wwPDB EM Validation Summary Report

Aug 5, 2026 – 02:14 AM EDT

PDB ID	:	7RH6 / pdb_00007rh6
EMDB ID	:	EMD-24456
Title	:	Mycobacterial CIII2CIV2 supercomplex, inhibitor free, -Lpqe cyt cc open
Authors	:	Di Trani, J.M.; Yanofsky, D.J.; Rubinstein, J.L.
Deposited on	:	2021-07-16
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

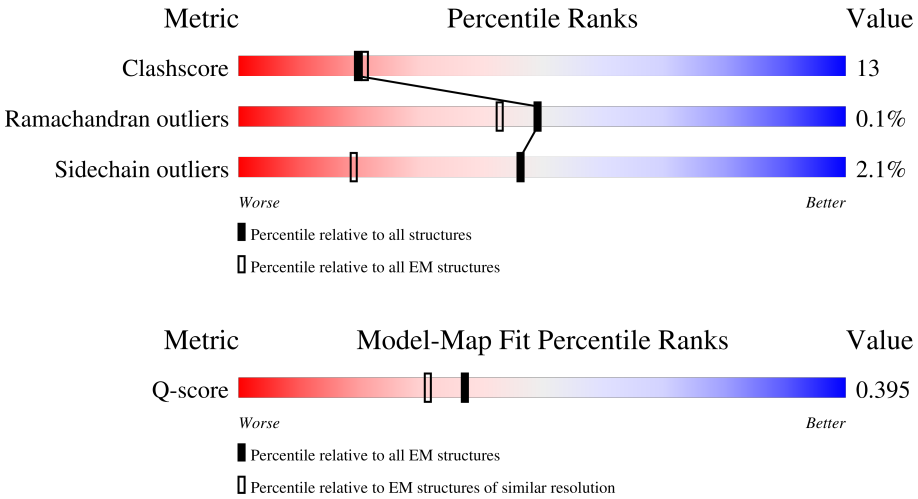
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	223	10% 80% 19%
1	O	223	63% 39% 39% 15% 6%
2	L	552	78% 22%
2	R	552	5% 79% 20%

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Mol	Chain	Length	Quality of chain
3	M	382	6% 85% 15%
3	Y	382	84% 16%
4	S	203	15% 84% 16%
4	X	203	14% 82% 17%
5	E	535	82% 18%
5	F	535	81% 19%
6	J	100	17% 72% 20% 8%
6	P	100	19% 83% 8% 8%
7	D	216	90% 97%
7	G	216	89% 99%
8	K	312	32% 83% 17%
8	Q	312	36% 80% 19%
9	T	139	8% 81% 19%
9	Z	139	13% 81% 19%
10	U	79	42% 81% 19%
10	a	79	28% 92% 8%
11	V	145	31% 84% 15%
11	b	145	19% 83% 17%
12	c	159	65% 84% 15%

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
13	HEC	I	302	X	-	-	-
13	HEC	O	301	X	-	-	-
13	HEC	O	302	X	-	X	-
18	CDL	L	604	-	-	X	-
18	CDL	S	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CDL	T	201	-	-	X	-
18	CDL	T	202	-	-	X	-
18	CDL	T	203	-	-	X	-
18	CDL	X	302	-	-	X	-
18	CDL	X	303	-	-	X	-
18	CDL	Z	202	-	-	X	-
18	CDL	Z	203	-	-	X	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 92757 atoms, of which 45318 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	O	210	Total	C	H	N	O	S	0	0
			3014	948	1483	276	295	12		
1	I	223	Total	C	H	N	O	S	0	0
			3187	1008	1564	289	314	12		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	R	552	Total	C	H	N	O	S	0	0
			8716	2937	4346	695	712	26		
2	L	552	Total	C	H	N	O	S	0	0
			8717	2937	4347	695	712	26		

- Molecule 3 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		
3	Y	382	Total	C	H	N	O	S	0	0
			5961	1924	2984	504	538	11		

- Molecule 4 is a protein called Cytochrome aa3 subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	S	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		
4	X	203	Total	C	H	N	O	S	0	0
			3108	1039	1548	253	260	8		

- Molecule 5 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	535	Total	C	H	N	O	S	0	0
			8384	2751	4203	711	701	18		
5	F	535	Total	C	H	N	O	S	0	0
			8381	2751	4200	711	701	18		

- Molecule 6 is a protein called Putative conserved transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	92	Total	C	H	N	O	S	0	0
			1454	471	718	136	124	5		
6	P	92	Total	C	H	N	O	S	0	0
			1453	471	717	136	124	5		

- Molecule 7 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		
7	G	216	Total	C	H	N	O	S	0	0
			1732	645	640	217	229	1		

- Molecule 8 is a protein called Cytochrome aa3 subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	Q	312	Total	C	H	N	O	S	0	0
			4856	1592	2391	412	451	10		
8	K	312	Total	C	H	N	O	S	0	0
			4857	1592	2392	412	451	10		

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	T	139	Total	C	H	N	O	S	0	0
			2136	719	1059	167	188	3		
9	Z	139	Total	C	H	N	O	S	0	0
			2135	719	1058	167	188	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	U	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	a	79	Total	C	H	N	O	S	0	0
			1167	381	576	107	101	2		

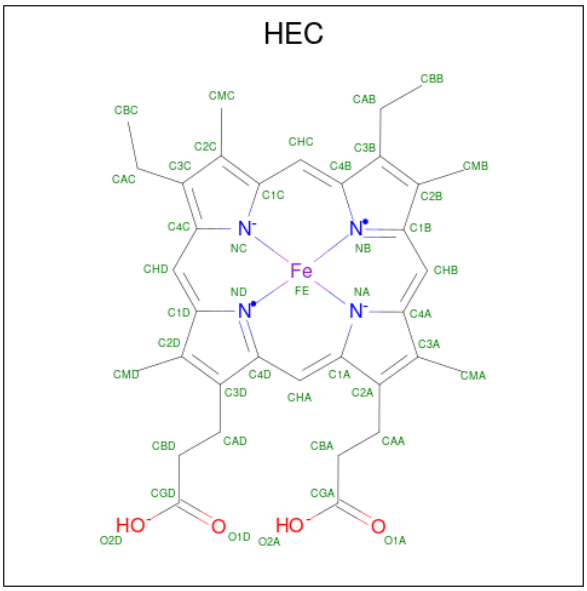
- Molecule 11 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	V	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		
11	b	145	Total	C	H	N	O	S	0	0
			2093	658	1052	176	205	2		

- Molecule 12 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	c	158	Total	C	H	N	O	S	0	0
			2259	708	1110	192	248	1		

- Molecule 13 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



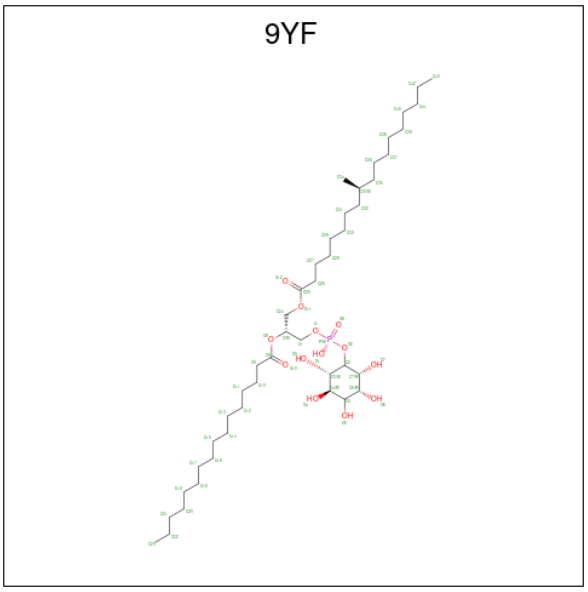
Mol	Chain	Residues	Atoms						AltConf
13	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
13	O	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
13	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

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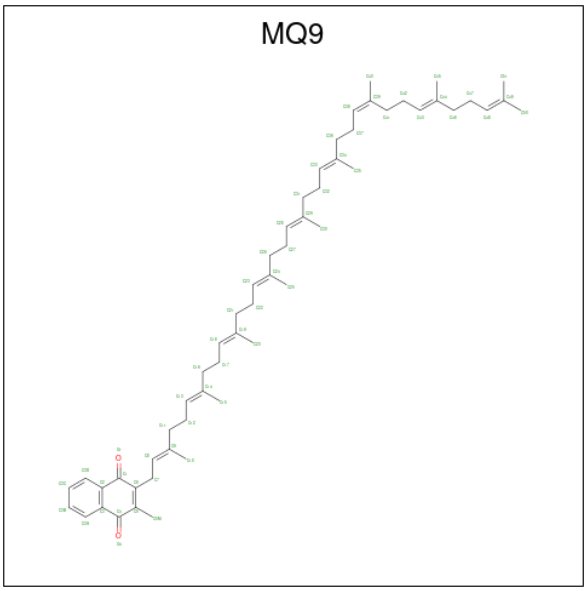
Mol	Chain	Residues	Atoms						AltConf
13	I	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

- Molecule 14 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



Mol	Chain	Residues	Atoms					AltConf
14	O	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	E	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	I	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
14	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	

- Molecule 15 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).

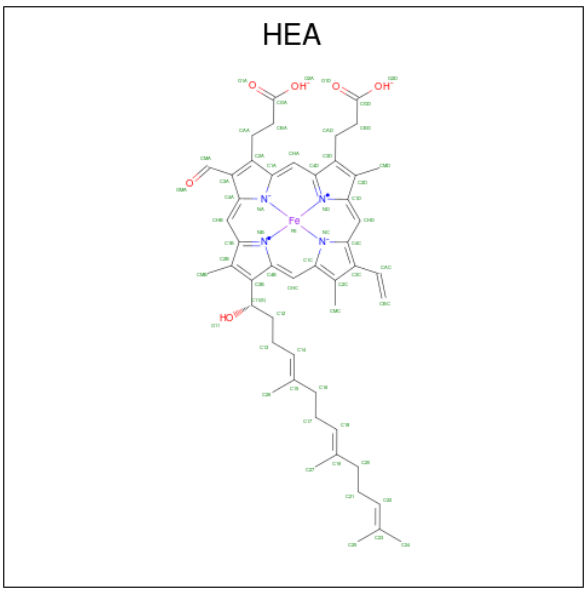


Mol	Chain	Residues	Atoms				AltConf
15	O	1	Total	C	H	O	0
			138	56	80	2	
15	E	1	Total	C	H	O	0
			138	56	80	2	
15	E	1	Total	C	H	O	0
			138	56	80	2	
15	F	1	Total	C	H	O	0
			138	56	80	2	
15	F	1	Total	C	H	O	0
			138	56	80	2	
15	T	1	Total	C	H	O	0
			138	56	80	2	
15	Z	1	Total	C	H	O	0
			138	56	80	2	
15	I	1	Total	C	H	O	0
			138	56	80	2	

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

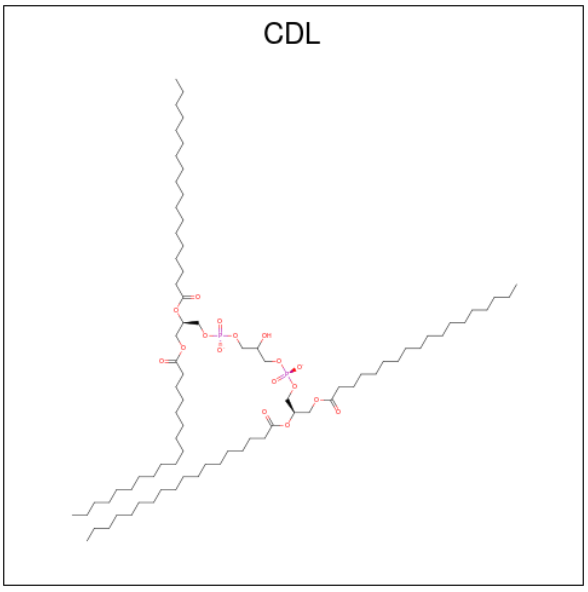
Mol	Chain	Residues	Atoms		AltConf
16	R	1	Total	Cu	0
			1	1	
16	L	1	Total	Cu	0
			1	1	
16	Q	2	Total	Cu	0
			2	2	
16	K	2	Total	Cu	0
			2	2	

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



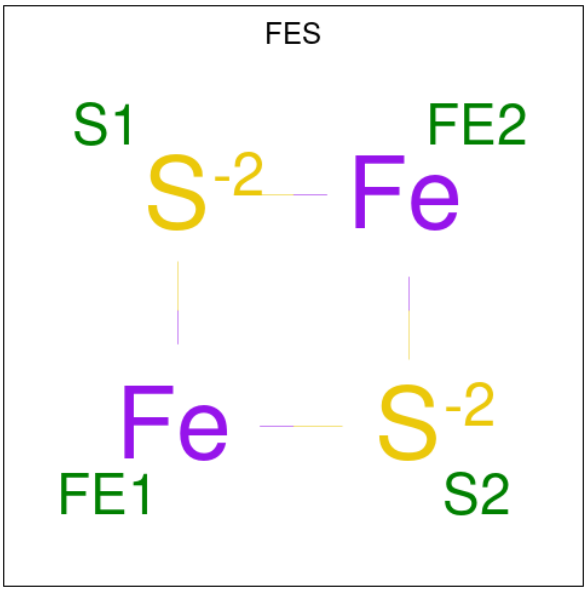
Mol	Chain	Residues	Atoms						AltConf
17	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
17	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
17	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
17	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



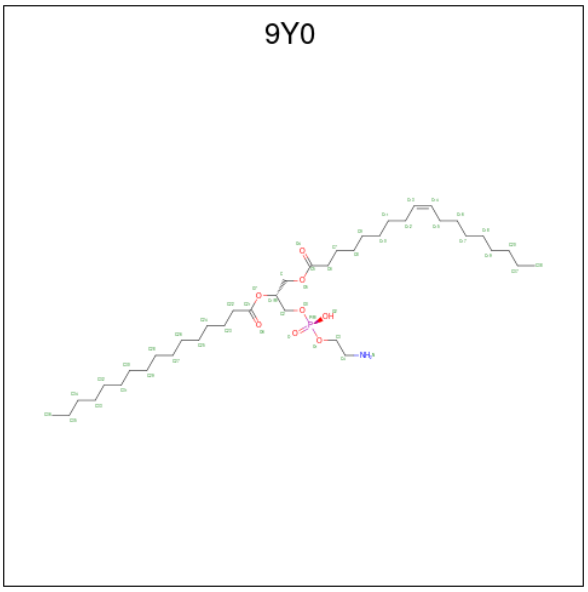
Mol	Chain	Residues	Atoms				AltConf
18	R	1	Total	C	O	P	0
			76	57	17	2	
18	S	1	Total	C	O	P	0
			76	57	17	2	
18	E	1	Total	C	O	P	0
			76	57	17	2	
18	E	1	Total	C	O	P	0
			76	57	17	2	
18	F	1	Total	C	O	P	0
			76	57	17	2	
18	F	1	Total	C	O	P	0
			76	57	17	2	
18	L	1	Total	C	O	P	0
			76	57	17	2	
18	J	1	Total	C	O	P	0
			76	57	17	2	
18	T	1	Total	C	O	P	0
			76	57	17	2	
18	T	1	Total	C	O	P	0
			76	57	17	2	
18	T	1	Total	C	O	P	0
			76	57	17	2	
18	P	1	Total	C	O	P	0
			76	57	17	2	
18	X	1	Total	C	O	P	0
			76	57	17	2	
18	X	1	Total	C	O	P	0
			76	57	17	2	
18	Z	1	Total	C	O	P	0
			76	57	17	2	
18	Z	1	Total	C	O	P	0
			76	57	17	2	

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
19	M	1	Total	Fe	S	0
			4	2	2	
19	Y	1	Total	Fe	S	0
			4	2	2	

- Molecule 20 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: $C_{39}H_{76}NO_8P$).



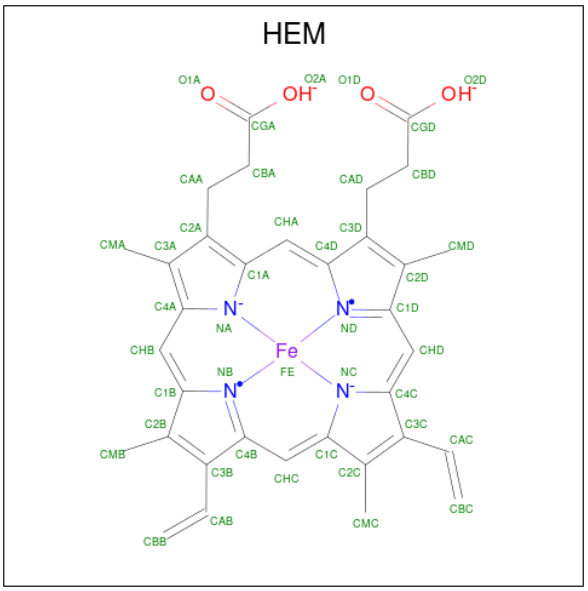
Mol	Chain	Residues	Atoms						AltConf
20	S	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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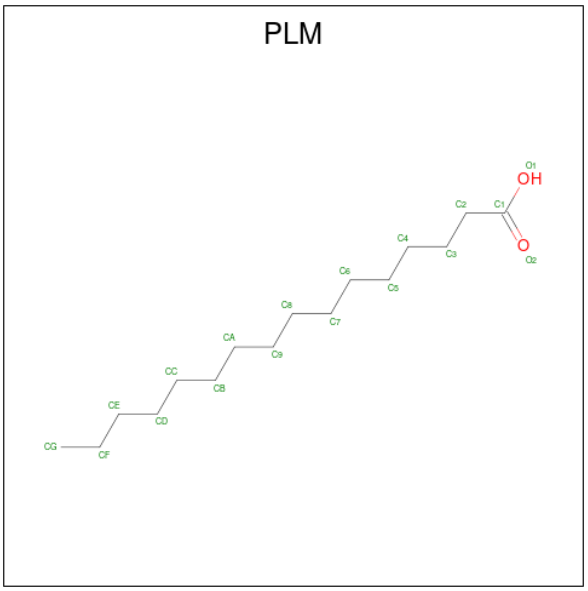
Mol	Chain	Residues	Atoms						AltConf
20	F	1	Total	C	H	N	O	P	0
			123	39	74	1	8	1	
20	J	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
20	J	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
20	X	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

- Molecule 21 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



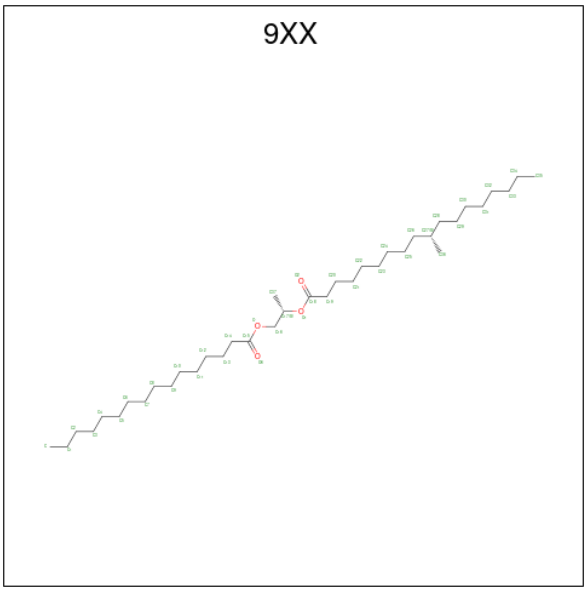
Mol	Chain	Residues	Atoms						AltConf
21	E	1	Total	C	Fe	H	N	O	0
			69	33	1	27	4	4	
21	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
21	F	1	Total	C	Fe	H	N	O	0
			69	33	1	27	4	4	
21	F	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 22 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms				AltConf
22	D	1	Total	C	H	O	0
			27	10	16	1	
22	G	1	Total	C	H	O	0
			27	10	16	1	
22	c	1	Total	C	H	O	0
			48	16	31	1	

- Molecule 23 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: $C_{38}H_{74}O_4$).



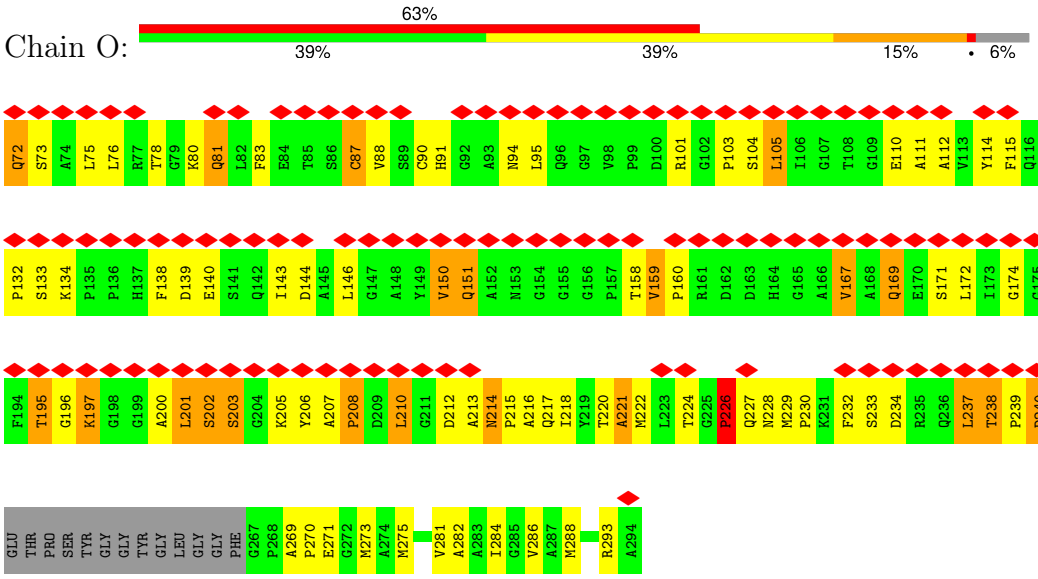
Mol	Chain	Residues	Atoms				AltConf
23	D	1	Total	C	H	O	0
			83	28	51	4	
23	G	1	Total	C	H	O	0
			83	28	51	4	
23	c	1	Total	C	H	O	0
			115	38	73	4	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

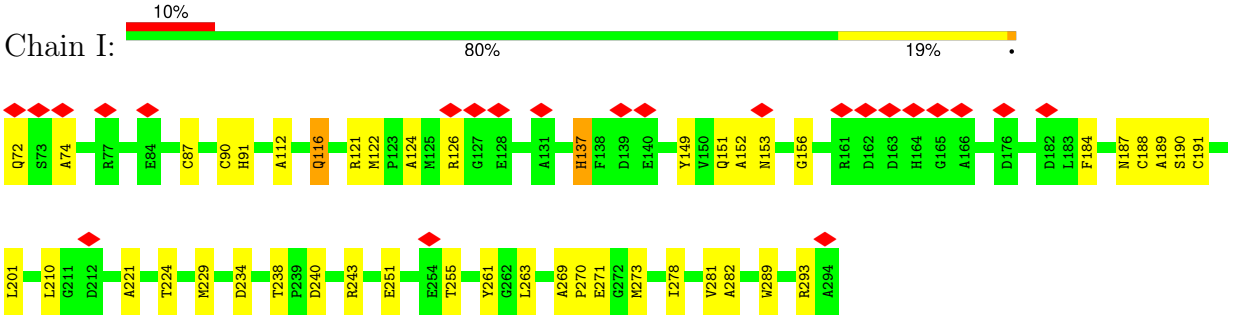
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

Chain O:



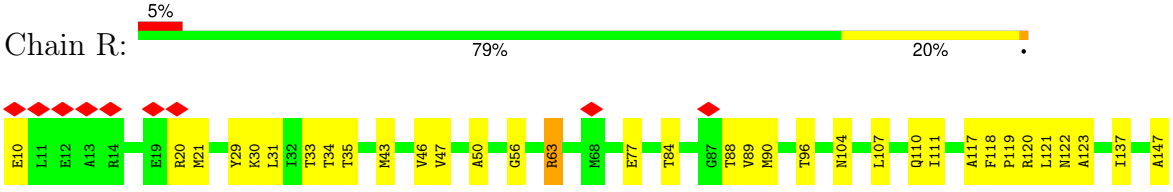
• Molecule 1: Cytochrome bc1 complex cytochrome c subunit

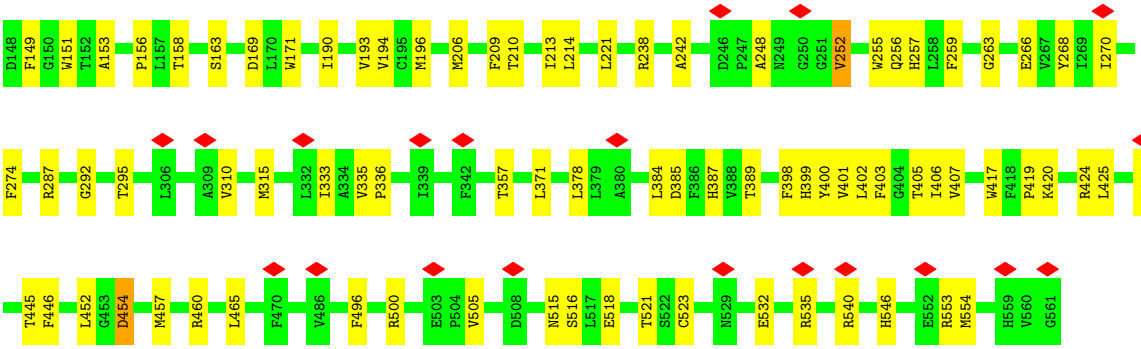
Chain I:



• Molecule 2: Cytochrome c oxidase subunit 1

Chain R:

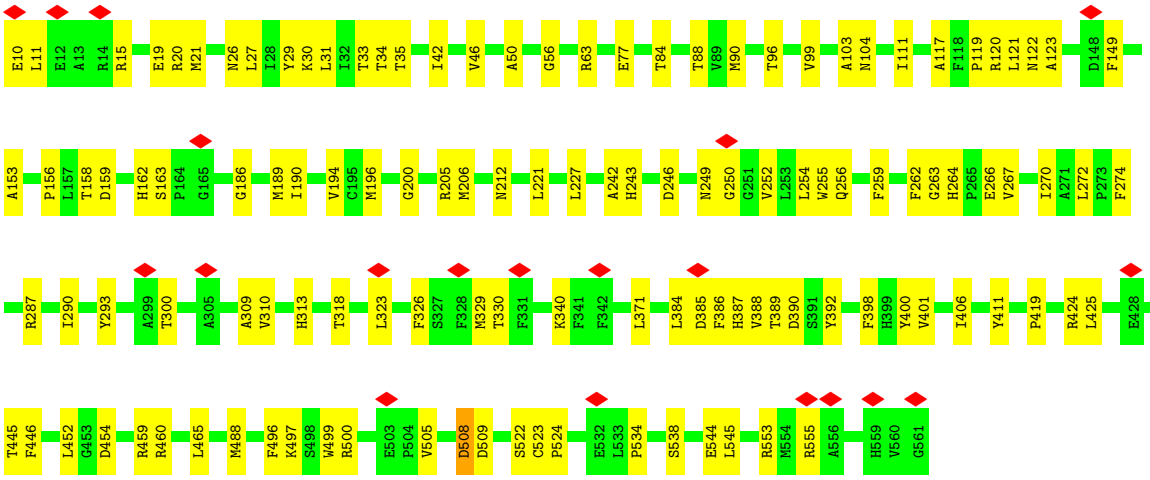




• Molecule 2: Cytochrome c oxidase subunit 1

Chain L:

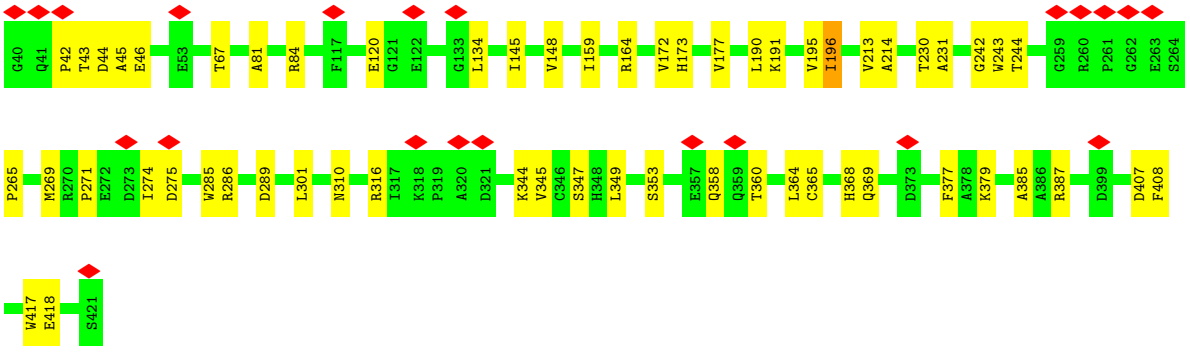




• Molecule 3: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain M:

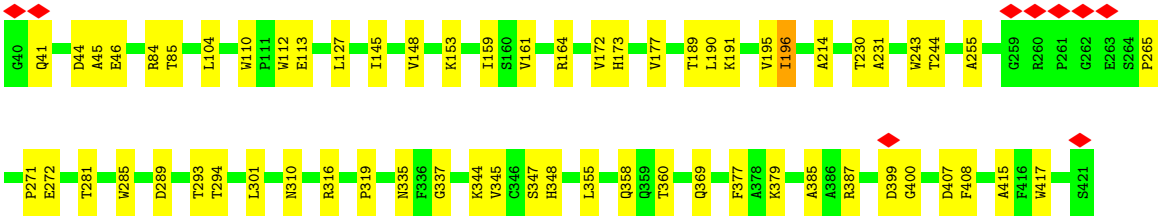




• Molecule 3: Cytochrome bc1 complex Rieske iron-sulfur subunit

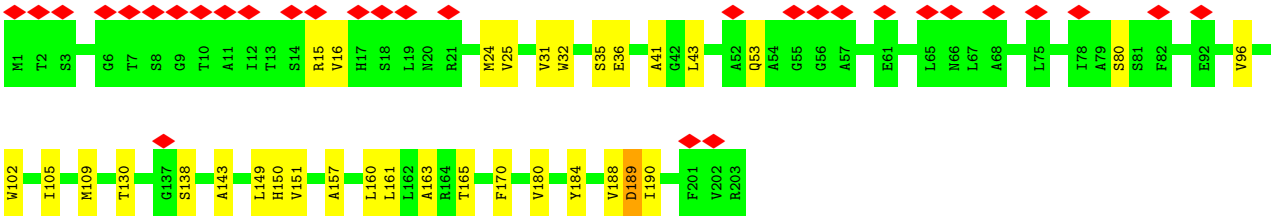
Chain Y:



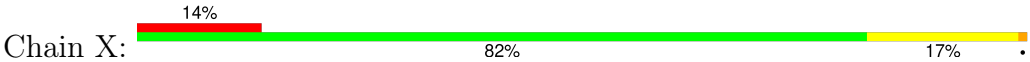


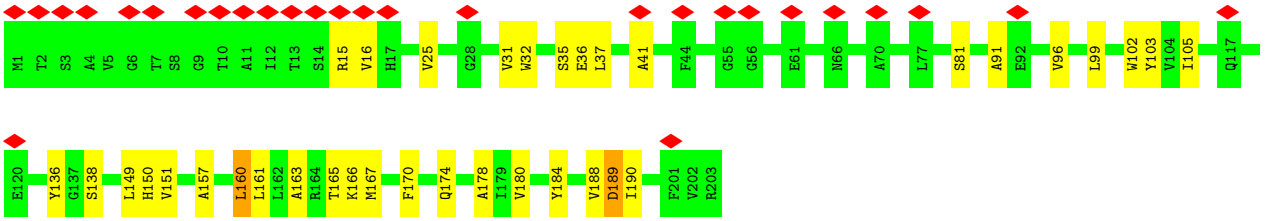
• Molecule 4: Cytochrome aa3 subunit 3



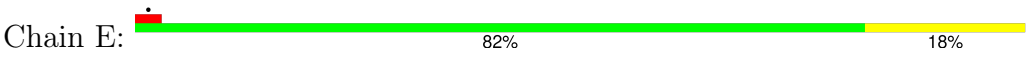


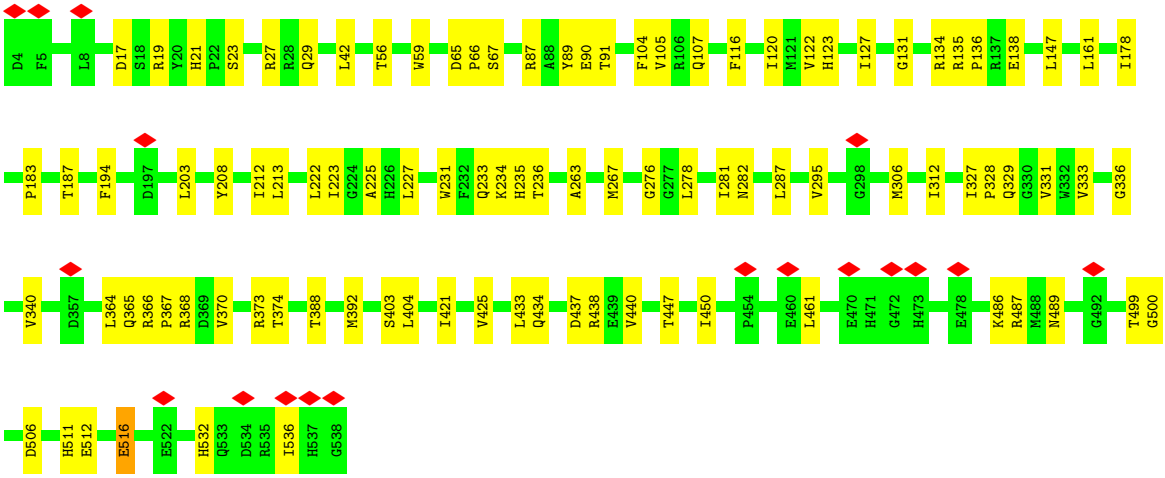
• Molecule 4: Cytochrome aa3 subunit 3





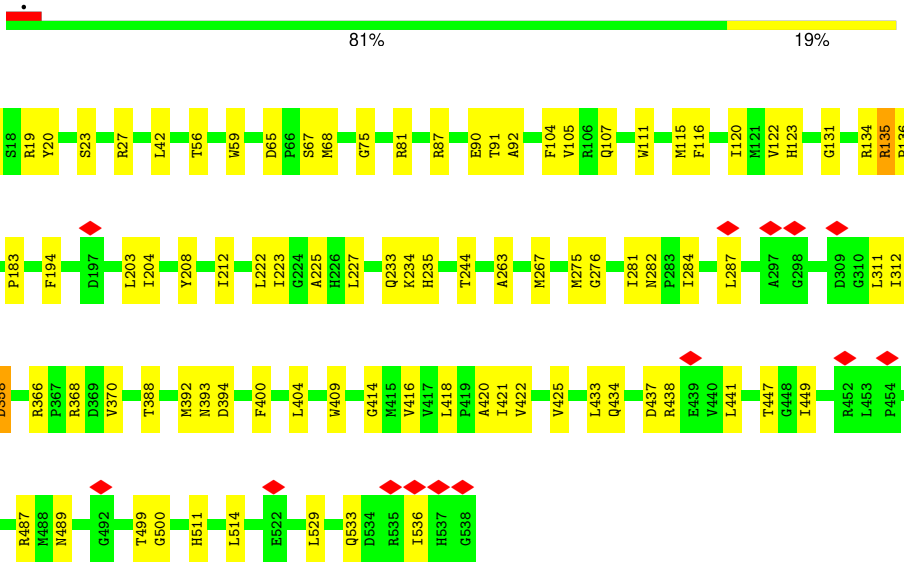
• Molecule 5: Cytochrome bc1 complex cytochrome b subunit





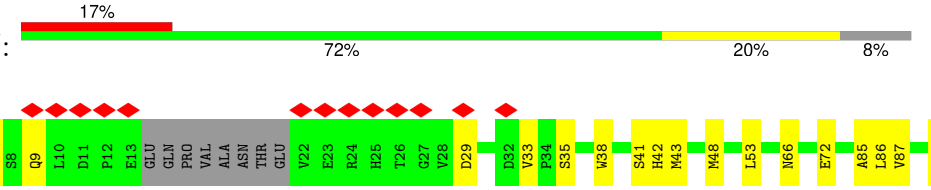
• Molecule 5: Cytochrome bc1 complex cytochrome b subunit

Chain F:



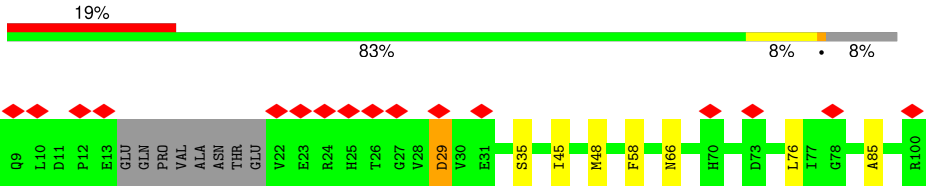
• Molecule 6: Putative conserved transmembrane protein

Chain J:



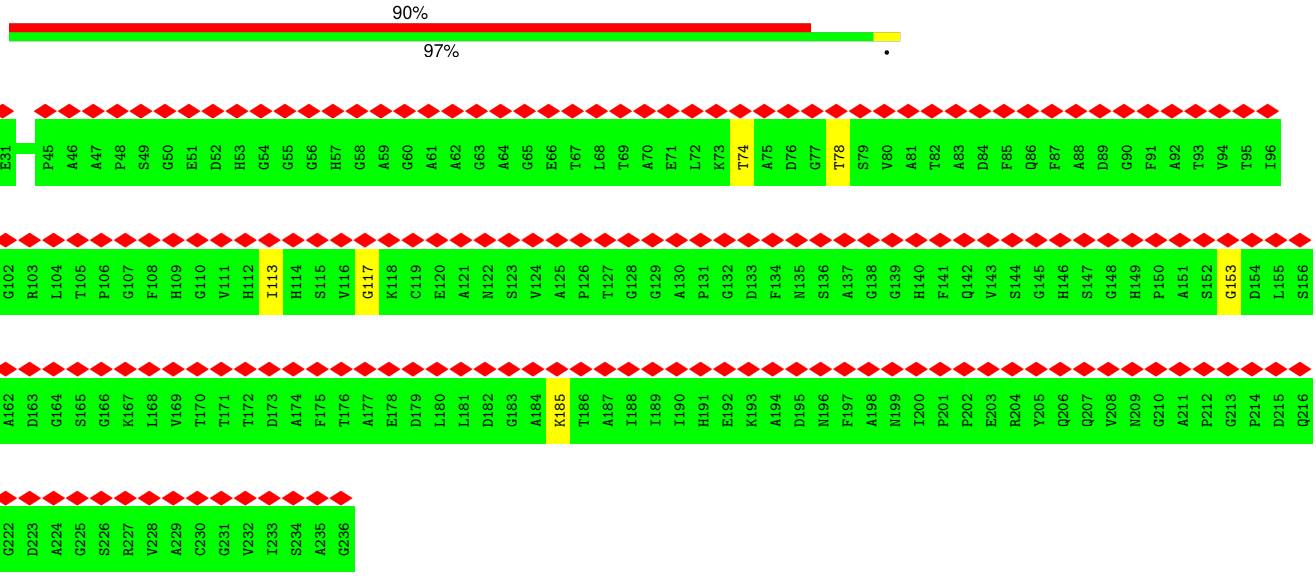
• Molecule 6: Putative conserved transmembrane protein

Chain P:



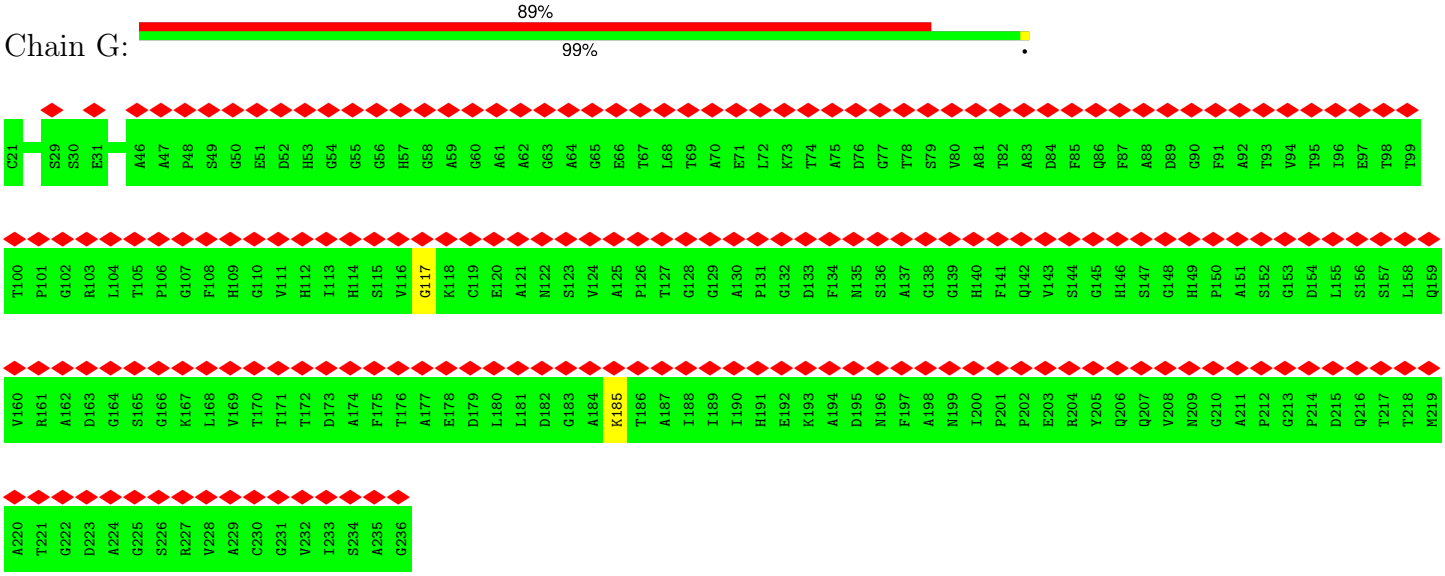
• Molecule 7: Superoxide dismutase [Cu-Zn]

Chain D:



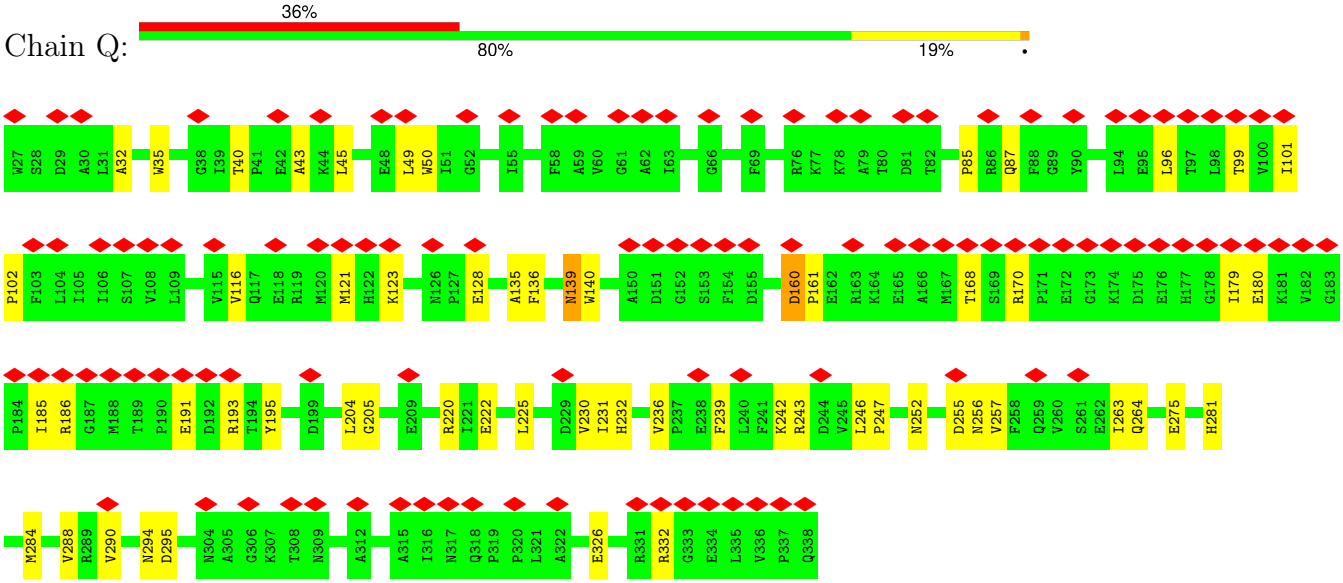
• Molecule 7: Superoxide dismutase [Cu-Zn]

Chain G:



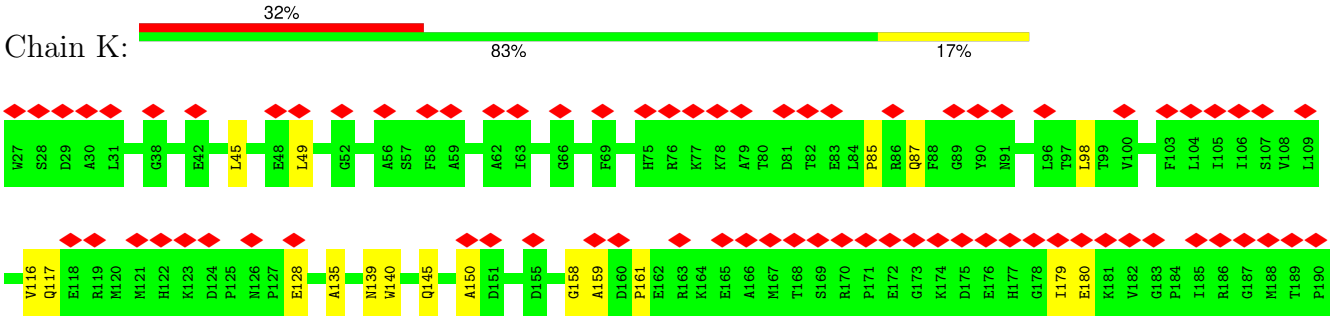
• Molecule 8: Cytochrome aa3 subunit 2

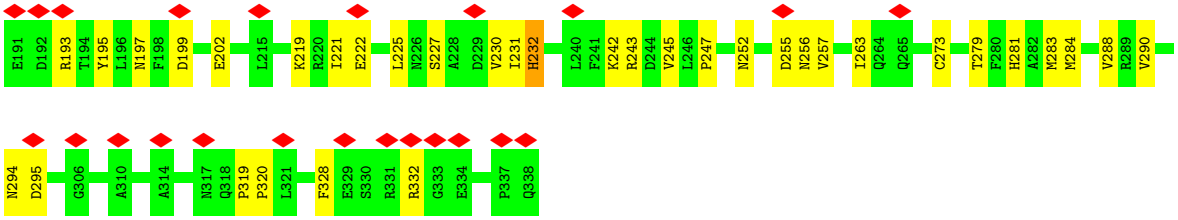
Chain Q:



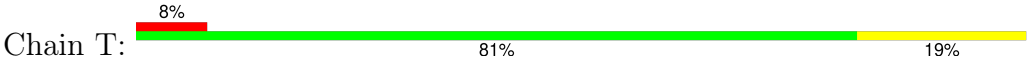
• Molecule 8: Cytochrome aa3 subunit 2

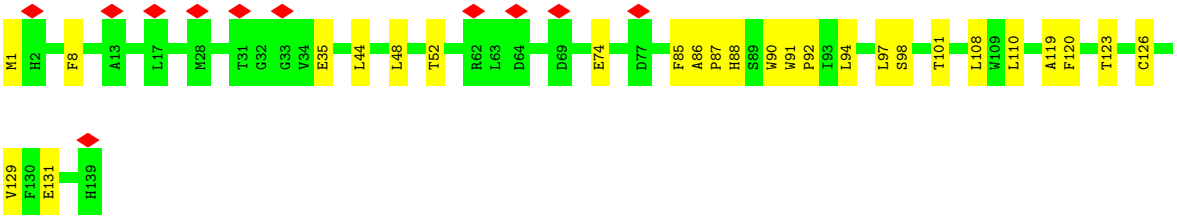
Chain K:



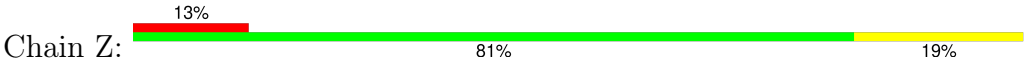


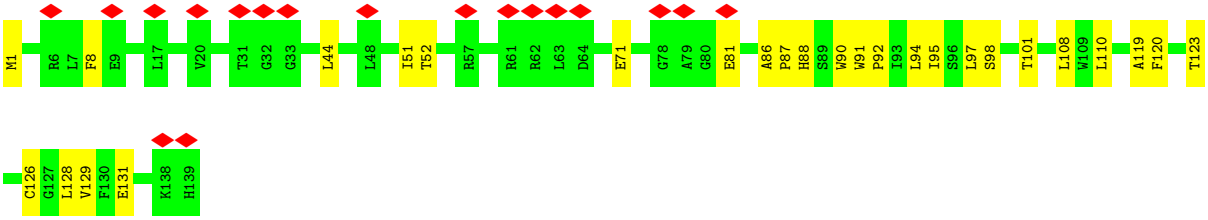
• Molecule 9: Cytochrome c oxidase polypeptide 4



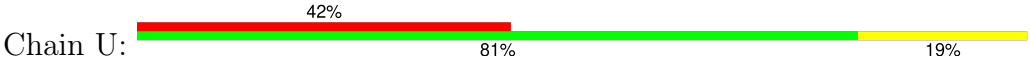


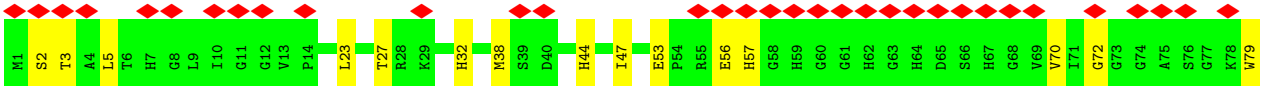
• Molecule 9: Cytochrome c oxidase polypeptide 4



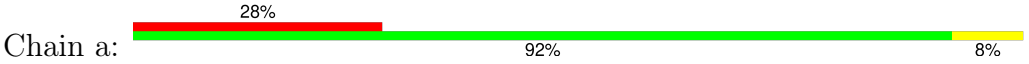


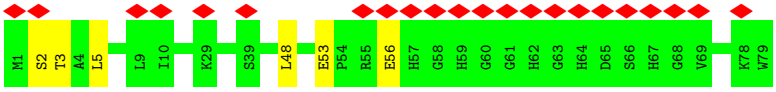
• Molecule 10: Cytochrome c oxidase subunit CtaJ



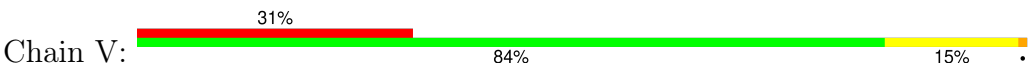


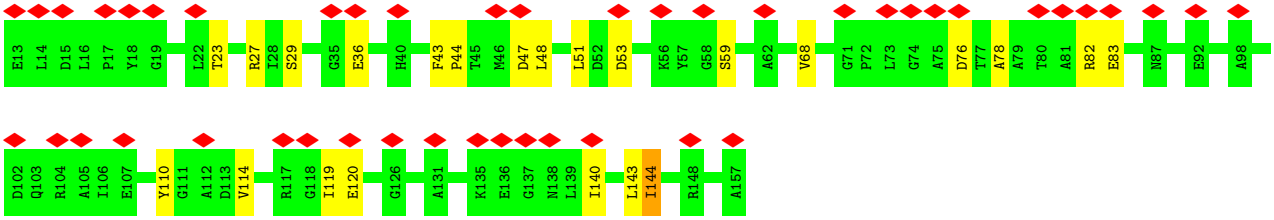
• Molecule 10: Cytochrome c oxidase subunit CtaJ





• Molecule 11: Uncharacterized protein MSMEG_4692/MSMEI_4575

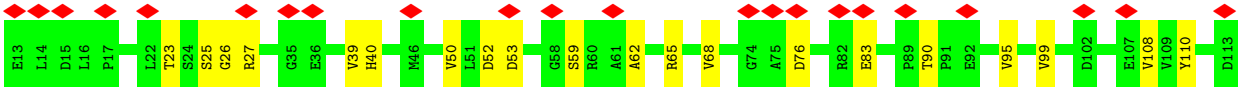




• Molecule 11: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain b:

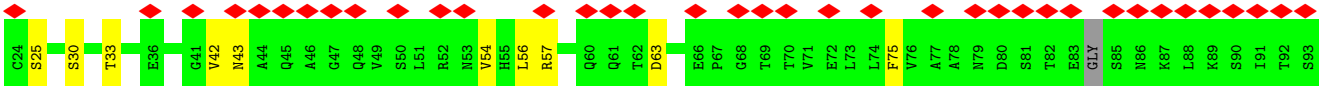




• Molecule 12: LpqE protein

Chain c:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.300	Depositor
Minimum map value	-1.965	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.634	Depositor
Map size (Å)	339.9, 339.9, 339.9	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

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: 9XX, HEM, 9YF, CDL, HEA, HEC, MQ9, PLM, FES, CU, 9Y0

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	I	0.18	0/1660	0.39	0/2250
1	O	0.95	1/1563 (0.1%)	1.49	12/2117 (0.6%)
2	L	0.17	0/4530	0.34	0/6188
2	R	0.17	0/4530	0.33	0/6188
3	M	0.17	0/3056	0.34	0/4142
3	Y	0.18	0/3056	0.33	0/4142
4	S	0.17	0/1608	0.32	0/2195
4	X	0.18	0/1608	0.32	0/2195
5	E	0.19	0/4314	0.35	0/5882
5	F	0.18	0/4314	0.34	0/5882
6	J	0.15	0/757	0.29	0/1027
6	P	0.15	0/757	0.29	0/1027
7	D	0.14	0/1099	0.33	0/1519
7	G	0.13	0/1099	0.34	0/1519
8	K	0.18	0/2534	0.37	0/3451
8	Q	0.19	0/2534	0.36	0/3451
9	T	0.15	0/1112	0.31	0/1524
9	Z	0.17	0/1112	0.31	0/1524
10	U	0.12	0/613	0.27	0/836
10	a	0.12	0/613	0.28	0/836
11	V	0.16	0/1059	0.34	0/1446
11	b	0.15	0/1059	0.35	0/1446
12	c	0.13	0/1166	0.33	0/1599
All	All	0.24	1/45753 (0.0%)	0.43	12/62386 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	208	PRO	C-O	-5.37	1.17	1.23

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	177	VAL	N-CA-C	-8.02	104.94	112.96
1	O	221	ALA	N-CA-C	-7.99	101.87	111.69
1	O	88	VAL	N-CA-C	-7.66	102.66	113.07
1	O	196	GLY	N-CA-C	-6.42	106.06	115.63
1	O	87	CYS	CB-CA-C	-5.89	101.48	111.02

There are no chirality outliers.

There are no planarity outliers.

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	I	1623	1564	1564	43	0
1	O	1531	1483	1484	208	0
2	L	4370	4347	4346	104	0
2	R	4370	4346	4345	106	0
3	M	2977	2984	2984	44	0
3	Y	2977	2984	2984	48	0
4	S	1560	1548	1547	64	0
4	X	1560	1548	1547	82	0
5	E	4181	4203	4202	81	0
5	F	4181	4200	4199	85	0
6	J	736	718	717	14	0
6	P	736	717	717	10	0
7	D	1092	640	640	3	0
7	G	1092	640	640	1	0
8	K	2465	2392	2392	39	0
8	Q	2465	2391	2391	70	0
9	T	1077	1059	1058	62	0
9	Z	1077	1058	1058	65	0
10	U	591	576	576	10	0
10	a	591	576	576	5	0
11	V	1041	1052	1052	18	0
11	b	1041	1052	1052	18	0
12	c	1149	1110	1110	20	0
13	I	86	64	64	13	0
13	O	86	64	64	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	E	58	84	0	0	0
14	I	58	84	0	0	0
14	O	58	84	0	0	0
14	Y	116	168	0	0	0
15	E	116	160	160	5	0
15	F	116	160	160	4	0
15	I	58	80	80	1	0
15	O	58	80	80	1	0
15	T	58	80	80	0	0
15	Z	58	80	80	3	0
16	K	2	0	0	0	0
16	L	1	0	0	0	0
16	Q	2	0	0	0	0
16	R	1	0	0	0	0
17	L	120	108	108	4	0
17	R	120	108	108	4	0
18	E	152	0	192	14	0
18	F	152	0	192	23	0
18	J	76	0	96	12	0
18	L	76	0	96	25	0
18	P	76	0	96	10	0
18	R	76	0	96	17	0
18	S	76	0	96	49	0
18	T	228	0	288	76	0
18	X	152	0	192	96	0
18	Z	152	0	192	77	0
19	M	4	0	0	0	0
19	Y	4	0	0	1	0
20	F	49	74	0	0	0
20	J	98	150	0	0	0
20	S	49	75	0	0	0
20	X	49	75	0	0	0
21	E	85	57	57	4	0
21	F	85	57	57	5	0
22	D	11	16	16	0	0
22	G	11	16	16	0	0
22	c	17	31	31	1	0
23	D	32	51	0	0	0
23	G	32	51	0	0	0
23	c	42	73	0	0	0
All	All	47439	45318	45878	1170	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 13.

The worst 5 of 1170 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)
4:X:166:LYS:NZ	18:X:302:CDL:H112	1.28	1.48
9:T:120:PHE:CB	18:T:201:CDL:H612	1.47	1.42
1:O:203:SER:CB	8:Q:170:ARG:HG3	1.46	1.41
9:T:120:PHE:HB3	18:T:201:CDL:C61	1.50	1.41
9:Z:120:PHE:CB	18:Z:202:CDL:H612	1.53	1.38

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 PDB entries followed by that with respect to all EM entries.

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	I	221/223 (99%)	199 (90%)	22 (10%)	0	100 100
1	O	206/223 (92%)	187 (91%)	16 (8%)	3 (2%)	8 37
2	L	550/552 (100%)	516 (94%)	34 (6%)	0	100 100
2	R	550/552 (100%)	518 (94%)	32 (6%)	0	100 100
3	M	380/382 (100%)	344 (90%)	36 (10%)	0	100 100
3	Y	380/382 (100%)	347 (91%)	33 (9%)	0	100 100
4	S	201/203 (99%)	193 (96%)	8 (4%)	0	100 100
4	X	201/203 (99%)	192 (96%)	9 (4%)	0	100 100
5	E	533/535 (100%)	490 (92%)	43 (8%)	0	100 100
5	F	533/535 (100%)	489 (92%)	43 (8%)	1 (0%)	43 74
6	J	88/100 (88%)	85 (97%)	3 (3%)	0	100 100
6	P	88/100 (88%)	83 (94%)	5 (6%)	0	100 100
7	D	214/216 (99%)	193 (90%)	20 (9%)	1 (0%)	24 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	214/216 (99%)	187 (87%)	27 (13%)	0	100 100
8	K	310/312 (99%)	282 (91%)	28 (9%)	0	100 100
8	Q	310/312 (99%)	282 (91%)	28 (9%)	0	100 100
9	T	137/139 (99%)	129 (94%)	8 (6%)	0	100 100
9	Z	137/139 (99%)	130 (95%)	7 (5%)	0	100 100
10	U	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9 39
10	a	77/79 (98%)	70 (91%)	7 (9%)	0	100 100
11	V	143/145 (99%)	139 (97%)	4 (3%)	0	100 100
11	b	143/145 (99%)	138 (96%)	5 (4%)	0	100 100
12	c	154/159 (97%)	135 (88%)	19 (12%)	0	100 100
All	All	5847/5931 (99%)	5398 (92%)	443 (8%)	6 (0%)	49 79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	226	PRO
5	F	135	ARG
1	O	202	SER
1	O	249	VAL
7	D	27	THR

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 PDB entries followed by that with respect to all EM entries.

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	I	163/163 (100%)	160 (98%)	3 (2%)	51 69
1	O	155/163 (95%)	111 (72%)	44 (28%)	0 2
2	L	452/453 (100%)	445 (98%)	7 (2%)	57 71
2	R	452/453 (100%)	447 (99%)	5 (1%)	65 74
3	M	312/312 (100%)	310 (99%)	2 (1%)	78 79
3	Y	312/312 (100%)	309 (99%)	3 (1%)	68 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	S	155/161 (96%)	153 (99%)	2 (1%)	61	72
4	X	155/161 (96%)	152 (98%)	3 (2%)	50	68
5	E	429/429 (100%)	424 (99%)	5 (1%)	63	73
5	F	429/429 (100%)	424 (99%)	5 (1%)	63	73
6	J	76/83 (92%)	73 (96%)	3 (4%)	28	54
6	P	76/83 (92%)	75 (99%)	1 (1%)	61	72
7	D	20/151 (13%)	20 (100%)	0	100	100
7	G	20/151 (13%)	20 (100%)	0	100	100
8	K	260/266 (98%)	257 (99%)	3 (1%)	63	73
8	Q	260/266 (98%)	258 (99%)	2 (1%)	73	77
9	T	106/106 (100%)	106 (100%)	0	100	100
9	Z	106/106 (100%)	106 (100%)	0	100	100
10	U	59/59 (100%)	59 (100%)	0	100	100
10	a	59/59 (100%)	59 (100%)	0	100	100
11	V	107/107 (100%)	105 (98%)	2 (2%)	50	68
11	b	107/107 (100%)	106 (99%)	1 (1%)	70	76
12	c	127/127 (100%)	126 (99%)	1 (1%)	73	77
All	All	4397/4707 (93%)	4305 (98%)	92 (2%)	46	66

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	516	GLU
6	J	43	MET
5	F	137	ARG
2	L	390	ASP
11	V	83	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
8	K	265	GLN
10	a	64	HIS
9	Z	139	HIS
12	c	31	GLN

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Mol	Chain	Res	Type
5	F	110	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 6 are monoatomic - leaving 54 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	$\#\|Z\| > 2$
13	HEC	O	302	1	50,50,50	2.95	30 (60%)	68,82,82	2.58	29 (42%)
15	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.63	16 (21%)
18	CDL	E	606	-	75,75,99	0.34	0	81,87,111	0.42	0
15	MQ9	F	707	-	59,59,59	2.43	22 (37%)	73,75,75	1.54	15 (20%)
17	HEA	L	602	2	67,67,67	1.42	11 (16%)	81,103,103	2.38	30 (37%)
15	MQ9	F	701	-	59,59,59	2.45	23 (38%)	73,75,75	1.38	15 (20%)
18	CDL	T	201	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
14	9YF	Y	503	-	58,58,58	1.13	8 (13%)	68,71,71	1.49	9 (13%)
18	CDL	T	202	-	75,75,99	0.33	0	81,87,111	0.40	0
23	9XX	D	302	-	31,31,41	1.11	3 (9%)	34,34,44	1.44	4 (11%)
15	MQ9	I	303	-	59,59,59	2.39	22 (37%)	73,75,75	1.43	17 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	9YF	I	304	-	58,58,58	1.08	5 (8%)	68,71,71	1.07	2 (2%)
18	CDL	J	203	-	75,75,99	0.33	0	81,87,111	0.45	0
15	MQ9	E	603	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	14 (19%)
18	CDL	F	706	-	75,75,99	0.37	0	81,87,111	0.46	1 (1%)
22	PLM	G	301	7	9,10,17	0.54	0	8,9,17	0.43	0
20	9Y0	S	301	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
18	CDL	Z	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
23	9XX	c	202	18,12	41,41,41	0.96	3 (7%)	44,44,44	1.18	4 (9%)
21	HEM	F	703	5	50,50,50	1.40	6 (12%)	67,82,82	1.11	3 (4%)
20	9Y0	J	201	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
22	PLM	D	301	7	9,10,17	0.53	0	8,9,17	0.43	0
14	9YF	O	303	-	58,58,58	1.03	5 (8%)	68,71,71	1.06	3 (4%)
15	MQ9	E	604	-	59,59,59	2.42	22 (37%)	73,75,75	1.53	16 (21%)
15	MQ9	T	204	-	59,59,59	2.39	22 (37%)	73,75,75	1.59	16 (21%)
17	HEA	R	603	2	67,67,67	1.37	10 (14%)	81,103,103	2.04	18 (22%)
19	FES	M	501	3	0,4,4	-	-	-		
18	CDL	F	705	-	75,75,99	0.34	0	81,87,111	0.42	0
19	FES	Y	501	3	0,4,4	-	-	-		
13	HEC	O	301	-	50,50,50	2.90	27 (54%)	68,82,82	2.73	34 (50%)
18	CDL	T	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
21	HEM	E	601	5	49,49,50	1.38	7 (14%)	67,81,82	1.05	2 (2%)
17	HEA	L	603	2	67,67,67	1.37	10 (14%)	81,103,103	1.92	19 (23%)
18	CDL	X	302	-	75,75,99	0.33	0	81,87,111	0.40	0
18	CDL	Z	202	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
20	9Y0	F	704	5	48,48,48	1.17	3 (6%)	51,53,53	0.87	2 (3%)
20	9Y0	J	202	-	48,48,48	1.16	3 (6%)	51,53,53	0.78	2 (3%)
15	MQ9	O	304	-	59,59,59	2.40	22 (37%)	73,75,75	1.43	17 (23%)
18	CDL	E	607	-	75,75,99	0.36	0	81,87,111	0.42	0
17	HEA	R	602	2	67,67,67	1.44	10 (14%)	81,103,103	2.33	31 (38%)
13	HEC	I	301	-	50,50,50	1.78	5 (10%)	68,82,82	1.32	5 (7%)
18	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.60	2 (2%)
18	CDL	L	604	23	75,75,99	0.33	0	81,87,111	0.60	2 (2%)
13	HEC	I	302	1	50,50,50	1.73	6 (12%)	68,82,82	1.65	11 (16%)
20	9Y0	X	301	-	48,48,48	1.16	3 (6%)	51,53,53	0.90	2 (3%)
22	PLM	c	201	12	15,16,17	0.47	0	14,15,17	0.35	0
14	9YF	Y	502	-	58,58,58	1.09	6 (10%)	68,71,71	1.29	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	HEM	F	702	5	49,49,50	1.37	5 (10%)	67,81,82	1.03	2 (2%)
18	CDL	S	302	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
18	CDL	P	201	-	75,75,99	0.33	0	81,87,111	0.45	0
14	9YF	E	605	-	58,58,58	1.02	5 (8%)	68,71,71	1.32	7 (10%)
18	CDL	X	303	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
23	9XX	G	302	7	31,31,41	1.12	3 (9%)	34,34,44	1.47	5 (14%)
21	HEM	E	602	5	50,50,50	1.42	7 (14%)	67,82,82	1.14	5 (7%)

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
13	HEC	O	302	1	1/1/7/7	10/14/54/54	-
15	MQ9	Z	201	-	-	11/53/73/73	0/2/2/2
18	CDL	E	606	-	-	49/86/86/110	-
15	MQ9	F	707	-	-	12/53/73/73	0/2/2/2
17	HEA	L	602	2	-	12/36/76/76	-
15	MQ9	F	701	-	-	6/53/73/73	0/2/2/2
18	CDL	T	201	-	-	34/86/86/110	-
14	9YF	Y	503	-	-	22/54/78/78	0/1/1/1
18	CDL	T	202	-	-	46/86/86/110	-
23	9XX	D	302	-	-	9/33/33/43	-
15	MQ9	I	303	-	-	8/53/73/73	0/2/2/2
14	9YF	I	304	-	-	22/54/78/78	0/1/1/1
18	CDL	J	203	-	-	48/86/86/110	-
15	MQ9	E	603	-	-	6/53/73/73	0/2/2/2
18	CDL	F	706	-	-	43/86/86/110	-
22	PLM	G	301	7	-	2/8/8/15	-
20	9Y0	S	301	-	-	19/52/52/52	-
18	CDL	Z	203	-	-	38/86/86/110	-
23	9XX	c	202	18,12	-	16/43/43/43	-
21	HEM	F	703	5	-	0/14/54/54	-
20	9Y0	J	201	-	-	19/52/52/52	-
22	PLM	D	301	7	-	3/8/8/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	9YF	O	303	-	-	29/54/78/78	0/1/1/1
15	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
15	MQ9	T	204	-	-	13/53/73/73	0/2/2/2
17	HEA	R	603	2	-	3/36/76/76	-
21	HEM	E	601	5	-	2/12/52/54	-
18	CDL	F	705	-	-	49/86/86/110	-
19	FES	M	501	3	-	-	0/1/1/1
13	HEC	O	301	-	1/1/7/7	7/14/54/54	-
18	CDL	T	203	-	-	38/86/86/110	-
19	FES	Y	501	3	-	-	0/1/1/1
17	HEA	L	603	2	-	3/36/76/76	-
18	CDL	X	302	-	-	46/86/86/110	-
18	CDL	Z	202	-	-	34/86/86/110	-
20	9Y0	F	704	5	-	16/52/52/52	-
20	9Y0	J	202	-	-	25/52/52/52	-
15	MQ9	O	304	-	-	7/53/73/73	0/2/2/2
18	CDL	E	607	-	-	40/86/86/110	-
17	HEA	R	602	2	-	7/36/76/76	-
13	HEC	I	301	-	-	6/14/54/54	-
18	CDL	R	604	-	-	47/86/86/110	-
18	CDL	L	604	23	-	47/86/86/110	-
13	HEC	I	302	1	1/1/7/7	5/14/54/54	-
20	9Y0	X	301	-	-	17/52/52/52	-
22	PLM	c	201	12	-	5/14/14/15	-
14	9YF	Y	502	-	-	22/54/78/78	0/1/1/1
21	HEM	F	702	5	-	4/12/52/54	-
18	CDL	S	302	-	-	43/86/86/110	-
18	CDL	P	201	-	-	48/86/86/110	-
14	9YF	E	605	-	-	17/54/78/78	0/1/1/1
18	CDL	X	303	-	-	43/86/86/110	-
23	9XX	G	302	7	-	10/33/33/43	-
21	HEM	E	602	5	-	2/14/54/54	-

The worst 5 of 411 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	707	MQ9	C6-C5	8.77	1.50	1.35
15	E	604	MQ9	C6-C5	8.77	1.50	1.35
15	F	701	MQ9	C6-C5	8.59	1.50	1.35
15	E	603	MQ9	C6-C5	8.53	1.50	1.35
15	I	303	MQ9	C6-C5	8.49	1.50	1.35

The worst 5 of 439 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	203	CDL	CB6-CB4-CB3	-9.91	88.68	111.78
18	Z	203	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
18	X	303	CDL	CB6-CB4-CB3	-9.67	89.23	111.78
18	S	302	CDL	CB6-CB4-CB3	-9.66	89.26	111.78
18	T	201	CDL	OB6-CB4-CB6	9.23	141.46	108.34

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	O	301	HEC	NA
13	O	302	HEC	NA
13	I	302	HEC	NA

5 of 1081 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	302	HEC	C1A-C2A-CAA-CBA
13	I	302	HEC	C2B-C3B-CAB-CBB
13	I	302	HEC	C4B-C3B-CAB-CBB
14	O	303	9YF	C-C1-O-P
14	O	303	9YF	C9-C8-O9-C

There are no ring outliers.

35 monomers are involved in 442 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	O	302	HEC	35	0
15	Z	201	MQ9	3	0
18	E	606	CDL	10	0
15	F	707	MQ9	4	0
17	L	602	HEA	2	0
18	T	201	CDL	35	0
18	T	202	CDL	29	0

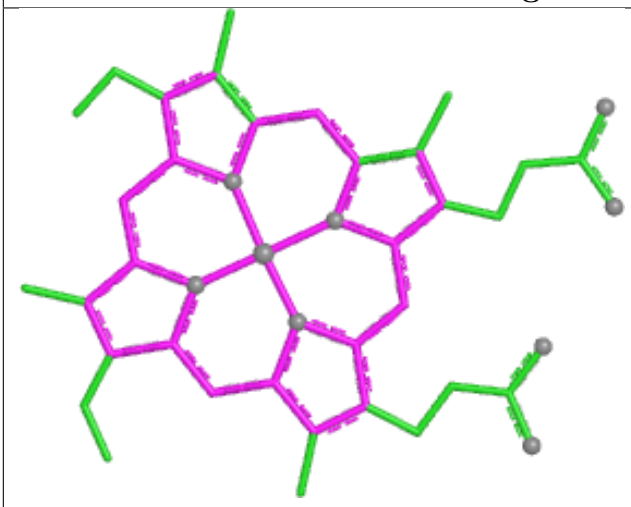
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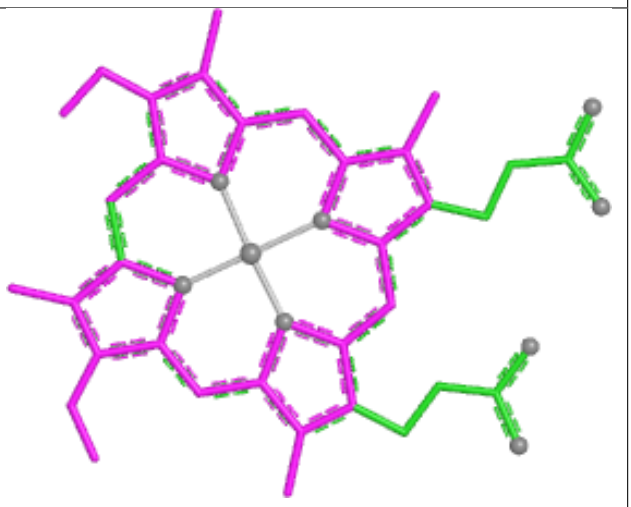
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	I	303	MQ9	1	0
18	J	203	CDL	12	0
15	E	603	MQ9	1	0
18	F	706	CDL	12	0
18	Z	203	CDL	42	0
21	F	703	HEM	4	0
15	E	604	MQ9	4	0
17	R	603	HEA	4	0
18	F	705	CDL	11	0
19	Y	501	FES	1	0
13	O	301	HEC	4	0
18	T	203	CDL	34	0
21	E	601	HEM	2	0
17	L	603	HEA	2	0
18	X	302	CDL	42	0
18	Z	202	CDL	35	0
15	O	304	MQ9	1	0
18	E	607	CDL	4	0
13	I	301	HEC	4	0
18	R	604	CDL	17	0
18	L	604	CDL	25	0
13	I	302	HEC	9	0
22	c	201	PLM	1	0
21	F	702	HEM	1	0
18	S	302	CDL	49	0
18	P	201	CDL	10	0
18	X	303	CDL	54	0
21	E	602	HEM	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.

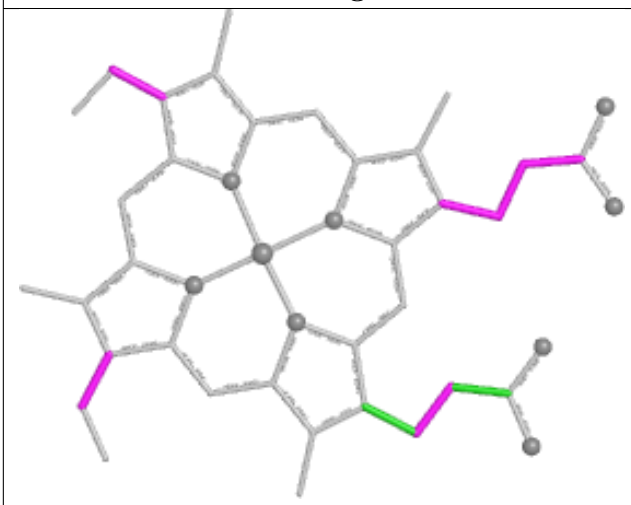
Ligand HEC O 302



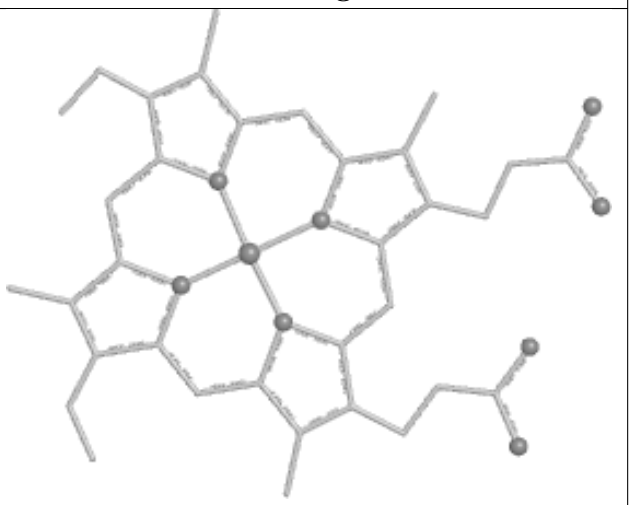
Bond lengths



Bond angles

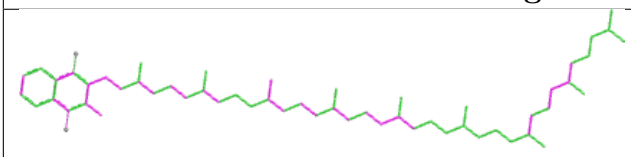


Torsions

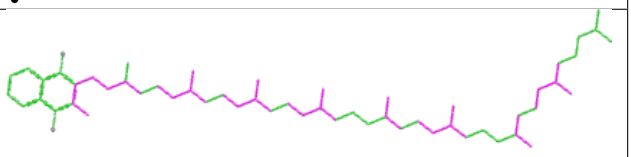


Rings

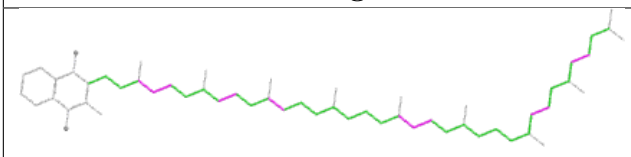
Ligand MQ9 Z 201



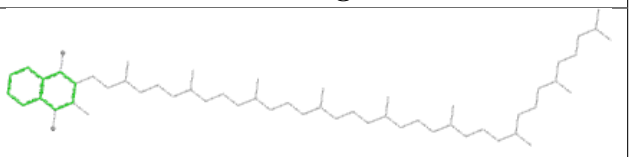
Bond lengths



Bond angles

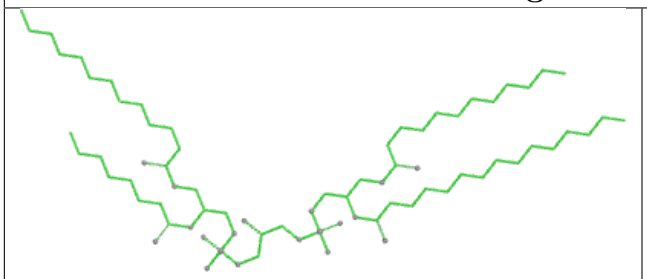


Torsions

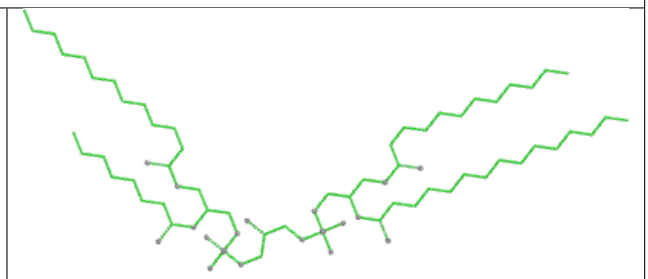


Rings

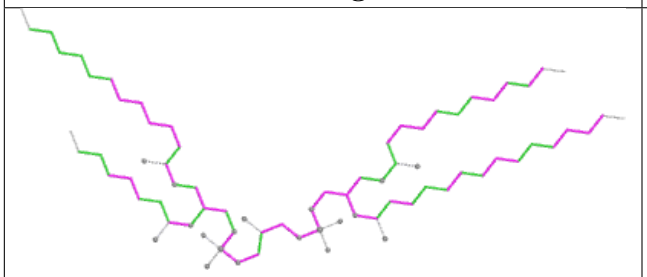
Ligand CDL E 606



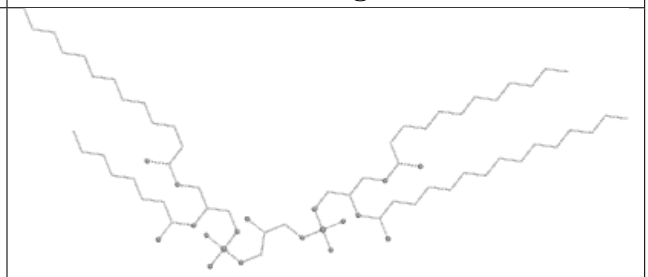
Bond lengths



Bond angles

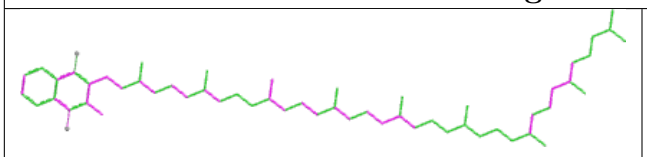


Torsions

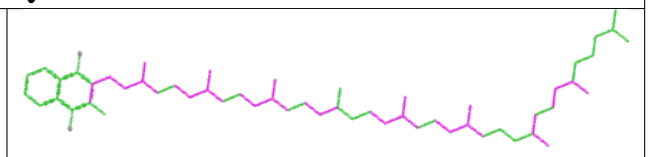


Rings

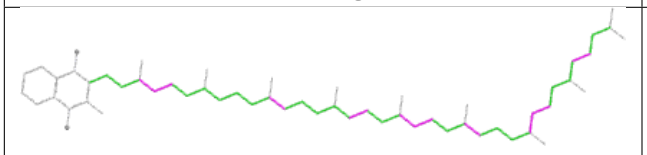
Ligand MQ9 F 707



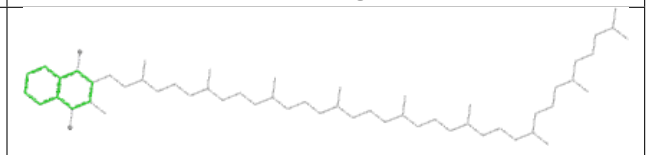
Bond lengths



Bond angles

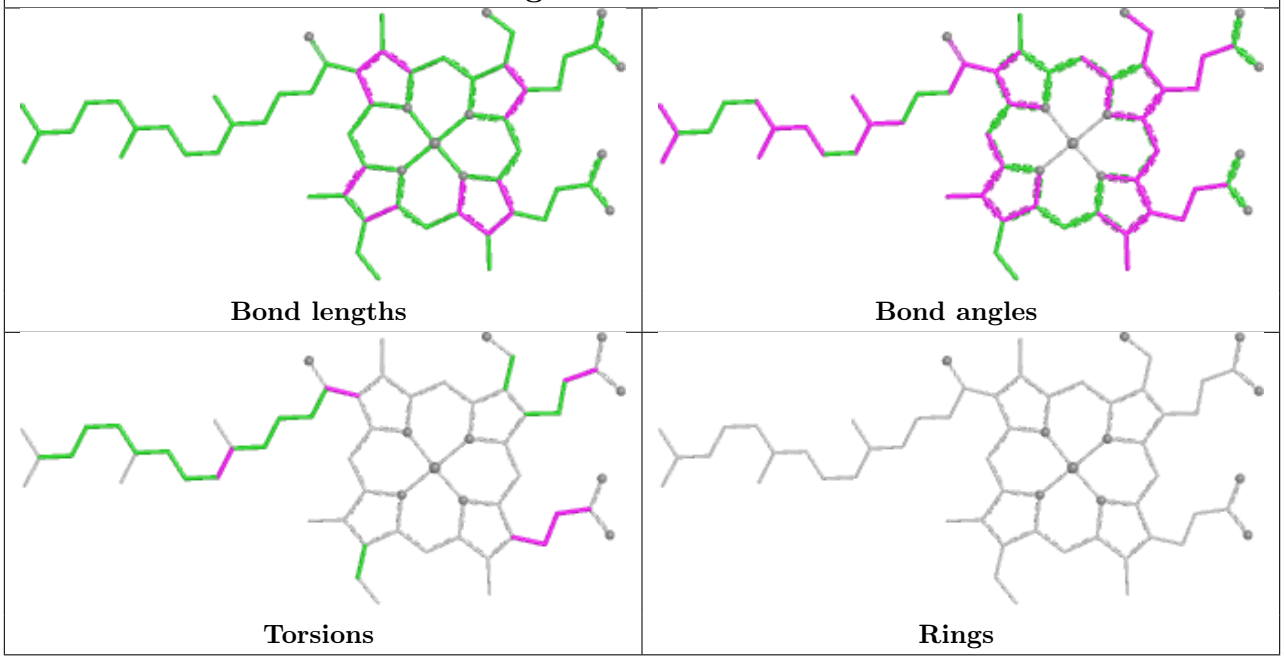


Torsions

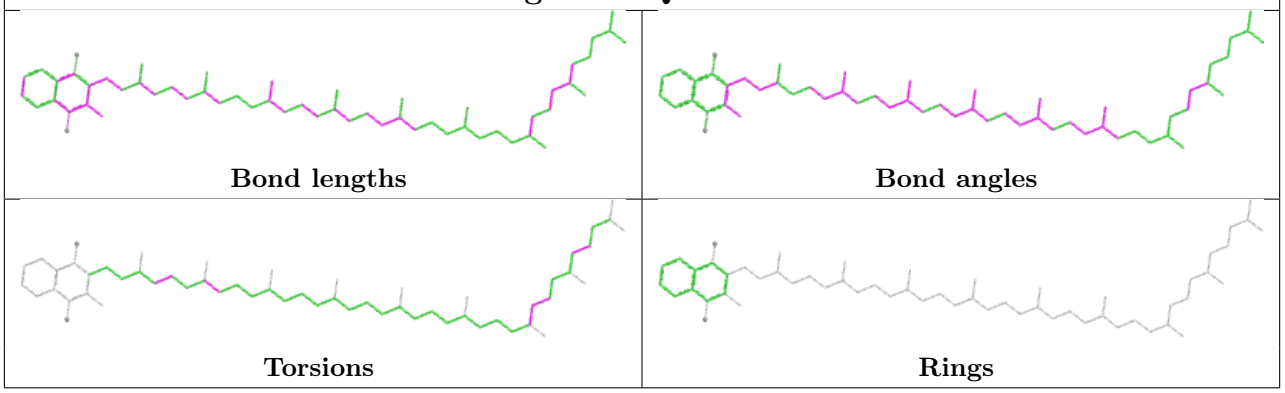


Rings

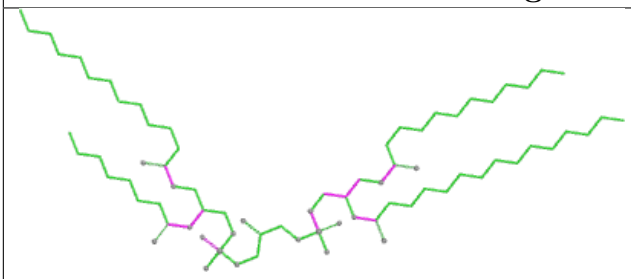
Ligand HEA L 602



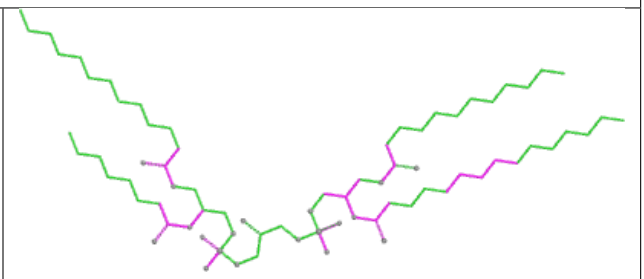
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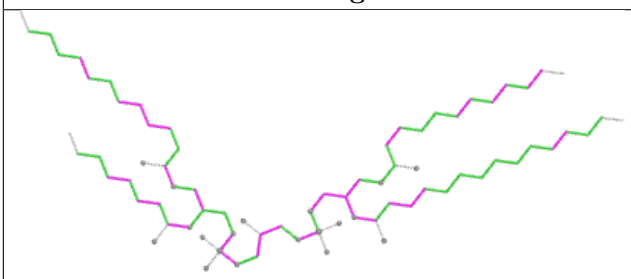
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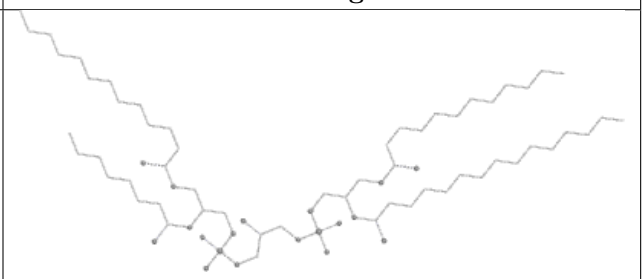
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Bond angles

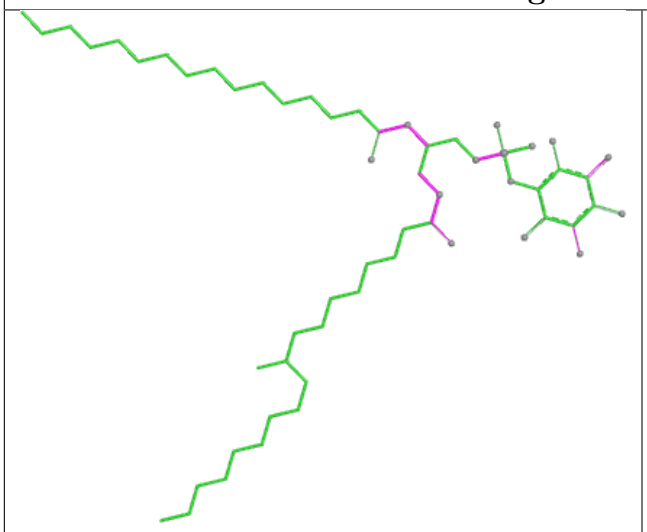


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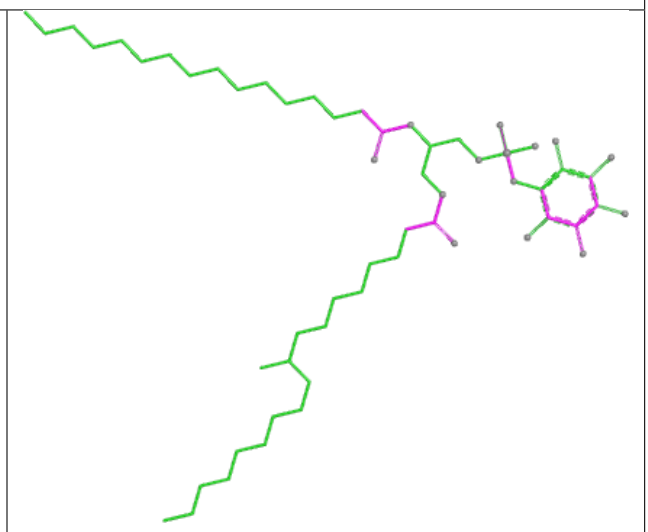


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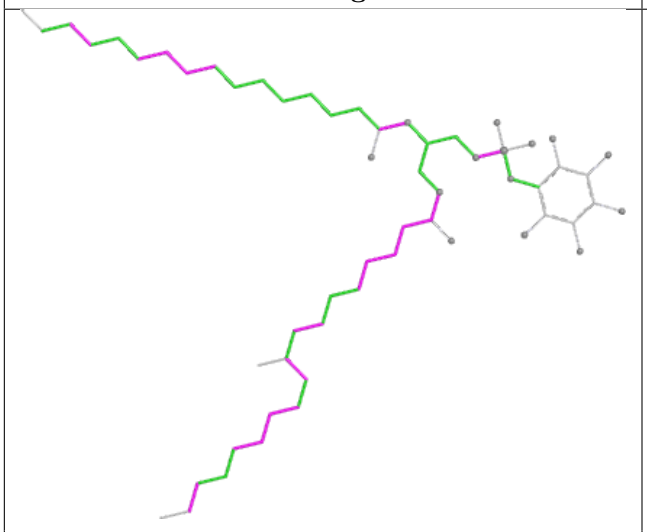
Ligand 9YF Y 503



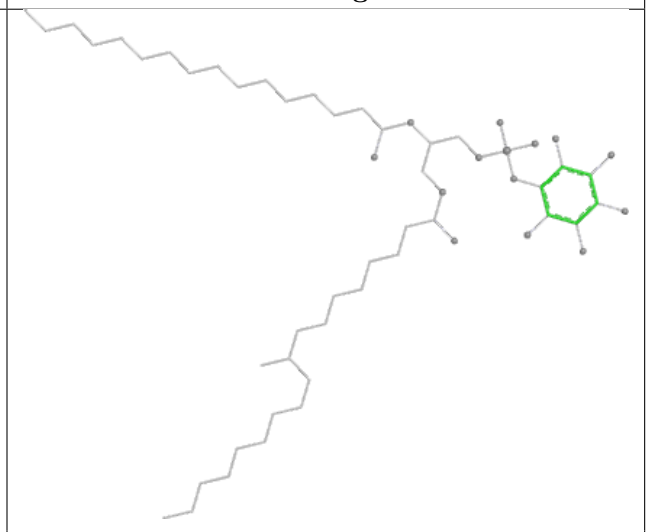
Bond lengths



Bond angles

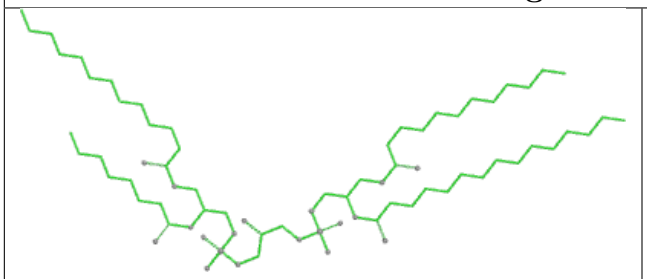


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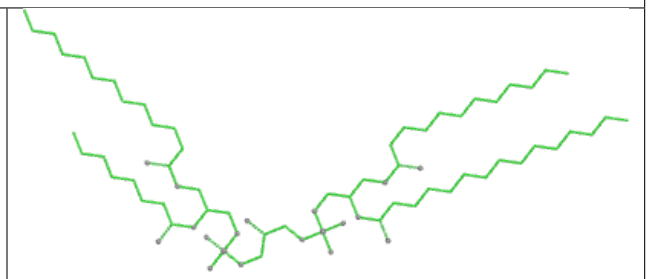


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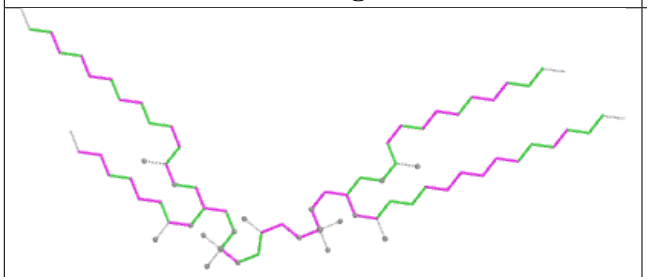
Ligand CDL T 202



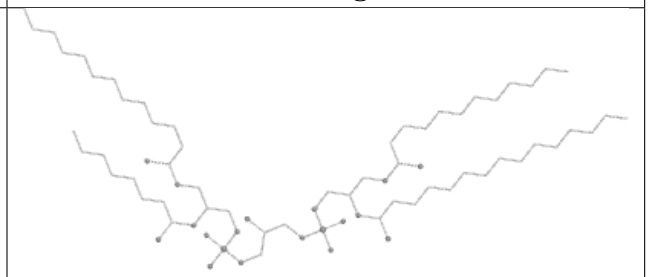
Bond lengths



Bond angles

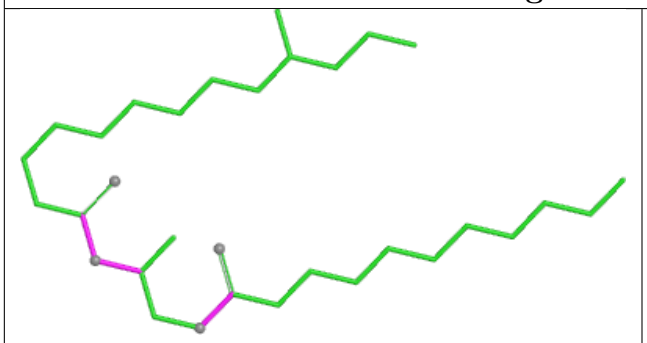


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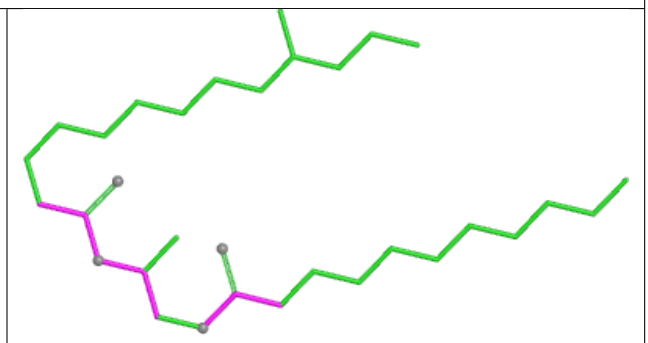


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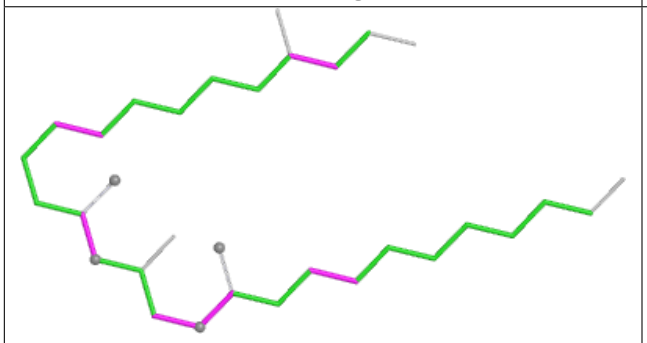
Ligand 9XX D 302



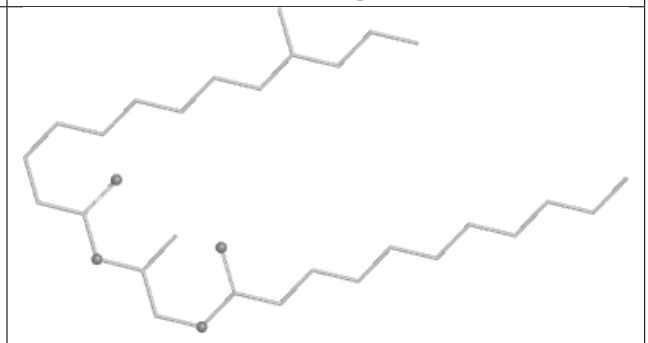
Bond lengths



Bond angles

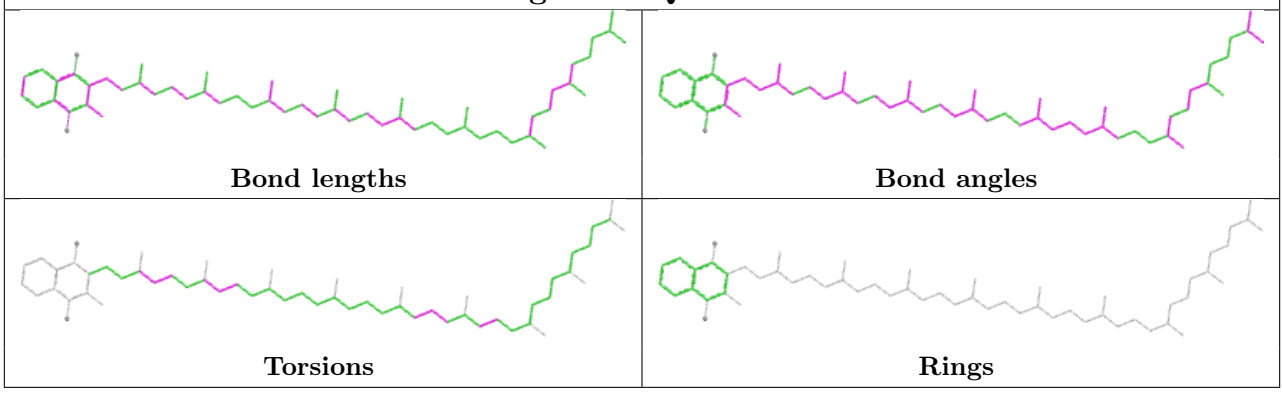


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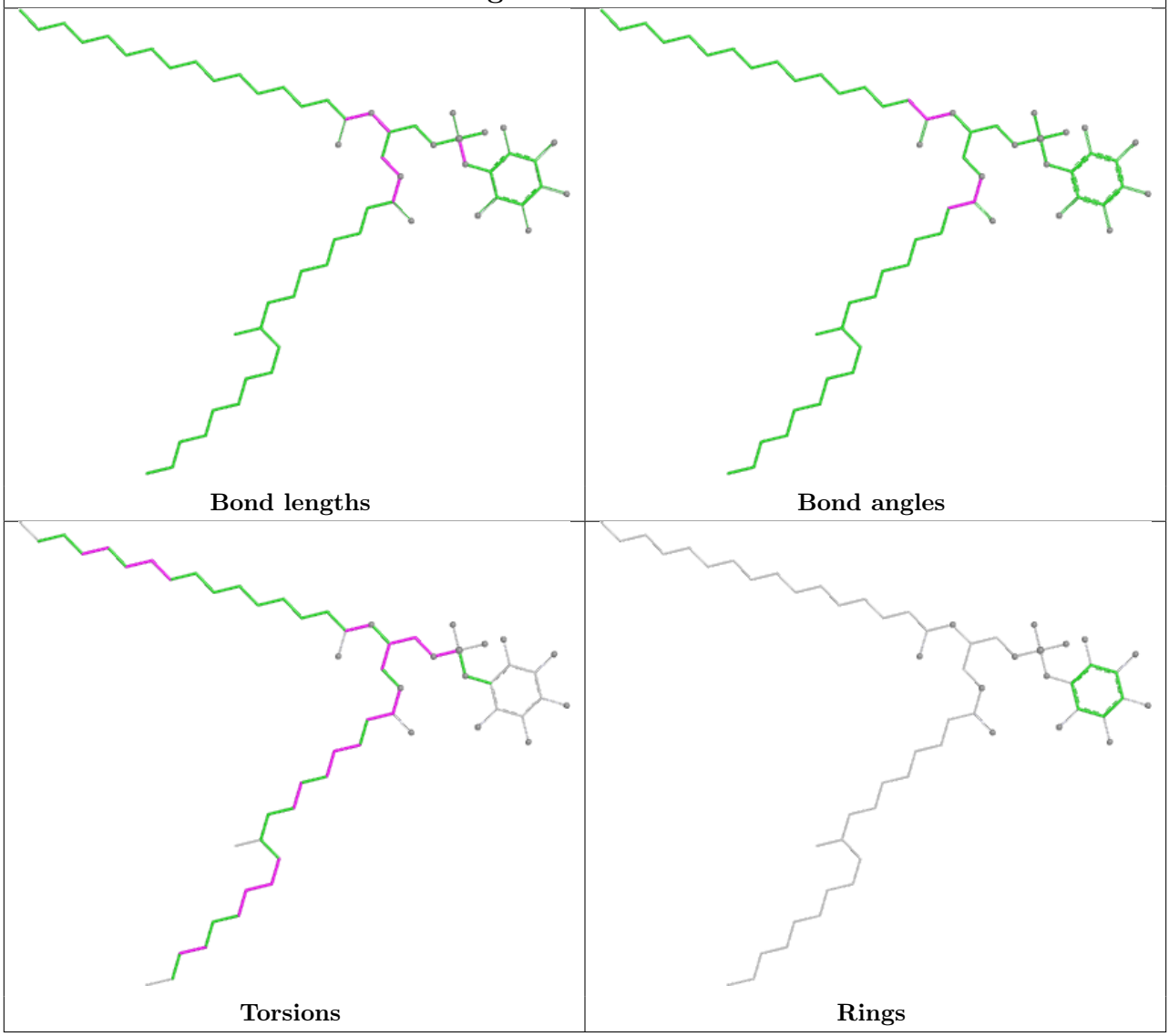


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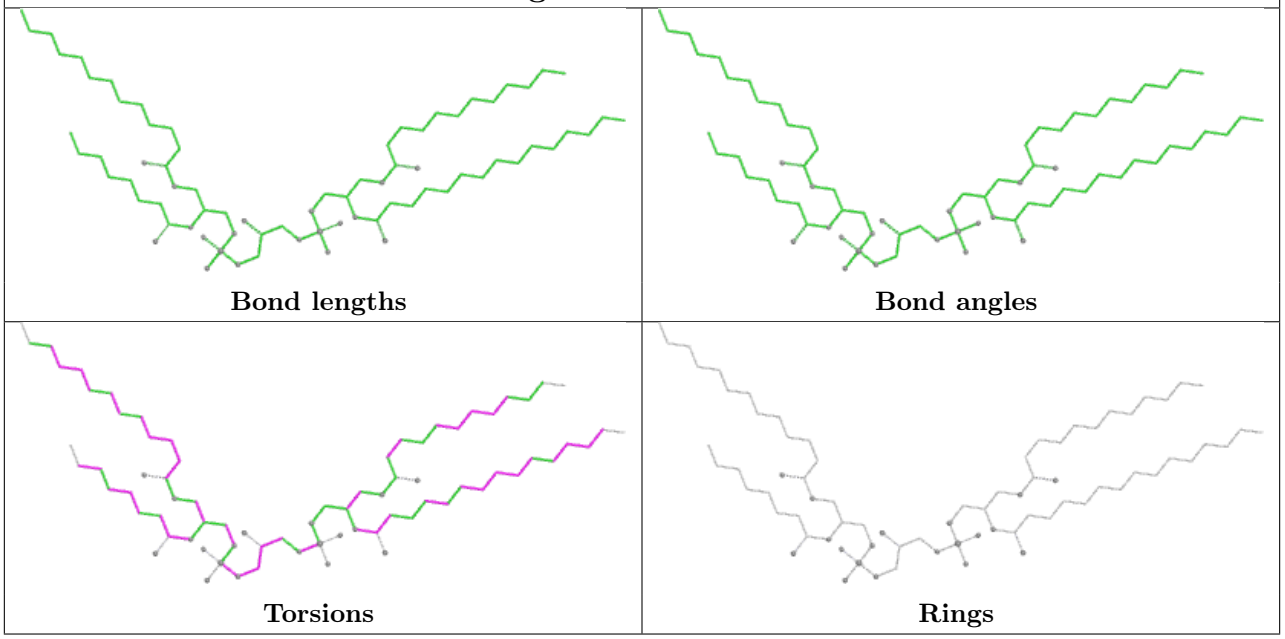
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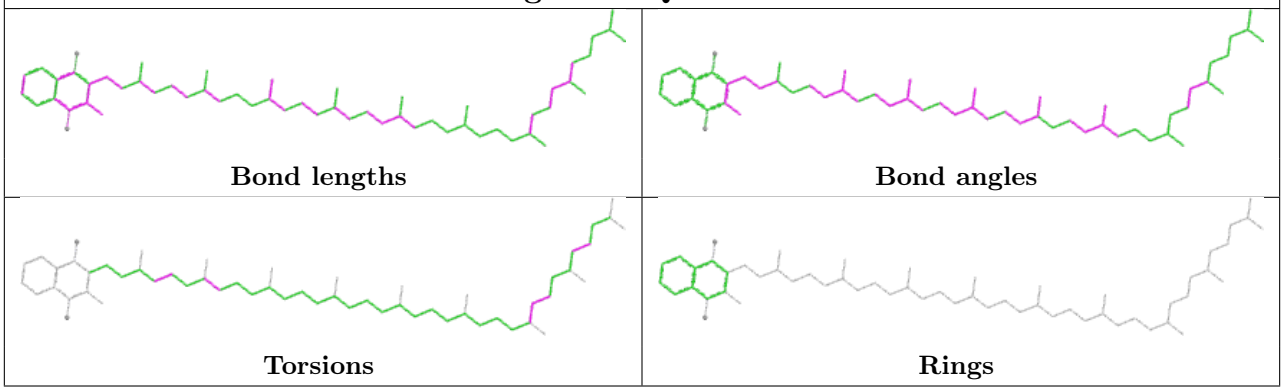
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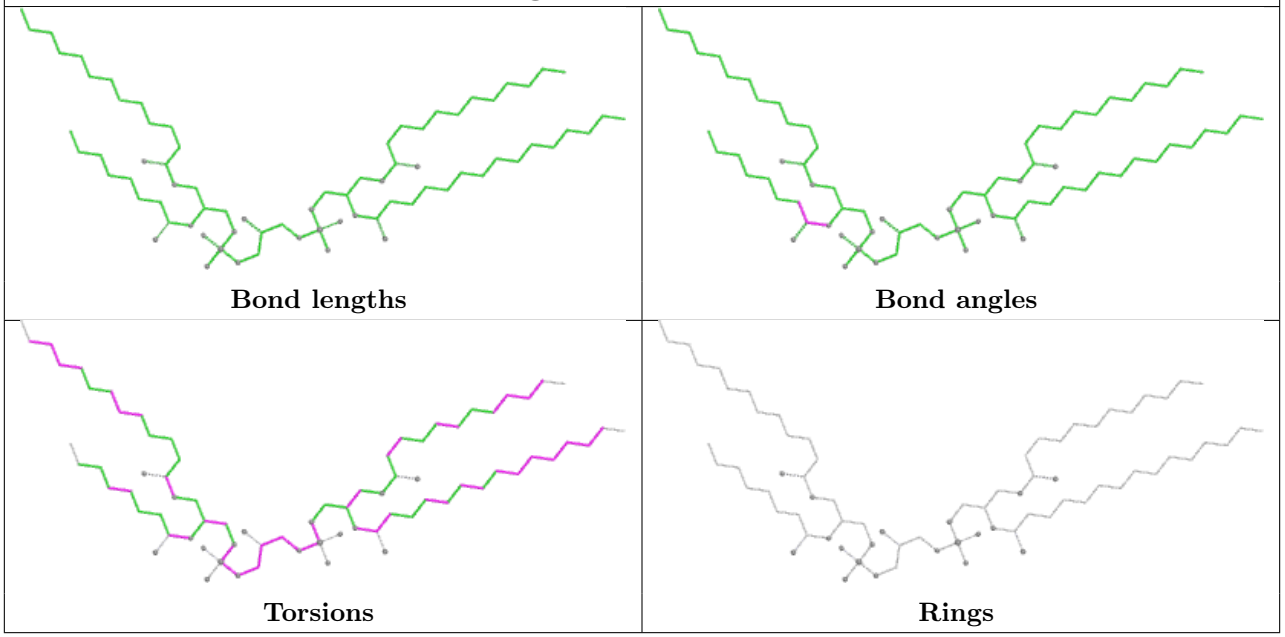
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Ligand MQ9 E 603



Ligand CDL F 706



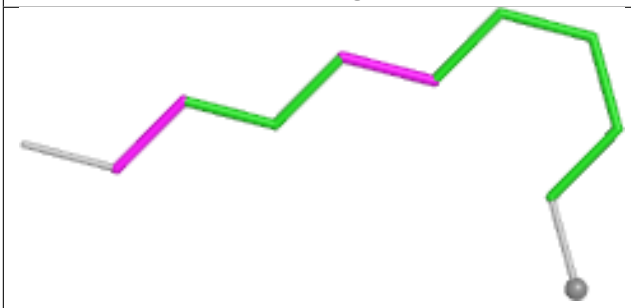
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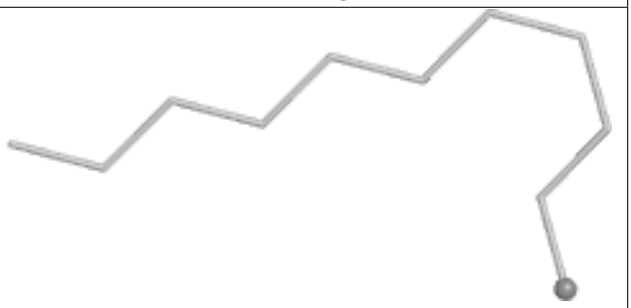
Bond lengths



Bond angles

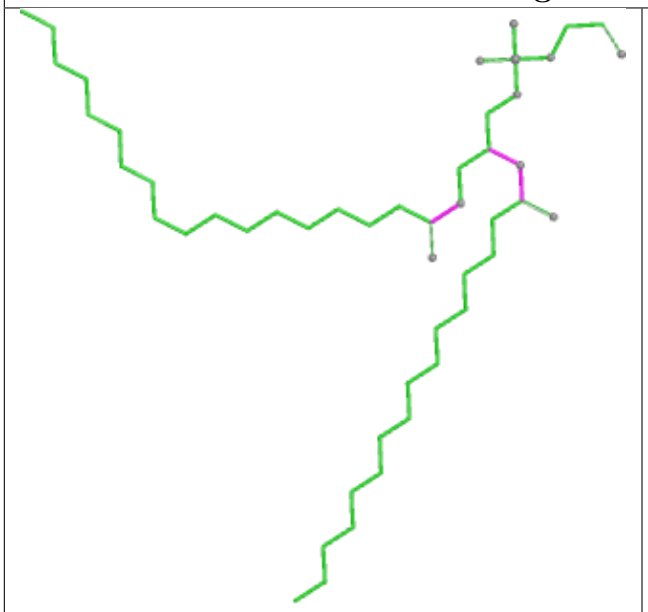


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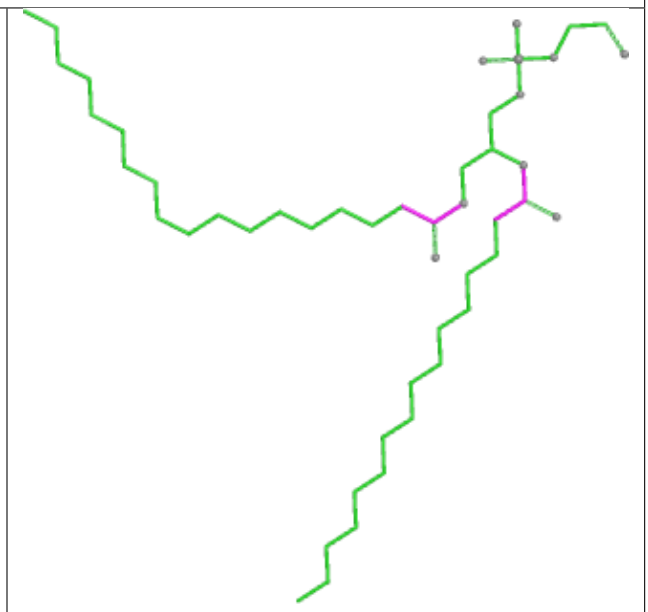


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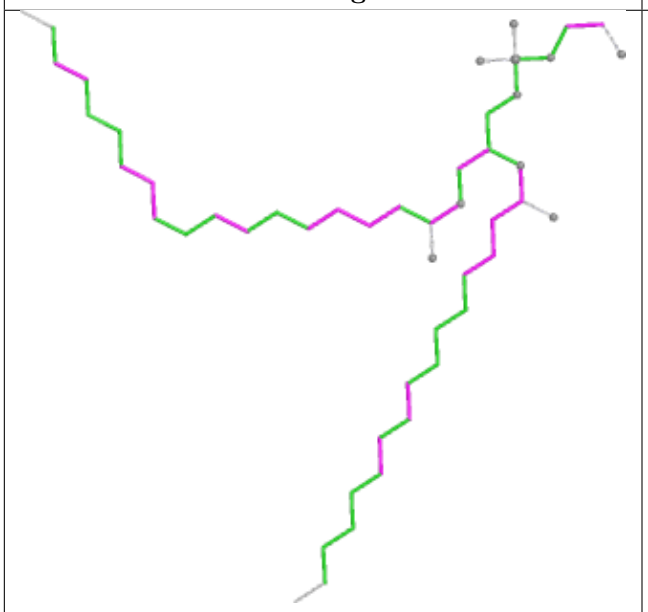
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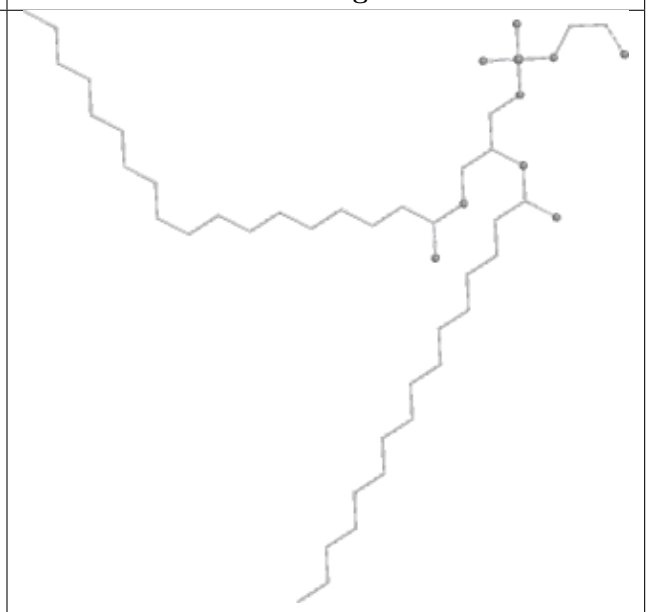
Bond lengths



Bond angles

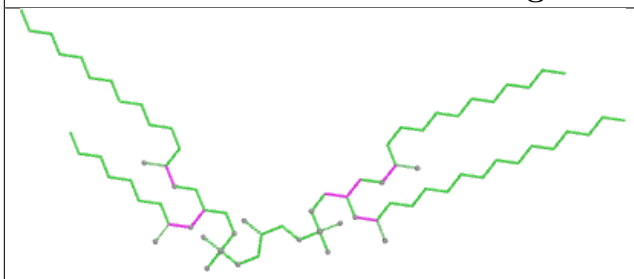


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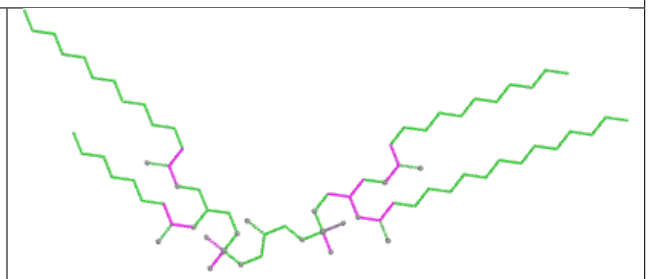


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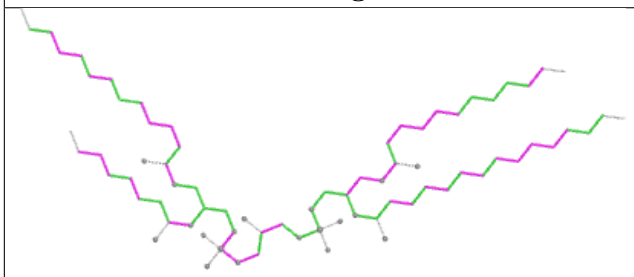
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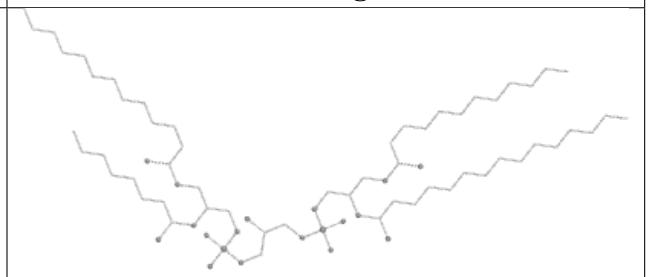
Bond lengths



Bond angles

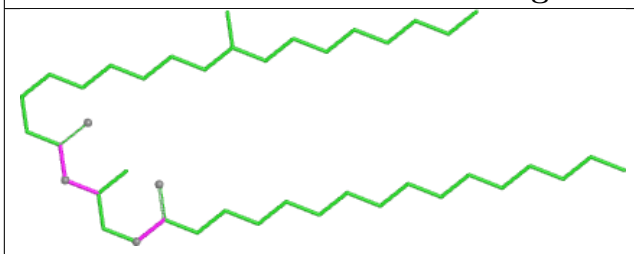


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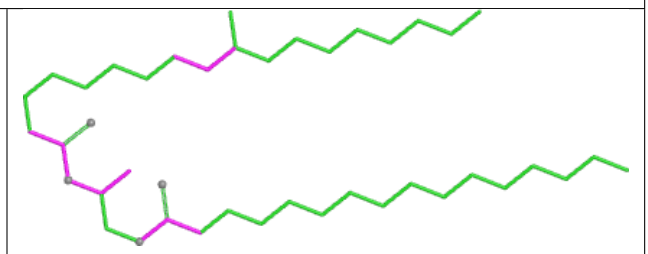


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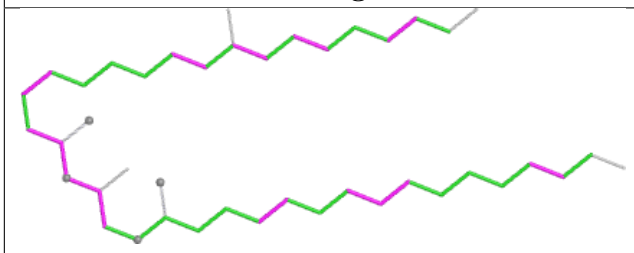
Ligand 9XX c 202



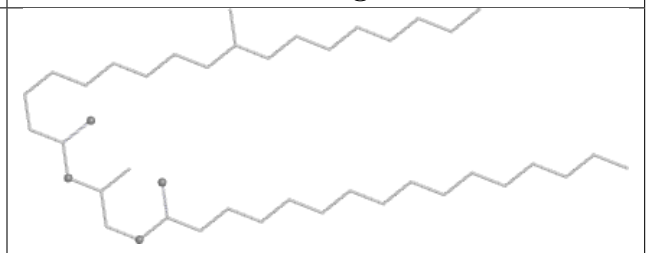
Bond lengths



Bond angles

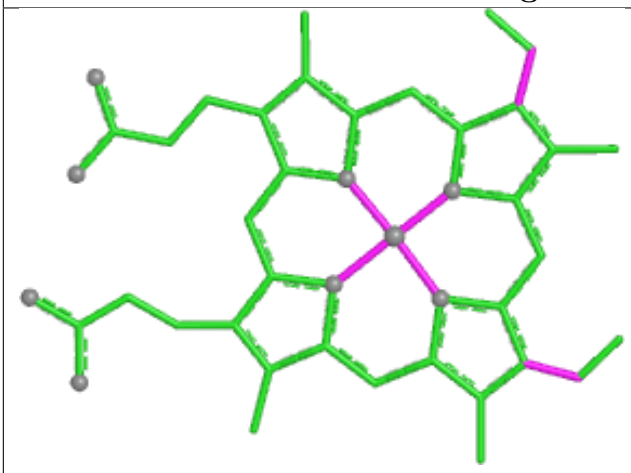


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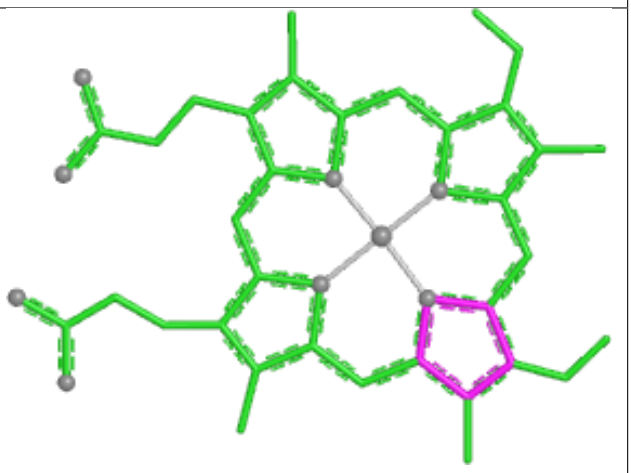


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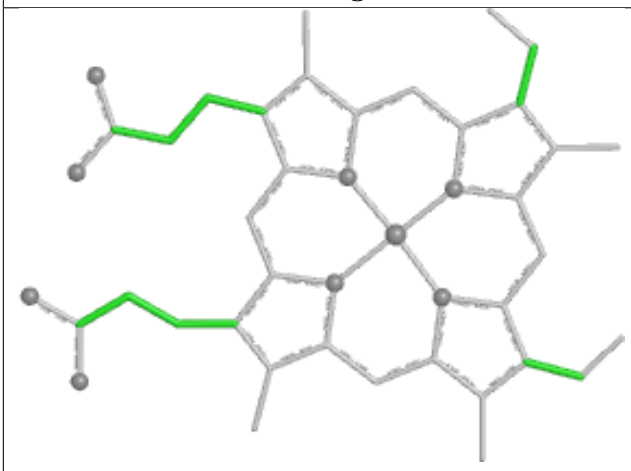
Ligand HEM F 703



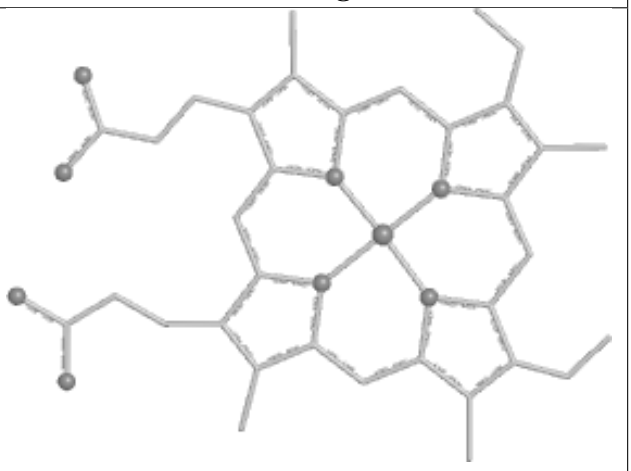
Bond lengths



Bond angles

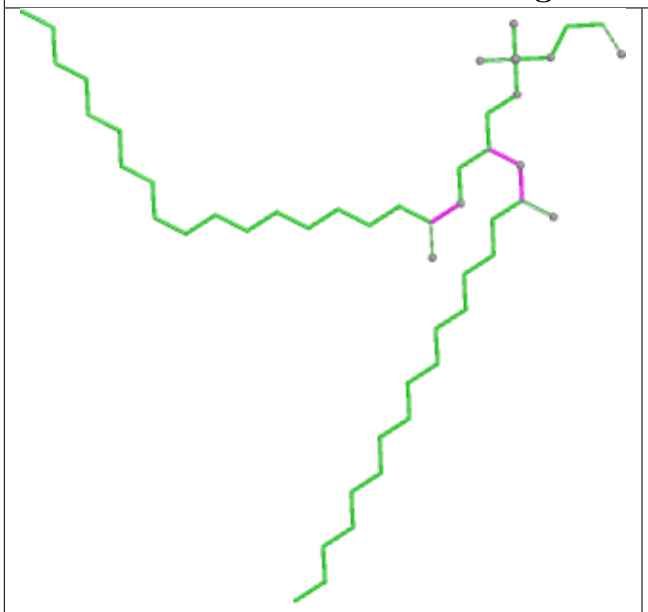


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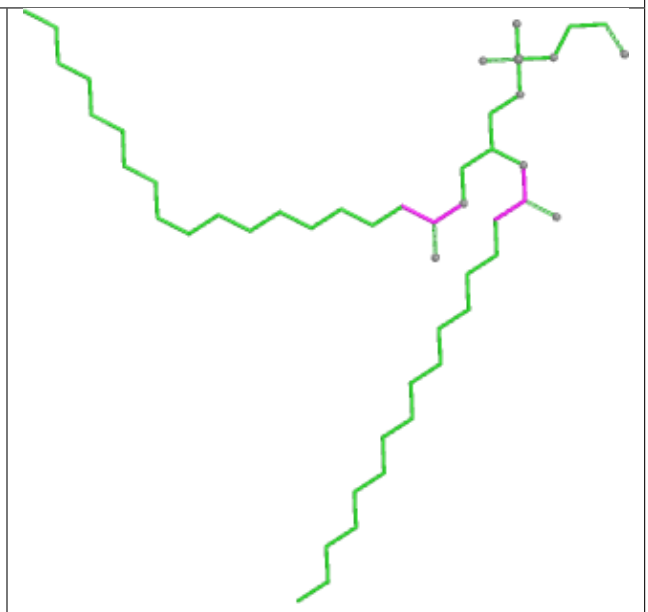


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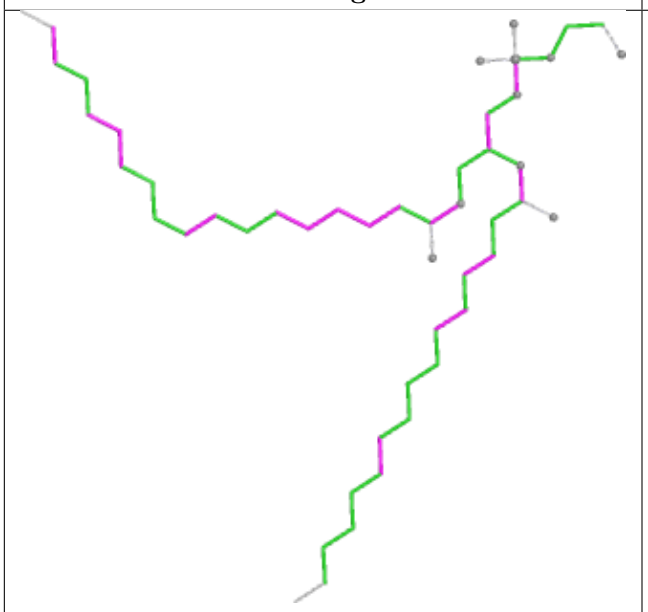
Ligand 9Y0 J 201



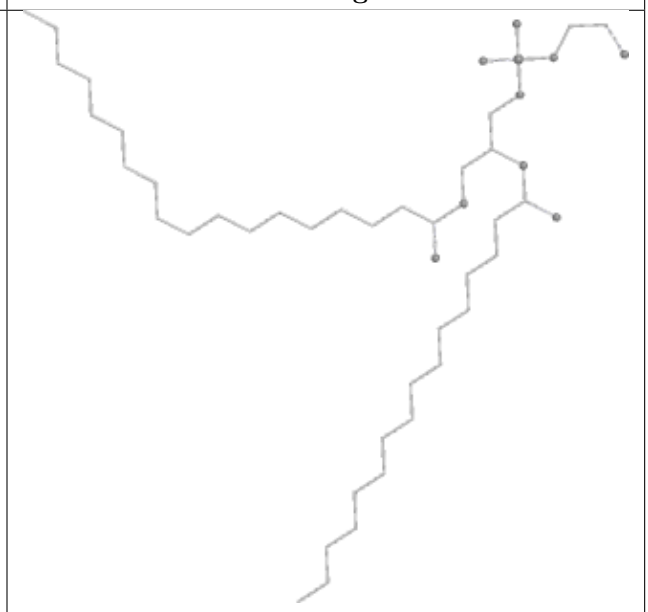
Bond lengths



Bond angles



Torsions



Rings

Ligand PLM D 301



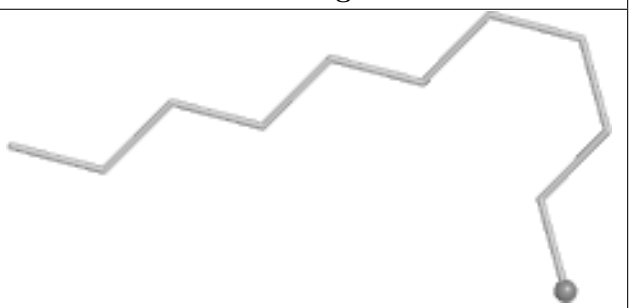
Bond lengths



Bond angles

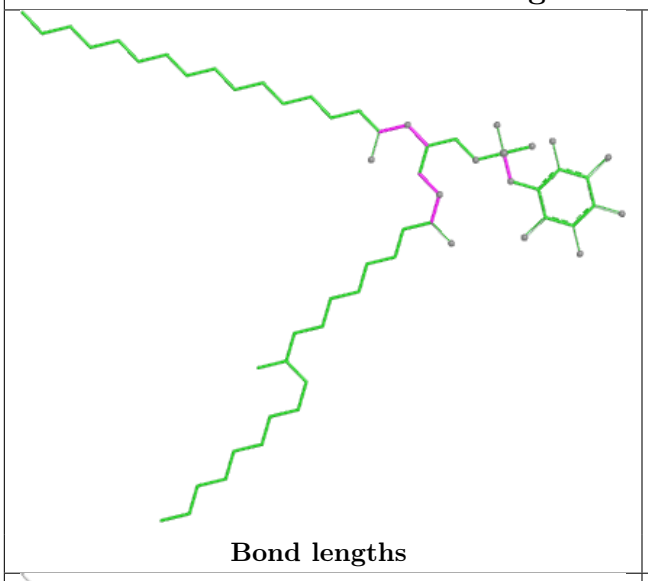


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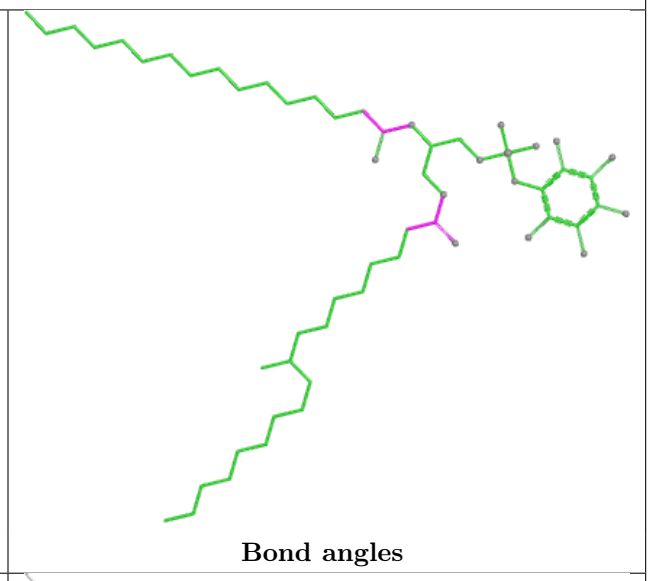


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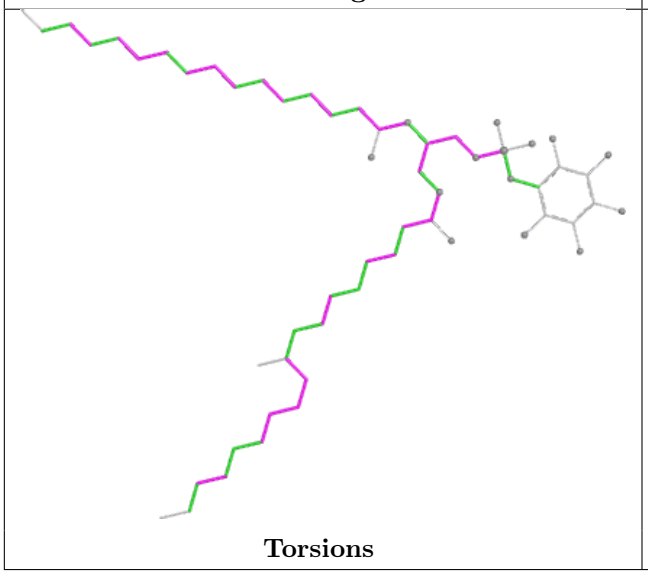
Ligand 9YF O 303



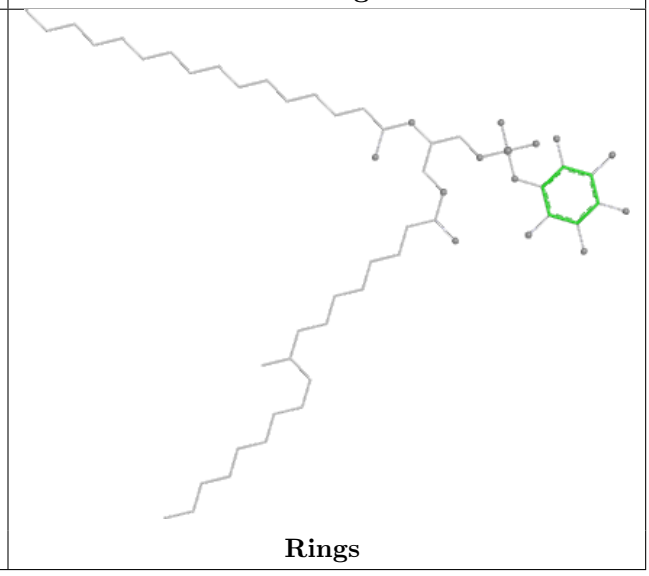
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Bond angles

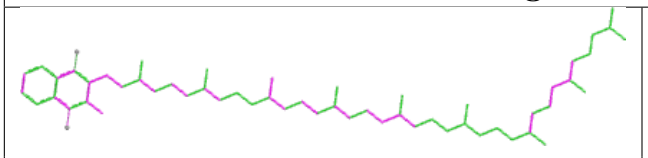


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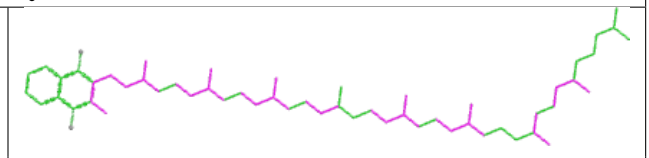


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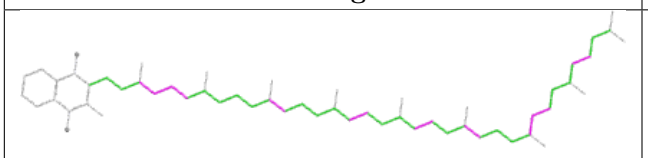
Ligand MQ9 E 604



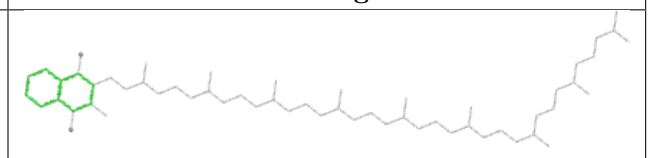
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Bond angles

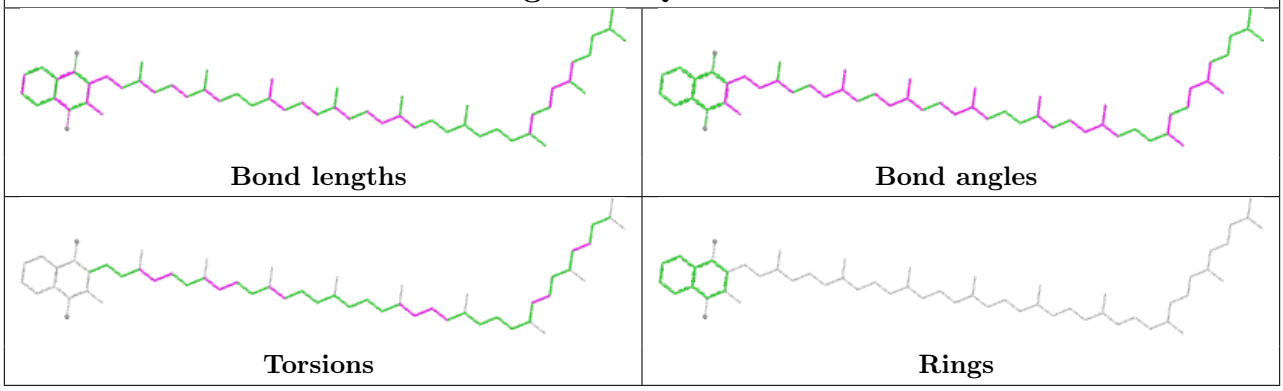


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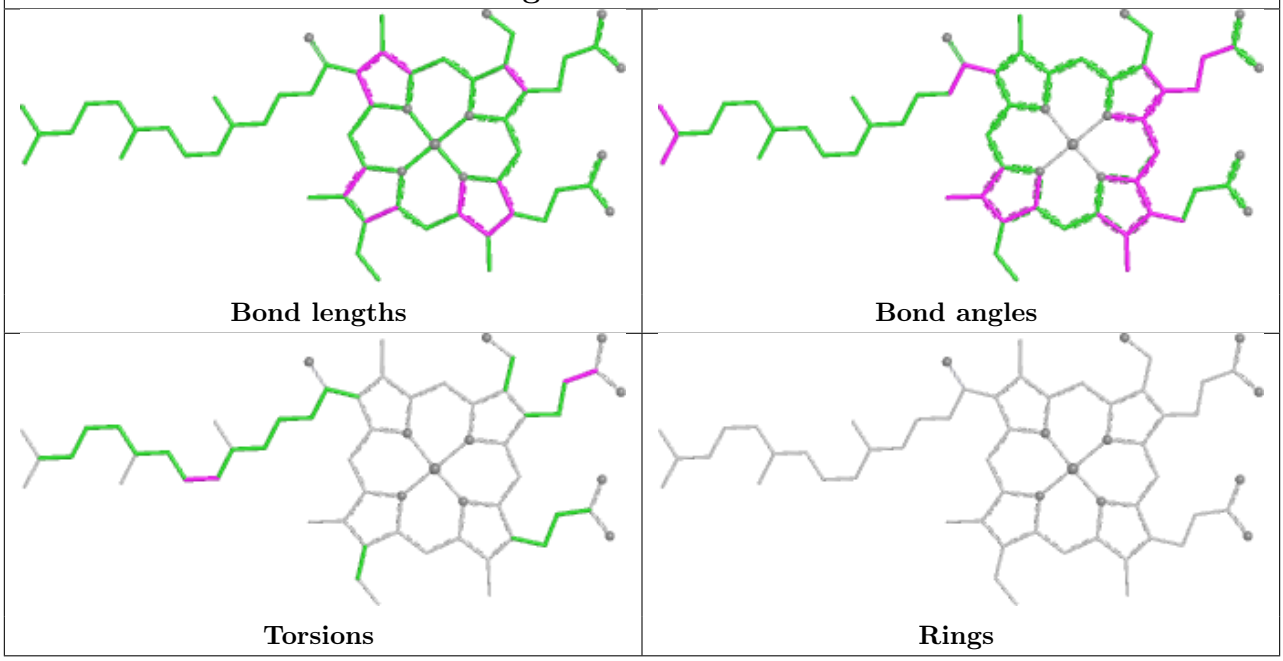


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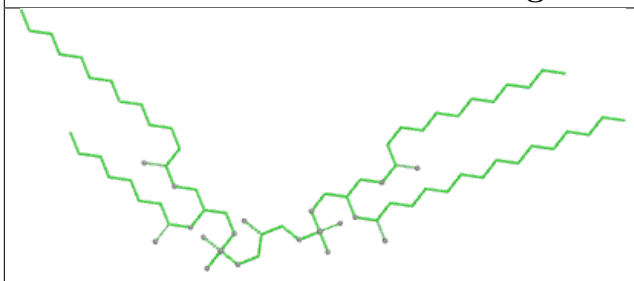
Ligand MQ9 T 204



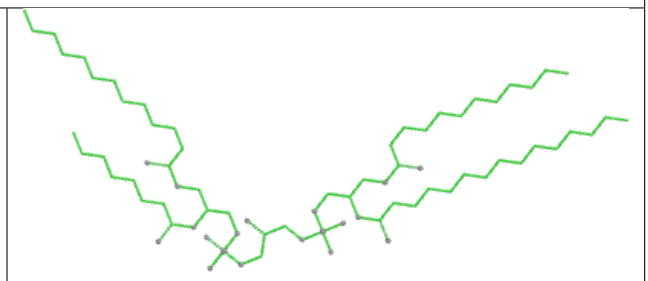
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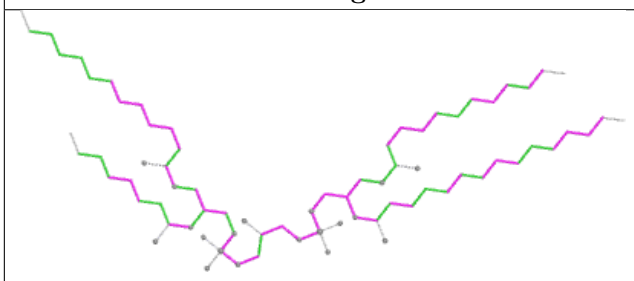
Ligand CDL F 705



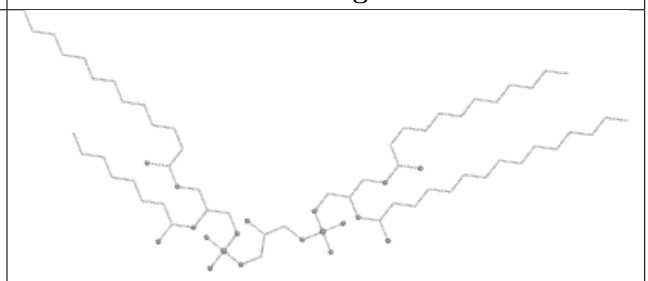
Bond lengths



Bond angles

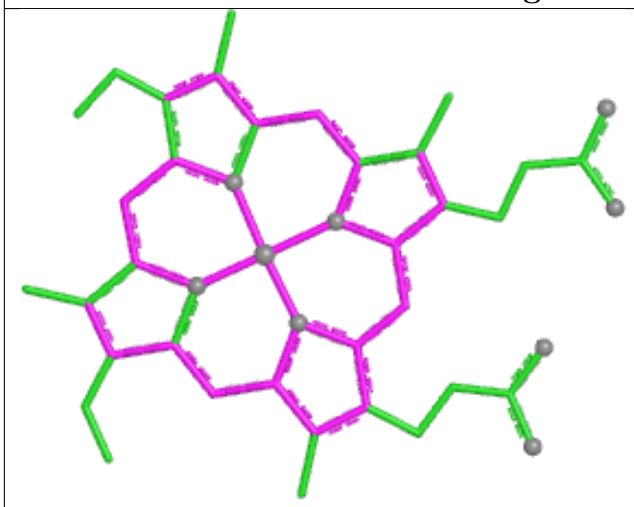


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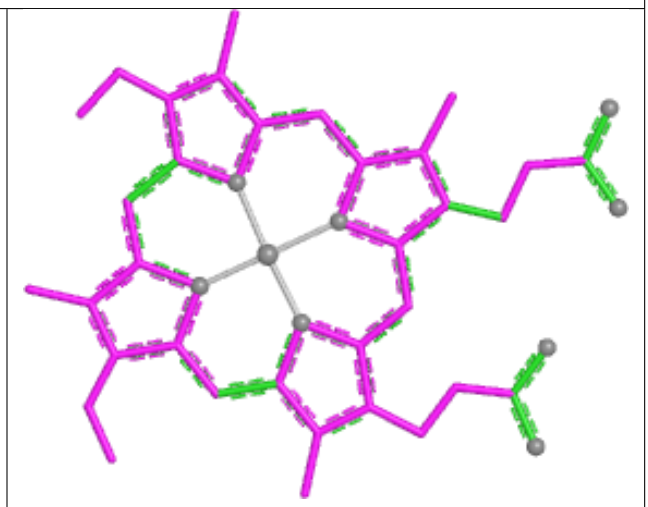


Rings

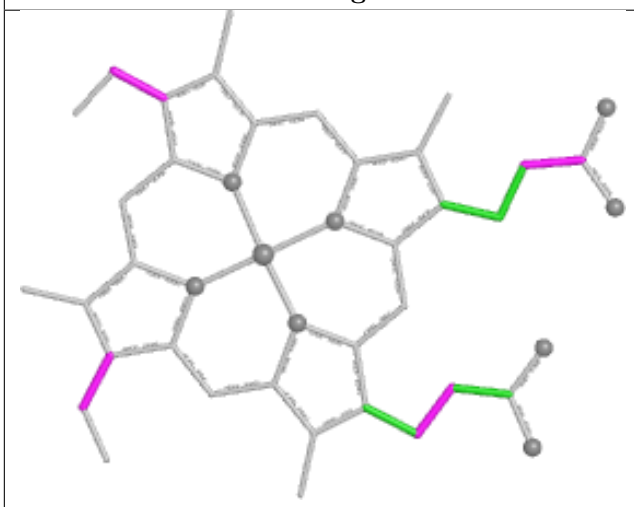
Ligand HEC O 301



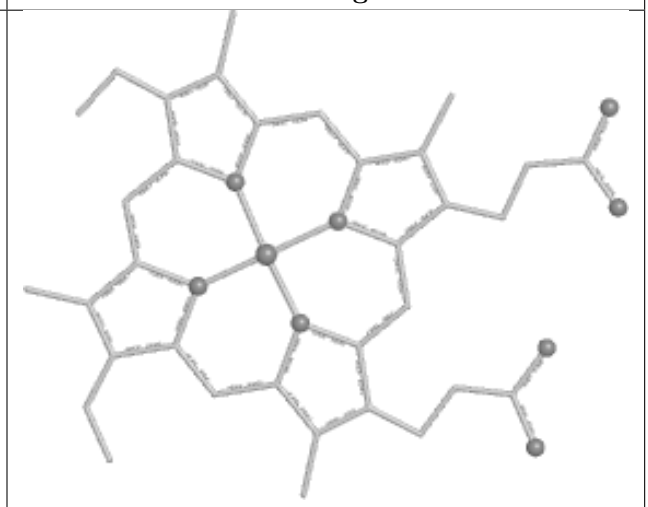
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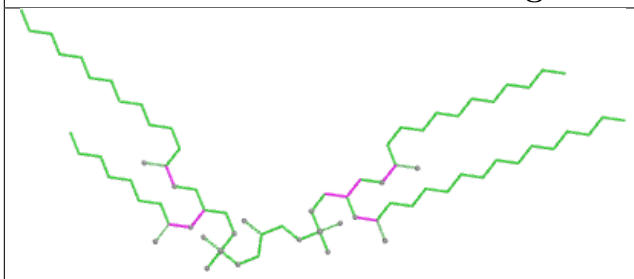


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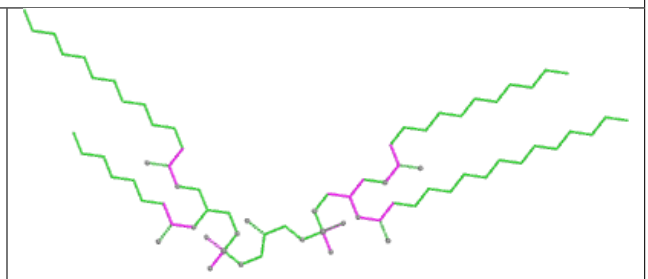


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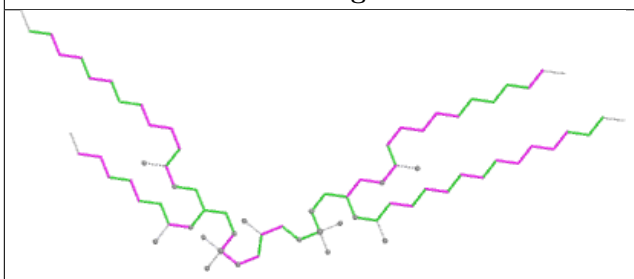
Ligand CDL T 203



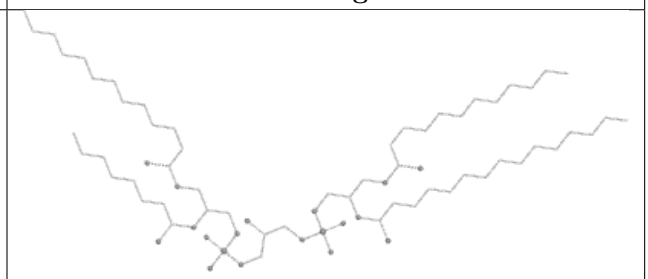
Bond lengths



Bond angles

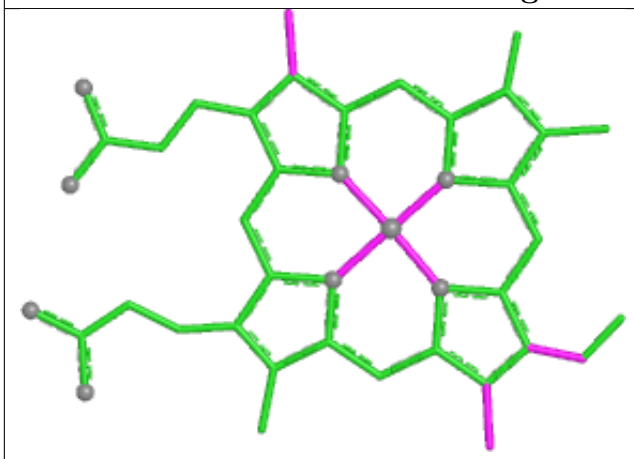


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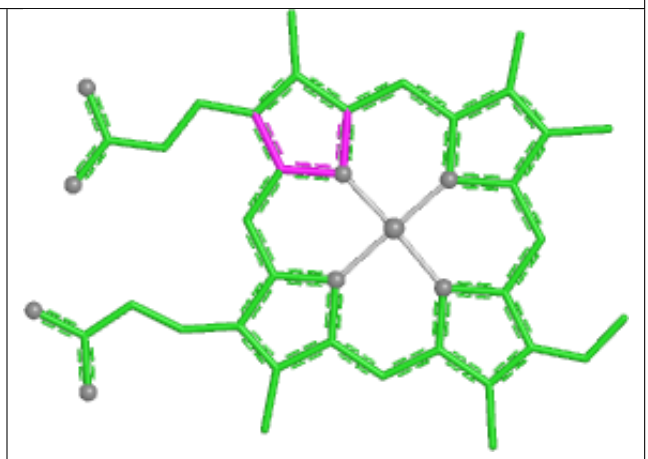


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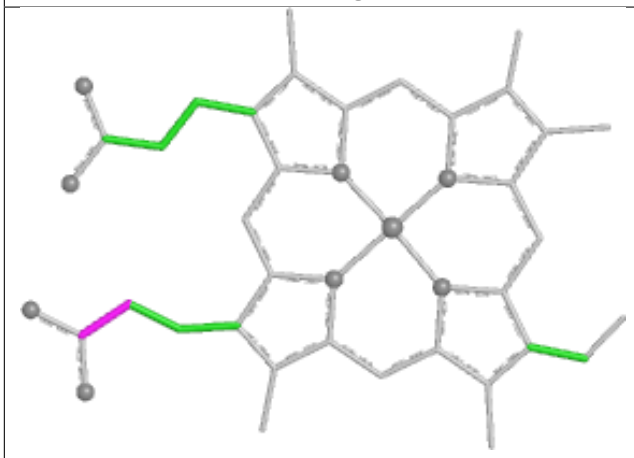
Ligand HEM E 601



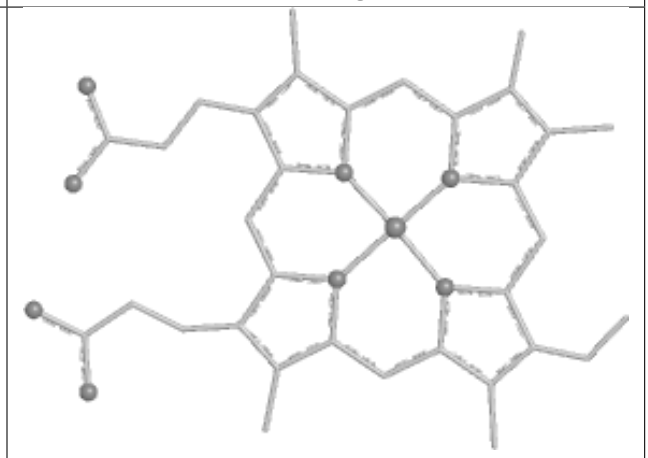
Bond lengths



Bond angles

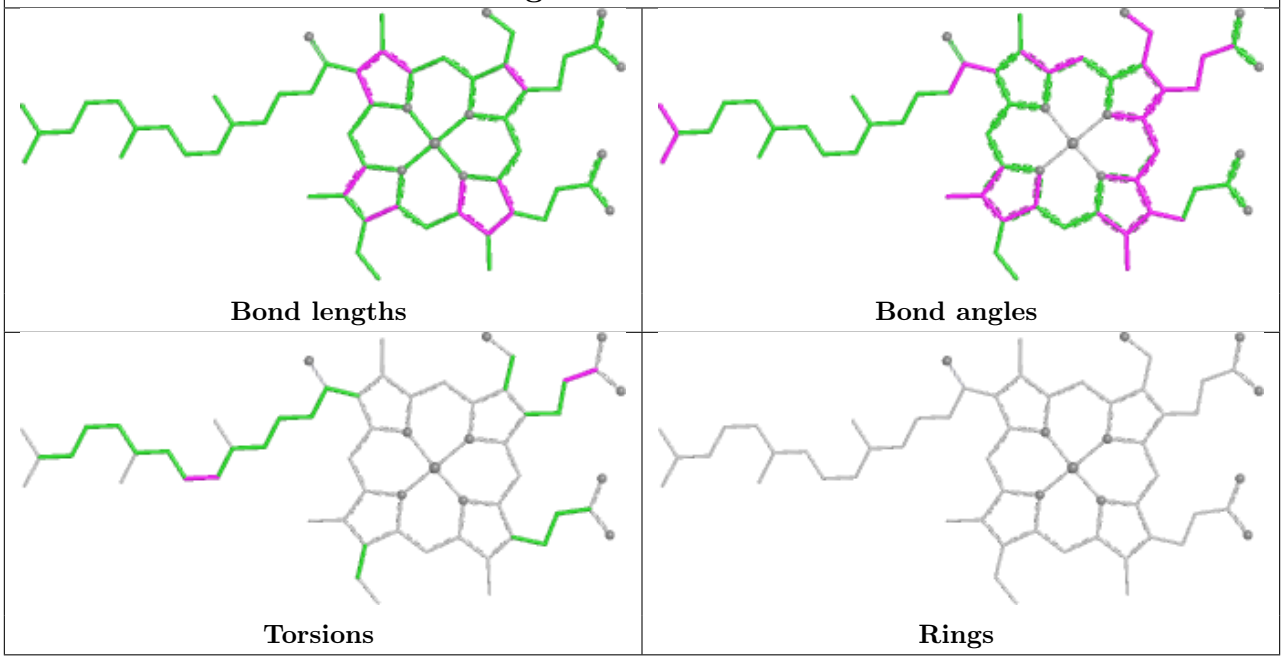


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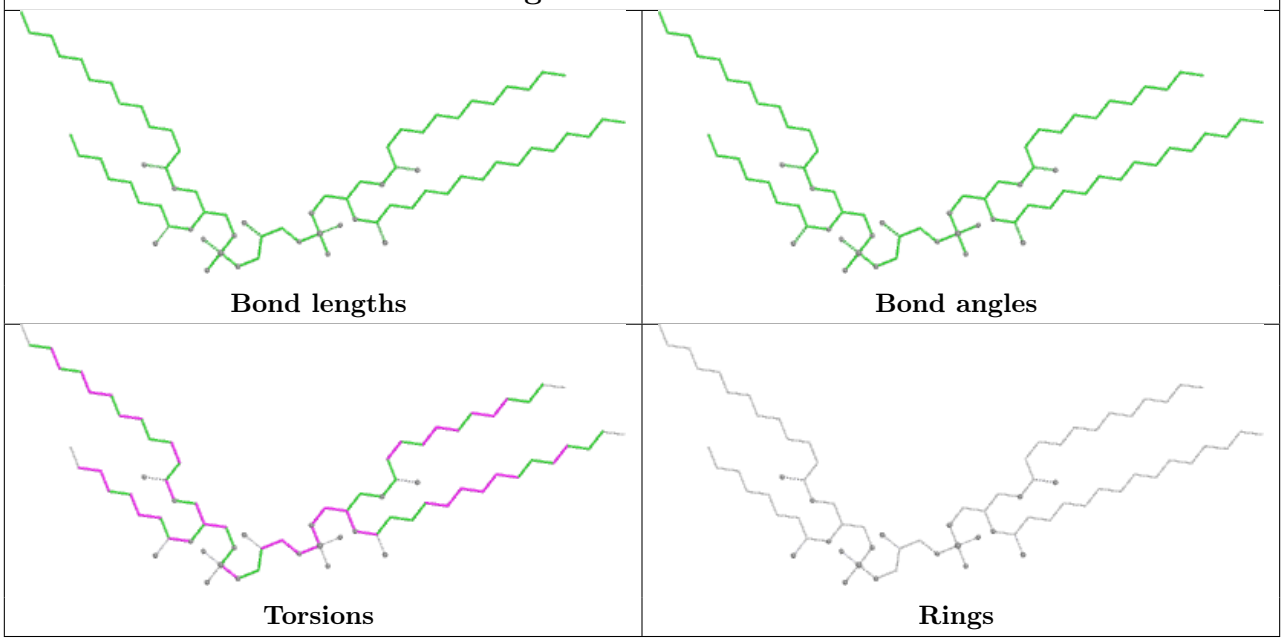


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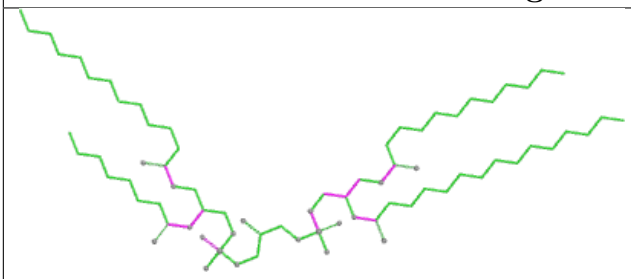
Ligand HEA L 603



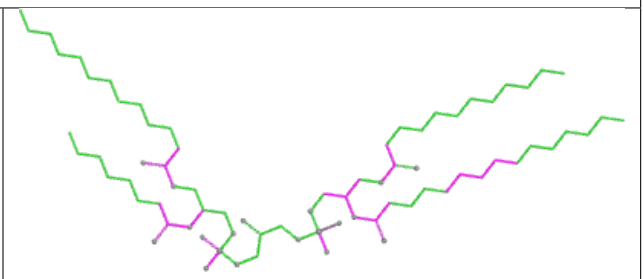
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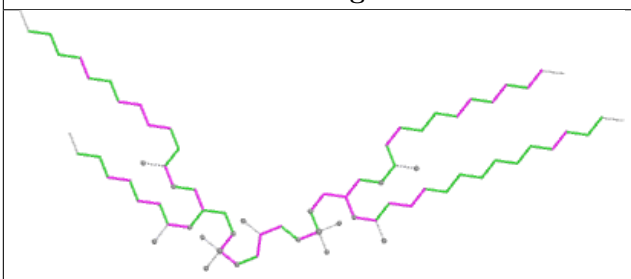
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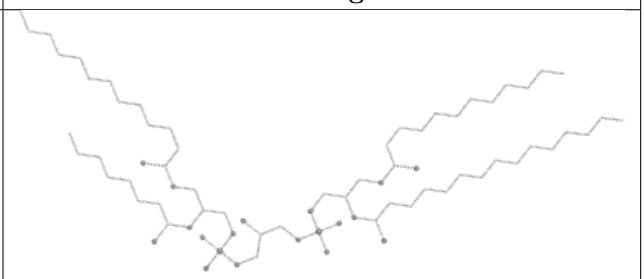
Bond lengths



Bond angles

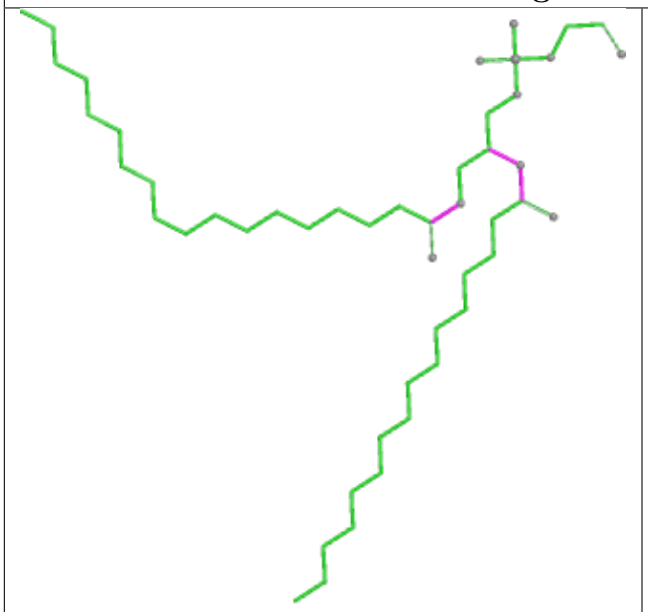


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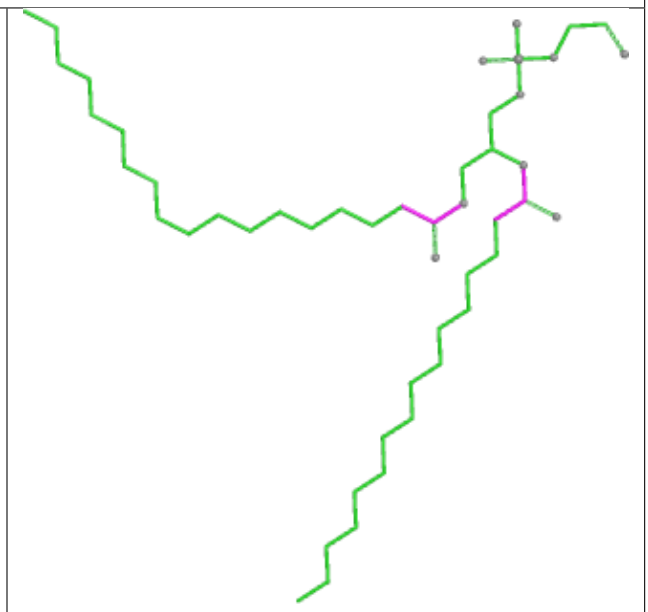


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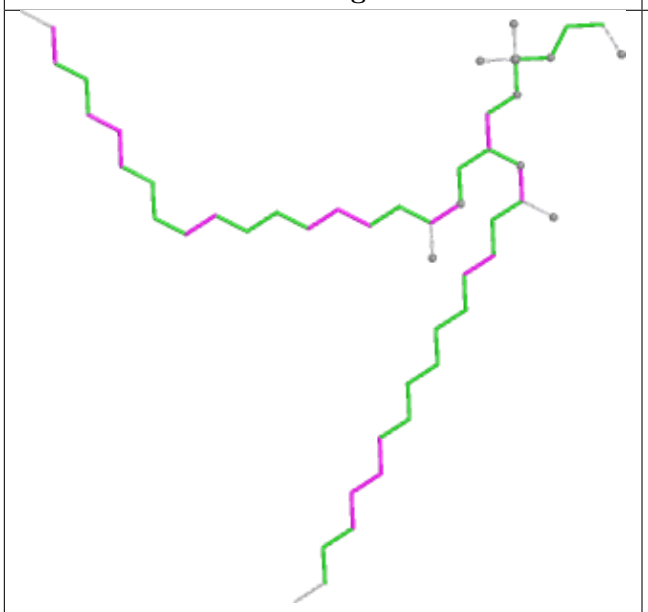
Ligand 9Y0 F 704



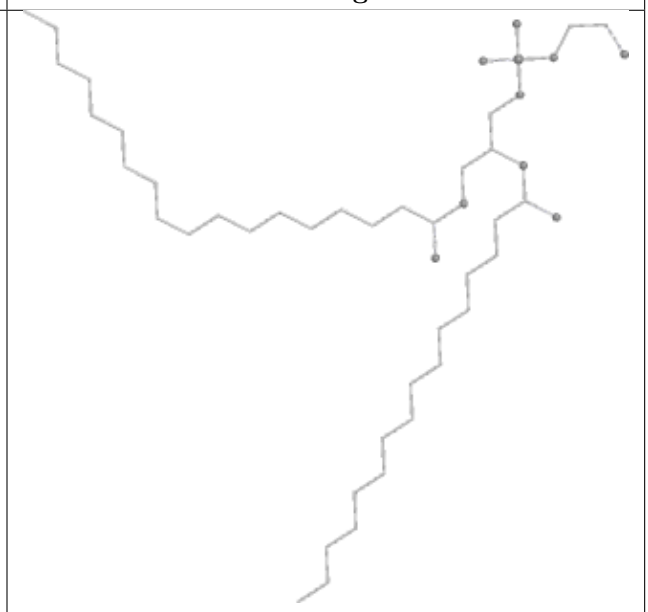
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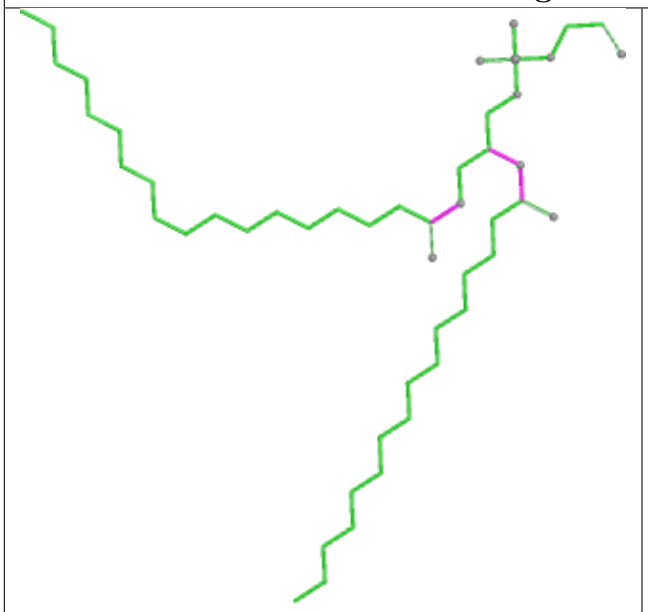


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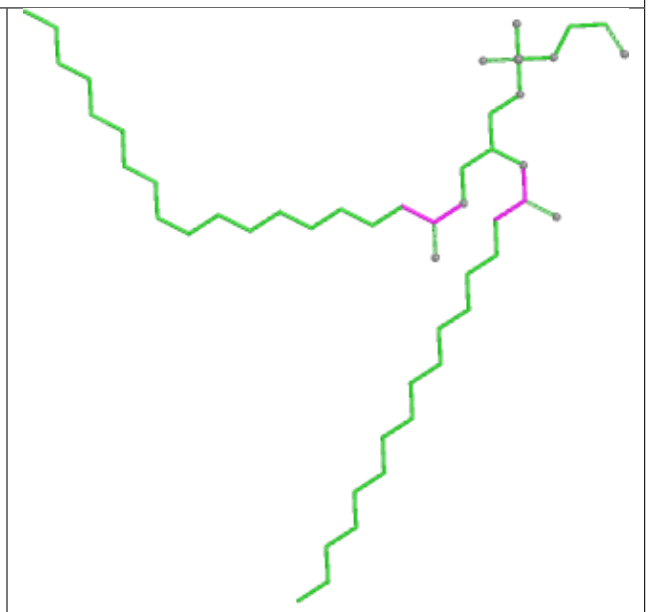


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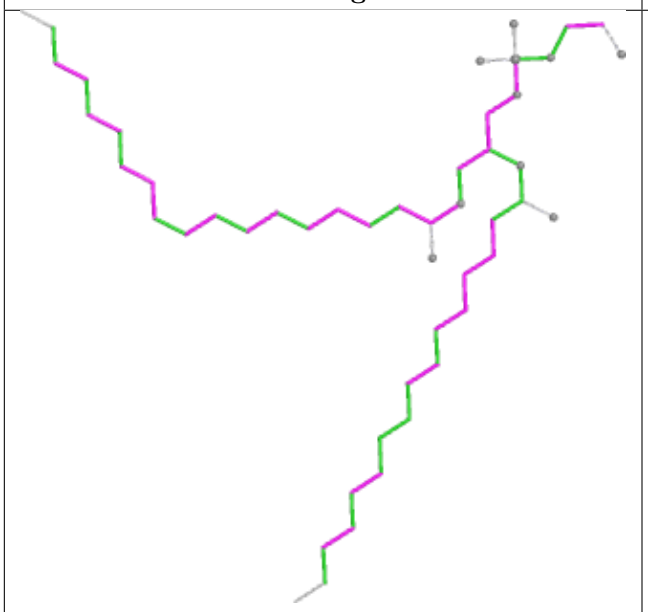
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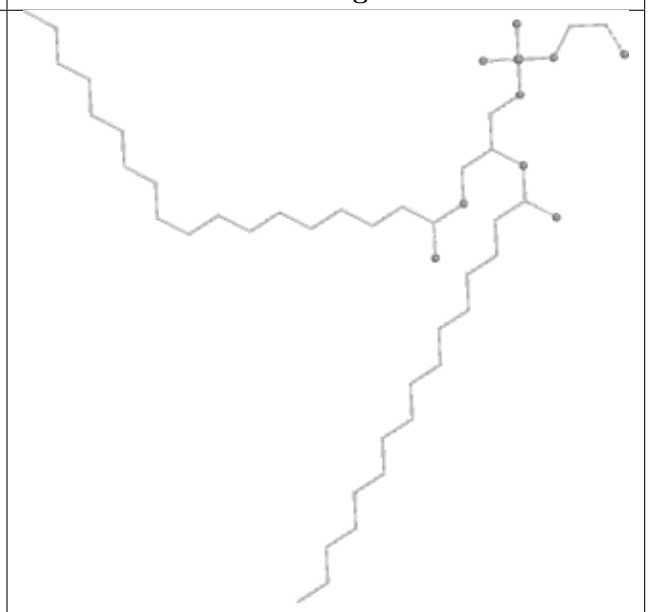
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Bond angles

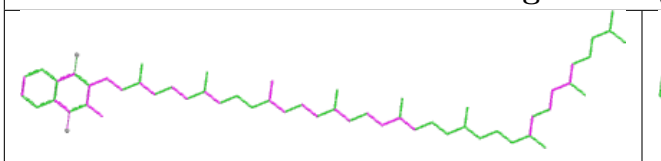


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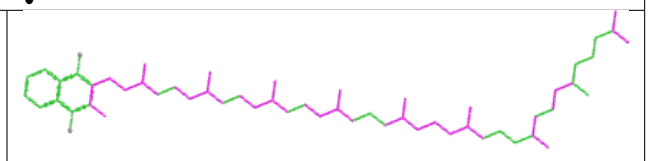


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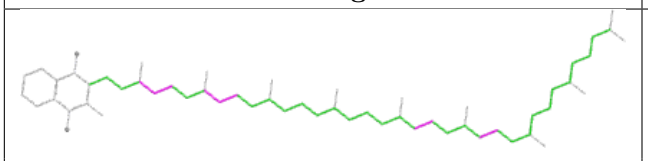
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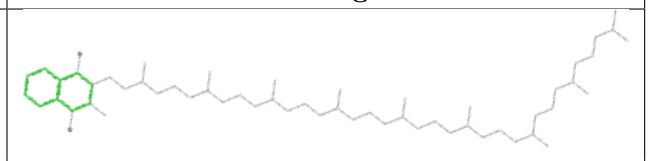
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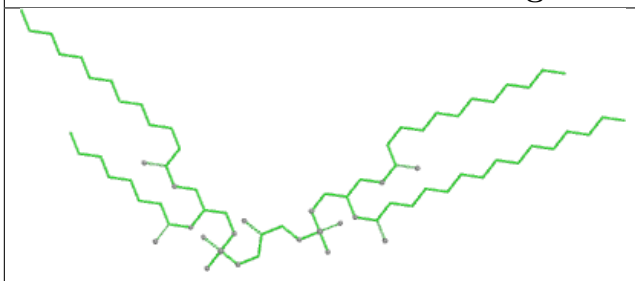


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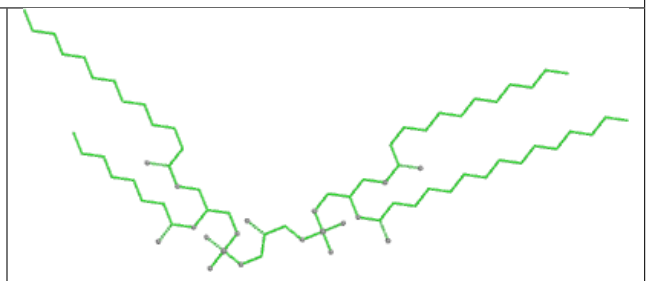


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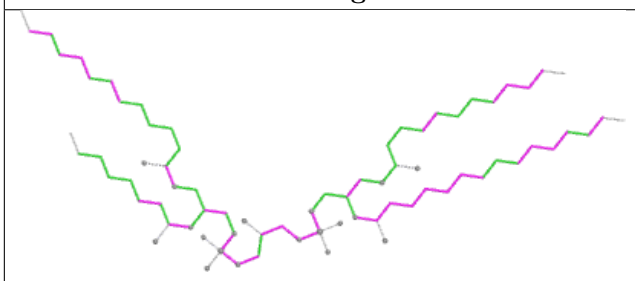
Ligand CDL E 607



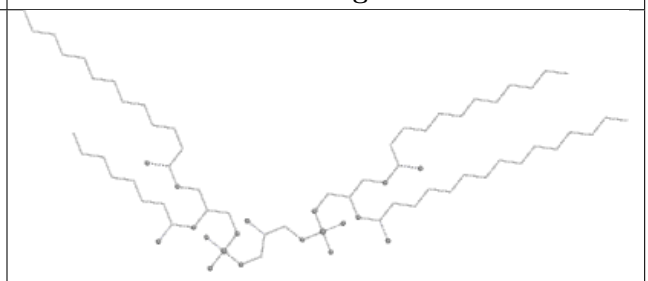
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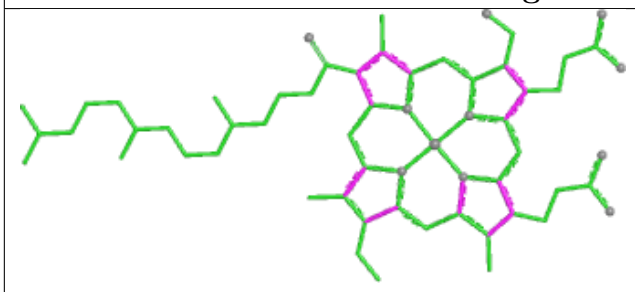


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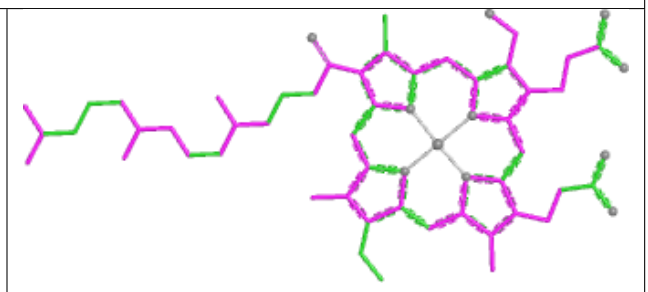


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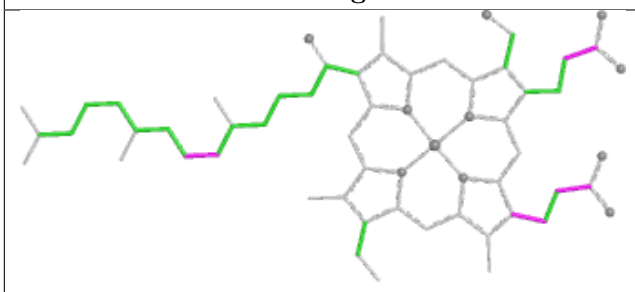
Ligand HEA R 602



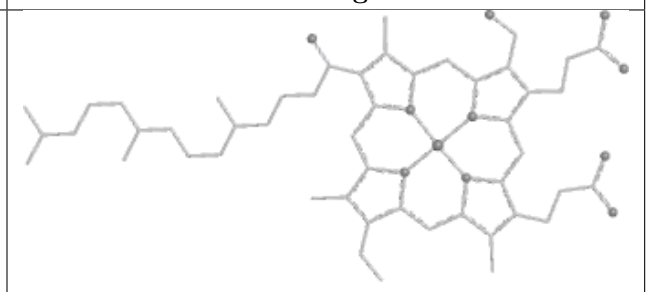
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Bond angles

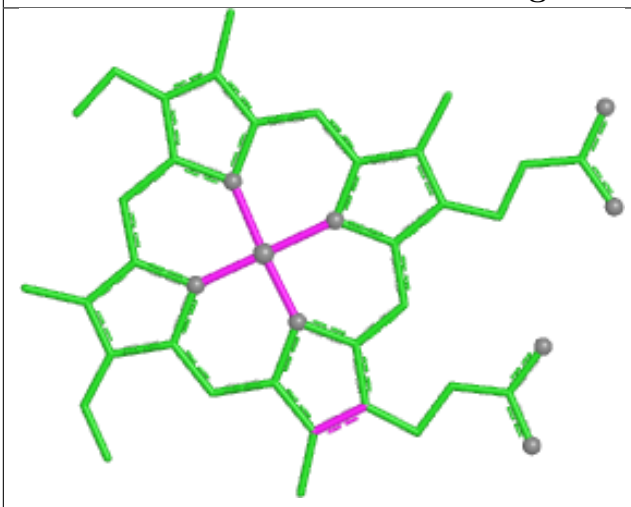


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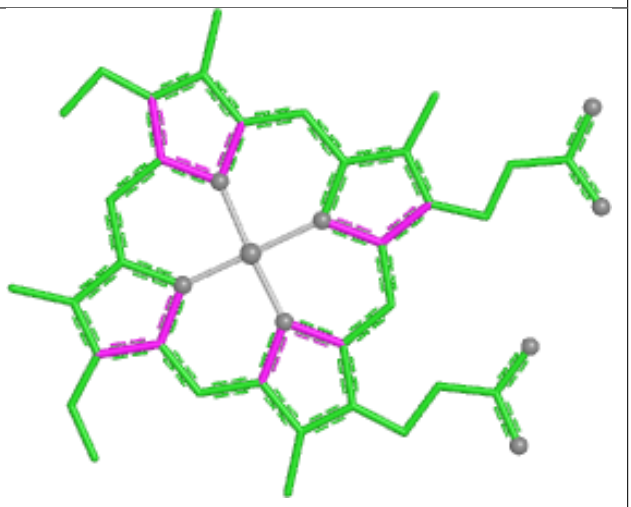


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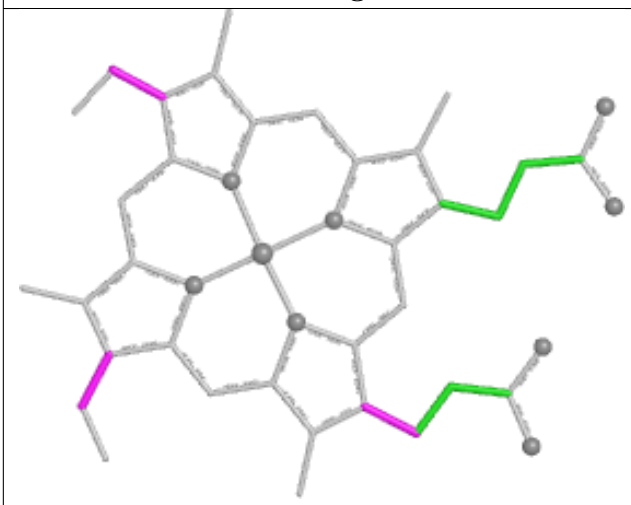
Ligand HEC I 301



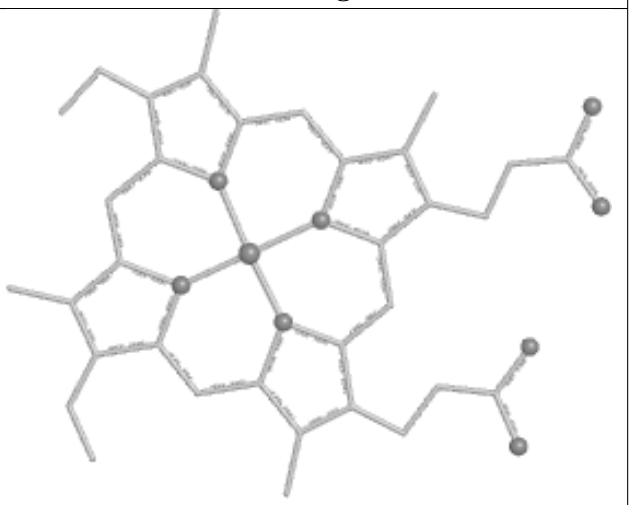
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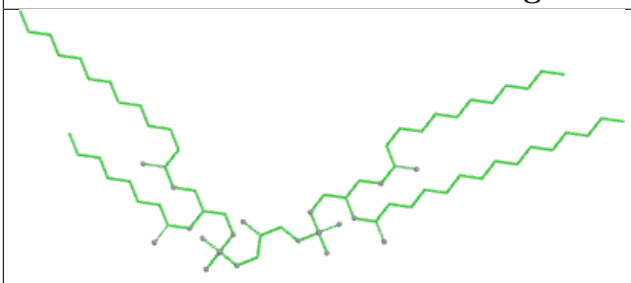


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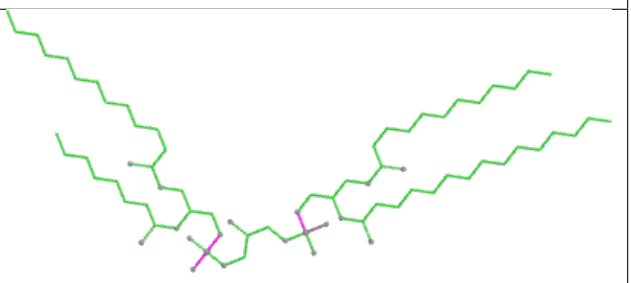


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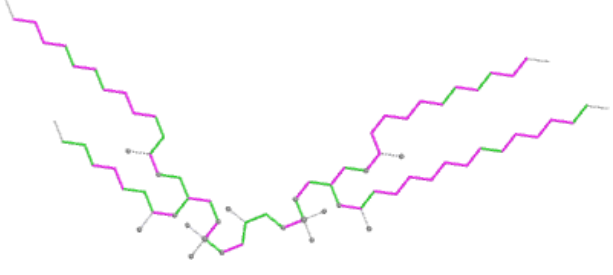
Ligand CDL R 604



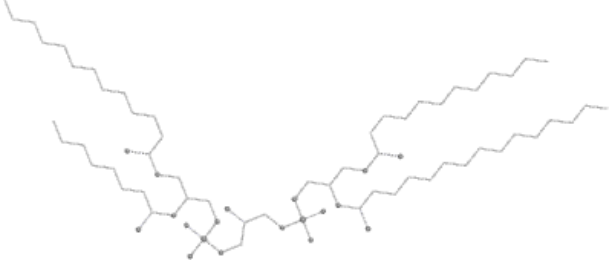
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Bond angles

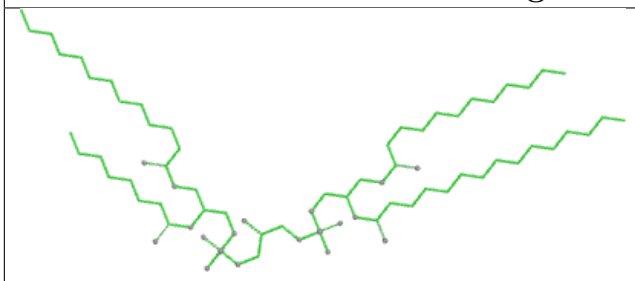


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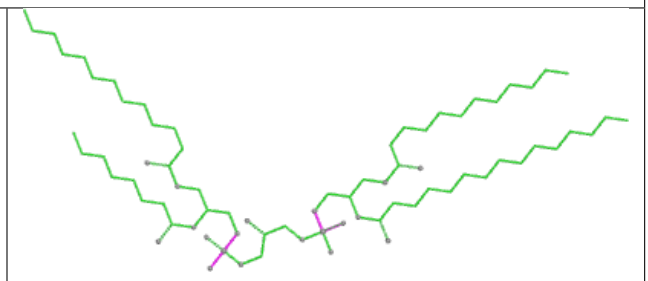


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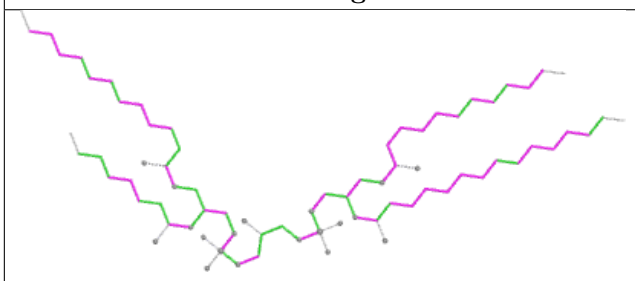
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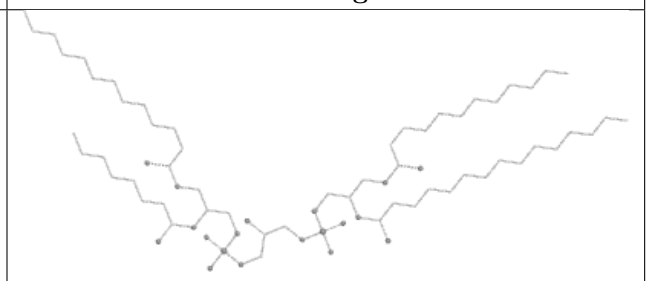
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Bond angles

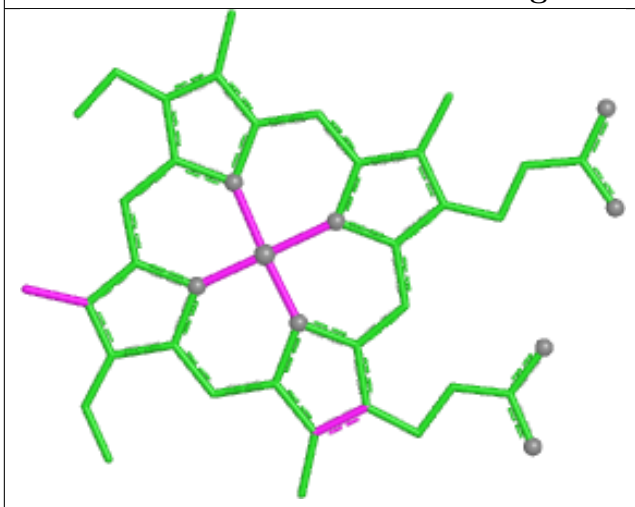


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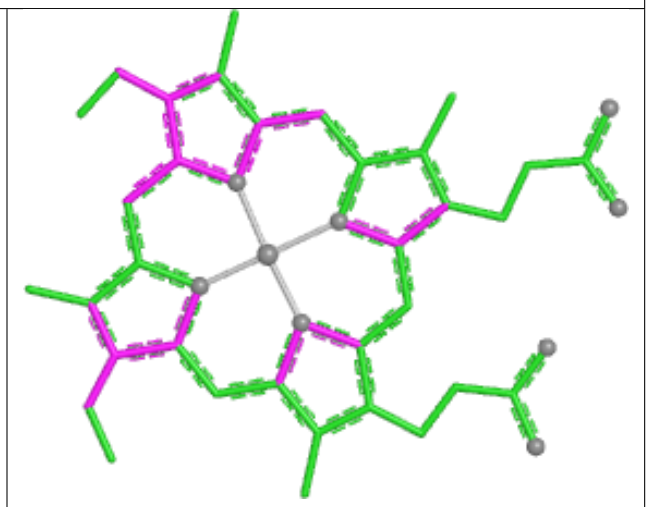


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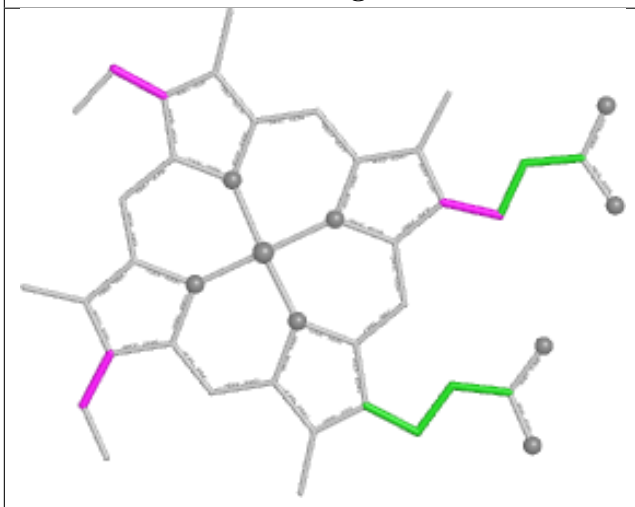
Ligand HEC I 302



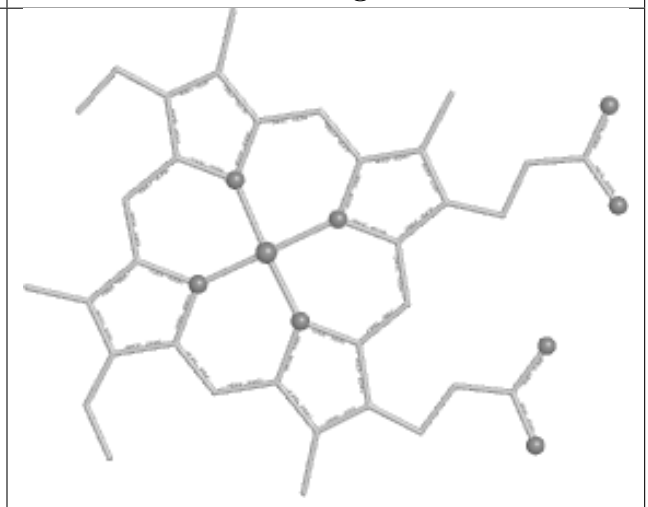
Bond lengths



Bond angles

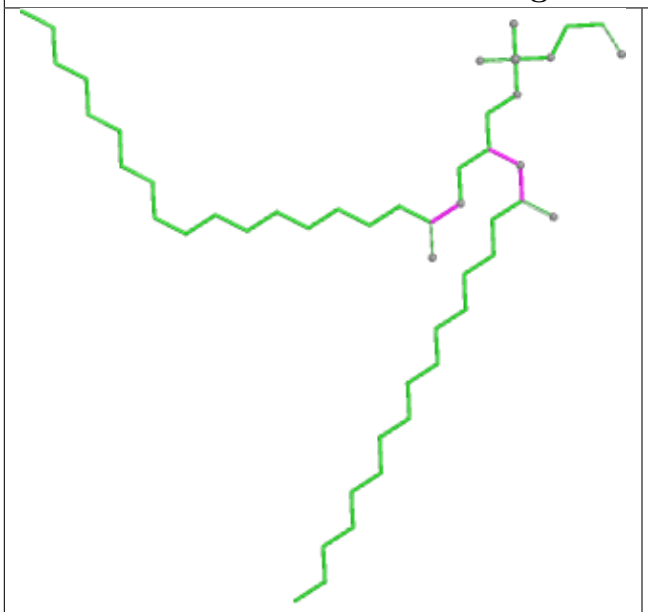


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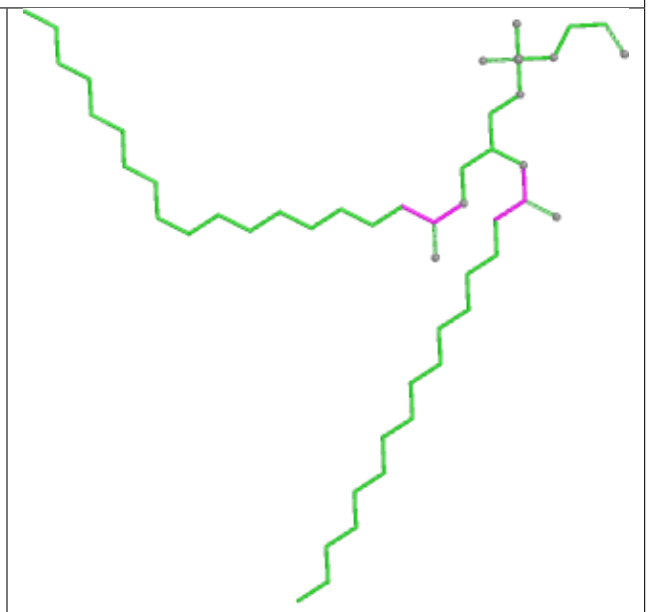


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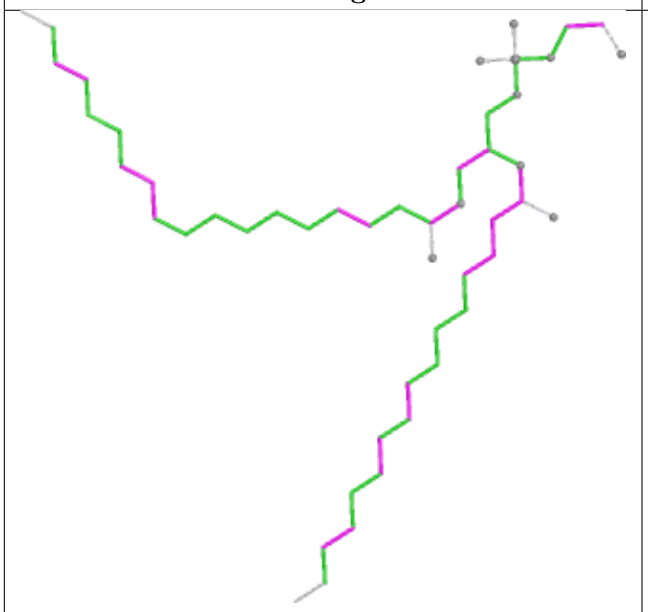
Ligand 9Y0 X 301



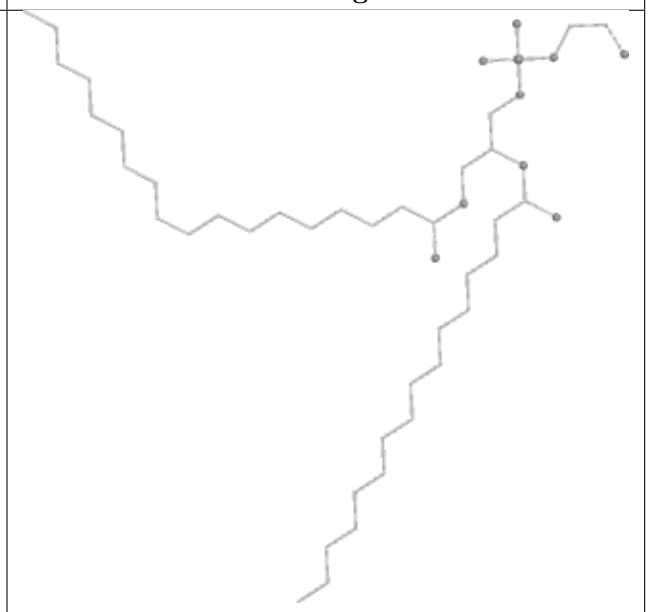
Bond lengths



Bond angles

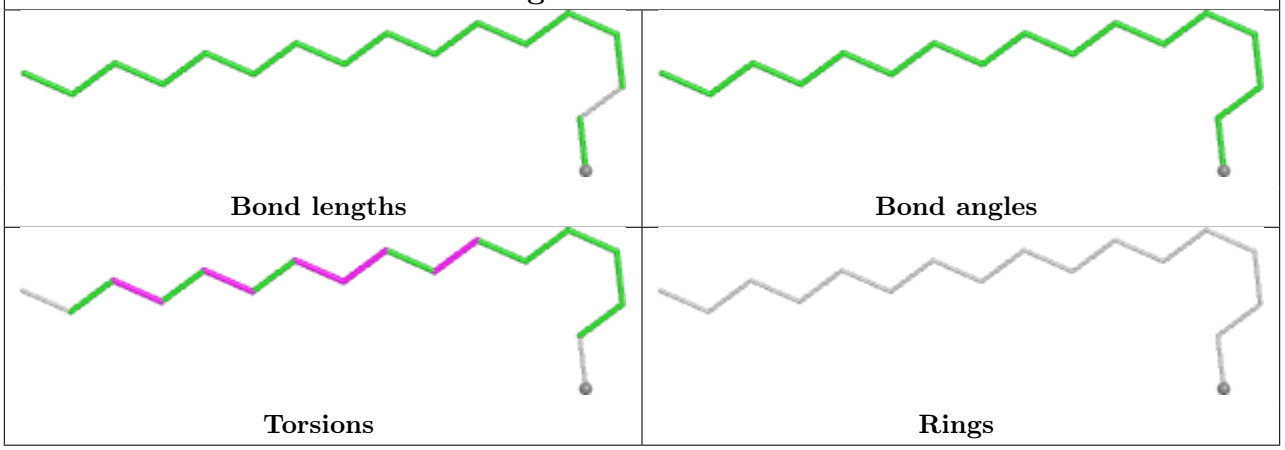


Torsions

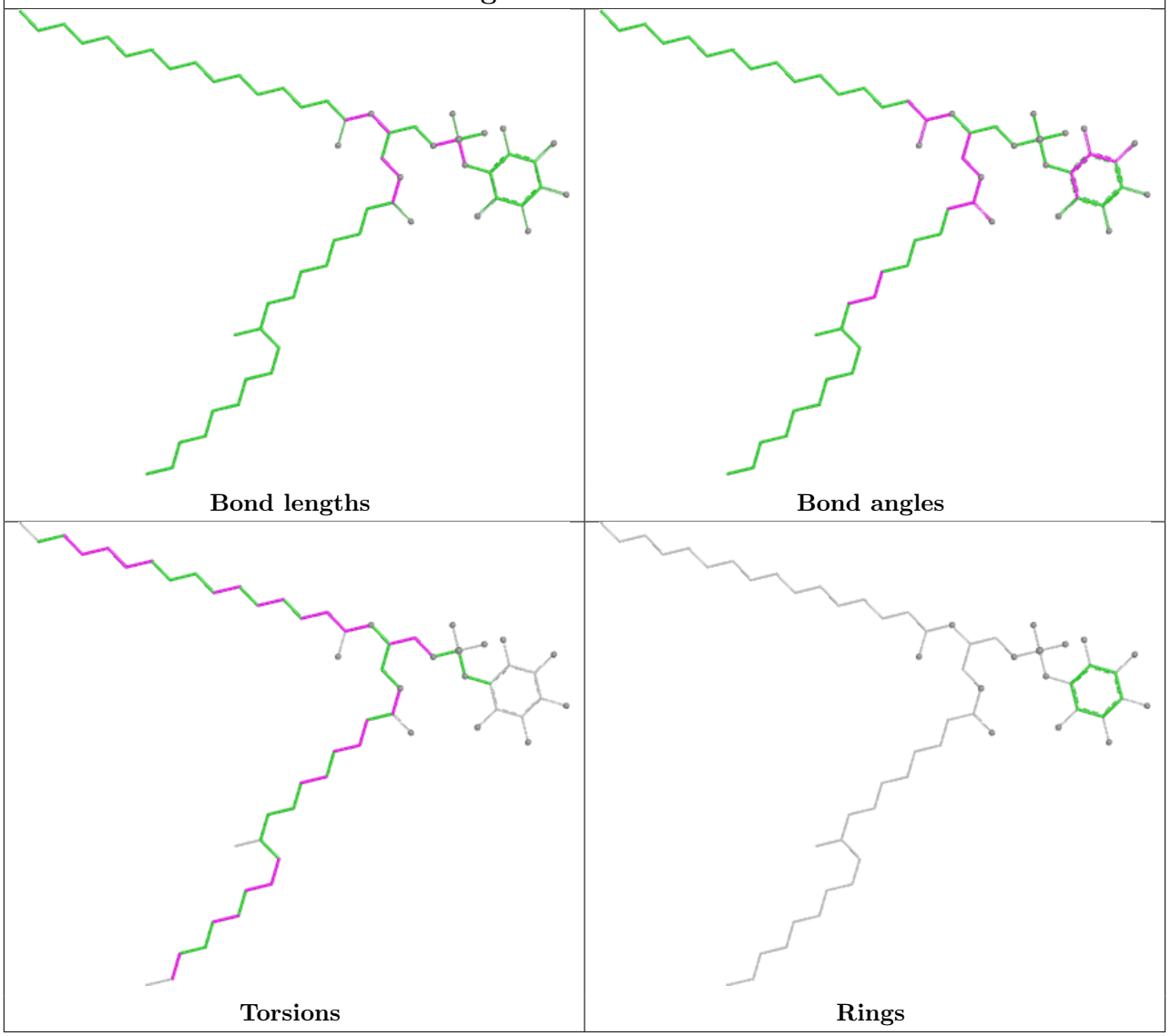


Rings

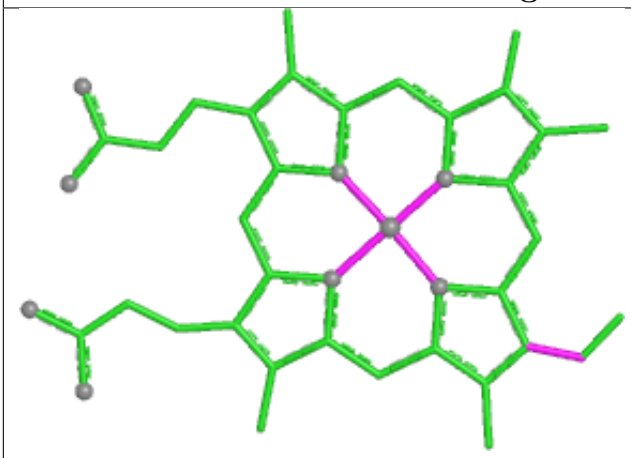
Ligand PLM c 201



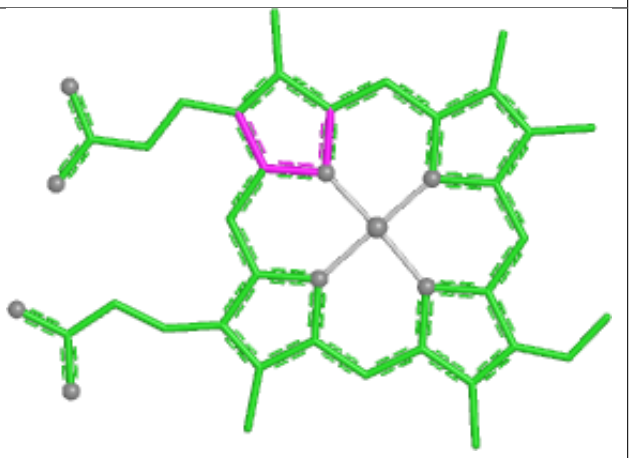
Ligand 9YF Y 502



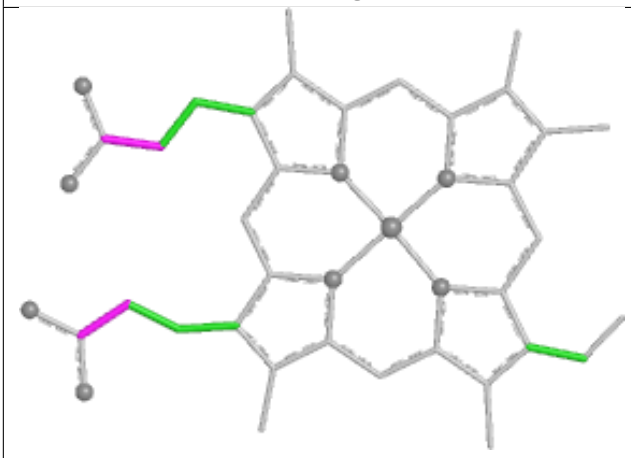
Ligand HEM F 702



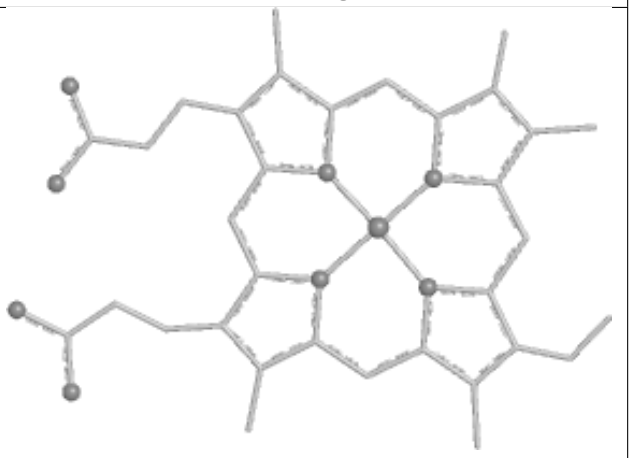
Bond lengths



Bond angles

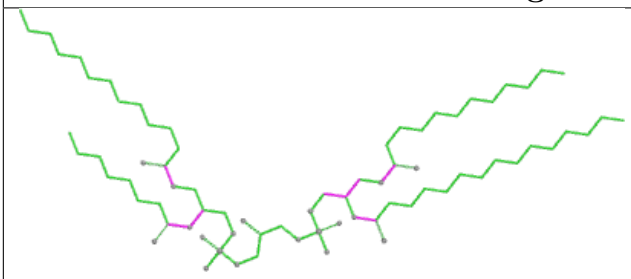


Torsions

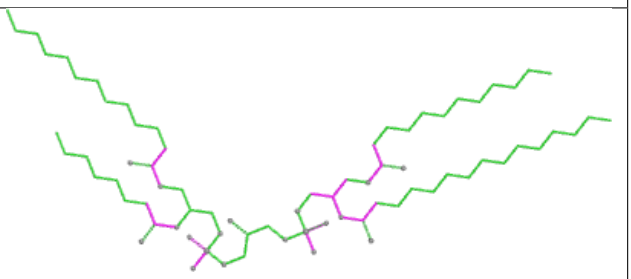


Rings

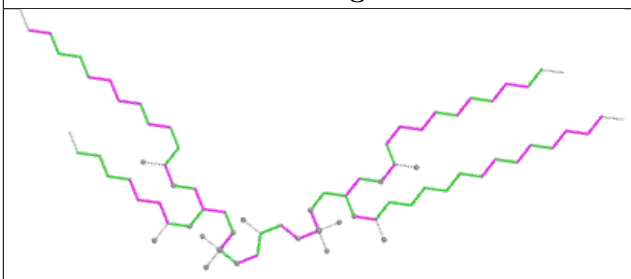
Ligand CDL S 302



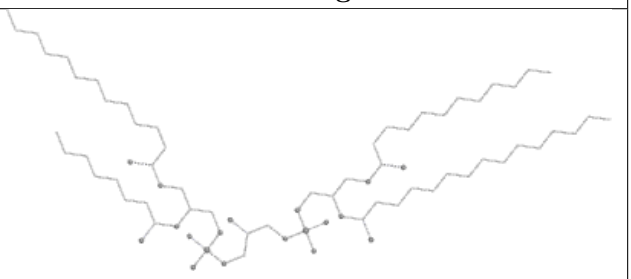
Bond lengths



Bond angles

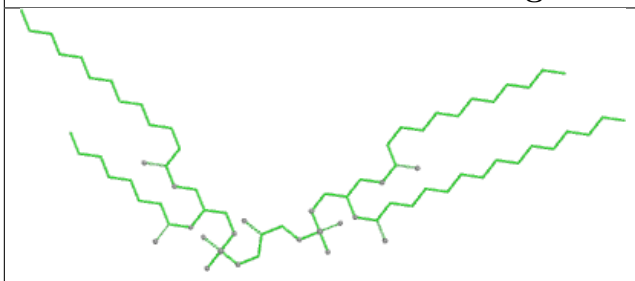


Torsions

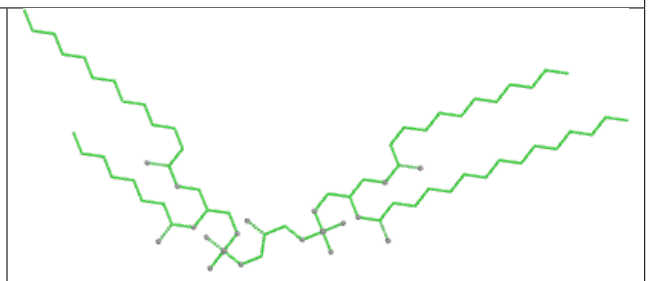


Rings

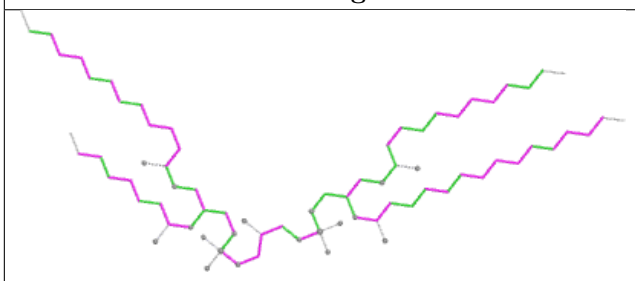
Ligand CDL P 201



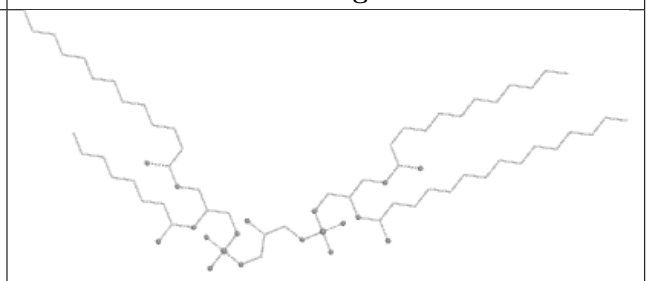
Bond lengths



Bond angles

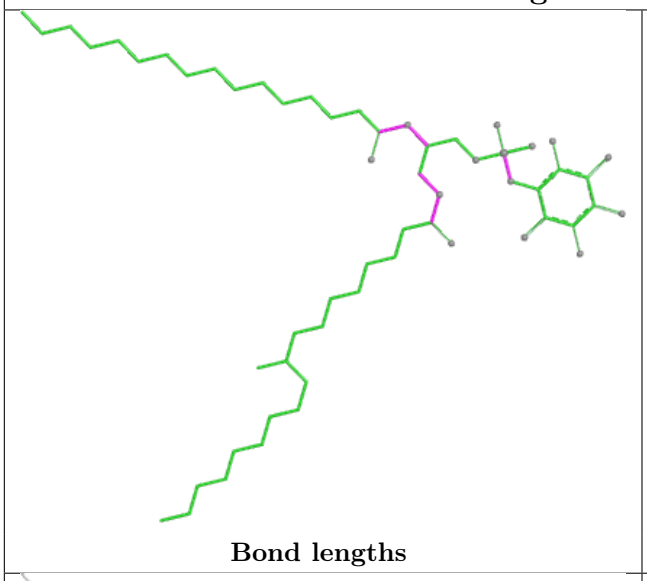


Torsions

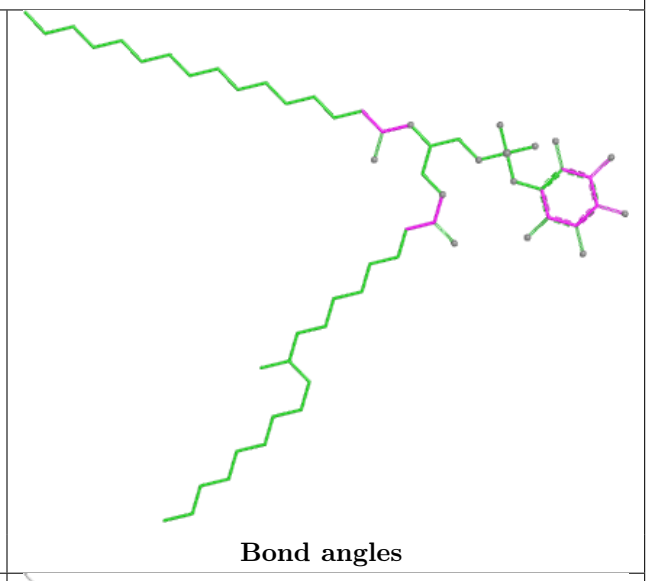


Rings

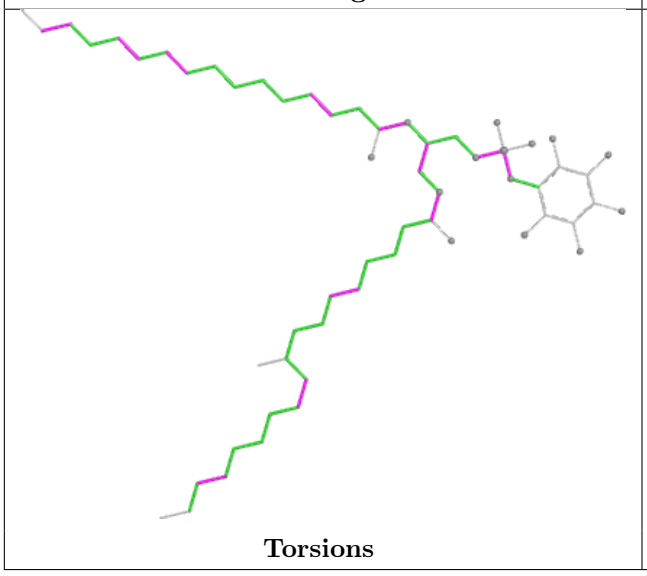
Ligand 9YF E 605



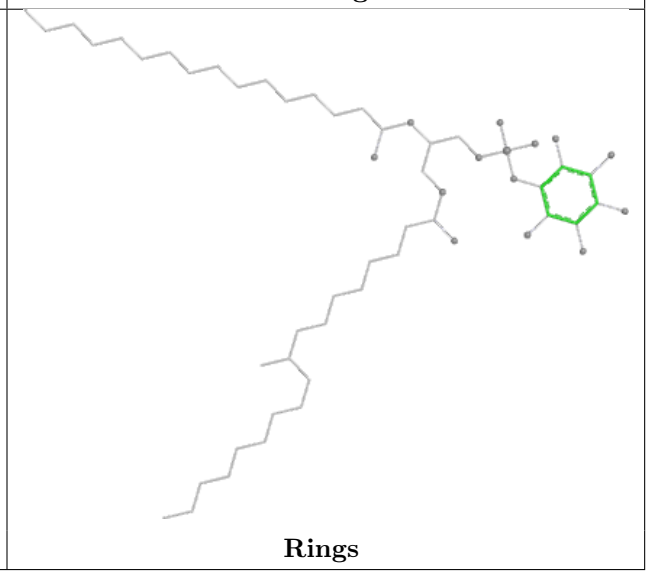
Bond lengths



Bond angles

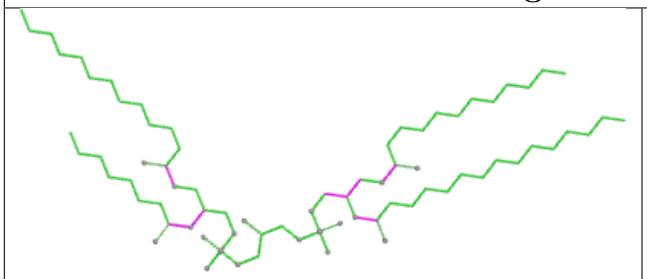


Torsions

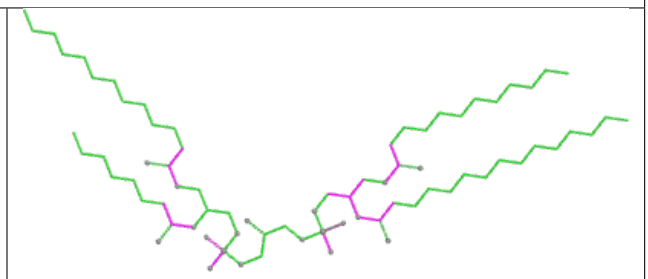


Rings

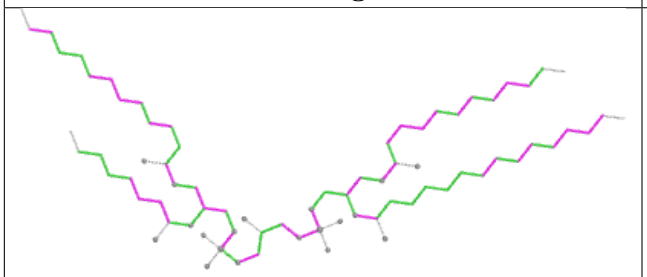
Ligand CDL X 303



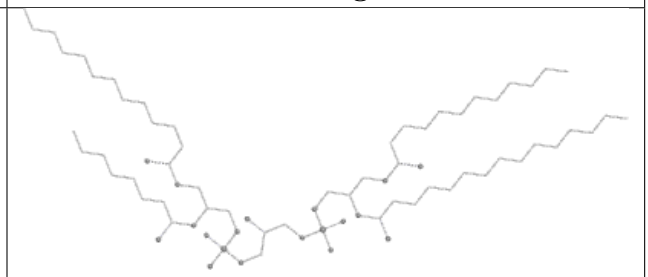
Bond lengths



Bond angles

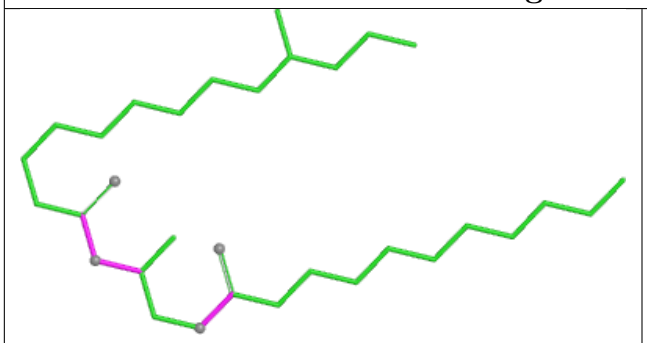


Torsions

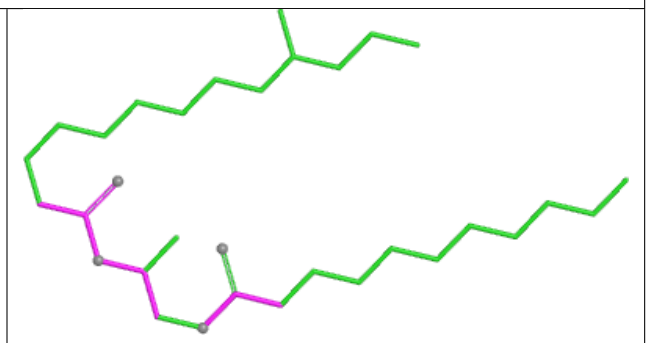


Rings

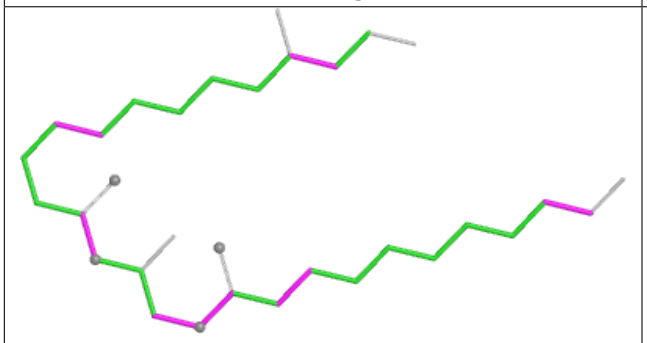
Ligand 9XX G 302



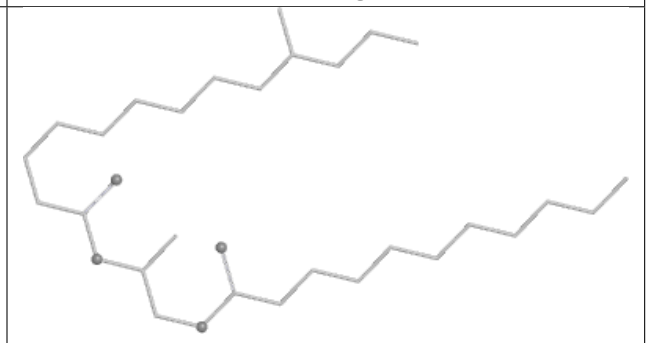
Bond lengths



Bond angles

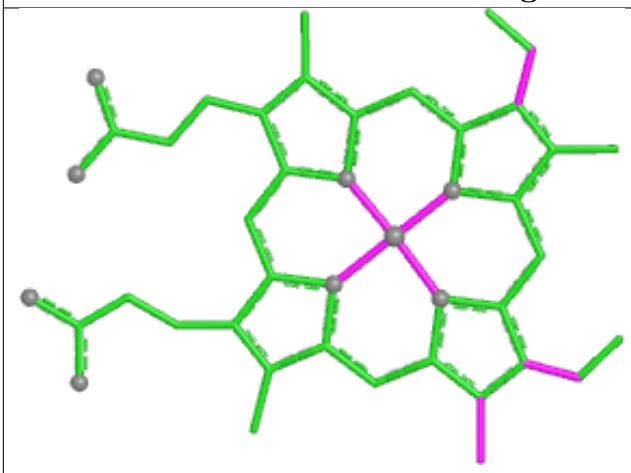


Torsions

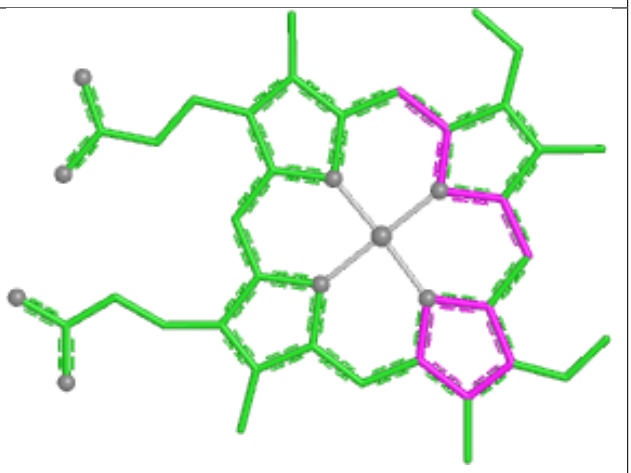


Rings

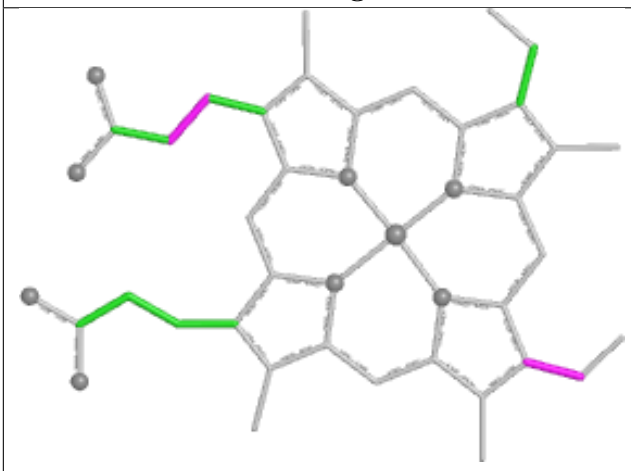
Ligand HEM E 602



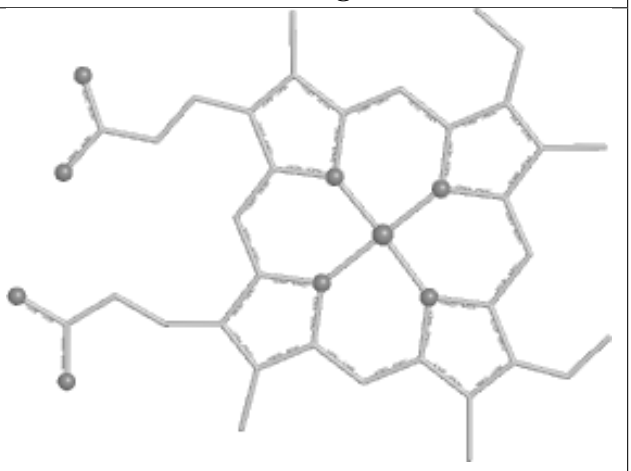
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

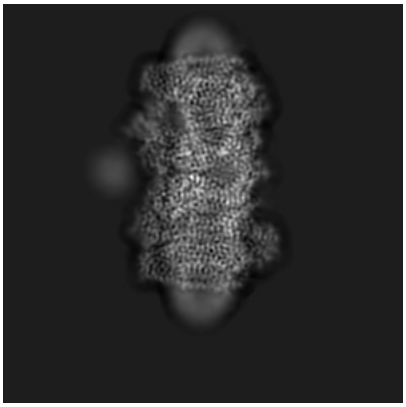
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24456. These allow visual inspection of the internal detail of the map and identification of artifacts.

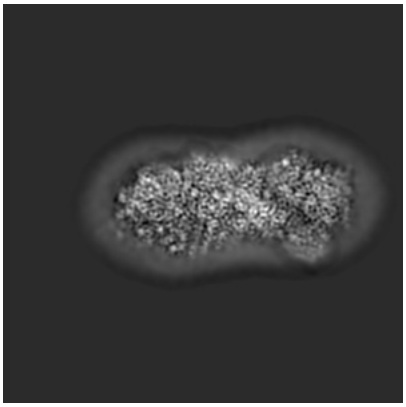
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

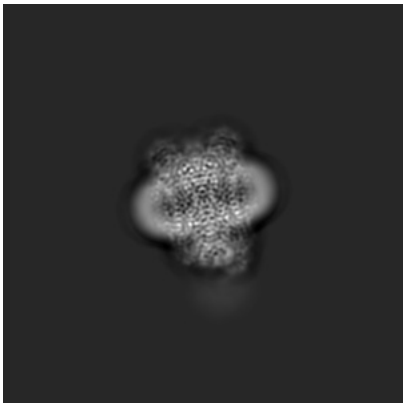
6.1.1 Primary map



X



Y

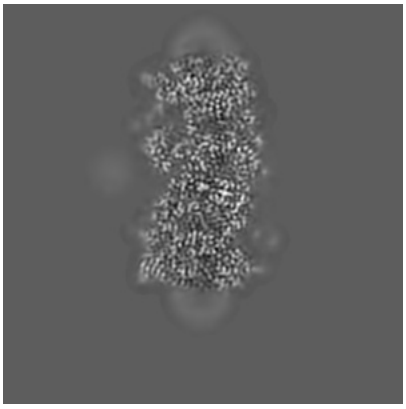


Z

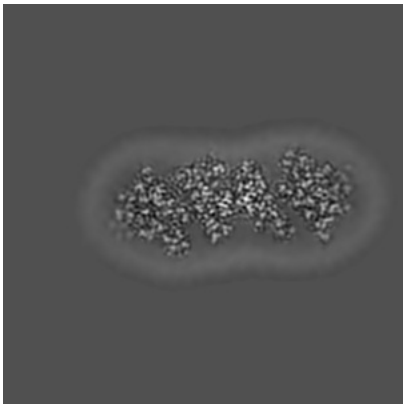
The images above show the map projected in three orthogonal directions.

6.2 Central slices

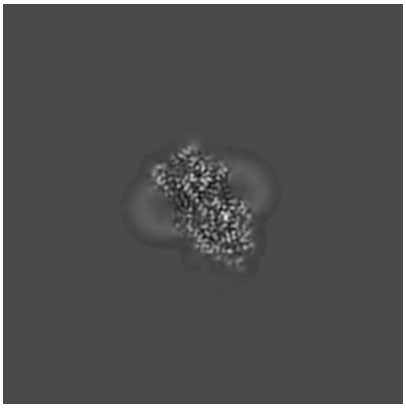
6.2.1 Primary map



X Index: 165



Y Index: 165

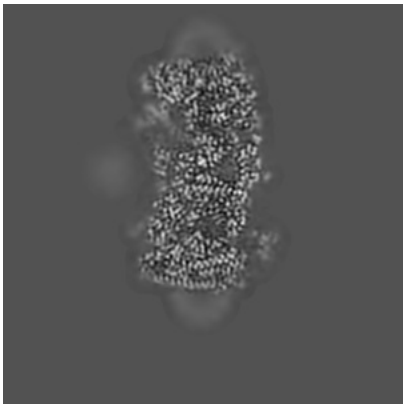


Z Index: 165

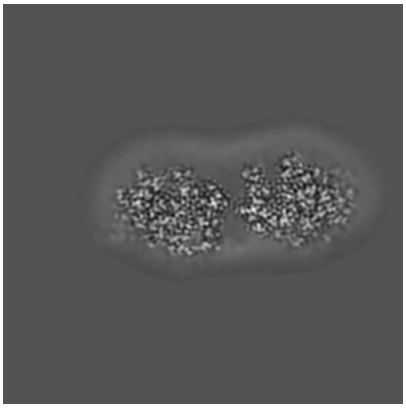
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

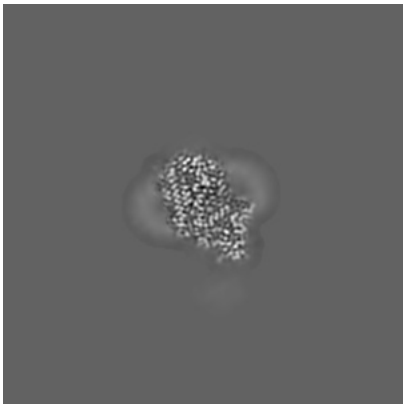
6.3.1 Primary map



X Index: 170



Y Index: 182

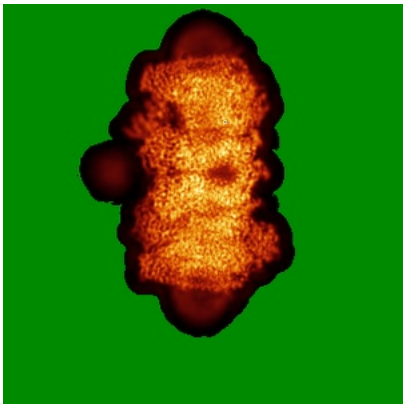


Z Index: 172

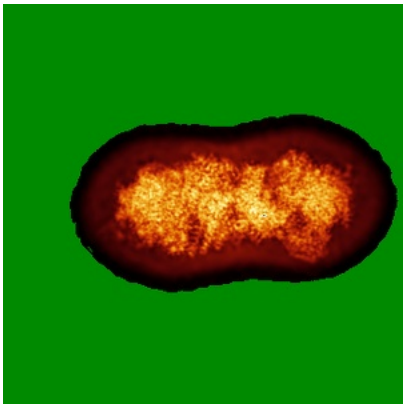
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

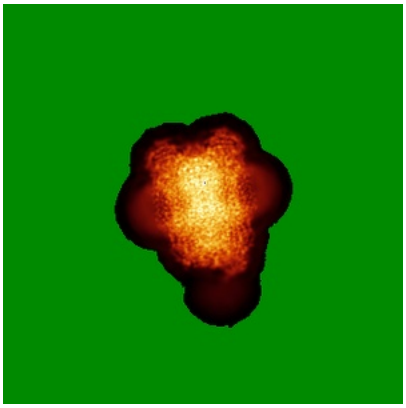
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.634. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

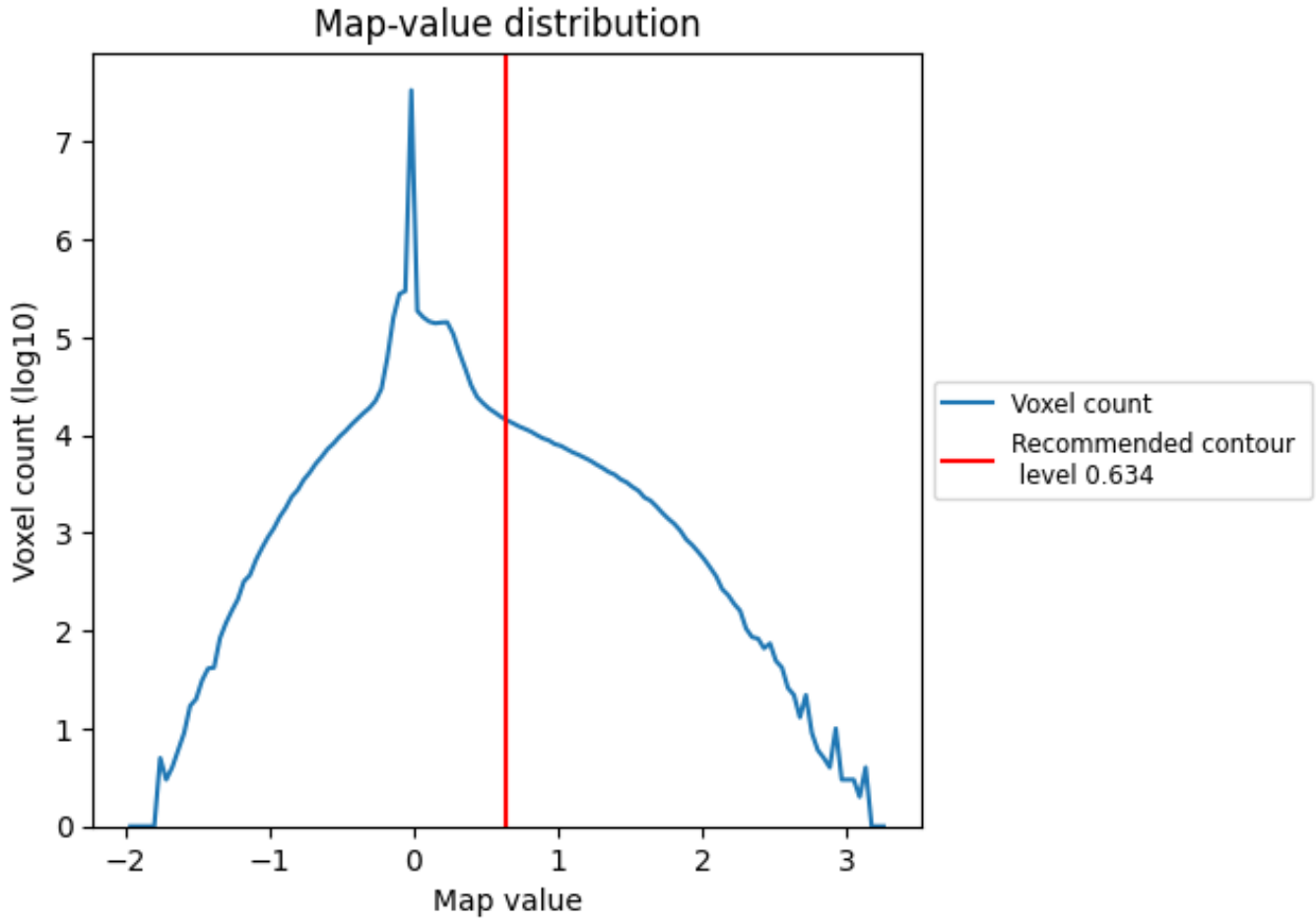
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

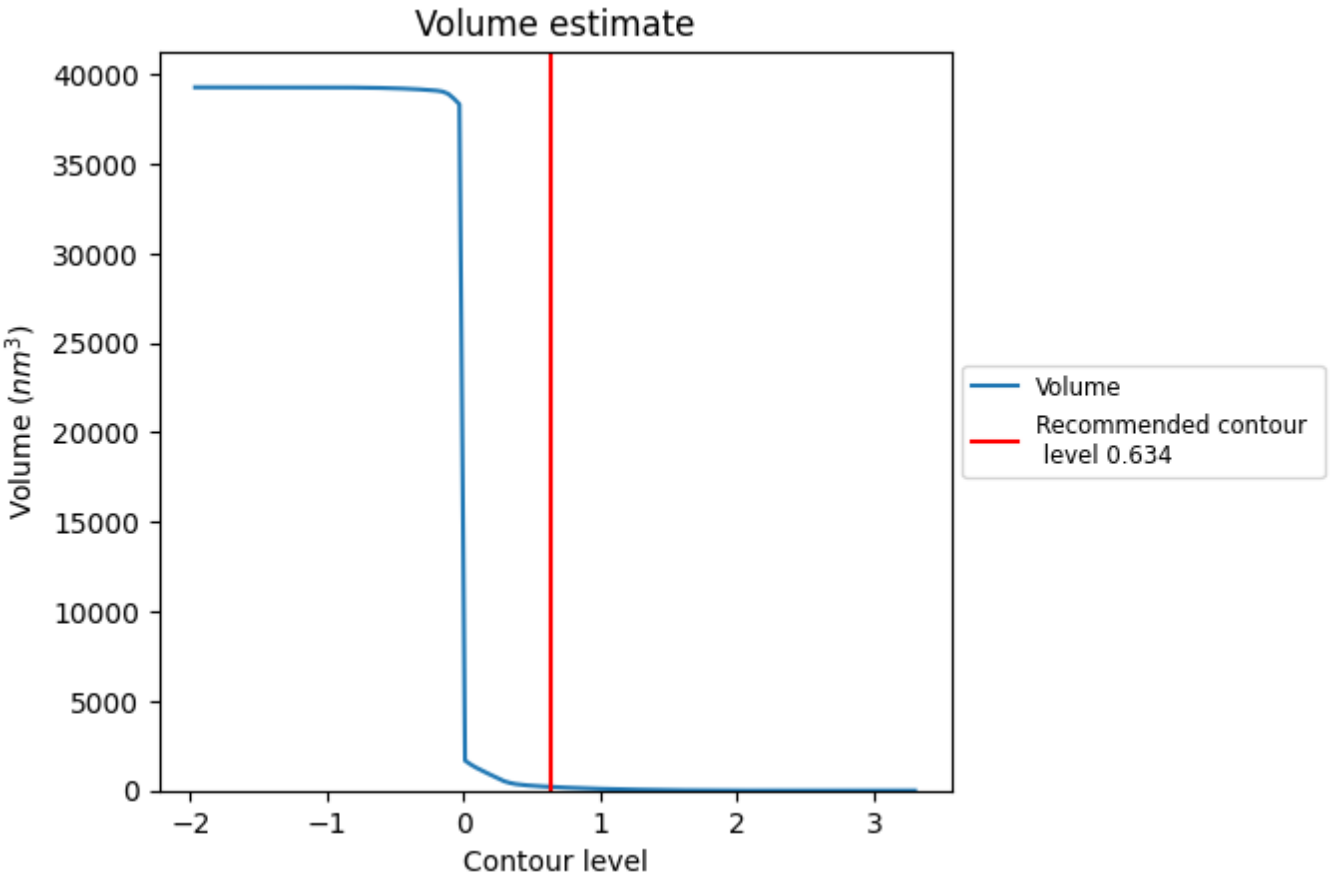
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

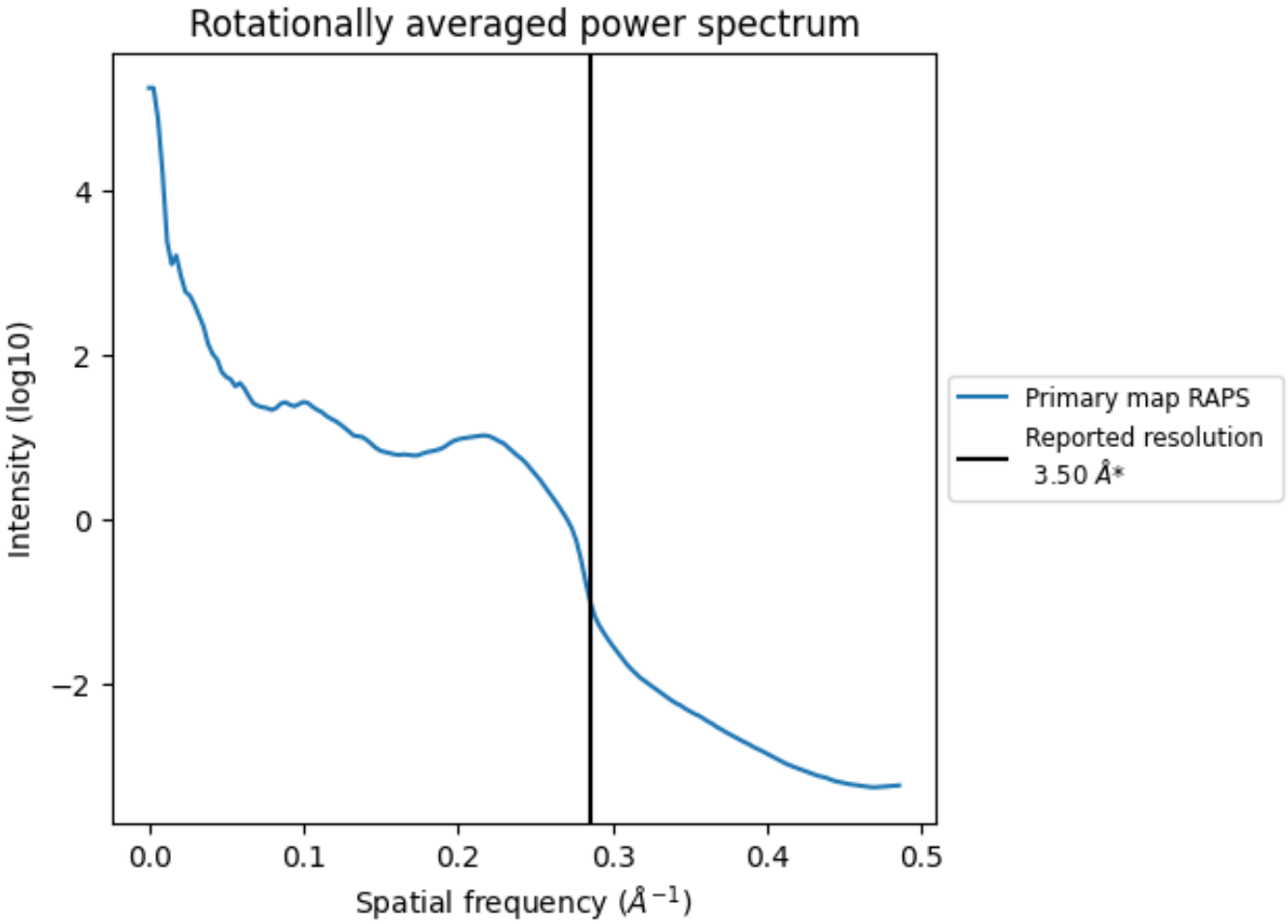
7.2 Volume estimate (i)



The volume at the recommended contour level is 206 nm^3; this corresponds to an approximate mass of 186 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

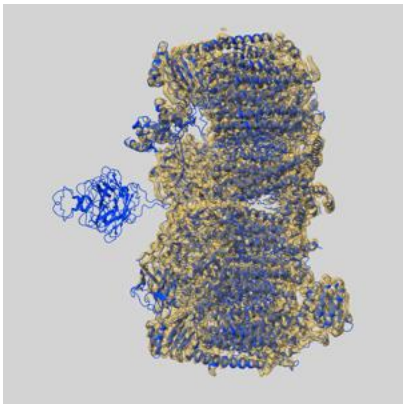
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

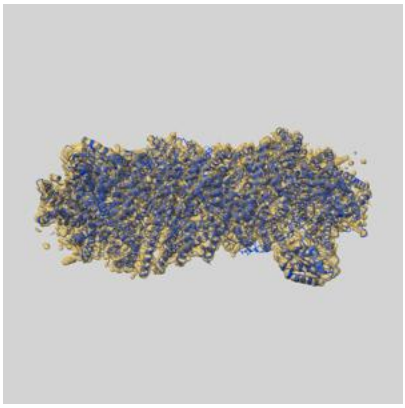
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24456 and PDB model 7RH6. Per-residue inclusion information can be found in section 3 on page 16.

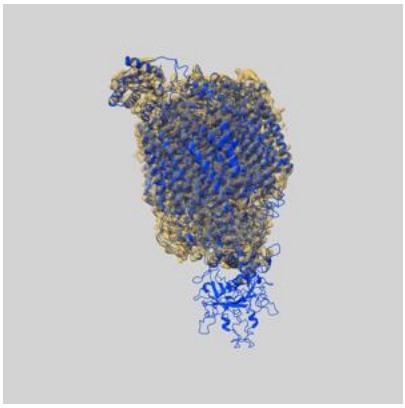
9.1 Map-model overlay



X



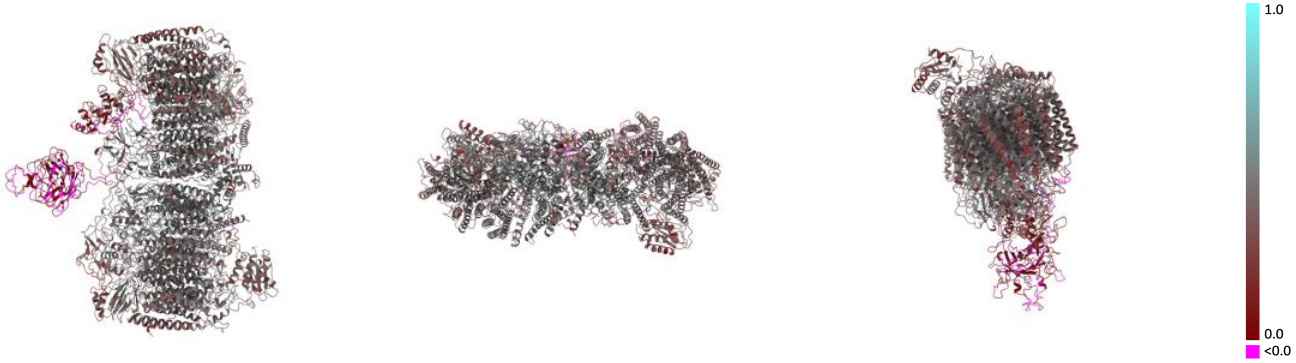
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.634 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

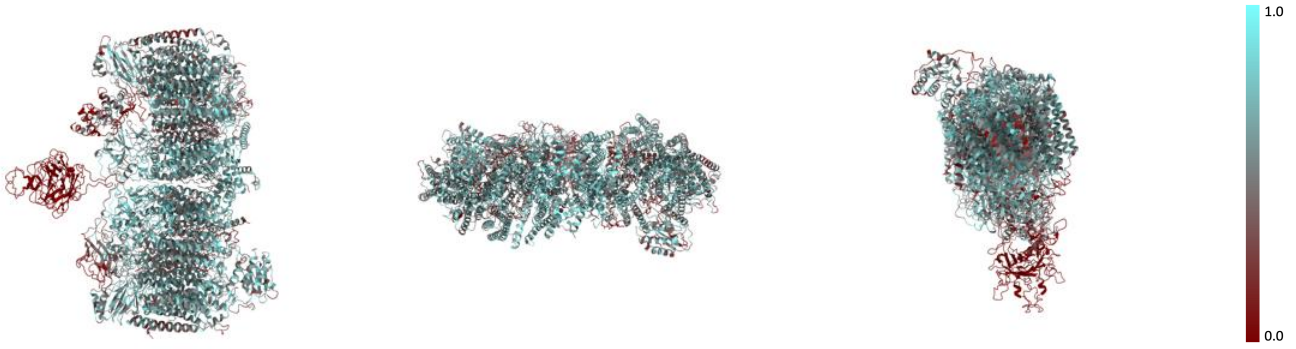
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

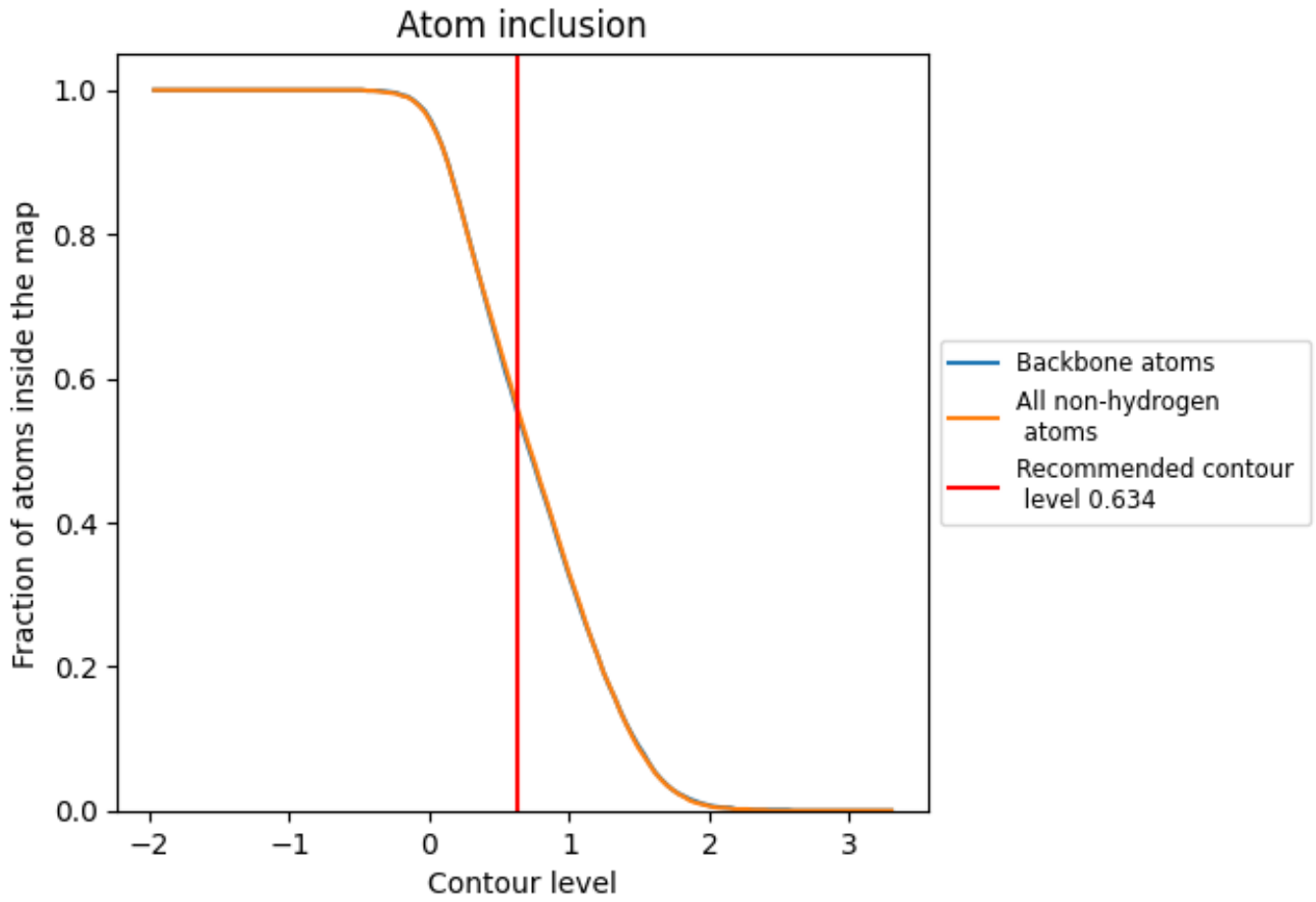
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.634).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.634) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5550	0.3950
D	0.1060	0.1100
E	0.6900	0.4680
F	0.6820	0.4590
G	0.1050	0.1110
I	0.6220	0.4400
J	0.4940	0.3960
K	0.5250	0.3690
L	0.6430	0.4400
M	0.6780	0.4330
O	0.2780	0.2240
P	0.5060	0.3970
Q	0.4680	0.3200
R	0.6210	0.4240
S	0.5620	0.3930
T	0.5170	0.3960
U	0.3950	0.3330
V	0.5040	0.3380
X	0.5640	0.4150
Y	0.6940	0.4470
Z	0.5570	0.4110
a	0.4750	0.3570
b	0.5690	0.3640
c	0.2700	0.3450

