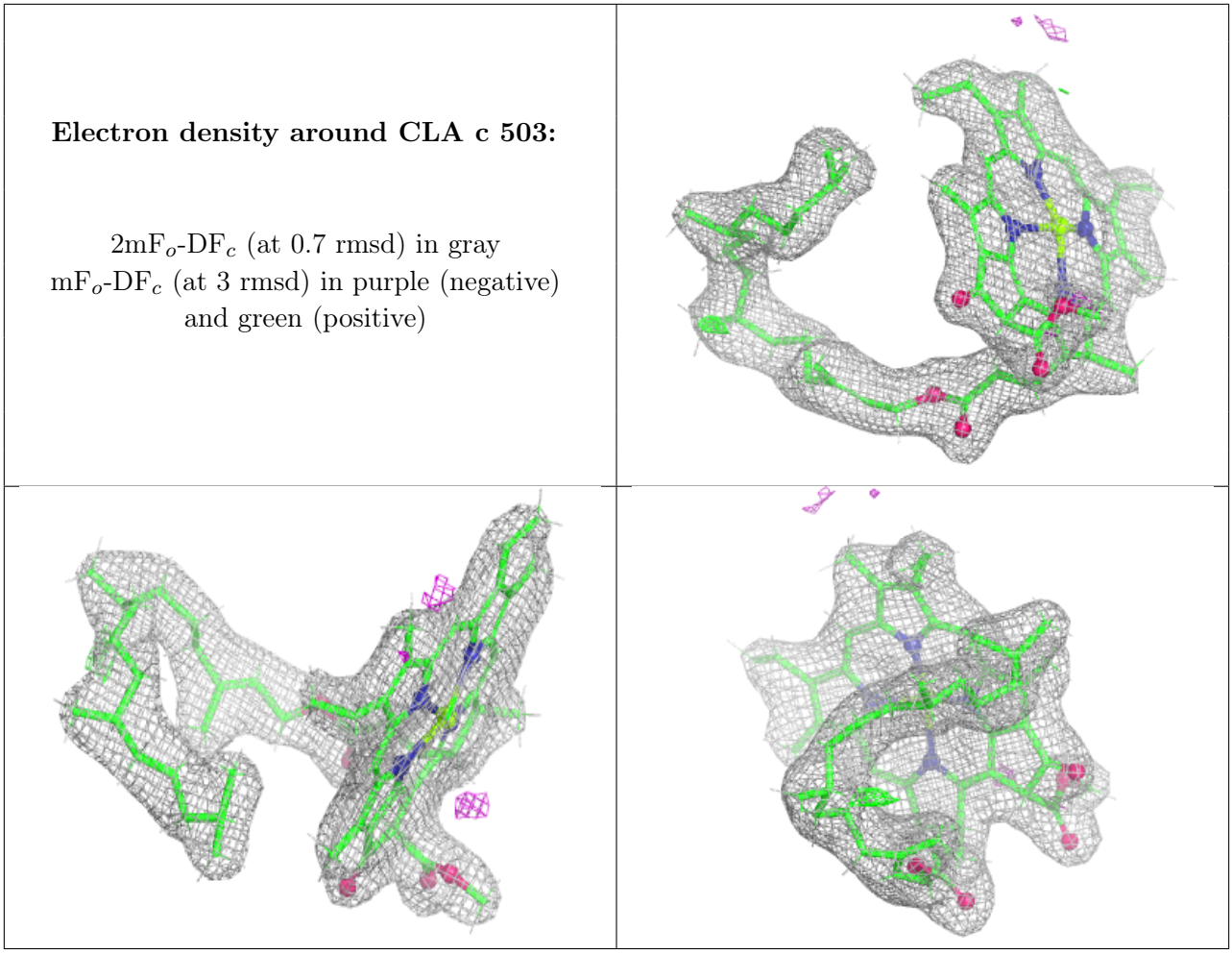
Electron density around CLA b 615:

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



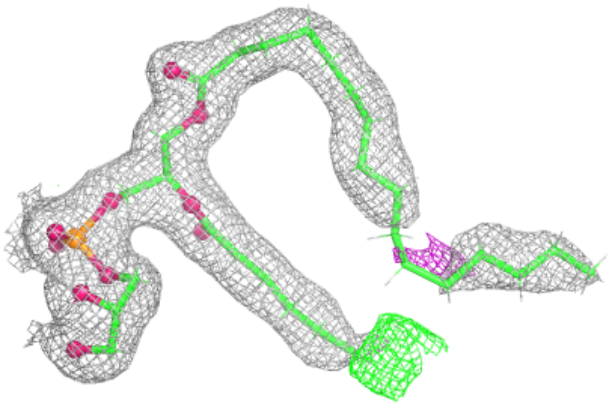
Electron density around CLA c 503:

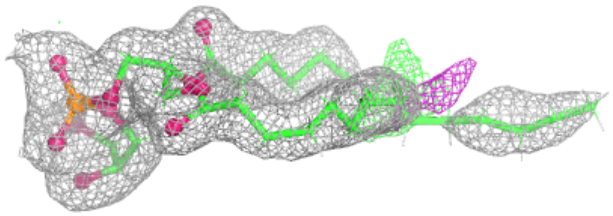
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

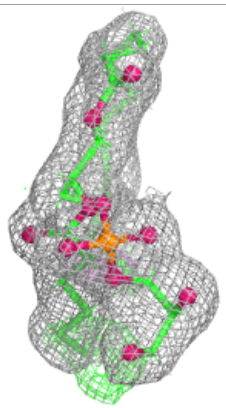


Electron density around LHG d 408:

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

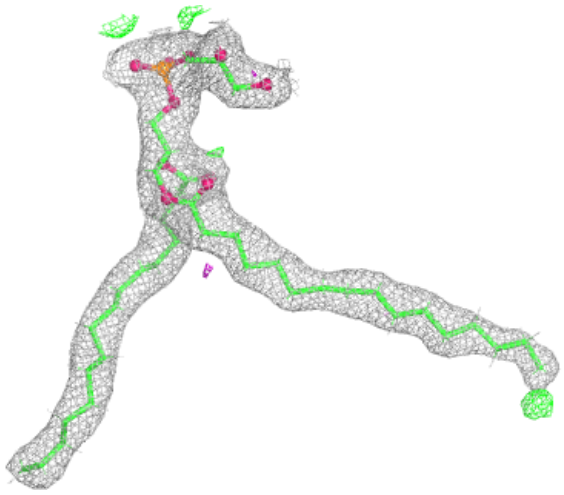


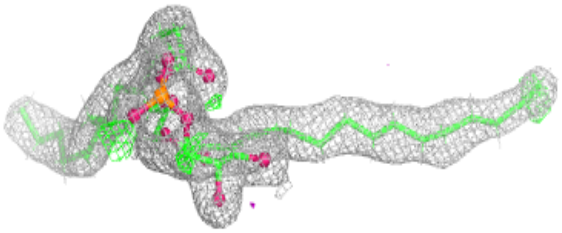


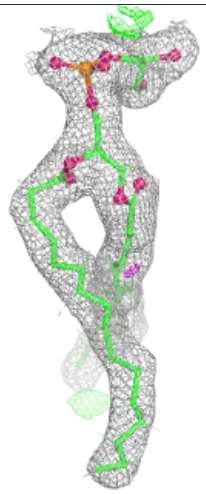


Electron density around LHG l 102:

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

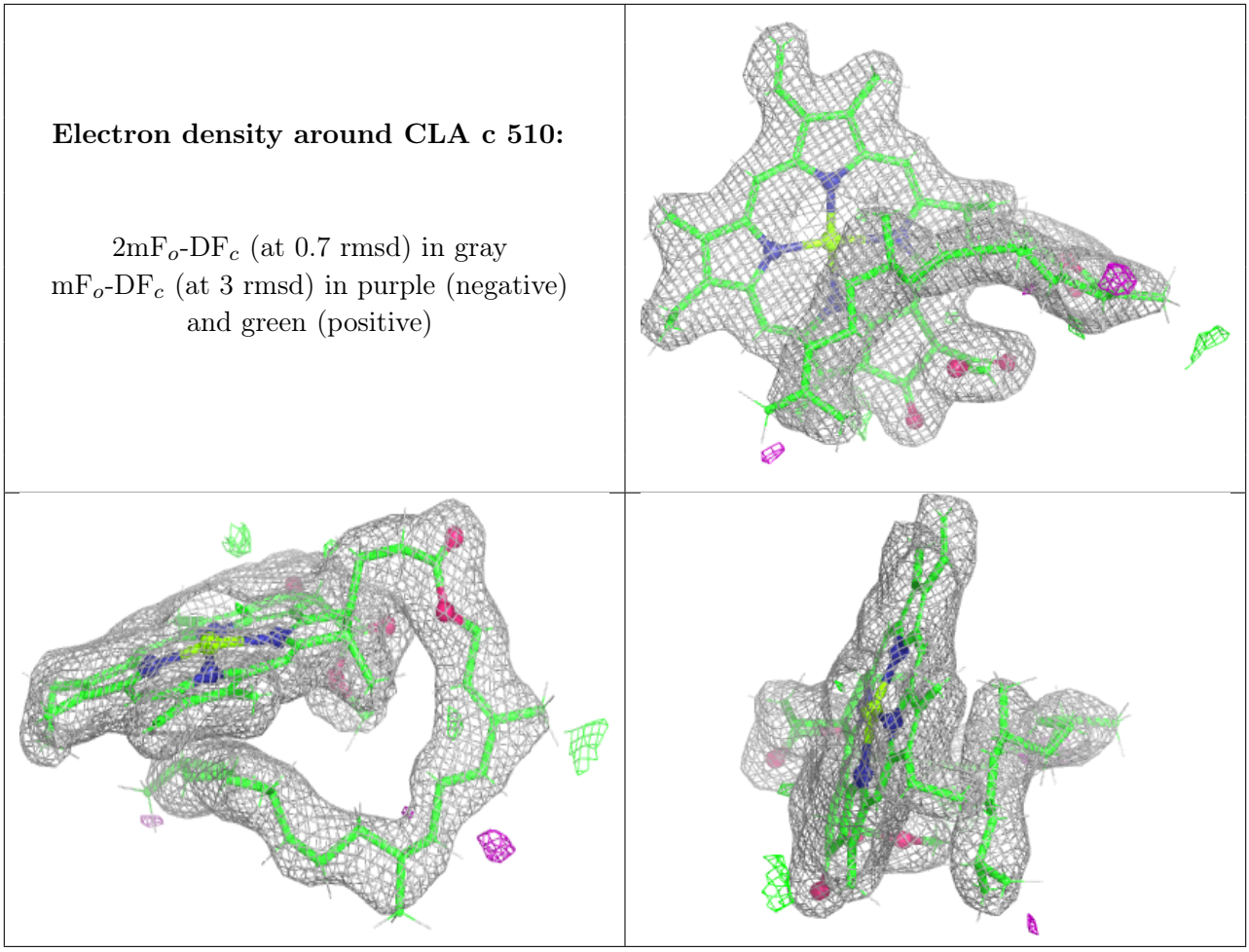






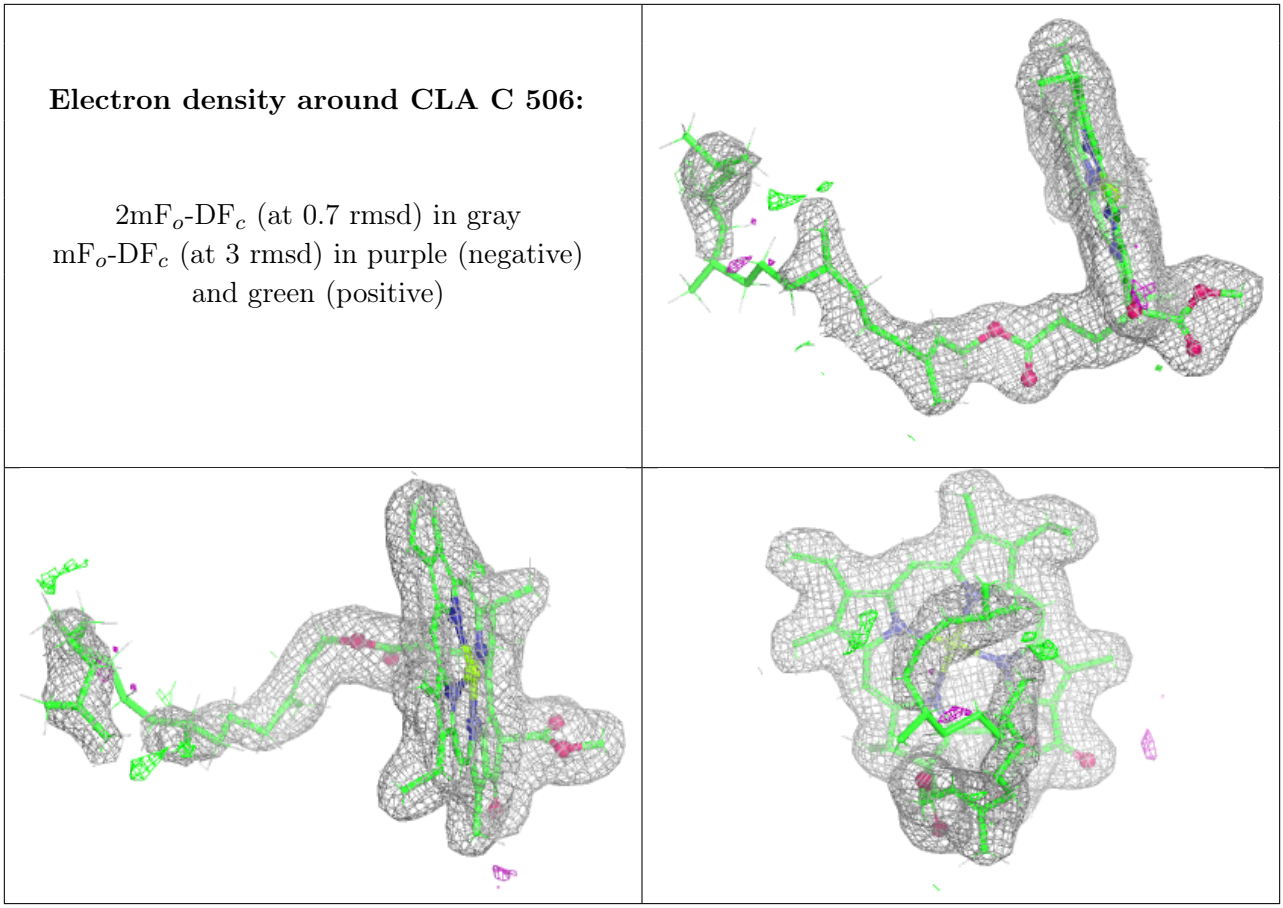
Electron density around CLA c 510:

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



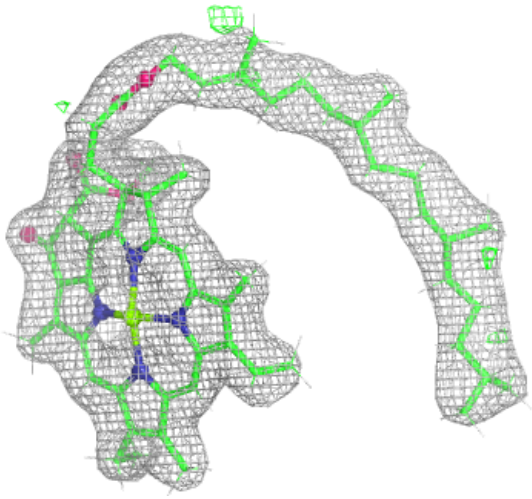
Electron density around CLA C 506:

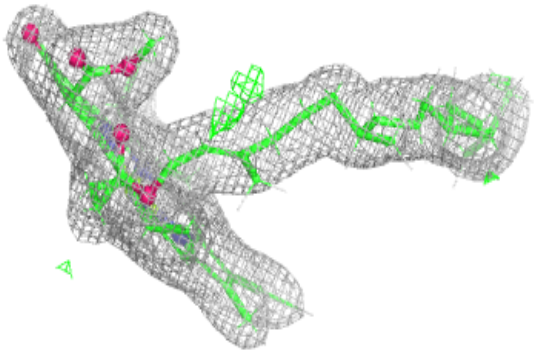
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

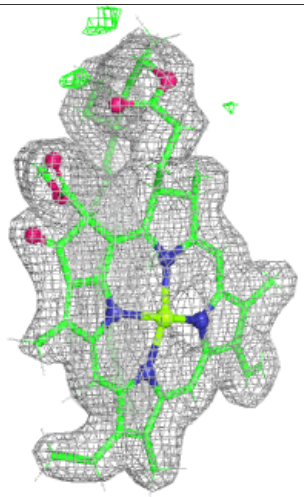


Electron density around CLA C 507:

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

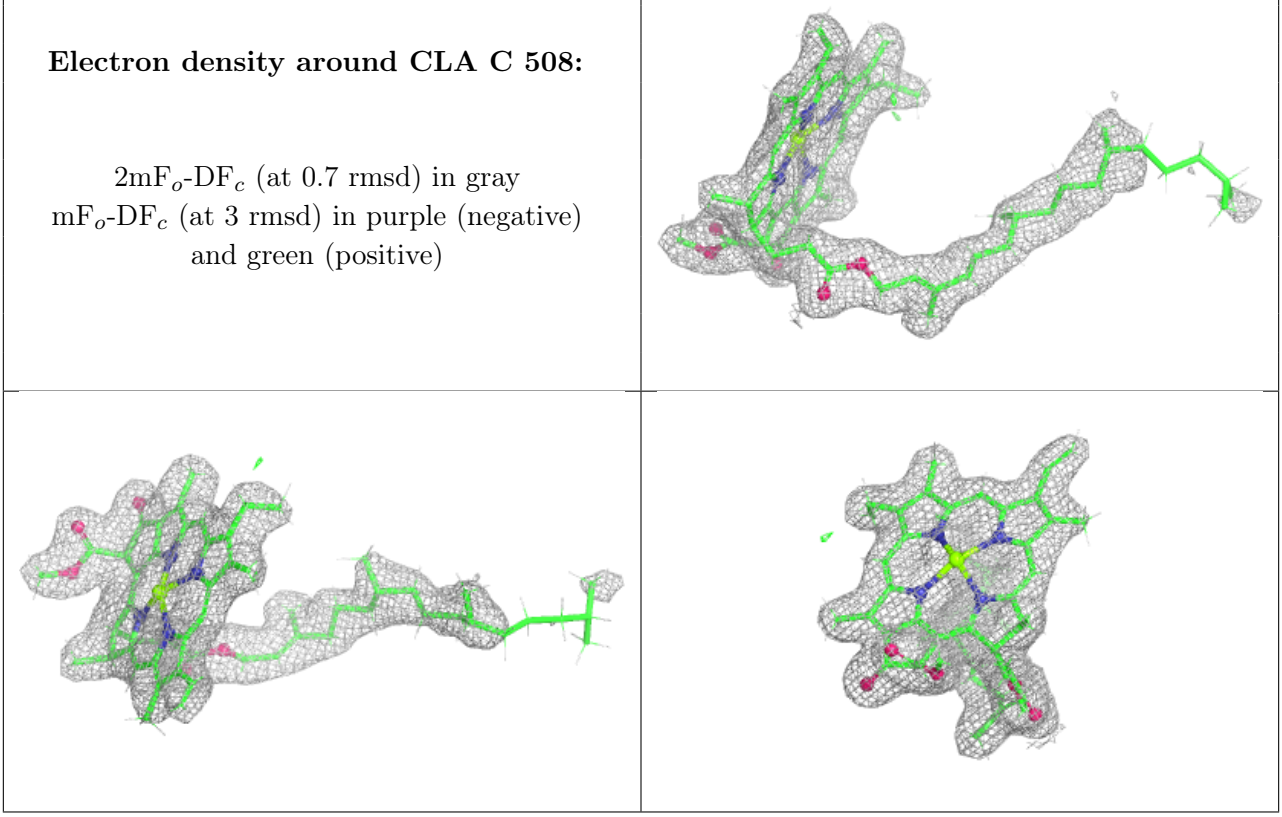






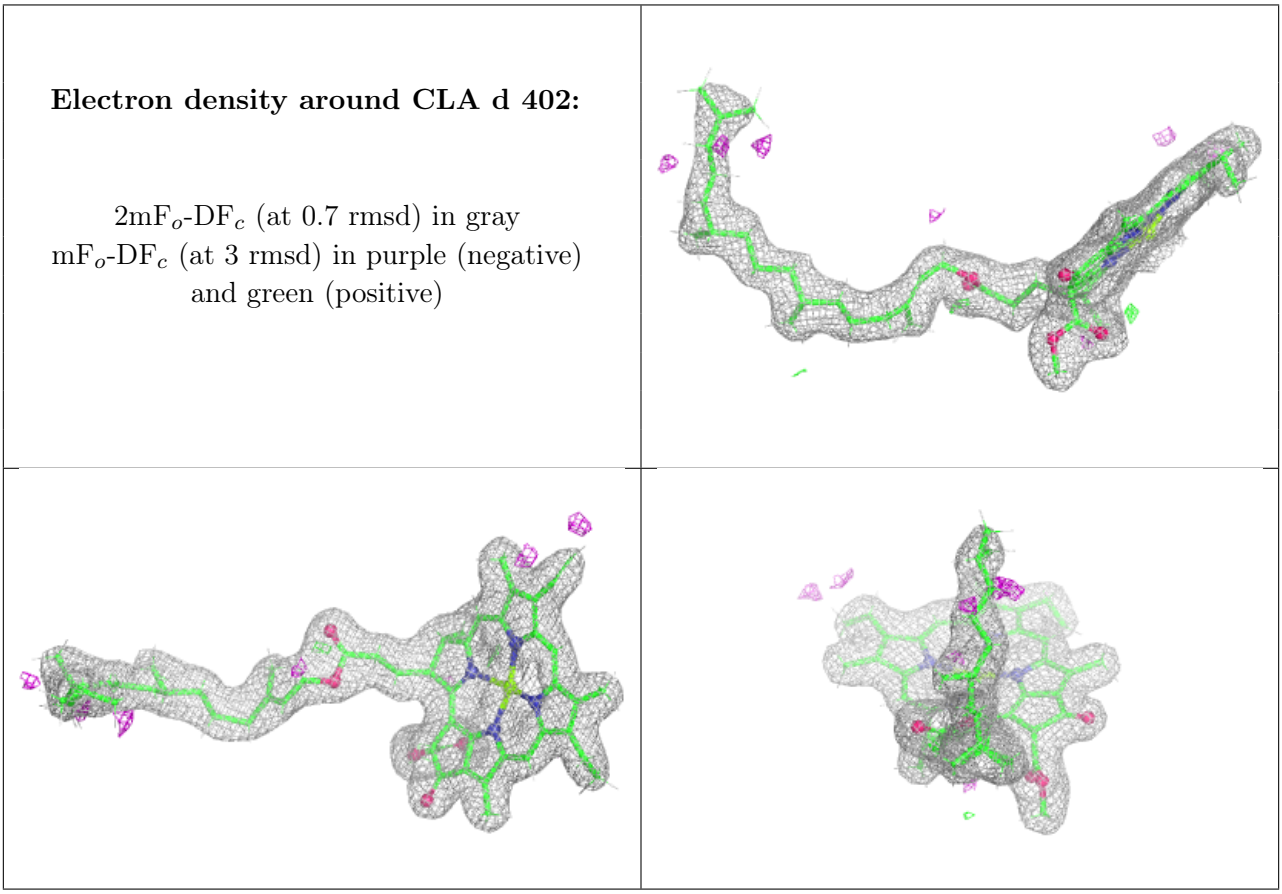
Electron density around CLA C 508:

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



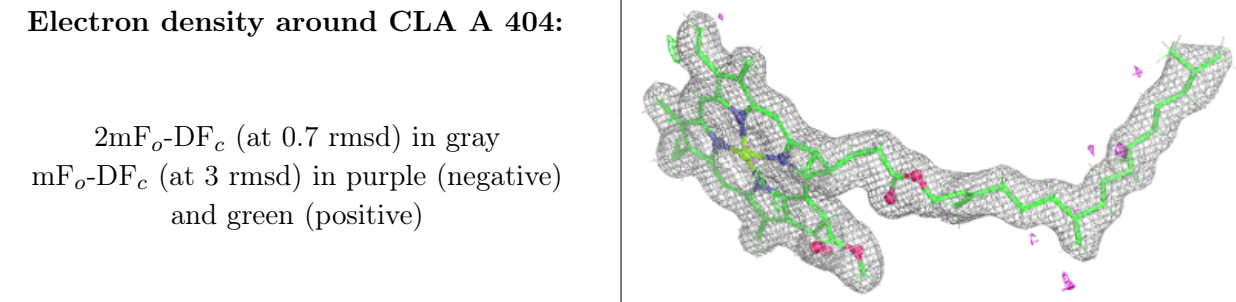
Electron density around CLA d 402:

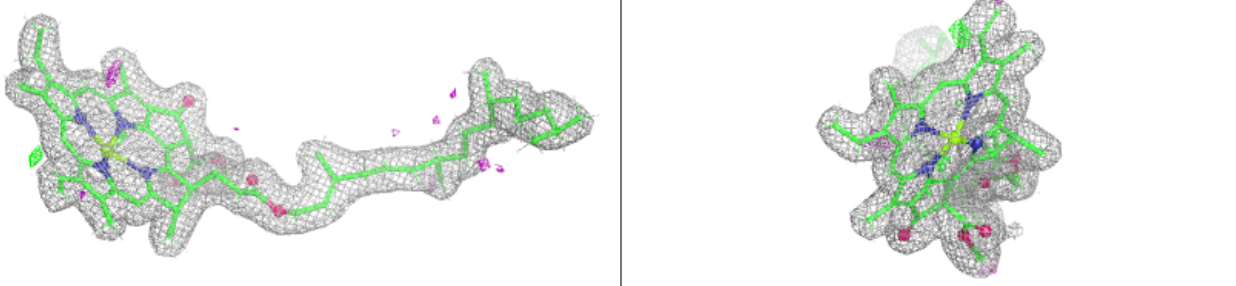
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 404:

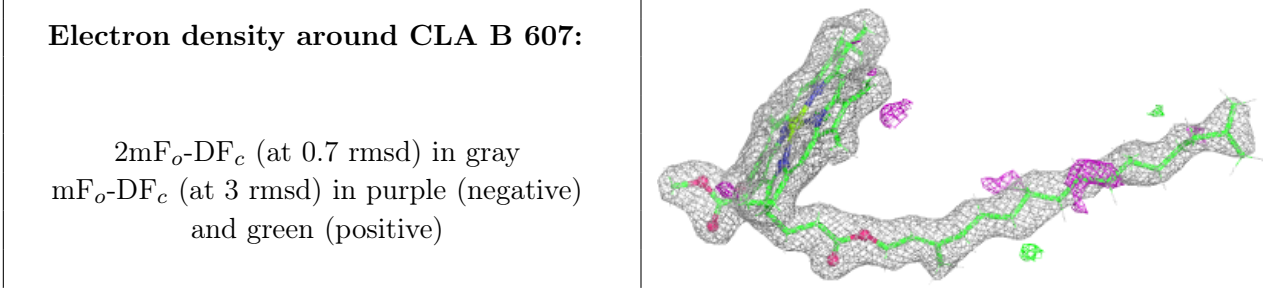
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

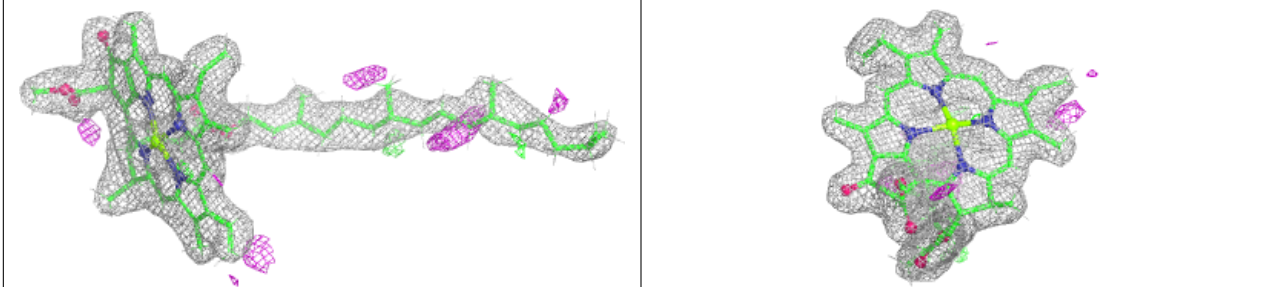




Electron density around CLA B 607:

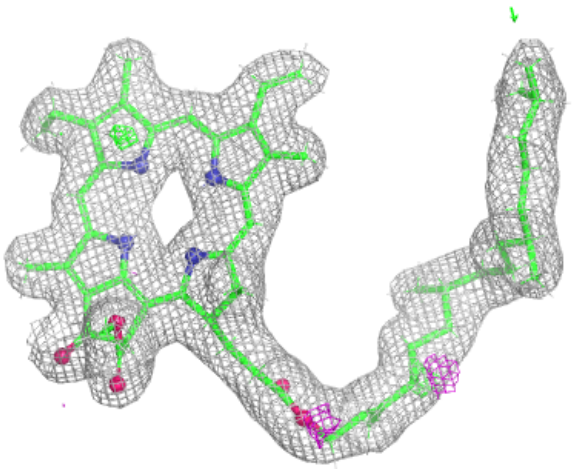
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

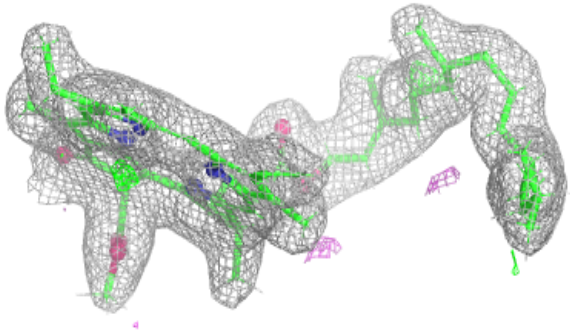


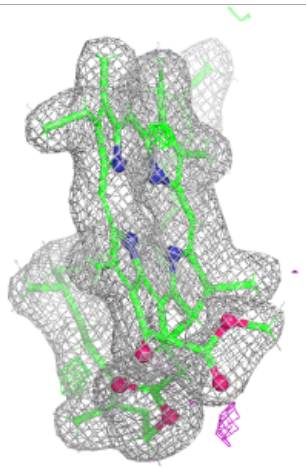


Electron density around PHO A 406:

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

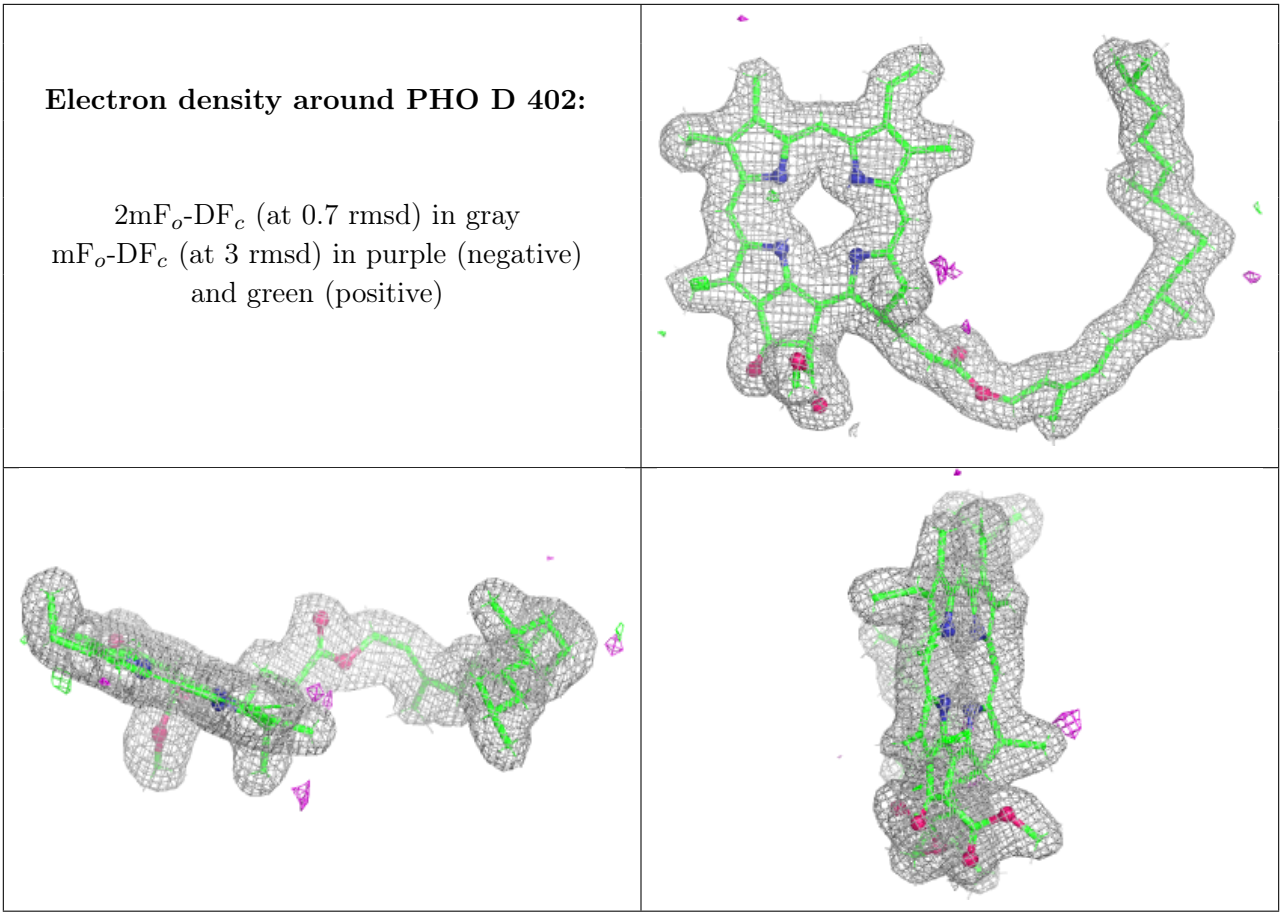






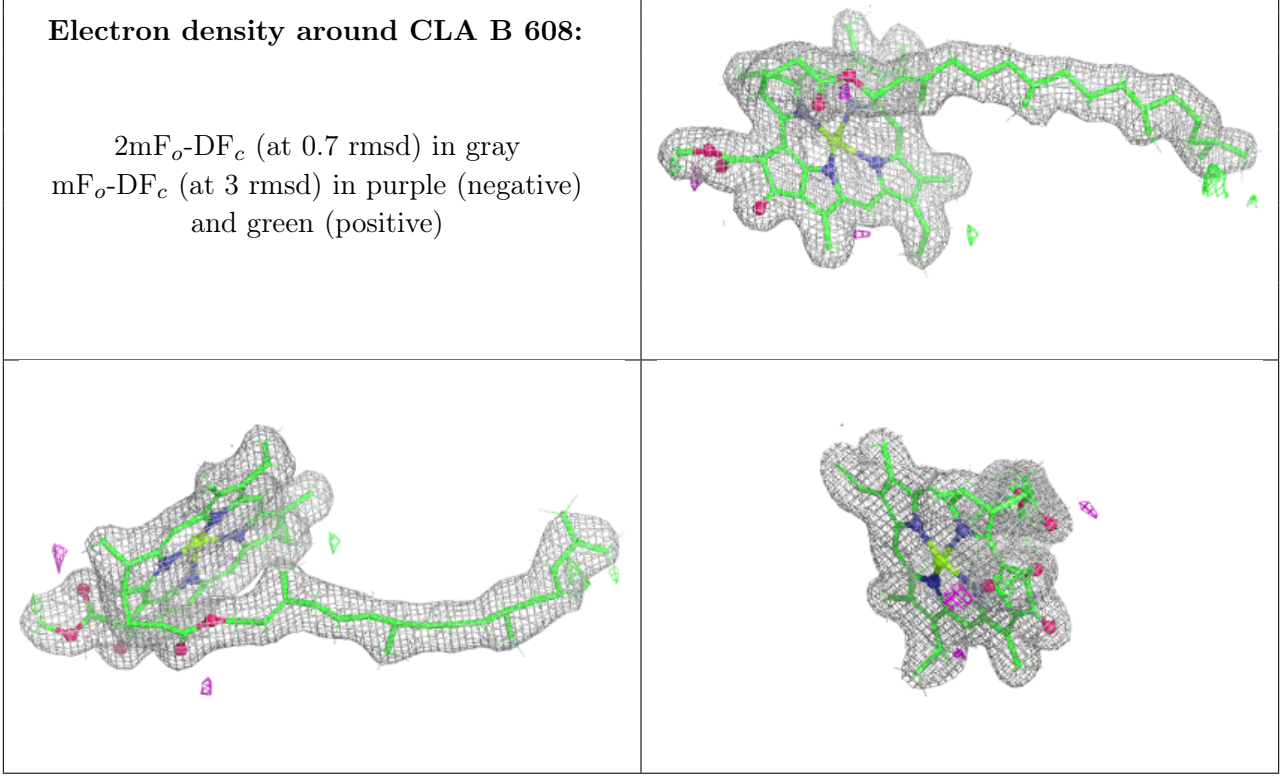
Electron density around PHO D 402:

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



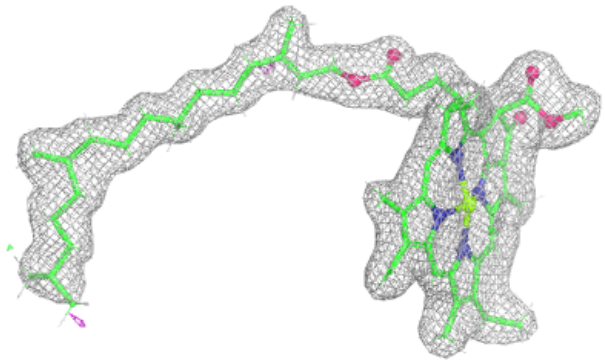
Electron density around CLA B 608:

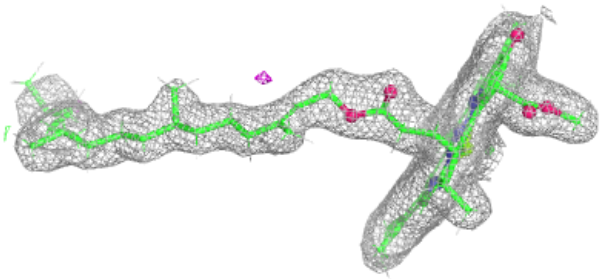
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

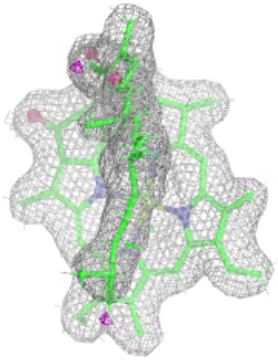


Electron density around CLA B 609:

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

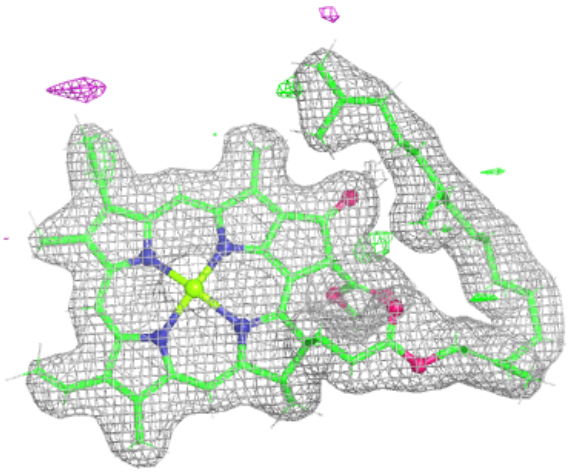


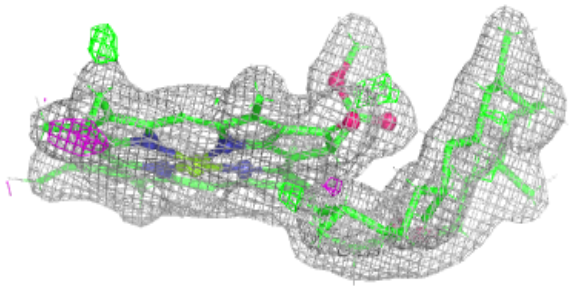


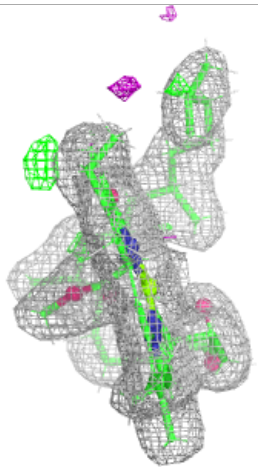


Electron density around CLA B 610:

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

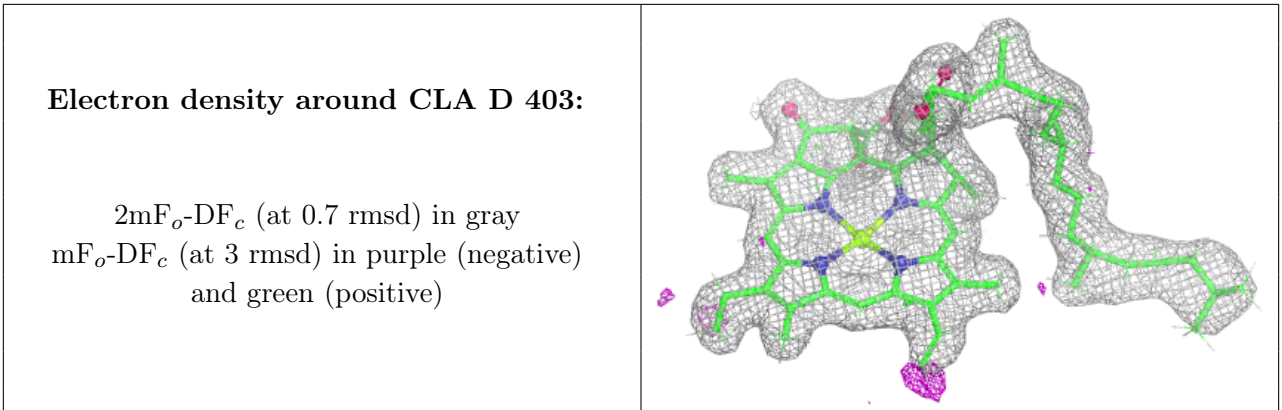


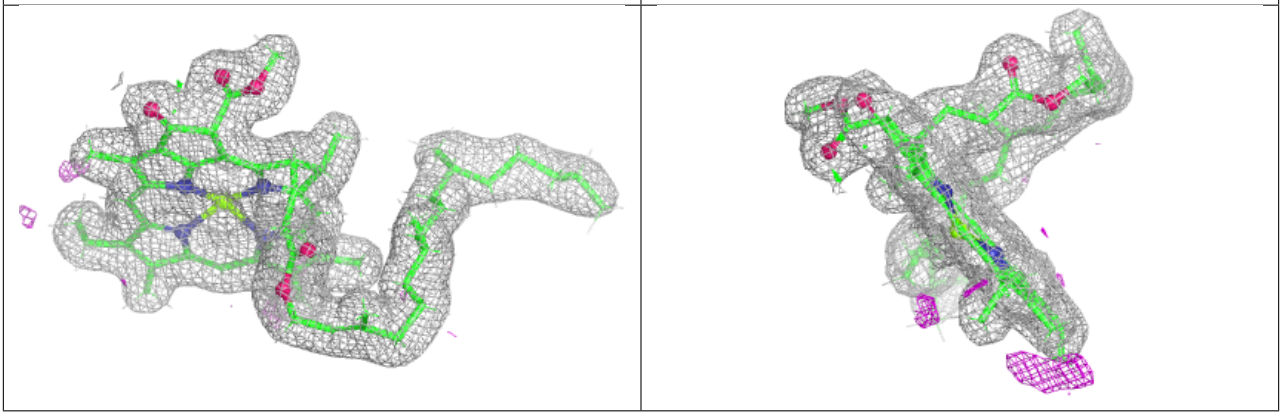




Electron density around CLA D 403:

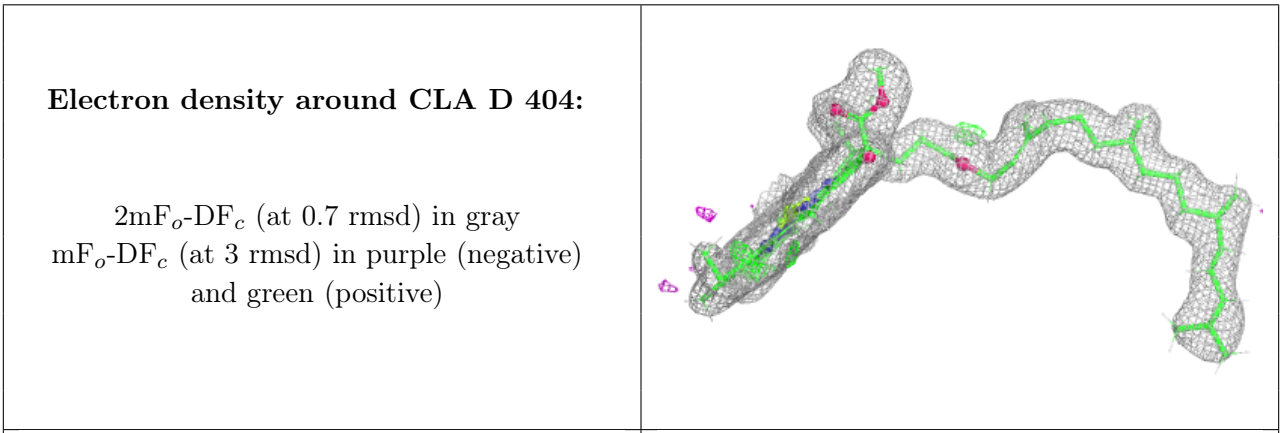
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

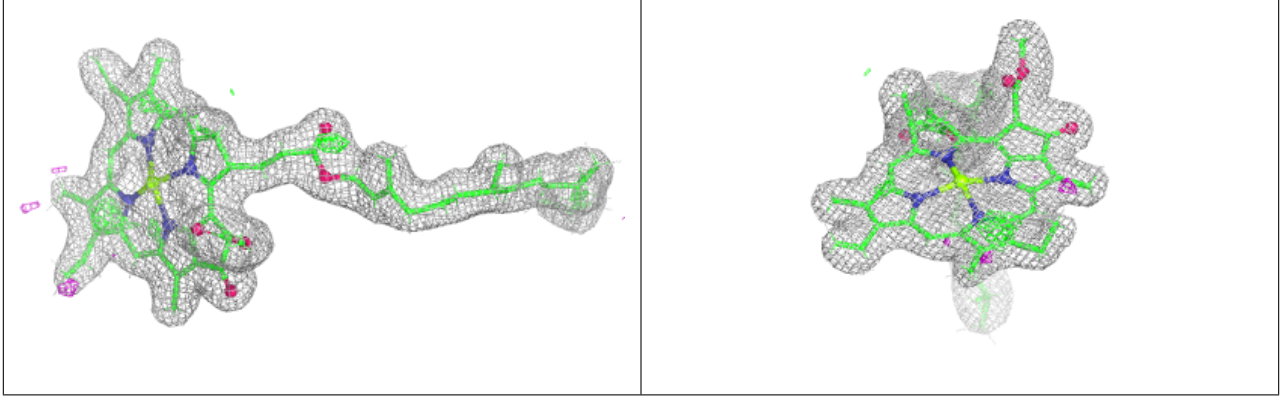




Electron density around CLA D 404:

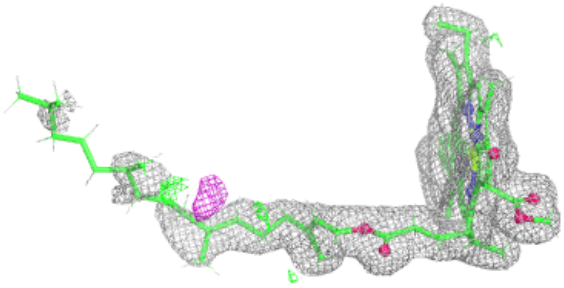
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

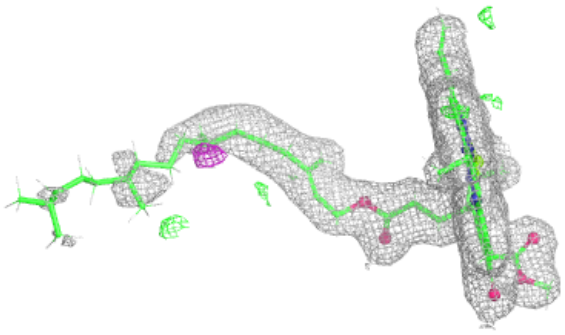


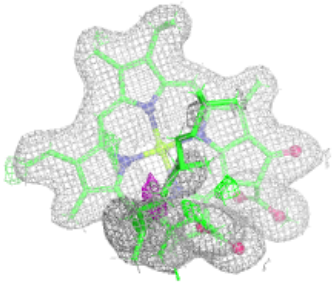


Electron density around CLA D 405:

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

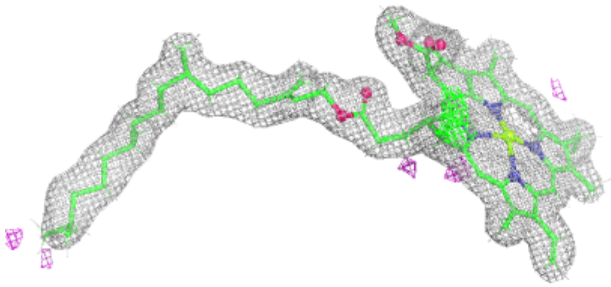


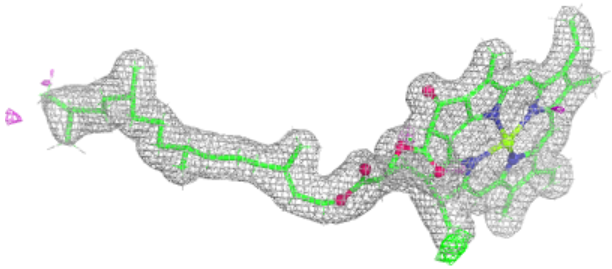


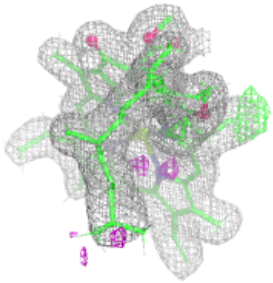


Electron density around CLA a 405:

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

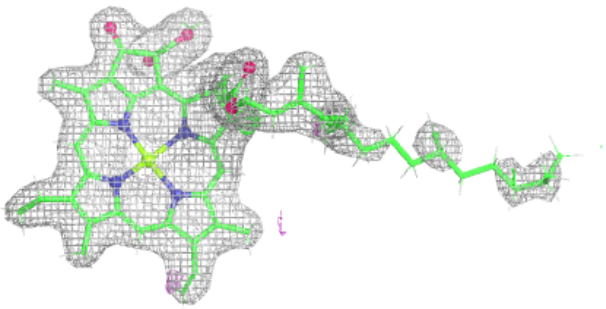


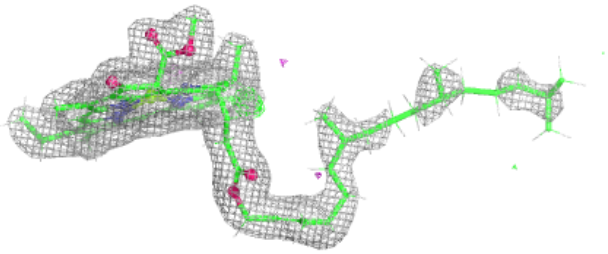


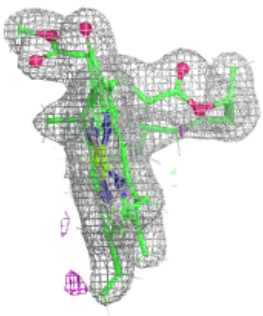


Electron density around CLA a 406:

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

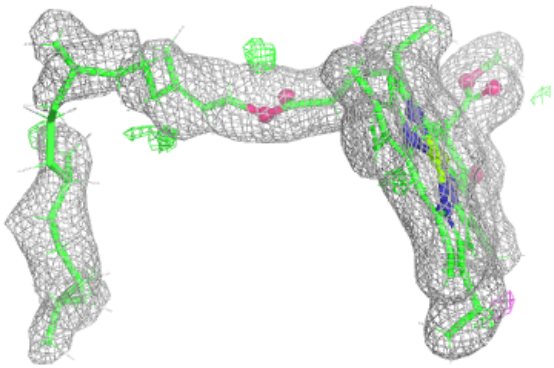


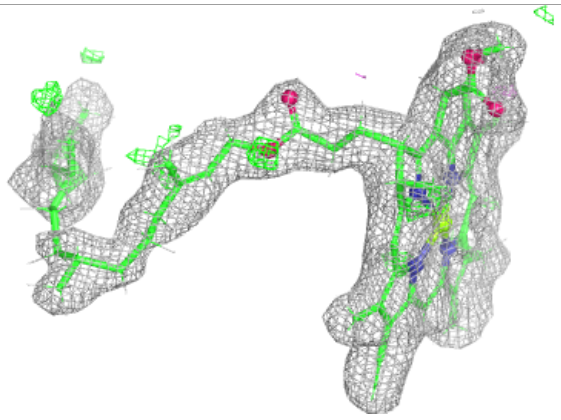


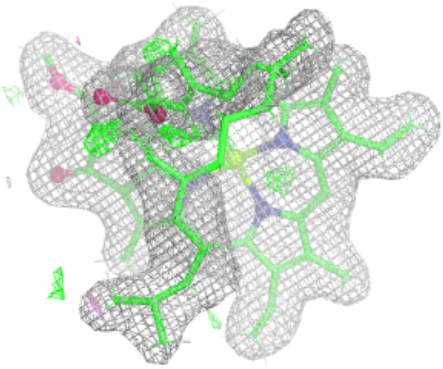


Electron density around CLA a 408:

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

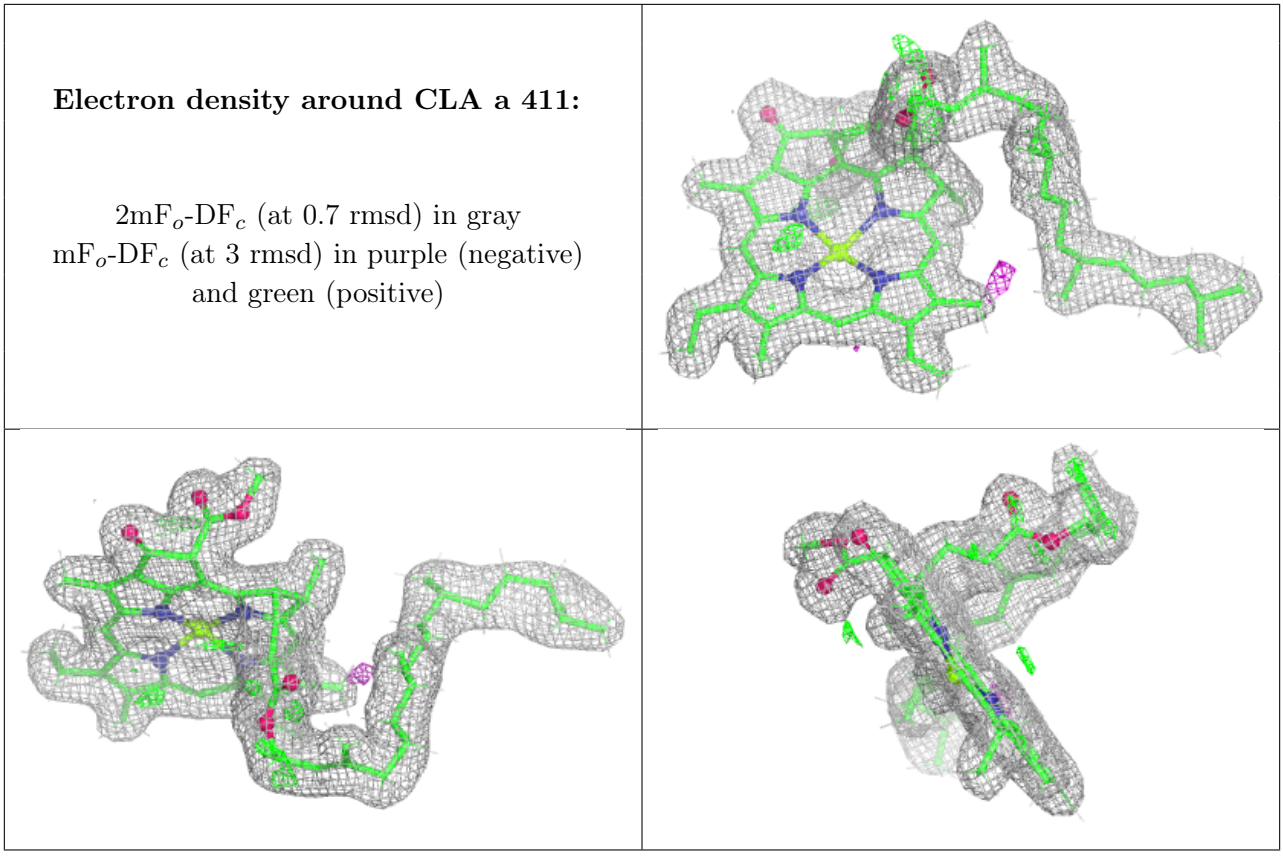






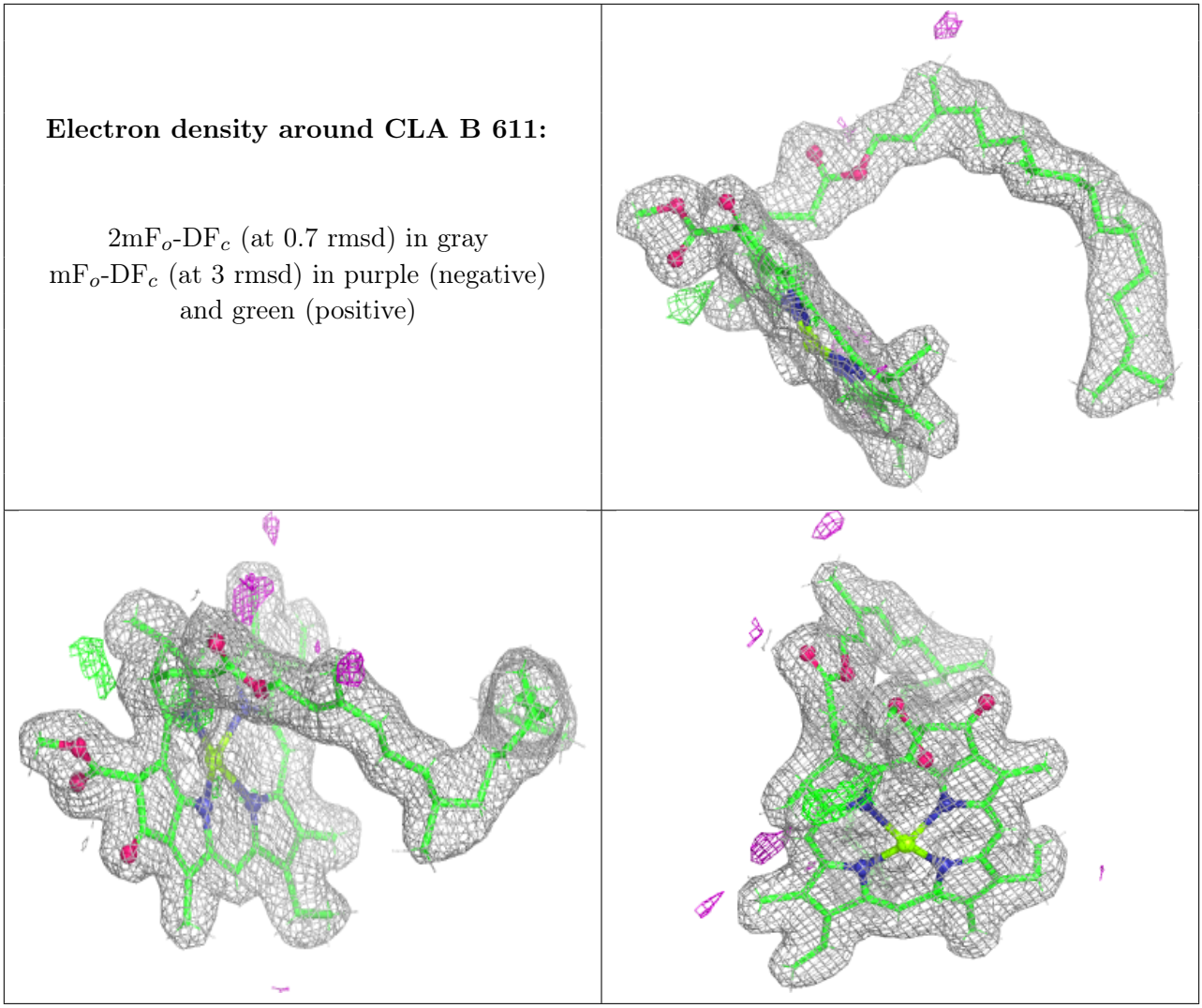
Electron density around CLA a 411:

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



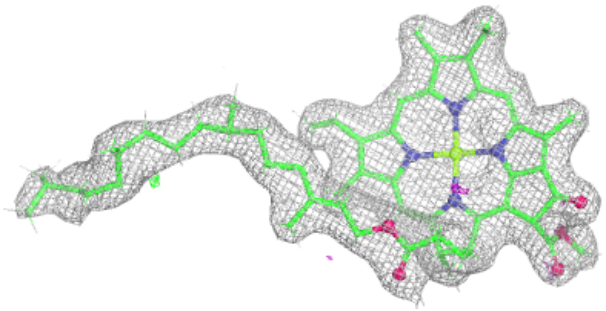
Electron density around CLA B 611:

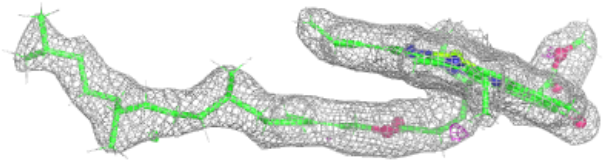
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

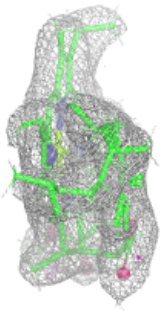


Electron density around CLA b 602:

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



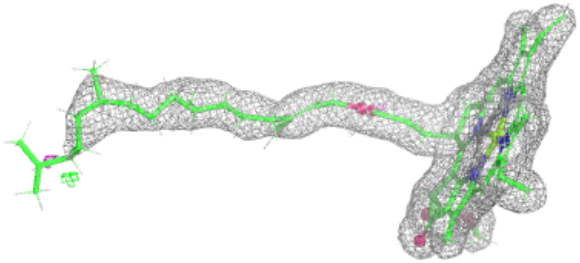


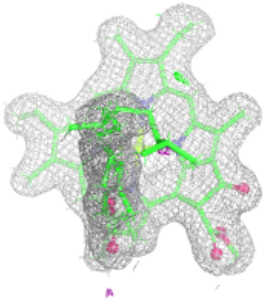


Electron density around CLA b 603:

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

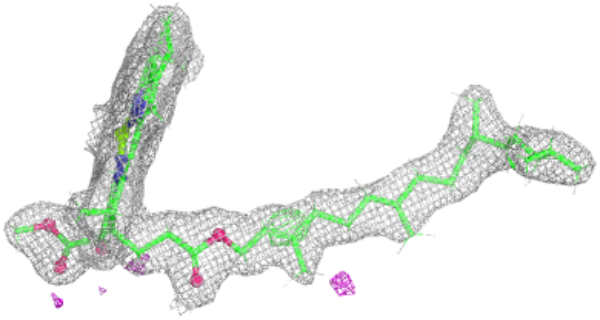


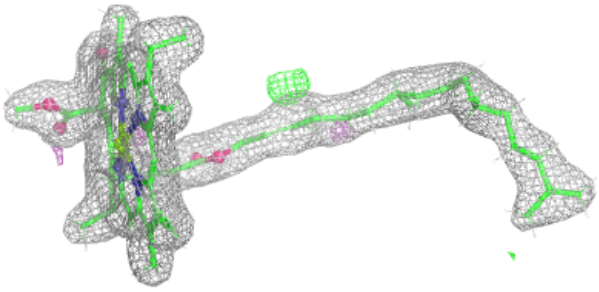


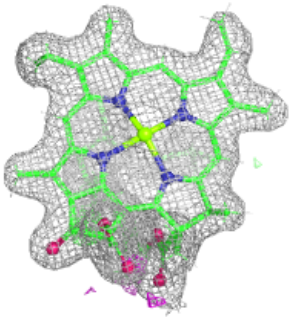


Electron density around CLA b 604:

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

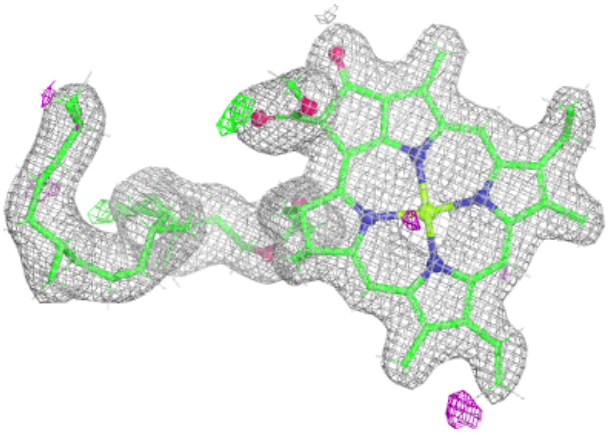


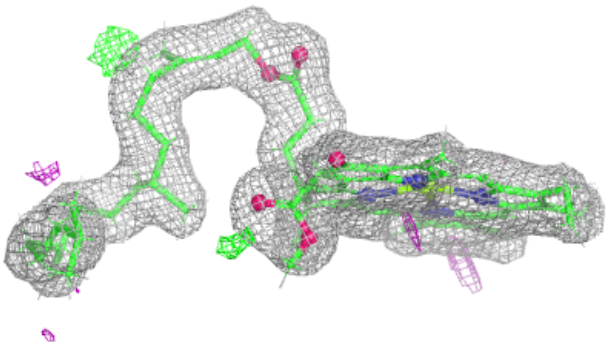


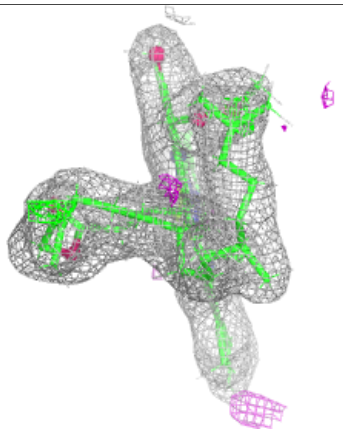


Electron density around CLA B 612:

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

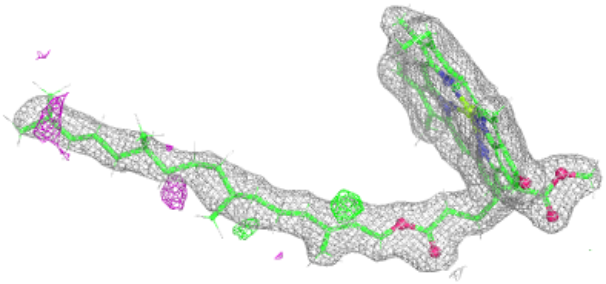


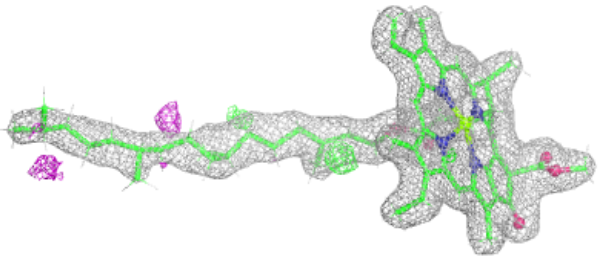


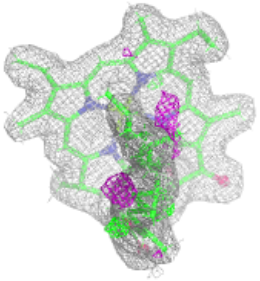


Electron density around CLA b 606:

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

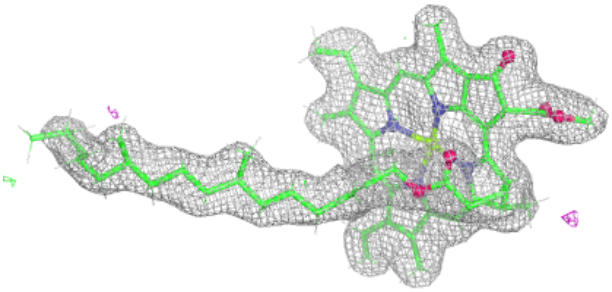


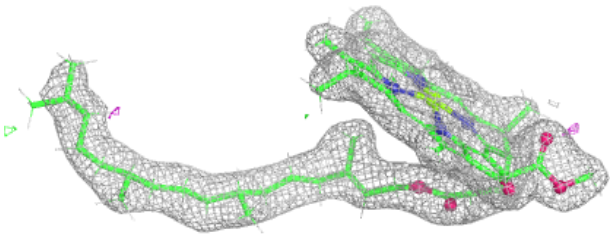


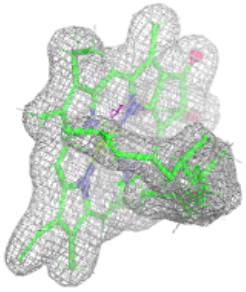


Electron density around CLA b 607:

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

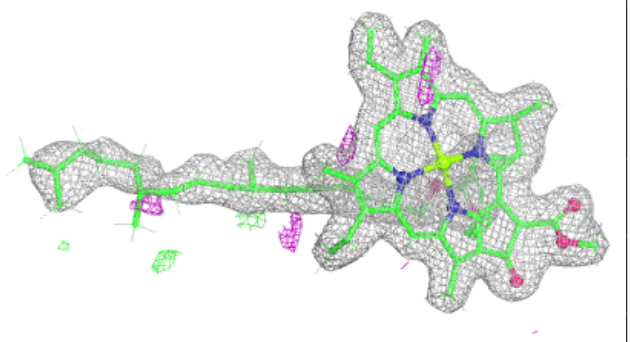


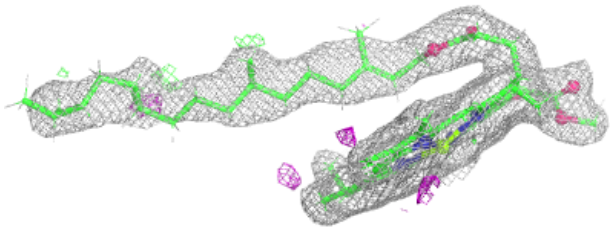


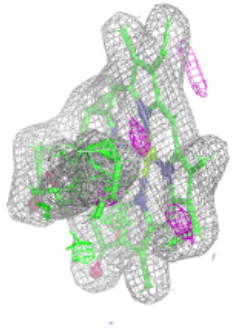


Electron density around CLA B 614:

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

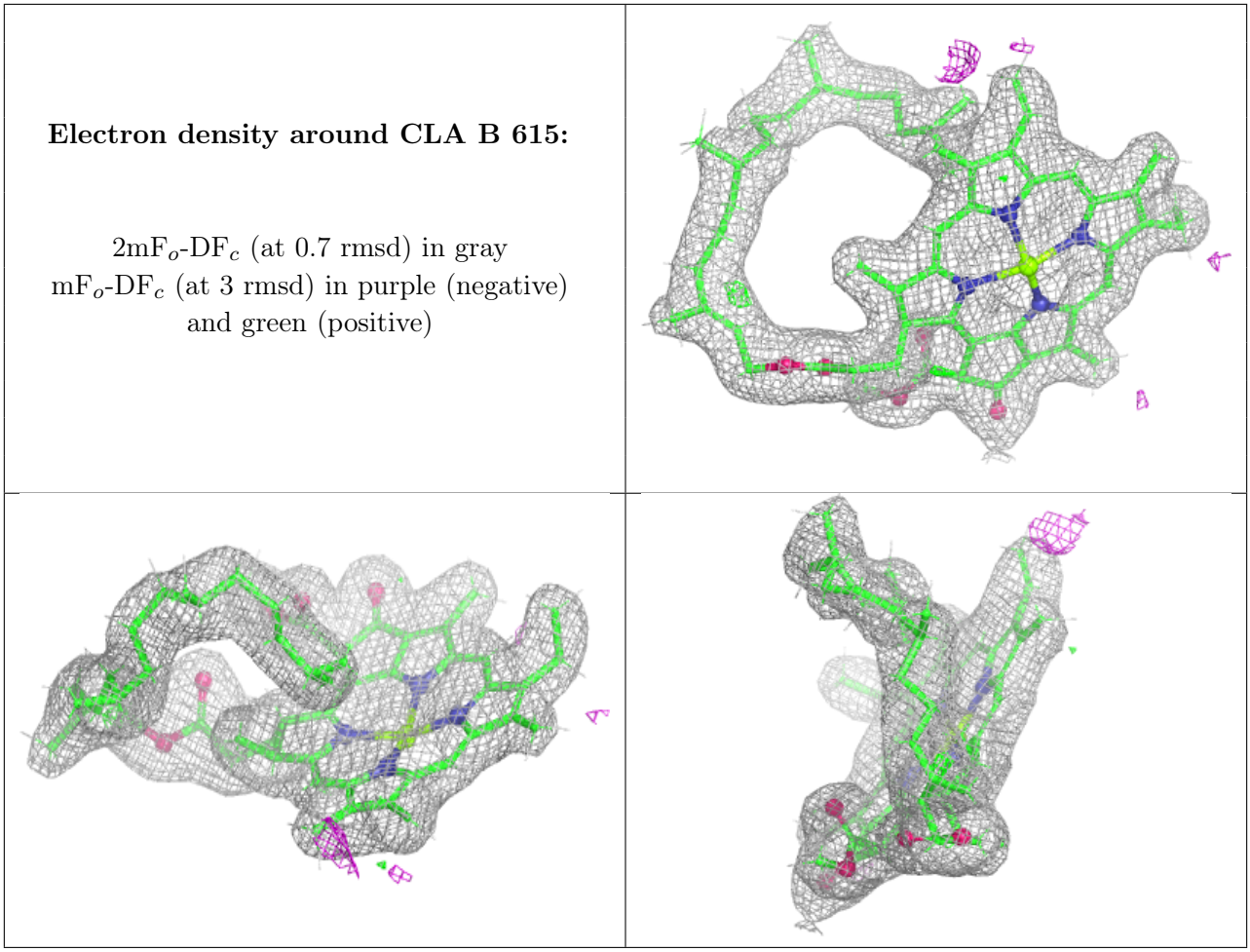






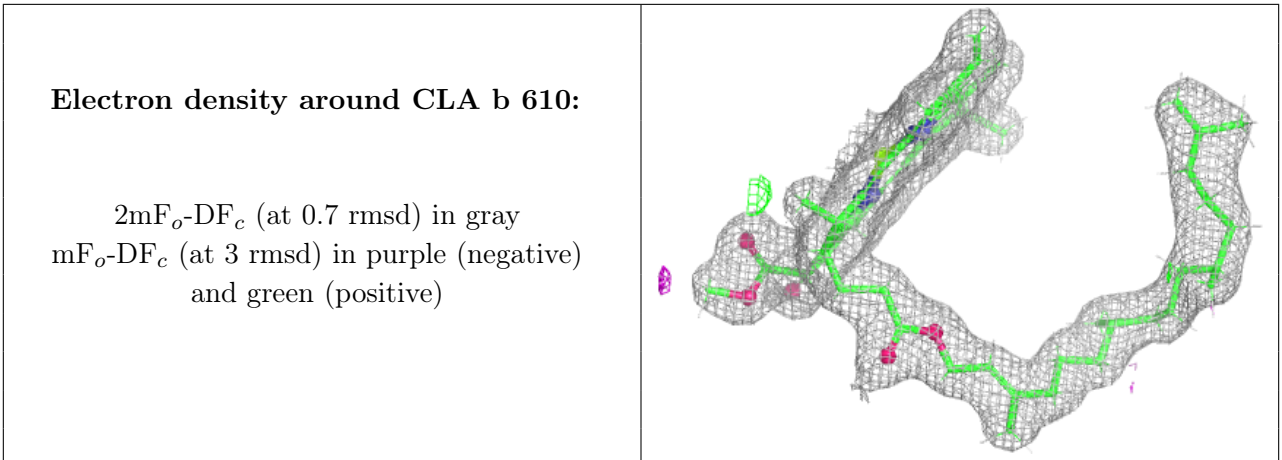
Electron density around CLA B 615:

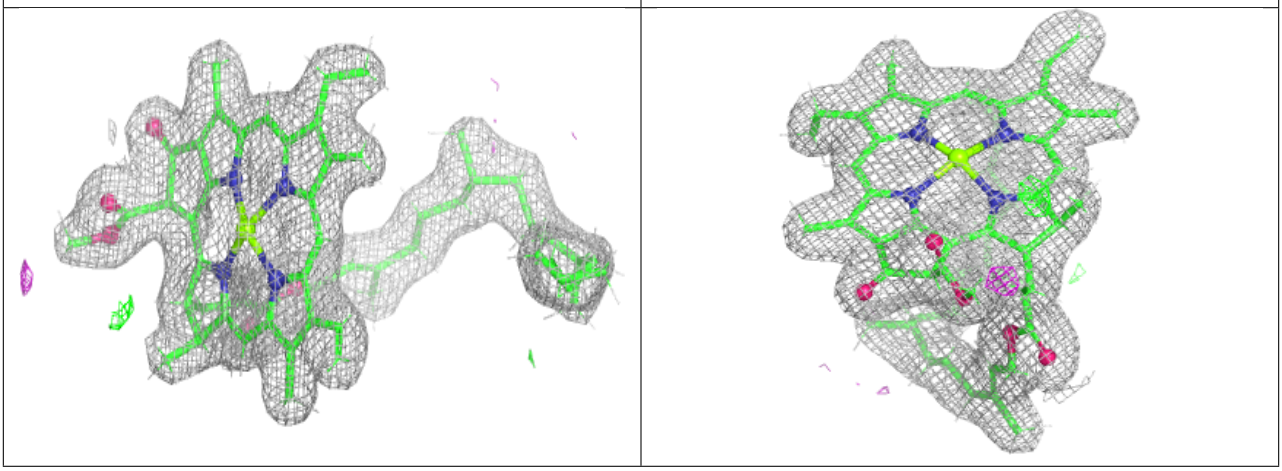
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 610:

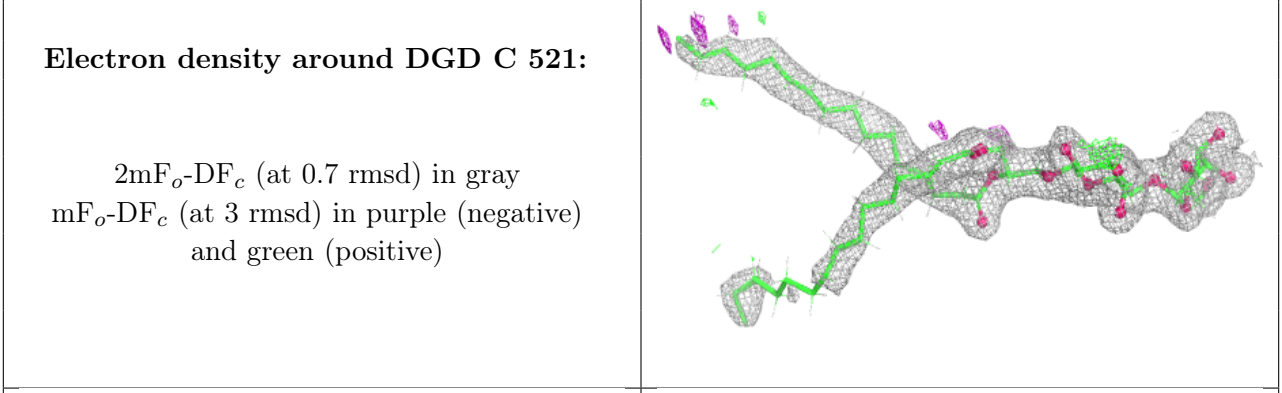
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

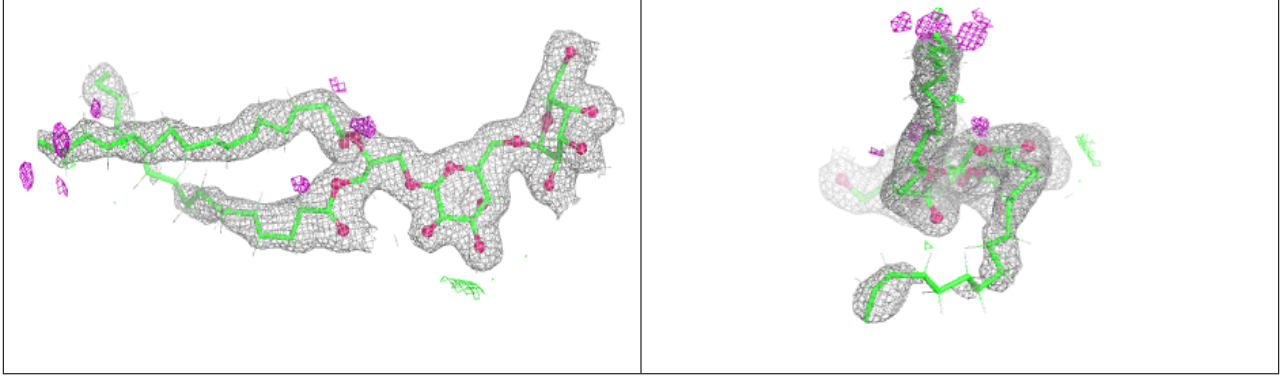




Electron density around DGD C 521:

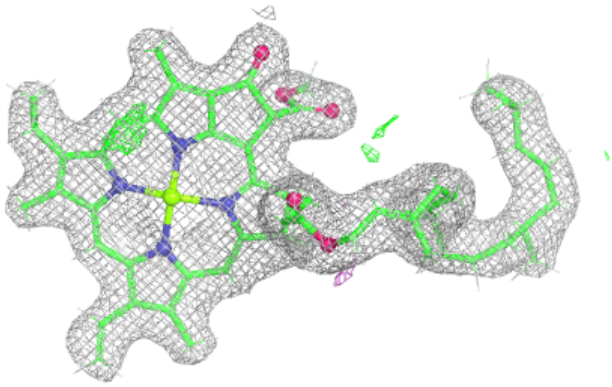
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

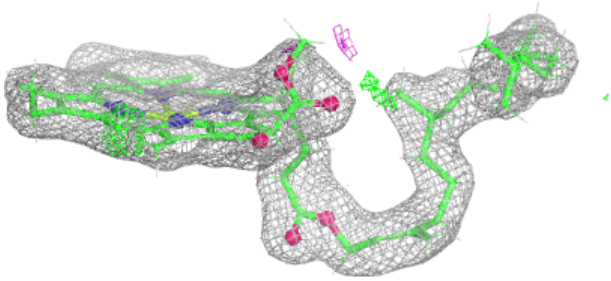


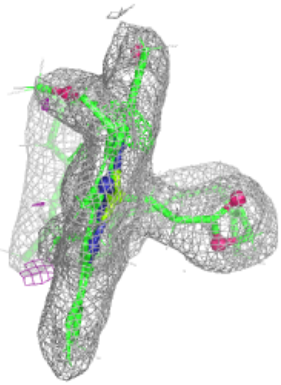


Electron density around CLA b 611:

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

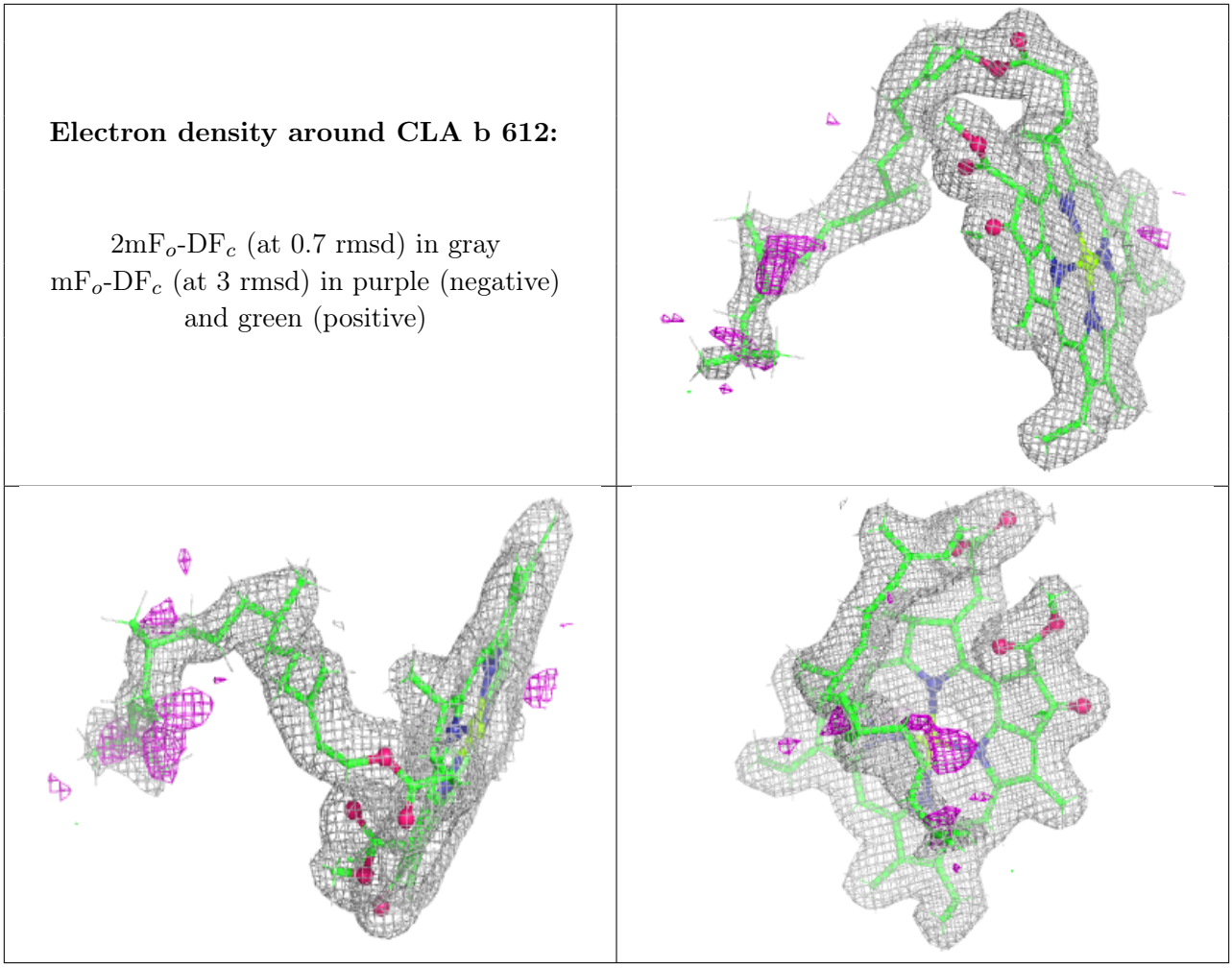






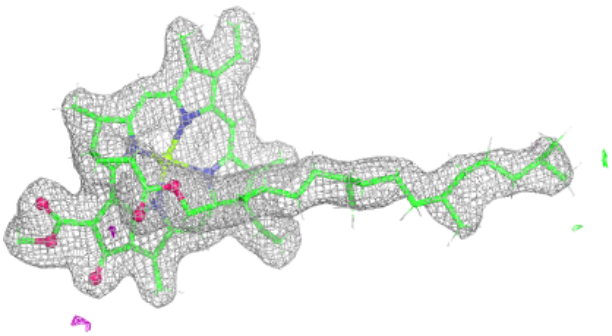
Electron density around CLA b 612:

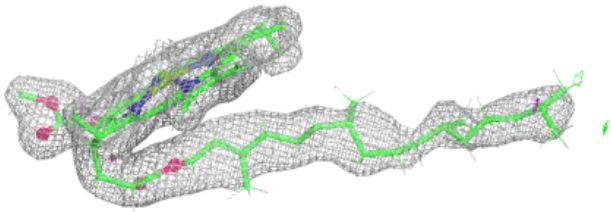
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 613:

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

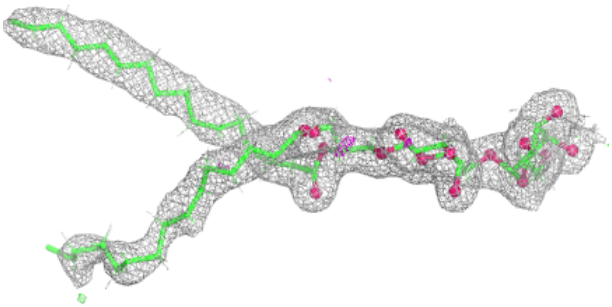


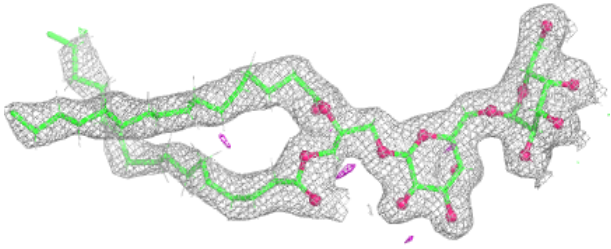


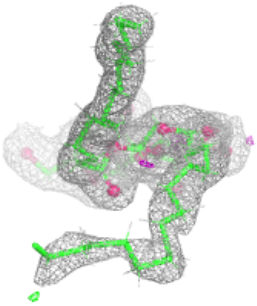


Electron density around DGD c 519:

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

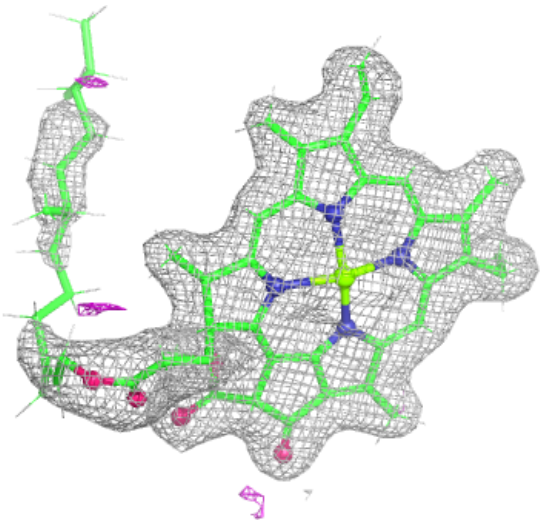


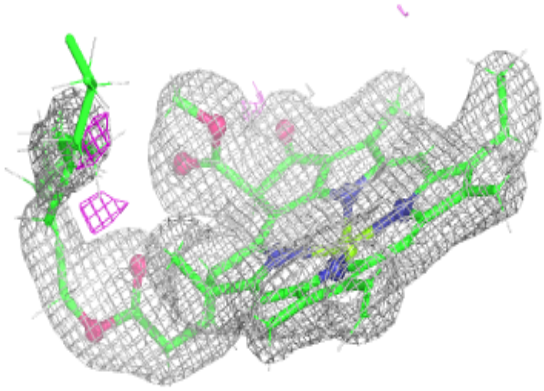




Electron density around CLA B 616:

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

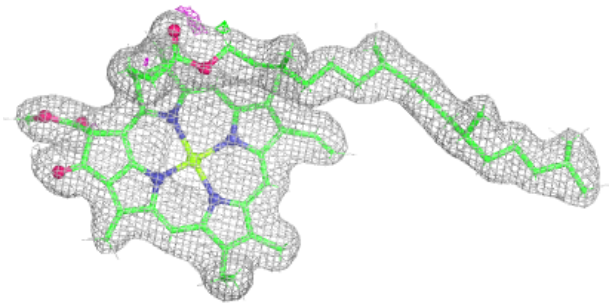


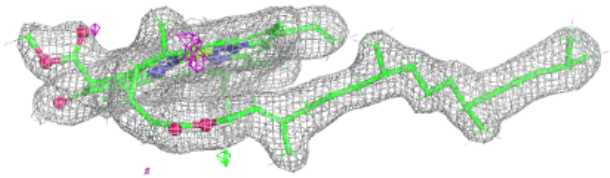


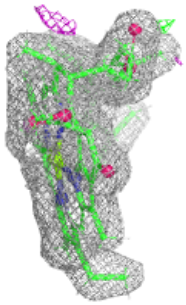


Electron density around CLA C 501:

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

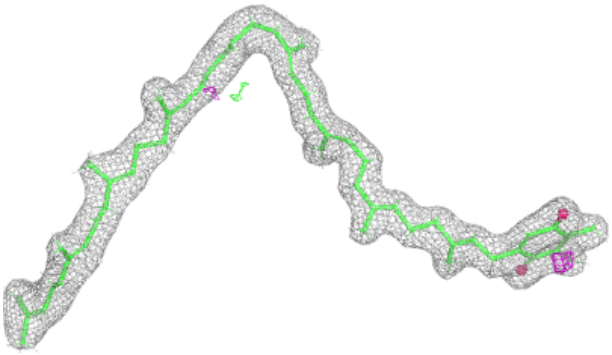


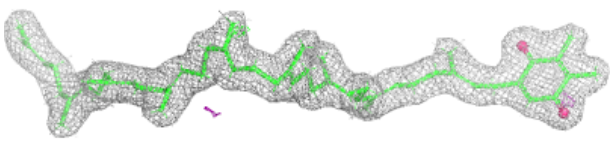


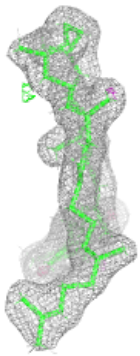


Electron density around PL9 D 407:

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

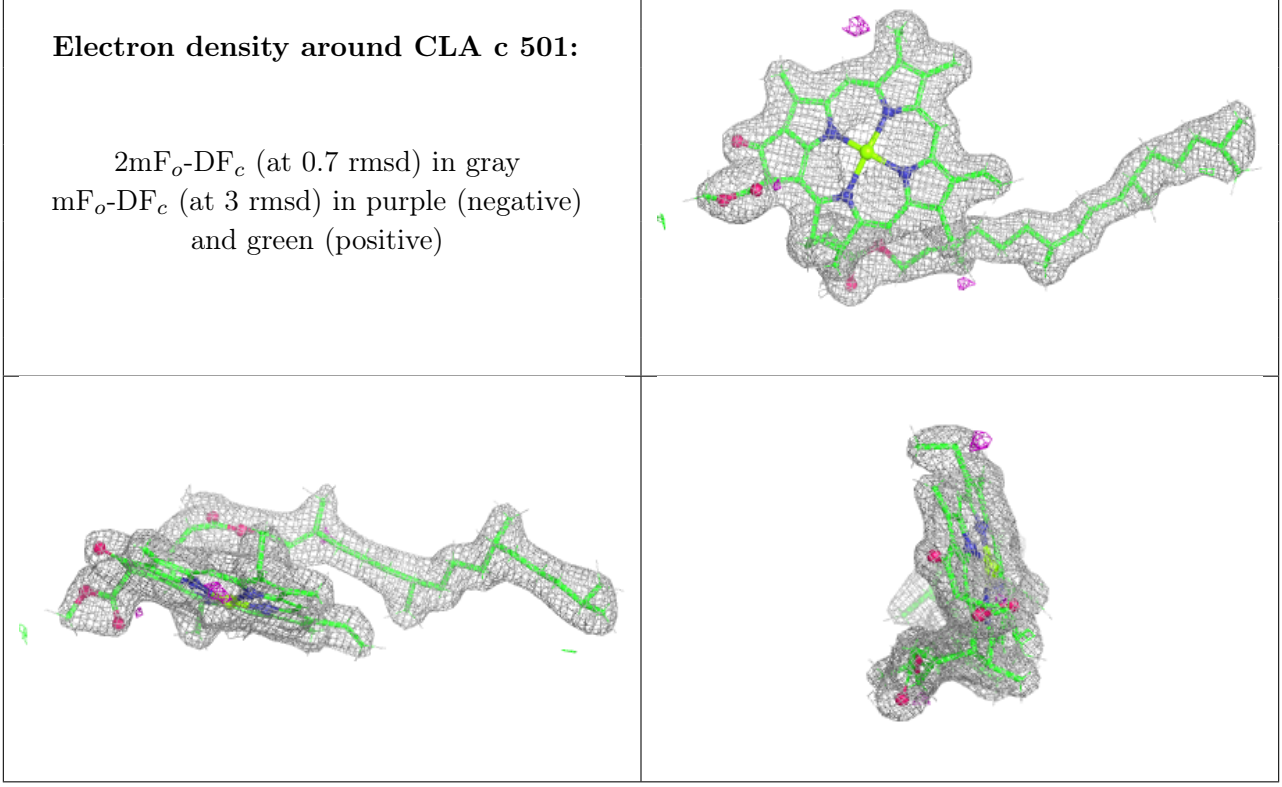






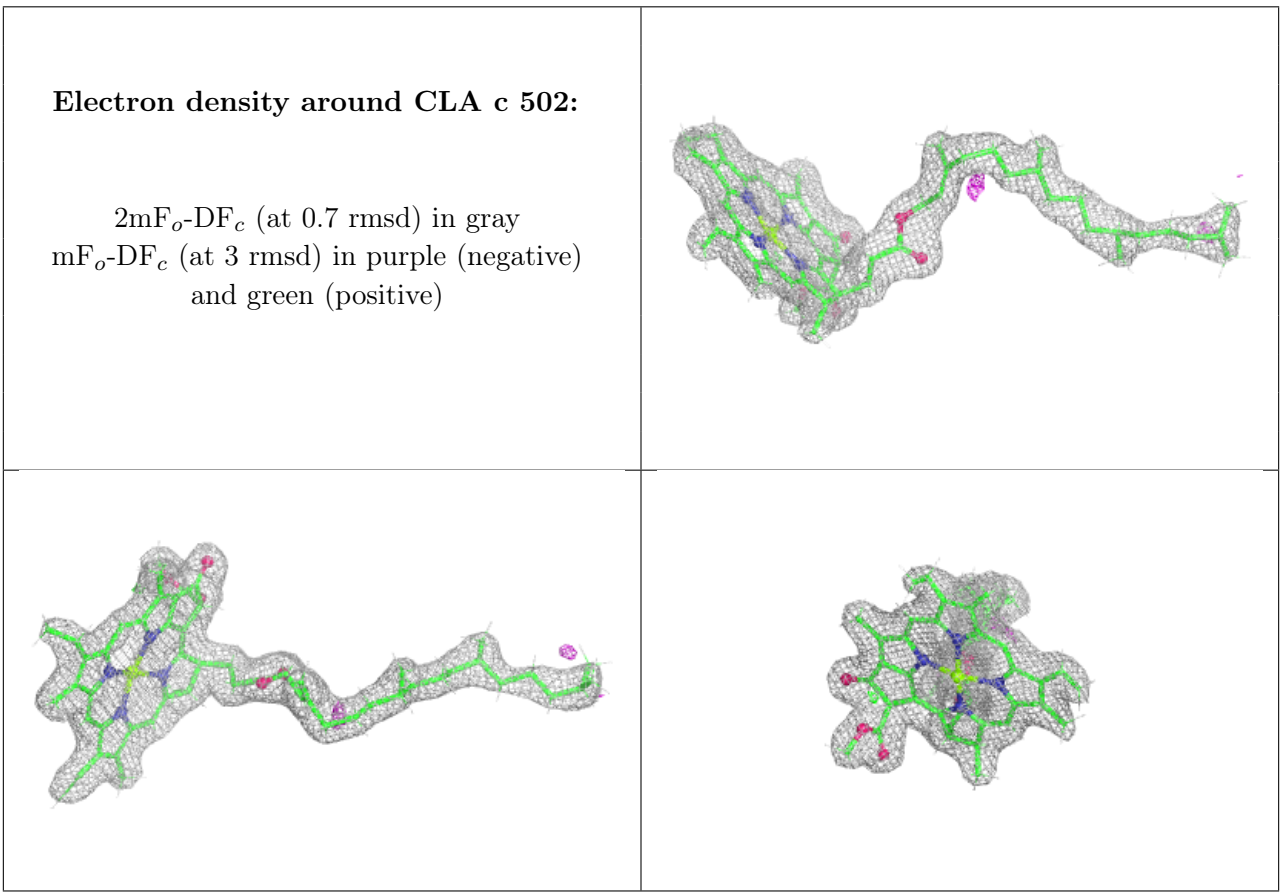
Electron density around CLA c 501:

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



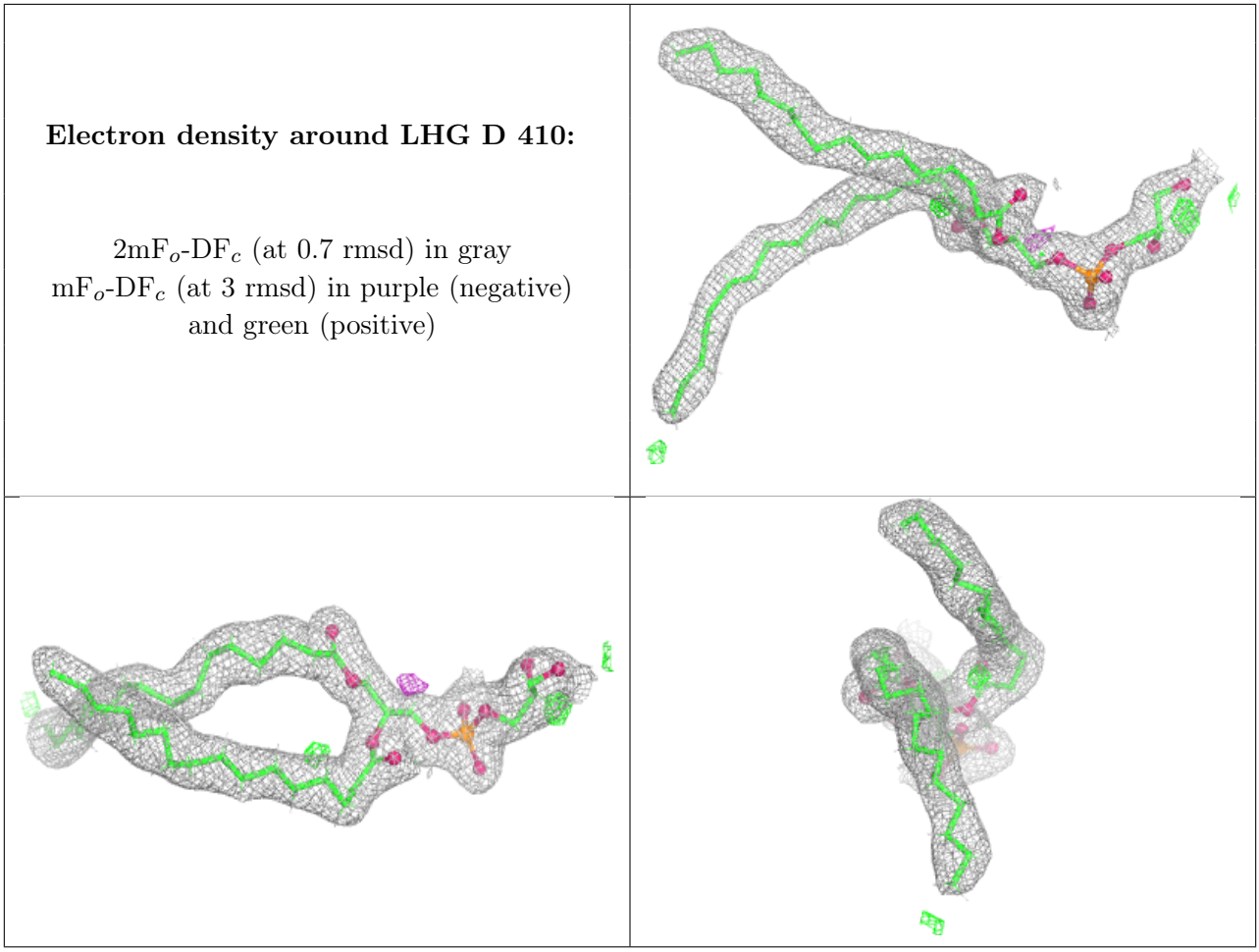
Electron density around CLA c 502:

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



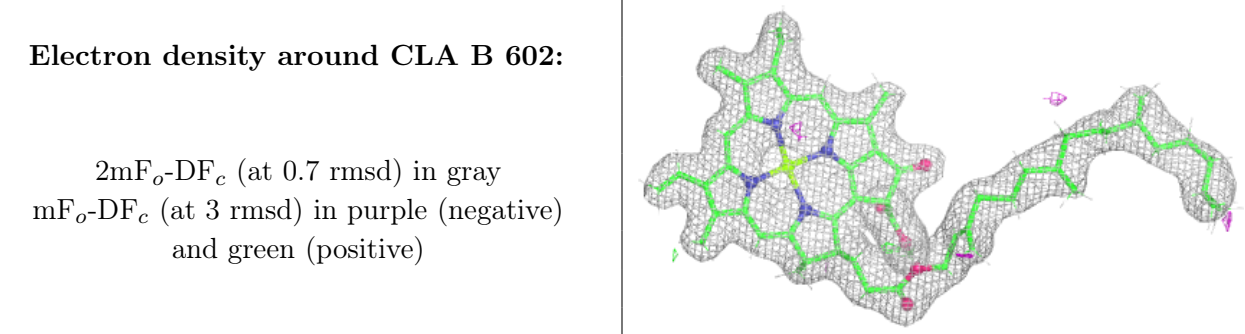
Electron density around LHG D 410:

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



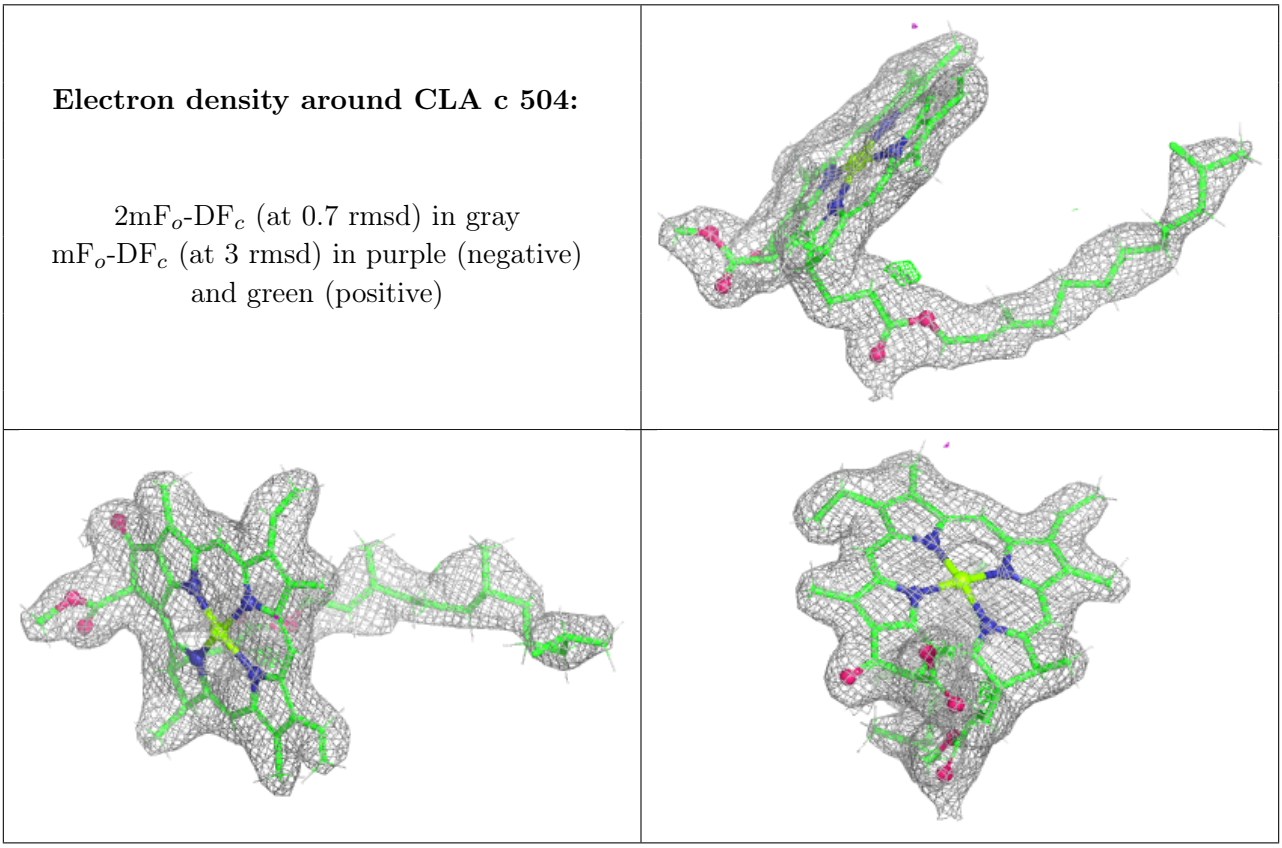
Electron density around CLA B 602:

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



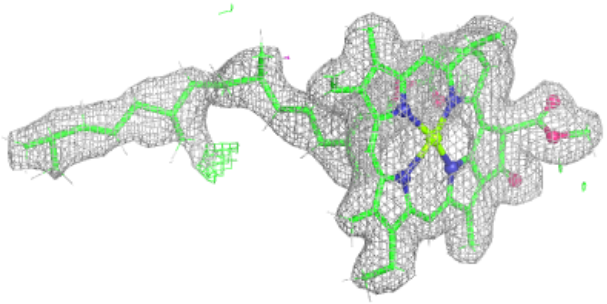
Electron density around CLA c 504:

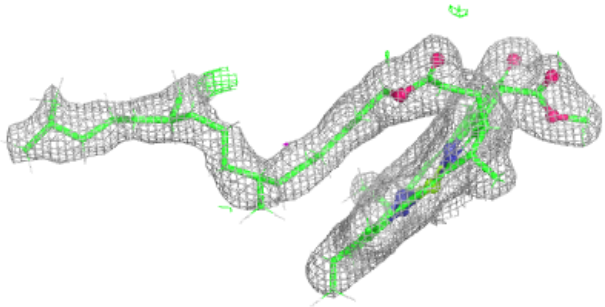
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

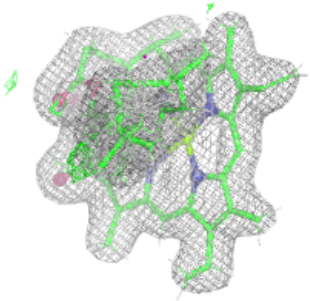


Electron density around CLA c 505:

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

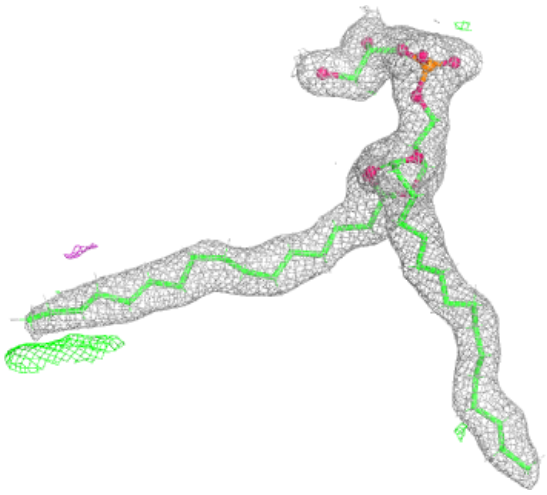




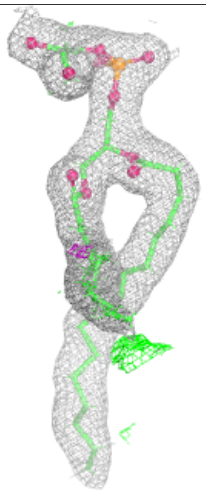


Electron density around LHG L 101:

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

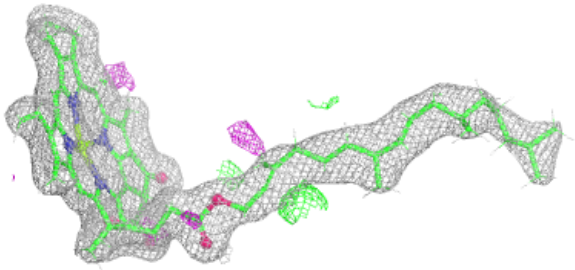


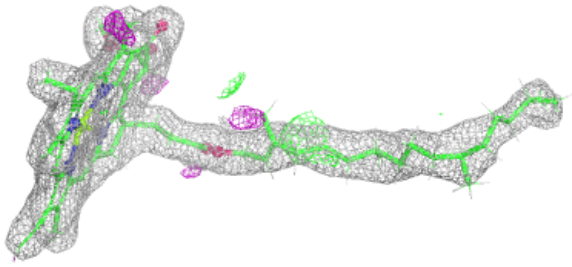


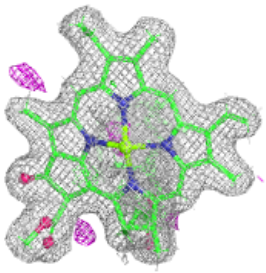


Electron density around CLA B 604:

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

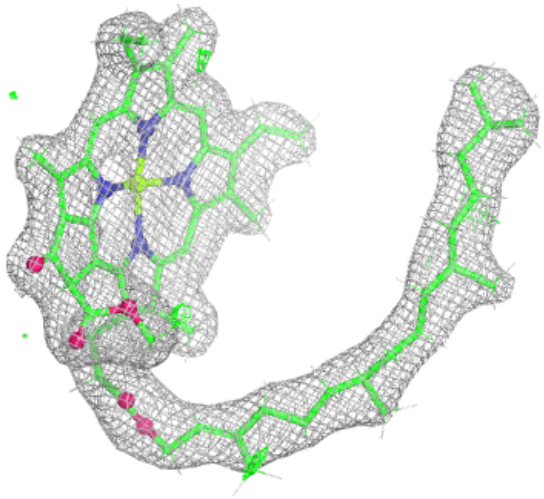


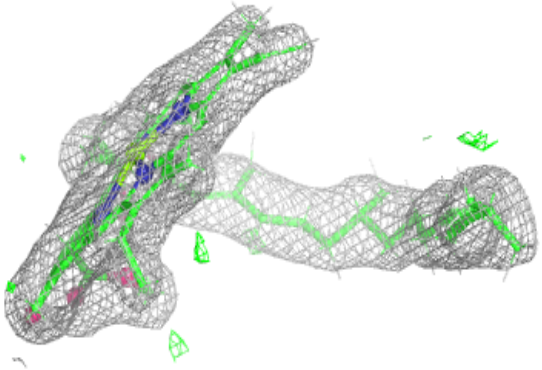


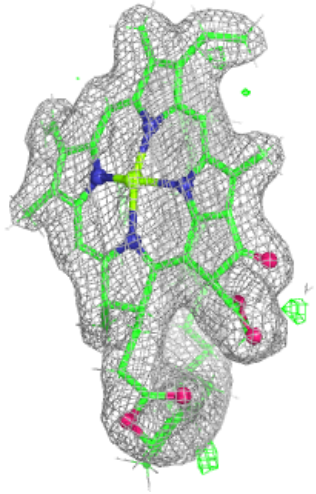


Electron density around CLA c 507:

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

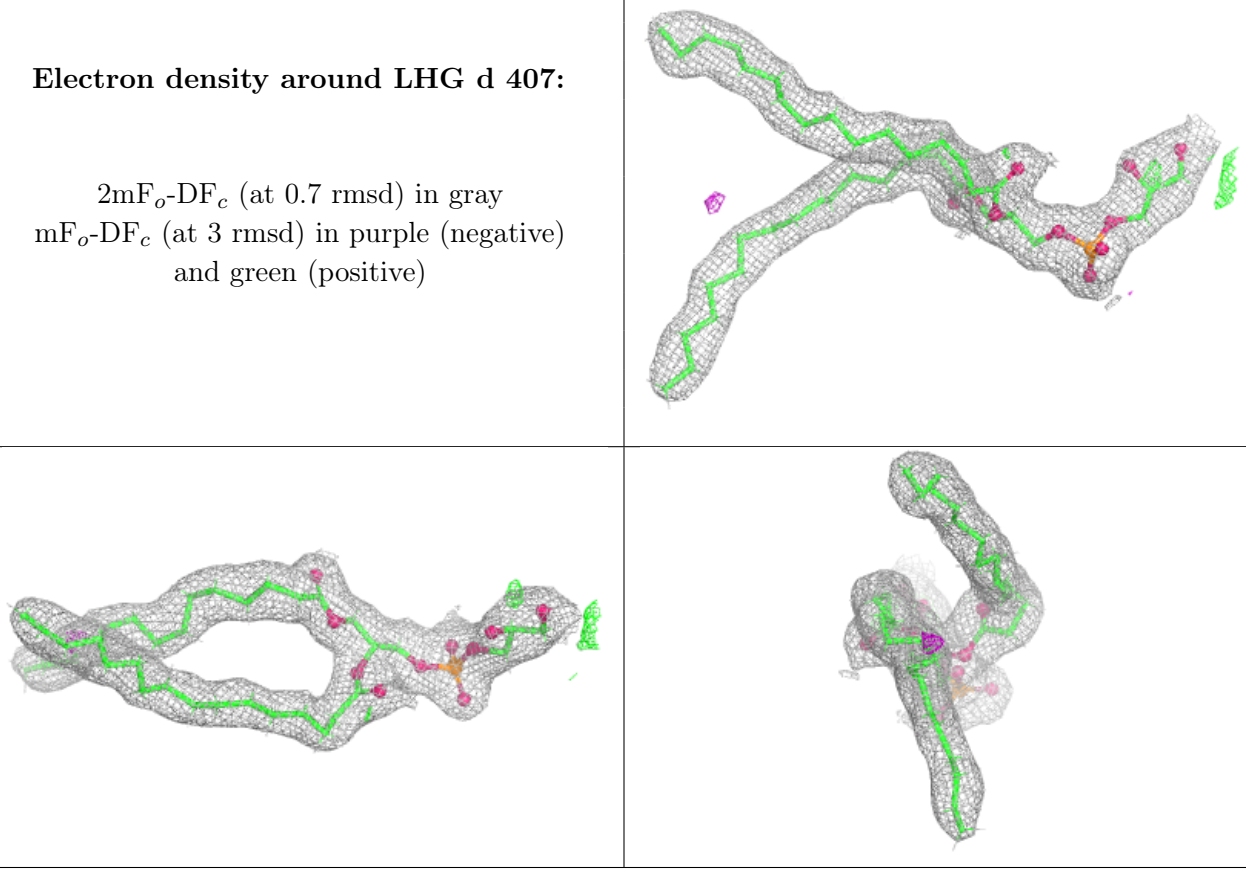






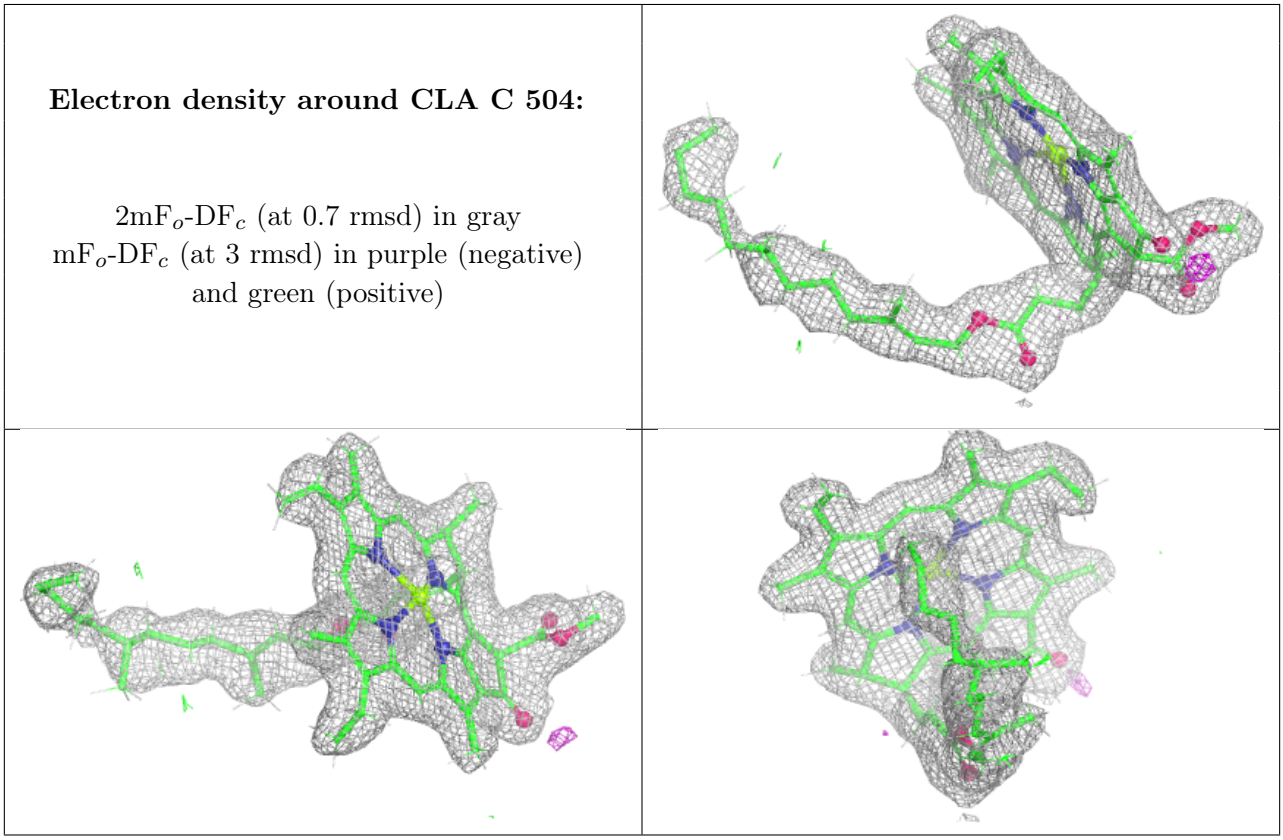
Electron density around LHG d 407:

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



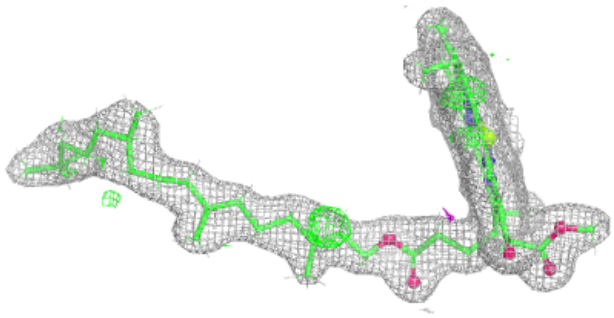
Electron density around CLA C 504:

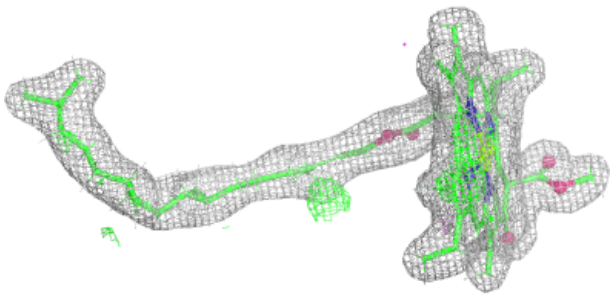
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

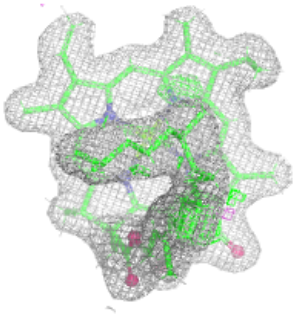


Electron density around CLA B 605:

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

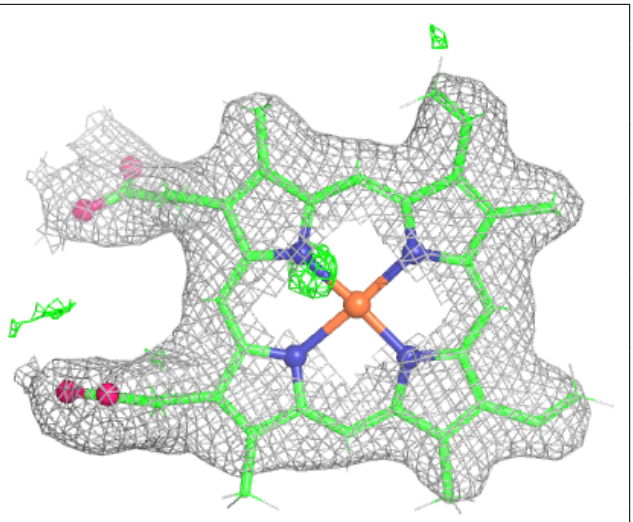


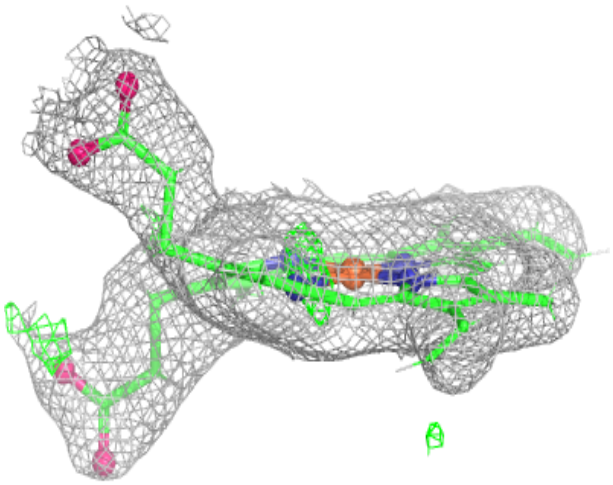


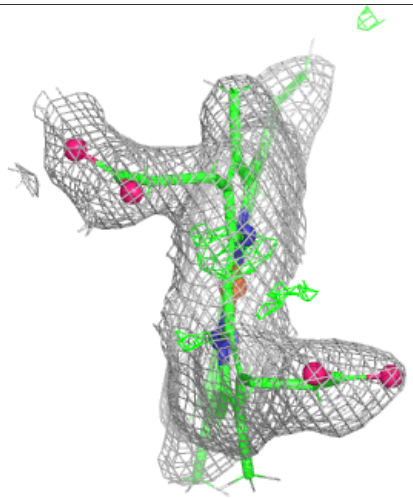


Electron density around HEM f 101:

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

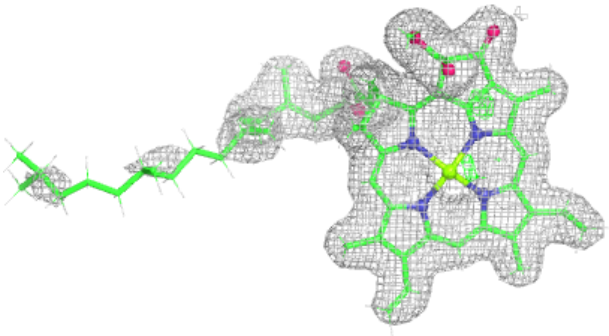


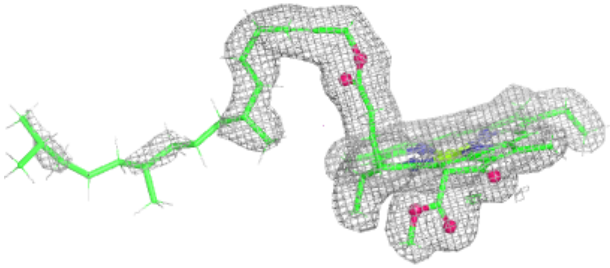


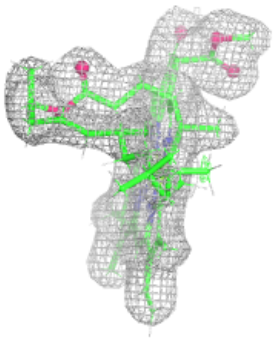


Electron density around CLA A 405:

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

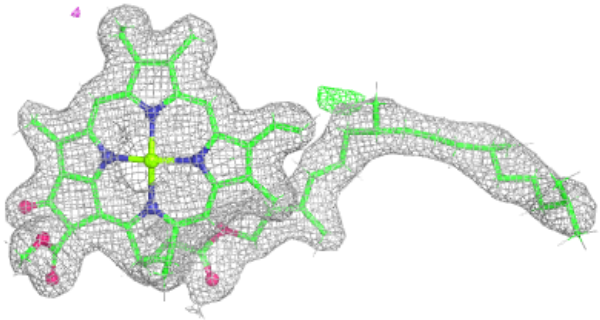


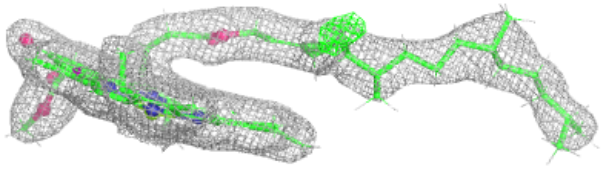


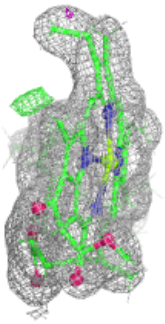


Electron density around CLA B 603:

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

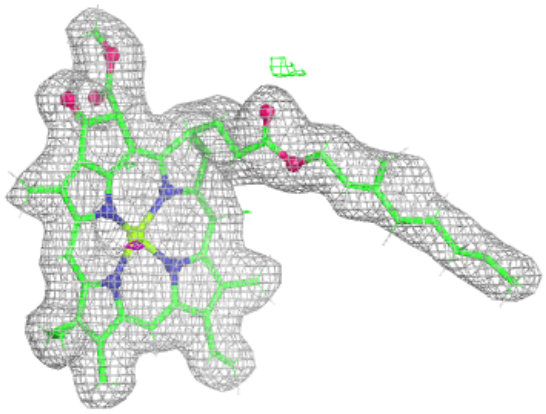


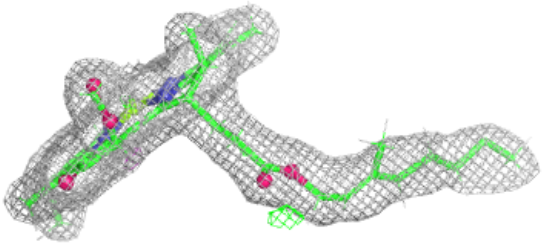


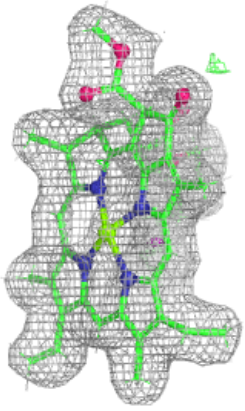


Electron density around CLA A 407:

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

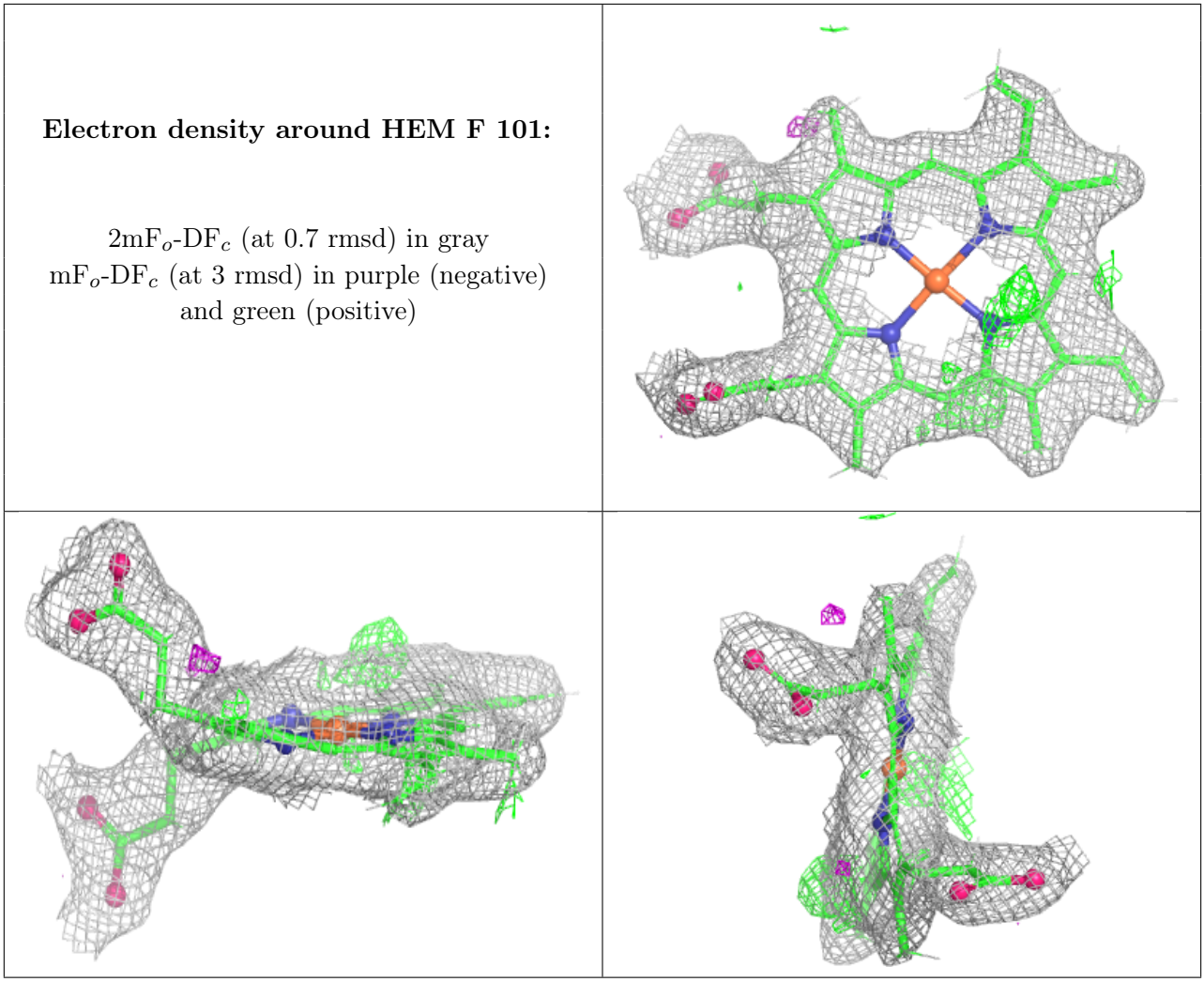






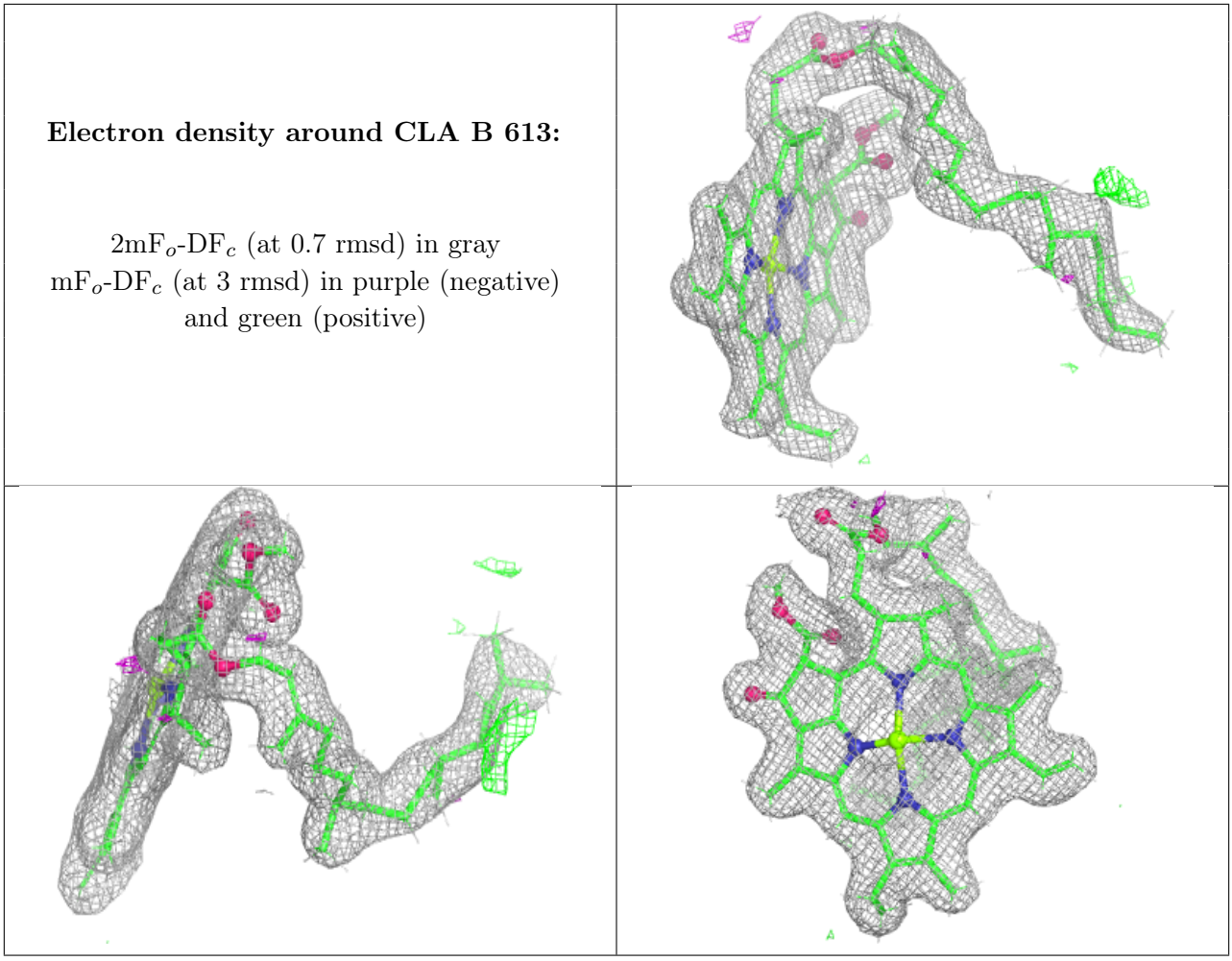
Electron density around HEM F 101:

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



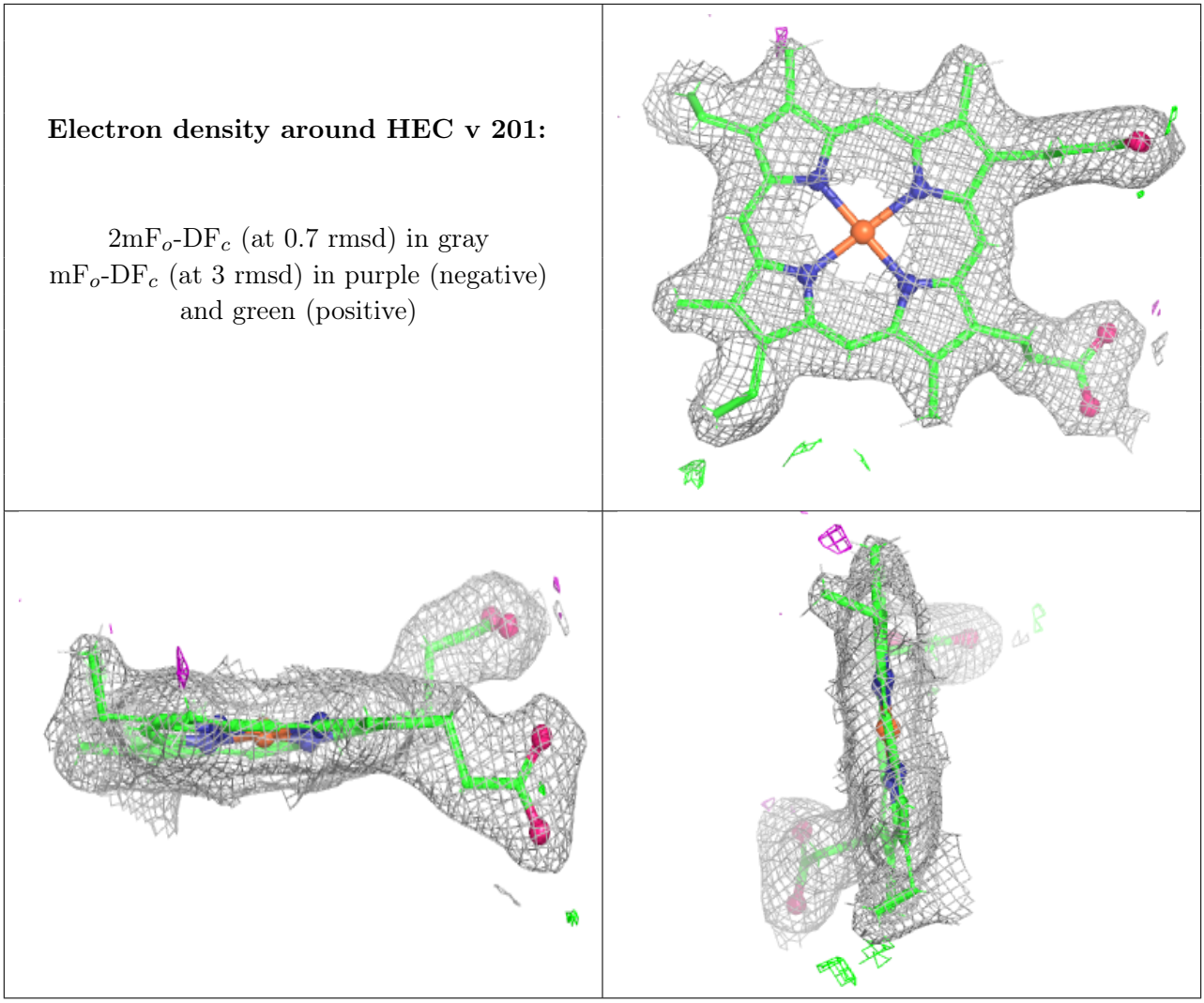
Electron density around CLA B 613:

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



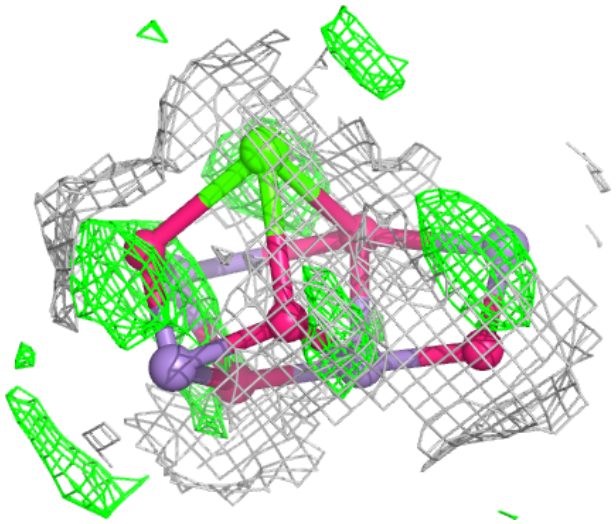
Electron density around HEC v 201:

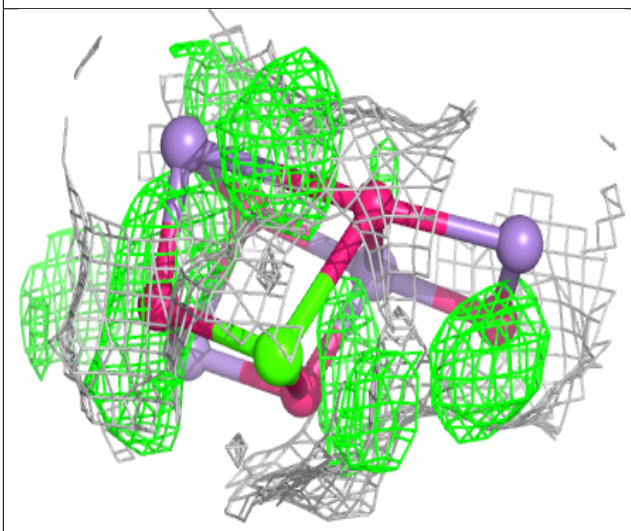
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

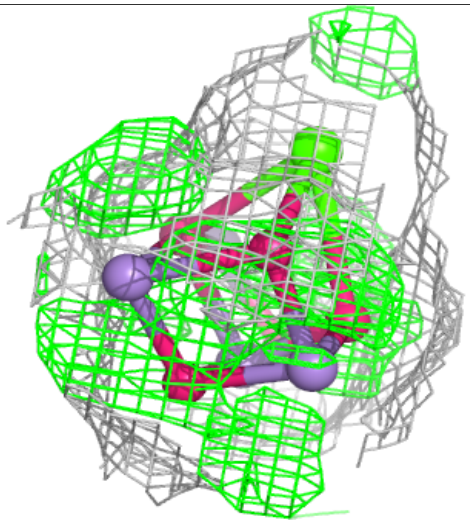


Electron density around OEX A 418:

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

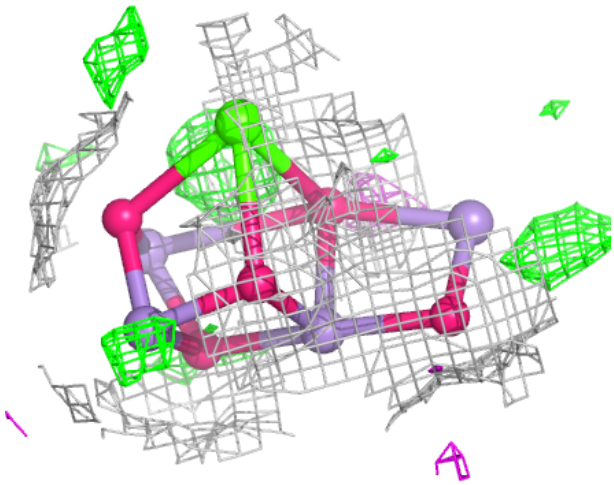


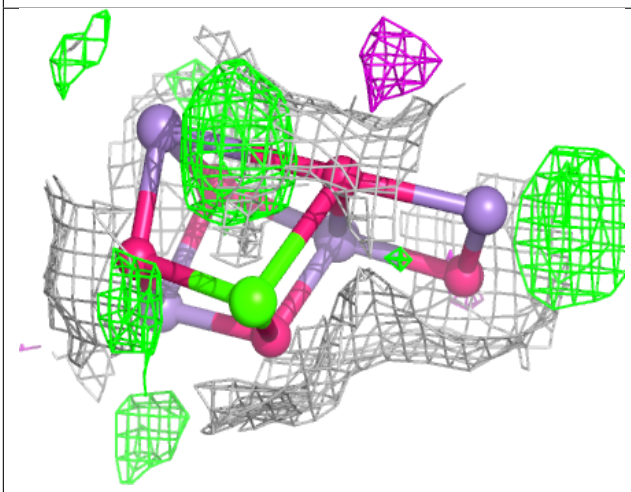


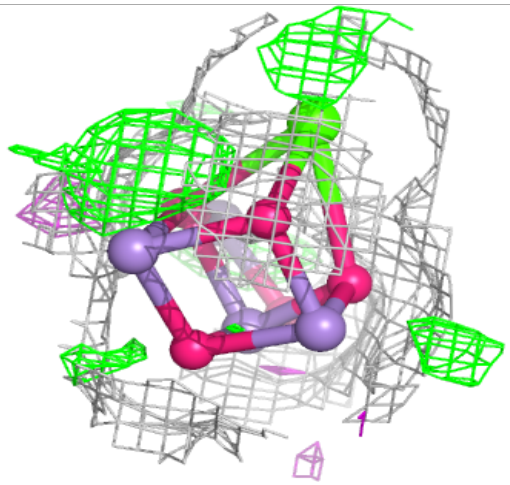


Electron density around OEX a 418:

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

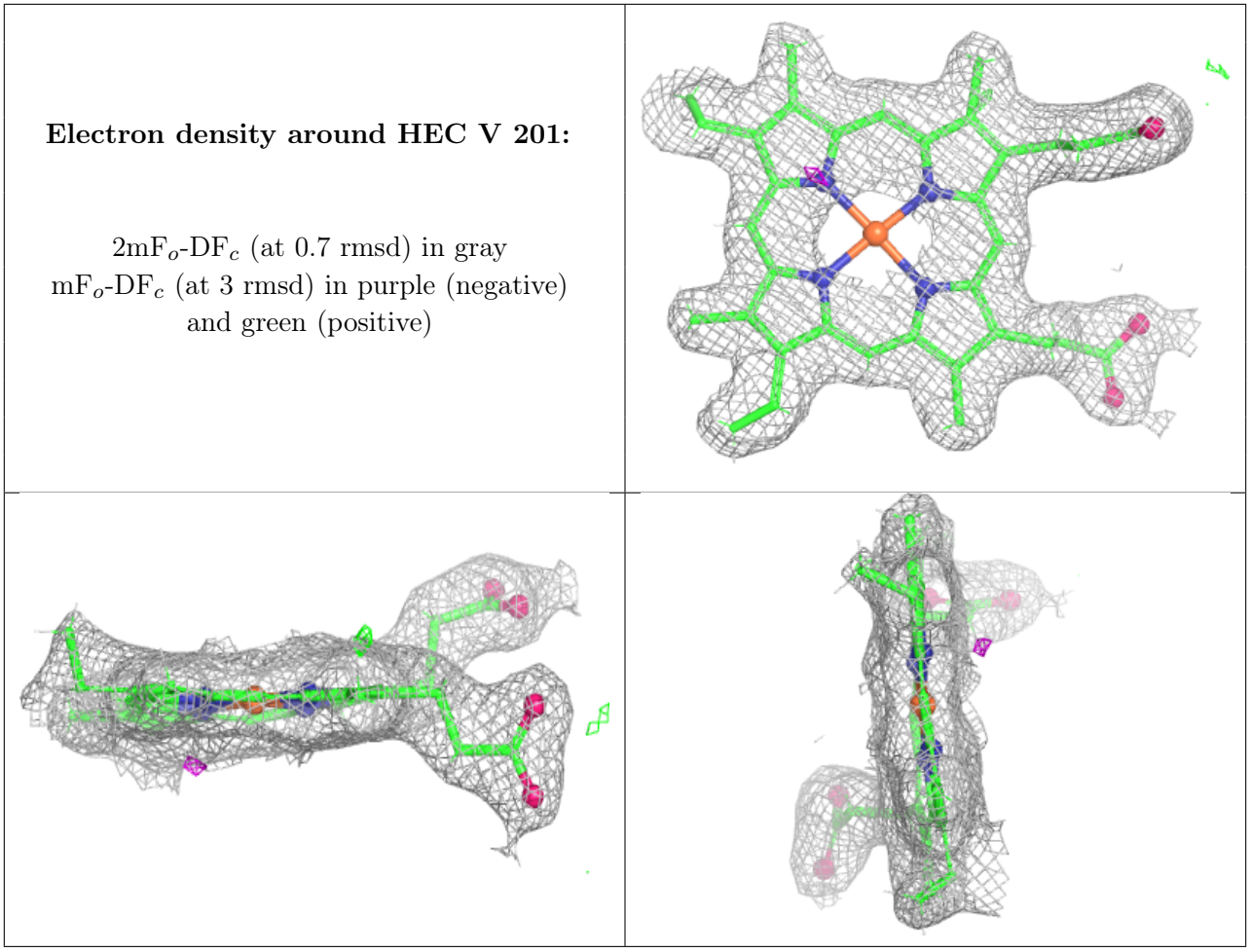






Electron density around HEC V 201:

$2mF_o$-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.