wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 05:55 AM EDT

PDB ID	:	7RH5 / pdb_00007rh5
EMDB ID	:	EMD-24455
Title	:	Mycobacterial CIII2CIV2 supercomplex, Inhibitor free
Authors	:	Di Trani, J.M.; Yanofsky, D.J.; Rubinstein, J.L.
Deposited on	:	2021-07-16
Resolution	:	3.00 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:

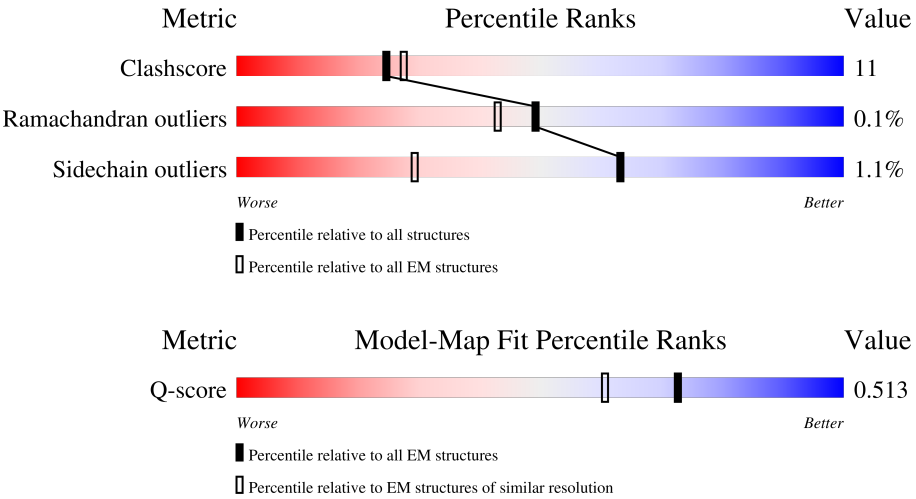
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	L	566	5% 76% 21%
1	R	566	77% 20%
2	E	535	5% 81% 18%
2	F	535	80% 19%

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Mol	Chain	Length	Quality of chain
3	D	216	91% 97%
3	G	216	91% 99%
4	K	341	31% 76% 15% 9%
4	Q	341	27% 74% 17% 9%
5	S	203	13% 84% 16%
5	X	203	13% 82% 17%
6	T	139	11% 83% 16%
6	Z	139	9% 81% 19%
7	U	79	48% 81% 19%
7	a	79	44% 92% 8%
8	V	145	23% 84% 15%
8	b	145	23% 83% 17%
9	J	100	15% 72% 20% 8%
9	P	100	14% 82% 9% 8%
10	I	223	13% 80% 19%
10	O	223	11% 78% 22%
11	W	159	60% 82% 17%
11	c	159	71% 84% 15%
12	M	382	7% 85% 15%
12	Y	382	6% 84% 16%

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
15	CDL	S	301	-	-	X	-
15	CDL	T	201	-	-	X	-
15	CDL	X	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CDL	X	302	-	-	X	-
15	CDL	Z	202	-	-	X	-
15	CDL	Z	203	-	-	X	-
21	HEC	I	302	X	-	-	-
21	HEC	O	302	X	-	-	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 95903 atoms, of which 46941 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 c oxidase subunit 1.

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

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

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

- Molecule 3 is a protein called Superoxide dismutase [Cu-Zn].

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

- Molecule 4 is a protein called Cytochrome aa3 subunit 2.

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

- Molecule 5 is a protein called Cytochrome aa3 subunit 3.

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

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide 4.

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

- Molecule 7 is a protein called Cytochrome c oxidase subunit CtaJ.

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

- Molecule 8 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

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

- Molecule 9 is a protein called Putative conserved transmembrane protein.

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

- Molecule 10 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	O	223	Total	C	H	N	O	S	0	0
			3187	1008	1564	289	314	12		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	223	Total	C	H	N	O	S	0	0
			3187	1008	1564	289	314	12		

- Molecule 11 is a protein called LpqE protein.

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

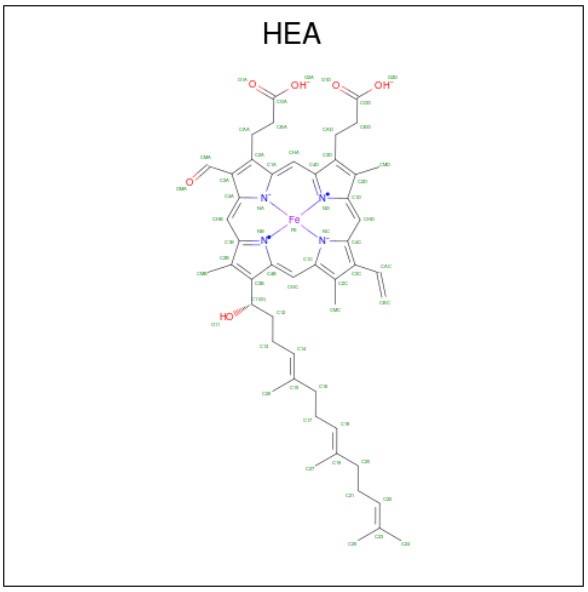
- Molecule 12 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

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

- Molecule 13 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

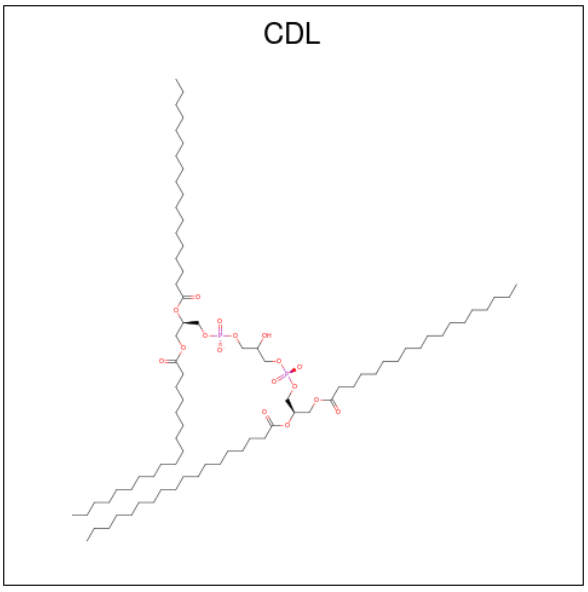
Mol	Chain	Residues	Atoms		AltConf
13	R	1	Total	Cu	0
			1	1	
13	L	1	Total	Cu	0
			1	1	
13	Q	2	Total	Cu	0
			2	2	
13	K	2	Total	Cu	0
			2	2	

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



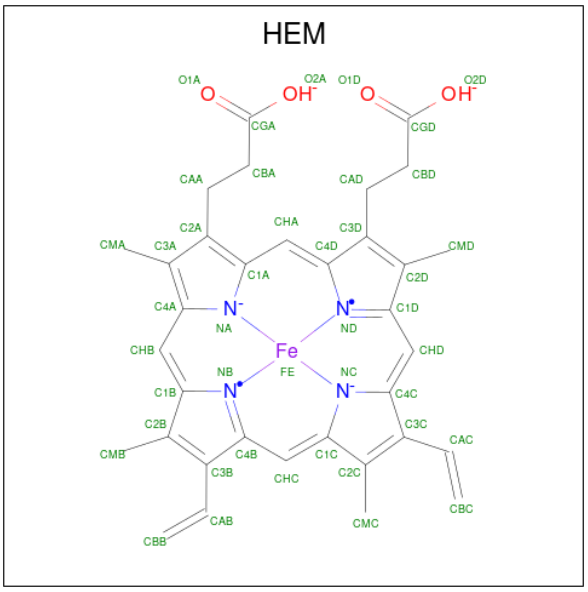
Mol	Chain	Residues	Atoms						AltConf
14	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
14	R	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
14	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
14	L	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



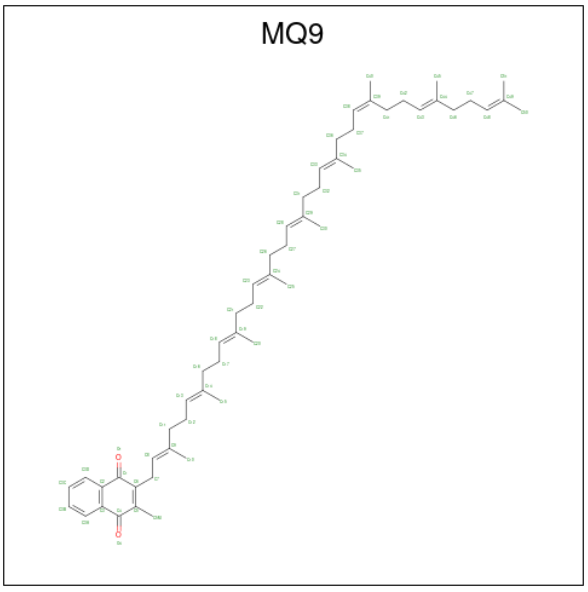
Mol	Chain	Residues	Atoms				AltConf
15	R	1	Total	C	O	P	0
			76	57	17	2	
15	E	1	Total	C	O	P	0
			76	57	17	2	
15	E	1	Total	C	O	P	0
			76	57	17	2	
15	F	1	Total	C	O	P	0
			76	57	17	2	
15	F	1	Total	C	O	P	0
			76	57	17	2	
15	L	1	Total	C	O	P	0
			76	57	17	2	
15	S	1	Total	C	O	P	0
			76	57	17	2	
15	T	1	Total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

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



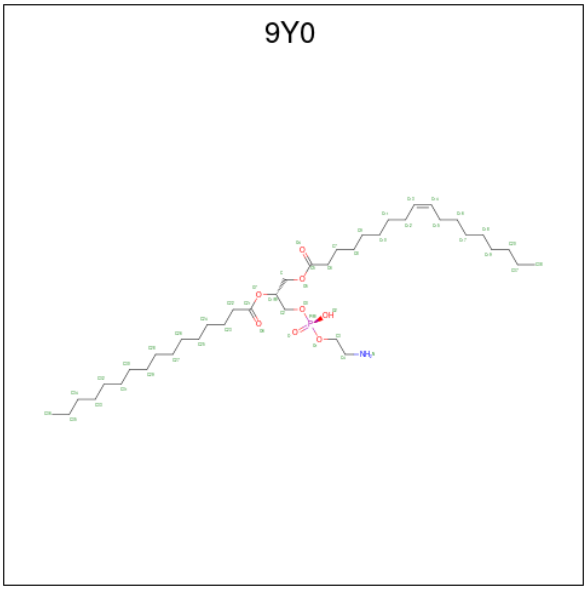
Mol	Chain	Residues	Atoms						AltConf
16	E	1	Total	C	Fe	H	N	O	0
			69	33	1	27	4	4	
16	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
16	F	1	Total	C	Fe	H	N	O	0
			69	33	1	27	4	4	
16	F	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 17 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



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

- Molecule 18 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: $C_{39}H_{76}NO_8P$).



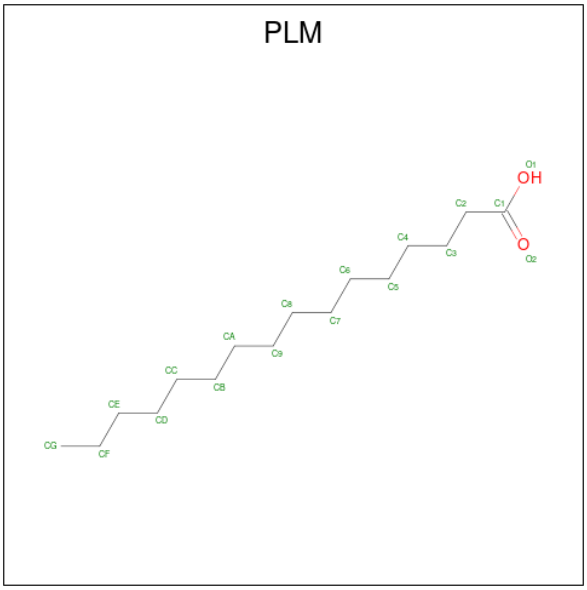
Mol	Chain	Residues	Atoms						AltConf
18	F	1	Total	C	H	N	O	P	0
			123	39	74	1	8	1	
18	S	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
18	P	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

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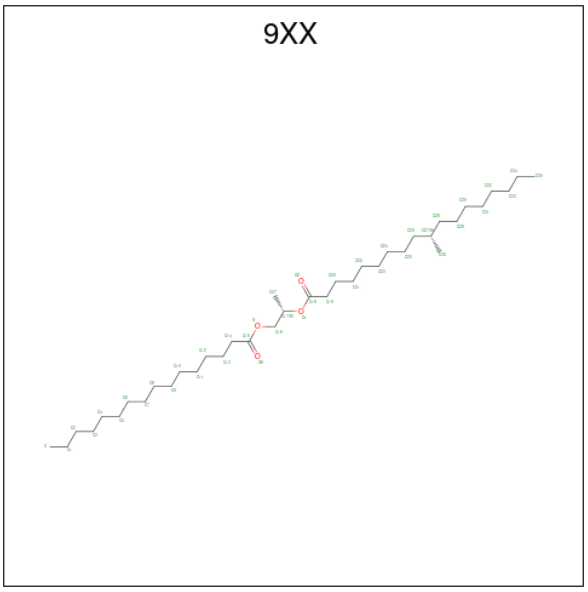
Mol	Chain	Residues	Atoms						AltConf
18	X	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
18	J	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
18	J	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	

- Molecule 19 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



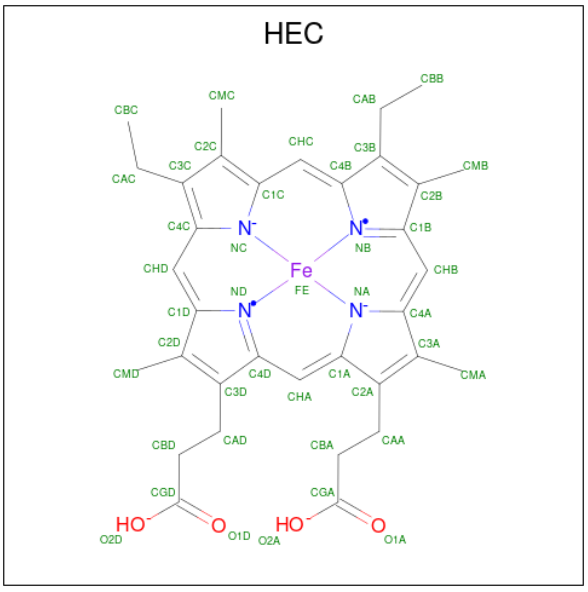
Mol	Chain	Residues	Atoms				AltConf
19	D	1	Total	C	H	O	0
			27	10	16	1	
19	G	1	Total	C	H	O	0
			27	10	16	1	
19	c	1	Total	C	H	O	0
			48	16	31	1	
19	W	1	Total	C	H	O	0
			48	16	31	1	

- Molecule 20 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: $C_{38}H_{74}O_4$).



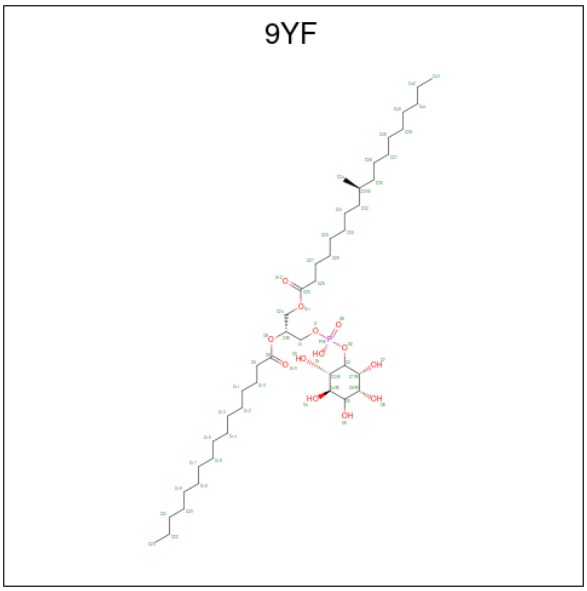
Mol	Chain	Residues	Atoms				AltConf
20	D	1	Total	C	H	O	0
			83	28	51	4	
20	G	1	Total	C	H	O	0
			83	28	51	4	
20	c	1	Total	C	H	O	0
			115	38	73	4	
20	W	1	Total	C	H	O	0
			115	38	73	4	

- Molecule 21 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 22 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: $C_{44}H_{85}O_{13}P$).



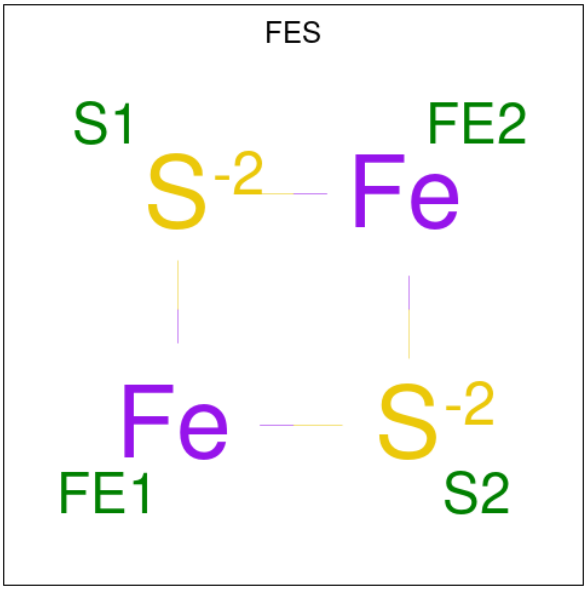
Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	H	O	P	0
			142	44	84	13	1	
22	c	1	Total	C	H	O	P	0
			142	44	84	13	1	
22	I	1	Total	C	H	O	P	0
			142	44	84	13	1	
22	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
22	Y	1	Total	C	H	O	P	0
			142	44	84	13	1	
22	W	1	Total	C	H	O	P	0
			142	44	84	13	1	
22	M	1	Total	C	H	O	P	0
			142	44	84	13	1	

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Mol	Chain	Residues	Atoms					AltConf
22	M	1	Total	C	H	O	P	0
			142	44	84	13	1	

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

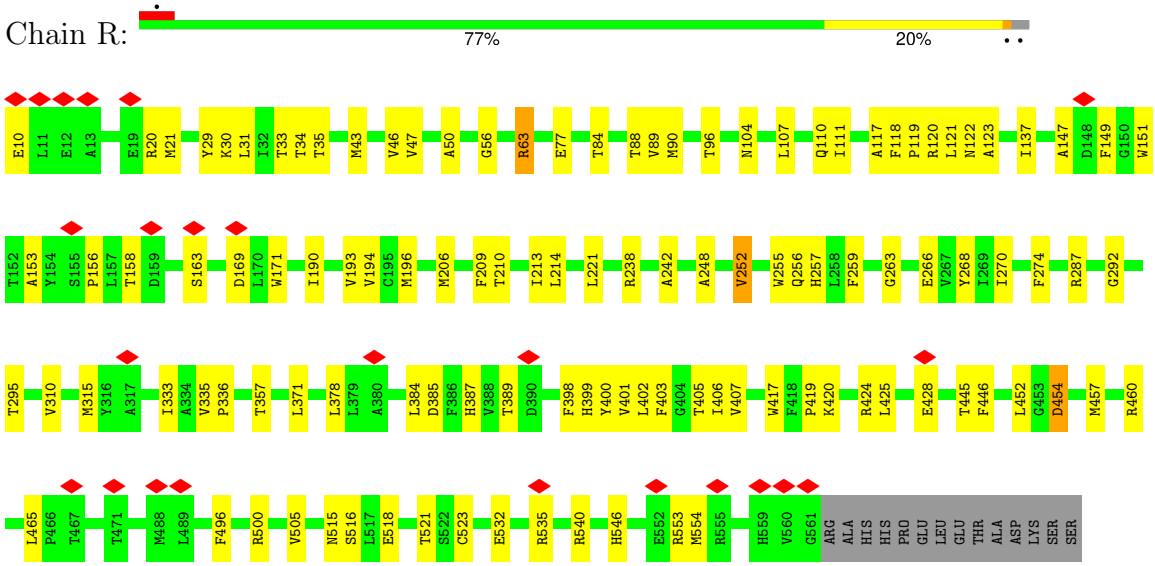


Mol	Chain	Residues	Atoms			AltConf
23	Y	1	Total	Fe	S	0
			4	2	2	
23	M	1	Total	Fe	S	0
			4	2	2	

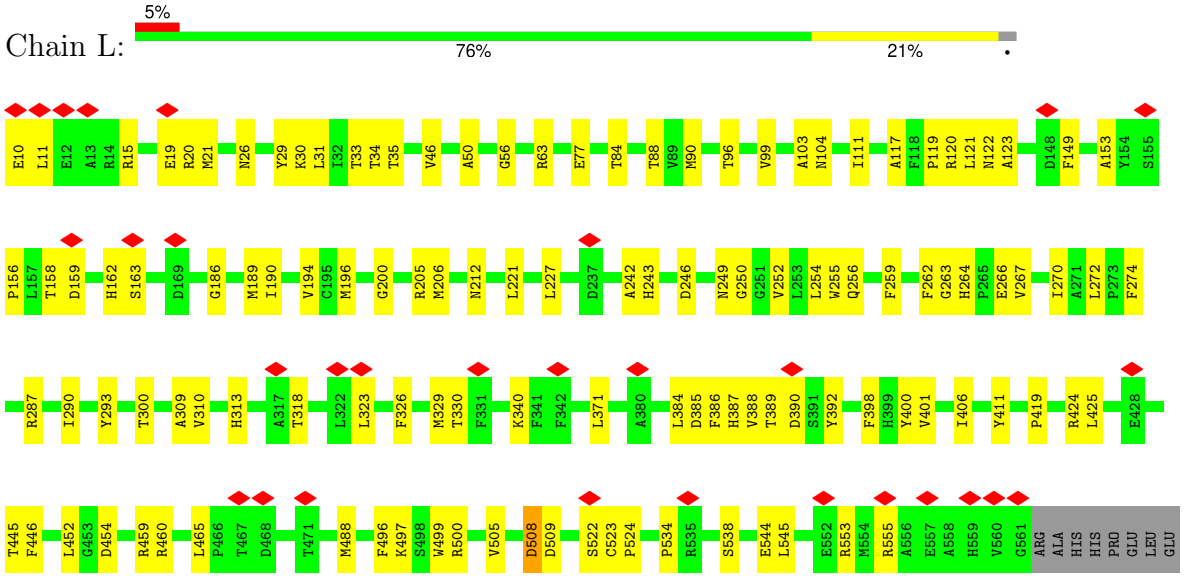
3 Residue-property plots (i)

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 c oxidase subunit 1



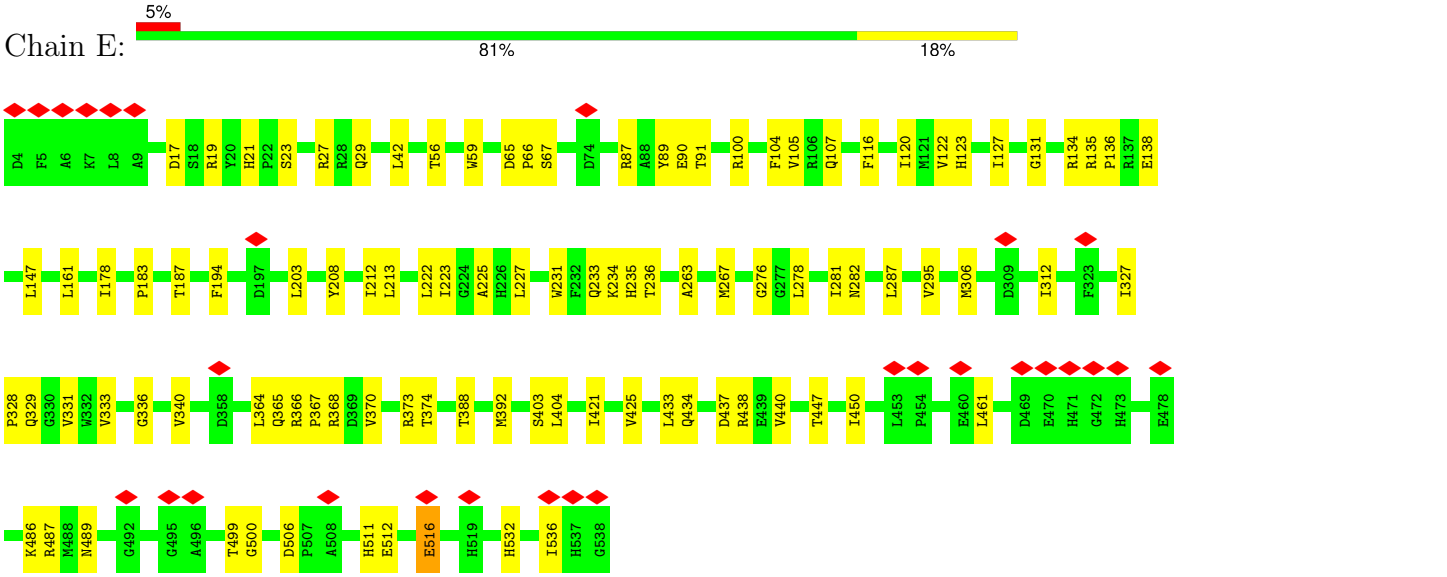
• Molecule 1: Cytochrome c oxidase subunit 1





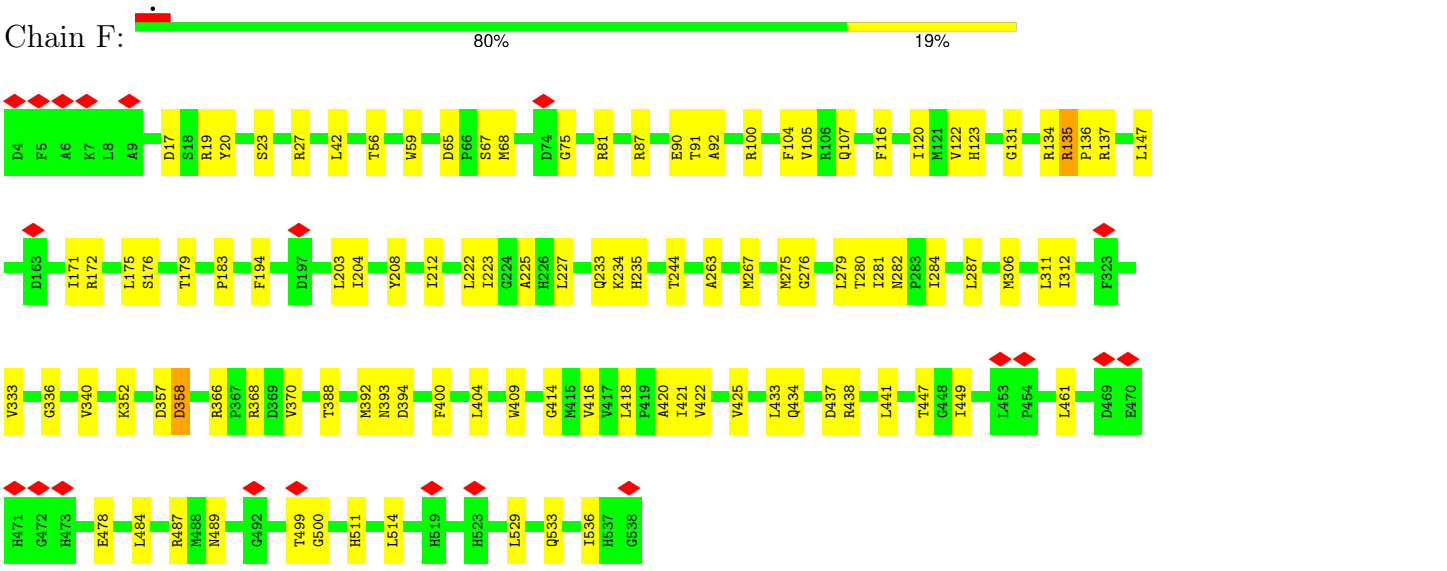
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain E:



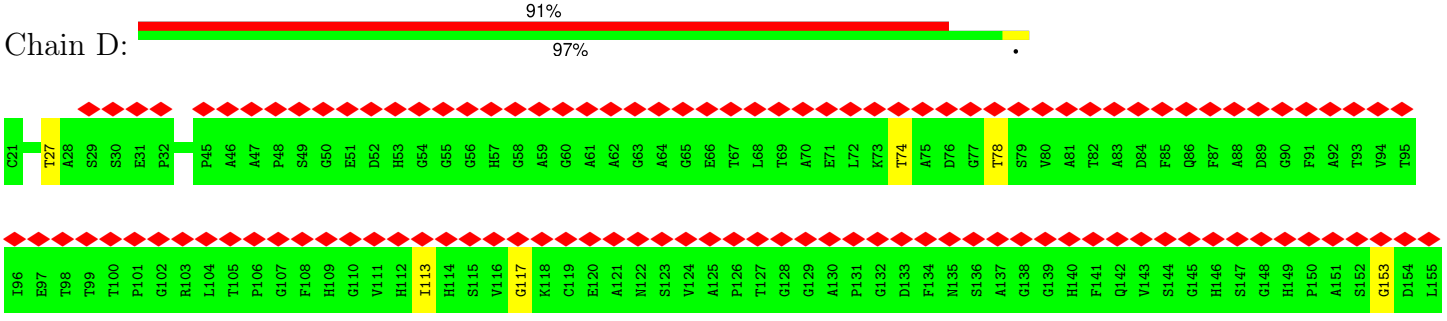
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

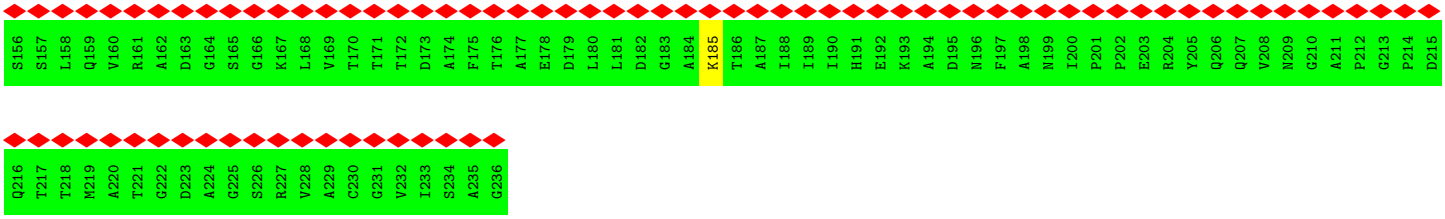
Chain F:



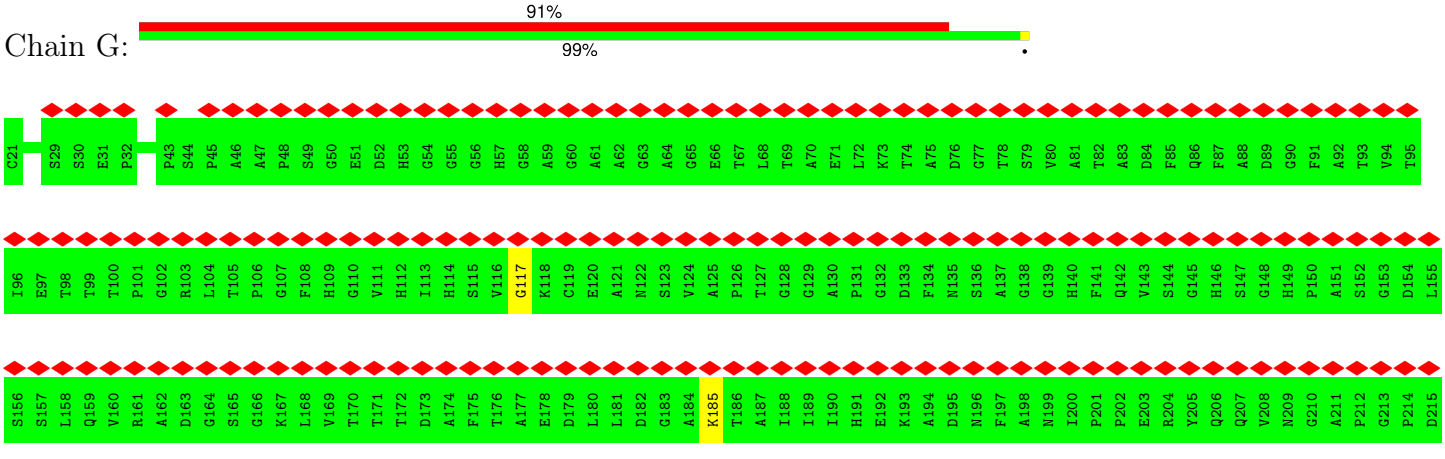
• Molecule 3: Superoxide dismutase [Cu-Zn]

Chain D:

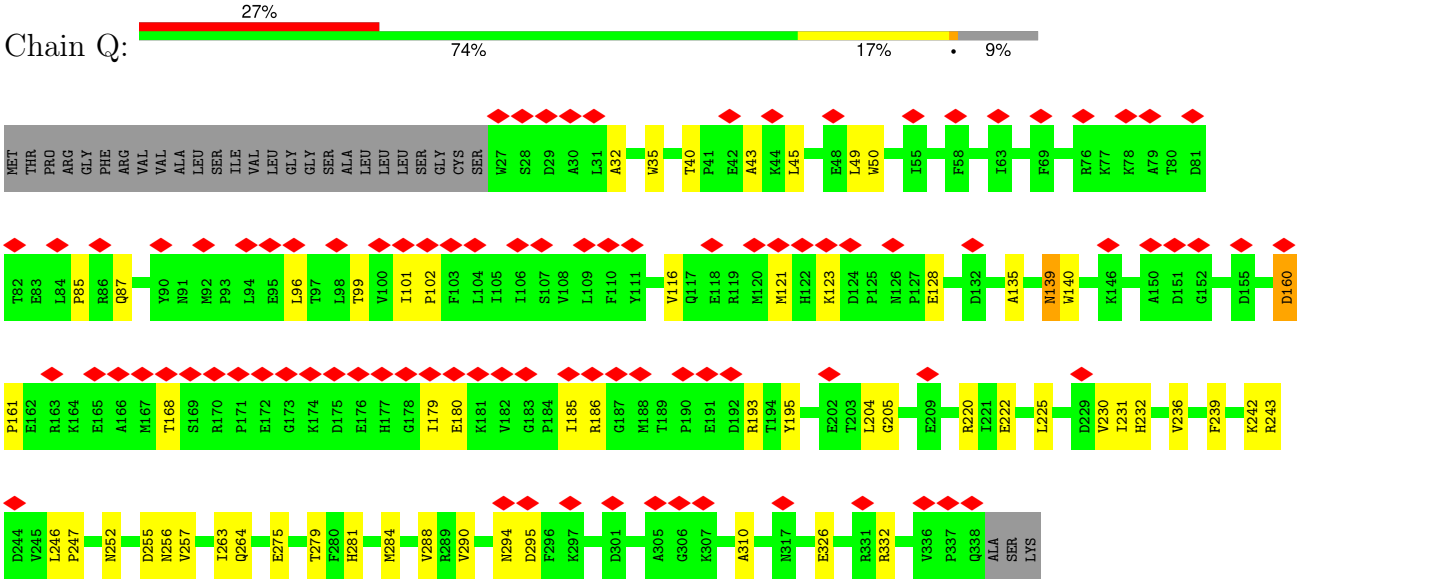




• Molecule 3: Superoxide dismutase [Cu-Zn]

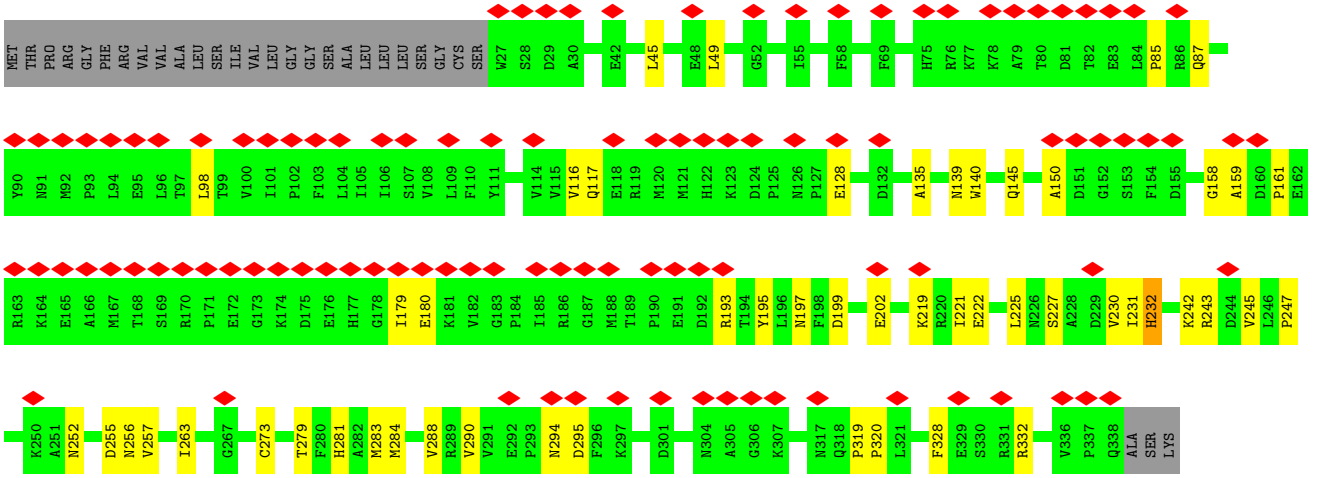


• Molecule 4: Cytochrome aa3 subunit 2

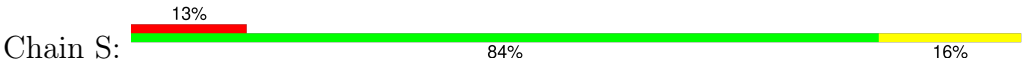


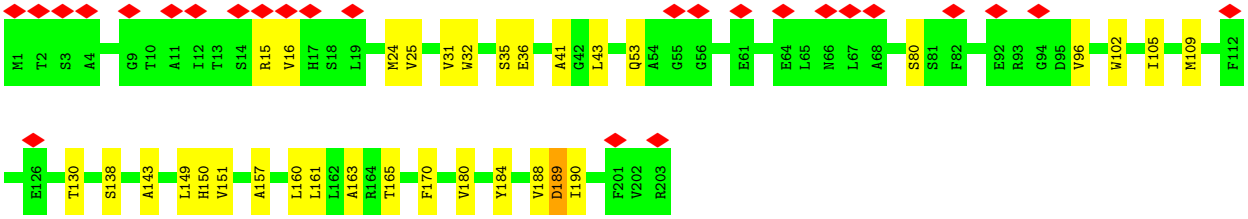
• Molecule 4: Cytochrome aa3 subunit 2



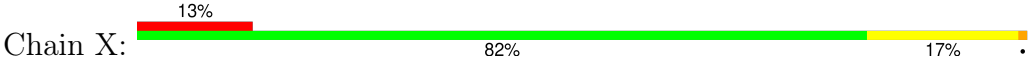


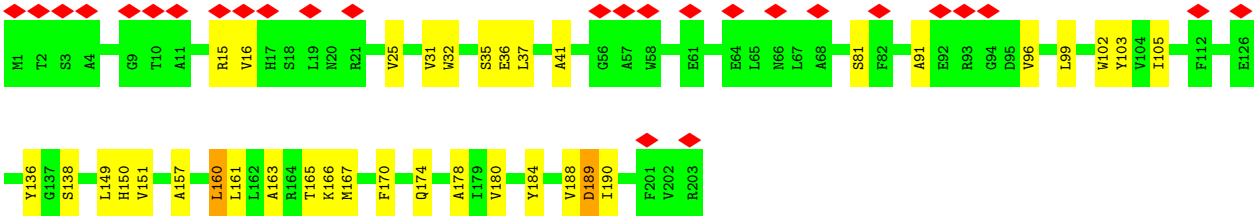
• Molecule 5: Cytochrome aa3 subunit 3



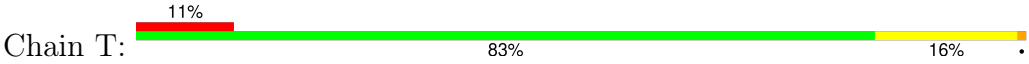


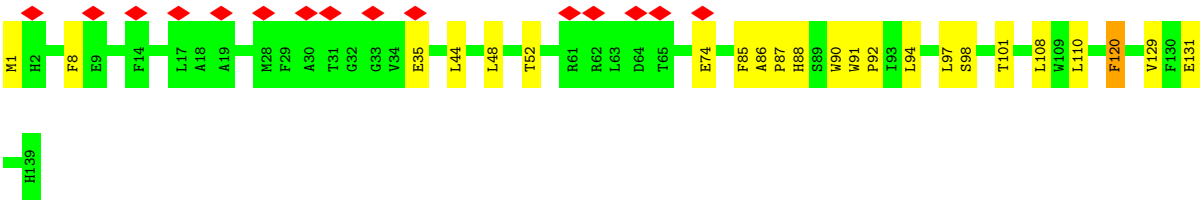
• Molecule 5: Cytochrome aa3 subunit 3





• Molecule 6: Cytochrome c oxidase polypeptide 4

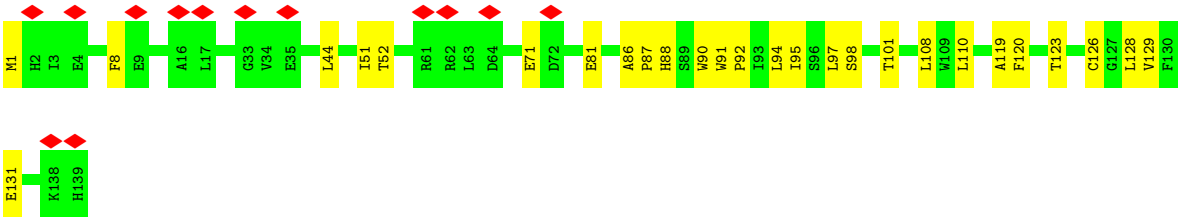




• Molecule 6: Cytochrome c oxidase polypeptide 4

Chain Z:

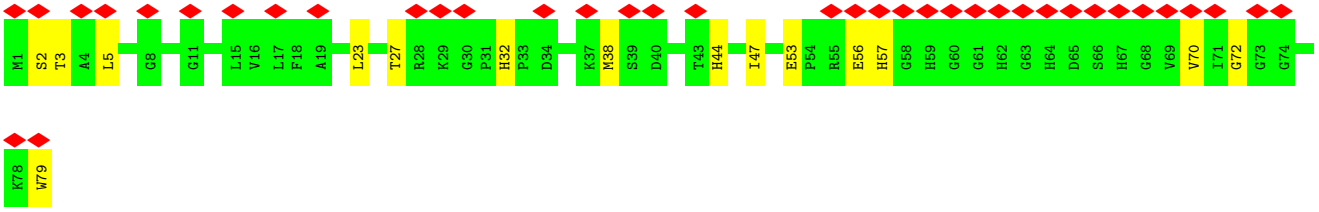




• Molecule 7: Cytochrome c oxidase subunit CtaJ

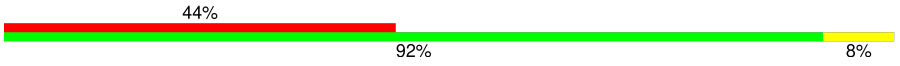
Chain U:

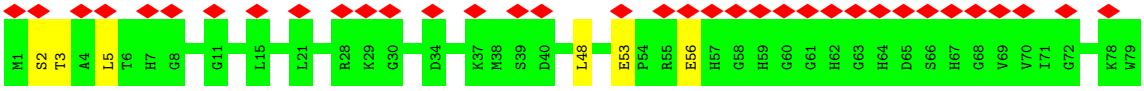




• Molecule 7: Cytochrome c oxidase subunit CtaJ

Chain a:

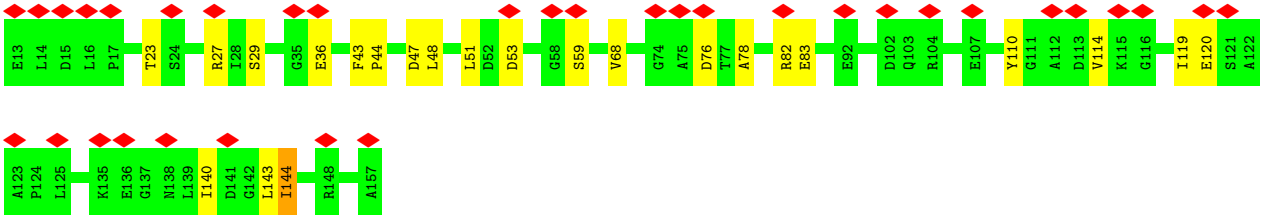




• Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:

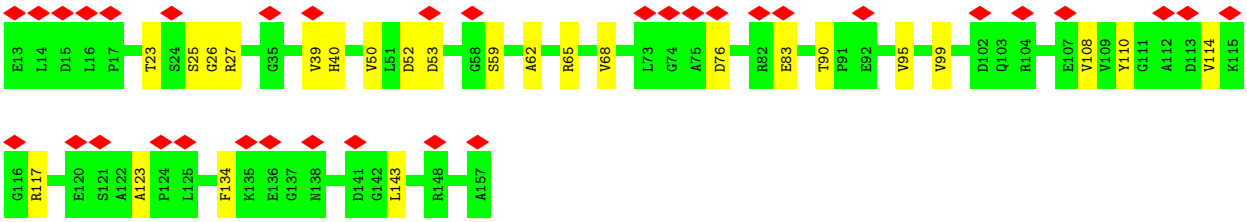




• Molecule 8: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain b:

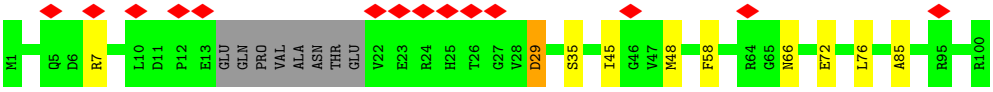




• Molecule 9: Putative conserved transmembrane protein

Chain P:

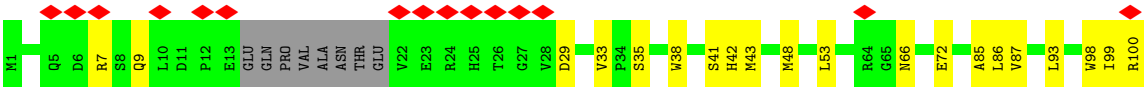




• Molecule 9: Putative conserved transmembrane protein

Chain J:

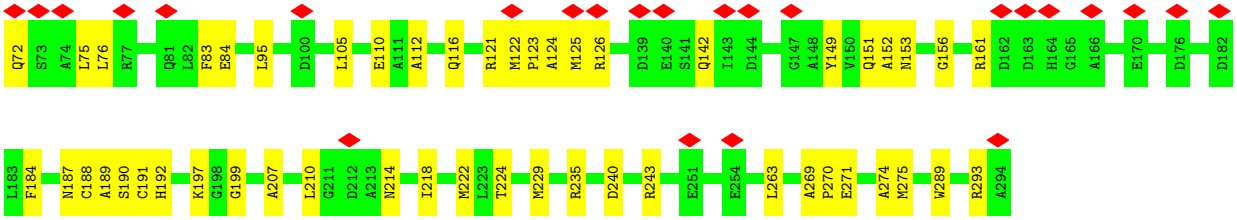




• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain O:

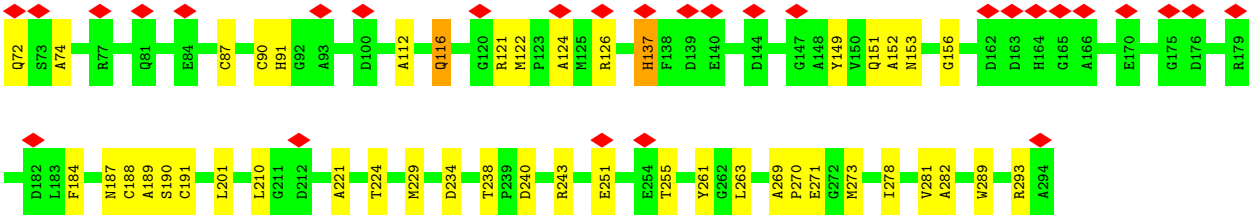




• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain I:

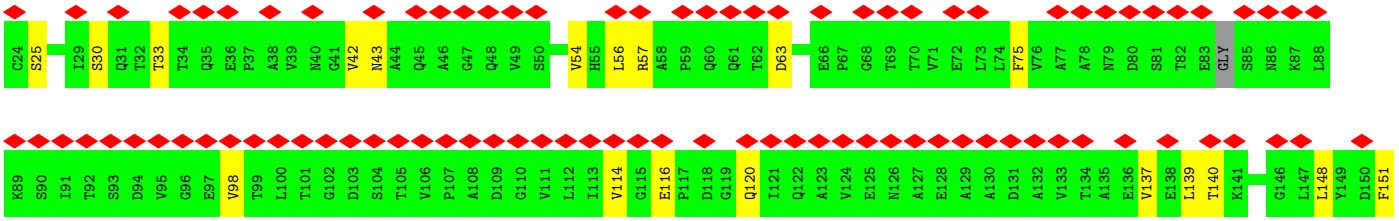


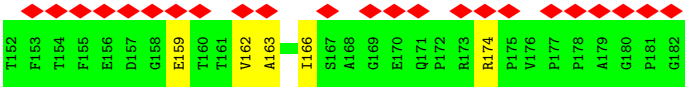


• Molecule 11: LpqE protein

Chain c:



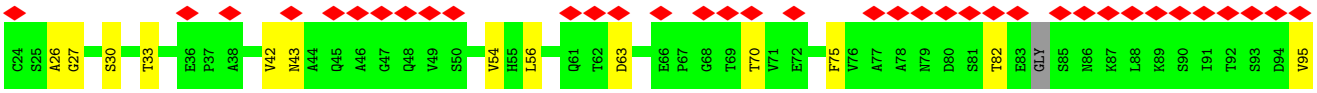


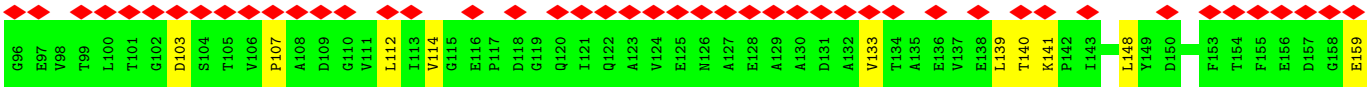


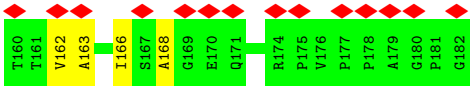
• Molecule 11: LpqE protein

Chain W:







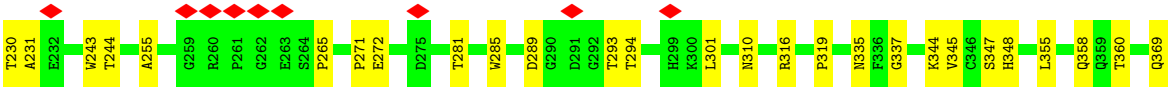


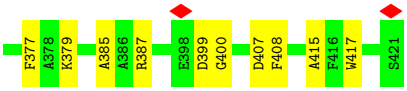
• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain Y:







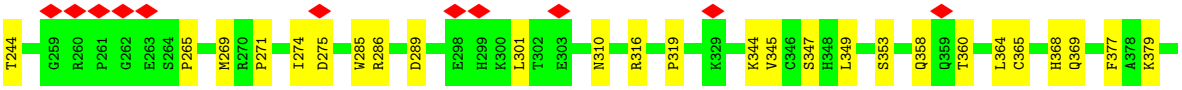


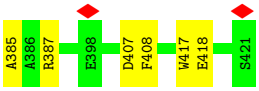
• Molecule 12: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain M:









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	5.732	Depositor
Minimum map value	-3.132	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.173	Depositor
Recommended contour level	1.1	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, PLM, CU, CDL, 9Y0, HEC, 9YF, 9XX, FES, MQ9, HEM

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	L	0.17	0/4530	0.34	0/6188
1	R	0.17	0/4530	0.33	0/6188
2	E	0.20	0/4314	0.38	0/5882
2	F	0.22	0/4314	0.40	0/5882
3	D	0.14	0/1099	0.33	0/1519
3	G	0.13	0/1099	0.34	0/1519
4	K	0.18	0/2534	0.37	0/3451
4	Q	0.16	0/2534	0.33	0/3451
5	S	0.17	0/1608	0.32	0/2195
5	X	0.18	0/1608	0.32	0/2195
6	T	0.39	1/1112 (0.1%)	0.64	4/1524 (0.3%)
6	Z	0.17	0/1112	0.31	0/1524
7	U	0.12	0/613	0.27	0/836
7	a	0.12	0/613	0.28	0/836
8	V	0.16	0/1059	0.34	0/1446
8	b	0.15	0/1059	0.35	0/1446
9	J	0.15	0/757	0.29	0/1027
9	P	0.24	0/757	0.33	0/1027
10	I	0.18	0/1660	0.39	0/2250
10	O	0.37	0/1660	0.64	2/2250 (0.1%)
11	W	0.14	0/1166	0.32	0/1599
11	c	0.13	0/1166	0.33	0/1599
12	M	0.26	0/3056	0.47	0/4142
12	Y	0.20	0/3056	0.38	1/4142 (0.0%)
All	All	0.20	1/47016 (0.0%)	0.38	7/64118 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	120	PHE	C-O	-7.60	1.15	1.24

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	120	PHE	CA-C-O	-9.17	111.09	120.90
6	T	120	PHE	CA-C-N	5.99	128.66	120.46
6	T	120	PHE	C-N-CA	5.99	128.66	120.46
10	O	197	LYS	N-CA-C	-5.48	103.39	110.19
10	O	274	ALA	N-CA-C	-5.37	105.50	111.36

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	L	4370	4347	4346	99	0
1	R	4370	4346	4345	106	0
2	E	4181	4203	4202	83	0
2	F	4181	4200	4199	86	0
3	D	1092	640	640	3	0
3	G	1092	640	640	1	0
4	K	2465	2392	2392	39	0
4	Q	2465	2392	2392	52	0
5	S	1560	1548	1547	64	0
5	X	1560	1548	1547	82	0
6	T	1077	1059	1058	52	0
6	Z	1077	1058	1058	65	0
7	U	591	576	576	10	0
7	a	591	576	576	5	0
8	V	1041	1052	1052	18	0
8	b	1041	1052	1052	18	0
9	J	736	718	717	14	0
9	P	736	717	717	11	0
10	I	1623	1564	1564	43	0
10	O	1623	1564	1564	46	0
11	W	1149	1110	1110	23	0
11	c	1149	1110	1110	20	0
12	M	2977	2984	2984	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	2977	2984	2984	47	0
13	K	2	0	0	0	0
13	L	1	0	0	0	0
13	Q	2	0	0	0	0
13	R	1	0	0	0	0
14	L	120	108	108	5	0
14	R	120	108	108	4	0
15	E	152	0	192	13	0
15	F	152	0	192	21	0
15	J	76	0	96	11	0
15	L	76	0	96	19	0
15	P	76	0	96	10	0
15	R	76	0	96	19	0
15	S	76	0	96	49	0
15	T	228	0	288	48	0
15	X	152	0	192	96	0
15	Z	152	0	192	81	0
16	E	85	57	57	4	0
16	F	85	57	57	5	0
17	E	116	160	160	4	0
17	F	232	320	320	5	0
17	I	58	80	80	1	0
17	Z	58	80	80	5	0
18	F	49	74	0	0	0
18	J	98	150	0	0	0
18	P	49	75	0	0	0
18	S	49	75	0	0	0
18	X	49	75	0	0	0
19	D	11	16	16	0	0
19	G	11	16	16	0	0
19	W	17	31	31	2	0
19	c	17	31	31	0	0
20	D	32	51	0	0	0
20	G	32	51	0	0	0
20	W	42	73	0	0	0
20	c	42	73	0	0	0
21	I	86	64	64	13	0
21	O	86	64	64	16	0
22	I	58	84	0	5	0
22	M	116	168	0	0	0
22	O	58	84	0	0	0
22	W	58	84	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Y	116	168	0	5	0
22	c	58	84	0	1	0
23	M	4	0	0	0	0
23	Y	4	0	0	1	0
All	All	48962	46941	47100	1013	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 11.

The worst 5 of 1013 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)
5:X:166:LYS:NZ	15:X:301:CDL:H112	1.28	1.48
15:Z:203:CDL:H631	22:I:304:9YF:C23	1.48	1.41
6:Z:120:PHE:CB	15:Z:202:CDL:H612	1.53	1.38
15:Z:203:CDL:C63	22:I:304:9YF:C23	2.03	1.35
6:Z:120:PHE:HB3	15:Z:202:CDL:C61	1.58	1.31

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	L	550/566 (97%)	516 (94%)	34 (6%)	0	100	100
1	R	550/566 (97%)	518 (94%)	32 (6%)	0	100	100
2	E	533/535 (100%)	490 (92%)	43 (8%)	0	100	100
2	F	533/535 (100%)	489 (92%)	43 (8%)	1 (0%)	43	76
3	D	214/216 (99%)	193 (90%)	20 (9%)	1 (0%)	24	60
3	G	214/216 (99%)	187 (87%)	27 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	310/341 (91%)	282 (91%)	28 (9%)	0	100	100
4	Q	310/341 (91%)	282 (91%)	28 (9%)	0	100	100
5	S	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
5	X	201/203 (99%)	192 (96%)	9 (4%)	0	100	100
6	T	137/139 (99%)	129 (94%)	8 (6%)	0	100	100
6	Z	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
7	U	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9	38
7	a	77/79 (98%)	70 (91%)	7 (9%)	0	100	100
8	V	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
8	b	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
9	J	88/100 (88%)	85 (97%)	3 (3%)	0	100	100
9	P	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
10	I	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
10	O	221/223 (99%)	199 (90%)	22 (10%)	0	100	100
11	W	154/159 (97%)	137 (89%)	17 (11%)	0	100	100
11	c	154/159 (97%)	135 (88%)	19 (12%)	0	100	100
12	M	380/382 (100%)	344 (90%)	36 (10%)	0	100	100
12	Y	380/382 (100%)	348 (92%)	31 (8%)	1 (0%)	36	70
All	All	6016/6176 (97%)	5549 (92%)	463 (8%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	135	ARG
12	Y	113	GLU
3	D	27	THR
7	U	70	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	L	452/465 (97%)	445 (98%)	7 (2%)	57	80
1	R	452/465 (97%)	447 (99%)	5 (1%)	65	83
2	E	429/429 (100%)	423 (99%)	6 (1%)	59	80
2	F	429/429 (100%)	423 (99%)	6 (1%)	59	80
3	D	20/151 (13%)	20 (100%)	0	100	100
3	G	20/151 (13%)	20 (100%)	0	100	100
4	K	260/288 (90%)	257 (99%)	3 (1%)	63	82
4	Q	260/288 (90%)	258 (99%)	2 (1%)	73	86
5	S	155/161 (96%)	153 (99%)	2 (1%)	61	81
5	X	155/161 (96%)	152 (98%)	3 (2%)	50	76
6	T	106/106 (100%)	106 (100%)	0	100	100
6	Z	106/106 (100%)	106 (100%)	0	100	100
7	U	59/59 (100%)	59 (100%)	0	100	100
7	a	59/59 (100%)	59 (100%)	0	100	100
8	V	107/107 (100%)	105 (98%)	2 (2%)	50	76
8	b	107/107 (100%)	106 (99%)	1 (1%)	70	85
9	J	76/83 (92%)	73 (96%)	3 (4%)	28	62
9	P	76/83 (92%)	75 (99%)	1 (1%)	61	81
10	I	163/163 (100%)	160 (98%)	3 (2%)	51	77
10	O	163/163 (100%)	162 (99%)	1 (1%)	78	88
11	W	127/127 (100%)	127 (100%)	0	100	100
11	c	127/127 (100%)	126 (99%)	1 (1%)	73	86
12	M	312/312 (100%)	310 (99%)	2 (1%)	78	88
12	Y	312/312 (100%)	309 (99%)	3 (1%)	68	84
All	All	4532/4902 (92%)	4481 (99%)	51 (1%)	63	83

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	V	83	GLU
5	X	160	LEU
12	M	120	GLU
8	V	144	ILE
4	K	139	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
7	a	64	HIS
10	I	137	HIS
12	M	331	GLN
10	I	169	GLN
10	I	81	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 66 ligands modelled in this entry, 6 are monoatomic - leaving 60 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	$\#\|Z\| > 2$
20	9XX	G	302	3	31,31,41	1.12	3 (9%)	34,34,44	1.47	5 (14%)
17	MQ9	I	303	-	59,59,59	2.39	22 (37%)	73,75,75	1.43	17 (23%)
19	PLM	W	201	11	15,16,17	0.49	0	14,15,17	0.33	0
22	9YF	W	203	-	58,58,58	1.01	5 (8%)	68,71,71	1.13	3 (4%)
15	CDL	L	604	-	75,75,99	0.34	0	81,87,111	0.72	3 (3%)
20	9XX	D	302	-	31,31,41	1.11	3 (9%)	34,34,44	1.44	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CDL	T	203	-	75,75,99	0.37	0	81,87,111	0.45	0
18	9Y0	X	303	-	48,48,48	1.16	3 (6%)	51,53,53	0.90	2 (3%)
22	9YF	Y	502	-	58,58,58	1.08	7 (12%)	68,71,71	1.30	7 (10%)
23	FES	Y	501	12	0,4,4	-	-	-		
16	HEM	E	602	2	50,50,50	1.42	7 (14%)	67,82,82	1.14	5 (7%)
16	HEM	F	702	2	49,49,50	1.37	5 (10%)	67,81,82	1.03	2 (2%)
15	CDL	S	301	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
15	CDL	R	604	-	75,75,99	0.34	0	81,87,111	0.60	2 (2%)
18	9Y0	J	202	-	48,48,48	1.17	3 (6%)	51,53,53	0.90	2 (3%)
16	HEM	E	601	2	49,49,50	1.38	7 (14%)	67,81,82	1.05	2 (2%)
22	9YF	M	501	-	58,58,58	1.08	7 (12%)	68,71,71	1.29	7 (10%)
17	MQ9	F	701	-	59,59,59	2.45	23 (38%)	73,75,75	1.38	15 (20%)
19	PLM	G	301	3	9,10,17	0.54	0	8,9,17	0.43	0
15	CDL	E	606	-	75,75,99	0.36	0	81,87,111	0.42	0
21	HEC	O	302	10	50,50,50	1.72	6 (12%)	68,82,82	1.43	7 (10%)
14	HEA	L	602	1	67,67,67	1.42	11 (16%)	81,103,103	2.38	30 (37%)
21	HEC	I	301	-	50,50,50	1.78	5 (10%)	68,82,82	1.32	5 (7%)
17	MQ9	E	603	-	59,59,59	2.44	23 (38%)	73,75,75	1.38	14 (19%)
20	9XX	W	202	-	41,41,41	1.10	4 (9%)	44,44,44	1.19	3 (6%)
16	HEM	F	703	2	50,50,50	1.40	6 (12%)	67,82,82	1.11	3 (4%)
17	MQ9	E	604	-	59,59,59	2.42	22 (37%)	73,75,75	1.53	16 (21%)
17	MQ9	F	708	-	59,59,59	2.30	22 (37%)	73,75,75	1.42	8 (10%)
15	CDL	Z	203	-	75,75,99	1.32	7 (9%)	81,87,111	2.04	9 (11%)
14	HEA	R	602	1	67,67,67	1.44	10 (14%)	81,103,103	2.33	31 (38%)
17	MQ9	F	709	-	59,59,59	2.43	22 (37%)	73,75,75	1.54	15 (20%)
18	9Y0	J	203	-	48,48,48	1.16	3 (6%)	51,53,53	0.78	2 (3%)
14	HEA	R	603	1	67,67,67	1.37	10 (14%)	81,103,103	2.04	18 (22%)
17	MQ9	Z	201	-	59,59,59	2.36	22 (37%)	73,75,75	1.63	16 (21%)
15	CDL	Z	202	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
22	9YF	I	304	-	58,58,58	1.05	5 (8%)	68,71,71	1.01	3 (4%)
21	HEC	O	301	10	50,50,50	1.81	5 (10%)	68,82,82	1.28	6 (8%)
18	9Y0	F	706	2	48,48,48	1.17	3 (6%)	51,53,53	0.87	2 (3%)
19	PLM	D	301	3	9,10,17	0.53	0	8,9,17	0.43	0
20	9XX	c	202	11	41,41,41	0.96	3 (7%)	44,44,44	1.18	4 (9%)
22	9YF	Y	503	-	58,58,58	1.09	5 (8%)	68,71,71	1.33	5 (7%)
15	CDL	P	201	-	75,75,99	0.33	0	81,87,111	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	CDL	F	704	-	75,75,99	0.34	0	81,87,111	0.42	0
15	CDL	J	201	-	75,75,99	0.33	0	81,87,111	0.45	0
15	CDL	T	202	-	75,75,99	0.33	0	81,87,111	0.40	0
19	PLM	c	201	11	15,16,17	0.47	0	14,15,17	0.35	0
18	9Y0	S	302	-	48,48,48	1.16	3 (6%)	51,53,53	0.87	2 (3%)
18	9Y0	P	202	-	48,48,48	1.20	3 (6%)	51,53,53	0.95	2 (3%)
15	CDL	E	605	-	75,75,99	0.34	0	81,87,111	0.42	0
15	CDL	X	302	-	75,75,99	1.33	7 (9%)	81,87,111	1.99	9 (11%)
22	9YF	c	203	-	58,58,58	1.01	5 (8%)	68,71,71	1.13	3 (4%)
15	CDL	T	201	-	75,75,99	1.26	9 (12%)	81,87,111	1.83	15 (18%)
22	9YF	M	502	-	58,58,58	1.10	5 (8%)	68,71,71	1.33	5 (7%)
17	MQ9	F	707	-	59,59,59	2.25	21 (35%)	73,75,75	1.73	22 (30%)
23	FES	M	503	12	0,4,4	-	-	-		
15	CDL	F	705	-	75,75,99	0.37	0	81,87,111	0.46	1 (1%)
21	HEC	I	302	10	50,50,50	1.73	6 (12%)	68,82,82	1.65	11 (16%)
22	9YF	O	303	-	58,58,58	1.05	5 (8%)	68,71,71	1.01	3 (4%)
14	HEA	L	603	1	67,67,67	1.37	10 (14%)	81,103,103	1.92	19 (23%)
15	CDL	X	301	-	75,75,99	0.33	0	81,87,111	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	9XX	G	302	3	-	10/33/33/43	-
17	MQ9	I	303	-	-	8/53/73/73	0/2/2/2
19	PLM	W	201	11	-	4/14/14/15	-
22	9YF	W	203	-	-	22/54/78/78	0/1/1/1
15	CDL	L	604	-	-	48/86/86/110	-
20	9XX	D	302	-	-	9/33/33/43	-
15	CDL	T	203	-	-	47/86/86/110	-
18	9Y0	X	303	-	-	17/52/52/52	-
22	9YF	Y	502	-	-	23/54/78/78	0/1/1/1
23	FES	Y	501	12	-	-	0/1/1/1
16	HEM	E	602	2	-	2/14/54/54	-
16	HEM	F	702	2	-	4/12/52/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	S	301	-	-	43/86/86/110	-
15	CDL	R	604	-	-	47/86/86/110	-
18	9Y0	J	202	-	-	19/52/52/52	-
16	HEM	E	601	2	-	2/12/52/54	-
22	9YF	M	501	-	-	23/54/78/78	0/1/1/1
17	MQ9	F	701	-	-	6/53/73/73	0/2/2/2
19	PLM	G	301	3	-	2/8/8/15	-
15	CDL	E	606	-	-	40/86/86/110	-
21	HEC	O	302	10	1/1/7/7	6/14/54/54	-
14	HEA	L	602	1	-	12/36/76/76	-
21	HEC	I	301	-	-	6/14/54/54	-
17	MQ9	E	603	-	-	6/53/73/73	0/2/2/2
20	9XX	W	202	-	-	15/43/43/43	-
16	HEM	F	703	2	-	0/14/54/54	-
17	MQ9	E	604	-	-	11/53/73/73	0/2/2/2
17	MQ9	F	708	-	-	11/53/73/73	0/2/2/2
15	CDL	Z	203	-	-	38/86/86/110	-
14	HEA	R	602	1	-	7/36/76/76	-
17	MQ9	F	709	-	-	12/53/73/73	0/2/2/2
18	9Y0	J	203	-	-	25/52/52/52	-
14	HEA	R	603	1	-	3/36/76/76	-
17	MQ9	Z	201	-	-	11/53/73/73	0/2/2/2
15	CDL	Z	202	-	-	34/86/86/110	-
22	9YF	I	304	-	-	27/54/78/78	0/1/1/1
21	HEC	O	301	10	-	6/14/54/54	-
18	9Y0	F	706	2	-	16/52/52/52	-
19	PLM	D	301	3	-	3/8/8/15	-
20	9XX	c	202	11	-	16/43/43/43	-
22	9YF	Y	503	-	-	27/54/78/78	0/1/1/1
15	CDL	P	201	-	-	48/86/86/110	-
15	CDL	F	704	-	-	49/86/86/110	-
15	CDL	J	201	-	-	48/86/86/110	-
15	CDL	T	202	-	-	46/86/86/110	-
19	PLM	c	201	11	-	5/14/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	9Y0	S	302	-	-	19/52/52/52	-
18	9Y0	P	202	-	-	22/52/52/52	-
15	CDL	E	605	-	-	49/86/86/110	-
15	CDL	X	302	-	-	43/86/86/110	-
22	9YF	c	203	-	-	22/54/78/78	0/1/1/1
15	CDL	T	201	-	-	34/86/86/110	-
22	9YF	M	502	-	-	27/54/78/78	0/1/1/1
17	MQ9	F	707	-	-	17/53/73/73	0/2/2/2
23	FES	M	503	12	-	-	0/1/1/1
15	CDL	F	705	-	-	43/86/86/110	-
21	HEC	I	302	10	1/1/7/7	5/14/54/54	-
22	9YF	O	303	-	-	27/54/78/78	0/1/1/1
14	HEA	L	603	1	-	3/36/76/76	-
15	CDL	X	301	-	-	46/86/86/110	-

The worst 5 of 379 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	709	MQ9	C6-C5	8.77	1.50	1.35
17	E	604	MQ9	C6-C5	8.77	1.50	1.35
17	F	701	MQ9	C6-C5	8.59	1.50	1.35
17	F	708	MQ9	C6-C5	8.56	1.50	1.35
17	E	603	MQ9	C6-C5	8.53	1.50	1.35

The worst 5 of 389 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	Z	203	CDL	CB6-CB4-CB3	-9.90	88.70	111.78
15	X	302	CDL	CB6-CB4-CB3	-9.67	89.23	111.78
15	S	301	CDL	CB6-CB4-CB3	-9.66	89.26	111.78
15	T	201	CDL	OB6-CB4-CB6	9.23	141.46	108.34
15	Z	202	CDL	OB6-CB4-CB6	9.23	141.46	108.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	O	302	HEC	NA
21	I	302	HEC	NA

5 of 1221 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	R	602	HEA	C2D-C3D-CAD-CBD
14	R	602	HEA	C4D-C3D-CAD-CBD
14	L	602	HEA	C12-C11-C3B-C2B
15	R	604	CDL	CA3-OA5-PA1-OA2
15	R	604	CDL	CA3-OA5-PA1-OA3

There are no ring outliers.

40 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	I	303	MQ9	1	0
19	W	201	PLM	2	0
22	W	203	9YF	1	0
15	L	604	CDL	19	0
15	T	203	CDL	8	0
22	Y	502	9YF	2	0
23	Y	501	FES	1	0
16	E	602	HEM	2	0
16	F	702	HEM	1	0
15	S	301	CDL	49	0
15	R	604	CDL	19	0
16	E	601	HEM	2	0
15	E	606	CDL	3	0
21	O	302	HEC	11	0
14	L	602	HEA	2	0
21	I	301	HEC	4	0
17	E	603	MQ9	1	0
16	F	703	HEM	4	0
17	E	604	MQ9	3	0
17	F	708	MQ9	1	0
15	Z	203	CDL	46	0
17	F	709	MQ9	4	0
14	R	603	HEA	4	0
17	Z	201	MQ9	5	0
15	Z	202	CDL	35	0
22	I	304	9YF	5	0
21	O	301	HEC	5	0
22	Y	503	9YF	3	0
15	P	201	CDL	10	0
15	F	704	CDL	11	0
15	J	201	CDL	11	0

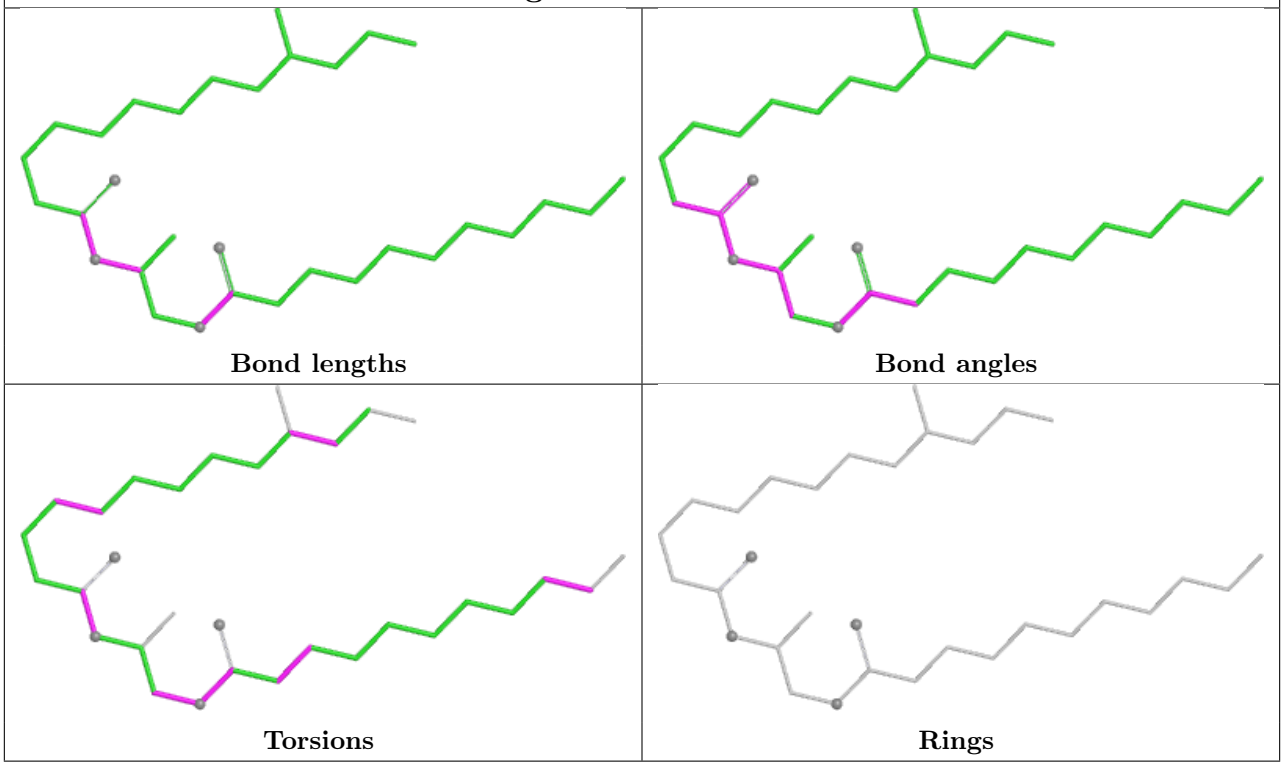
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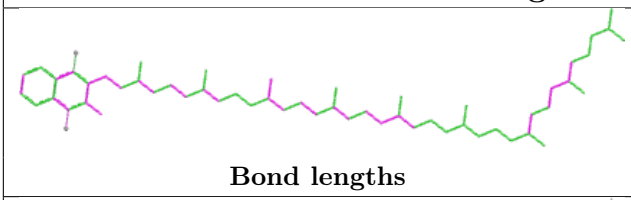
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	202	CDL	9	0
15	E	605	CDL	10	0
15	X	302	CDL	54	0
22	c	203	9YF	1	0
15	T	201	CDL	33	0
15	F	705	CDL	10	0
21	I	302	HEC	9	0
14	L	603	HEA	3	0
15	X	301	CDL	42	0

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.

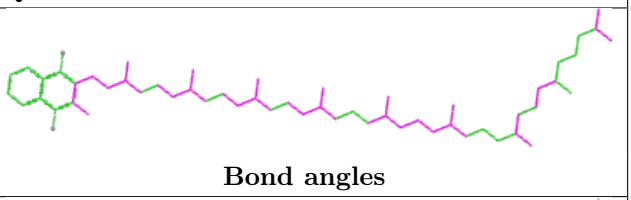
Ligand 9XX G 302



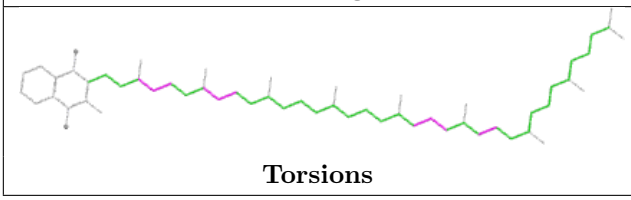
Ligand MQ9 I 303



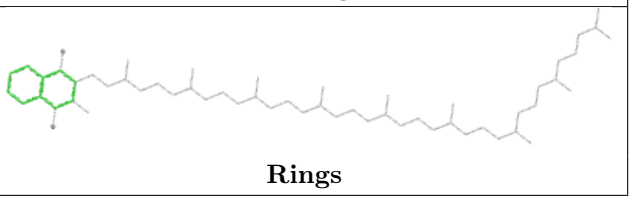
Bond lengths



Bond angles

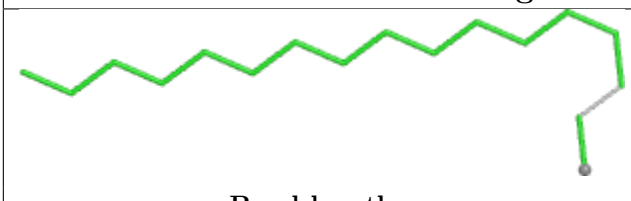


Torsions

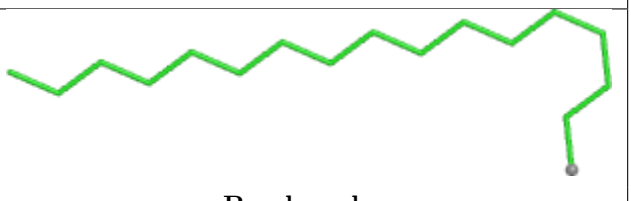


Rings

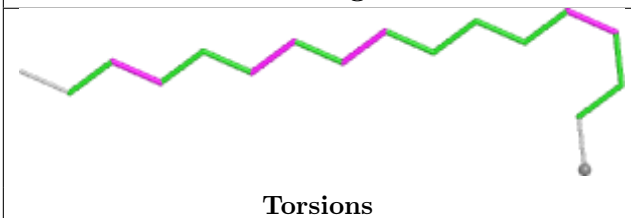
Ligand PLM W 201



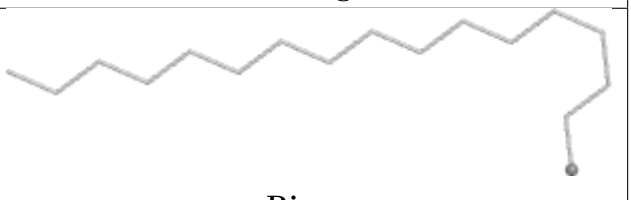
Bond lengths



Bond angles

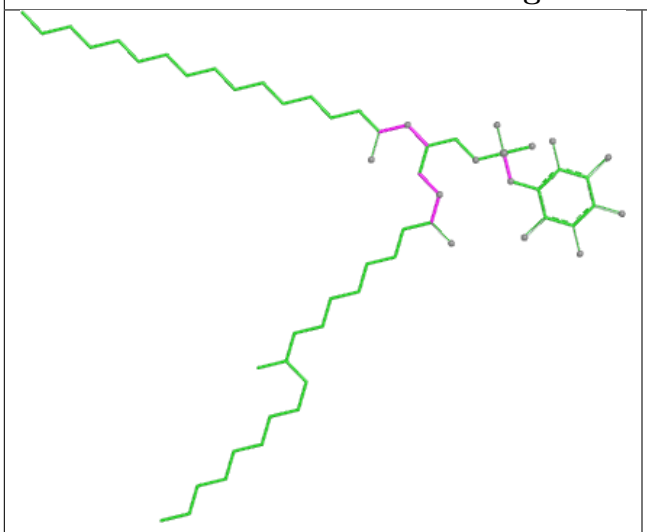


Torsions

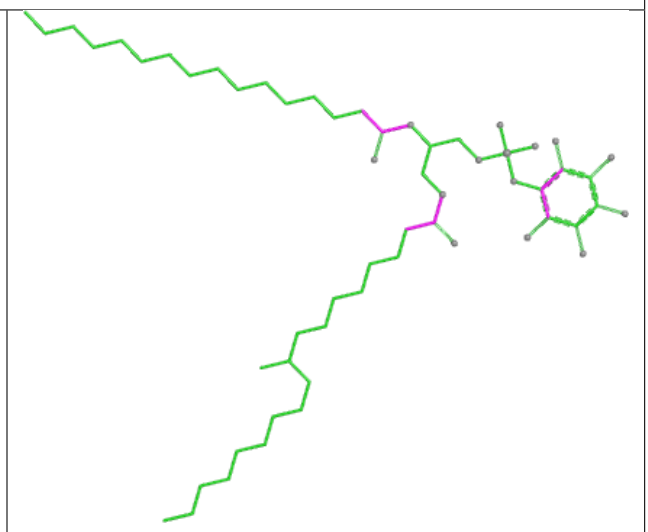


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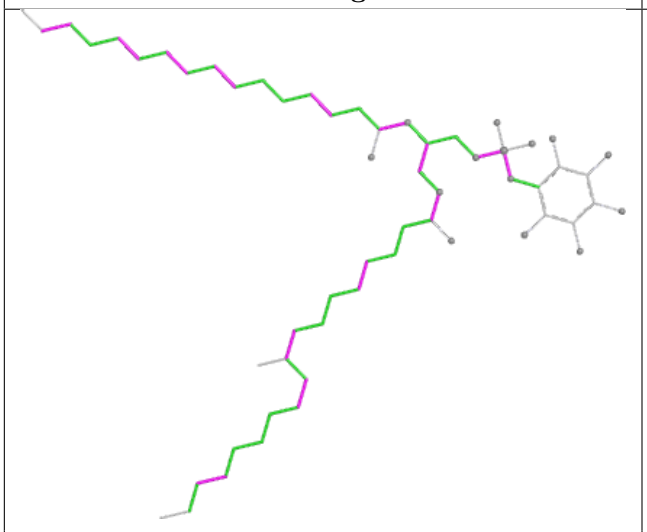
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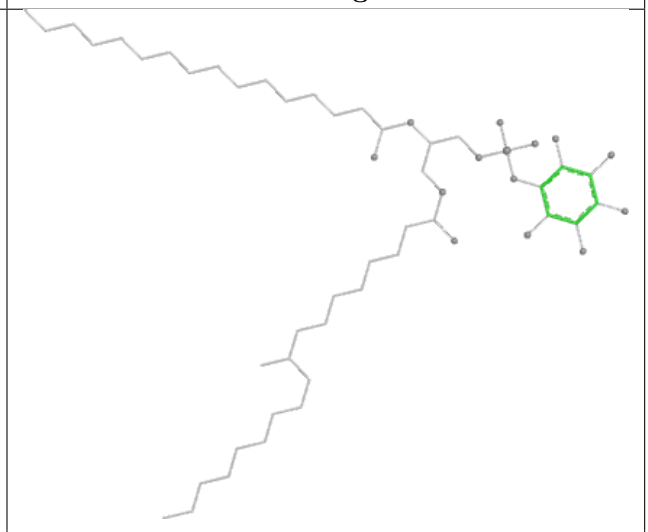
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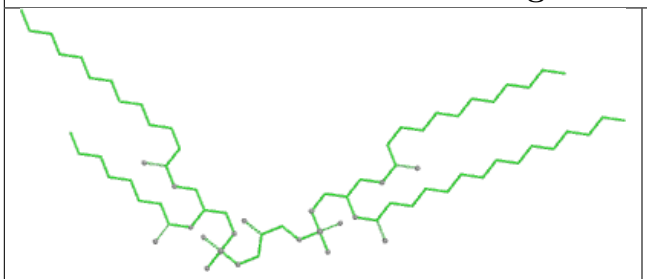


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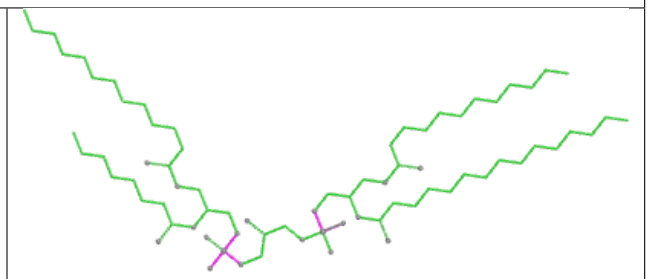


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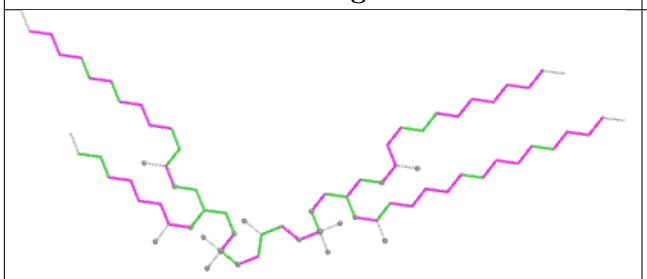
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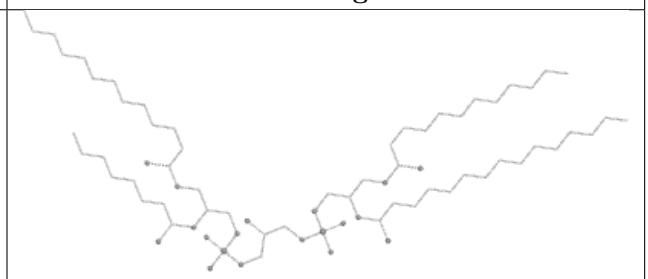
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Bond angles

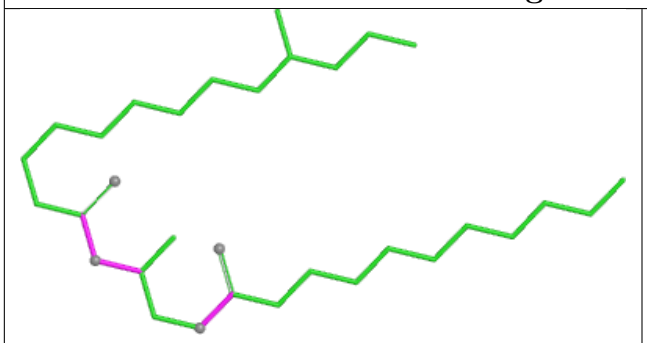


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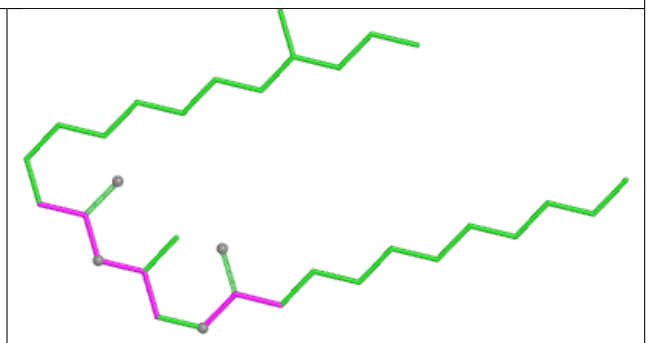


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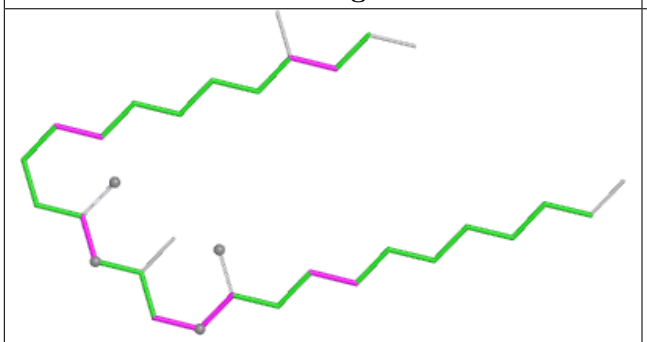
Ligand 9XX D 302



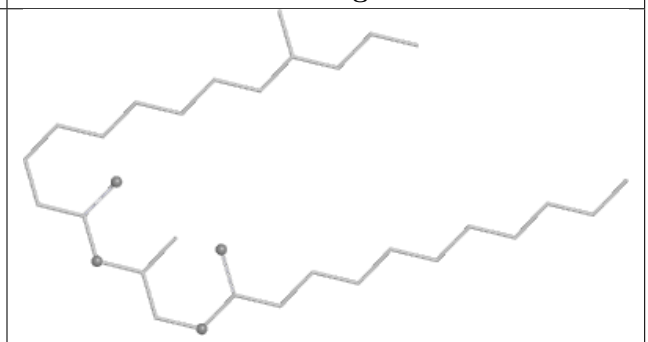
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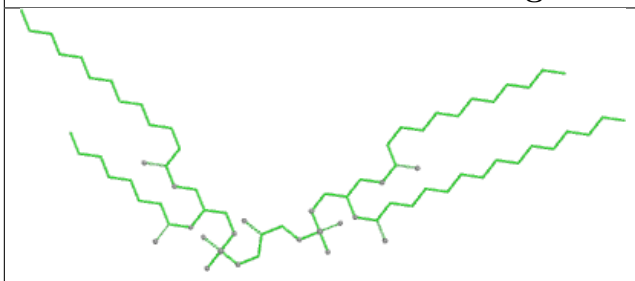


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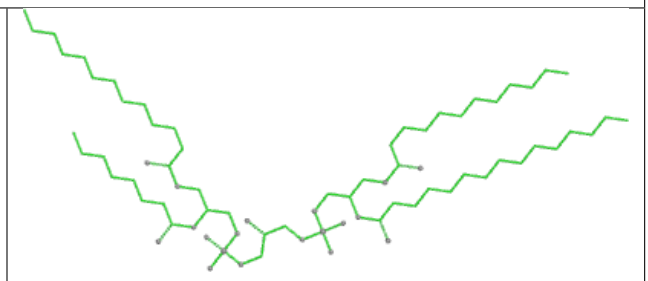


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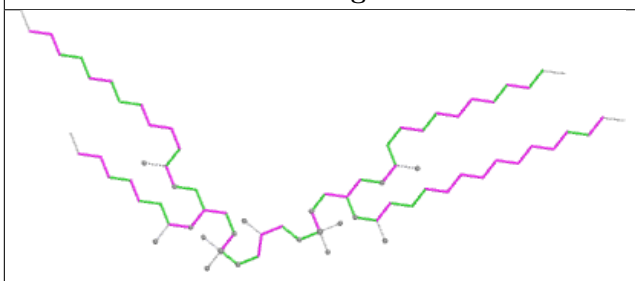
Ligand CDL T 203



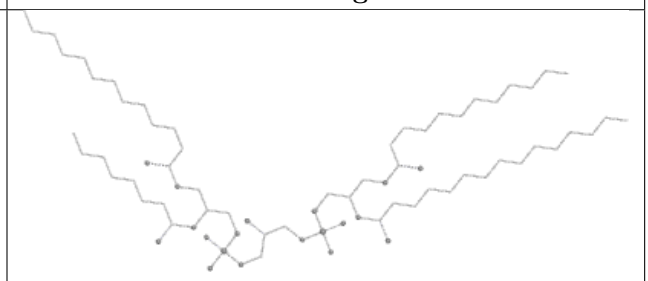
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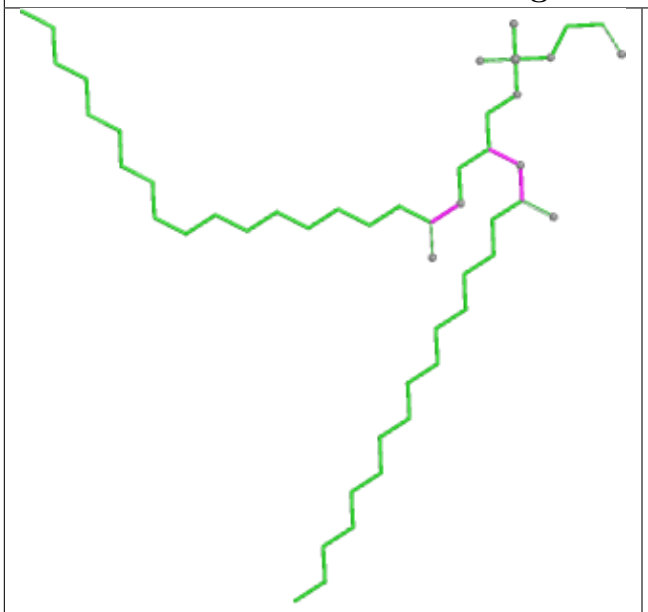


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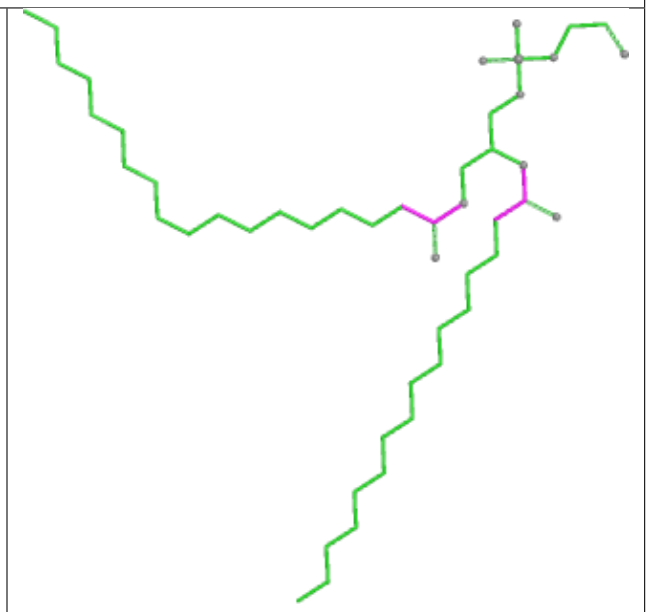


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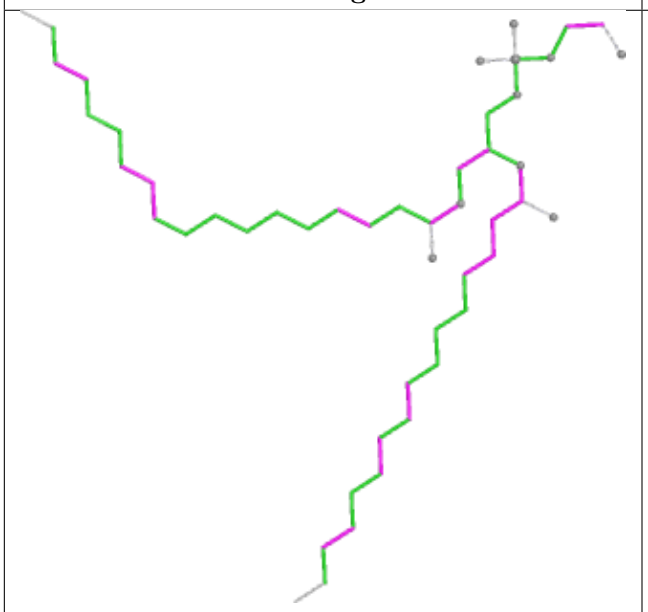
Ligand 9Y0 X 303



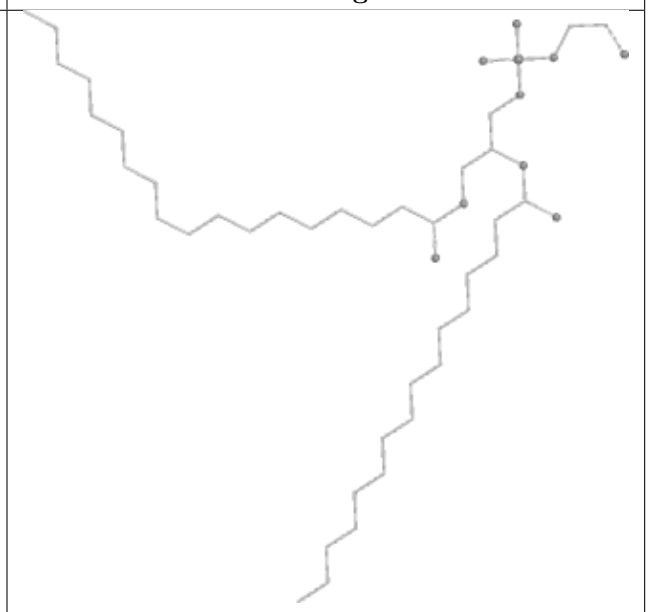
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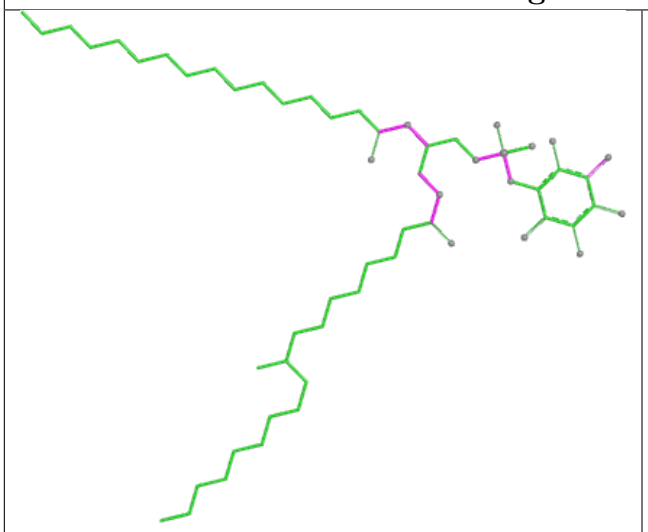


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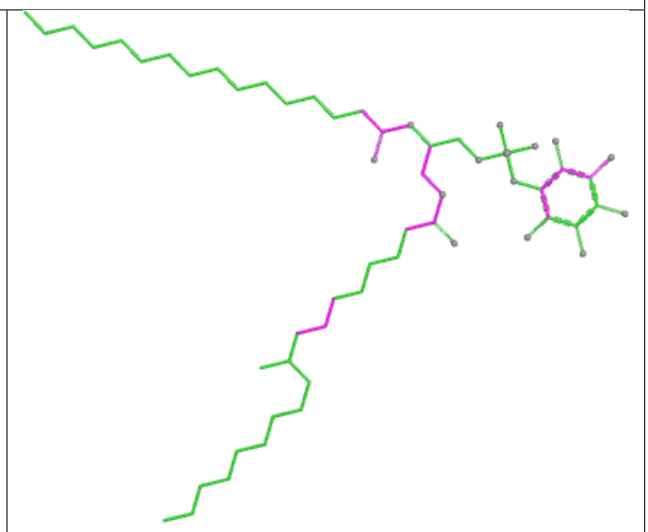


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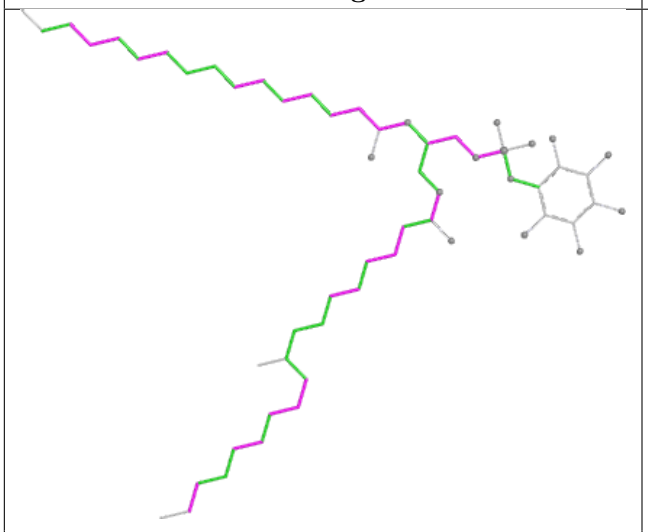
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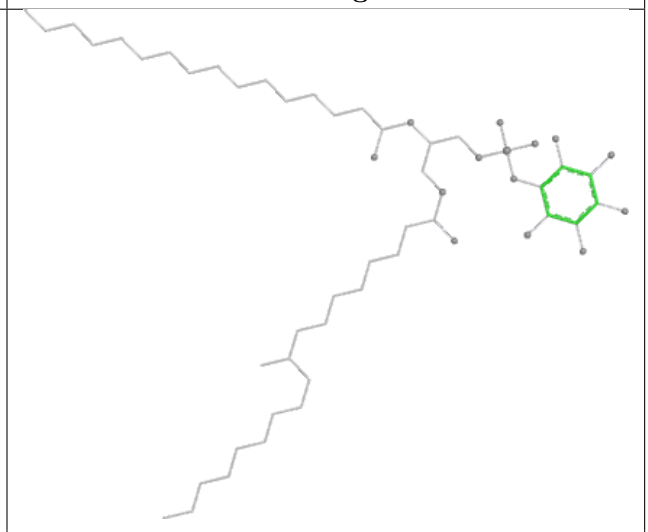
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Bond angles

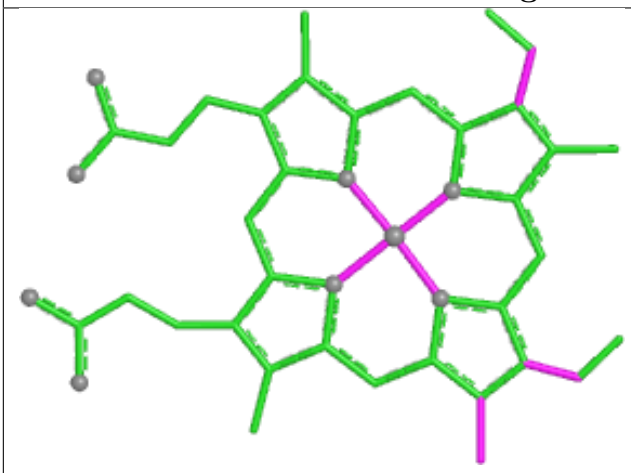


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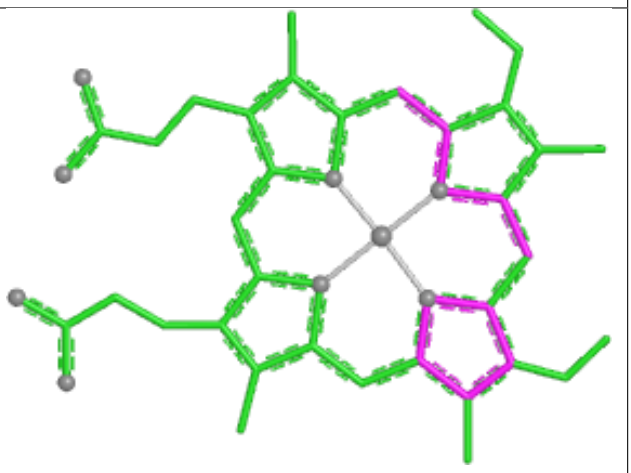


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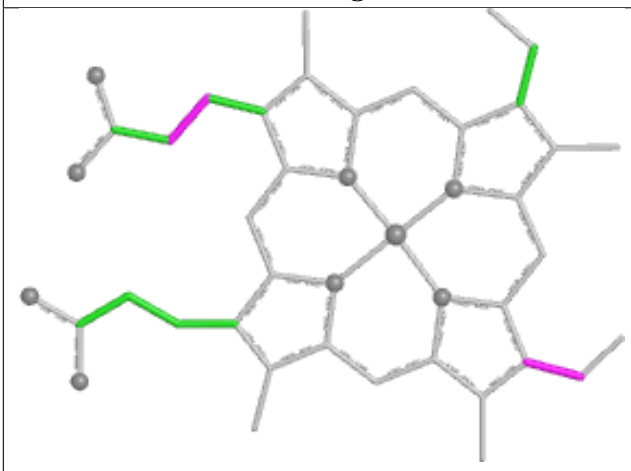
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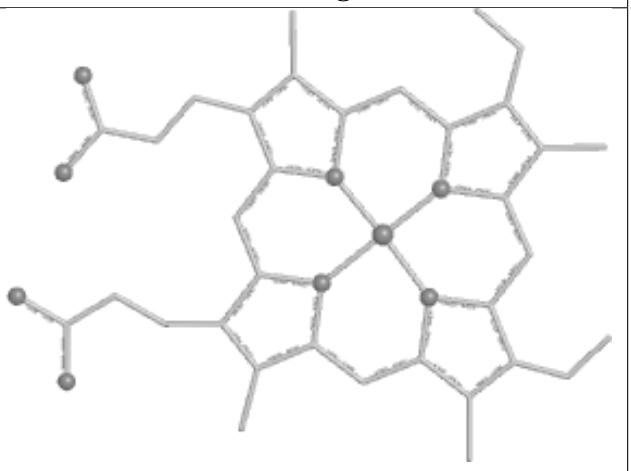
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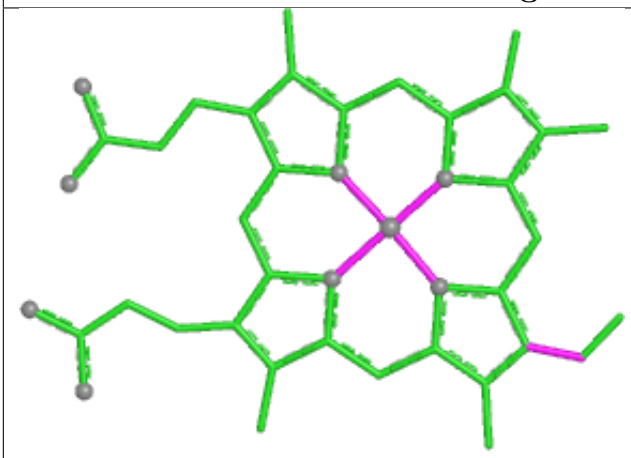


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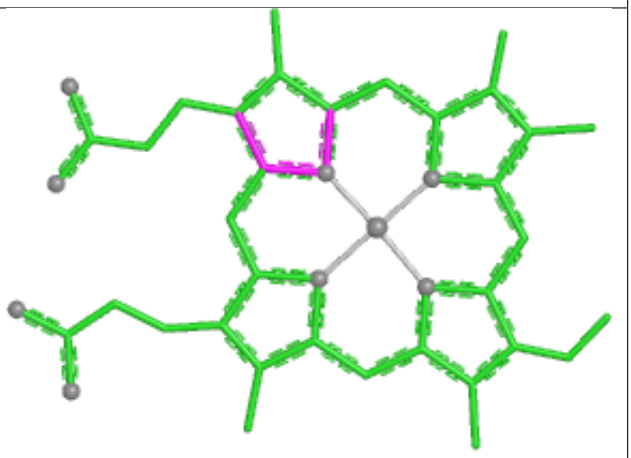


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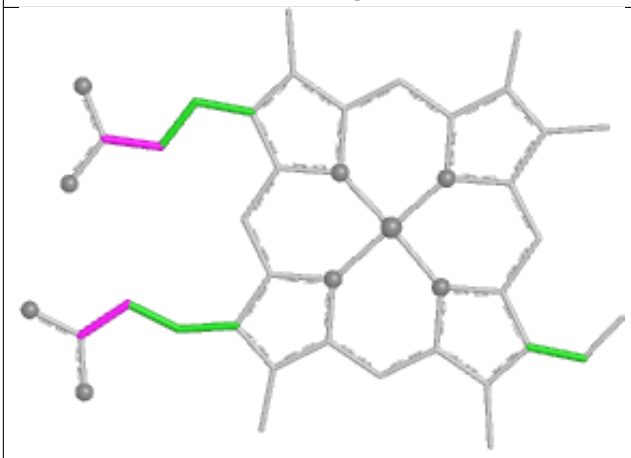
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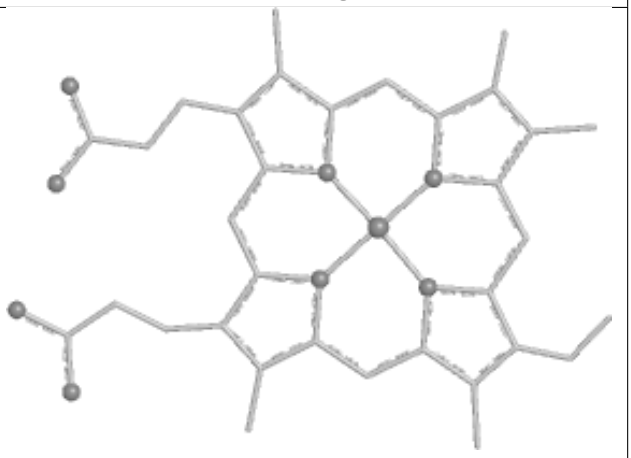
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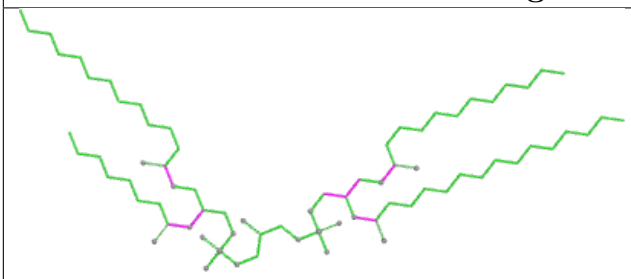


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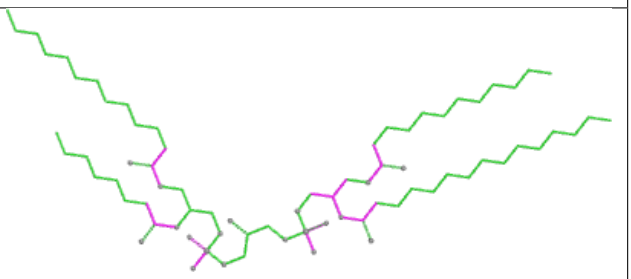


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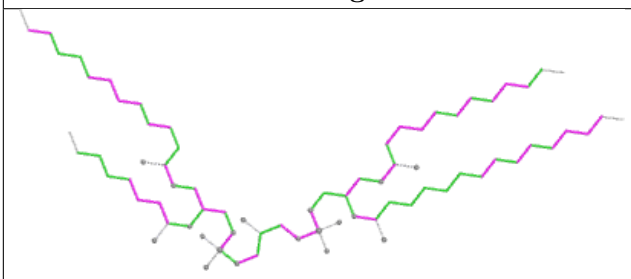
Ligand CDL S 301



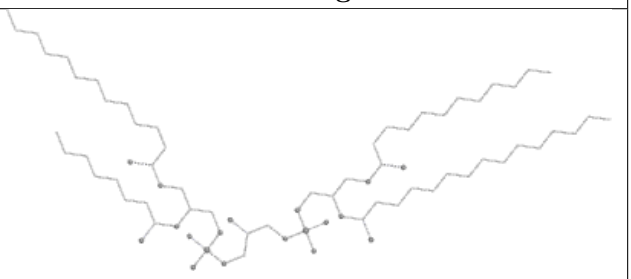
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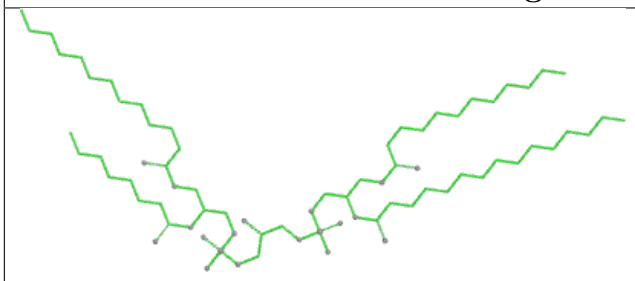


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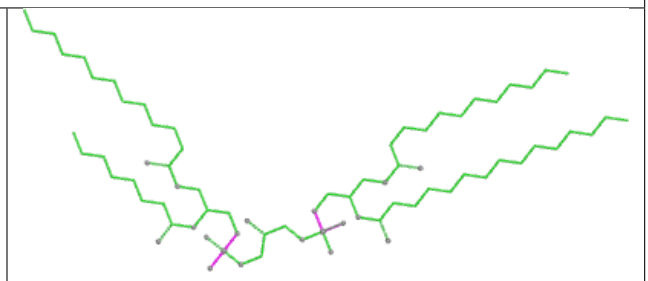


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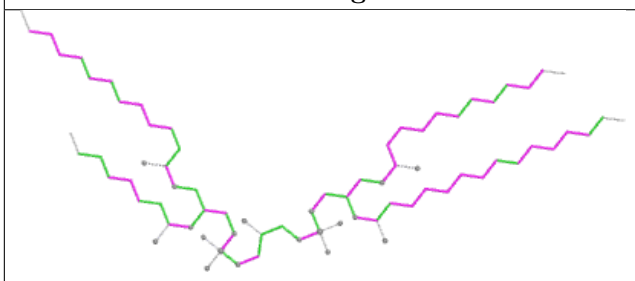
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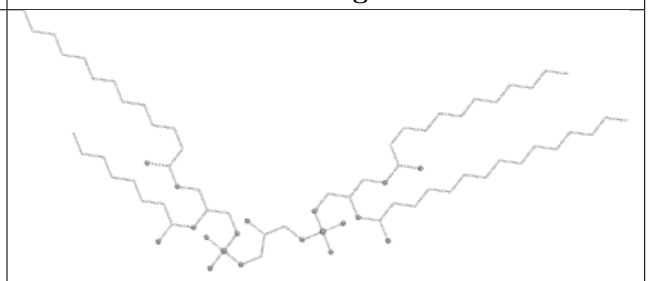
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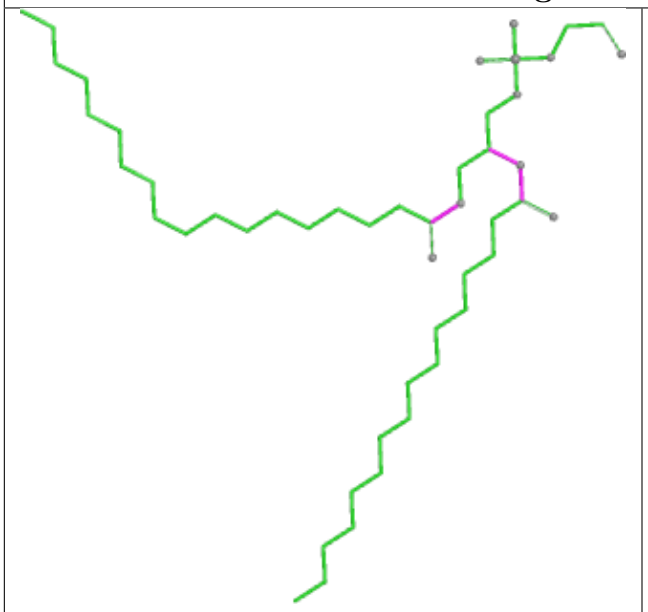


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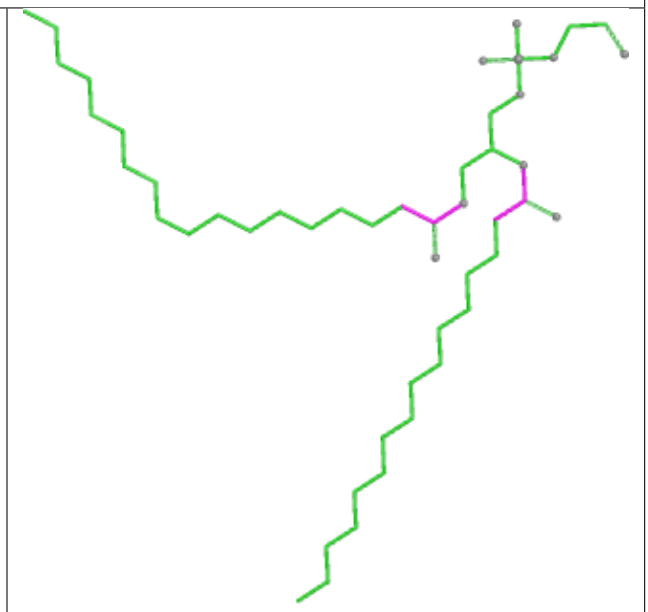


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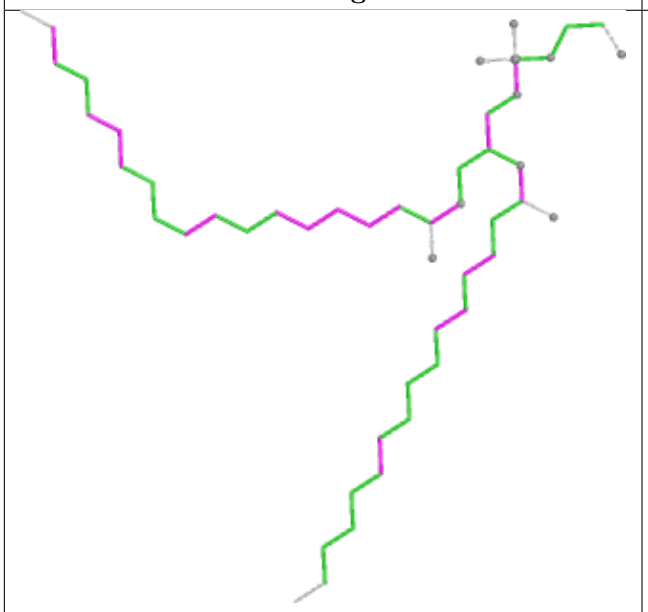
Ligand 9Y0 J 202



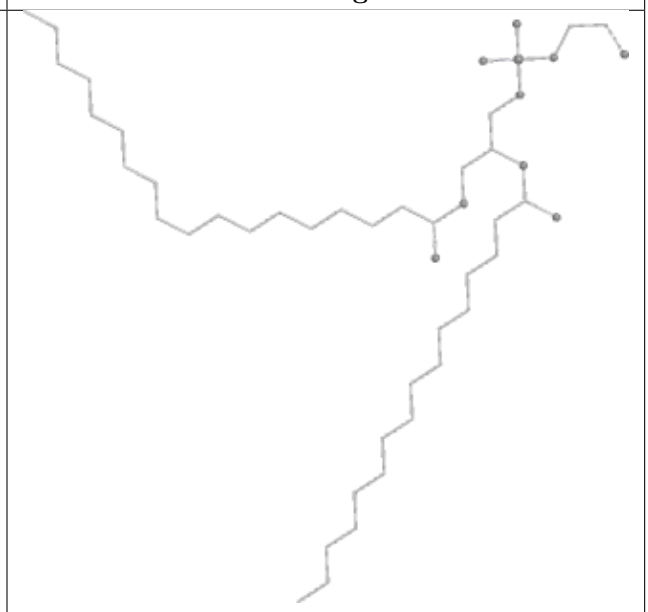
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Bond angles

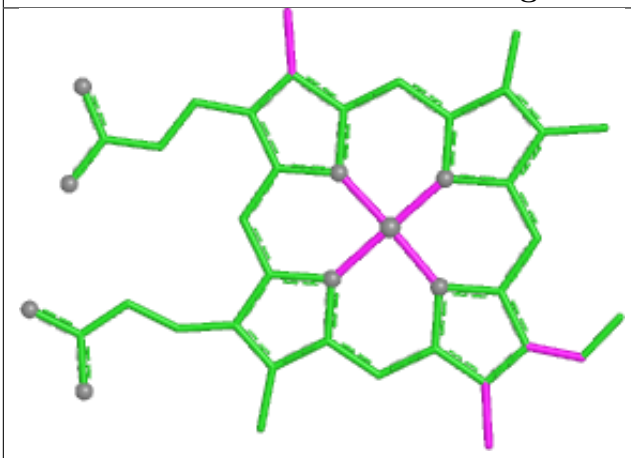


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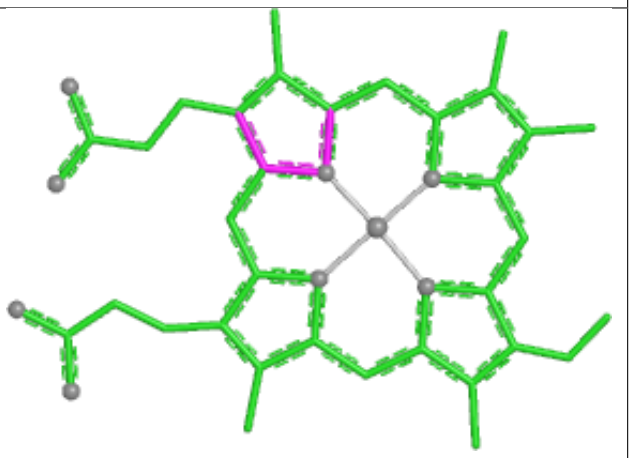


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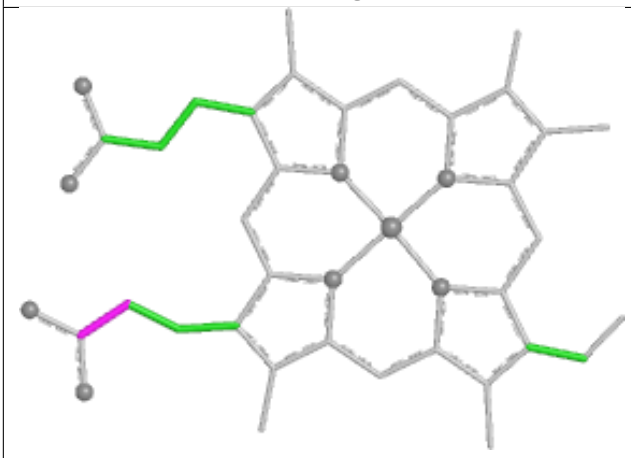
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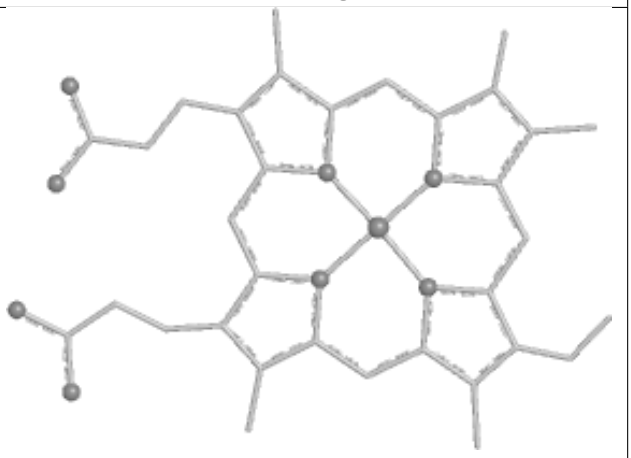
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Bond angles

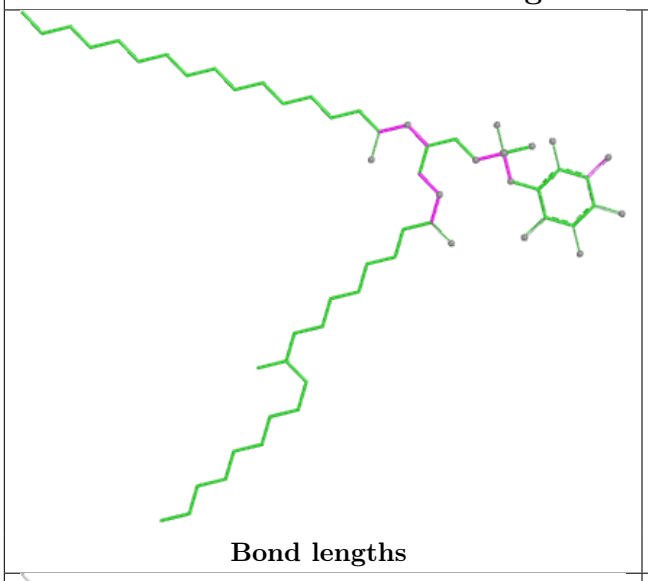


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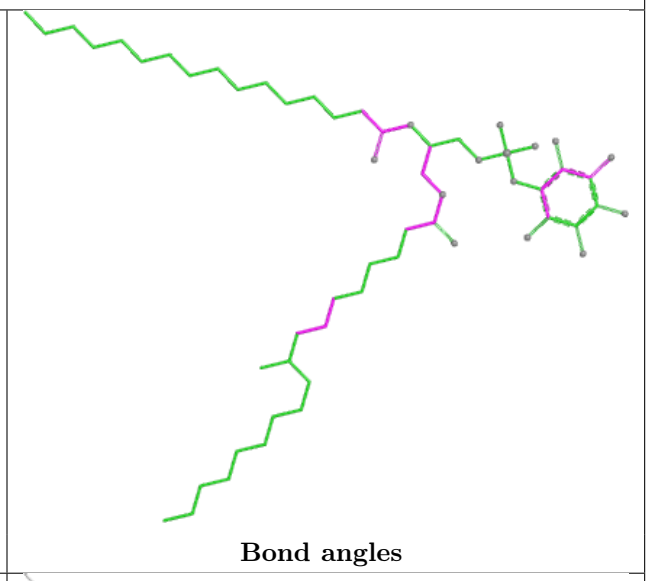


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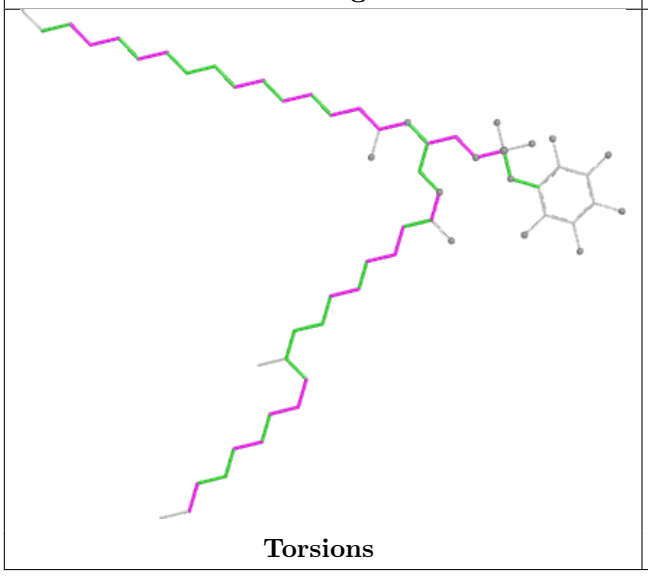
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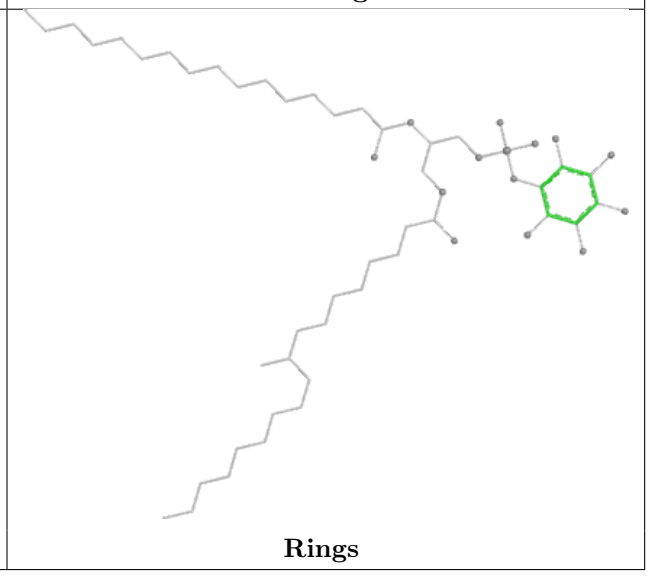
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Bond angles

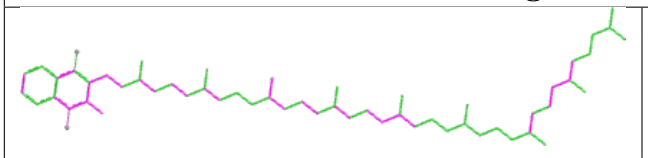


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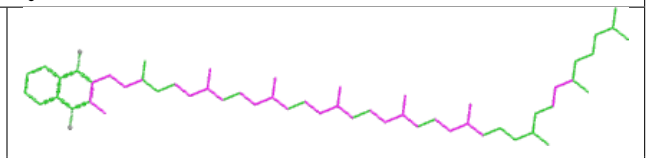


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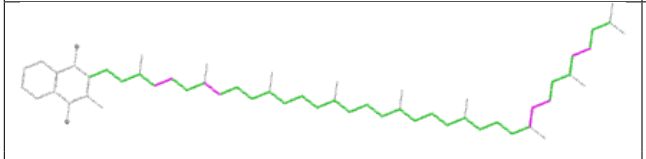
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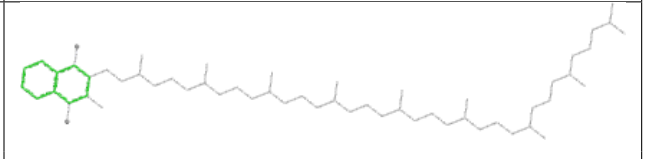
Bond lengths



Bond angles

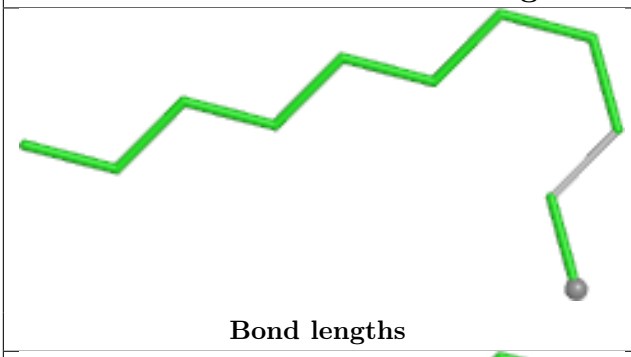


Torsions

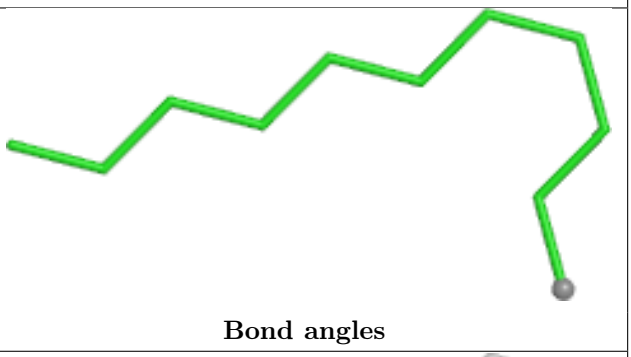


Rings

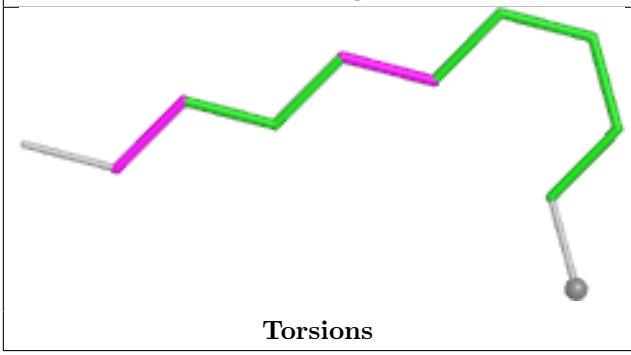
Ligand PLM G 301



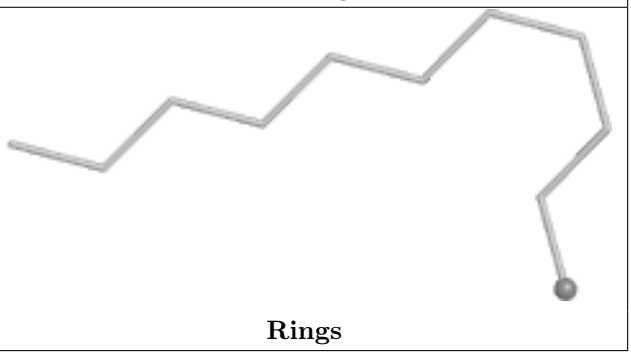
Bond lengths



Bond angles

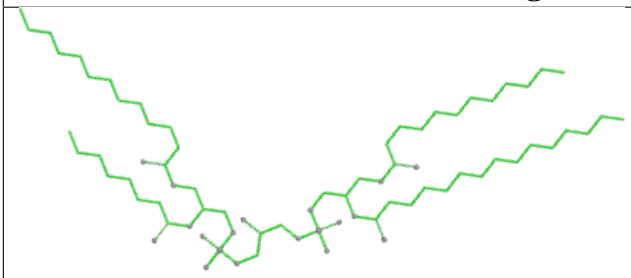


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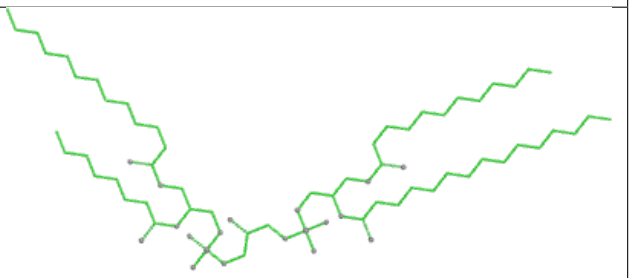


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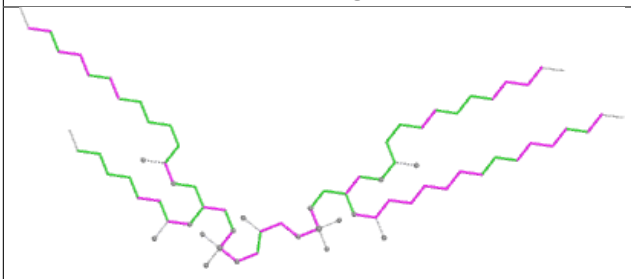
Ligand CDL E 606



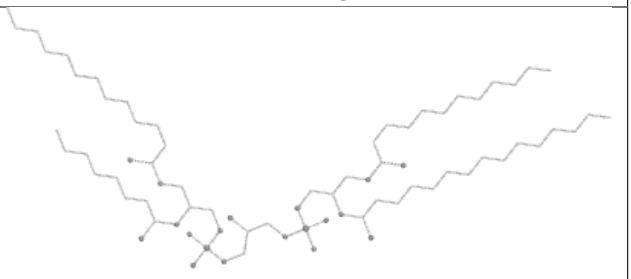
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Bond angles

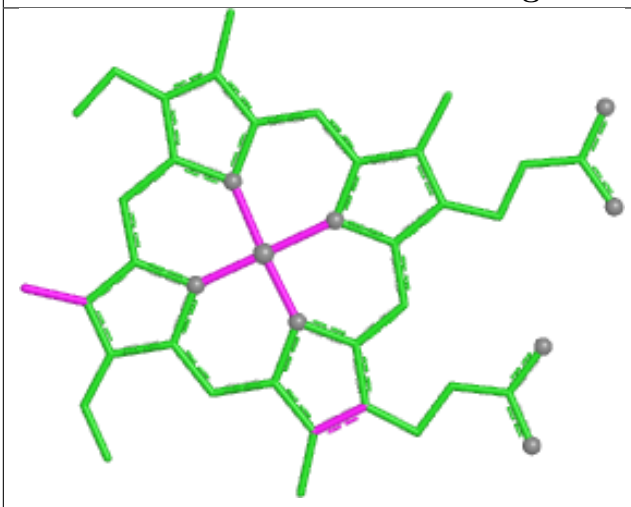


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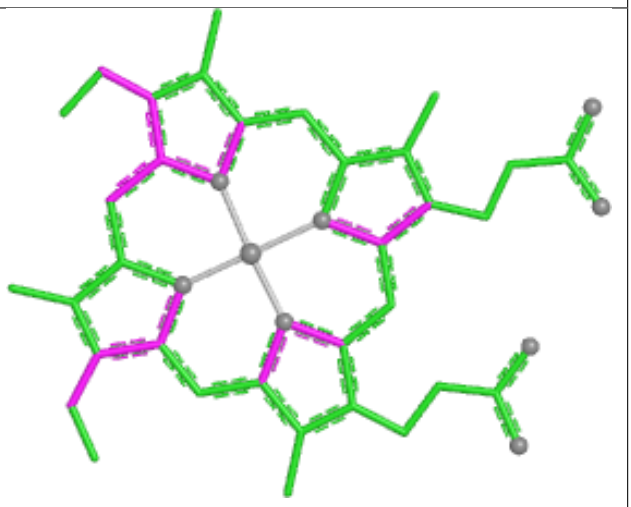


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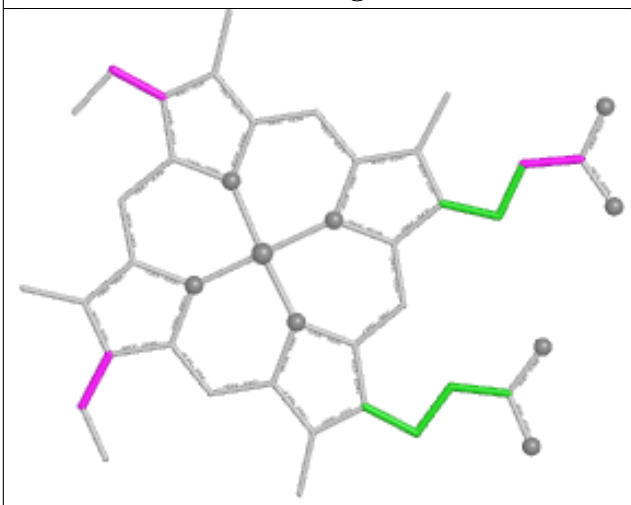
Ligand HEC O 302



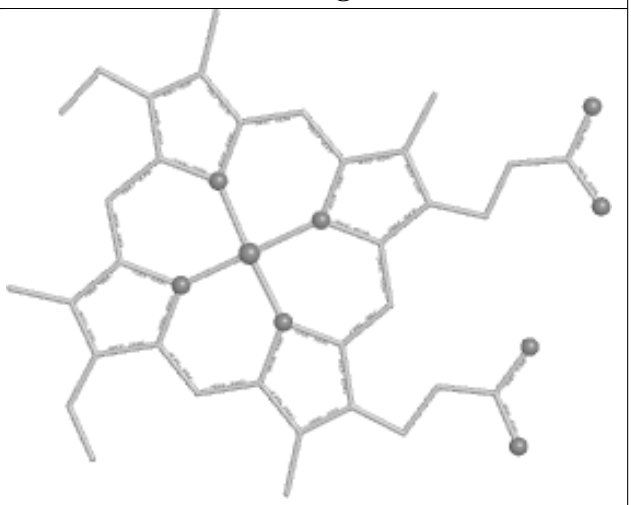
Bond lengths



Bond angles

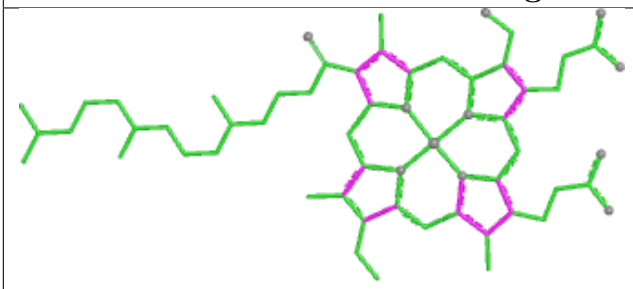


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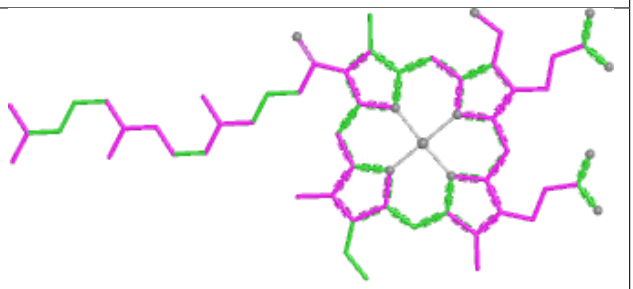


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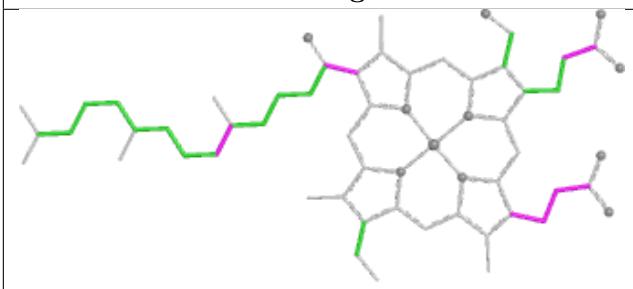
Ligand HEA L 602



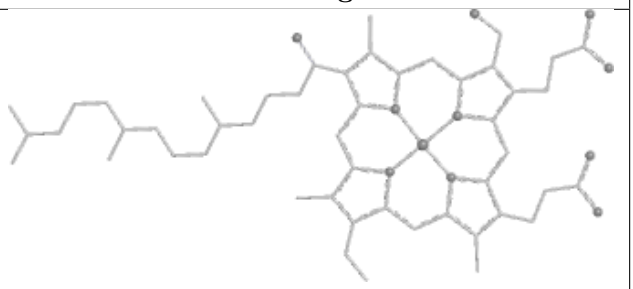
Bond lengths



Bond angles

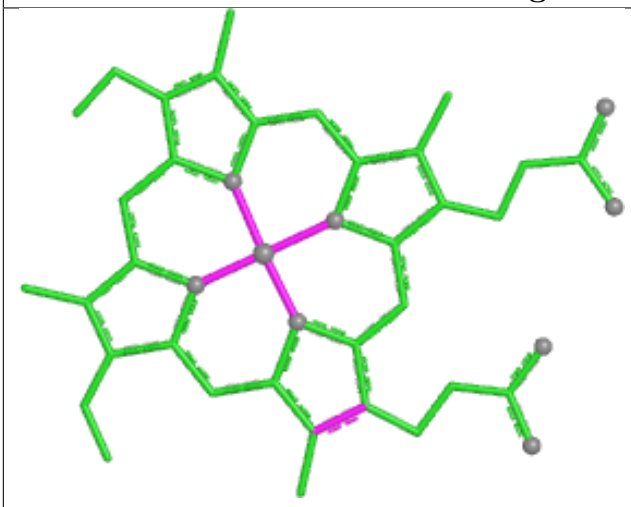


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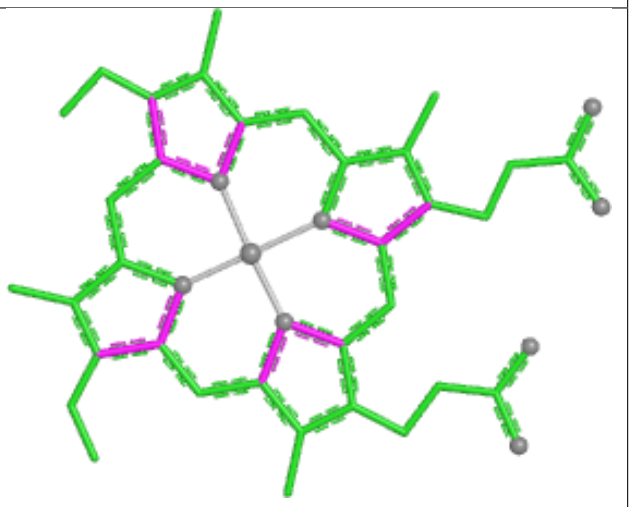


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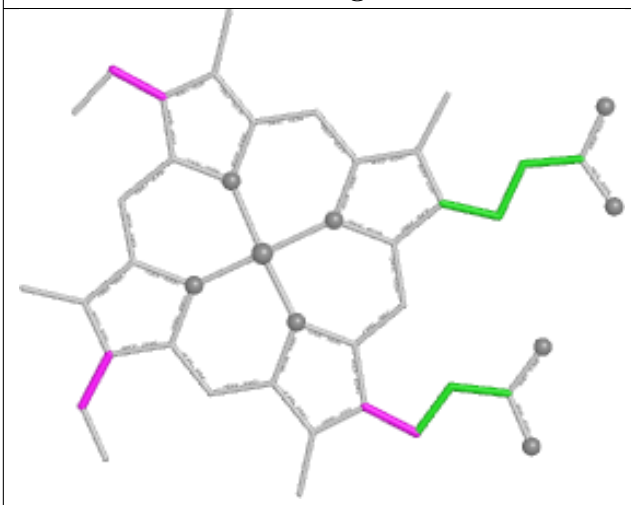
Ligand HEC I 301



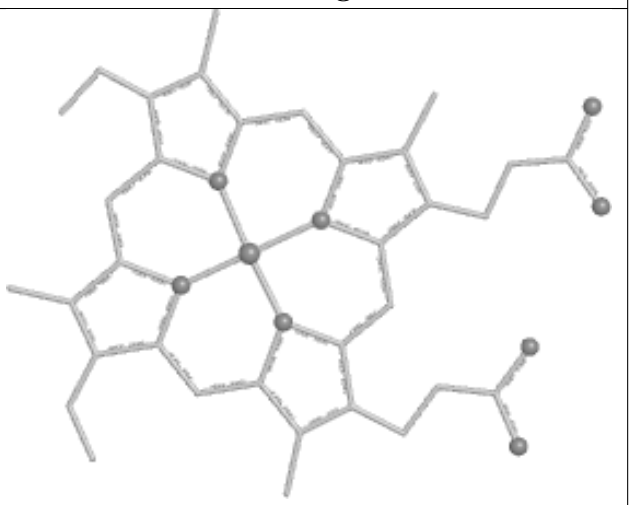
Bond lengths



Bond angles

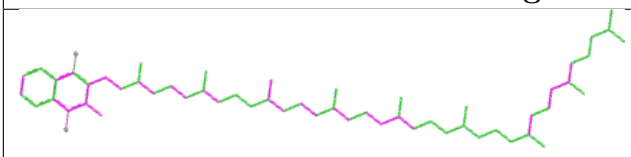


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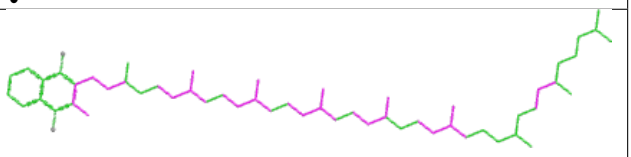


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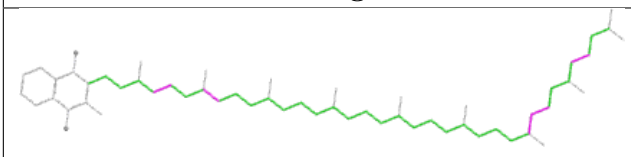
Ligand MQ9 E 603



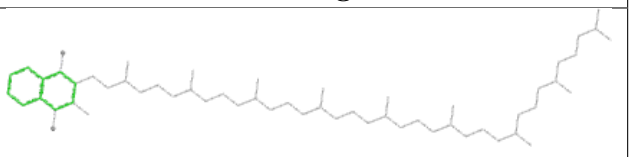
Bond lengths



Bond angles

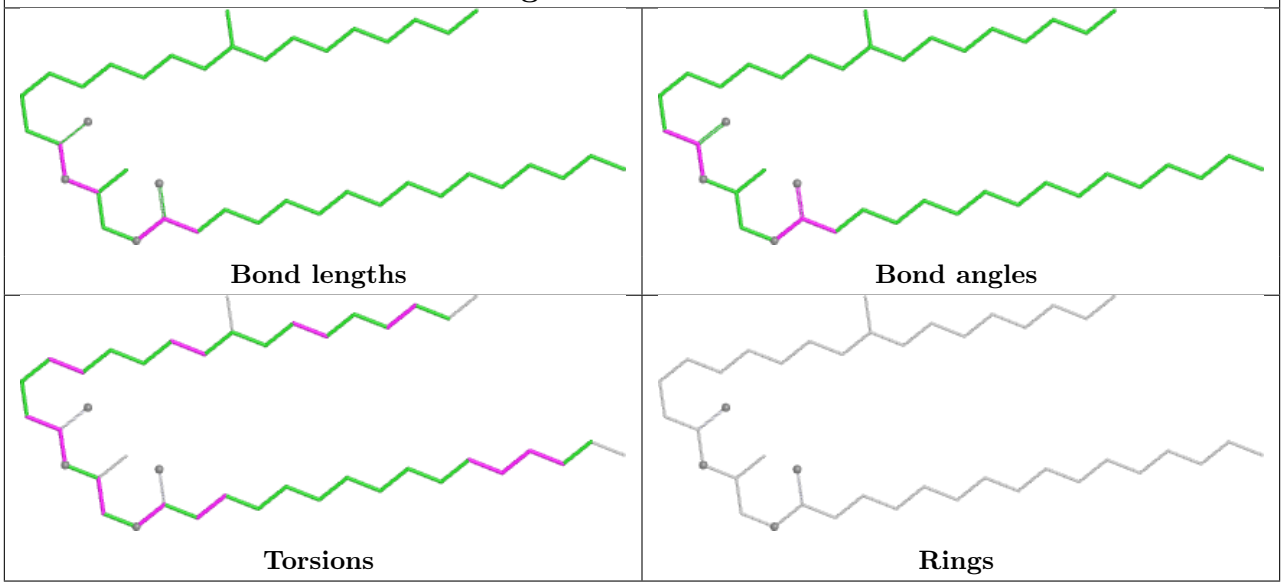


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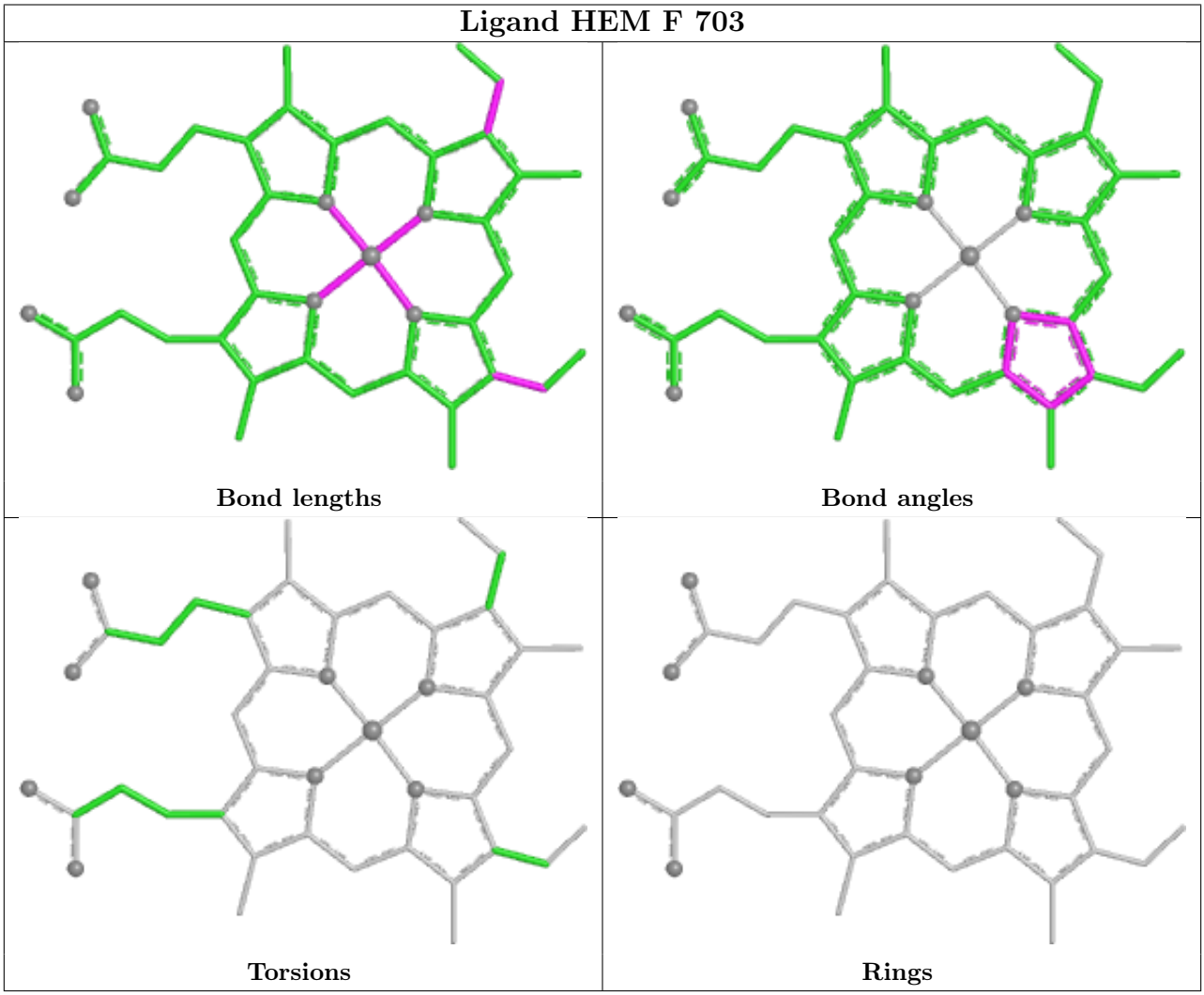


Rings

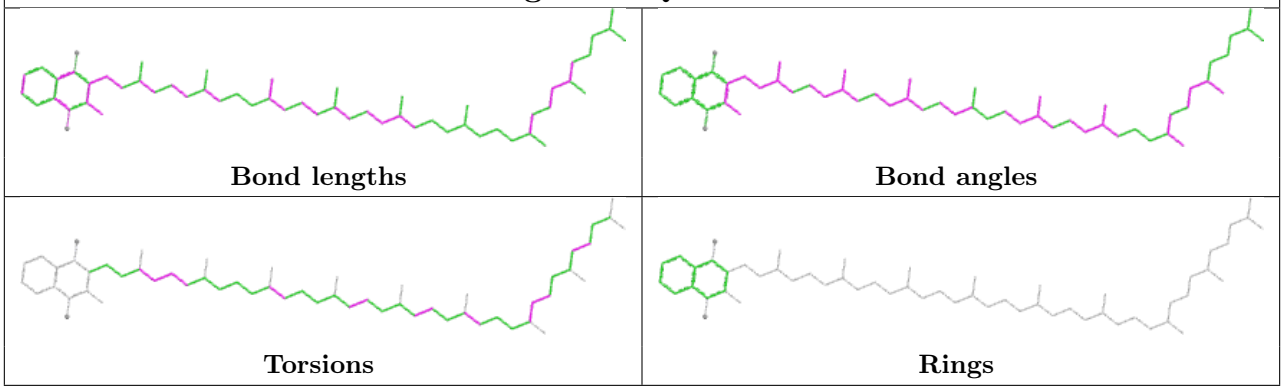
Ligand 9XX W 202



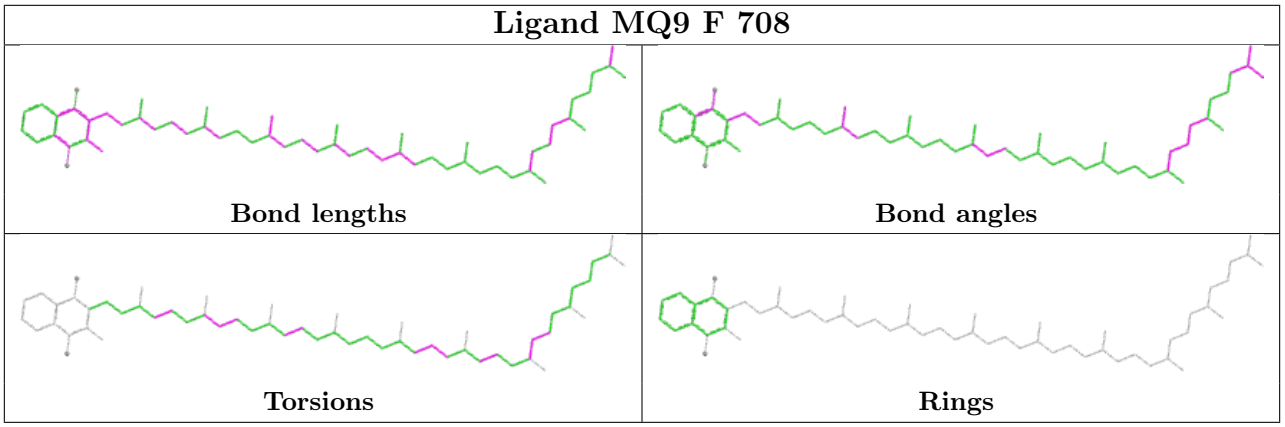
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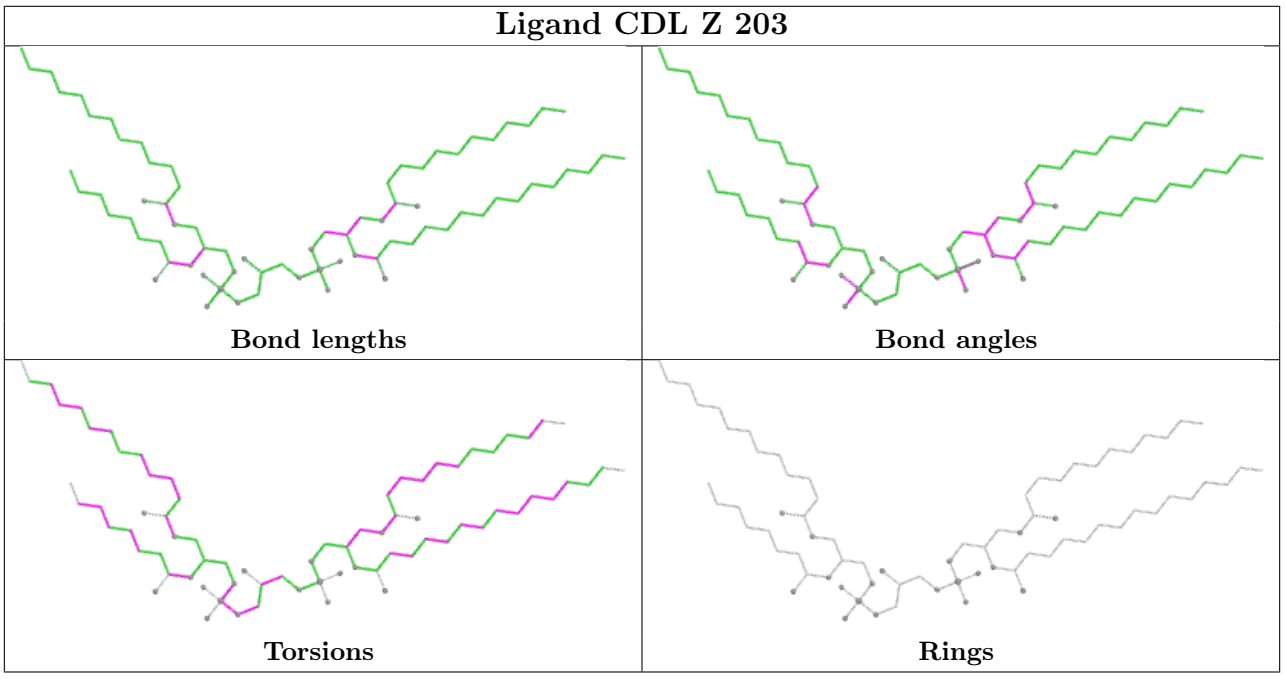
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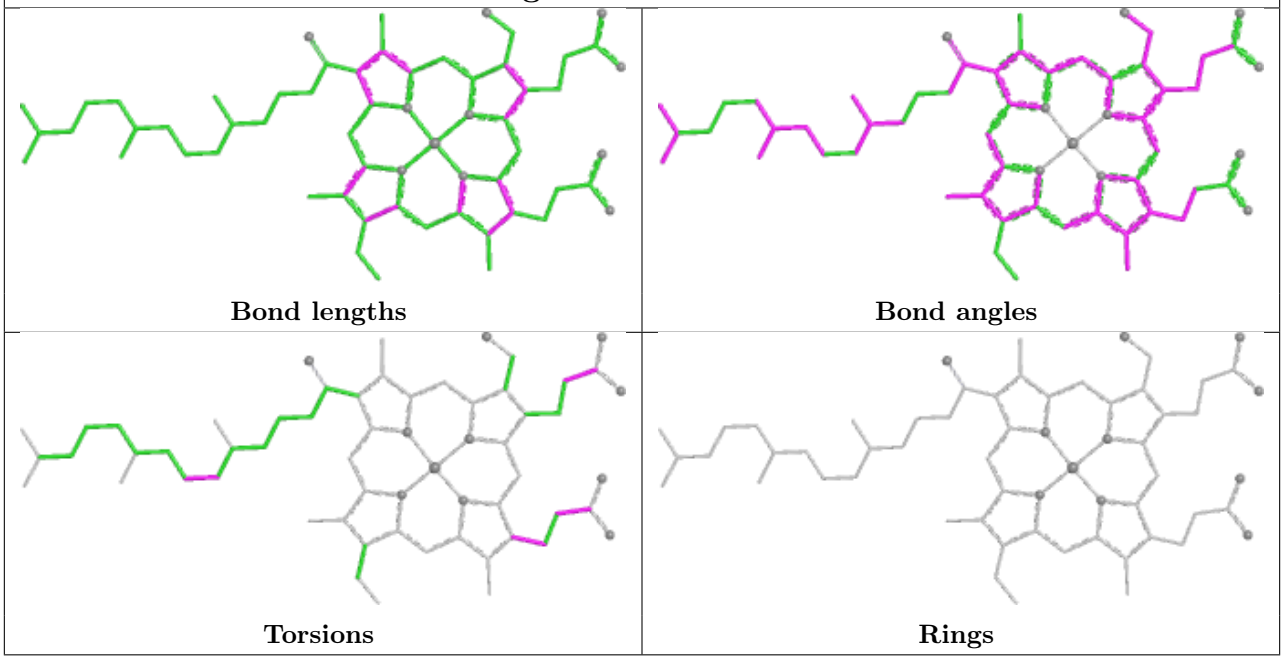
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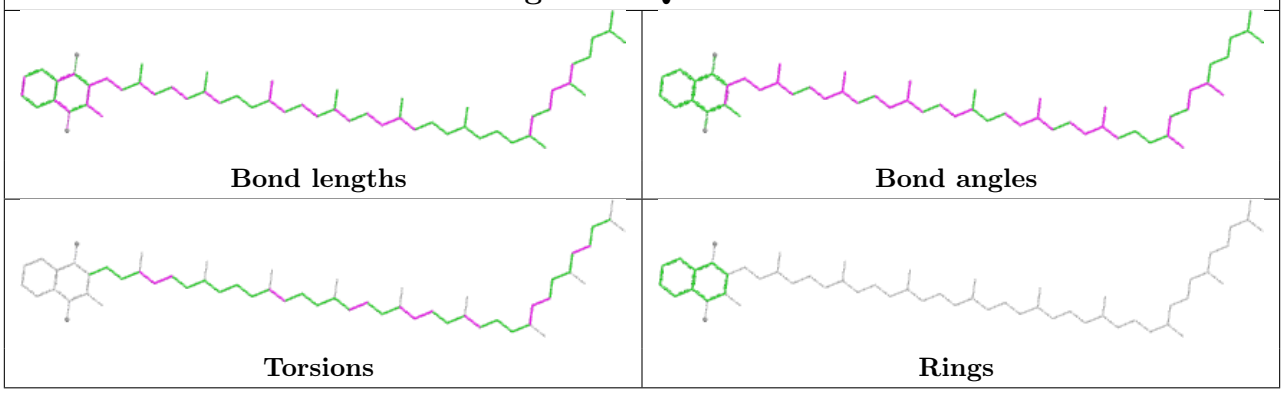
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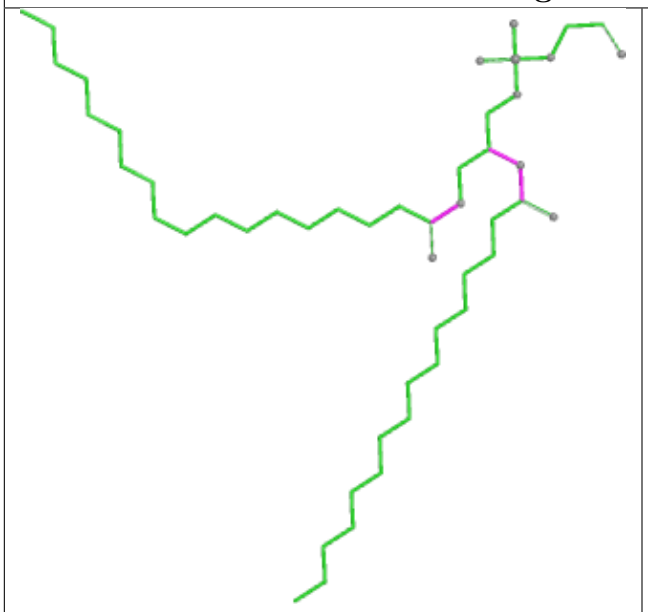
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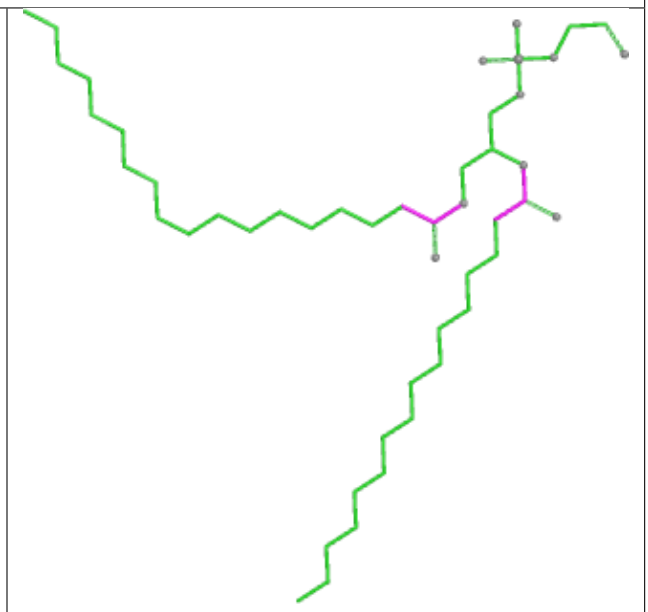
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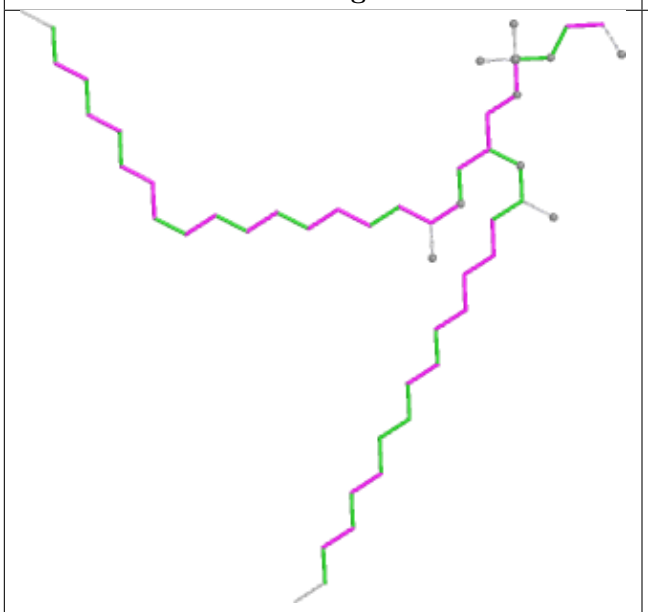
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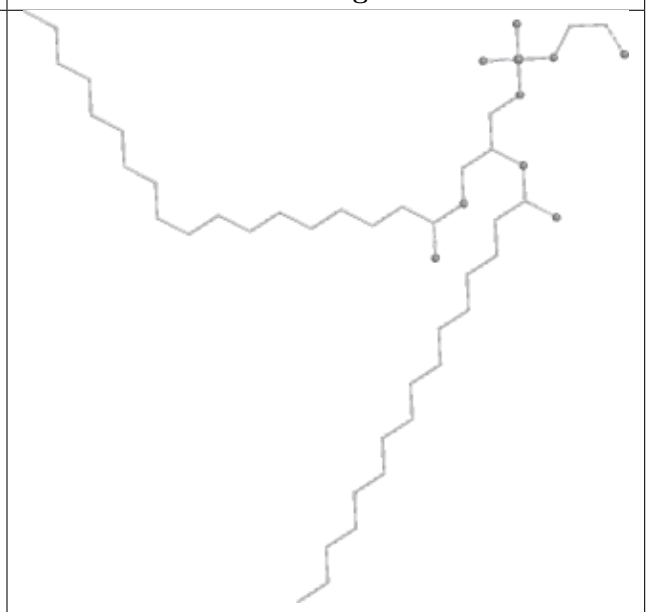
Bond lengths



Bond angles

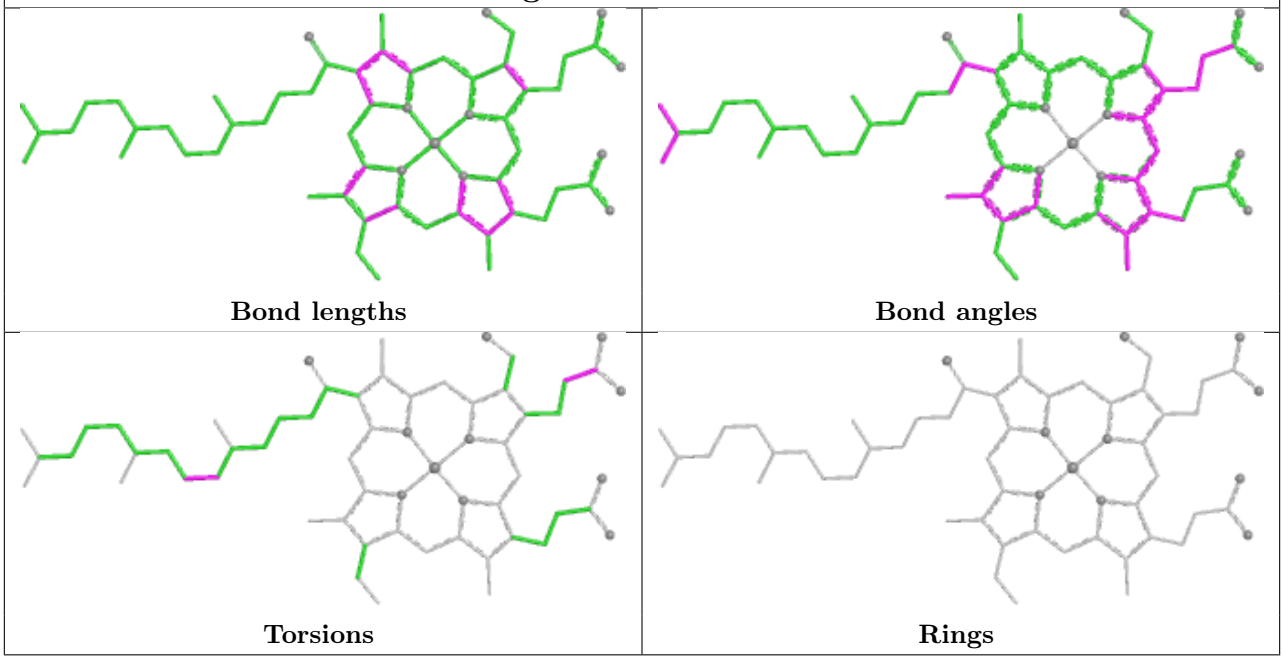


Torsions

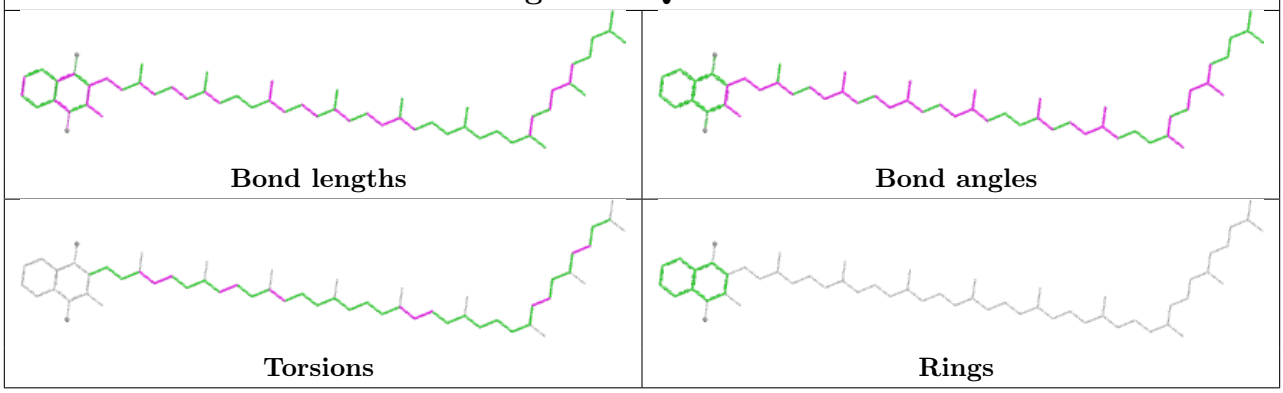


Rings

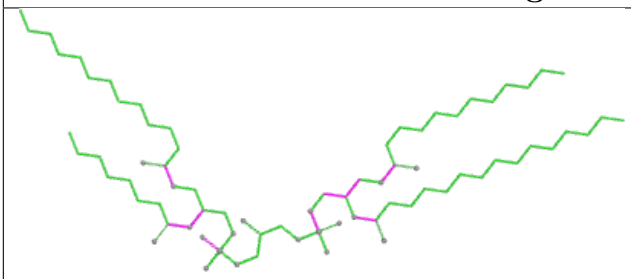
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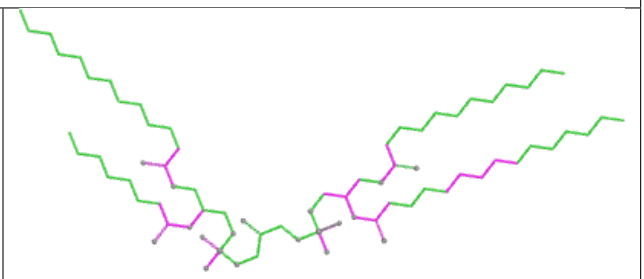
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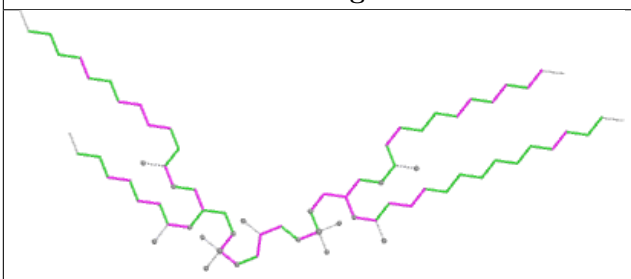
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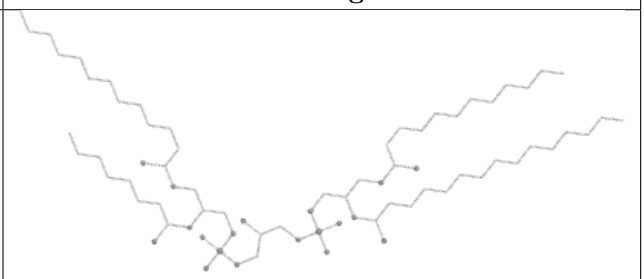
Bond lengths



Bond angles

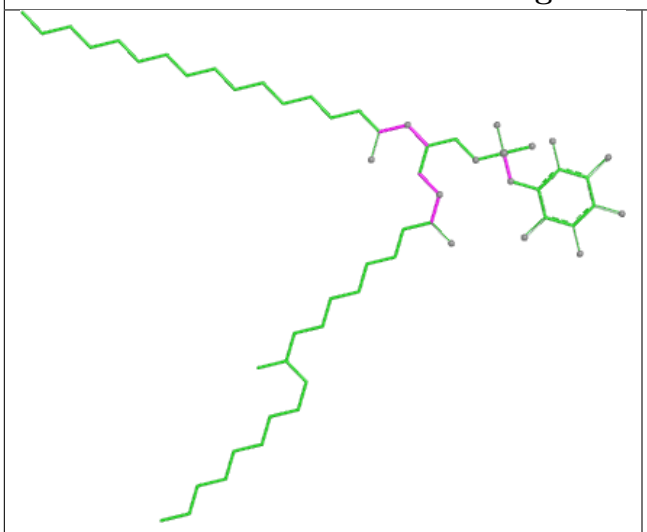


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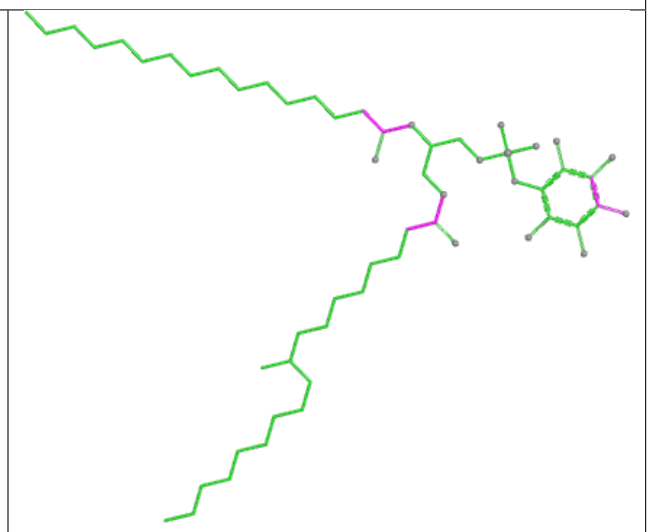


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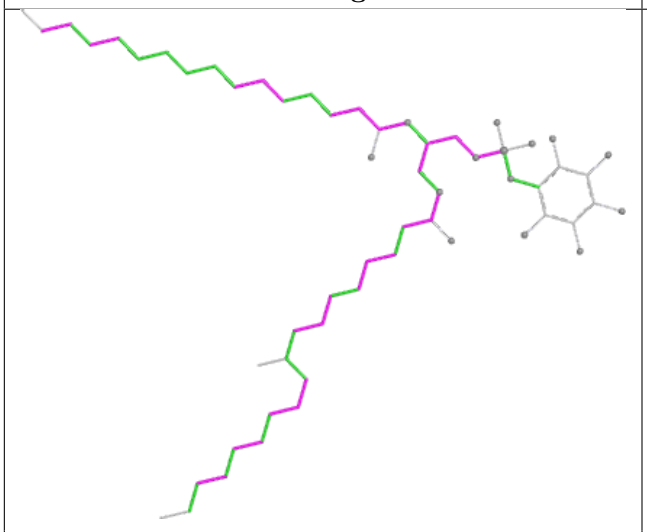
Ligand 9YF I 304



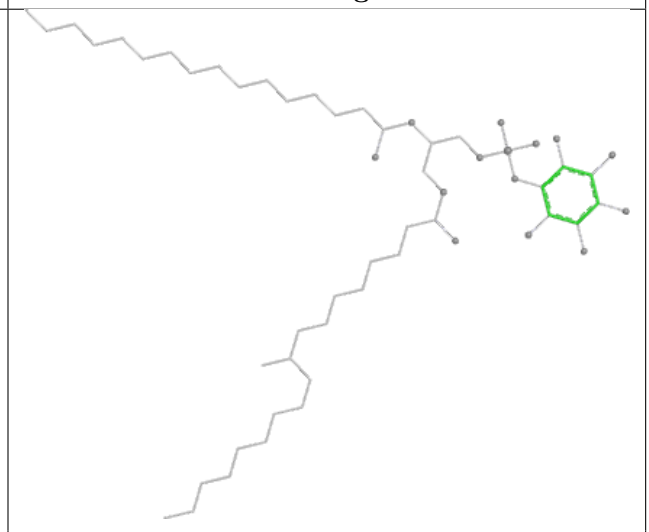
Bond lengths



Bond angles

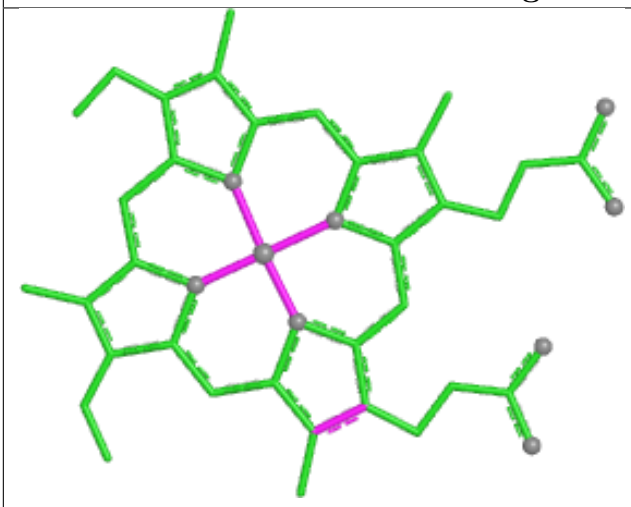


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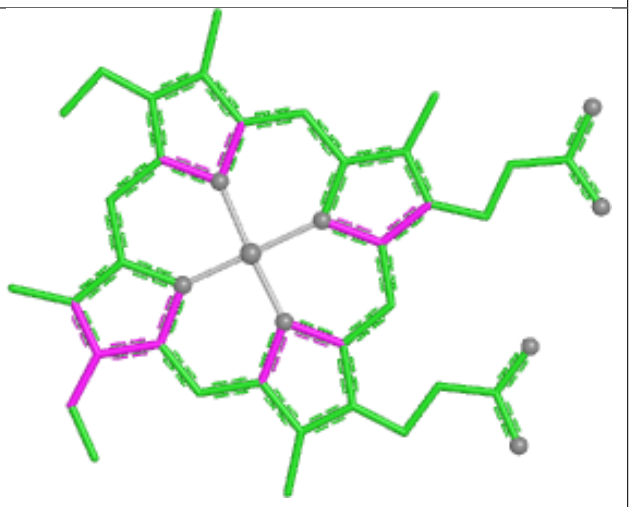


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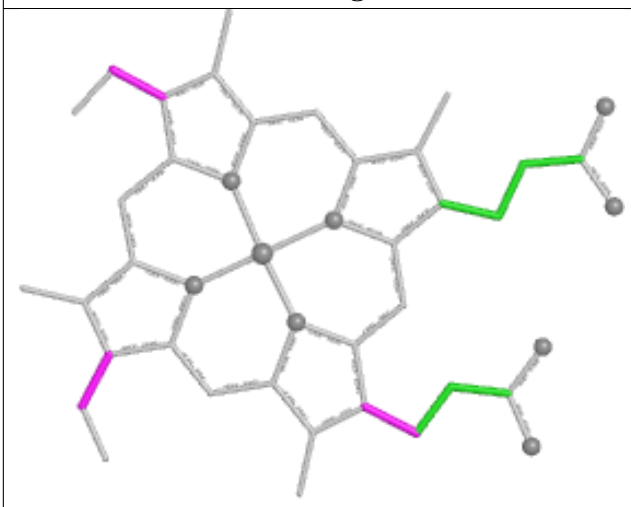
Ligand HEC O 301



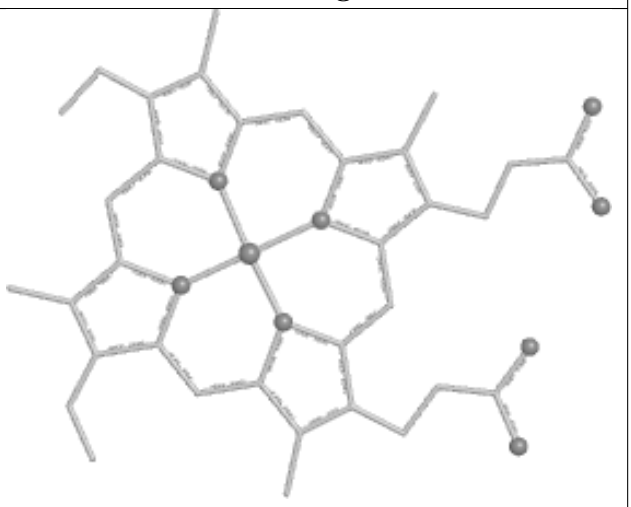
Bond lengths



Bond angles

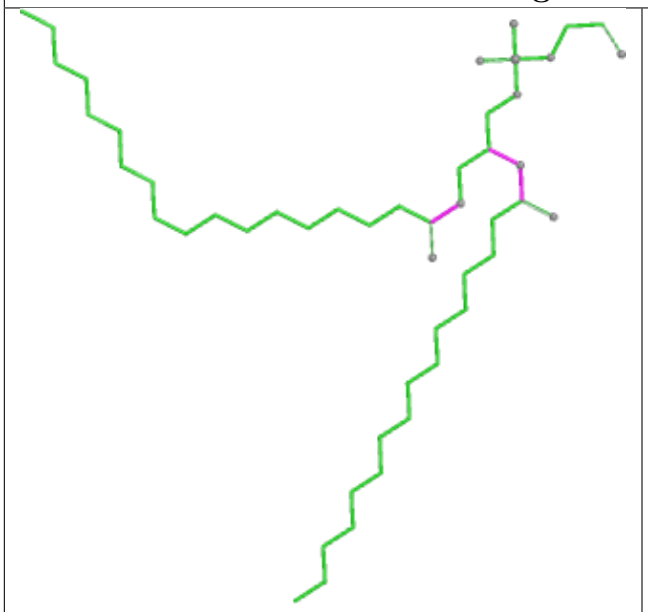


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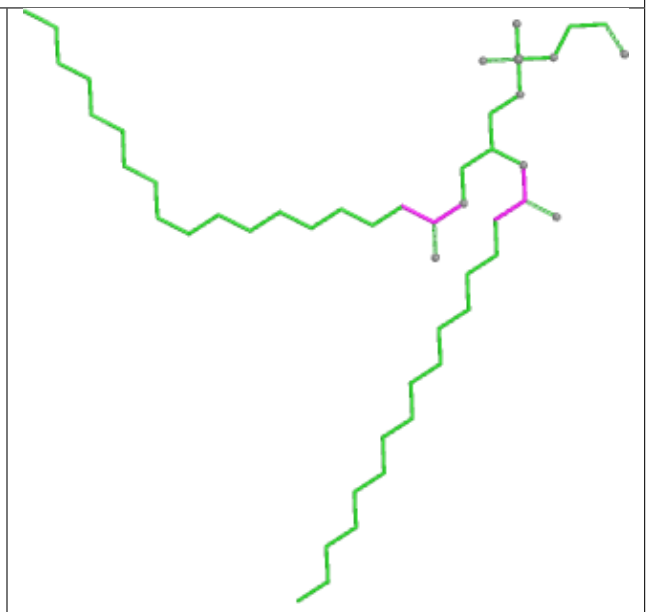


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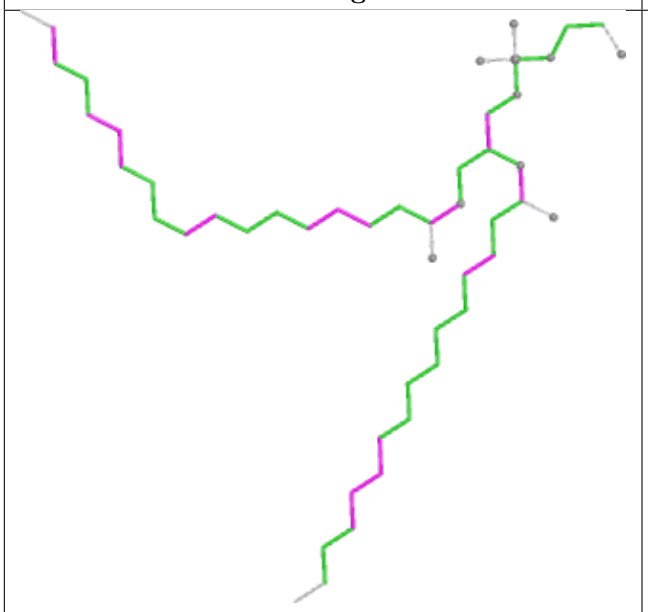
Ligand 9Y0 F 706



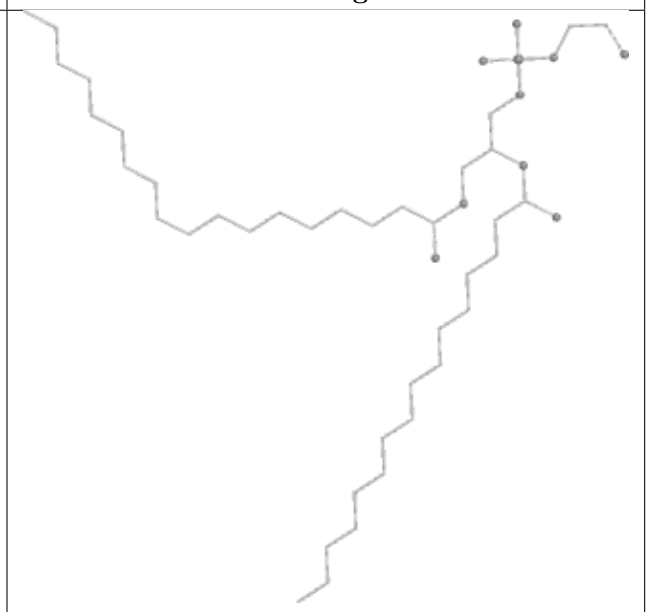
Bond lengths



Bond angles

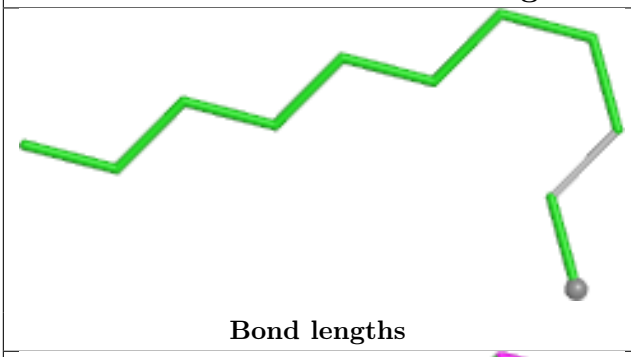


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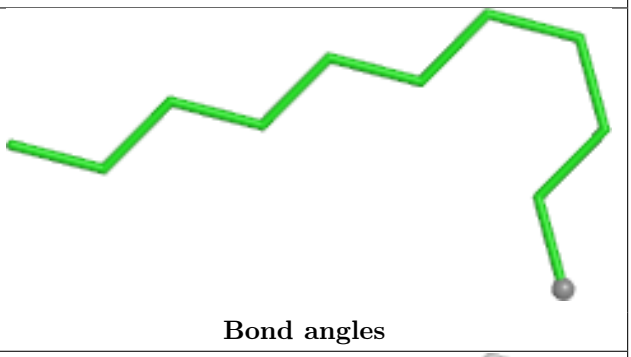


Rings

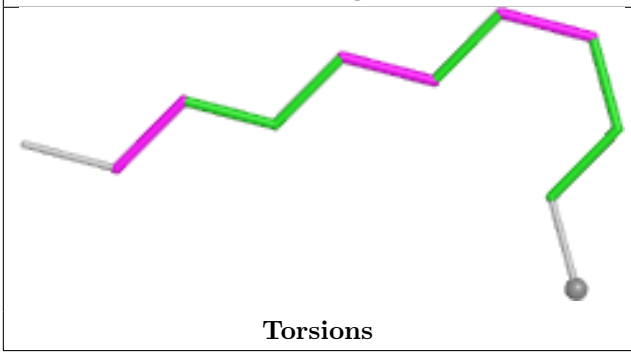
Ligand PLM D 301



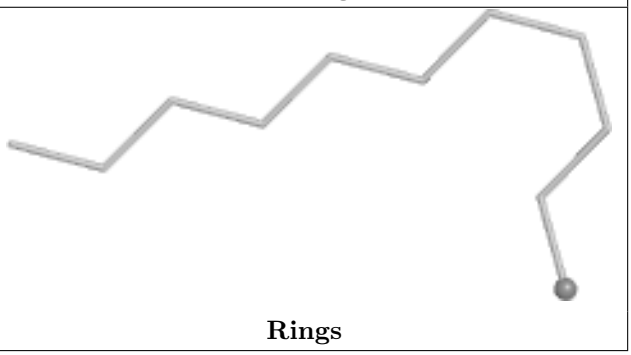
Bond lengths



Bond angles

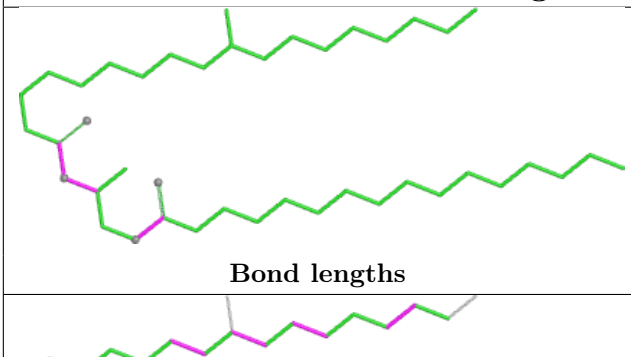


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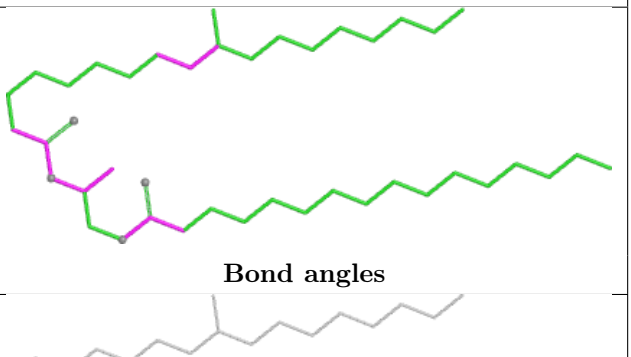


Rings

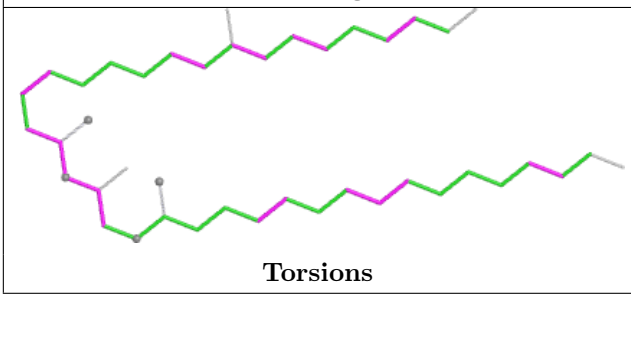
Ligand 9XX c 202



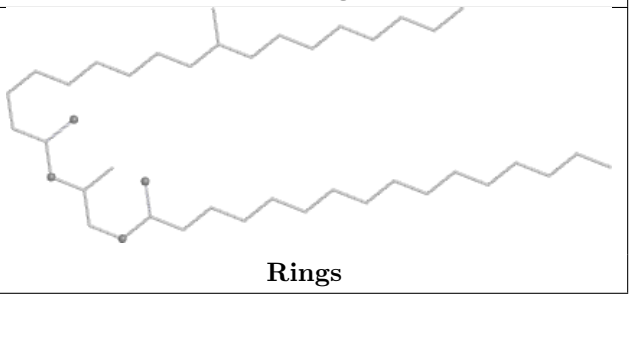
Bond lengths



Bond angles

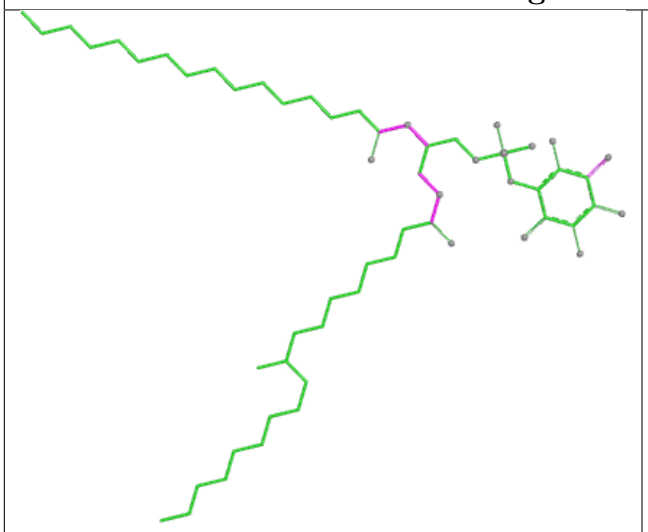


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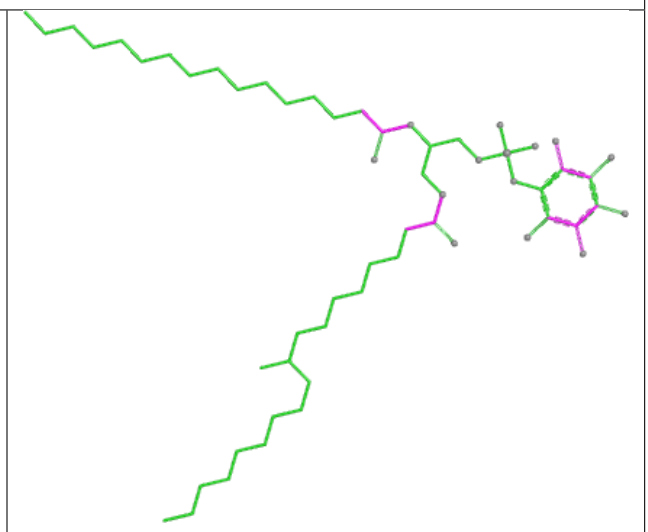


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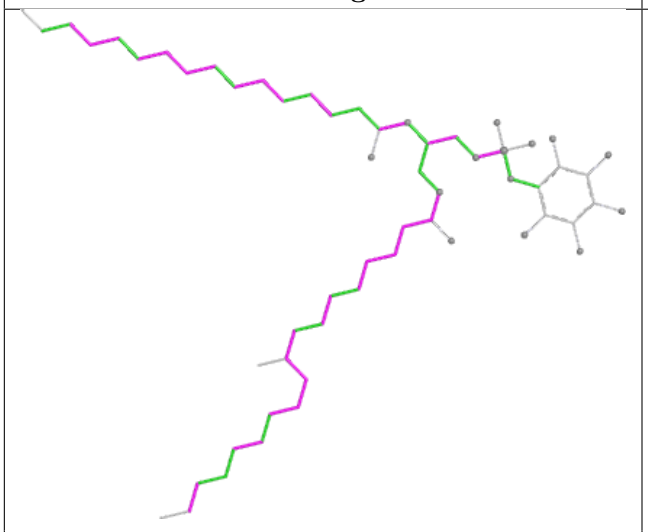
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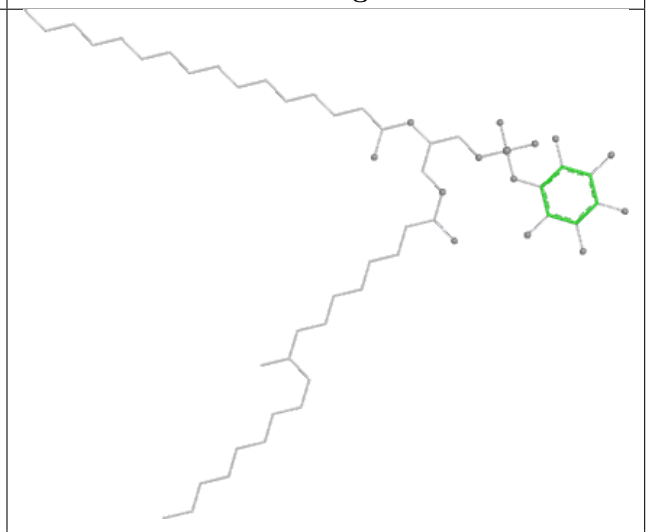
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Bond angles

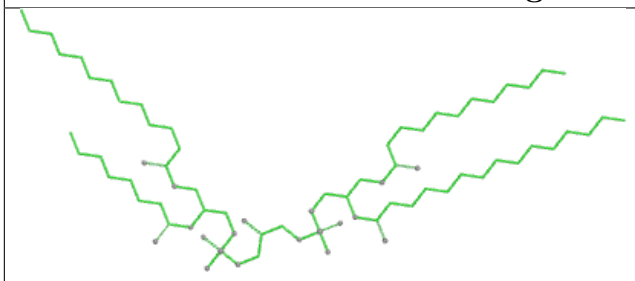


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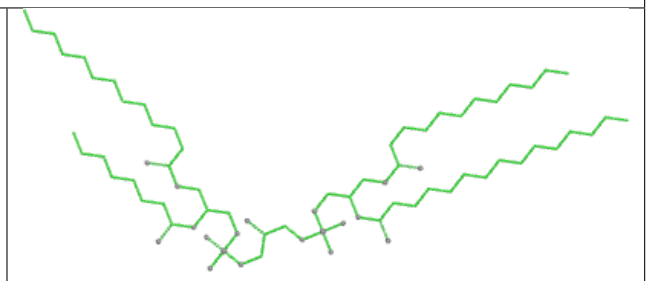


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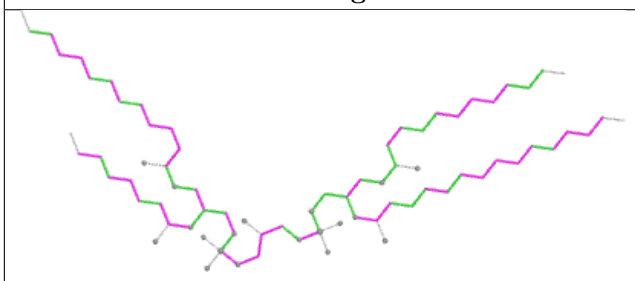
Ligand CDL P 201



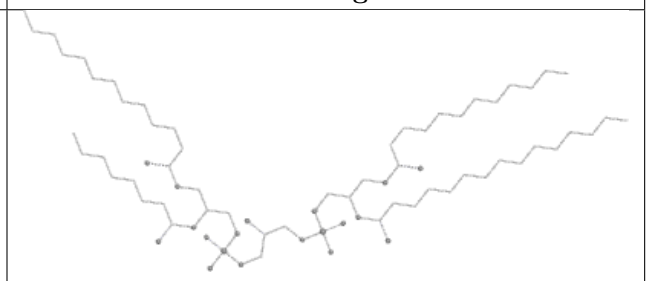
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Bond angles

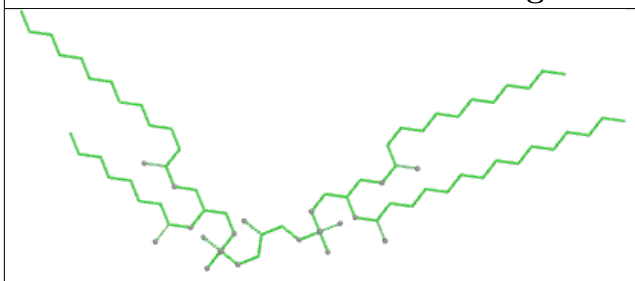


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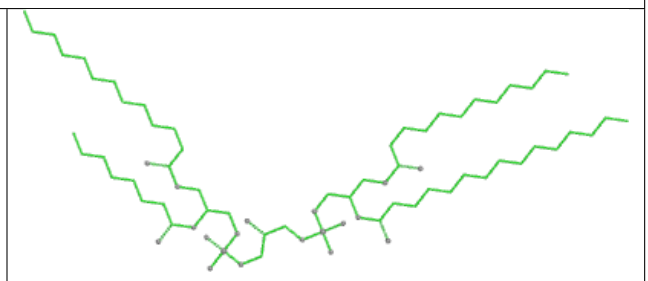


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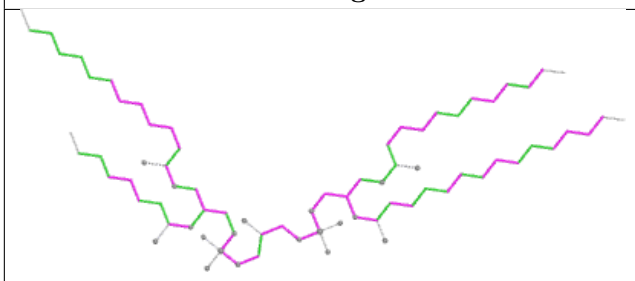
Ligand CDL F 704



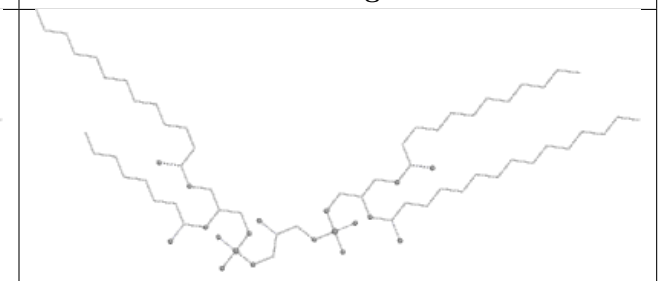
Bond lengths



Bond angles

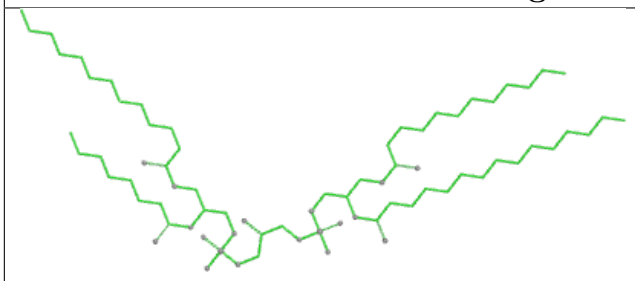


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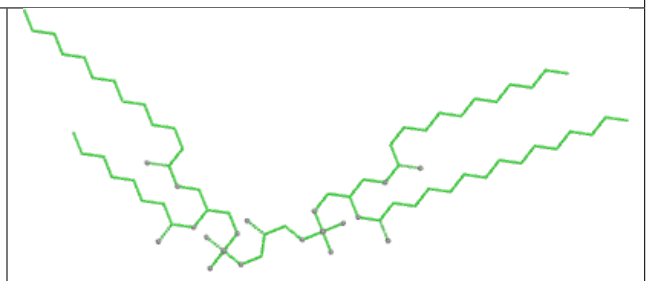


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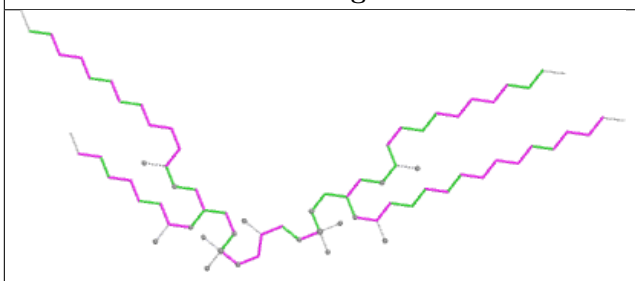
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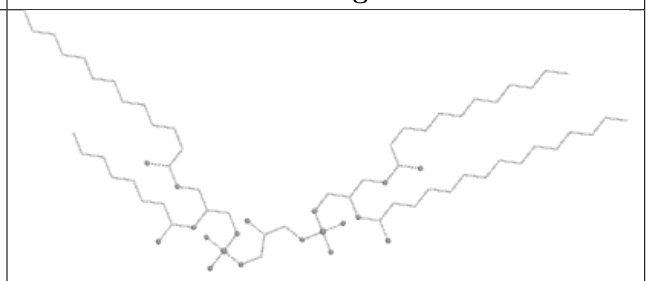
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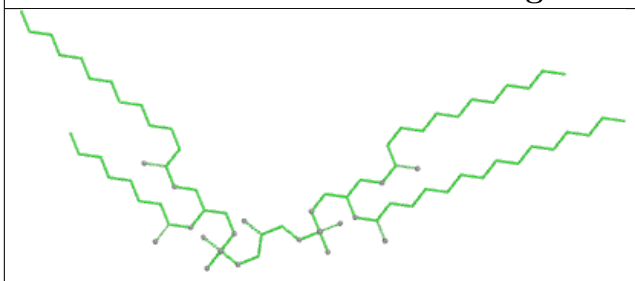


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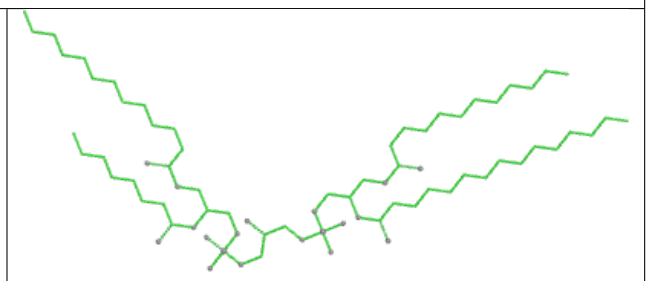


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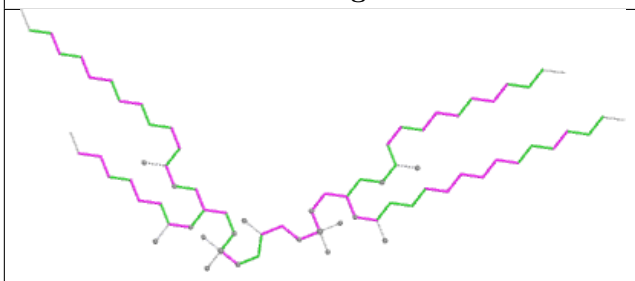
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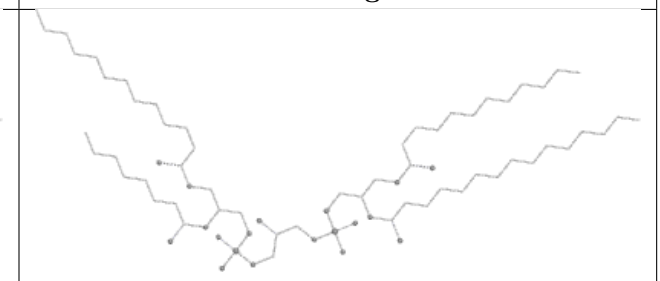
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Bond angles

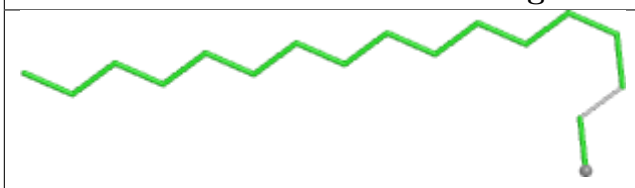


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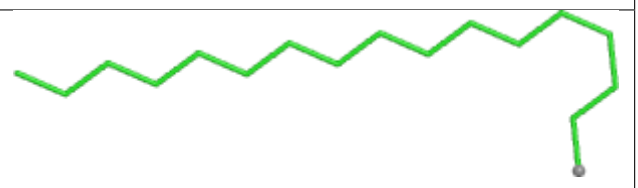


Rings

Ligand PLM c 201



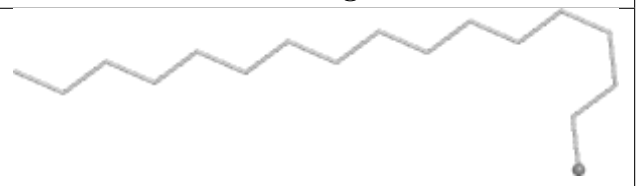
Bond lengths



Bond angles

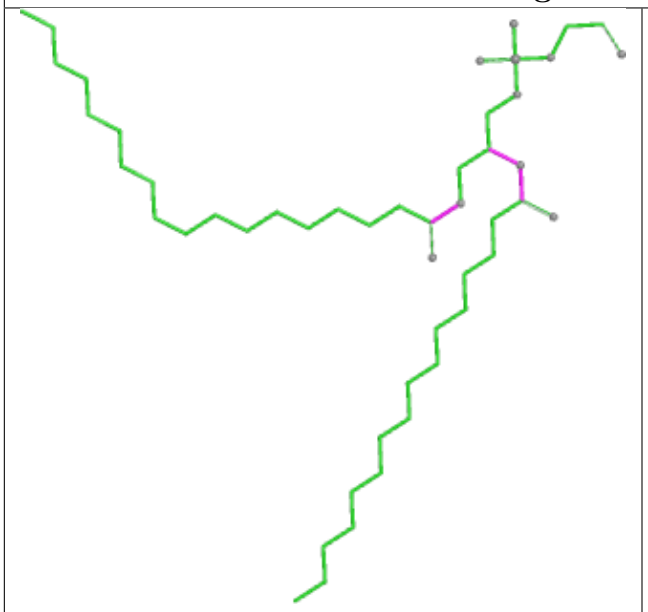


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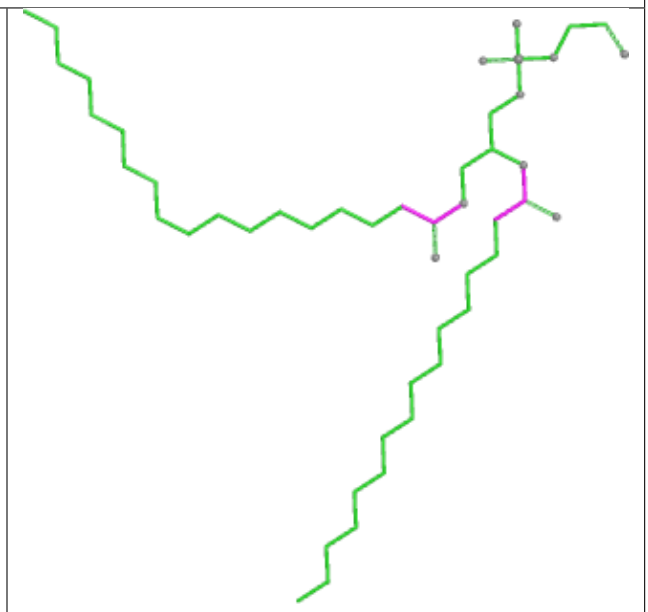


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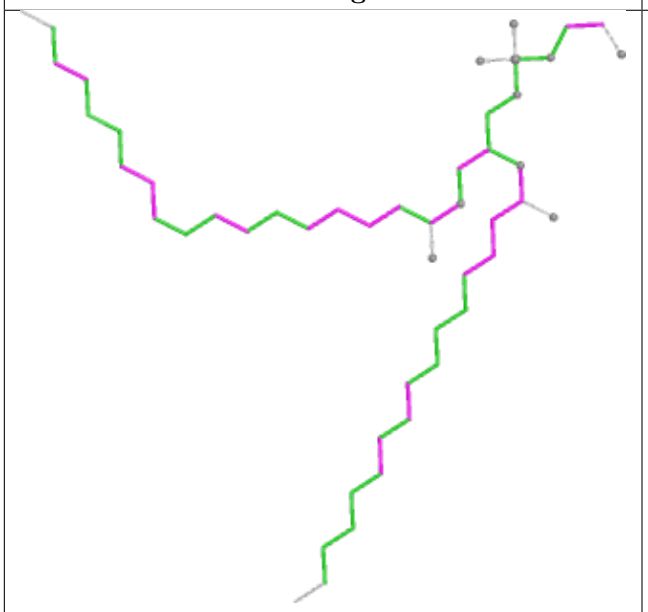
Ligand 9Y0 S 302



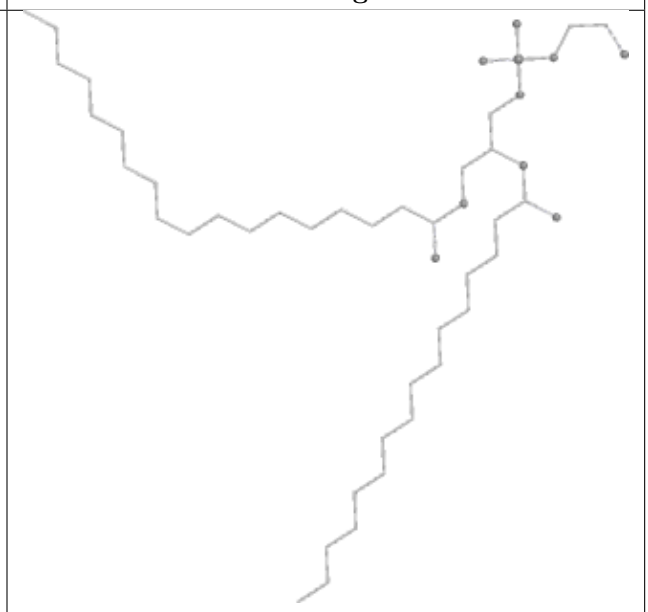
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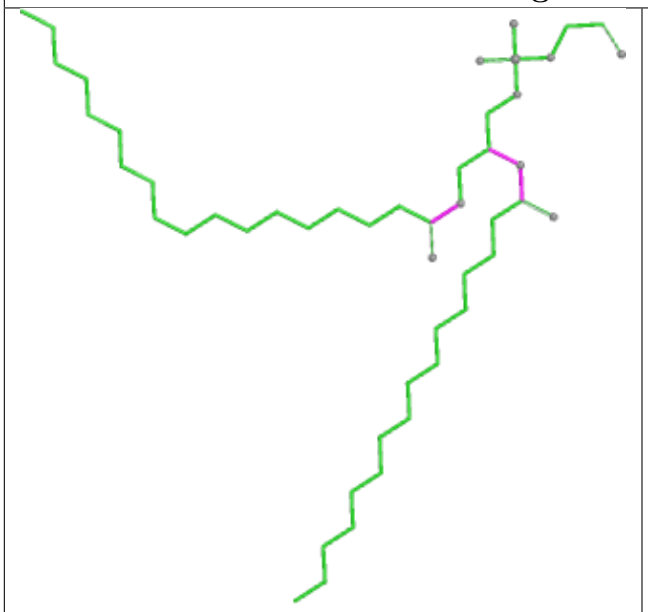


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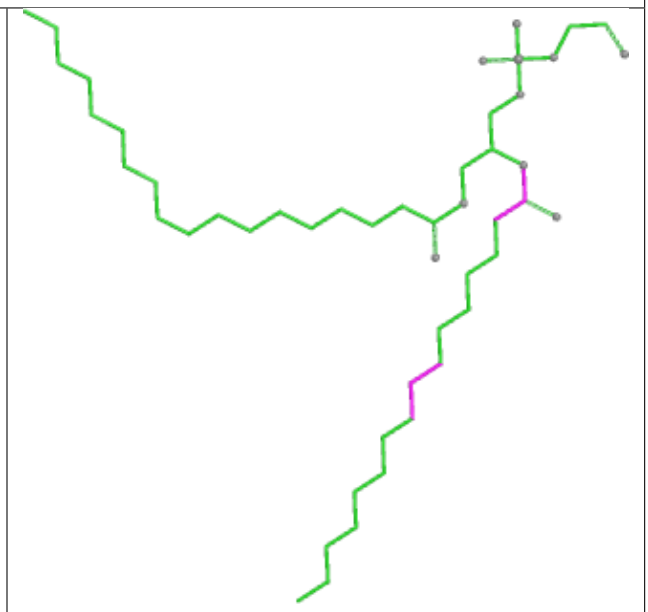


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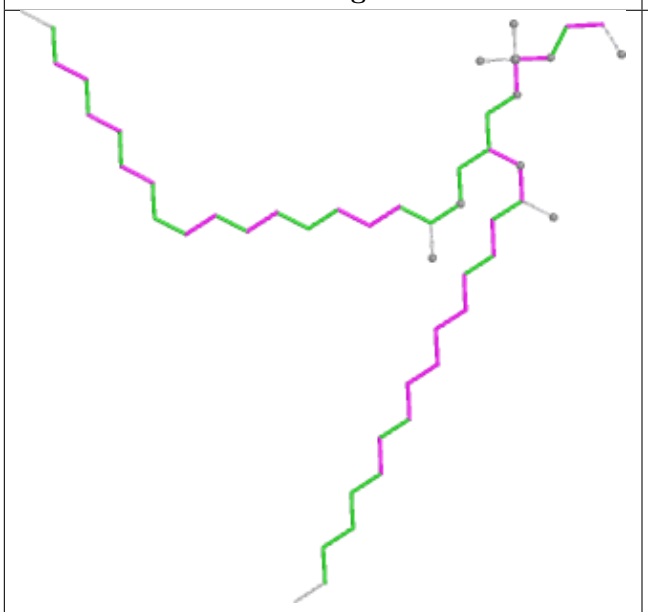
Ligand 9Y0 P 202



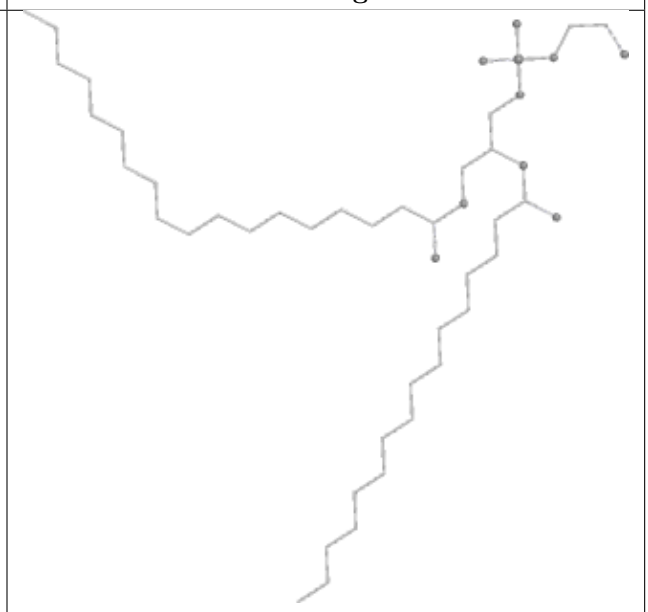
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Bond angles

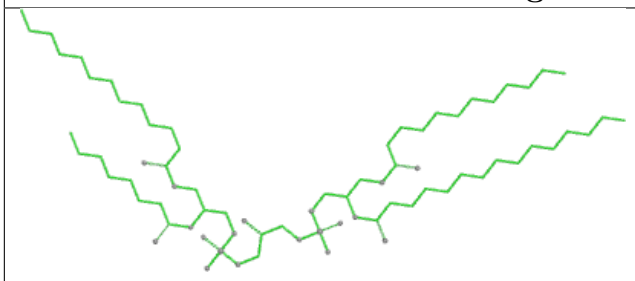


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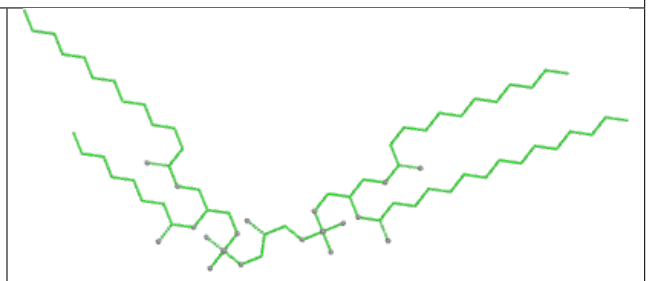


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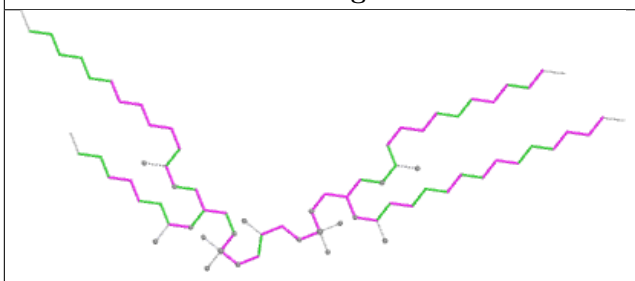
Ligand CDL E 605



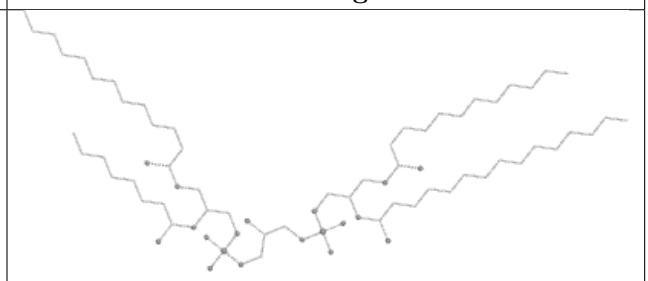
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Bond angles

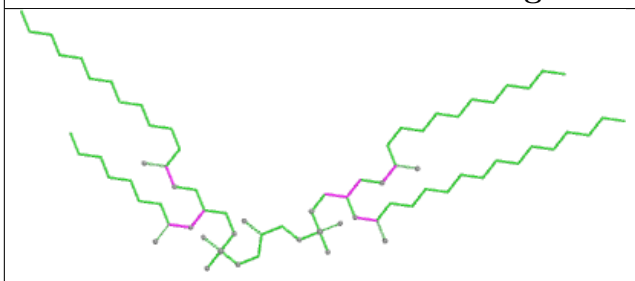


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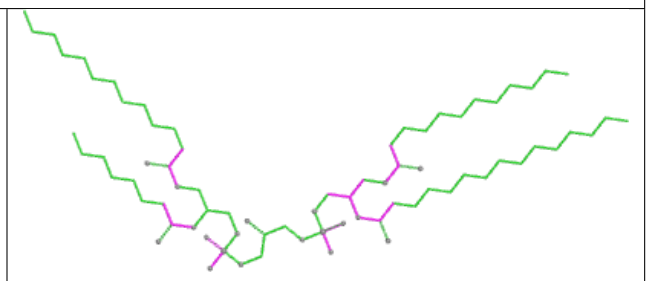


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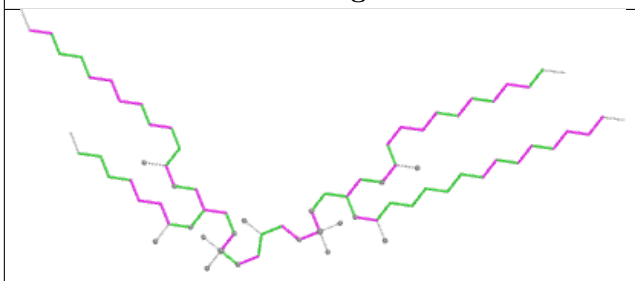
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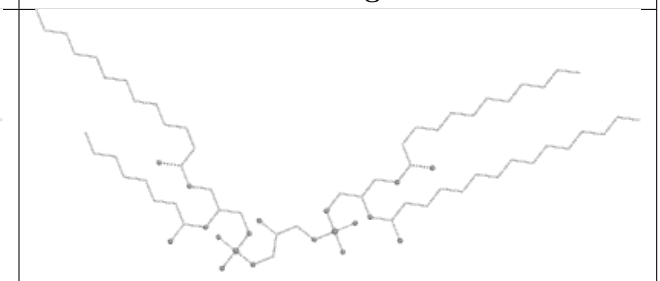
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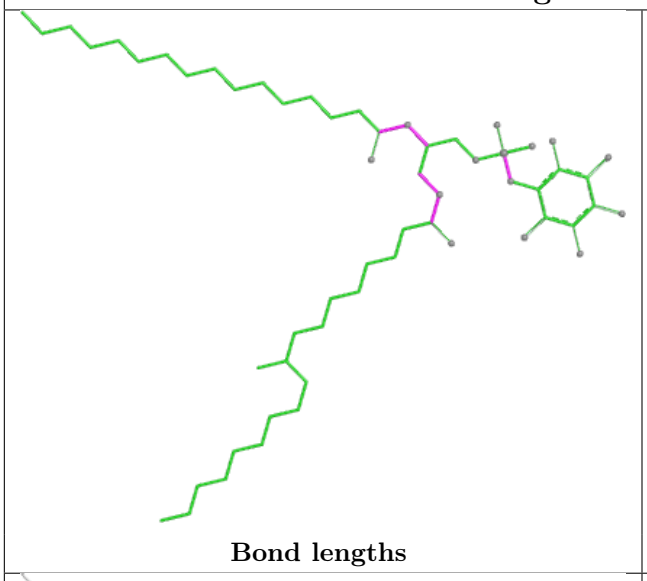


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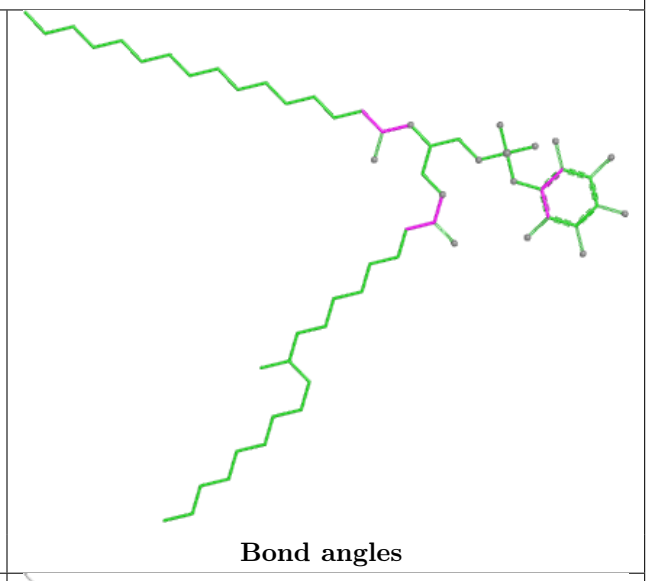


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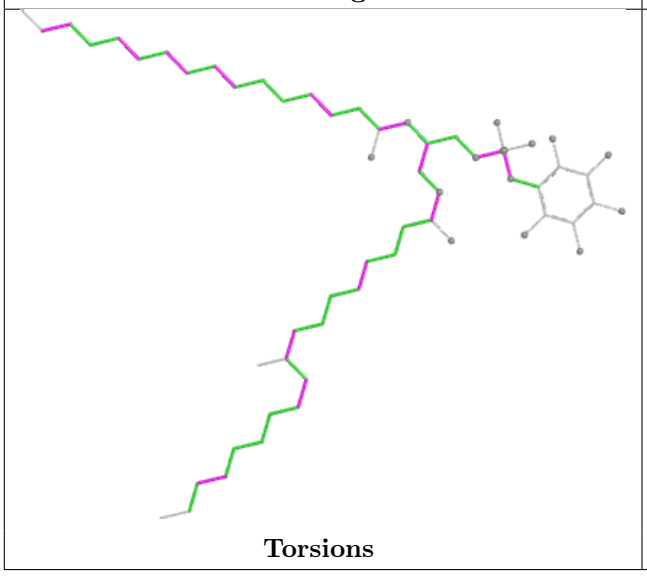
Ligand 9YF c 203



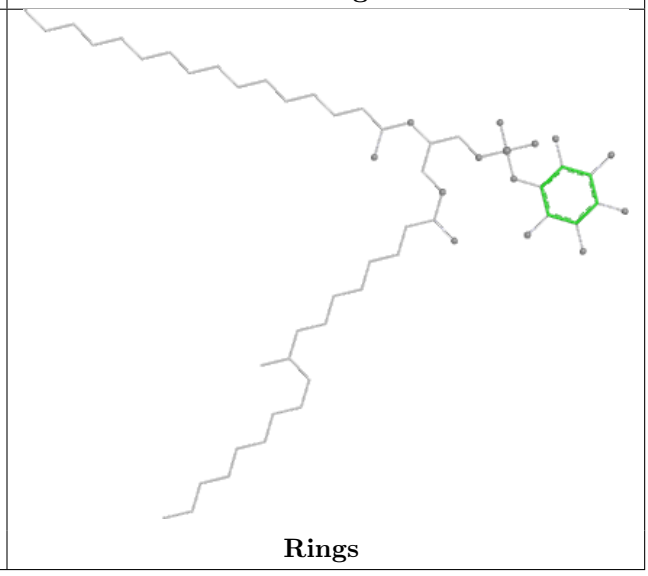
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Bond angles

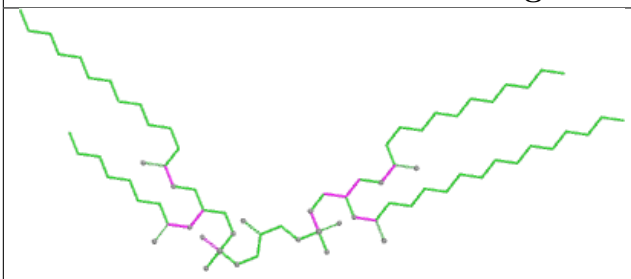


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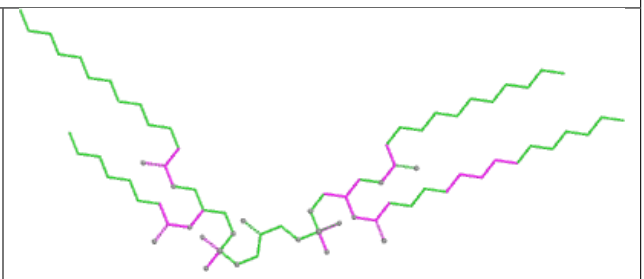


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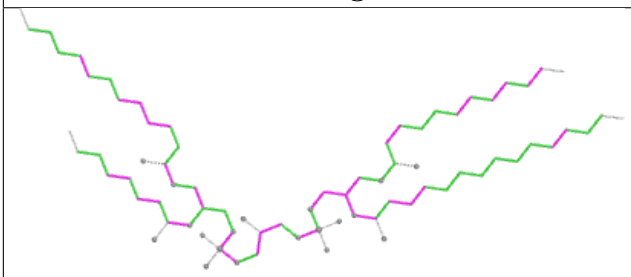
Ligand CDL T 201



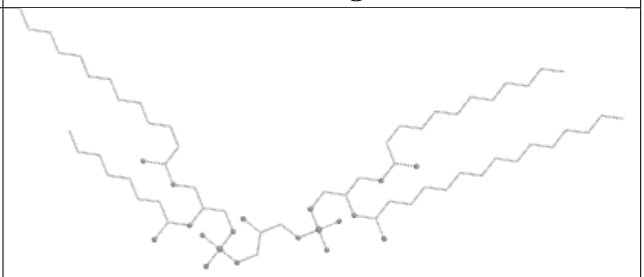
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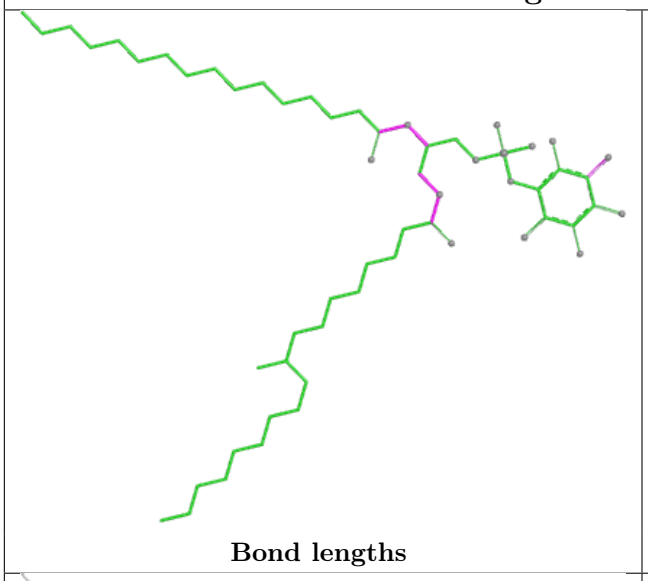


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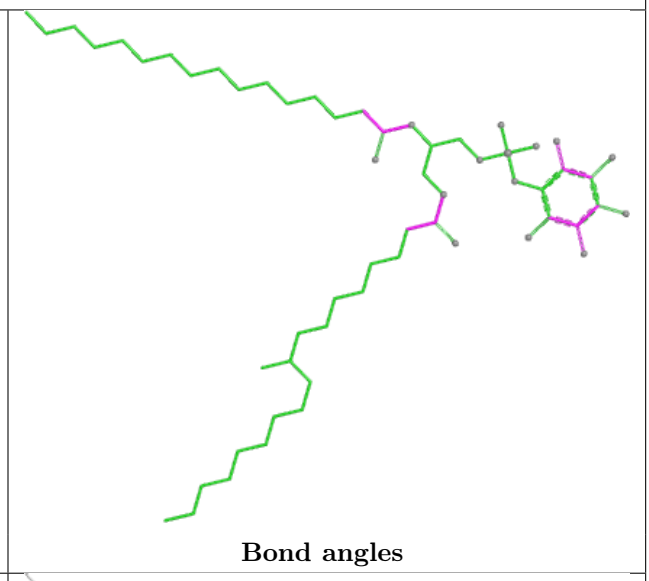


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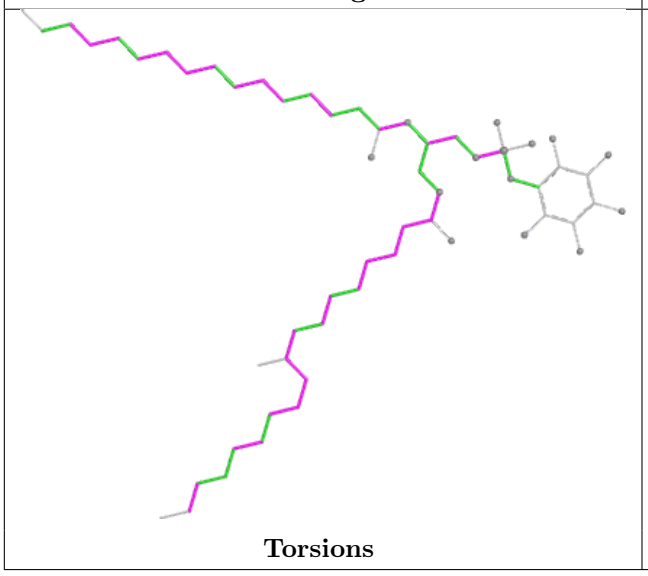
Ligand 9YF M 502



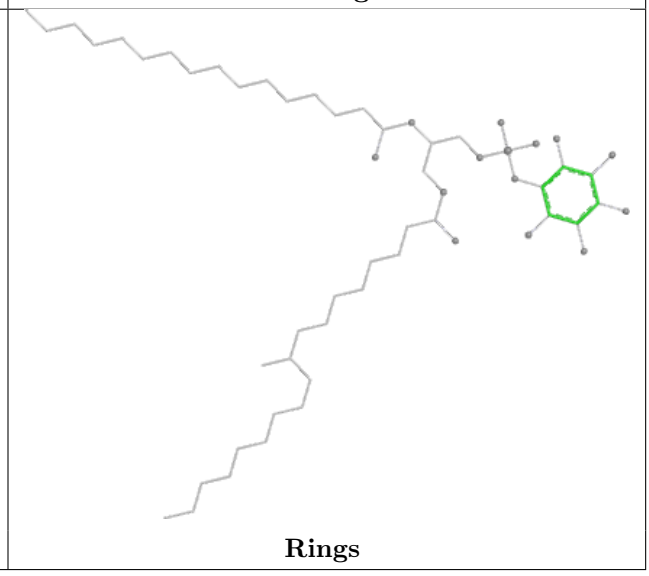
Bond lengths



Bond angles

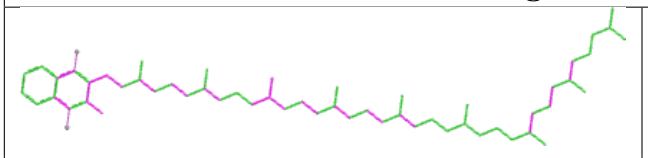


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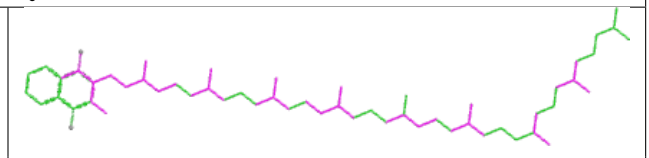


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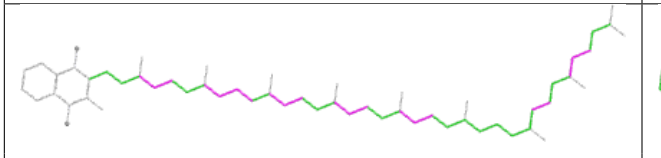
Ligand MQ9 F 707



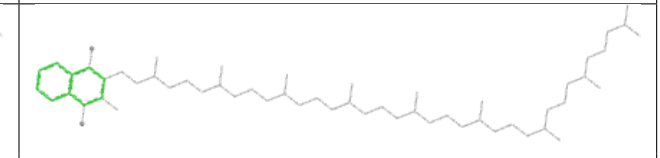
Bond lengths



Bond angles

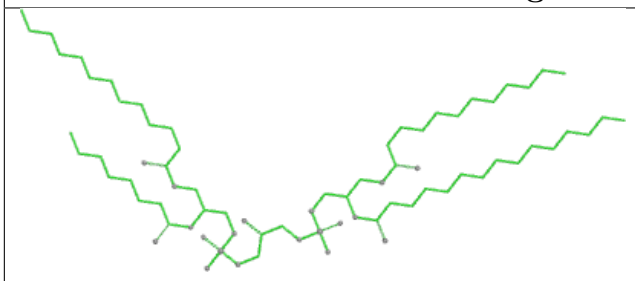


Torsions

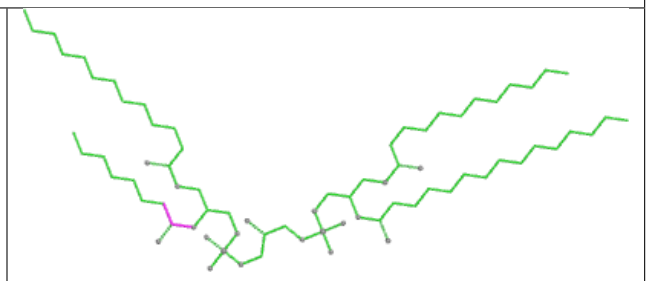


Rings

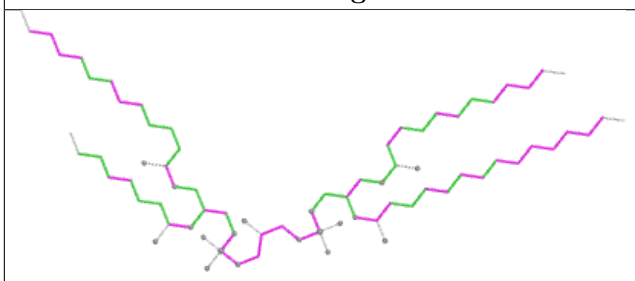
Ligand CDL F 705



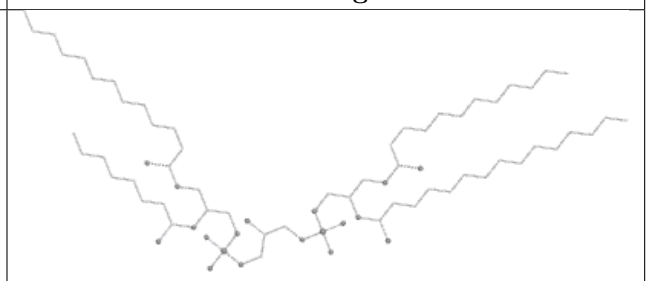
Bond lengths



Bond angles

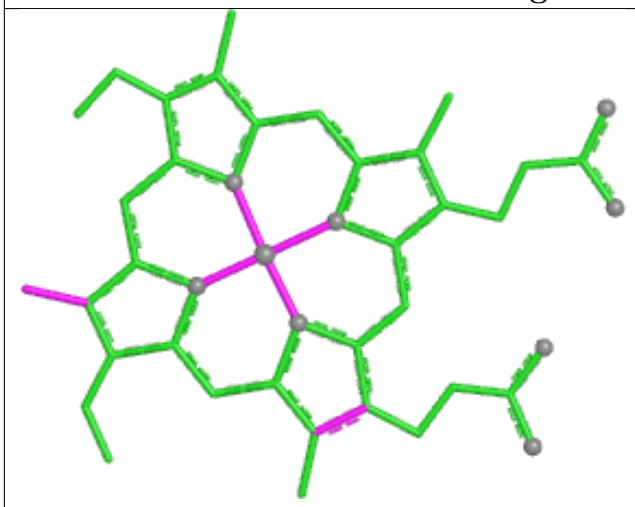


Torsions

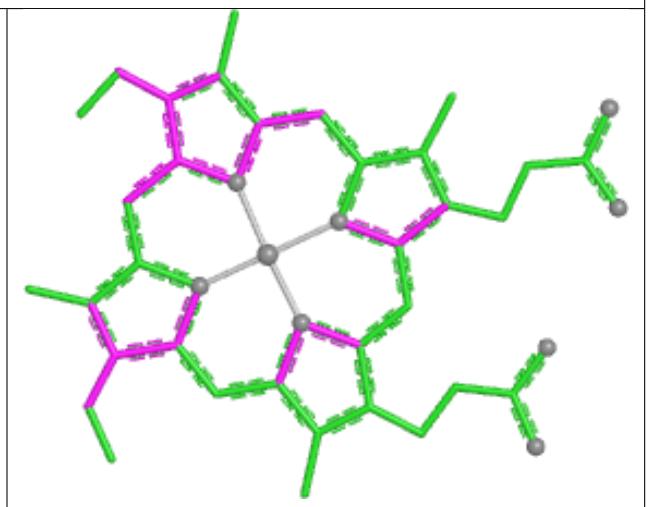


Rings

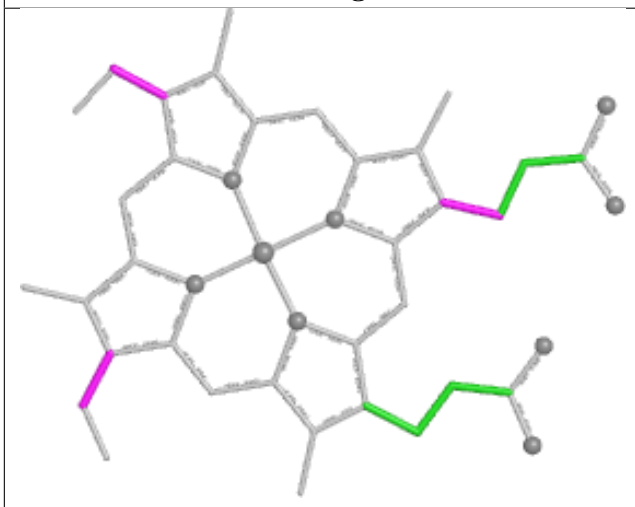
Ligand HEC I 302



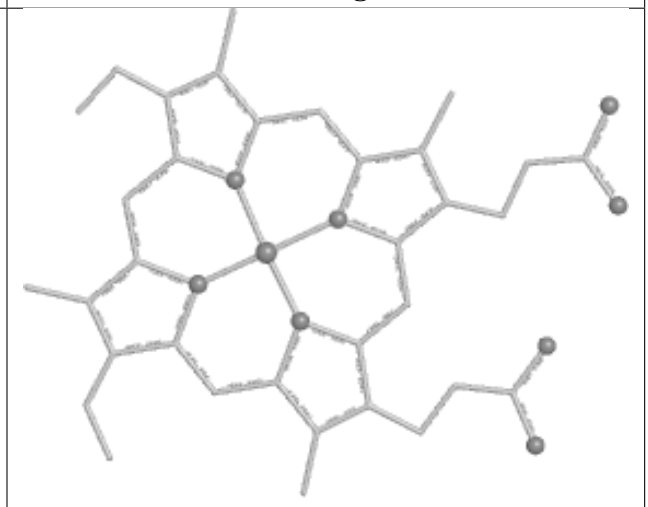
Bond lengths



Bond angles

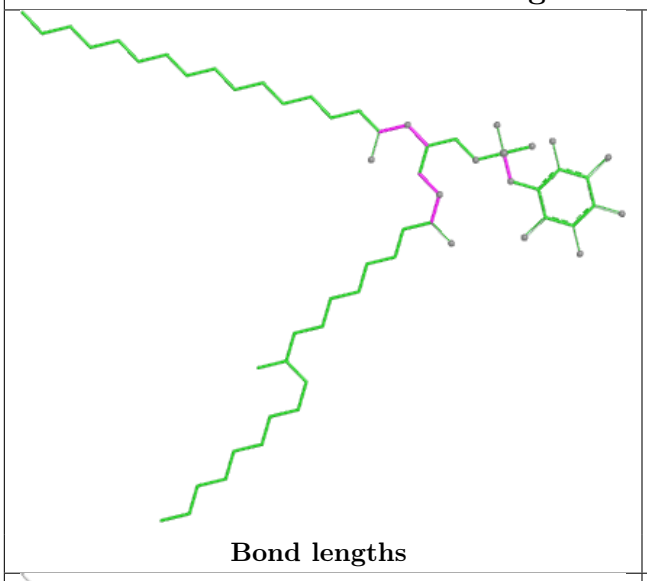


Torsions

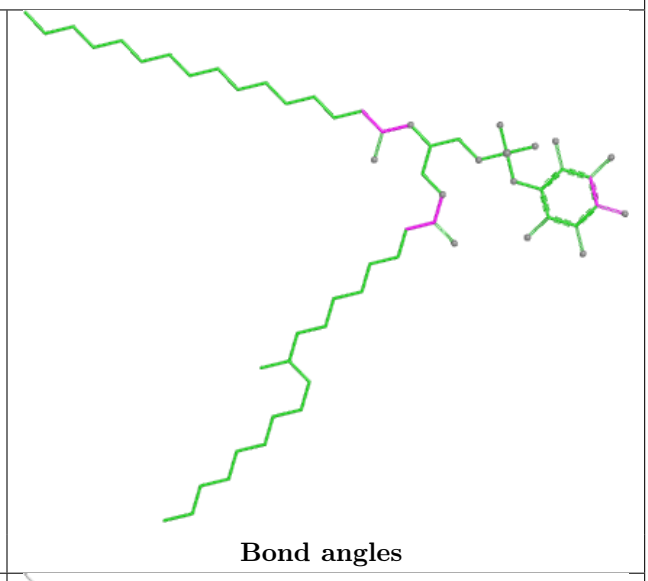


Rings

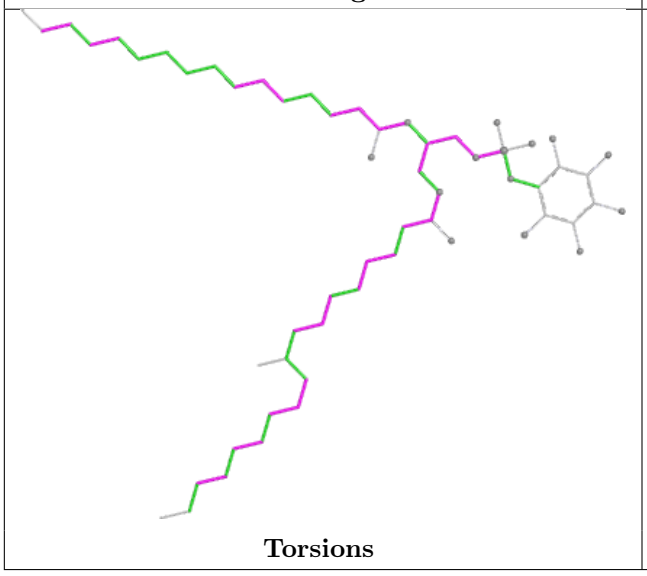
Ligand 9YF O 303



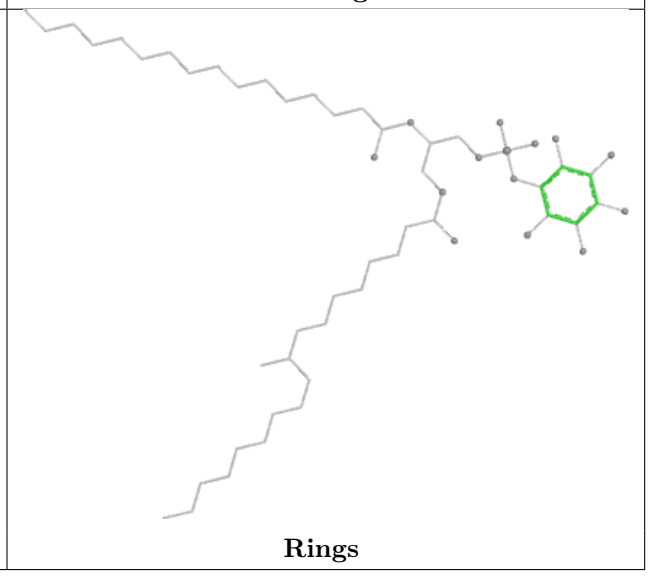
Bond lengths



Bond angles

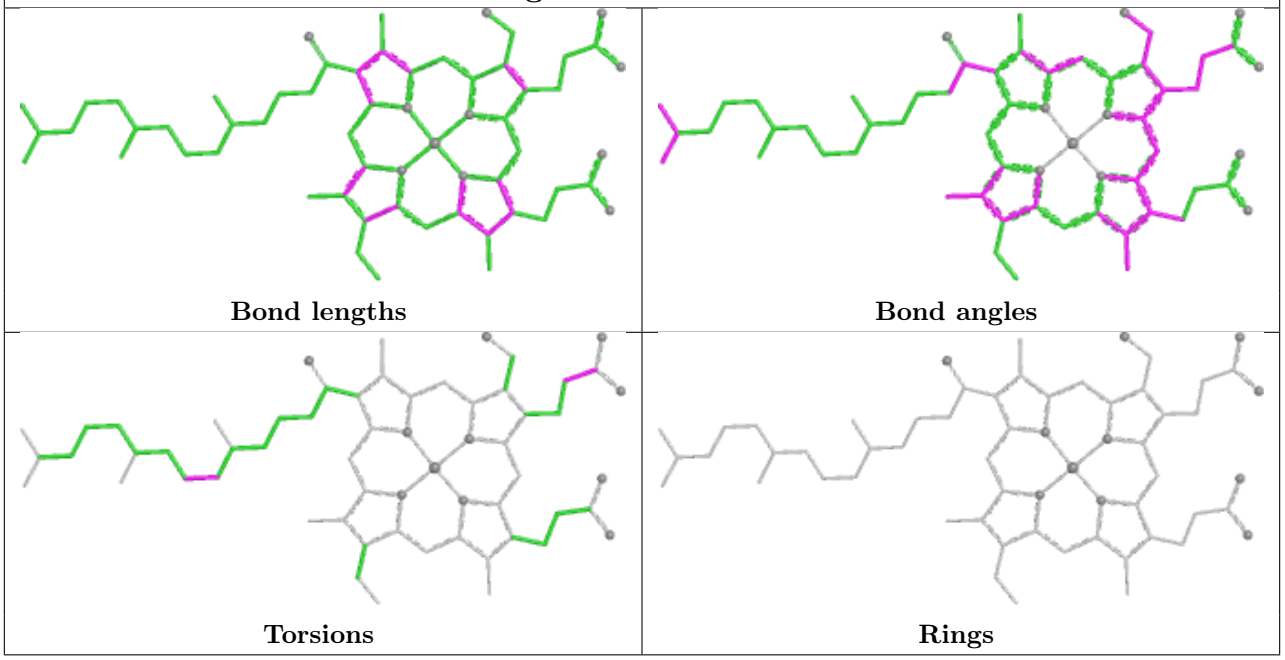


Torsions

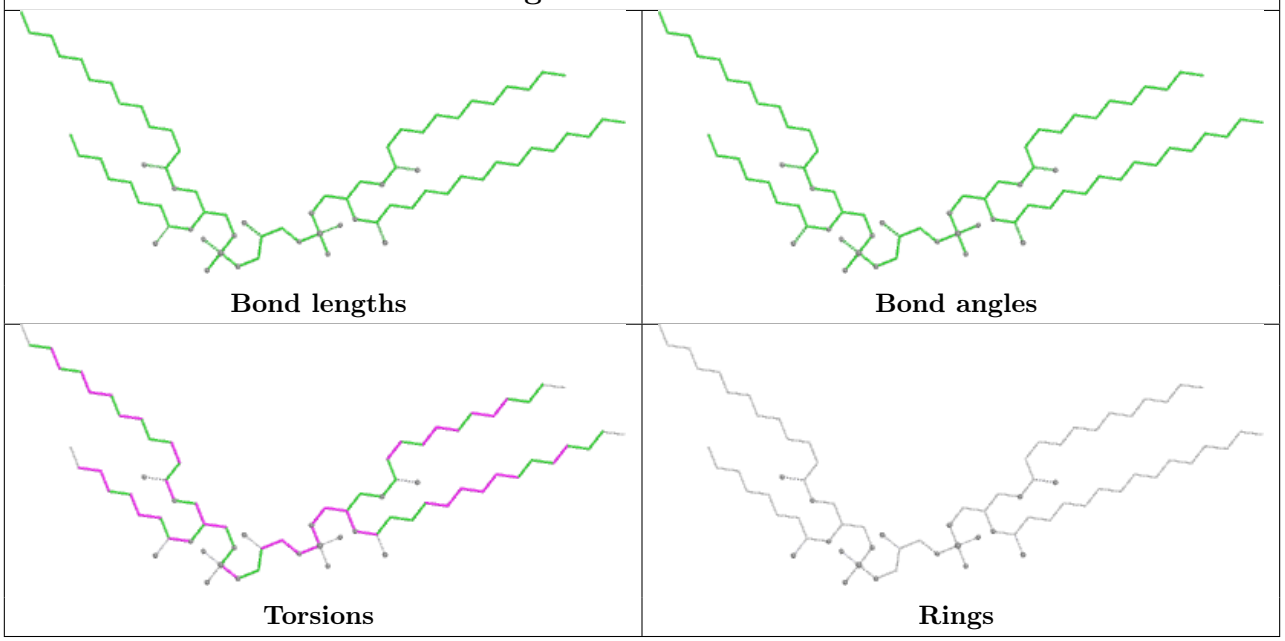


Rings

Ligand HEA L 603



Ligand CDL X 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

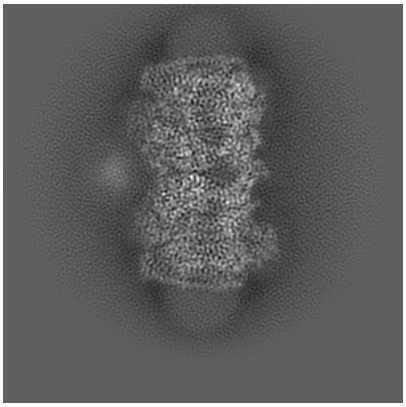
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24455. These allow visual inspection of the internal detail of the map and identification of artifacts.

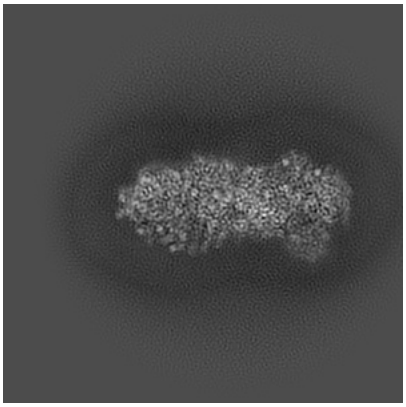
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

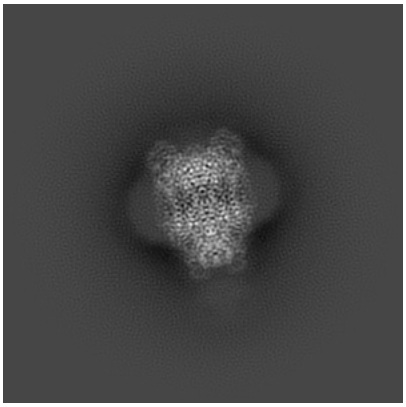
6.1.1 Primary map



X



Y

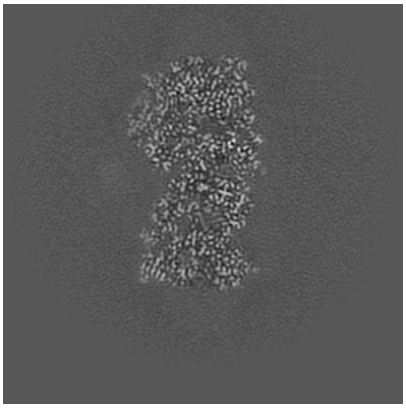


Z

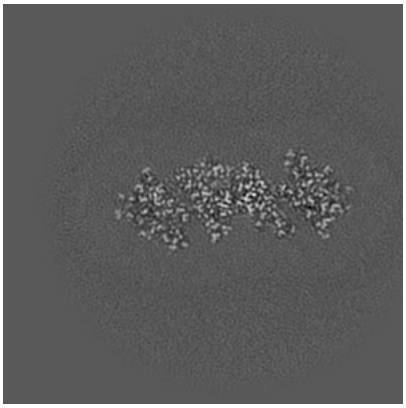
The images above show the map projected in three orthogonal directions.

6.2 Central slices

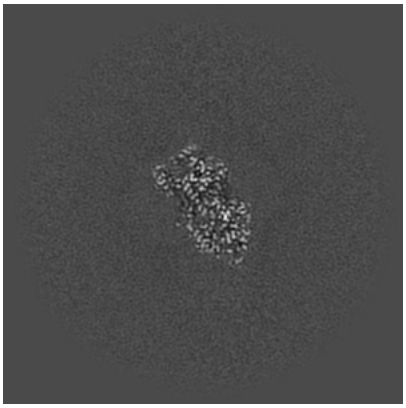
6.2.1 Primary map



X Index: 165



Y Index: 165

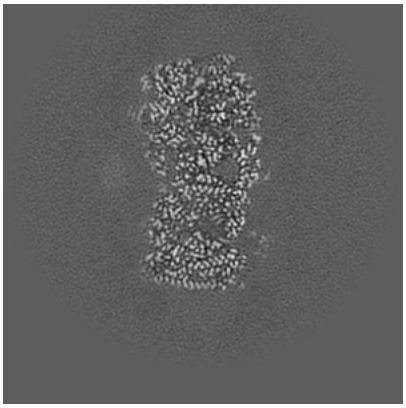


Z Index: 165

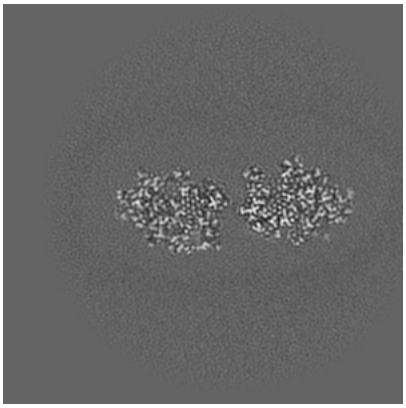
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

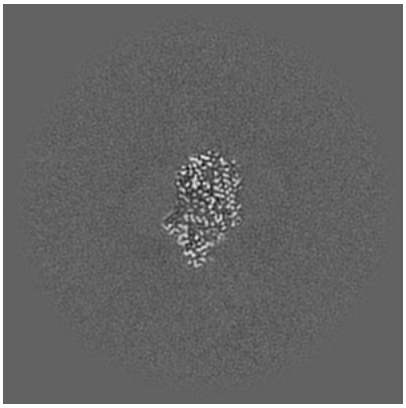
6.3.1 Primary map



X Index: 170



Y Index: 182

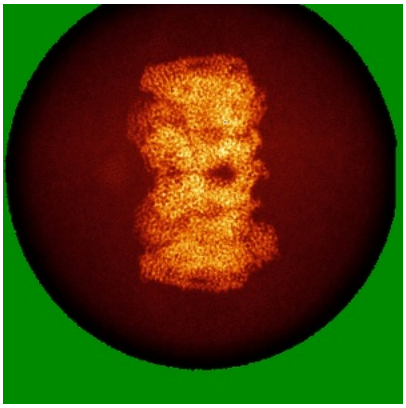


Z Index: 208

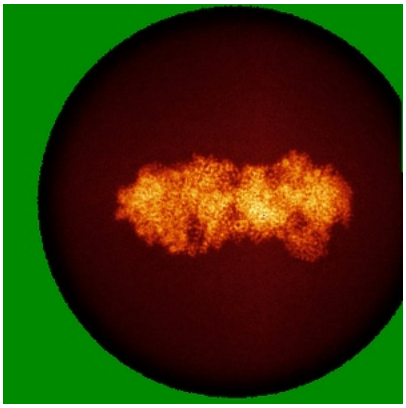
The images above show the largest variance slices of the map in three orthogonal directions.

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

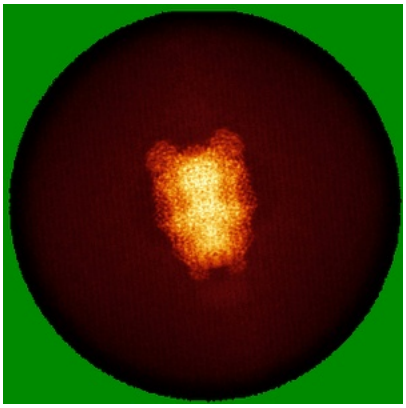
6.4.1 Primary map



X



Y

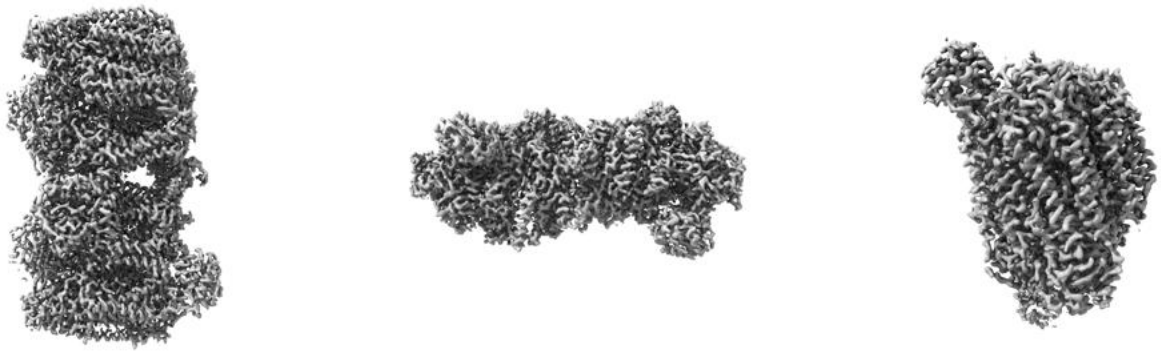


Z

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 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

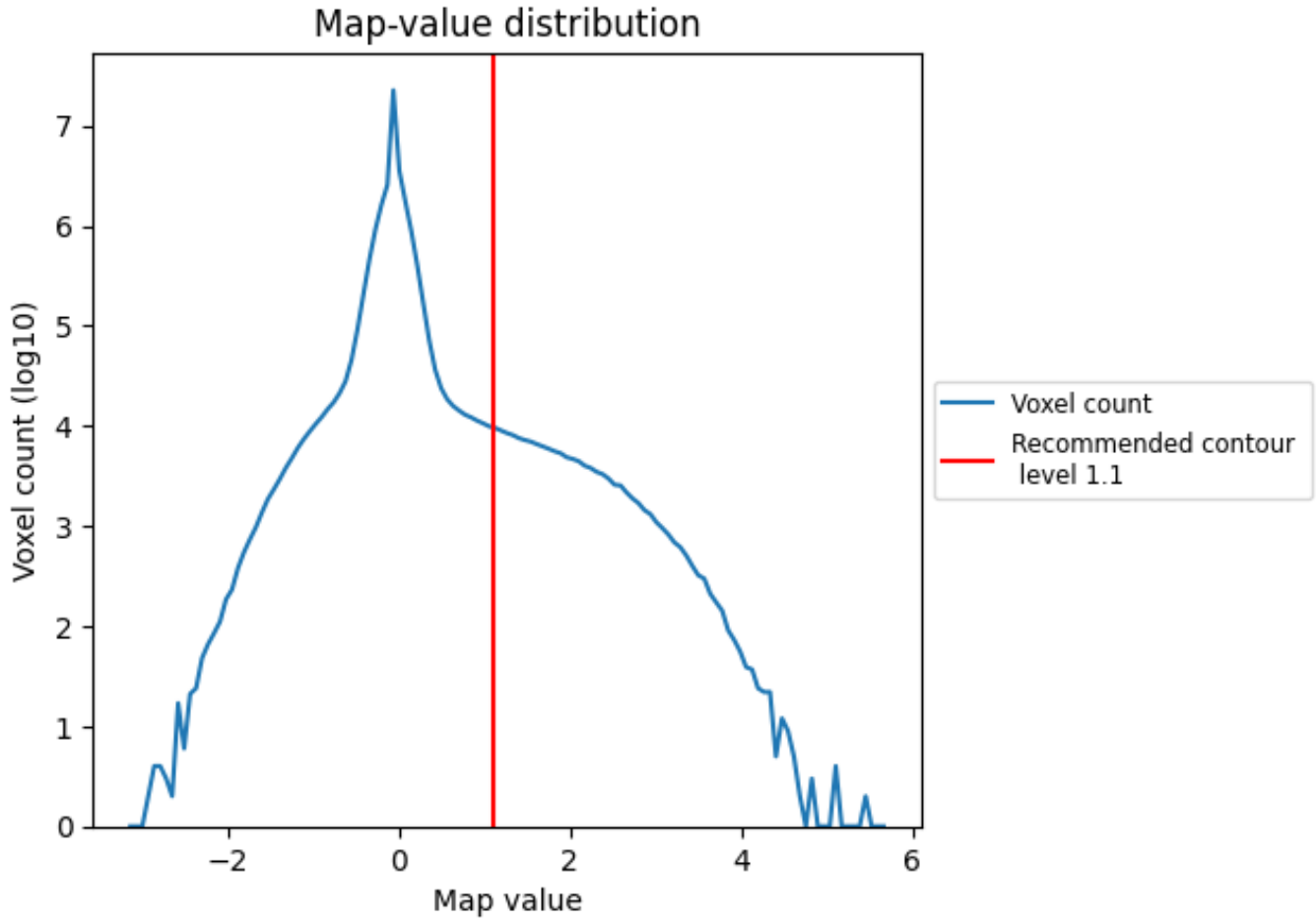
6.6 Mask visualisation (i)

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

7 Map analysis

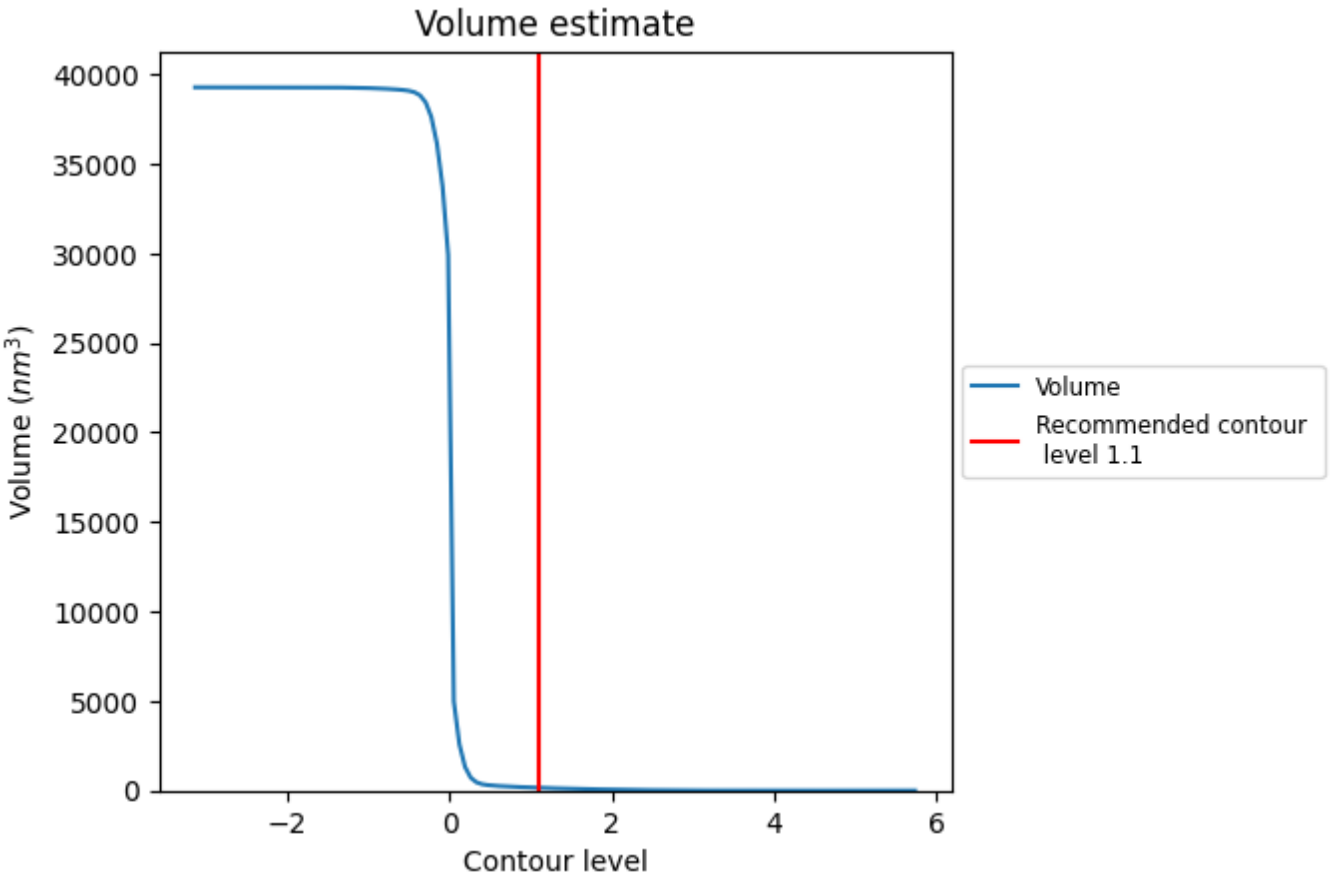
This section contains the results of statistical analysis of the map.

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.

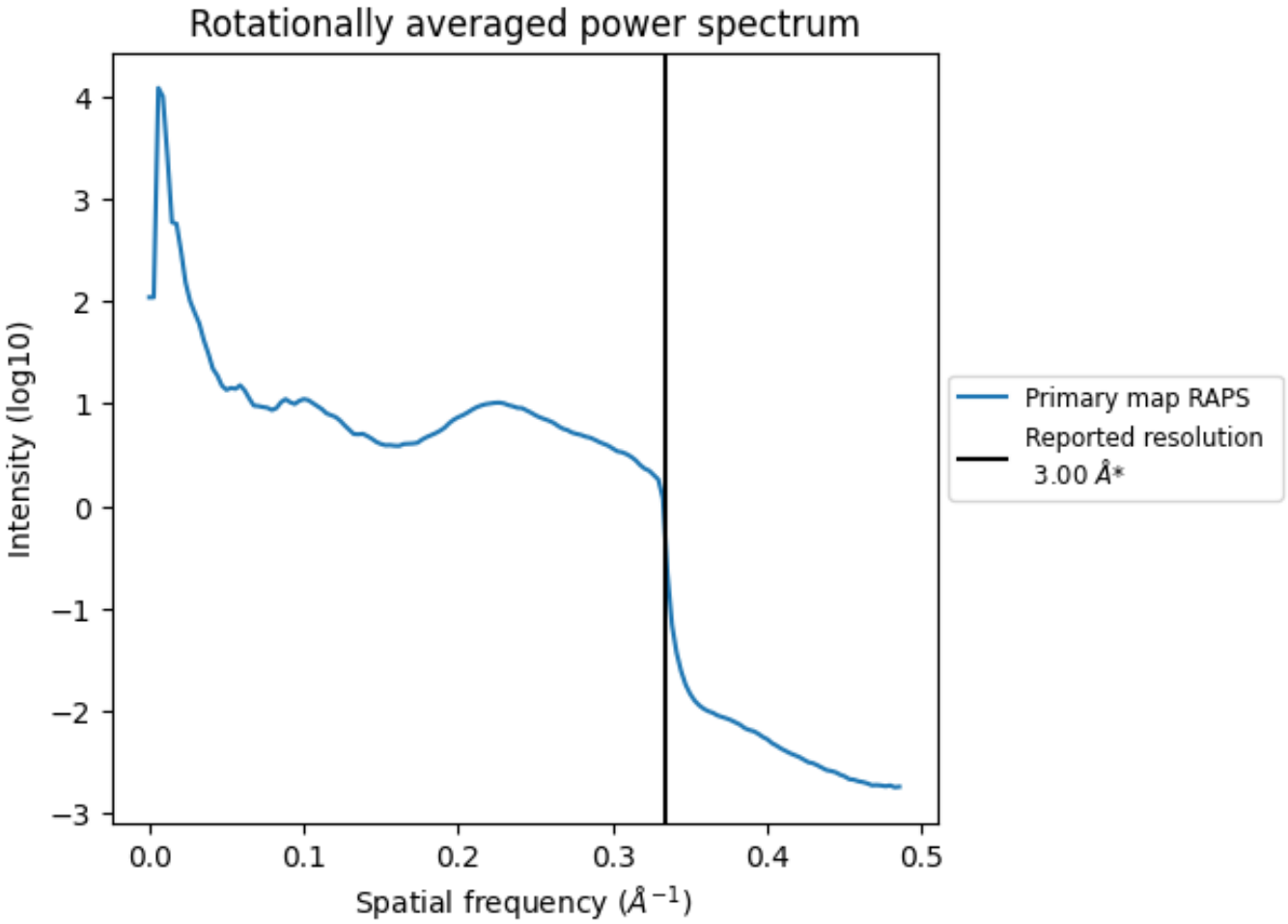
7.2 Volume estimate



The volume at the recommended contour level is 155 nm^3; this corresponds to an approximate mass of 140 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 0.333 Å^{-1}

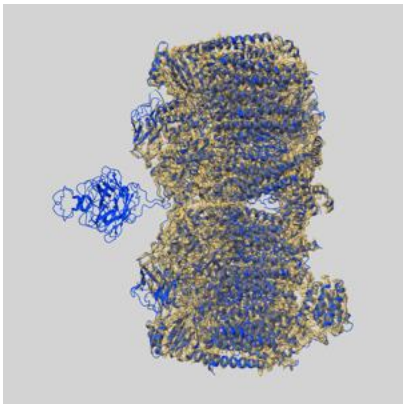
8 Fourier-Shell correlation (i)

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

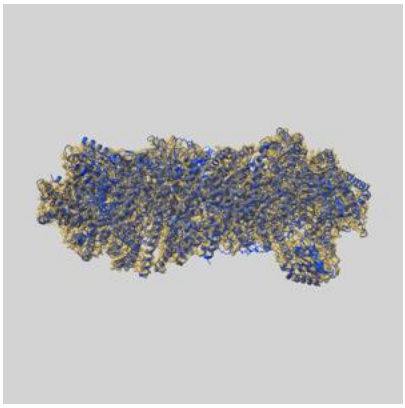
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24455 and PDB model 7RH5. Per-residue inclusion information can be found in section 3 on page 16.

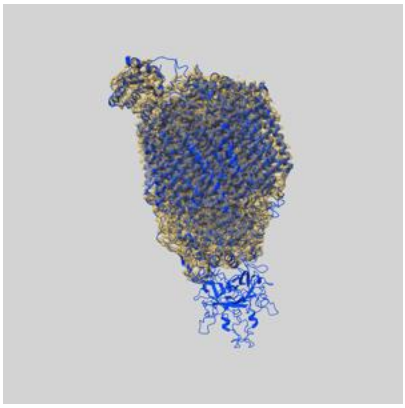
9.1 Map-model overlay



X



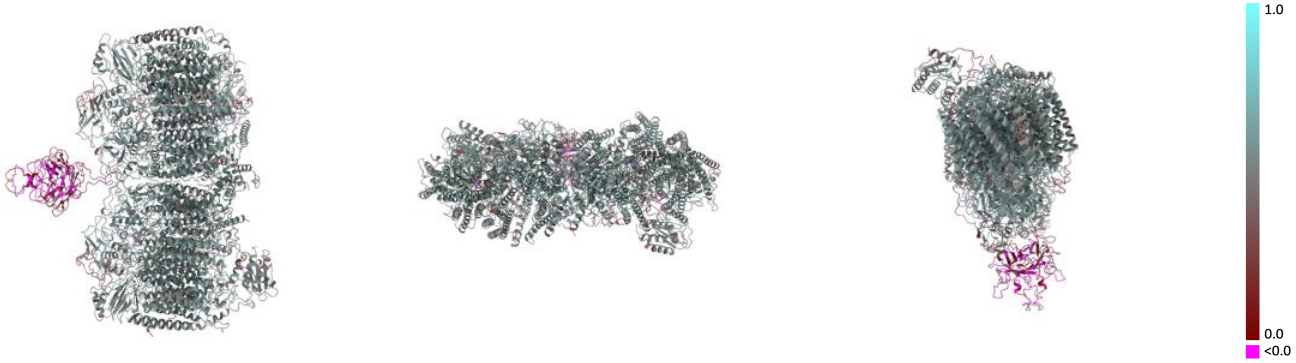
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.1 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.

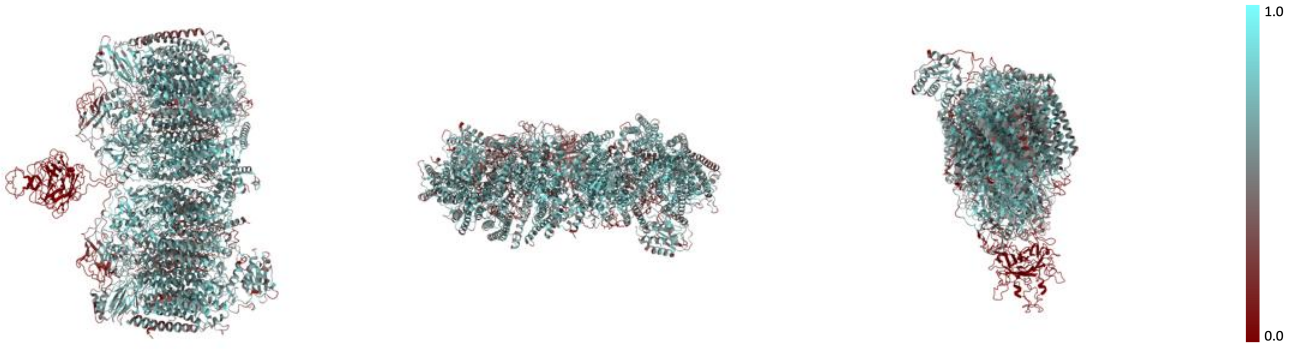
9.2 Q-score mapped to coordinate model



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.

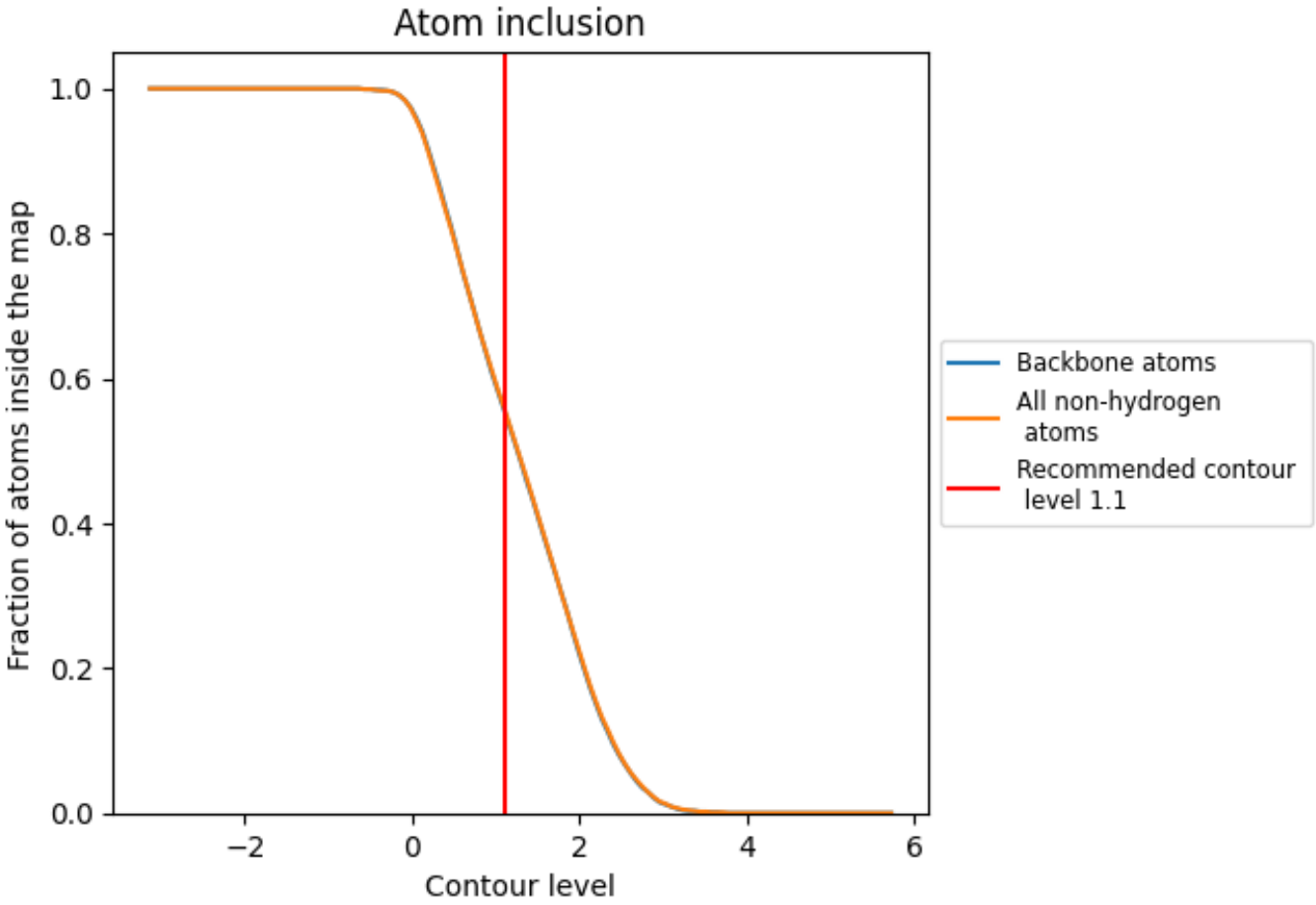
9.3 Atom inclusion mapped to coordinate model



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 (1.1).

9.4 Atom inclusion (i)



At the recommended contour level, 56% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.5130
D	0.0790	0.1670
E	0.6810	0.5580
F	0.6870	0.5560
G	0.0850	0.1590
I	0.6130	0.5480
J	0.4740	0.5050
K	0.5030	0.4900
L	0.6620	0.5560
M	0.6750	0.5500
O	0.6400	0.5460
P	0.5140	0.5020
Q	0.5170	0.4950
R	0.6770	0.5550
S	0.5920	0.5140
T	0.5580	0.5220
U	0.4030	0.4330
V	0.5340	0.4920
W	0.2870	0.4550
X	0.5500	0.5160
Y	0.6710	0.5520
Z	0.5480	0.5110
a	0.4060	0.4380
b	0.5250	0.4980
c	0.2540	0.4560

