wwPDB EM Validation Summary Report (i)

Aug 13, 2026 – 12:59 AM JST

PDB ID	:	9WCY / pdb_00009wcy
EMDB ID	:	EMD-65879
Title	:	Cryo-EM structure of the Mycobacterium abscessus cytochrome bcc:aa3 supercomplex in the presence of ND-011458
Authors	:	Mathiyazakan, V.; Gruber, G.
Deposited on	:	2025-08-18
Resolution	:	2.26 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:

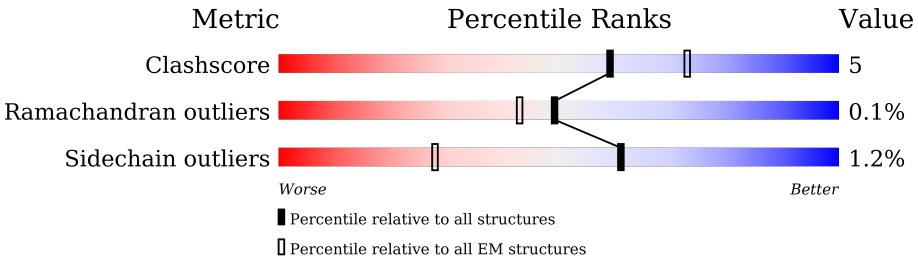
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

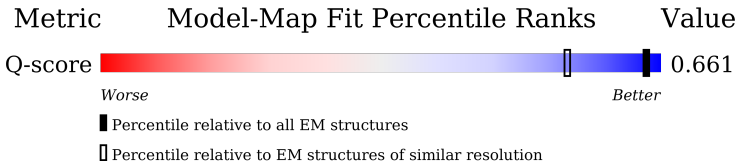
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.26 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	3535 (1.76 - 2.76)

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	G	99	75% • 23%
1	b	99	75% • 23%
2	I	564	84% 13% •
2	L	564	84% 13% •

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Mol	Chain	Length	Quality of chain
3	J	86	73% 6% 21%
3	h	86	6% 71% 8% 21%
4	U	295	69% 5% 25%
4	o	295	68% 6% 25%
5	V	391	93% 5%
5	p	391	93% 5%
6	X	238	10% 89%
6	a	238	10% 89%
7	d	349	81% 9% 11%
7	e	349	82% 7% 11%
8	f	206	88% 11%
8	g	206	90% 9%
9	i	546	86% 10%
9	j	546	88% 8%
10	k	175	77% 6% 17%
10	l	175	78% 5% 17%
11	m	139	95% 5%
11	n	139	90% 10%
12	q	227	64% 5% 31%
12	r	227	62% 7% 31%

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
20	HEC	U	601	X	-	-	-
20	HEC	U	602	X	-	-	-
20	HEC	o	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	HEC	o	602	X	-	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 46789 atoms, of which 0 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 Prokaryotic respiratory supercomplex associate factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	76	575	372	103	98	2	0	0
1	b	76	575	372	103	98	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	551	4363	2936	696	707	24	0	0
2	L	551	4363	2936	696	707	24	0	0

- Molecule 3 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	68	509	333	86	87	3	0	0
3	h	68	509	333	86	87	3	0	0

- Molecule 4 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	U	221	1639	1015	296	318	10	0	0
4	o	221	1639	1015	296	318	10	0	0

- Molecule 5 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	V	381	2957	1900	511	534	12	0	0
5	p	381	2957	1900	511	534	12	0	0

- Molecule 6 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	X	25	171	104	28	38	1	0	0
6	a	25	171	104	28	38	1	0	0

- Molecule 7 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	d	312	2476	1604	418	445	9	0	0
7	e	312	2476	1604	418	445	9	0	0

- Molecule 8 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	f	206	1595	1053	259	275	8	0	0
8	g	206	1595	1053	259	275	8	0	0

- Molecule 9 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	527	4127	2716	693	696	22	0	0
9	j	527	4127	2716	693	696	22	0	0

- Molecule 10 is a protein called DUF5130 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	k	145	1068	672	185	210	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	l	145	1068	672	185	210	1	0	0

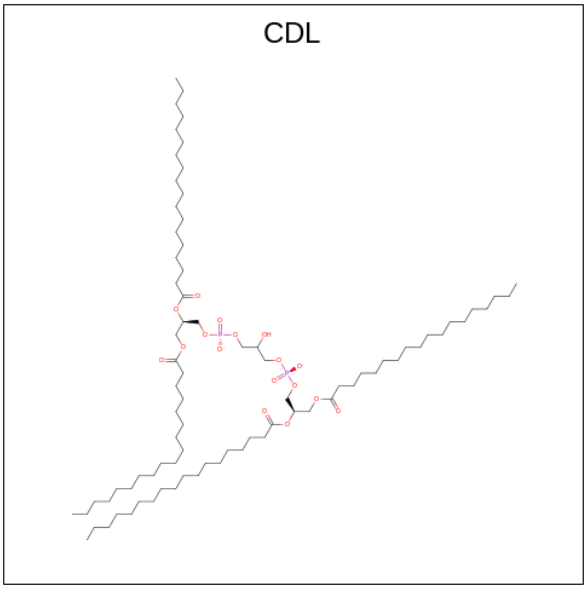
- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	m	139	1066	704	169	188	5	0	0
			Total	C	N	O	S		
11	n	139	1066	704	169	188	5	0	0

- Molecule 12 is a protein called Lipoprotein lpqE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	q	156	1129	696	201	231	1	0	0
			Total	C	N	O	S		
12	r	156	1129	696	201	231	1	0	0

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	G	1	88	69	17	2	0
			Total	C	O	P	
13	I	1	76	57	17	2	0

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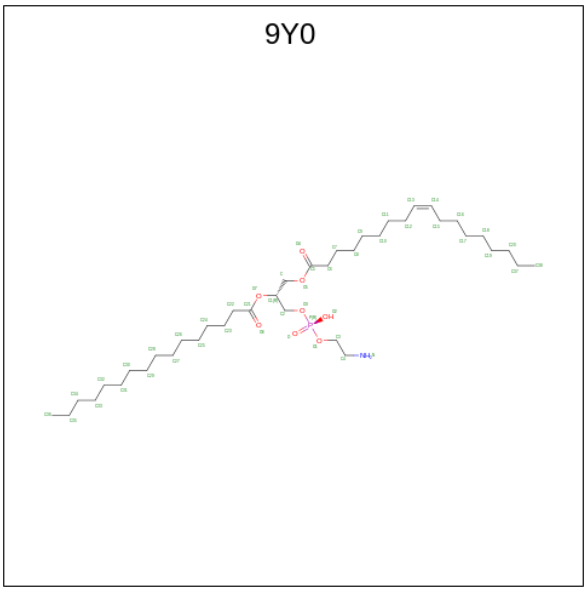
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	I	1	81	62	17	2	0
13	L	1	76	57	17	2	0
13	L	1	81	62	17	2	0
13	U	1	79	60	17	2	0
13	V	1	95	76	17	2	0
13	b	1	88	69	17	2	0
13	i	1	66	47	17	2	0
13	i	1	74	55	17	2	0
13	i	1	77	58	17	2	0
13	i	1	79	60	17	2	0
13	i	1	74	55	17	2	0
13	i	1	66	47	17	2	0
13	j	1	77	58	17	2	0
13	j	1	79	60	17	2	0
13	j	1	79	60	17	2	0
13	p	1	95	76	17	2	0

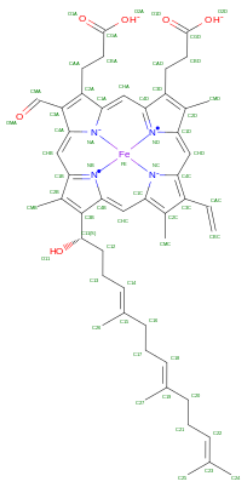
- Molecule 14 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: $C_{39}H_{76}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	N	O	P	0
			41	31	1	8	1	
14	I	1	Total	C	N	O	P	0
			38	28	1	8	1	
14	I	1	Total	C	N	O	P	0
			43	33	1	8	1	
14	L	1	Total	C	N	O	P	0
			38	28	1	8	1	
14	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
14	f	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 15 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).

HEA

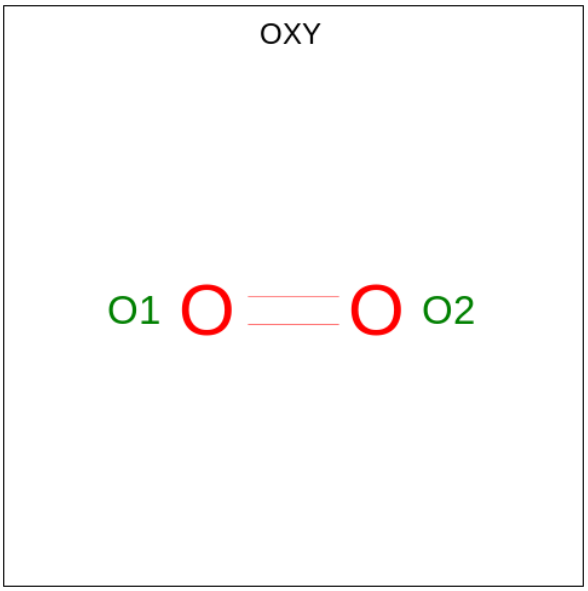


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
15	I	1	60	49	1	4	6	0
15	I	1	60	49	1	4	6	0
15	L	1	60	49	1	4	6	0
15	L	1	60	49	1	4	6	0

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

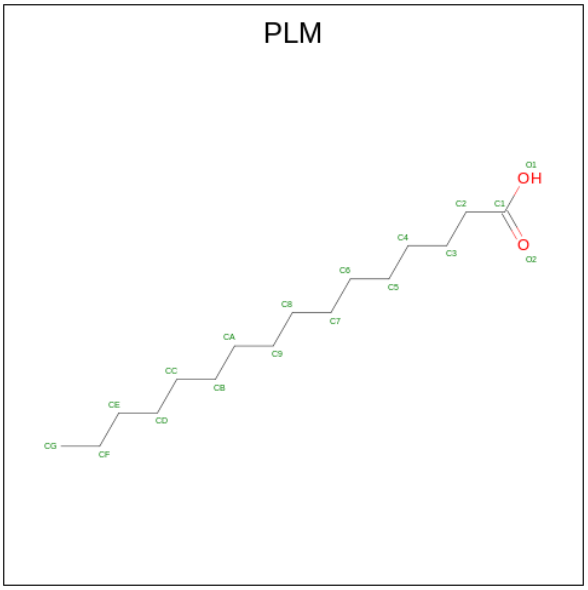
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
16	I	2	2	2	0
16	L	2	2	2	0
16	d	2	2	2	0
16	e	2	2	2	0

- Molecule 17 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total O 2 2	0
17	L	1	Total O 2 2	0

- Molecule 18 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	AltConf
18	I	1	Total C O 17 16 1	0
18	j	1	Total C O 11 10 1	0

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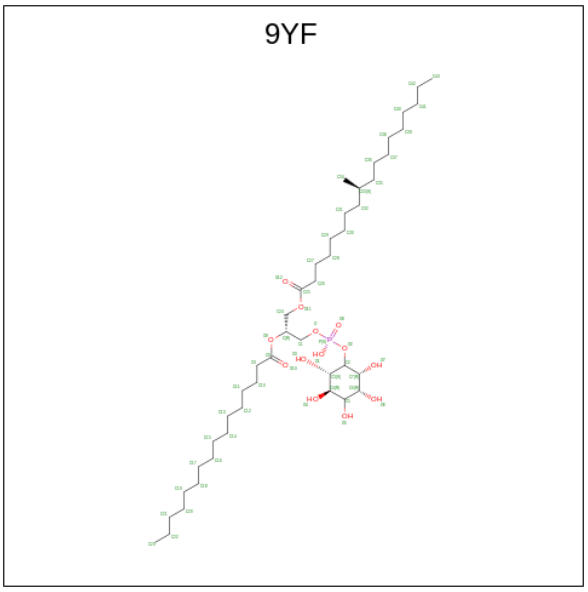
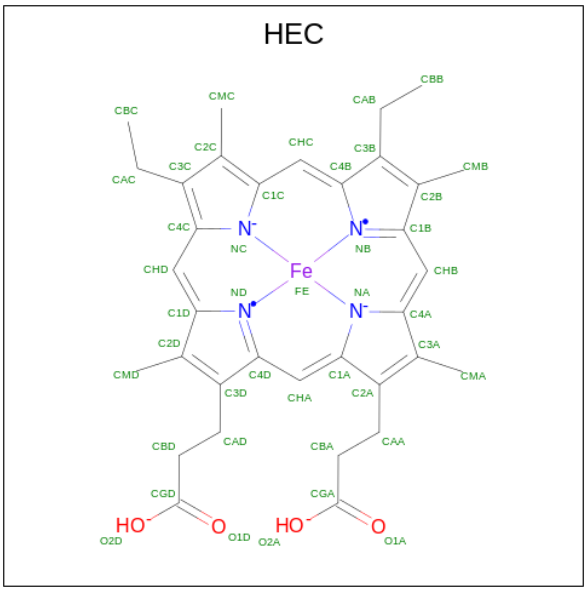
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	q	1	17	16	1	0

- Molecule 19 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: $C_{44}H_{85}O_{13}P$).



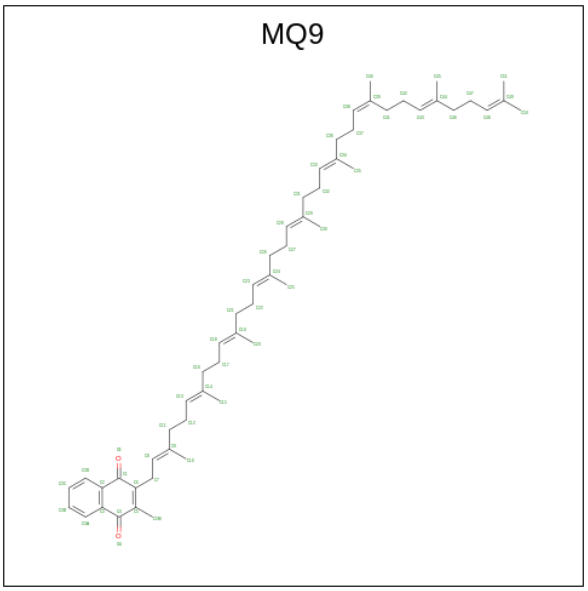
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	L	1	58	44	13	1	0
			Total	C	O	P	
19	V	1	58	44	13	1	0
			Total	C	O	P	
19	i	1	58	44	13	1	0
			Total	C	O	P	
19	j	1	58	44	13	1	0
			Total	C	O	P	
19	o	1	58	44	13	1	0
			Total	C	O	P	
19	p	1	58	44	13	1	0
			Total	C	O	P	
19	p	1	58	44	13	1	0

- Molecule 20 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



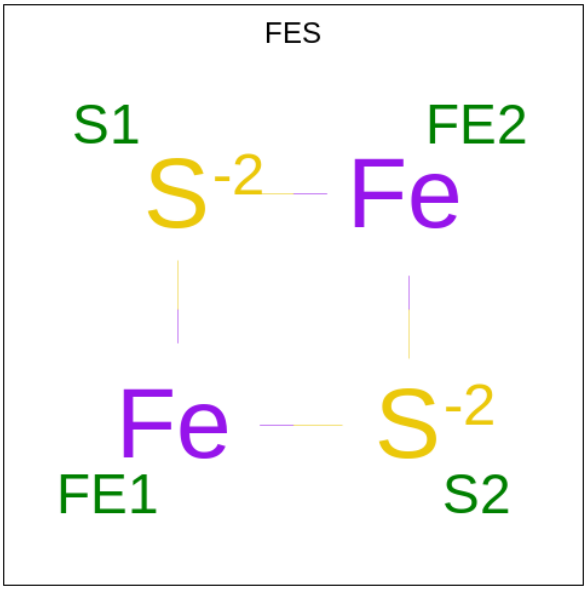
Mol	Chain	Residues	Atoms					AltConf
20	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	U	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	o	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	o	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 21 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	U	1	58	56	2	0
21	i	1	43	41	2	0
21	i	1	58	56	2	0
21	j	1	43	41	2	0
21	j	1	58	56	2	0
21	m	1	48	46	2	0
21	n	1	48	46	2	0
21	o	1	58	56	2	0

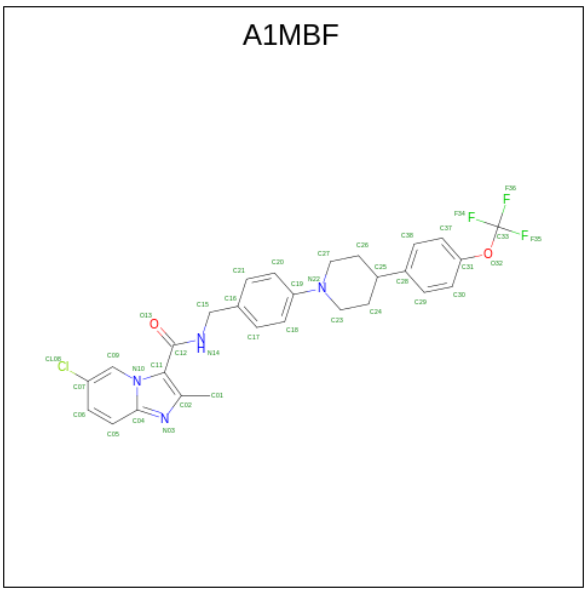
- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	V	1	4	2	2	0
22	p	1	4	2	2	0

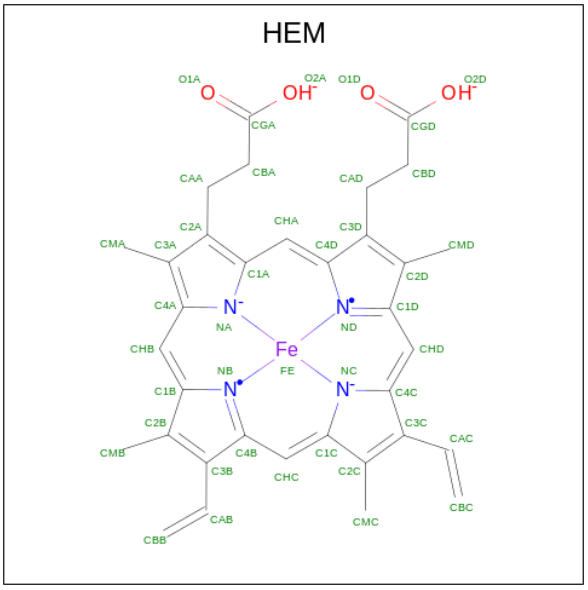
- Molecule 23 is 6-chloranyl-2-methyl- {N}-[[4-[4-[4-(trifluoromethyloxy)phenyl]piperidin -1-yl]phenyl]methyl]imidazo[1,2-a]pyridine-3-carboxamide (CCD ID: A1MBF) (formula:

$C_{28}H_{26}ClF_3N_4O_2$) (labeled as "Ligand of Interest" by depositor).



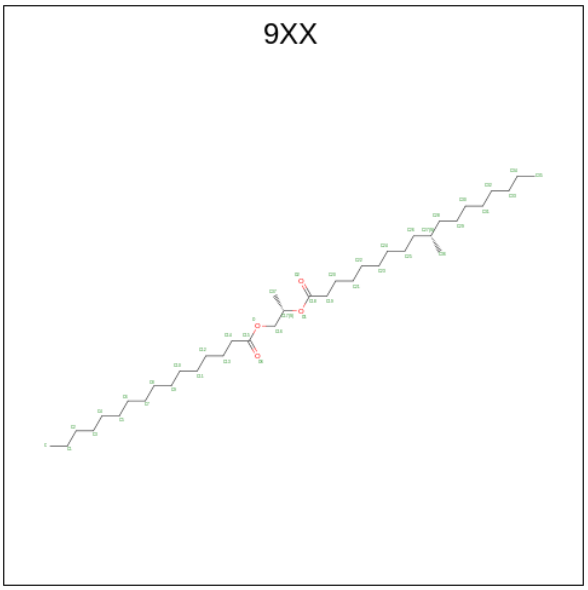
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	F	N	O	
23	i	1	38	28	1	3	4	2	0
			Total	C	Cl	F	N	O	
23	j	1	38	28	1	3	4	2	0

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	i	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
24	i	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	j	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
24	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 25 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
25	i	1	Total	C	O	0
			32	28	4	
25	j	1	Total	C	O	0
			32	28	4	
25	q	1	Total	C	O	0
			42	38	4	
25	r	1	Total	C	O	0
			42	38	4	

- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	I	18	Total	O	0
			18	18	

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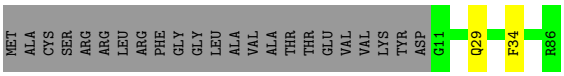
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
26	L	17	17	17	0
			Total	O	
26	U	5	5	5	0
			Total	O	
26	V	1	1	1	0
			Total	O	
26	d	2	2	2	0
			Total	O	
26	e	1	1	1	0
			Total	O	
26	i	8	8	8	0
			Total	O	
26	j	9	9	9	0
			Total	O	
26	m	2	2	2	0
			Total	O	
26	n	3	3	3	0
			Total	O	
26	o	6	6	6	0
			Total	O	
26	p	2	2	2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Prokaryotic respiratory supercomplex associate factor 1

Chain G:

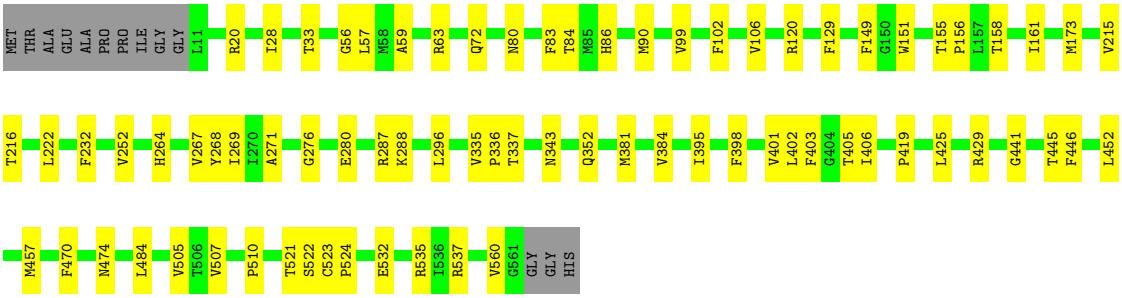


• Molecule 1: Prokaryotic respiratory supercomplex associate factor 1

Chain b:

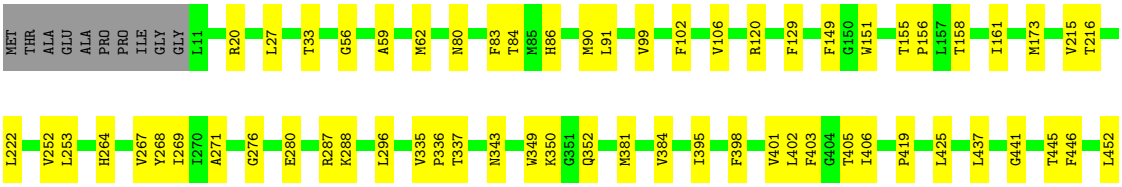
• Molecule 2: Cytochrome c oxidase subunit 1

Chain I:



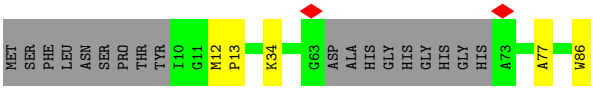
• Molecule 2: Cytochrome c oxidase subunit 1

Chain L:



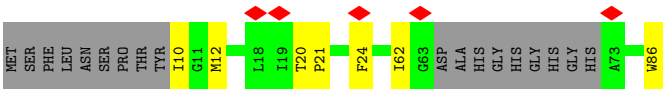
• Molecule 3: Cytochrome c oxidase subunit CtaJ

Chain J:



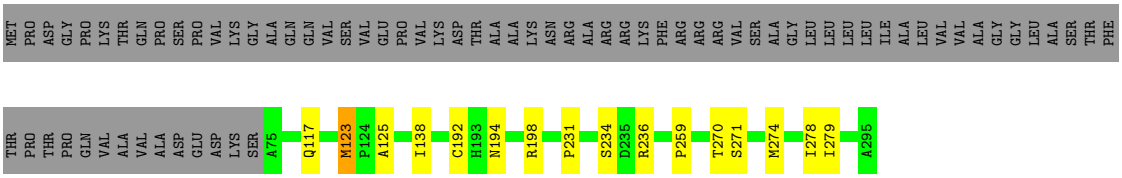
• Molecule 3: Cytochrome c oxidase subunit CtaJ

Chain h:



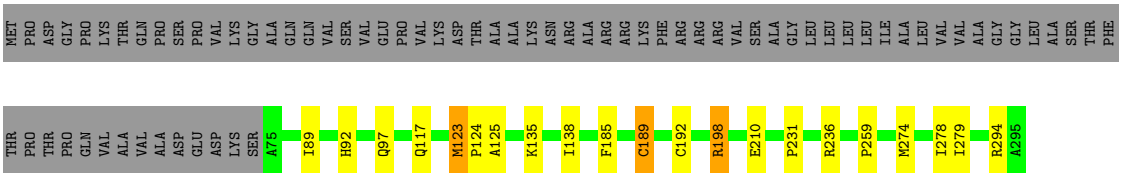
• Molecule 4: Cytochrome bc1 complex cytochrome c subunit

Chain U:



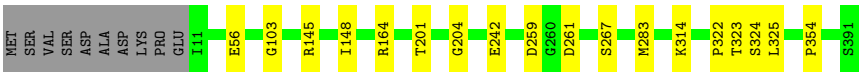
• Molecule 4: Cytochrome bc1 complex cytochrome c subunit

Chain o:



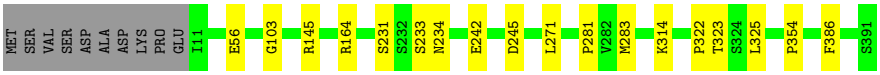
• Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain V:



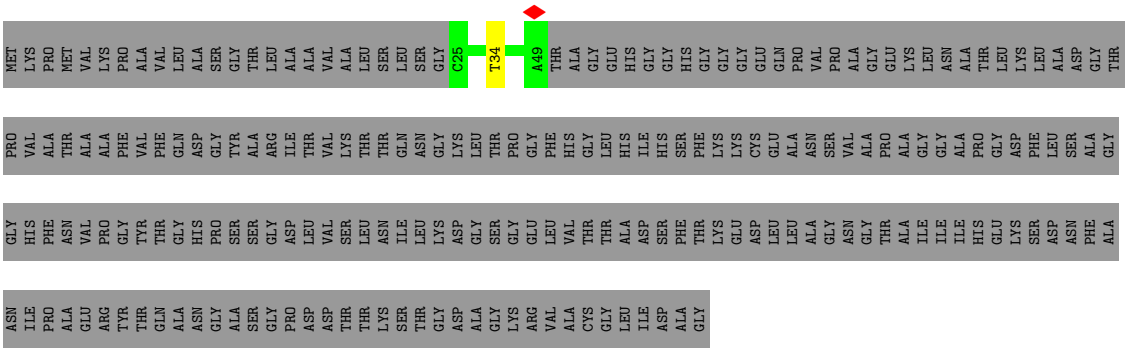
• Molecule 5: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain p:



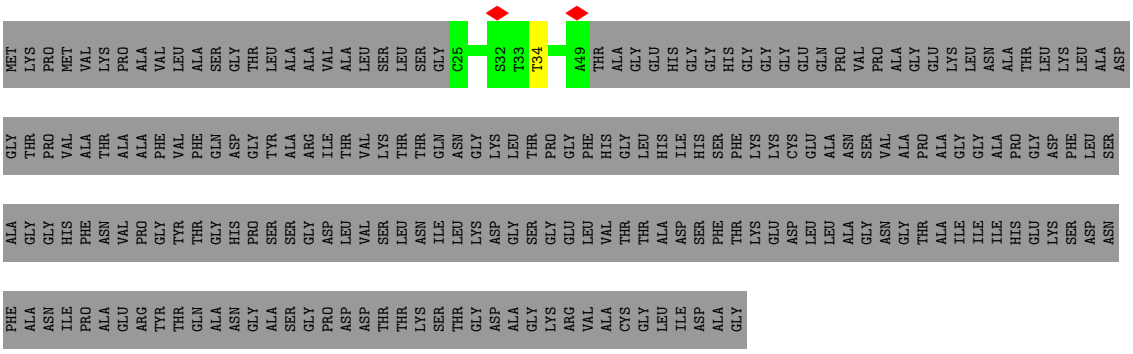
• Molecule 6: Superoxide dismutase [Cu-Zn]

Chain X:



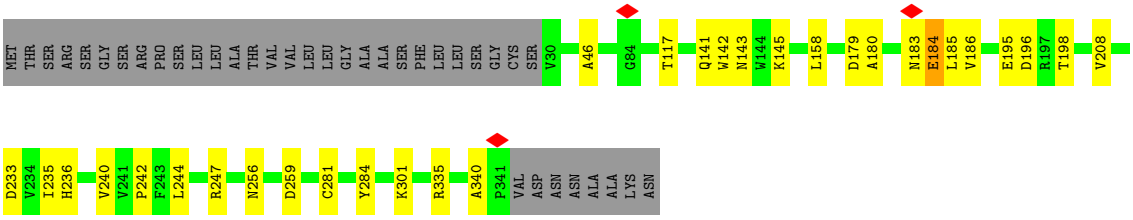
• Molecule 6: Superoxide dismutase [Cu-Zn]

Chain a:



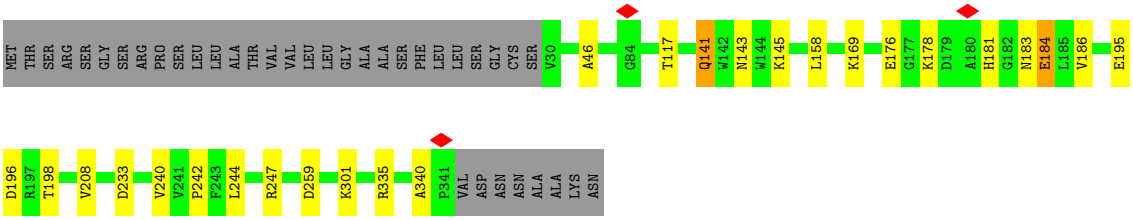
• Molecule 7: cytochrome-c oxidase

Chain d:



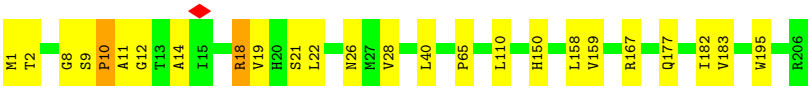
• Molecule 7: cytochrome-c oxidase

Chain e:



• Molecule 8: Probable cytochrome c oxidase subunit 3

Chain f:

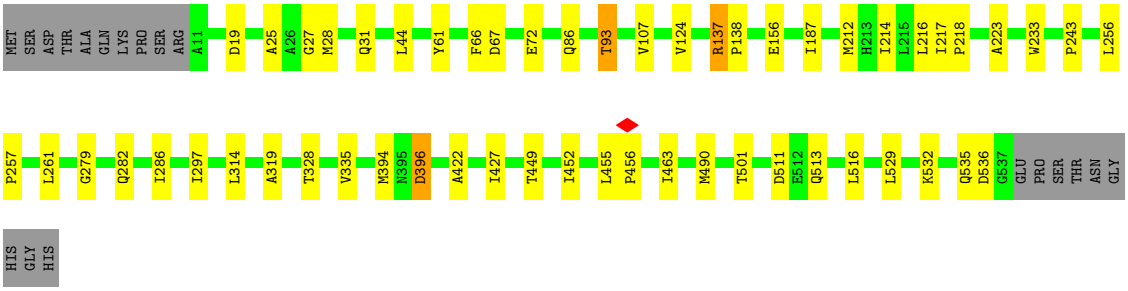


• Molecule 8: Probable cytochrome c oxidase subunit 3

Chain g:

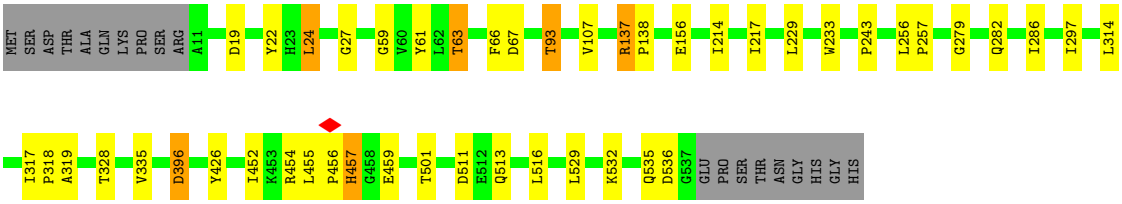
• Molecule 9: Cytochrome bc1 complex cytochrome b subunit

Chain i:



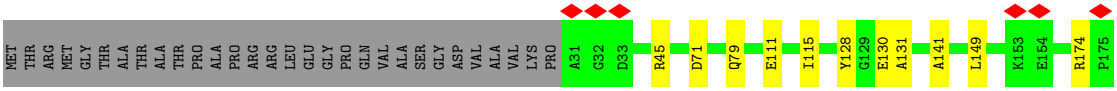
• Molecule 9: Cytochrome bc1 complex cytochrome b subunit

Chain j:



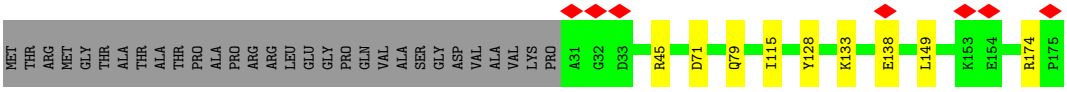
• Molecule 10: DUF5130 domain-containing protein

Chain k:



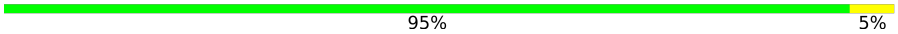
• Molecule 10: DUF5130 domain-containing protein

Chain l:



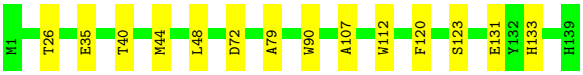
• Molecule 11: Cytochrome c oxidase polypeptide 4

Chain m:



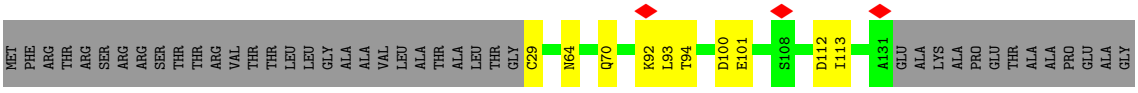
• Molecule 11: Cytochrome c oxidase polypeptide 4

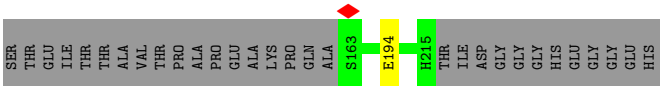
Chain n:



• Molecule 12: Lipoprotein lpqE

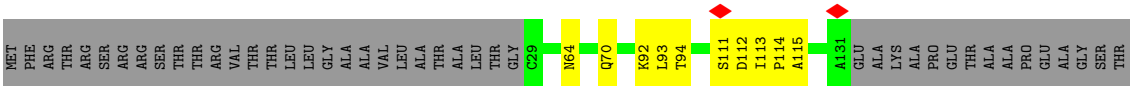
Chain q:

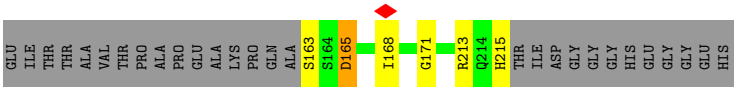




• Molecule 12: Lipoprotein lpqE

Chain r:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136434	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.342	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0332	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, FES, HEC, CU, CDL, 9Y0, PLM, OXY, 9YF, 9XX, A1MBF, HEM, MQ9

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	G	0.12	0/585	0.23	0/789
1	b	0.13	0/585	0.29	0/789
2	I	0.16	0/4526	0.36	0/6181
2	L	0.16	0/4526	0.35	0/6181
3	J	0.11	0/526	0.25	0/718
3	h	0.11	0/526	0.29	0/718
4	U	0.13	0/1669	0.35	0/2257
4	o	0.19	0/1669	0.40	1/2257 (0.0%)
5	V	0.13	0/3033	0.30	0/4120
5	p	0.12	0/3033	0.29	0/4120
6	X	0.14	0/177	0.45	0/248
6	a	0.11	0/177	0.36	0/248
7	d	0.13	0/2547	0.31	0/3466
7	e	0.12	0/2547	0.30	0/3466
8	f	0.17	0/1644	0.32	0/2244
8	g	0.17	0/1644	0.35	0/2244
9	i	0.14	0/4252	0.33	0/5785
9	j	0.14	0/4252	0.33	0/5785
10	k	0.08	0/1088	0.23	0/1481
10	l	0.09	0/1088	0.26	0/1481
11	m	0.12	0/1097	0.28	0/1499
11	n	0.13	0/1097	0.28	0/1499
12	q	0.11	0/1144	0.31	0/1551
12	r	0.12	0/1144	0.33	0/1551
All	All	0.14	0/44576	0.32	1/60678 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	o	89	ILE	N-CA-C	-6.67	107.37	113.71

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	G	575	0	591	1	0
1	b	575	0	591	1	0
2	I	4363	0	4322	70	0
2	L	4363	0	4322	64	0
3	J	509	0	500	5	0
3	h	509	0	500	6	0
4	U	1639	0	1598	14	0
4	o	1639	0	1600	17	0
5	V	2957	0	2964	14	0
5	p	2957	0	2964	15	0
6	X	171	0	156	0	0
6	a	171	0	156	0	0
7	d	2476	0	2445	19	0
7	e	2476	0	2445	13	0
8	f	1595	0	1581	19	0
8	g	1595	0	1581	15	0
9	i	4127	0	4157	41	0
9	j	4127	0	4158	32	0
10	k	1068	0	1054	7	0
10	l	1068	0	1054	6	0
11	m	1066	0	1052	7	0
11	n	1066	0	1052	13	0
12	q	1129	0	1126	10	0
12	r	1129	0	1126	10	0
13	G	88	0	126	8	0
13	I	157	0	208	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	157	0	208	4	0
13	U	79	0	105	2	0
13	V	95	0	143	14	0
13	b	88	0	126	6	0
13	i	436	0	539	14	0
13	j	235	0	308	2	0
13	p	95	0	143	4	0
14	G	41	0	0	0	0
14	I	81	0	0	11	0
14	L	38	0	0	1	0
14	b	41	0	0	0	0
14	f	43	0	0	0	0
15	I	120	0	108	9	0
15	L	120	0	108	8	0
16	I	2	0	0	0	0
16	L	2	0	0	0	0
16	d	2	0	0	0	0
16	e	2	0	0	0	0
17	I	2	0	0	0	0
17	L	2	0	0	0	0
18	I	17	0	31	1	0
18	j	11	0	16	0	0
18	q	17	0	31	5	0
19	L	58	0	0	0	0
19	V	58	0	0	0	0
19	i	58	0	0	0	0
19	j	58	0	0	0	0
19	o	58	0	0	0	0
19	p	116	0	0	0	0
20	U	86	0	62	4	0
20	o	86	0	64	4	0
21	U	58	0	80	1	0
21	i	101	0	133	17	0
21	j	101	0	130	11	0
21	m	48	0	61	2	0
21	n	48	0	61	5	0
21	o	58	0	80	3	0
22	V	4	0	0	0	0
22	p	4	0	0	0	0
23	i	38	0	0	0	0
23	j	38	0	0	0	0
24	i	85	0	57	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	j	85	0	57	3	0
25	i	32	0	0	0	0
25	j	32	0	0	0	0
25	q	42	0	0	3	0
25	r	42	0	0	0	0
26	I	18	0	0	0	0
26	L	17	0	0	0	0
26	U	5	0	0	0	0
26	V	1	0	0	0	0
26	d	2	0	0	0	0
26	e	1	0	0	0	0
26	i	8	0	0	0	0
26	j	9	0	0	0	0
26	m	2	0	0	0	0
26	n	3	0	0	0	0
26	o	6	0	0	0	0
26	p	2	0	0	0	0
All	All	46789	0	46080	426	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 426 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)
13:i:607:CDL:C42	25:q:302:9XX:C35	1.78	1.57
2:I:232:PHE:CZ	14:I:610:9Y0:C15	1.85	1.56
2:I:155:THR:CG2	2:I:156:PRO:HD3	1.65	1.25
2:L:472:PHE:CZ	2:L:476:PHE:CE2	2.27	1.22
2:L:472:PHE:CE2	2:L:476:PHE:CE2	2.31	1.18

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	G	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
1	b	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
2	I	549/564 (97%)	530 (96%)	19 (4%)	0	100	100
2	L	549/564 (97%)	530 (96%)	19 (4%)	0	100	100
3	J	64/86 (74%)	62 (97%)	2 (3%)	0	100	100
3	h	64/86 (74%)	62 (97%)	2 (3%)	0	100	100
4	U	219/295 (74%)	208 (95%)	11 (5%)	0	100	100
4	o	219/295 (74%)	206 (94%)	13 (6%)	0	100	100
5	V	379/391 (97%)	372 (98%)	7 (2%)	0	100	100
5	p	379/391 (97%)	369 (97%)	10 (3%)	0	100	100
6	X	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
6	a	23/238 (10%)	20 (87%)	3 (13%)	0	100	100
7	d	310/349 (89%)	290 (94%)	20 (6%)	0	100	100
7	e	310/349 (89%)	295 (95%)	14 (4%)	1 (0%)	36	40
8	f	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	24	24
8	g	204/206 (99%)	195 (96%)	7 (3%)	2 (1%)	12	10
9	i	525/546 (96%)	499 (95%)	25 (5%)	1 (0%)	43	50
9	j	525/546 (96%)	500 (95%)	24 (5%)	1 (0%)	43	50
10	k	143/175 (82%)	141 (99%)	2 (1%)	0	100	100
10	l	143/175 (82%)	141 (99%)	2 (1%)	0	100	100
11	m	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
11	n	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
12	q	152/227 (67%)	141 (93%)	11 (7%)	0	100	100
12	r	152/227 (67%)	140 (92%)	12 (8%)	0	100	100
All	All	5558/6630 (84%)	5320 (96%)	232 (4%)	6 (0%)	49	56

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	f	10	PRO
8	g	19	VAL
9	i	137	ARG

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Mol	Chain	Res	Type
9	j	137	ARG
8	g	15	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	G	59/77 (77%)	59 (100%)	0	100	100
1	b	59/77 (77%)	59 (100%)	0	100	100
2	I	448/455 (98%)	442 (99%)	6 (1%)	61	72
2	L	448/455 (98%)	444 (99%)	4 (1%)	70	79
3	J	49/63 (78%)	49 (100%)	0	100	100
3	h	49/63 (78%)	48 (98%)	1 (2%)	48	59
4	U	164/223 (74%)	161 (98%)	3 (2%)	51	63
4	o	164/223 (74%)	161 (98%)	3 (2%)	51	63
5	V	312/321 (97%)	311 (100%)	1 (0%)	86	90
5	p	312/321 (97%)	311 (100%)	1 (0%)	86	90
6	X	20/173 (12%)	19 (95%)	1 (5%)	22	24
6	a	20/173 (12%)	19 (95%)	1 (5%)	22	24
7	d	269/298 (90%)	265 (98%)	4 (2%)	57	68
7	e	269/298 (90%)	263 (98%)	6 (2%)	45	56
8	f	163/163 (100%)	162 (99%)	1 (1%)	78	84
8	g	163/163 (100%)	161 (99%)	2 (1%)	63	74
9	i	421/437 (96%)	415 (99%)	6 (1%)	59	70
9	j	421/437 (96%)	412 (98%)	9 (2%)	47	58
10	k	108/130 (83%)	107 (99%)	1 (1%)	70	79
10	l	108/130 (83%)	107 (99%)	1 (1%)	70	79
11	m	103/103 (100%)	103 (100%)	0	100	100
11	n	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	q	121/171 (71%)	120 (99%)	1 (1%)	73	80
12	r	121/171 (71%)	119 (98%)	2 (2%)	53	65
All	All	4474/5228 (86%)	4420 (99%)	54 (1%)	61	74

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	g	145	LEU
9	i	529	LEU
4	o	198	ARG
3	h	62	ILE
9	i	286	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
9	i	86	GLN
9	j	109	GLN
12	q	70	GLN
9	i	109	GLN
9	i	535	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 72 ligands modelled in this entry, 8 are monoatomic - leaving 64 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	$\#\|Z\| > 2$
14	9Y0	L	601	-	37,37,48	0.40	0	40,42,53	0.47	0
14	9Y0	I	608	-	37,37,48	0.37	0	40,42,53	0.35	0
25	9XX	j	610	-	31,31,41	0.38	0	34,34,44	0.65	1 (2%)
13	CDL	L	606	-	75,75,99	0.36	0	81,87,111	0.23	0
15	HEA	L	603	2	66,67,67	1.18	7 (10%)	78,103,103	1.40	11 (14%)
13	CDL	b	101	-	87,87,99	0.33	0	93,99,111	0.23	0
18	PLM	I	609	-	16,16,17	0.51	0	15,15,17	0.44	0
13	CDL	I	604	-	75,75,99	0.36	0	81,87,111	0.23	0
13	CDL	i	613	-	65,65,99	0.36	0	71,77,111	0.23	0
13	CDL	i	606	-	73,73,99	0.35	0	79,85,111	0.23	0
21	MQ9	n	201	-	49,49,59	0.32	0	60,63,75	0.47	0
19	9YF	p	604	-	58,58,58	1.28	4 (6%)	69,71,71	1.12	3 (4%)
19	9YF	i	601	-	58,58,58	0.34	0	69,71,71	0.52	0
15	HEA	I	601	2	66,67,67	1.19	7 (10%)	78,103,103	1.47	15 (19%)
18	PLM	j	609	-	10,10,17	0.65	0	9,9,17	0.53	0
21	MQ9	i	609	9	44,44,59	0.34	0	54,57,75	0.65	2 (3%)
17	OXY	I	607	-	1,1,1	0.15	0	-		
19	9YF	j	601	-	58,58,58	1.25	4 (6%)	69,71,71	1.19	5 (7%)
19	9YF	o	603	-	58,58,58	0.27	0	69,71,71	0.32	0
21	MQ9	i	610	-	59,59,59	0.35	0	72,75,75	0.34	0
22	FES	V	601	5	0,4,4	-	-	-		
24	HEM	j	603	9	49,49,50	1.43	5 (10%)	66,81,82	1.14	5 (7%)
13	CDL	I	605	-	80,80,99	0.34	0	86,92,111	0.36	0
13	CDL	U	604	-	78,78,99	0.35	0	84,90,111	0.21	0
13	CDL	j	606	-	78,78,99	0.36	0	84,90,111	0.23	0
15	HEA	I	602	2	66,67,67	1.18	6 (9%)	78,103,103	1.40	12 (15%)
13	CDL	j	605	-	76,76,99	0.36	0	82,88,111	0.21	0
20	HEC	o	601	4	50,50,50	1.85	4 (8%)	68,82,82	1.56	5 (7%)
13	CDL	p	603	-	94,94,99	0.31	0	100,106,111	0.20	0
21	MQ9	j	608	-	59,59,59	0.41	0	72,75,75	0.32	0
19	9YF	p	601	-	58,58,58	1.27	4 (6%)	69,71,71	1.13	3 (4%)
25	9XX	i	611	-	31,31,41	0.40	0	34,34,44	0.38	0
25	9XX	r	301	-	41,41,41	0.38	0	44,44,44	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	HEM	i	604	9	49,49,50	1.45	5 (10%)	66,81,82	1.13	5 (7%)
23	A1MBF	i	602	-	42,42,42	2.68	13 (30%)	58,61,61	1.32	5 (8%)
15	HEA	L	602	2	66,67,67	1.19	7 (10%)	78,103,103	1.47	15 (19%)
24	HEM	j	604	9	50,50,50	1.44	7 (14%)	66,82,82	1.16	6 (9%)
13	CDL	L	607	-	80,80,99	0.35	0	86,92,111	0.21	0
20	HEC	o	602	4	50,50,50	1.74	5 (10%)	68,82,82	1.49	7 (10%)
23	A1MBF	j	602	-	42,42,42	2.68	14 (33%)	58,61,61	1.30	5 (8%)
21	MQ9	j	607	9	44,44,59	0.32	0	54,57,75	0.49	0
18	PLM	q	301	-	16,16,17	0.40	0	15,15,17	0.39	0
14	9Y0	f	601	-	42,42,48	0.52	0	44,47,53	0.47	0
20	HEC	U	601	4	50,50,50	1.80	5 (10%)	68,82,82	1.45	6 (8%)
21	MQ9	o	604	-	59,59,59	0.31	0	72,75,75	0.50	1 (1%)
13	CDL	j	611	-	78,78,99	0.35	0	84,90,111	0.22	0
13	CDL	i	612	9	73,73,99	0.34	0	79,85,111	0.24	0
14	9Y0	G	102	-	40,40,48	0.52	0	43,45,53	0.46	0
21	MQ9	U	603	-	59,59,59	0.31	0	72,75,75	0.48	1 (1%)
17	OXY	L	608	-	1,1,1	0.15	0	-		
13	CDL	i	608	-	78,78,99	0.36	0	84,90,111	0.23	0
20	HEC	U	602	4	50,50,50	1.76	5 (10%)	68,82,82	1.50	8 (11%)
13	CDL	i	607	-	76,76,99	0.36	0	82,88,111	0.21	0
14	9Y0	I	610	-	42,42,48	0.52	0	44,47,53	0.48	0
14	9Y0	b	102	-	40,40,48	0.51	0	43,45,53	0.59	1 (2%)
13	CDL	V	602	-	94,94,99	0.30	0	100,106,111	0.33	0
24	HEM	i	605	9	50,50,50	1.44	8 (16%)	66,82,82	1.16	5 (7%)
21	MQ9	m	201	-	49,49,59	0.38	0	60,63,75	1.15	3 (5%)
22	FES	p	602	5	0,4,4	-	-	-		
13	CDL	i	603	-	65,65,99	0.36	0	71,77,111	0.23	0
25	9XX	q	302	-	41,41,41	0.31	0	44,44,44	0.39	0
19	9YF	V	603	-	58,58,58	1.27	4 (6%)	69,71,71	1.14	3 (4%)
13	CDL	G	101	-	87,87,99	0.33	0	93,99,111	0.21	0
19	9YF	L	609	-	58,58,58	1.28	4 (6%)	69,71,71	1.19	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	9Y0	L	601	-	-	23/41/41/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	9Y0	I	608	-	-	18/41/41/52	-
25	9XX	j	610	-	-	12/33/33/43	-
13	CDL	L	606	-	-	45/86/86/110	-
15	HEA	L	603	2	-	18/36/76/76	-
13	CDL	b	101	-	-	68/98/98/110	-
18	PLM	I	609	-	-	4/13/14/15	-
13	CDL	I	604	-	-	46/86/86/110	-
13	CDL	i	613	-	-	35/76/76/110	-
13	CDL	i	606	-	-	44/84/84/110	-
21	MQ9	n	201	-	-	21/41/61/73	0/2/2/2
19	9YF	p	604	-	-	34/54/78/78	0/1/1/1
19	9YF	i	601	-	-	22/54/78/78	0/1/1/1
15	HEA	I	601	2	-	14/36/76/76	-
18	PLM	j	609	-	-	0/7/8/15	-
21	MQ9	i	609	9	-	11/35/55/73	0/2/2/2
19	9YF	j	601	-	-	26/54/78/78	0/1/1/1
19	9YF	o	603	-	-	24/54/78/78	0/1/1/1
21	MQ9	i	610	-	-	31/53/73/73	0/2/2/2
24	HEM	j	603	9	-	2/12/52/54	-
22	FES	V	601	5	-	-	0/1/1/1
13	CDL	I	605	-	-	44/91/91/110	-
13	CDL	U	604	-	-	43/89/89/110	-
13	CDL	j	606	-	-	55/89/89/110	-
15	HEA	I	602	2	-	17/36/76/76	-
20	HEC	o	601	4	1/1/3/7	4/14/54/54	-
13	CDL	j	605	-	-	36/87/87/110	-
13	CDL	p	603	-	-	62/105/105/110	-
21	MQ9	j	608	-	-	27/53/73/73	0/2/2/2
19	9YF	p	601	-	-	26/54/78/78	0/1/1/1
25	9XX	i	611	-	-	5/33/33/43	-
25	9XX	r	301	-	-	19/43/43/43	-
24	HEM	i	604	9	-	3/12/52/54	-
23	A1MBF	i	602	-	-	3/22/32/32	0/5/5/5
15	HEA	L	602	2	-	14/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	HEM	j	604	9	-	3/14/54/54	-
20	HEC	o	602	4	1/1/3/7	4/14/54/54	-
13	CDL	L	607	-	-	58/91/91/110	-
23	A1MBF	j	602	-	-	2/22/32/32	0/5/5/5
21	MQ9	j	607	9	-	9/35/55/73	0/2/2/2
18	PLM	q	301	-	-	9/13/14/15	-
20	HEC	U	601	4	1/1/3/7	4/14/54/54	-
14	9Y0	f	601	-	-	21/46/46/52	-
21	MQ9	o	604	-	-	19/53/73/73	0/2/2/2
13	CDL	i	612	9	-	46/84/84/110	-
13	CDL	j	611	-	-	46/89/89/110	-
14	9Y0	G	102	-	-	18/44/44/52	-
21	MQ9	U	603	-	-	20/53/73/73	0/2/2/2
13	CDL	i	608	-	-	57/89/89/110	-
20	HEC	U	602	4	1/1/3/7	3/14/54/54	-
13	CDL	i	607	-	-	38/87/87/110	-
14	9Y0	I	610	-	-	18/46/46/52	-
14	9Y0	b	102	-	-	13/44/44/52	-
13	CDL	V	602	-	-	52/105/105/110	-
24	HEM	i	605	9	-	3/14/54/54	-
21	MQ9	m	201	-	-	12/41/61/73	0/2/2/2
25	9XX	q	302	-	-	32/43/43/43	-
13	CDL	i	603	-	-	42/76/76/110	-
22	FES	p	602	5	-	-	0/1/1/1
19	9YF	V	603	-	-	22/54/78/78	0/1/1/1
13	CDL	G	101	-	-	64/98/98/110	-
19	9YF	L	609	-	-	25/54/78/78	0/1/1/1

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	i	602	A1MBF	C12-N14	8.35	1.47	1.33
23	j	602	A1MBF	C12-N14	8.33	1.47	1.33
20	o	601	HEC	C3D-C2D	8.19	1.54	1.36
20	U	601	HEC	C3D-C2D	8.00	1.53	1.36
20	o	602	HEC	C3D-C2D	7.92	1.53	1.36

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	o	601	HEC	C1D-ND-C4D	7.59	112.91	105.07
21	m	201	MQ9	C7-C6-C1	-6.94	111.07	118.50
20	o	602	HEC	C1D-ND-C4D	6.36	111.65	105.07
20	U	601	HEC	C1D-ND-C4D	6.27	111.55	105.07
20	U	602	HEC	C1D-ND-C4D	6.26	111.54	105.07

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	U	601	HEC	NA
20	U	602	HEC	NA
20	o	601	HEC	NA
20	o	602	HEC	NA

5 of 1496 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	101	CDL	CA2-OA2-PA1-OA3
13	G	101	CDL	C11-CA5-OA6-CA4
13	G	101	CDL	CB2-OB2-PB2-OB3
13	I	604	CDL	CB2-OB2-PB2-OB3
13	I	604	CDL	CB2-OB2-PB2-OB4

There are no ring outliers.

43 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L	601	9Y0	1	0
14	I	608	9Y0	3	0
13	L	606	CDL	1	0
15	L	603	HEA	6	0
13	b	101	CDL	6	0
18	I	609	PLM	1	0
13	I	604	CDL	1	0
13	i	613	CDL	1	0
13	i	606	CDL	4	0
21	n	201	MQ9	5	0
15	I	601	HEA	1	0
21	i	609	MQ9	4	0
21	i	610	MQ9	13	0
24	j	603	HEM	1	0

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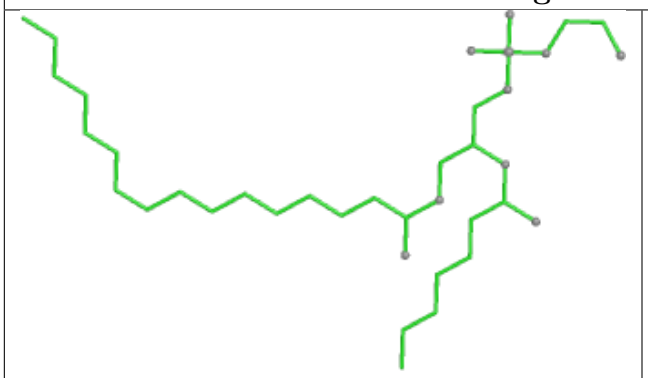
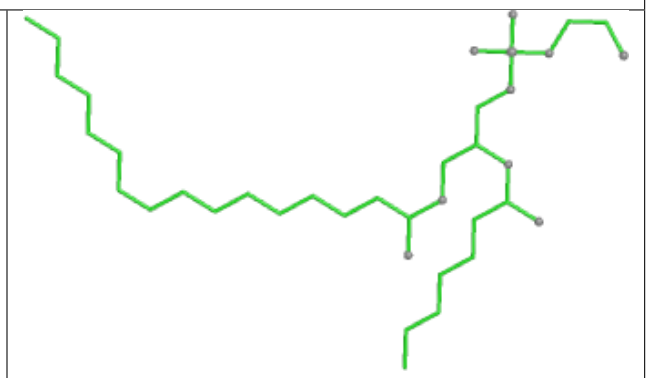
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	I	605	CDL	7	0
13	U	604	CDL	2	0
15	I	602	HEA	8	0
13	j	605	CDL	1	0
20	o	601	HEC	2	0
13	p	603	CDL	4	0
21	j	608	MQ9	10	0
24	i	604	HEM	1	0
15	L	602	HEA	2	0
24	j	604	HEM	2	0
13	L	607	CDL	3	0
20	o	602	HEC	2	0
21	j	607	MQ9	1	0
18	q	301	PLM	5	0
20	U	601	HEC	3	0
21	o	604	MQ9	3	0
13	j	611	CDL	1	0
13	i	612	CDL	2	0
21	U	603	MQ9	1	0
13	i	608	CDL	2	0
20	U	602	HEC	1	0
13	i	607	CDL	2	0
14	I	610	9Y0	8	0
13	V	602	CDL	14	0
24	i	605	HEM	2	0
21	m	201	MQ9	2	0
13	i	603	CDL	3	0
25	q	302	9XX	3	0
13	G	101	CDL	8	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.

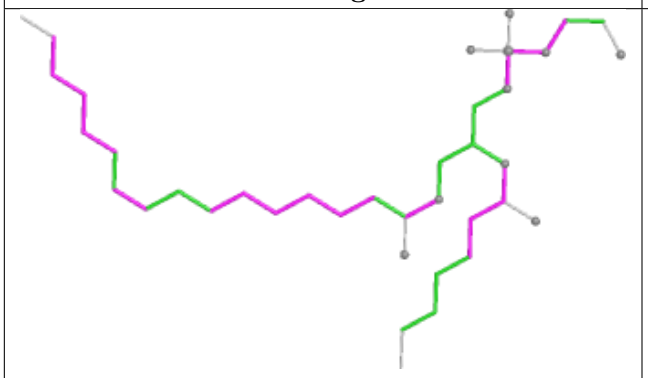
Ligand 9Y0 L 601



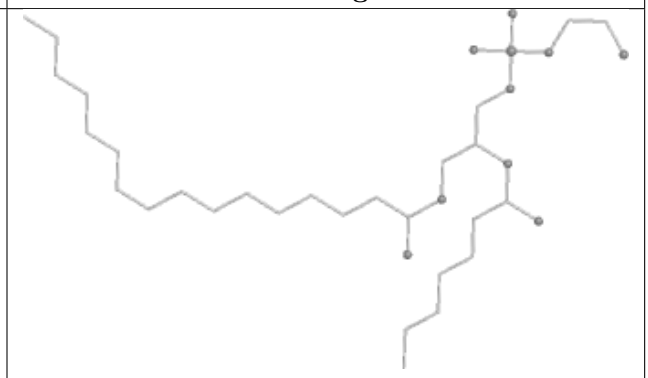
Bond lengths



Bond angles

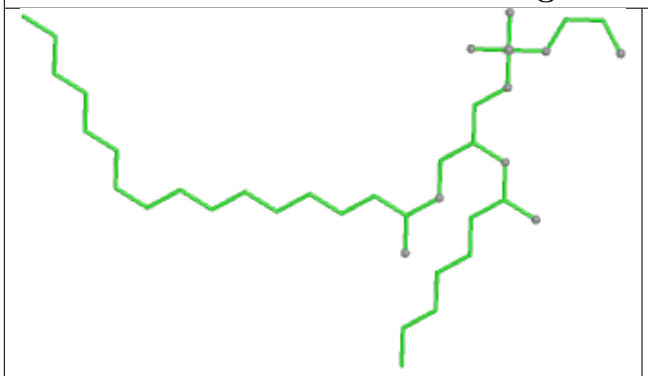


Torsions

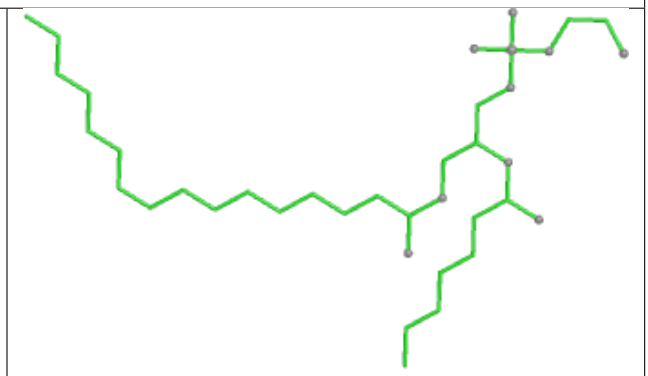


Rings

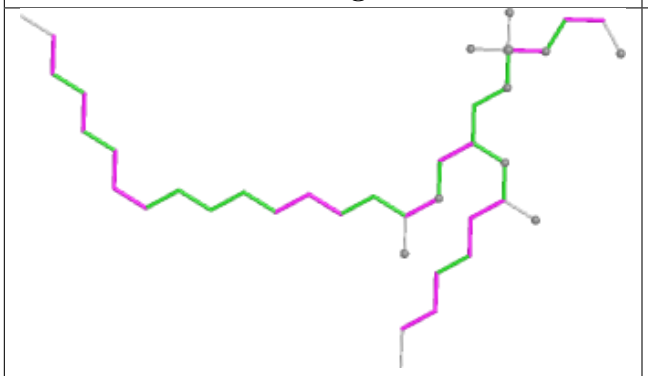
Ligand 9Y0 I 608



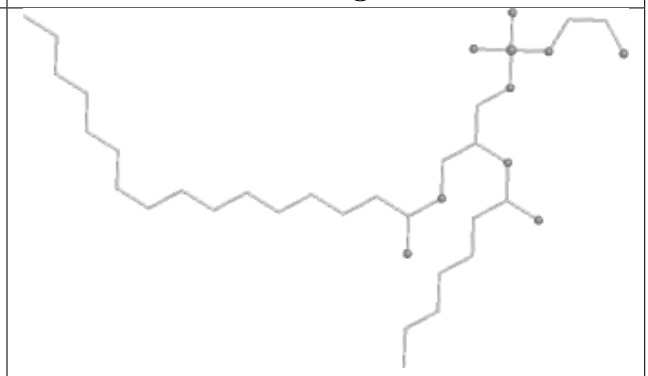
Bond lengths



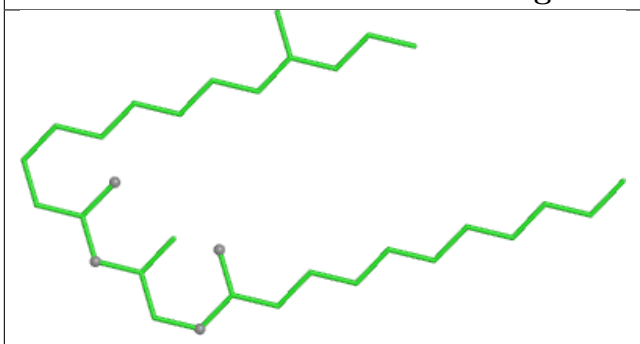
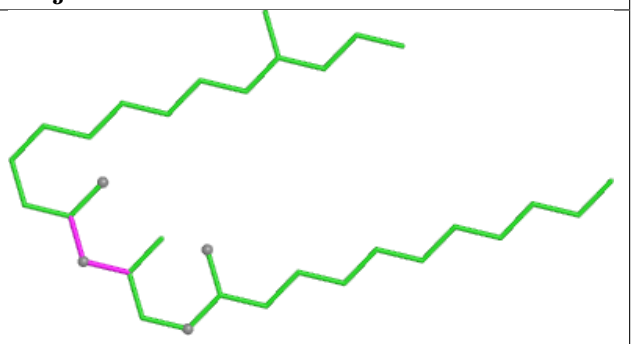
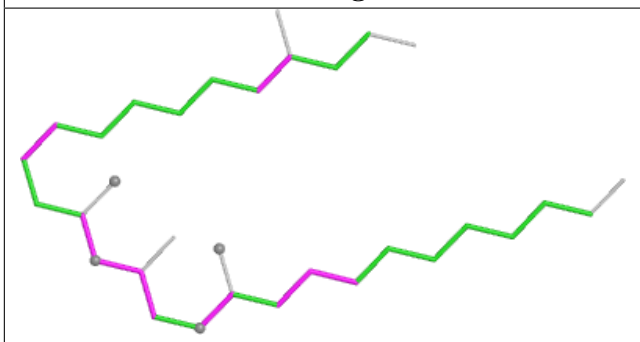
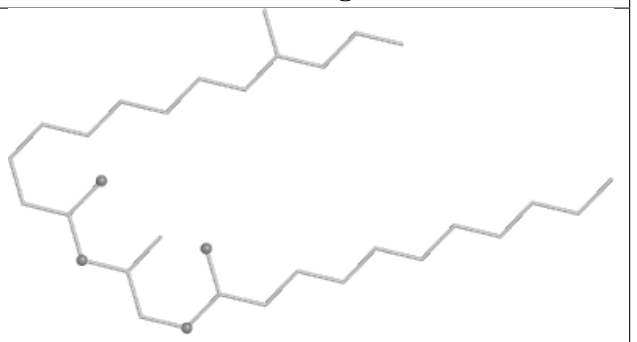
Bond angles

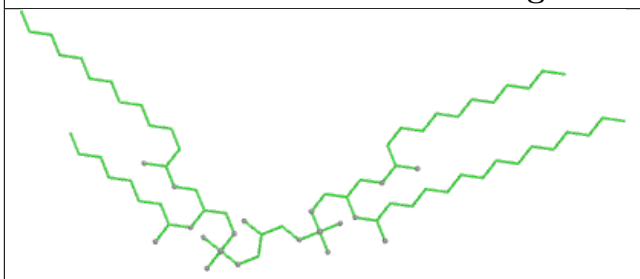
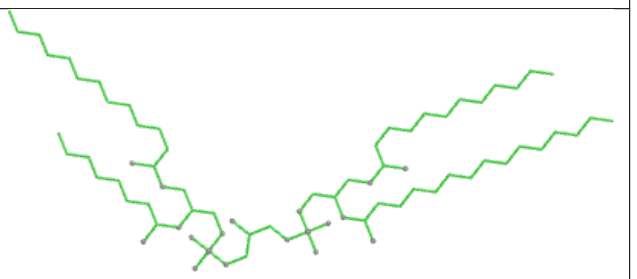
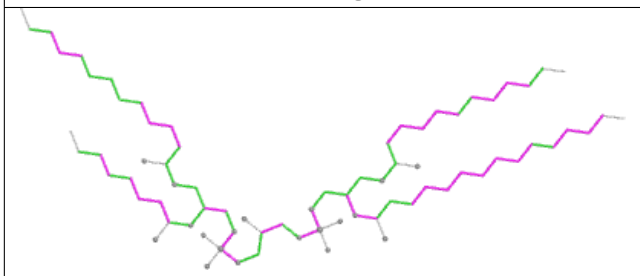
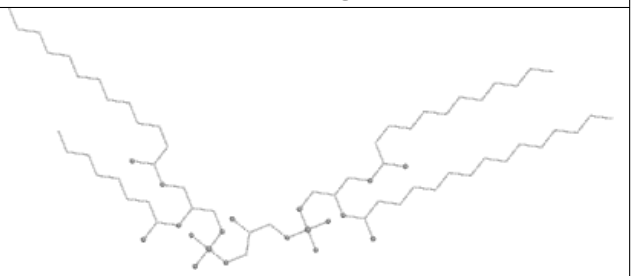


Torsions

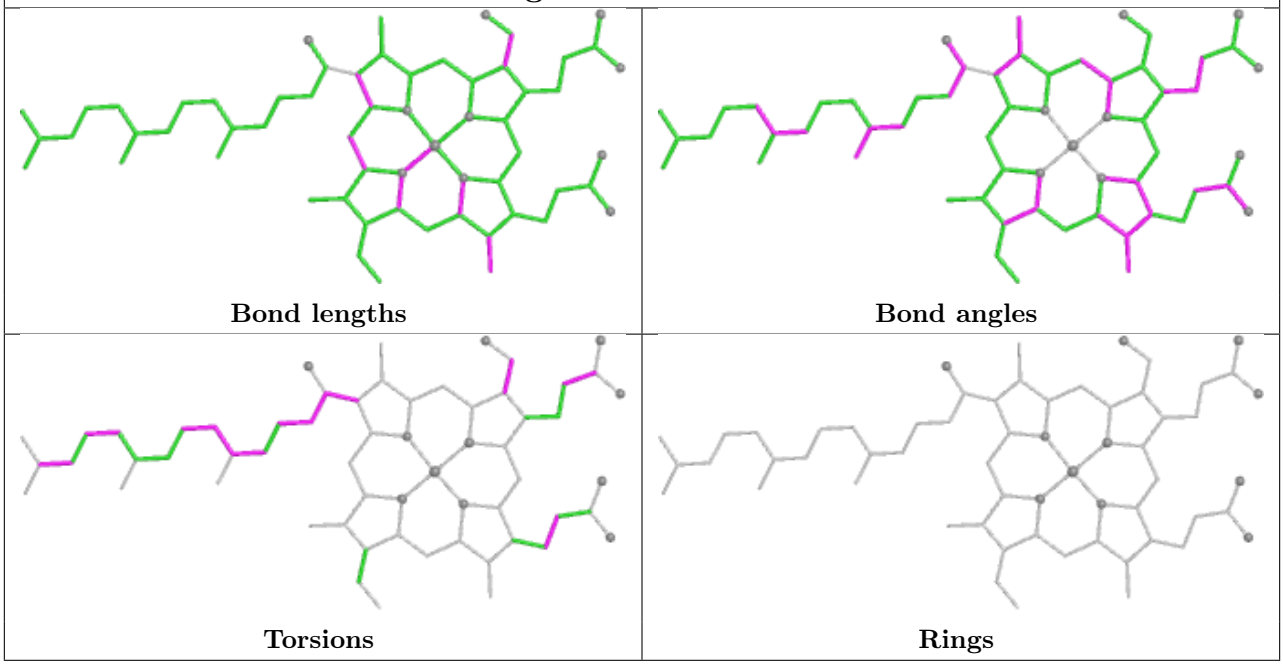


Rings

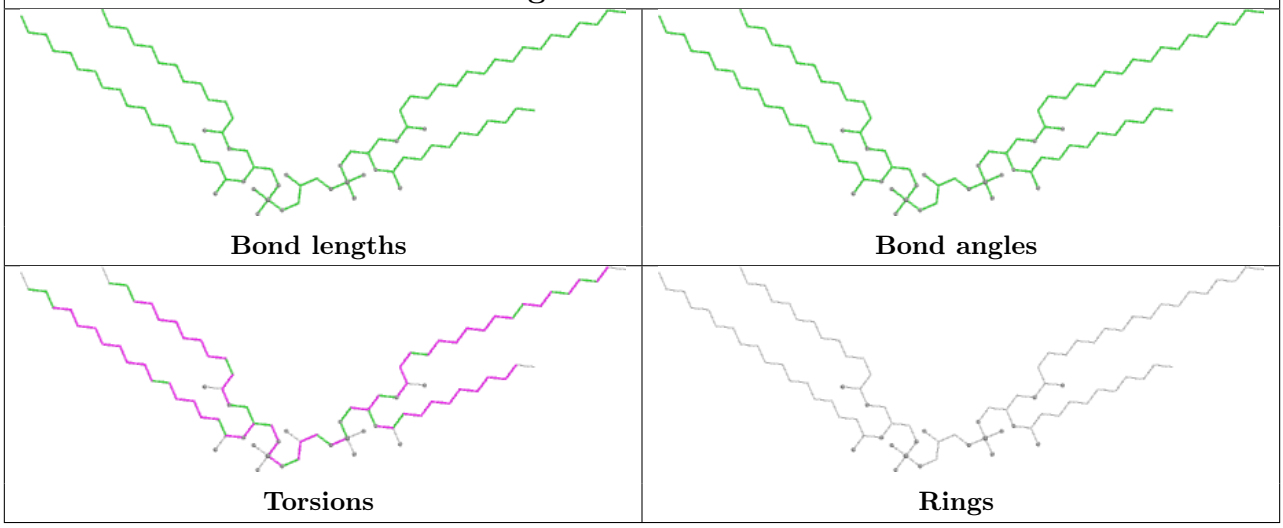
Ligand 9XX j 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL L 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

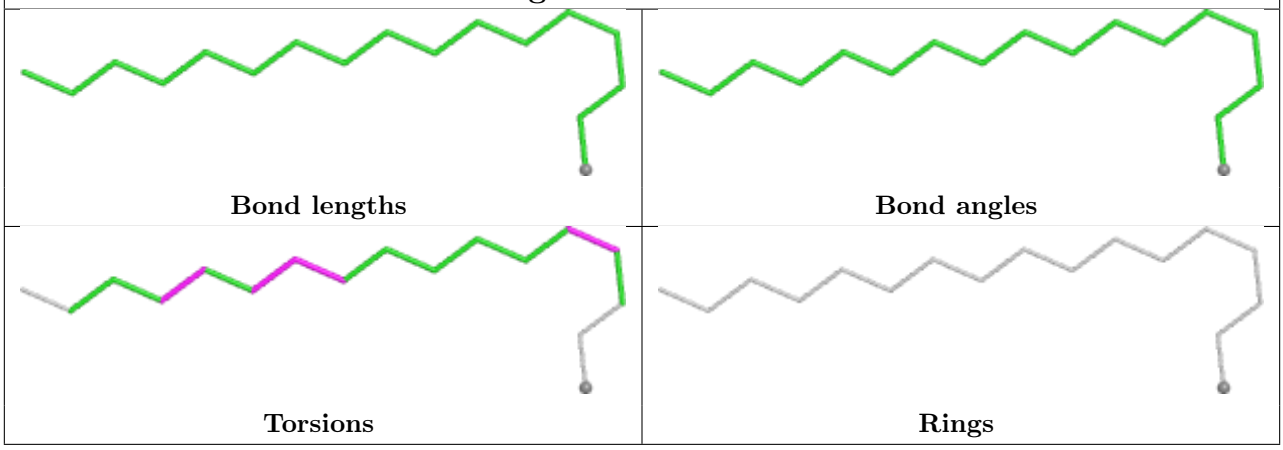
Ligand HEA L 603

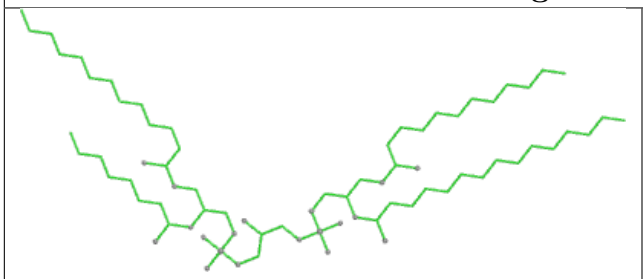
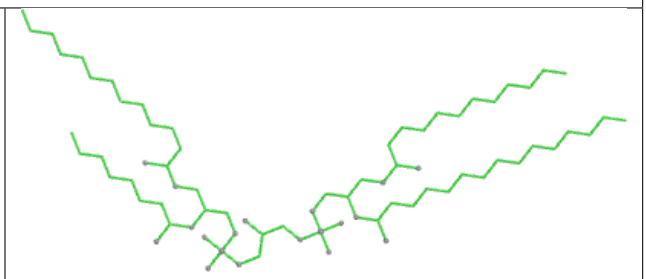
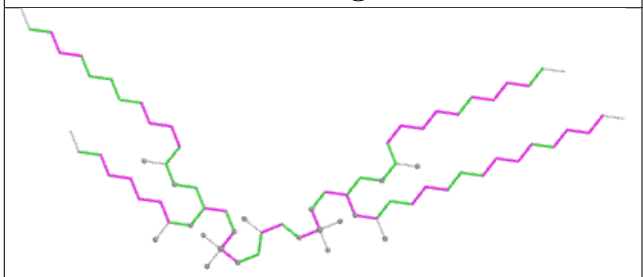
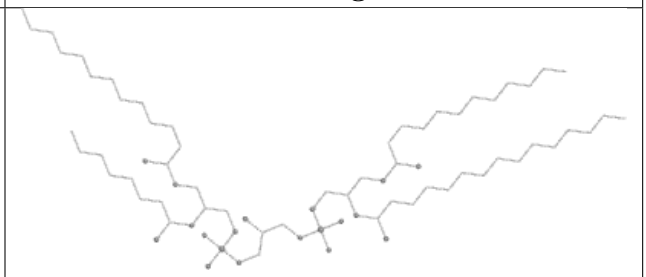


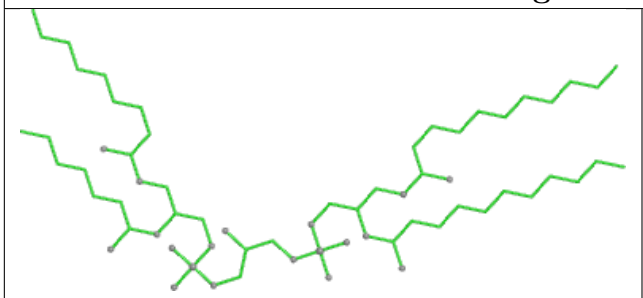
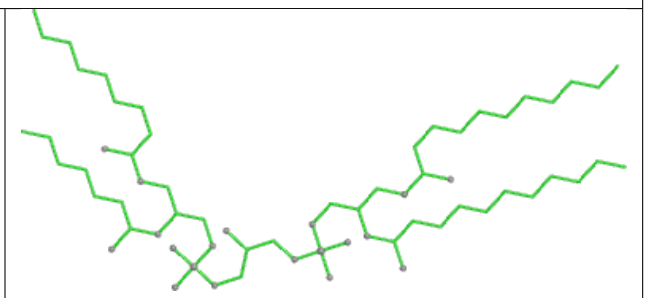
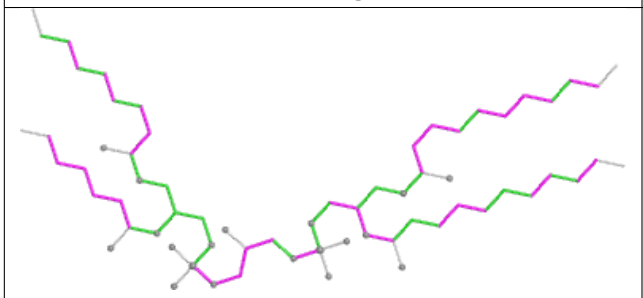
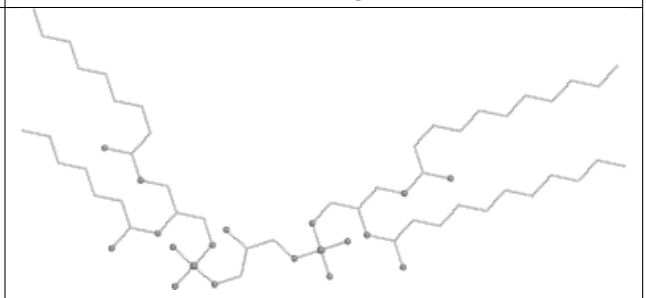
Ligand CDL b 101



Ligand PLM I 609



Ligand CDL I 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL i 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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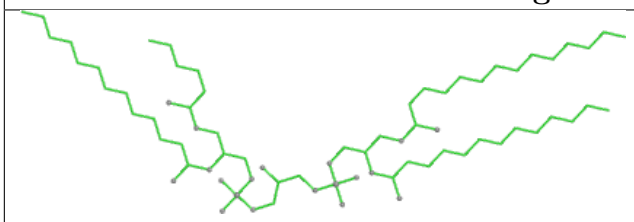
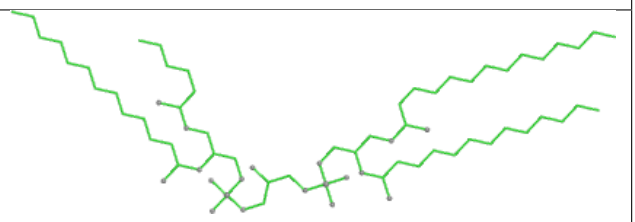
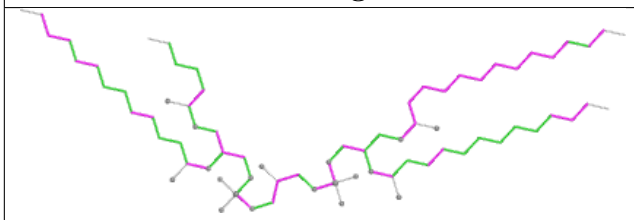
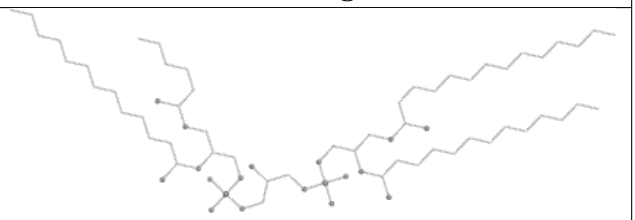
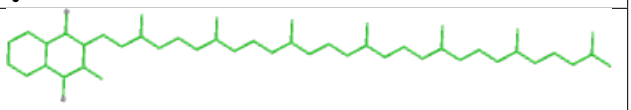
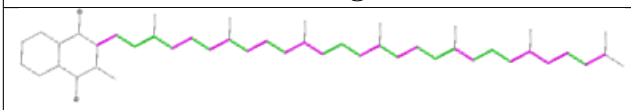
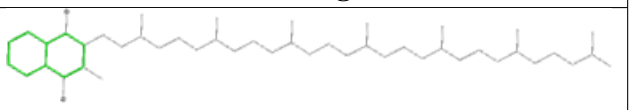
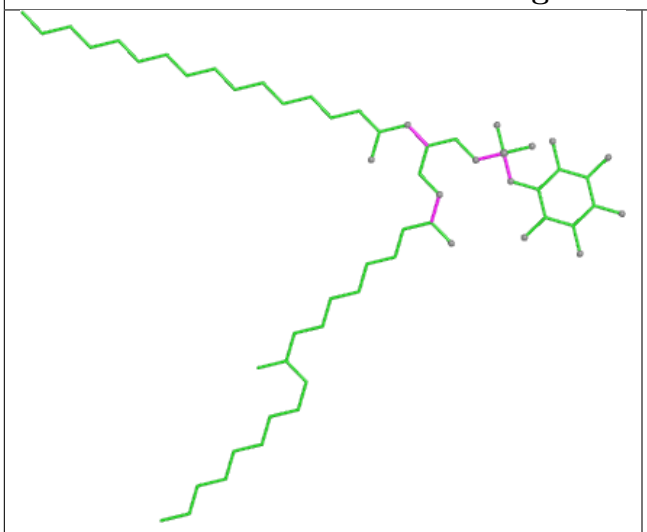
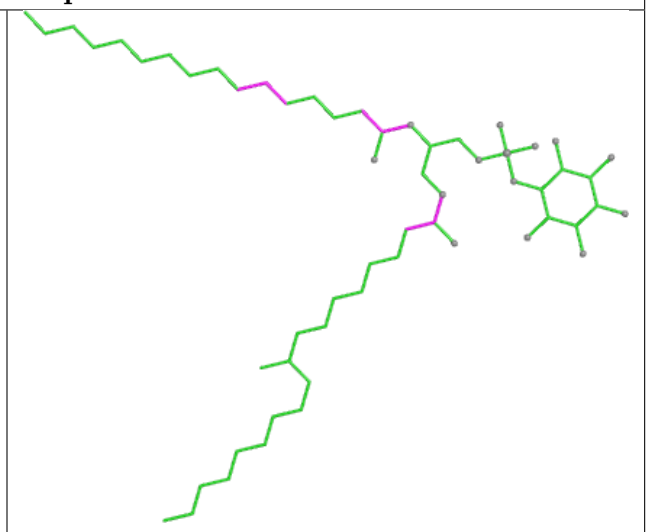
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 n 201	
Bond lengths	 Bond angles
 Torsions	 Rings

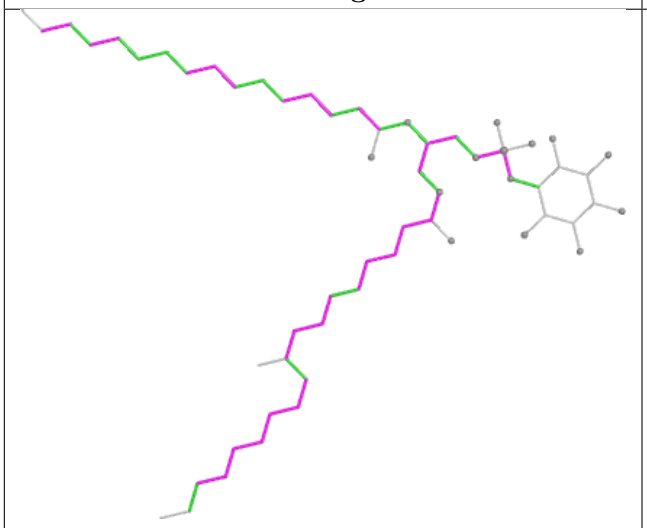
Ligand 9YF p 604



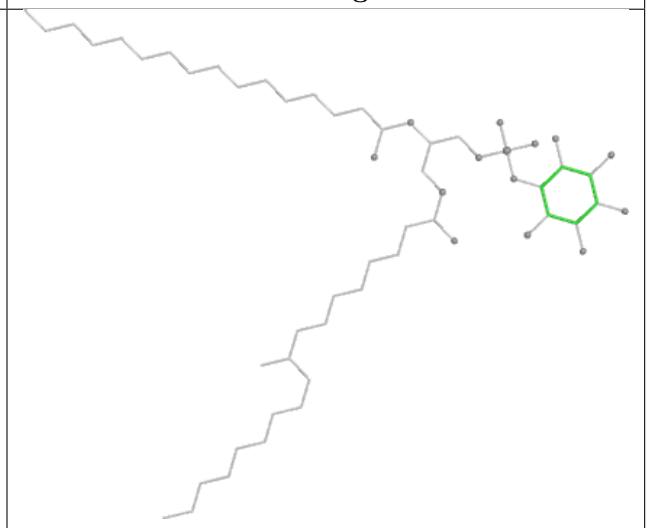
Bond lengths



Bond angles

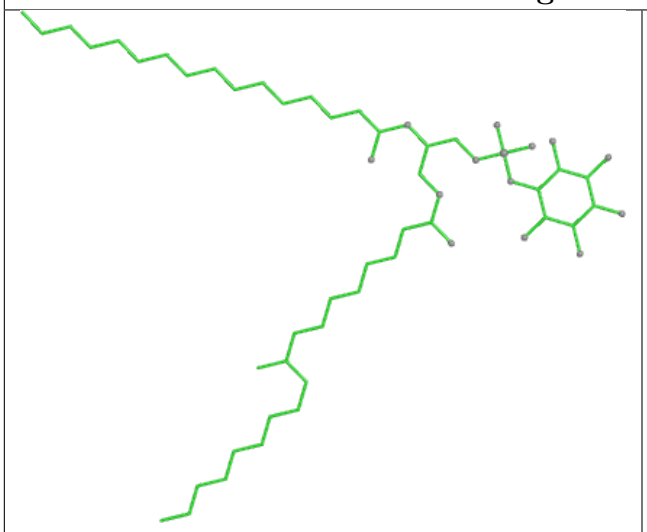


Torsions



Rings

Ligand 9YF i 601



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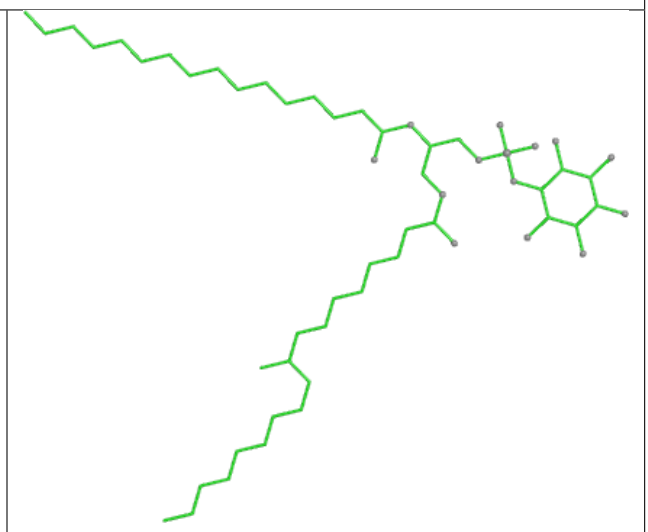

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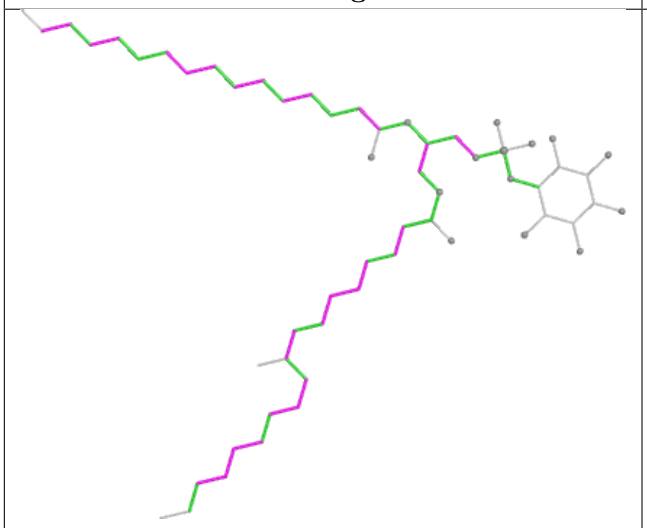

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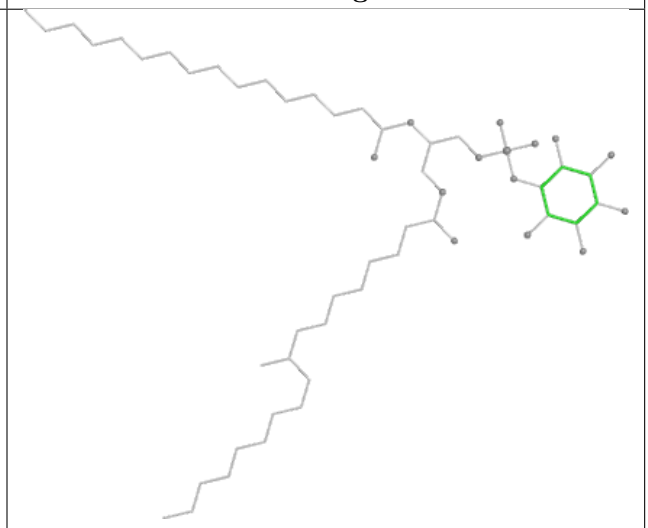
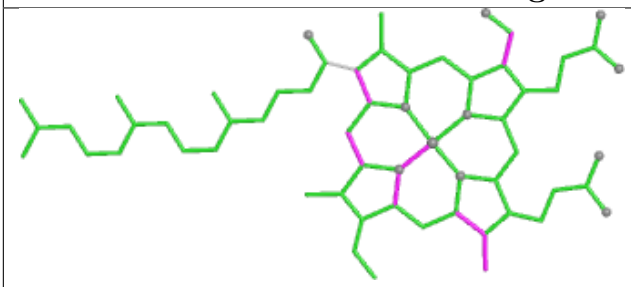
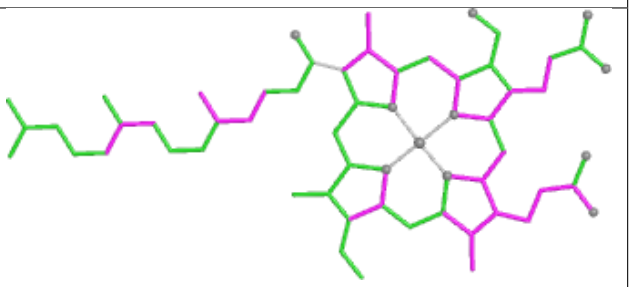
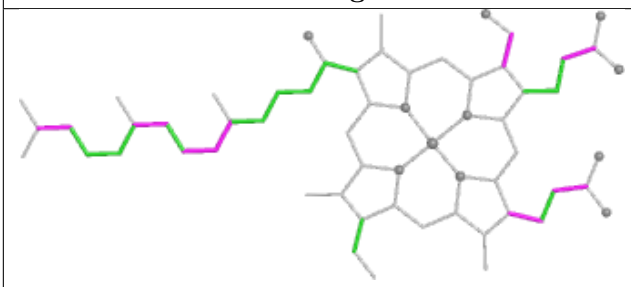
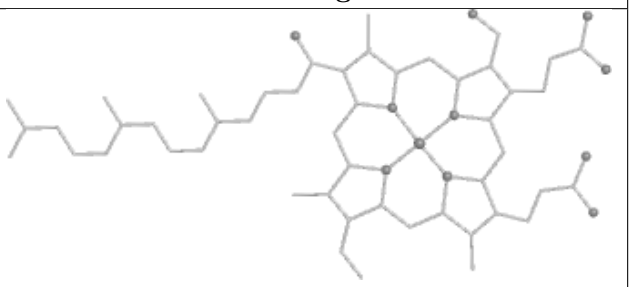
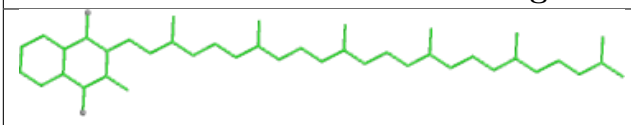
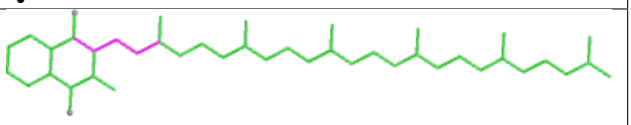
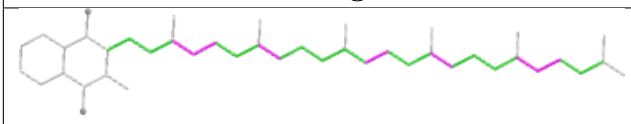
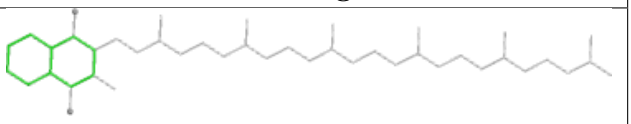
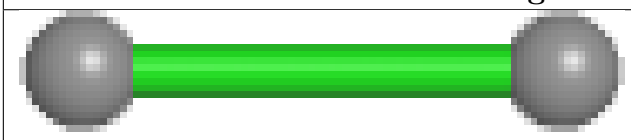
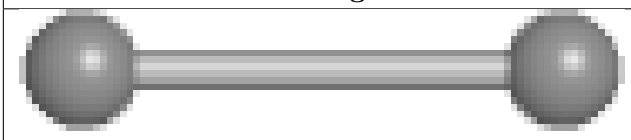
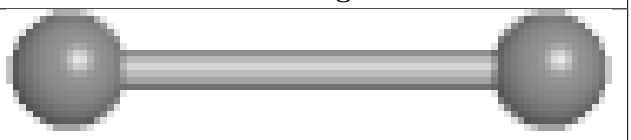


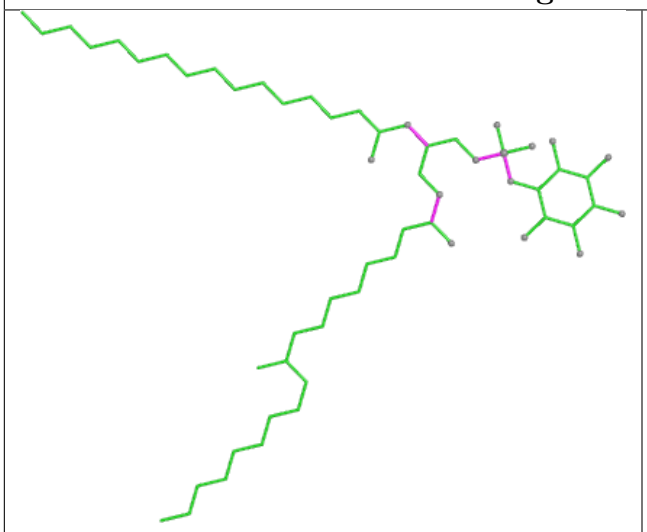
Rings

Ligand HEA I 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 i 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OXY I 607	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand 9YF j 601



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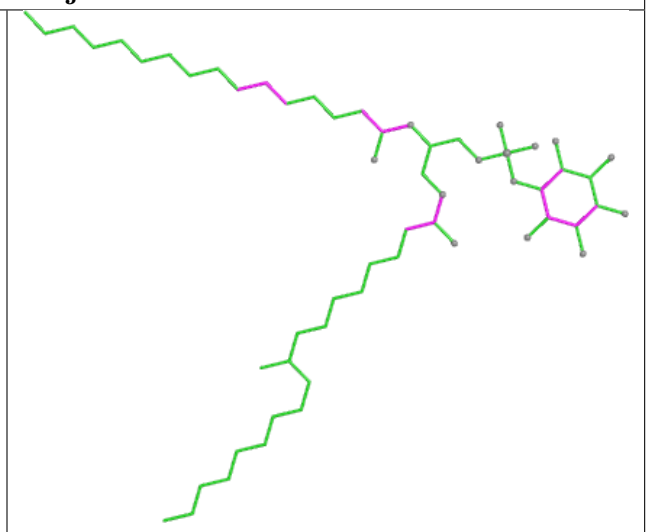

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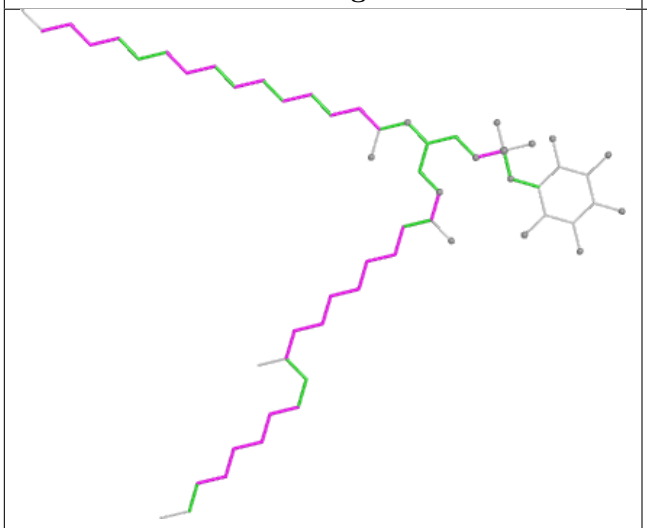

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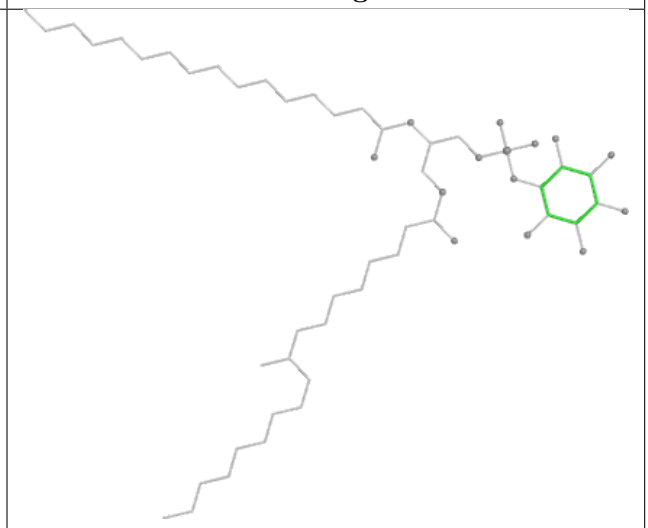
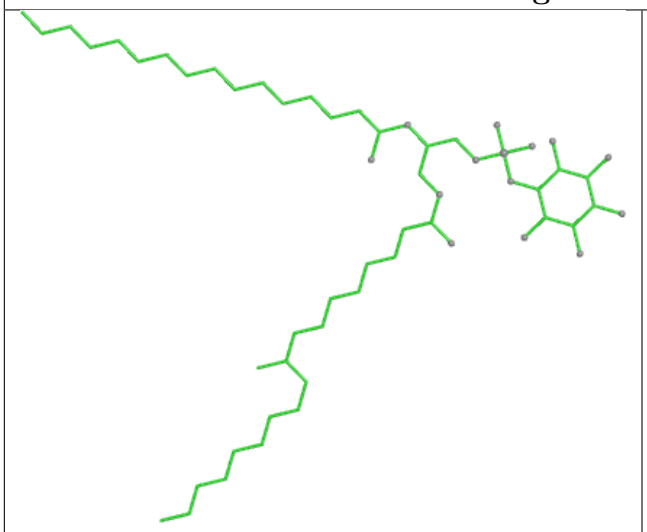


Rings

Ligand 9YF o 603



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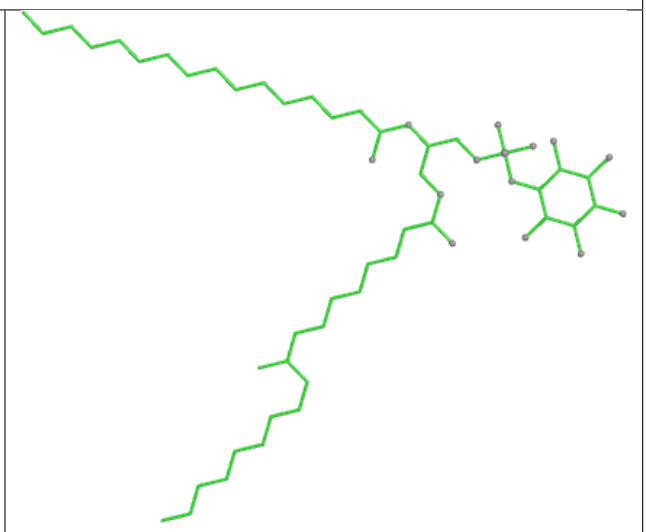
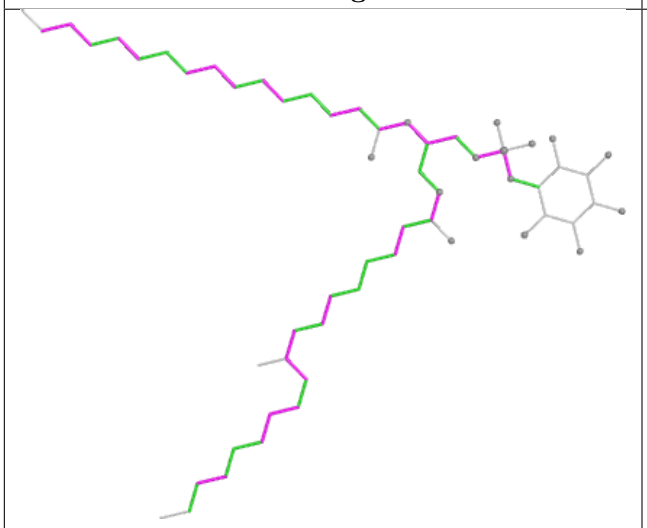


Bond angles



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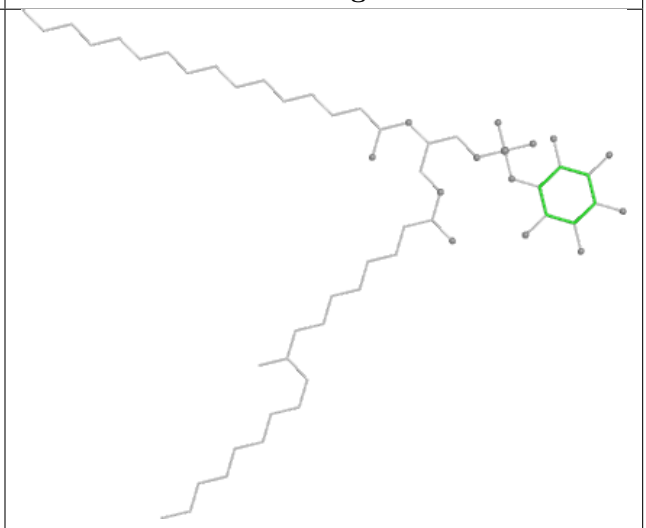
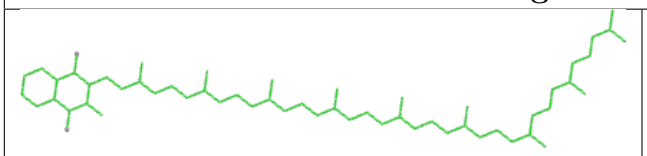


Rings

Ligand MQ9 i 610



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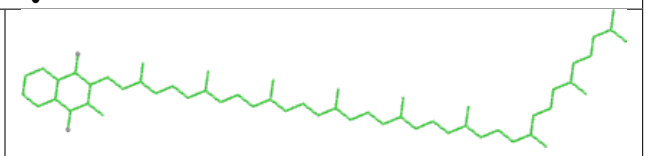
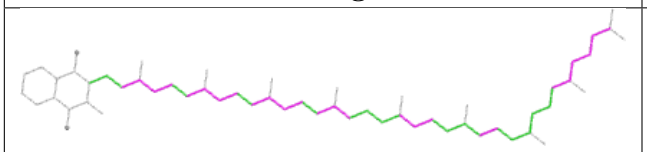
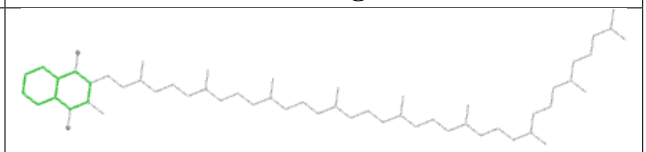


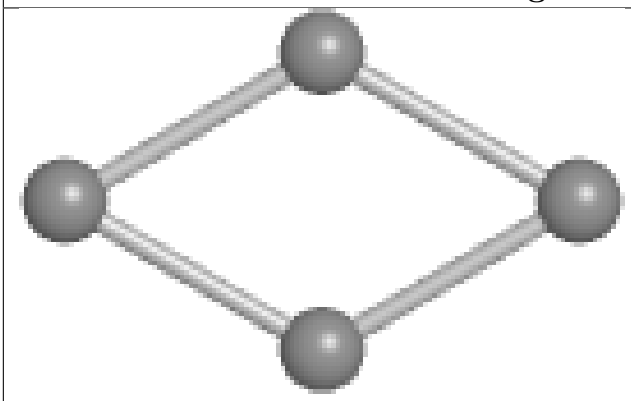
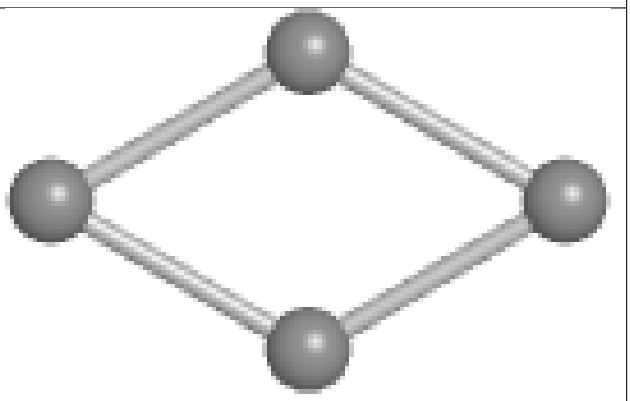
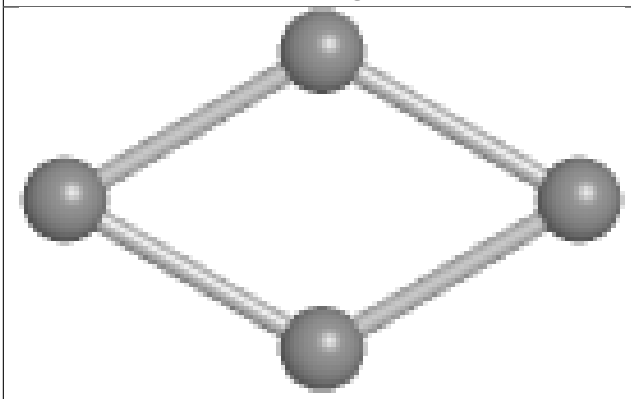
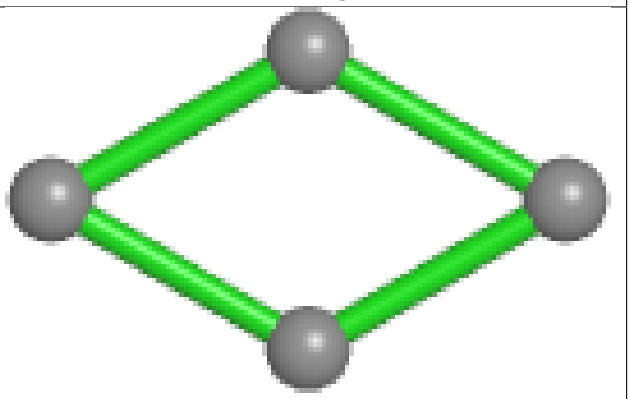
Bond angles



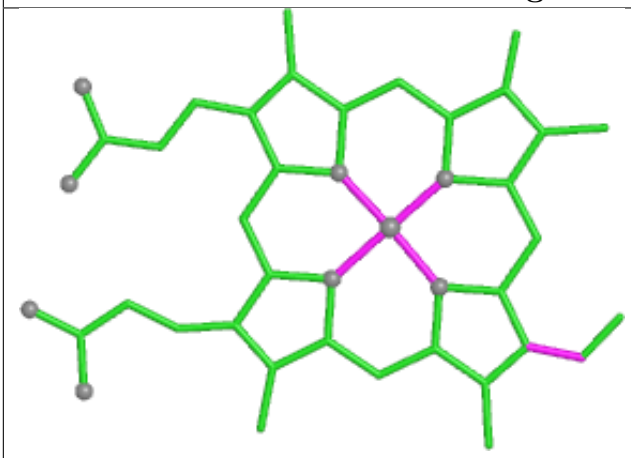
Torsions



Rings

Ligand FES V 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM j 603



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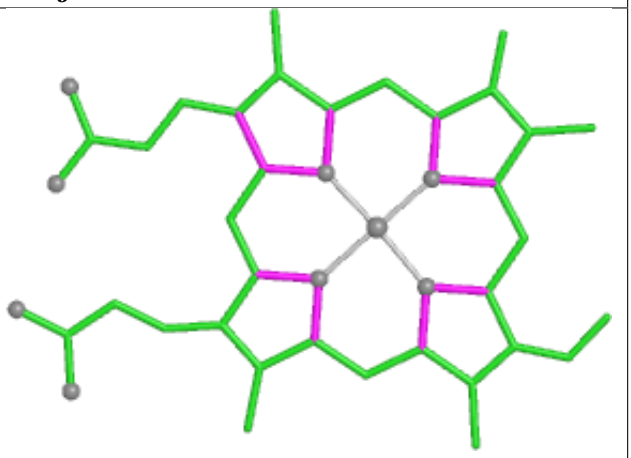

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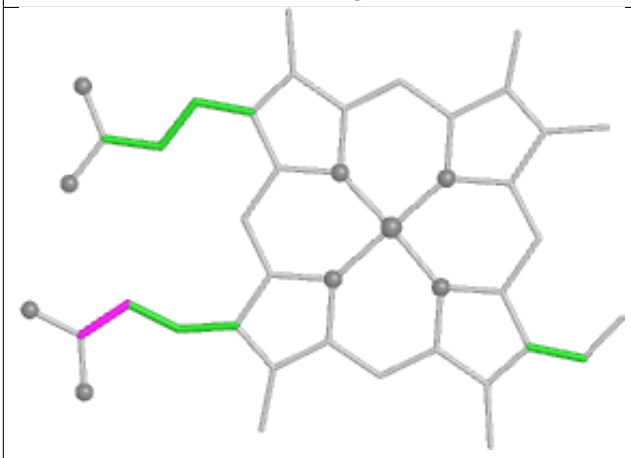

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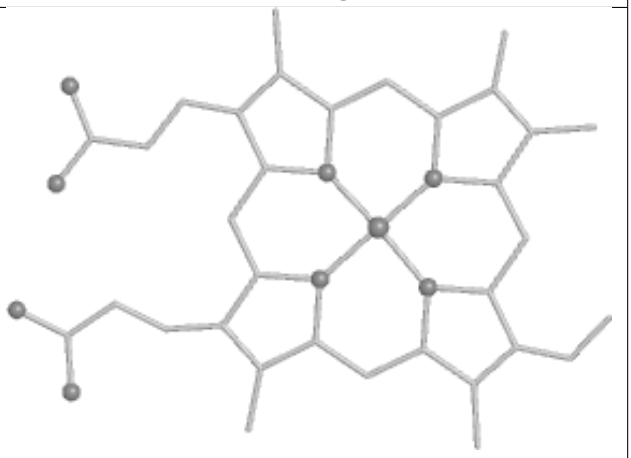
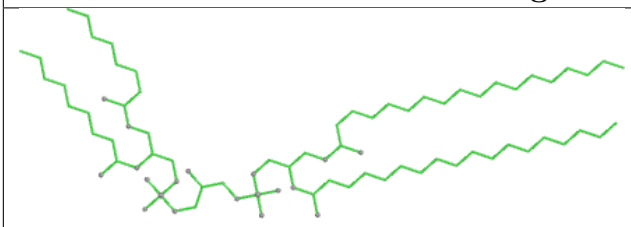


Rings

Ligand CDL I 605



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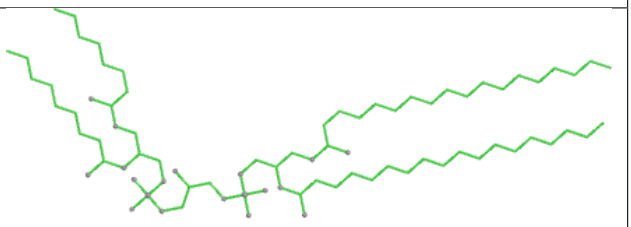

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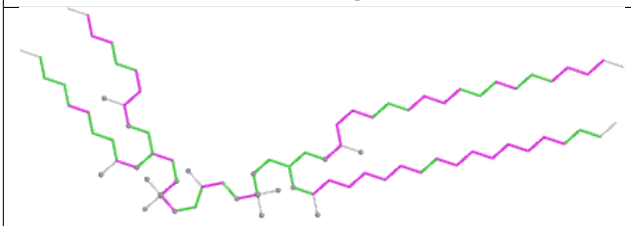

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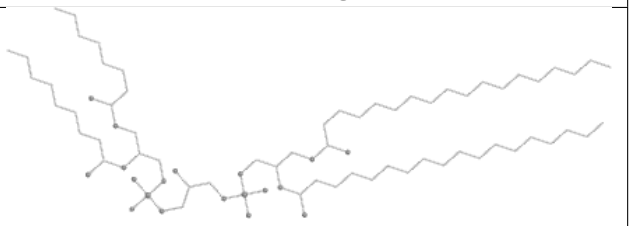

Rings

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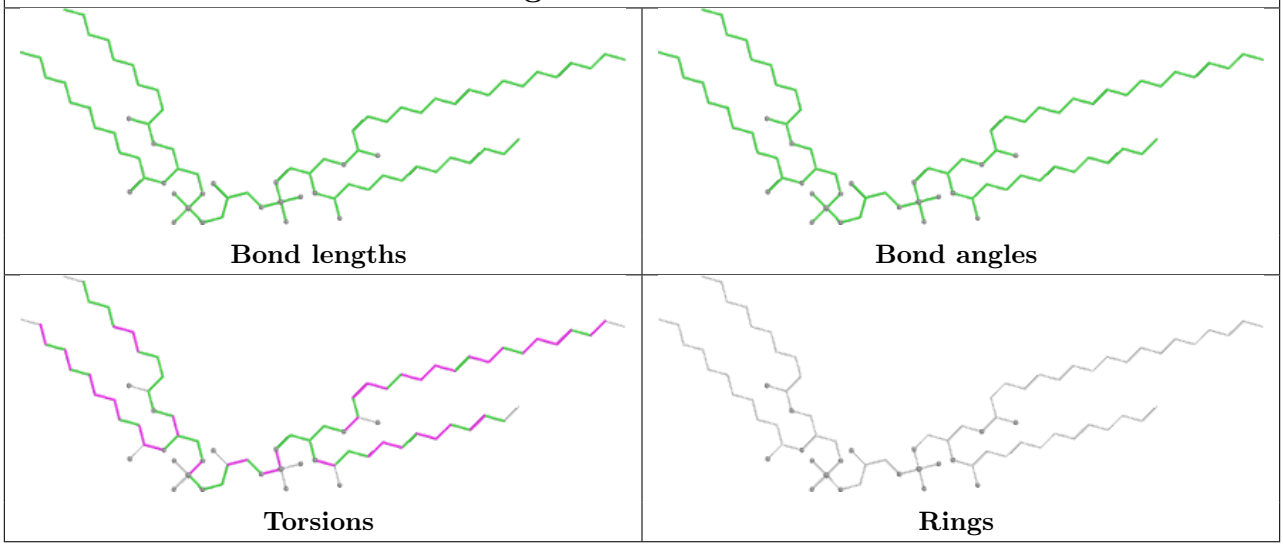

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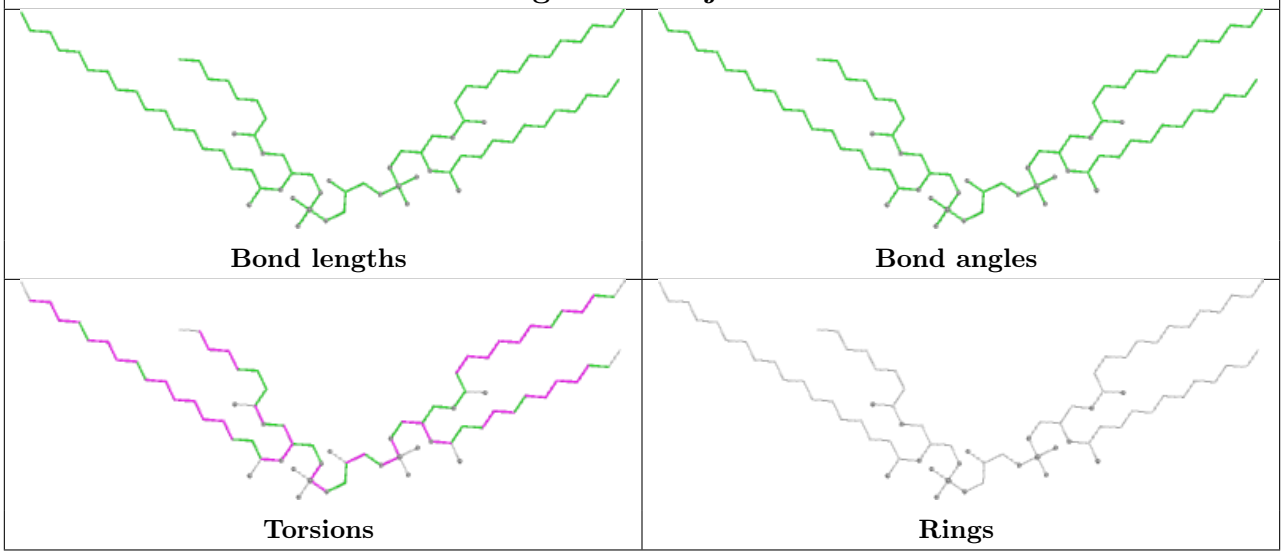

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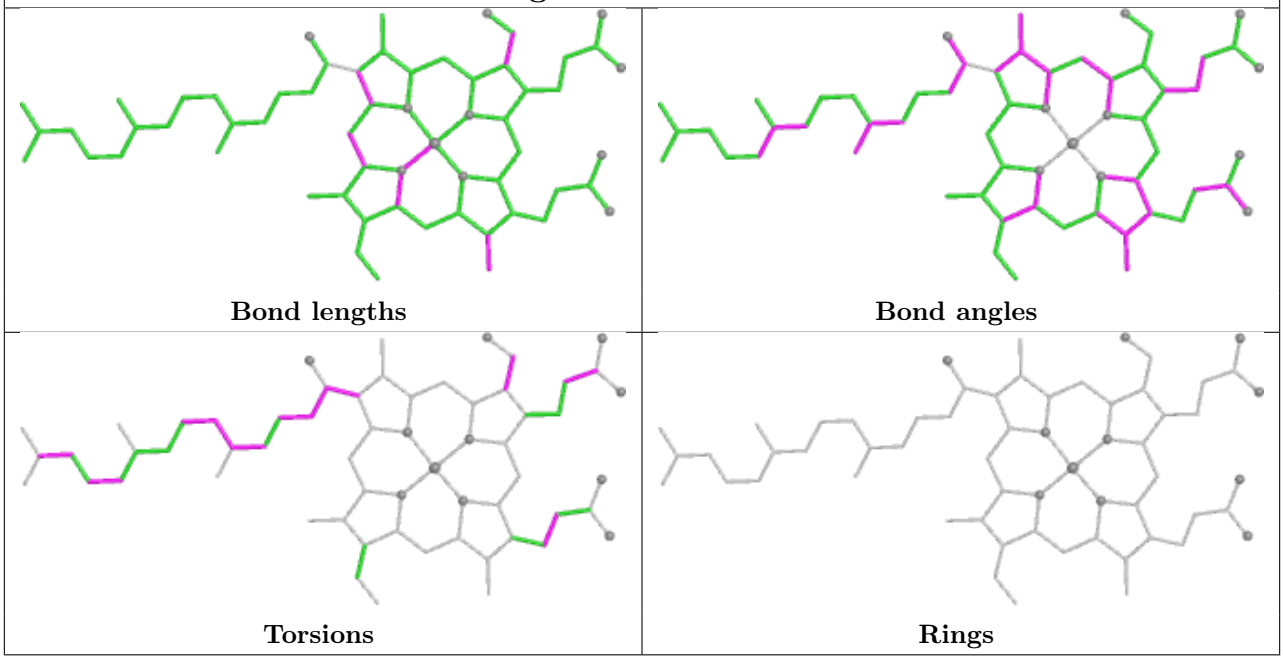

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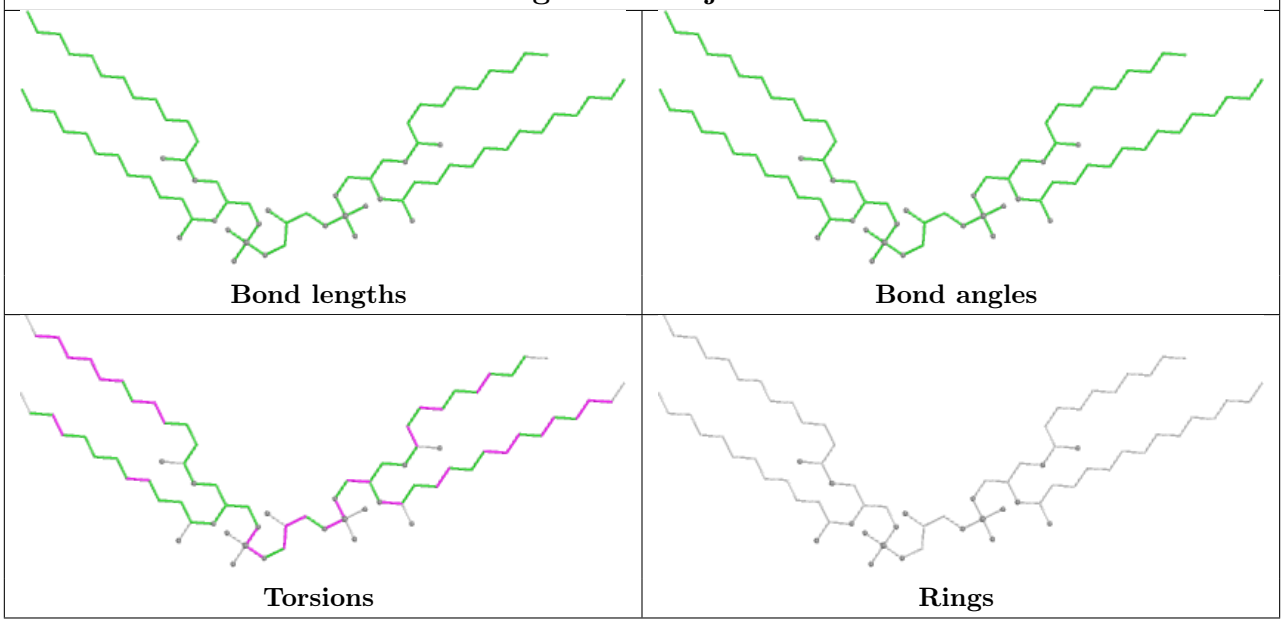

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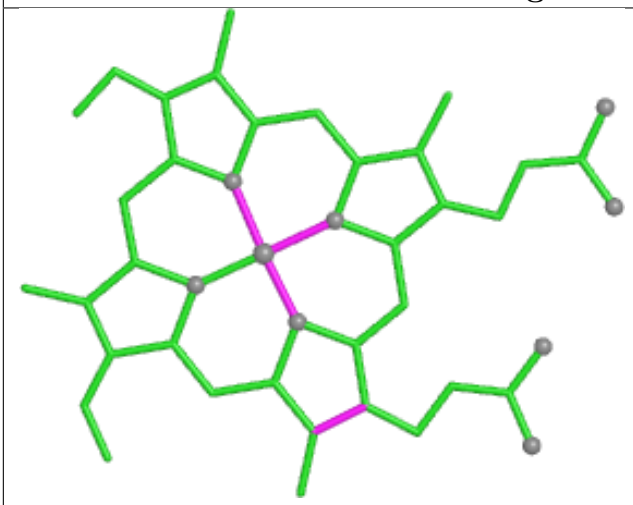

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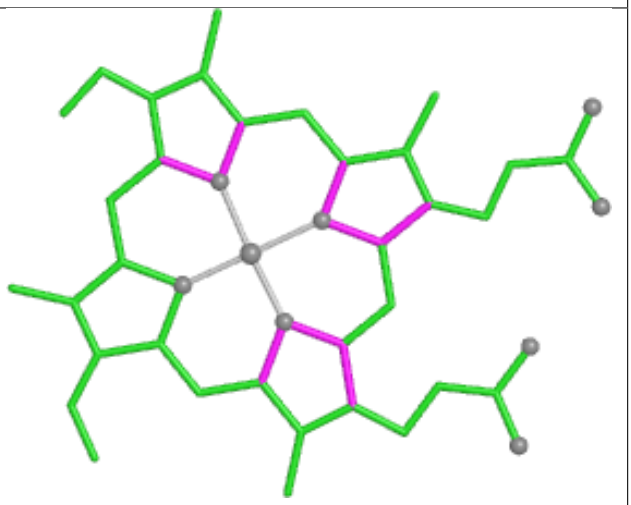

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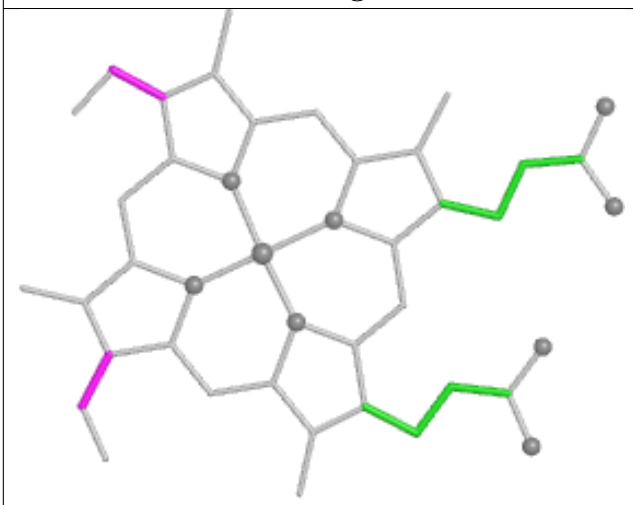

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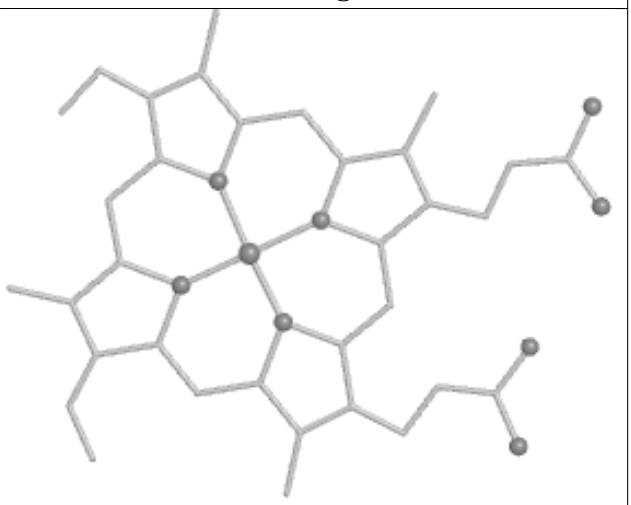
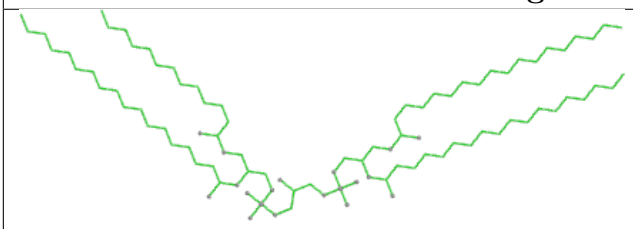


Rings

Ligand CDL p 603



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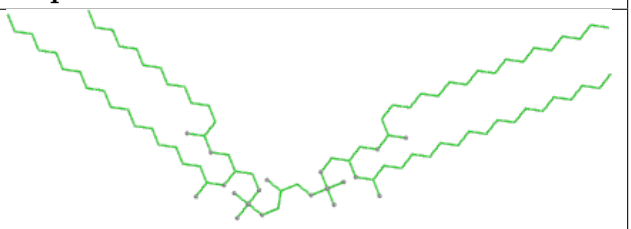

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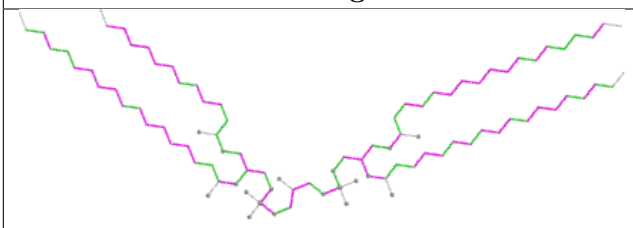

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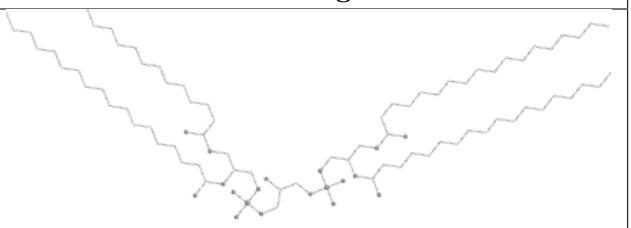
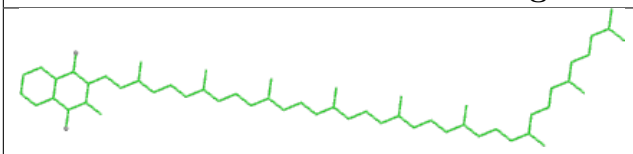


Rings

Ligand MQ9 j 608



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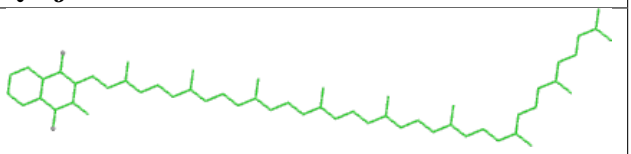

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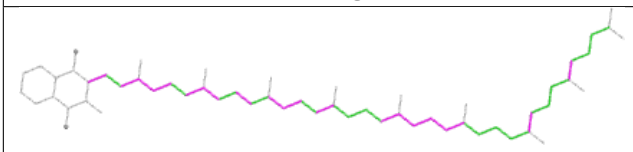

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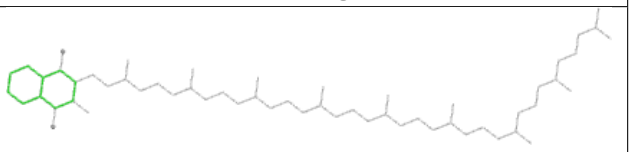
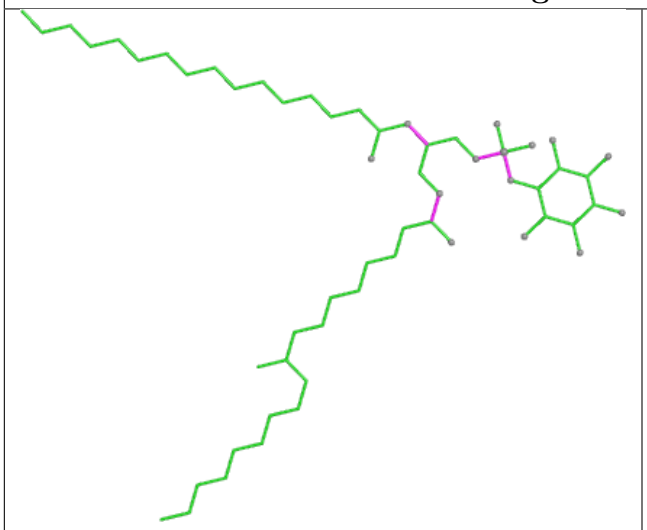


Rings

Ligand 9YF p 601



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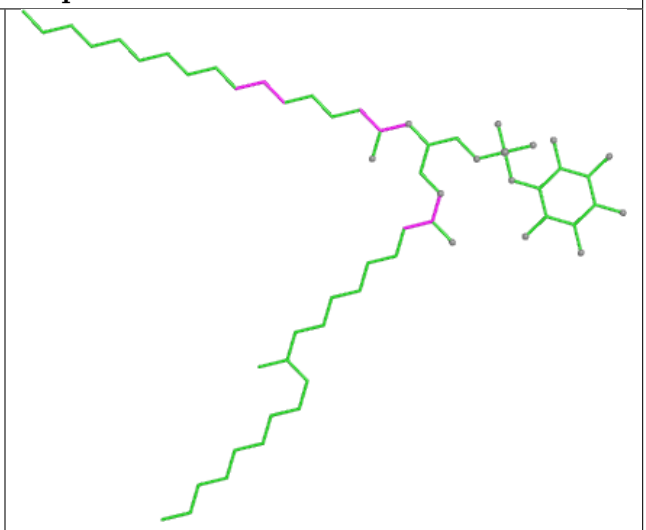

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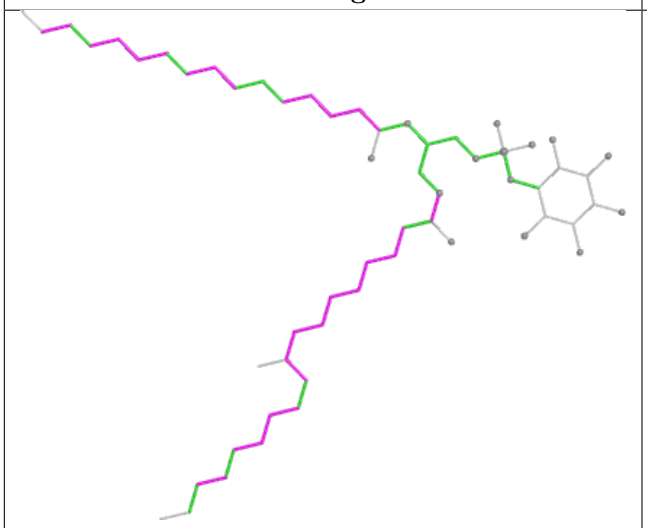

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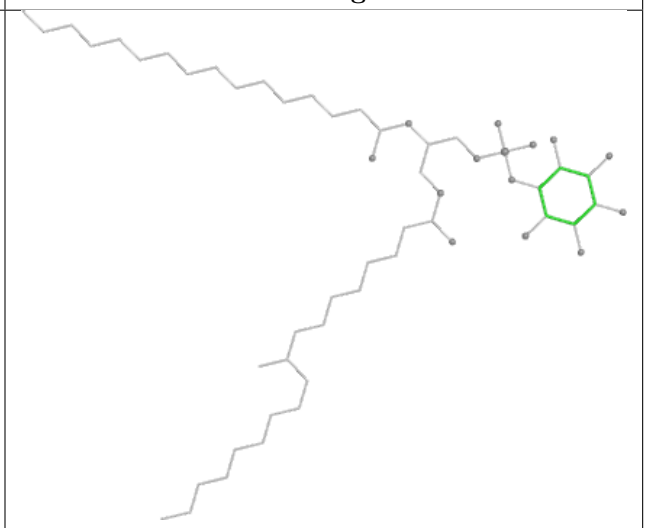
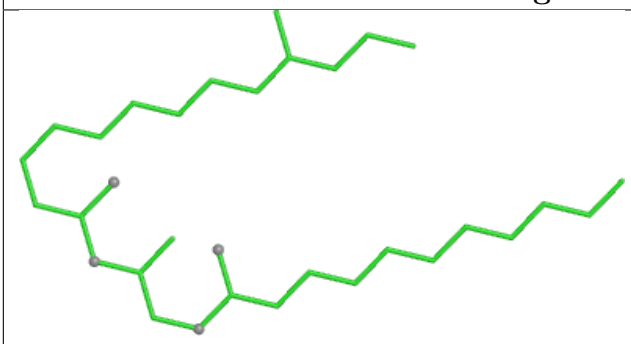
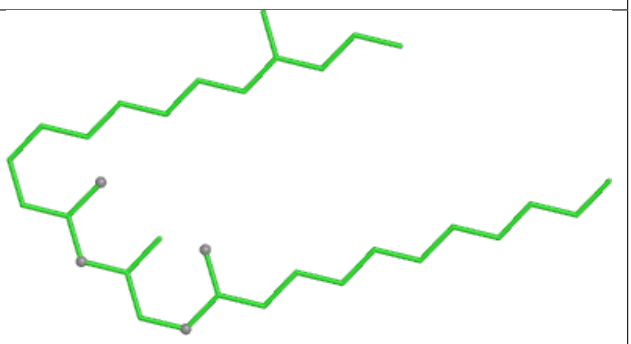
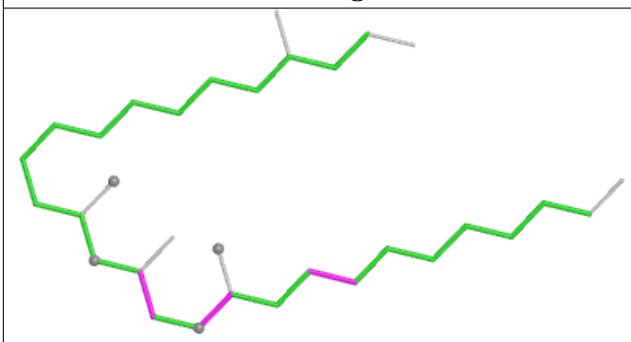
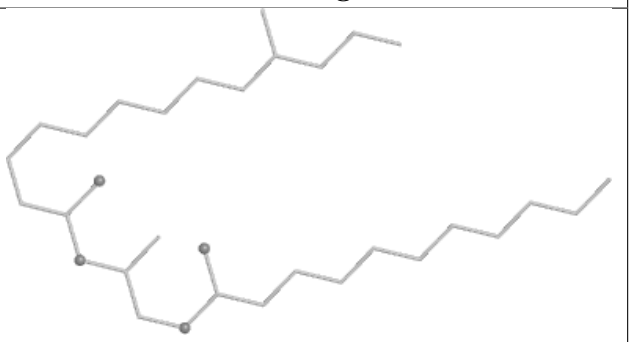
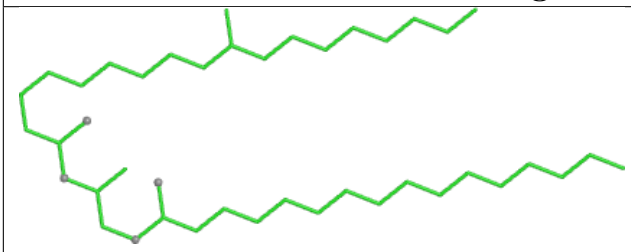
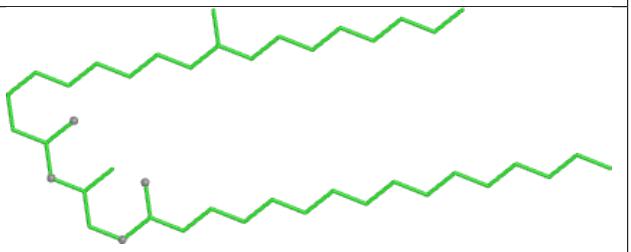
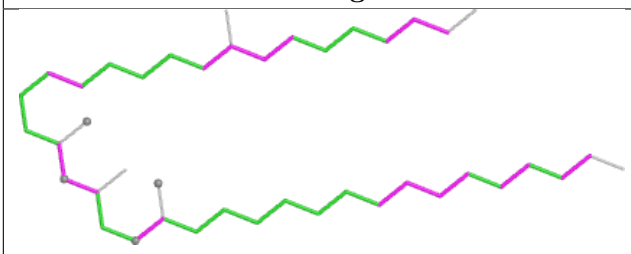
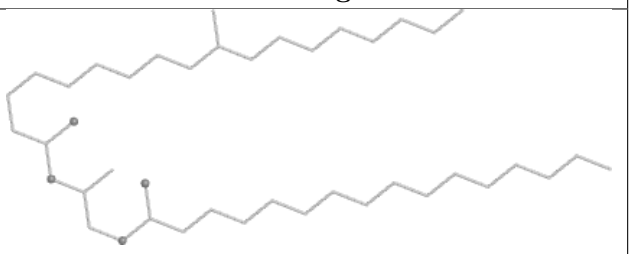
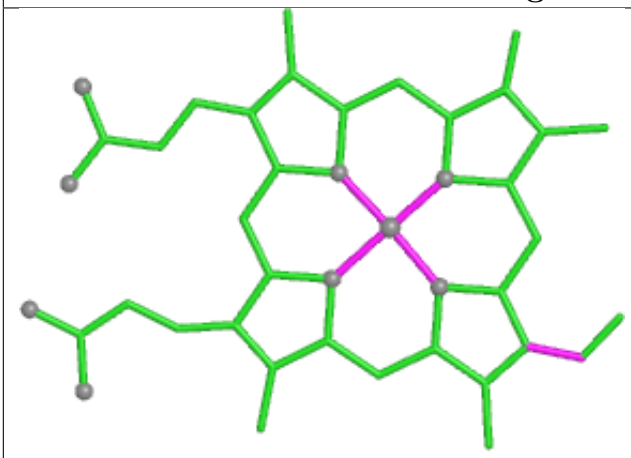


Rings

Ligand 9XX i 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9XX r 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM i 604



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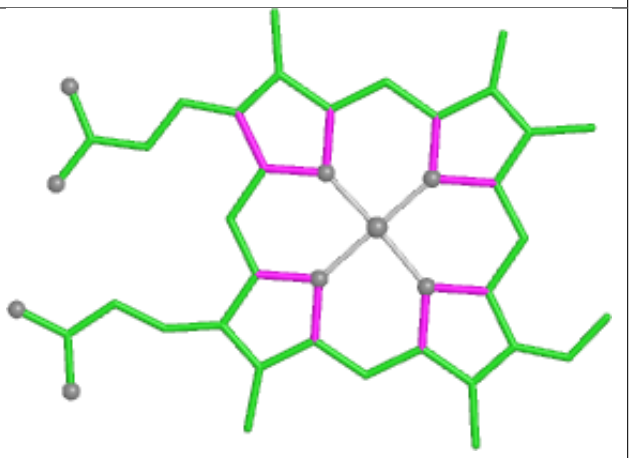

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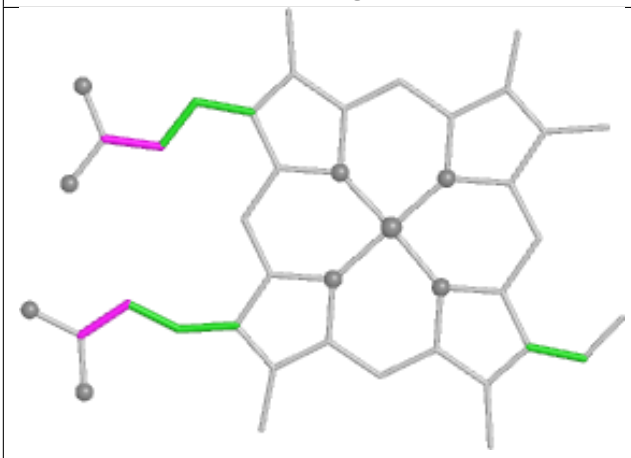

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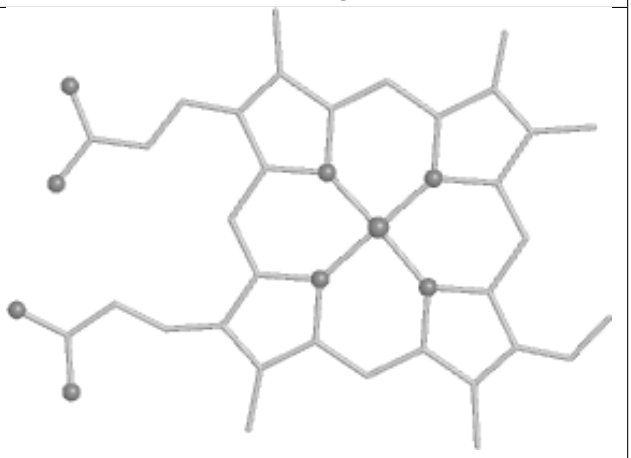
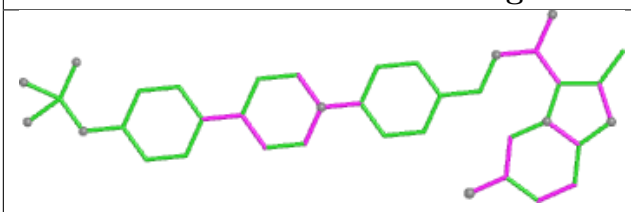


Rings

Ligand A1MBF i 602



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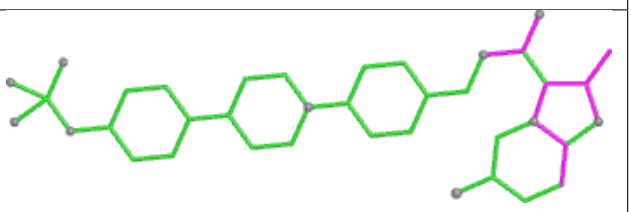

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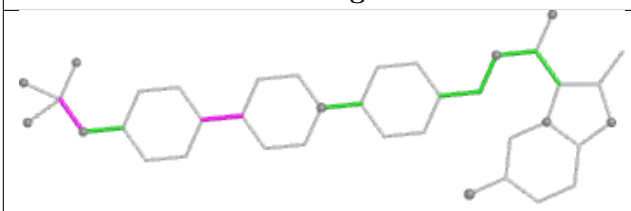

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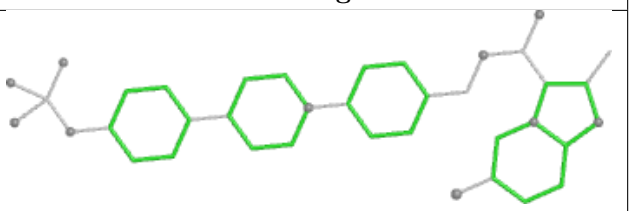
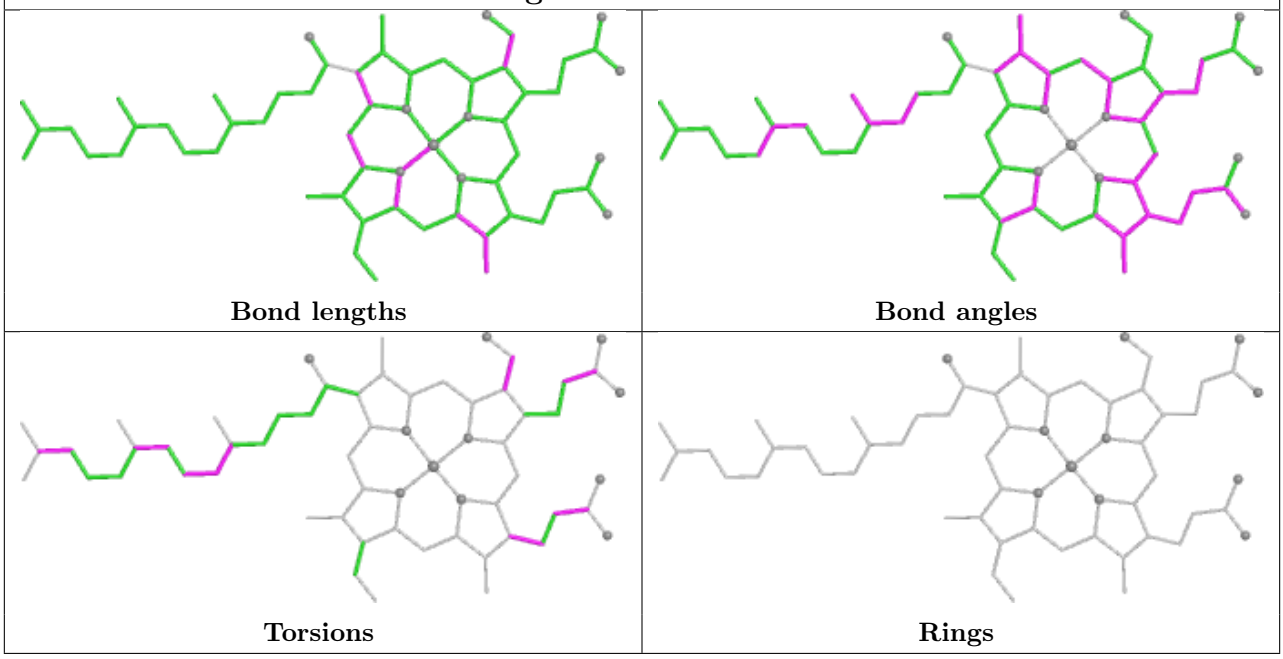
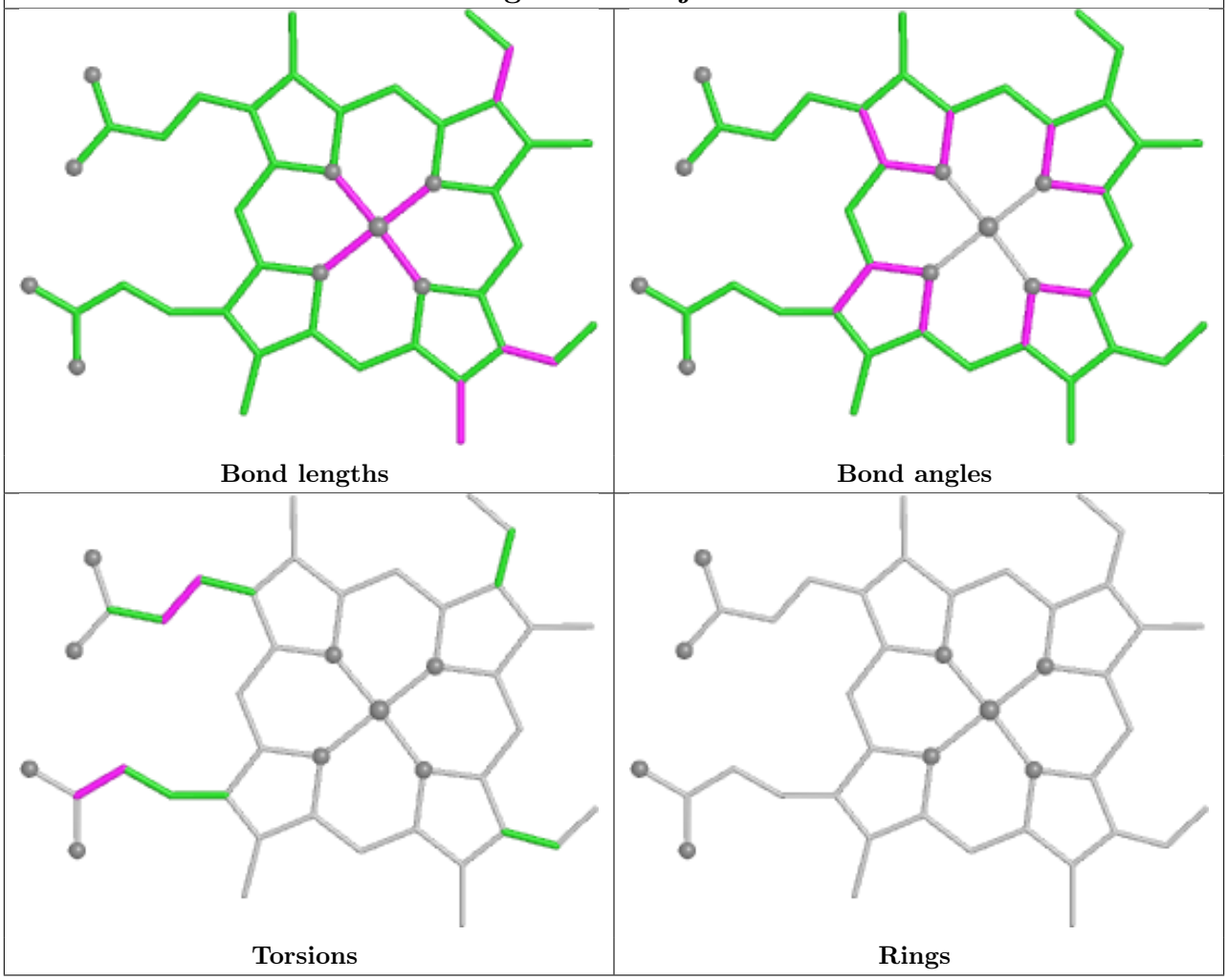


Rings

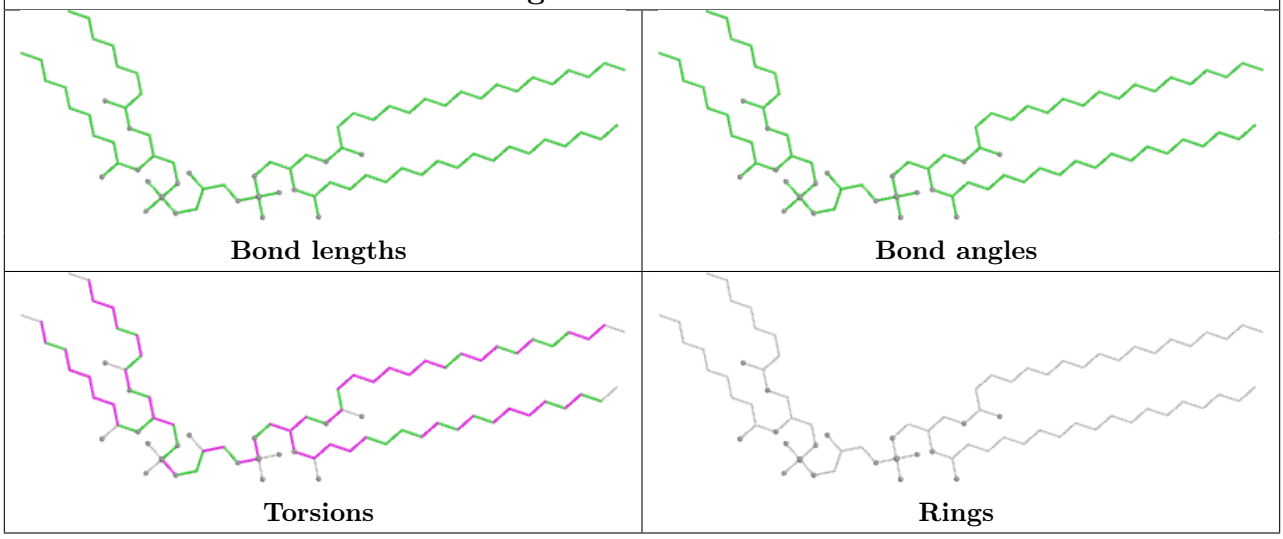
Ligand HEA L 602



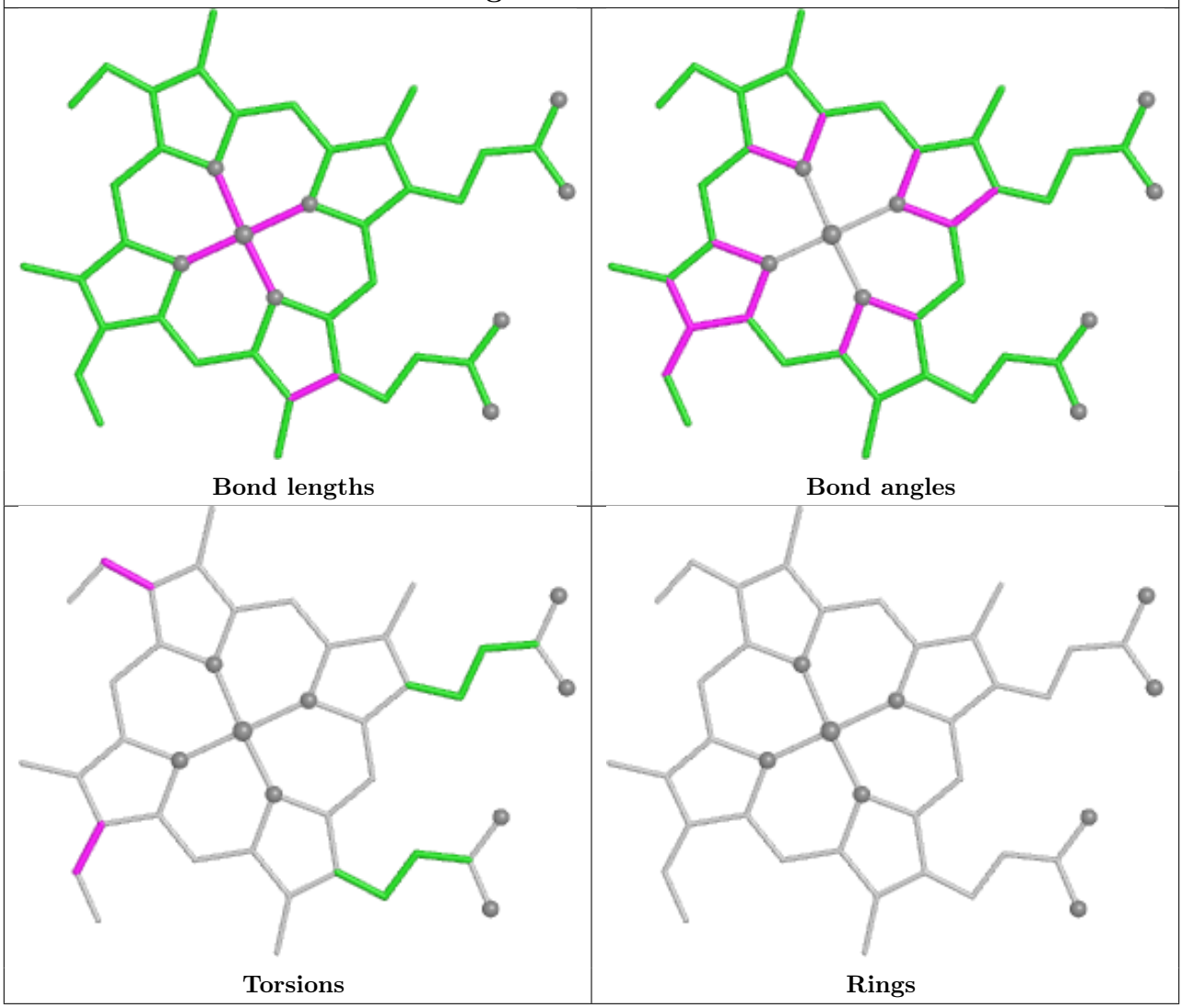
Ligand HEM j 604



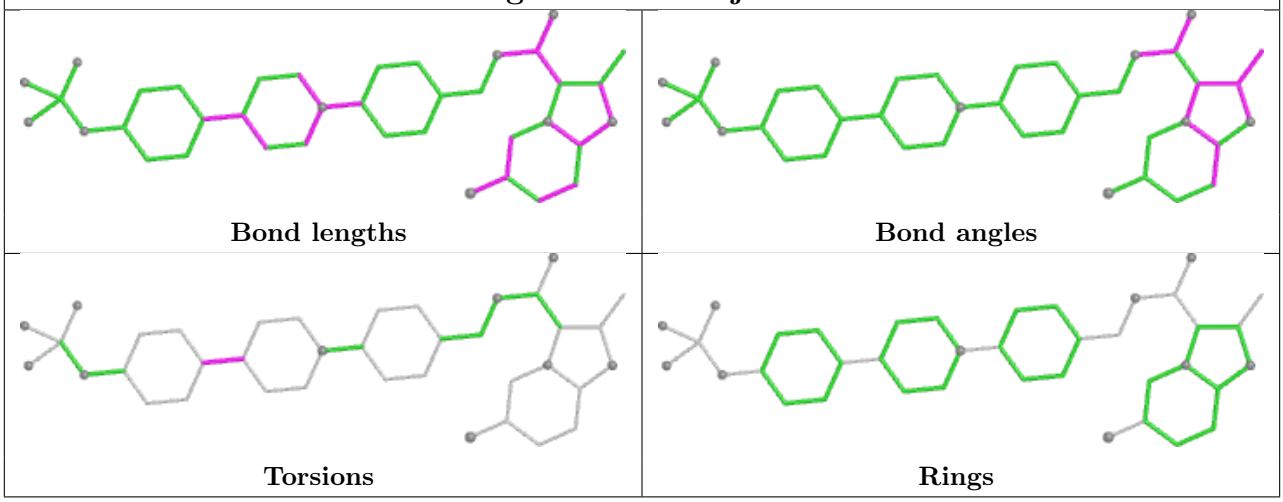
Ligand CDL L 607



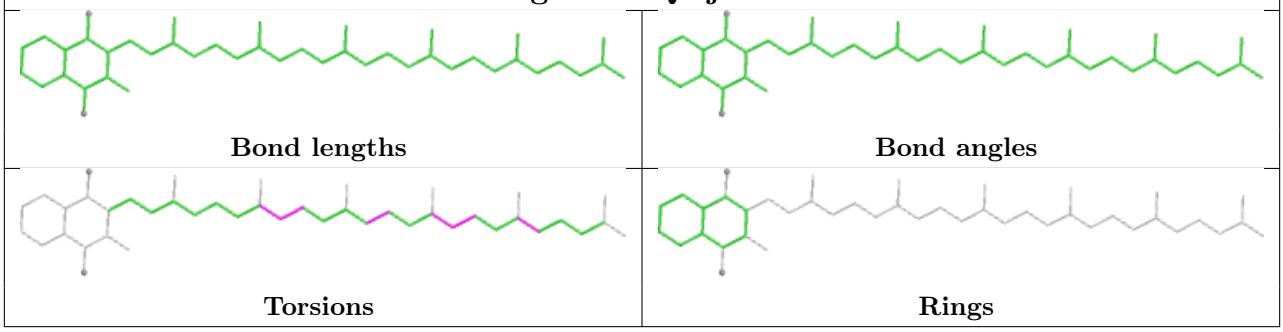
Ligand HEC o 602



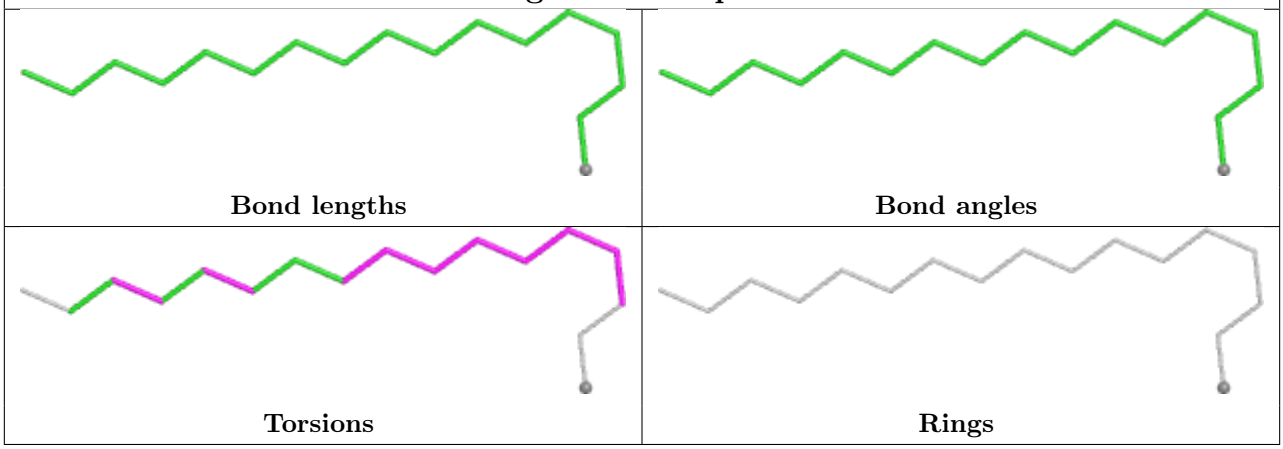
Ligand A1MBF j 602



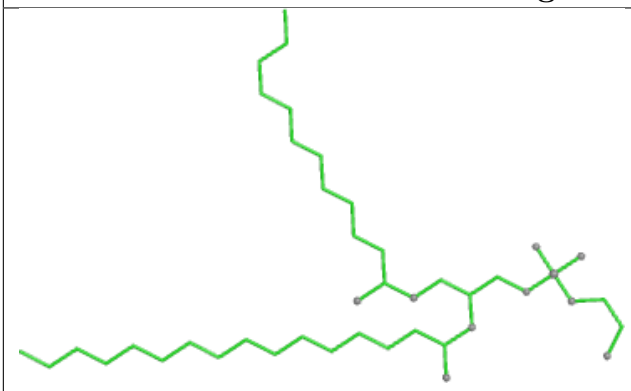
Ligand MQ9 j 607



Ligand PLM q 301

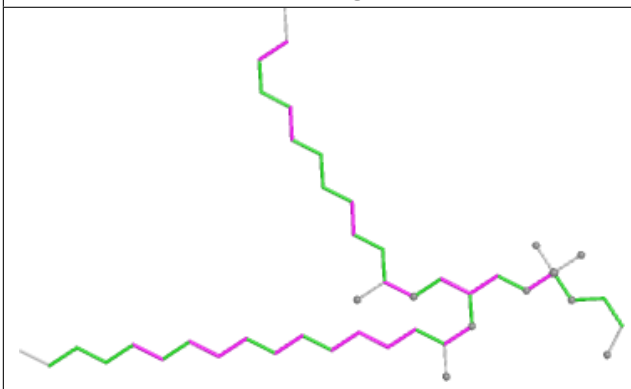


Ligand 9Y0 f 601

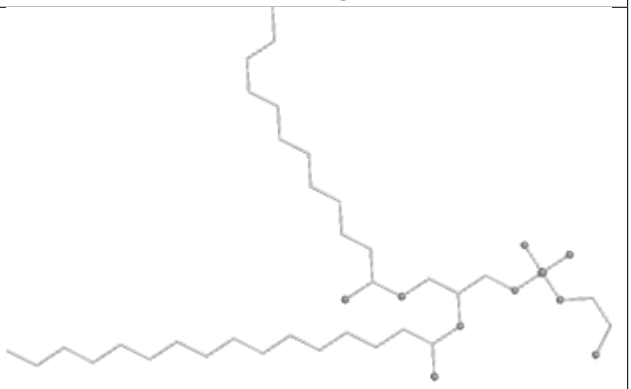


Bond lengths

Bond angles

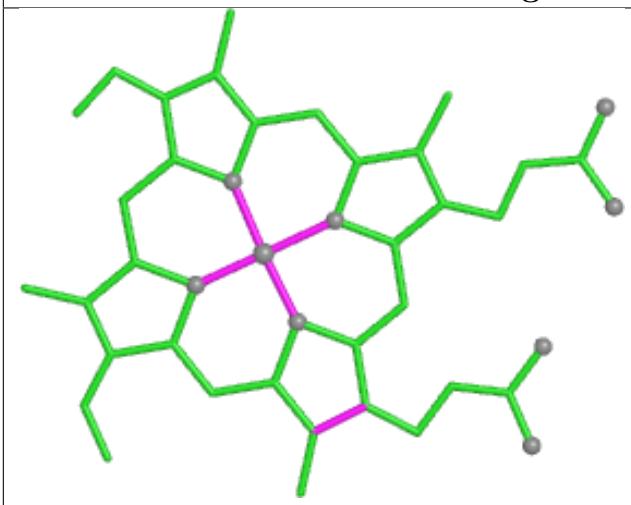


Torsions



Rings

Ligand HEC U 601



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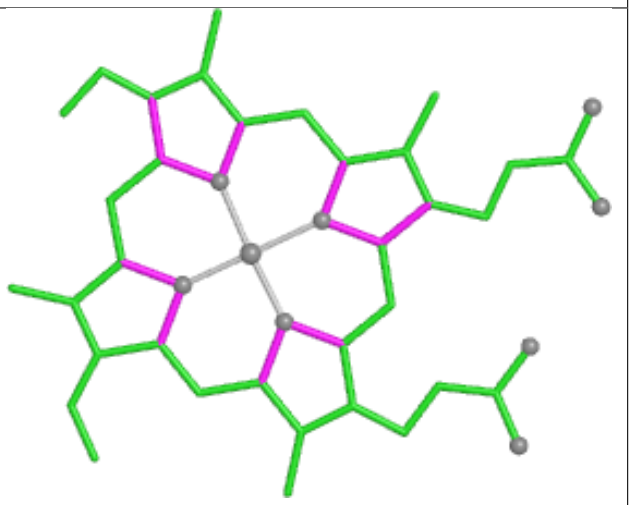

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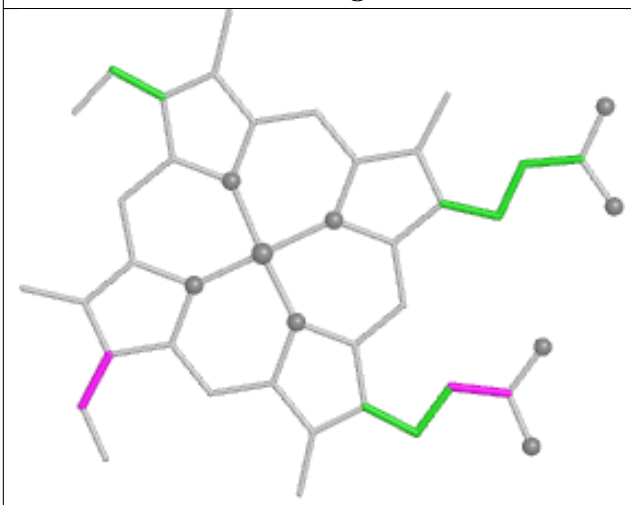

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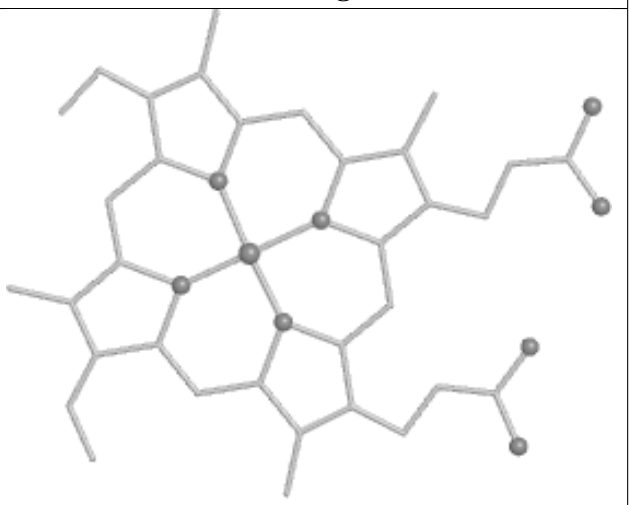
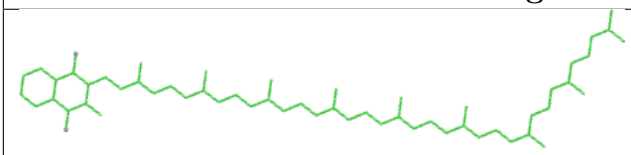
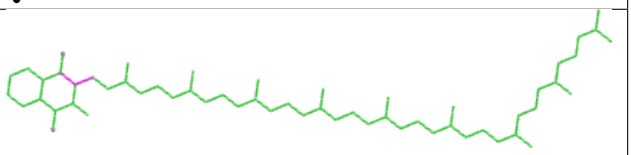


Rings

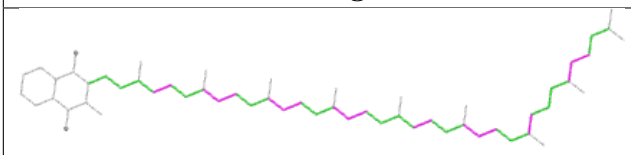
Ligand MQ9 o 604



Bond lengths



Bond angles



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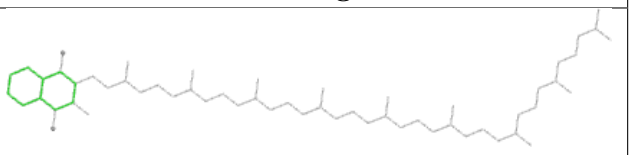
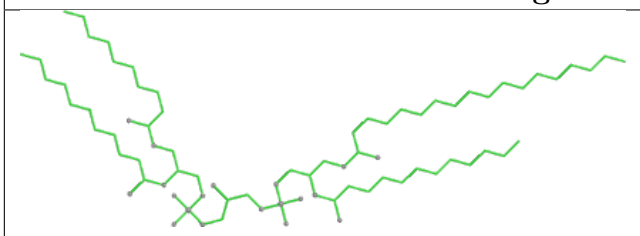
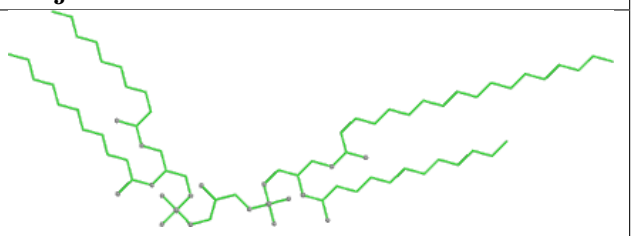
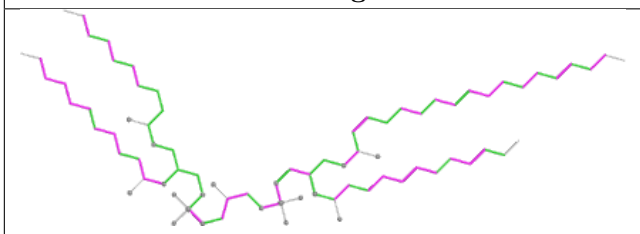
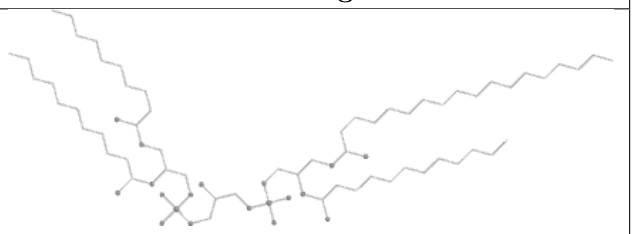


Rings

Ligand CDL j 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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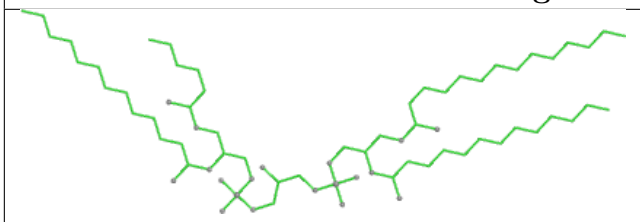
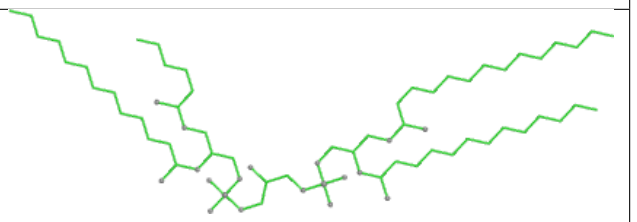
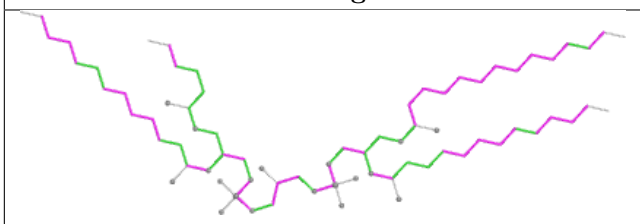
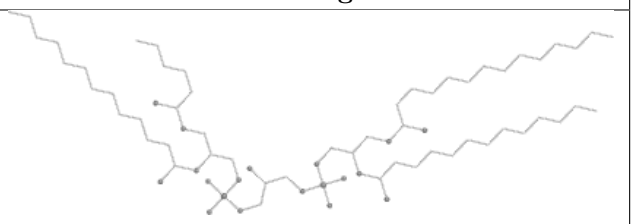
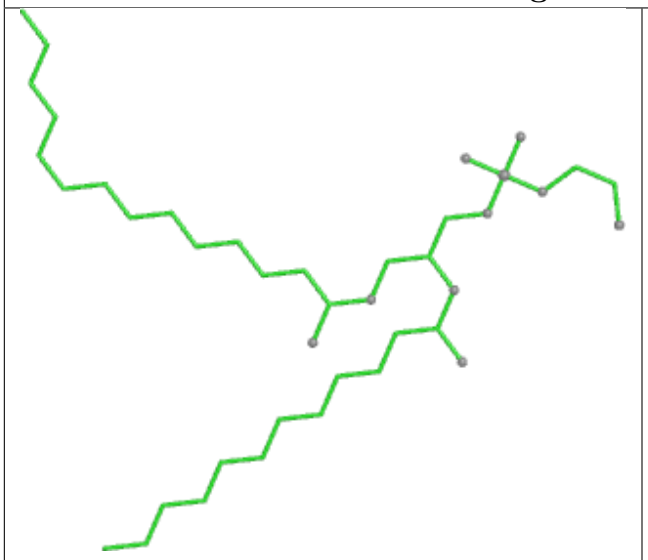
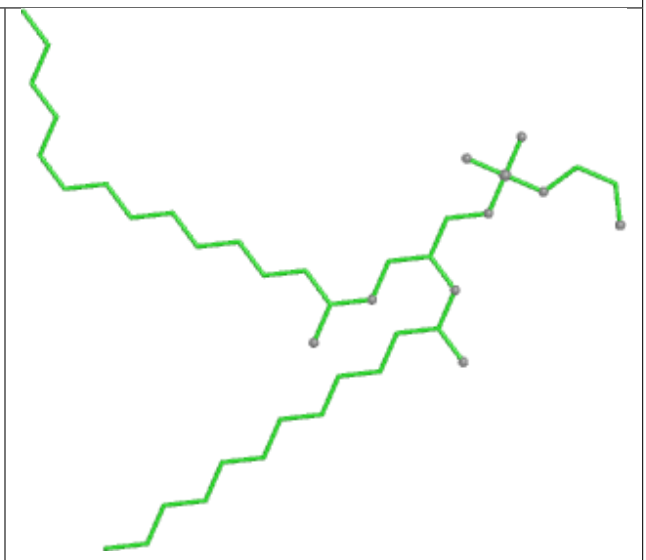
 Bond lengths	 Bond angles
 Torsions	 Rings

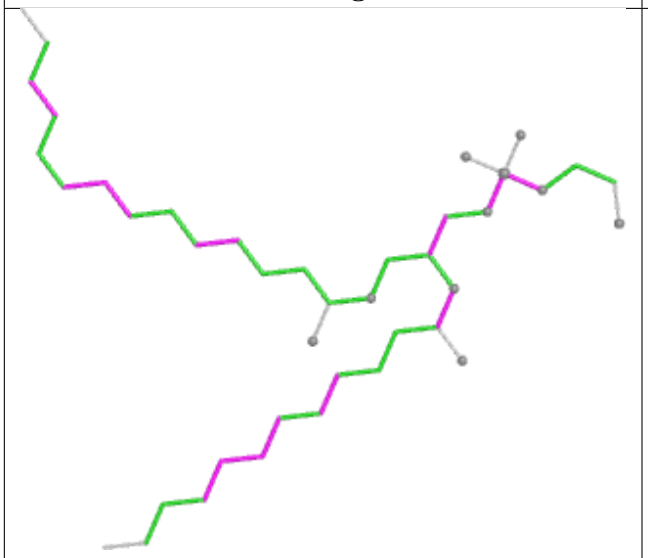
Ligand 9Y0 G 102



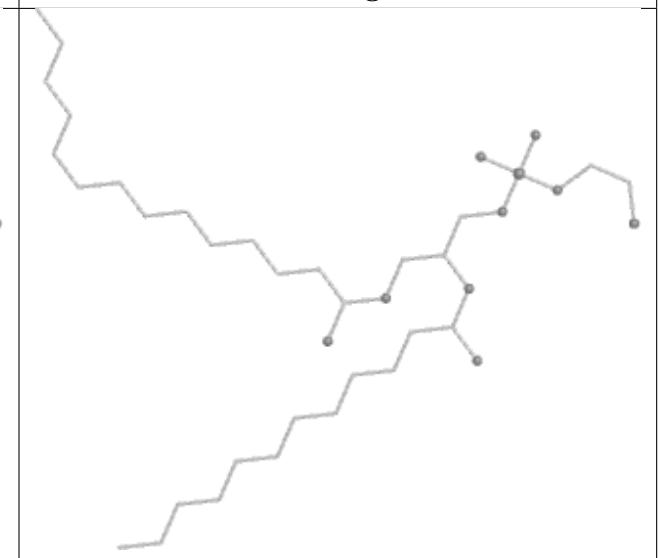
Bond lengths



Bond angles



Torsions

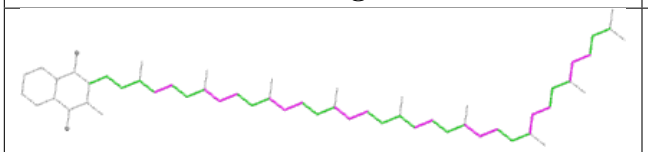


Rings

Ligand MQ9 U 603

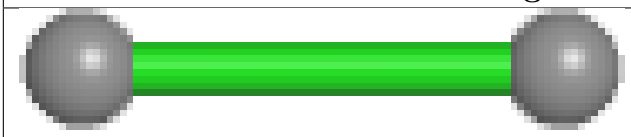
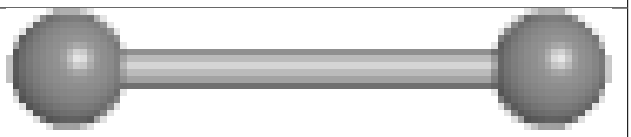
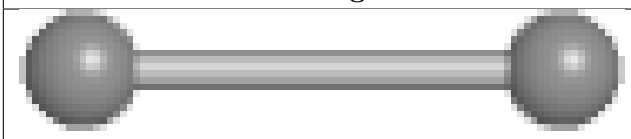
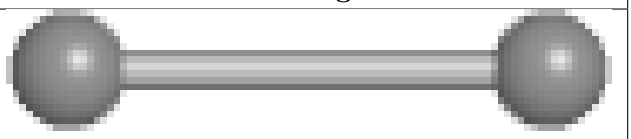
Bond lengths

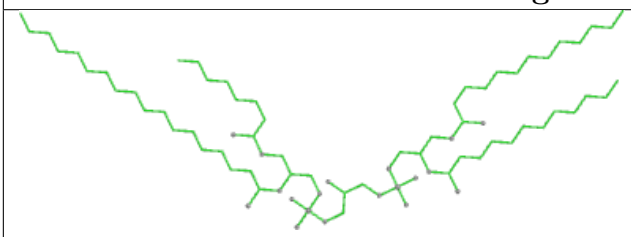
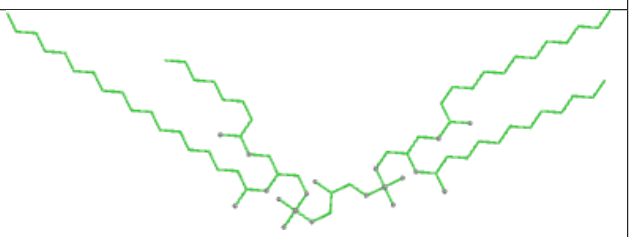
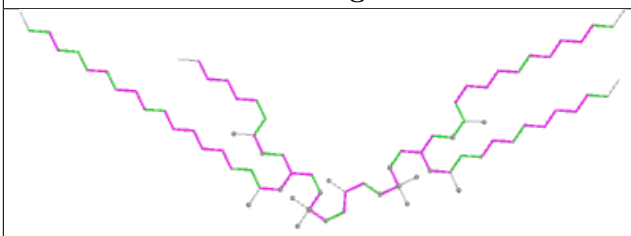
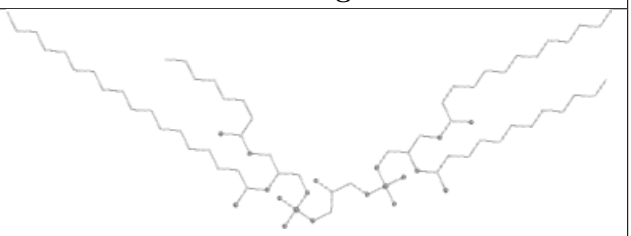
Bond angles



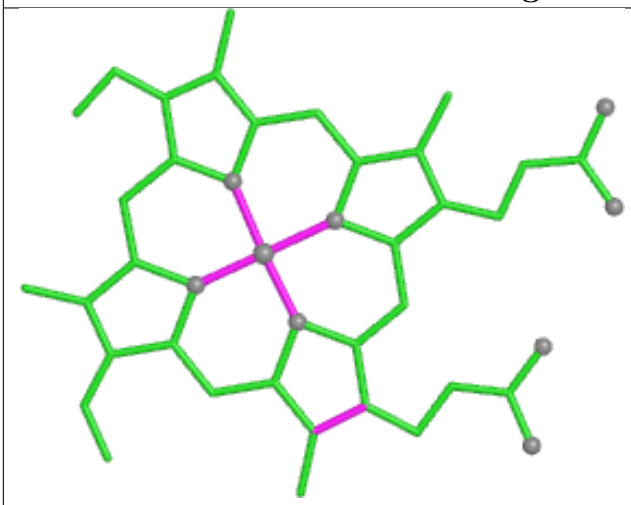
Torsions

Rings

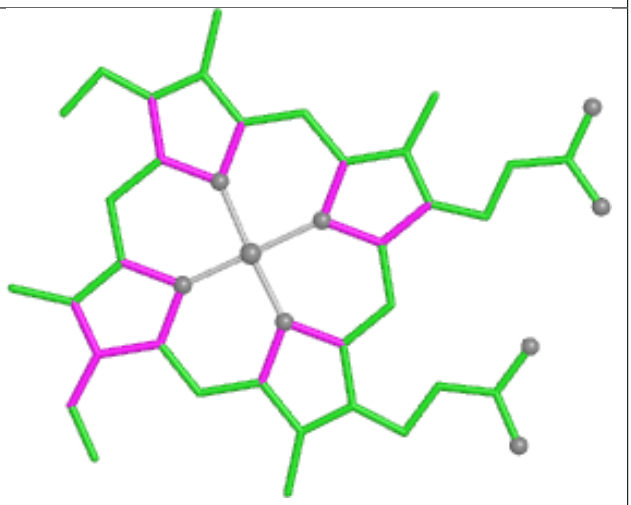
Ligand OXY L 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL i 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

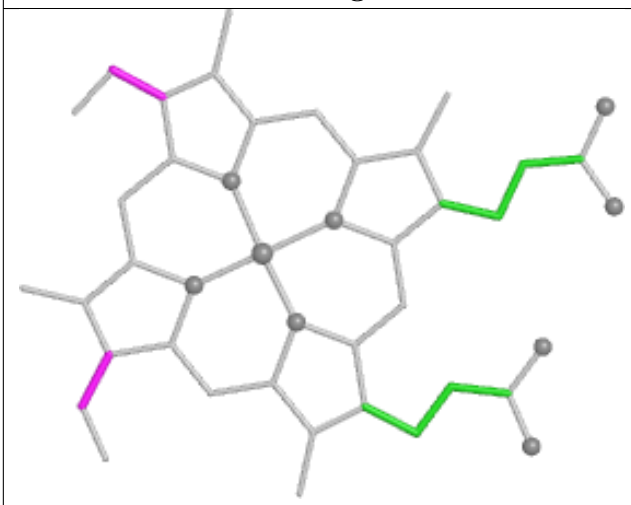
Ligand HEC U 602



Bond lengths



Bond angles



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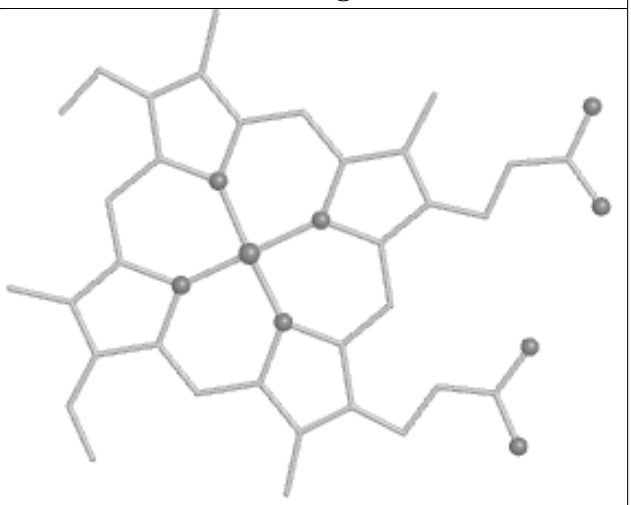
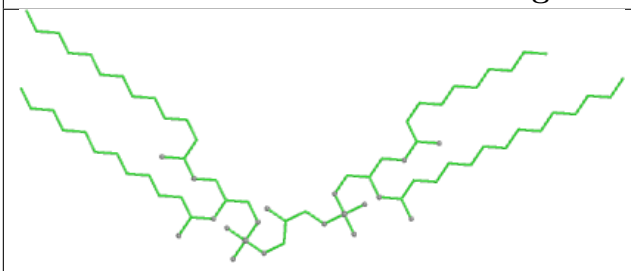


Rings

Ligand CDL i 607



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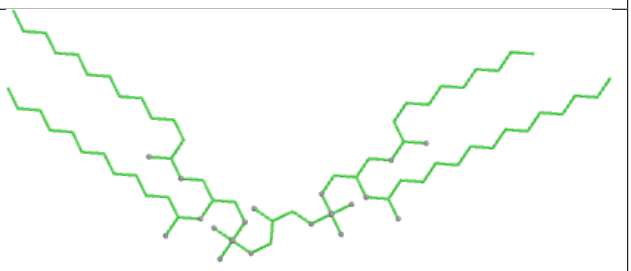
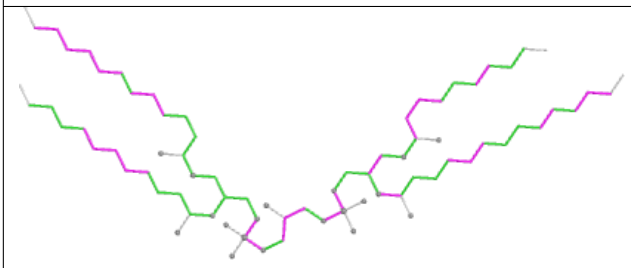


Bond angles



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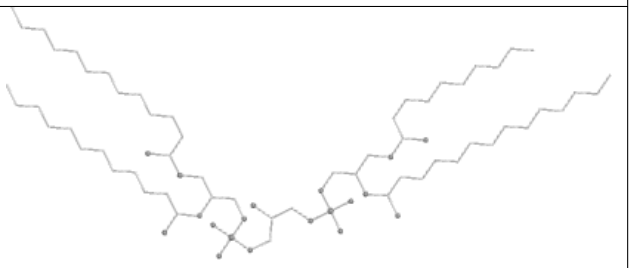
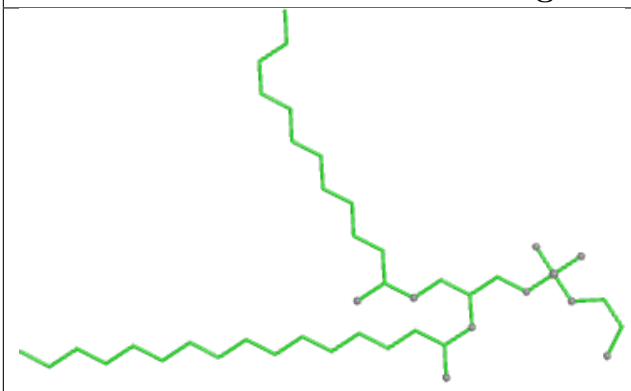


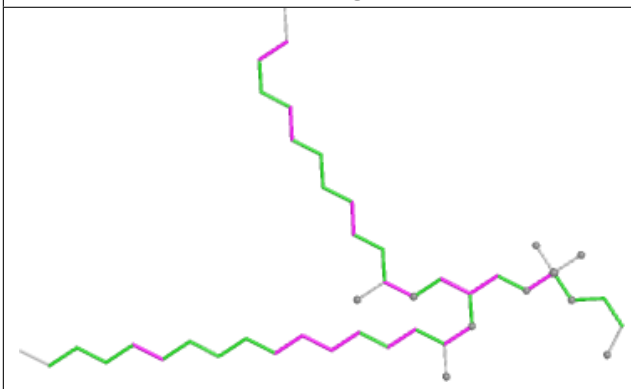
Rings

Ligand 9Y0 I 610



Bond lengths

Bond angles



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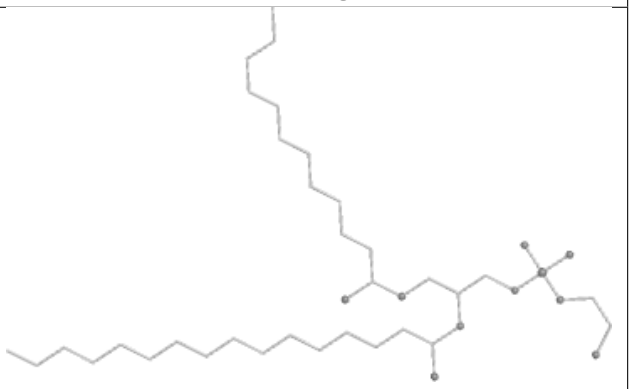
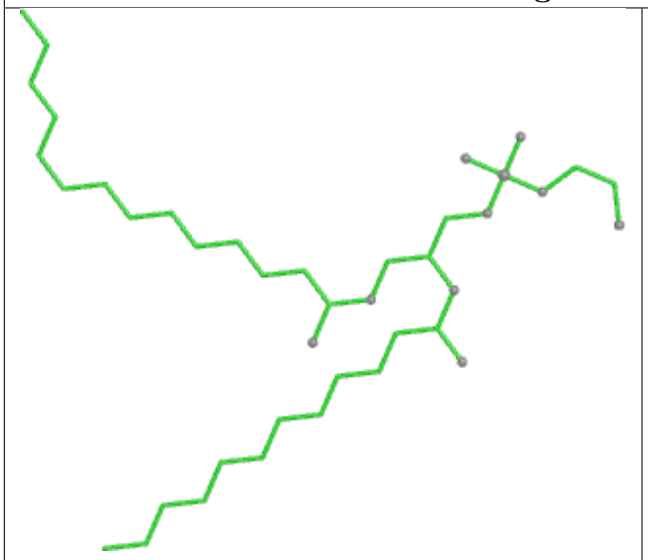


Rings

Ligand 9Y0 b 102



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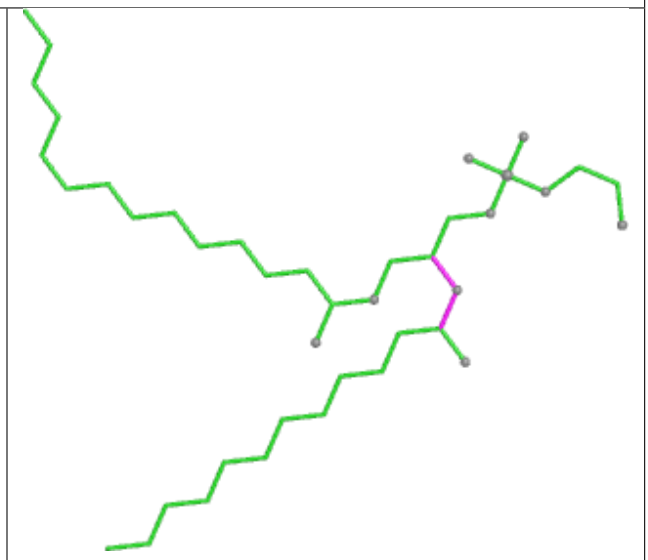
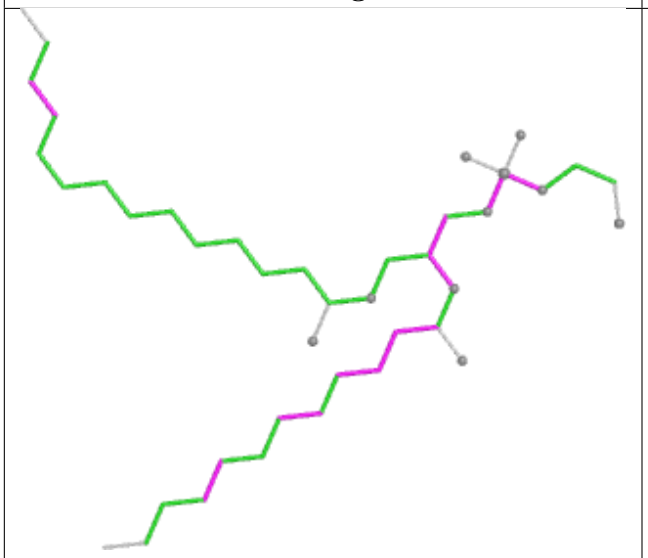


Bond angles



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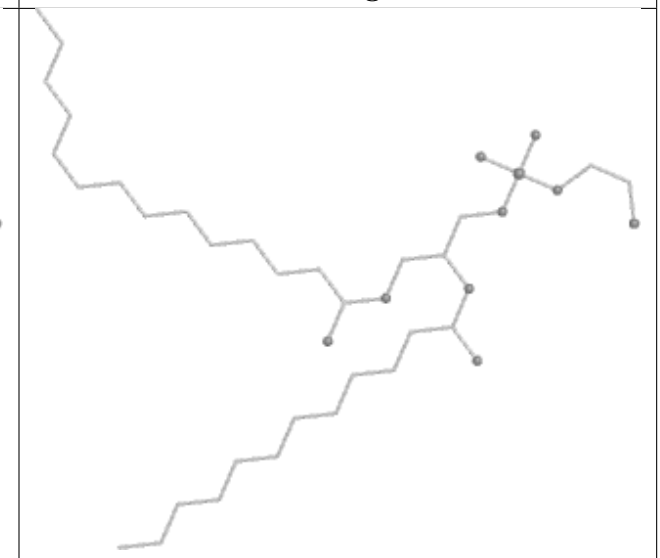
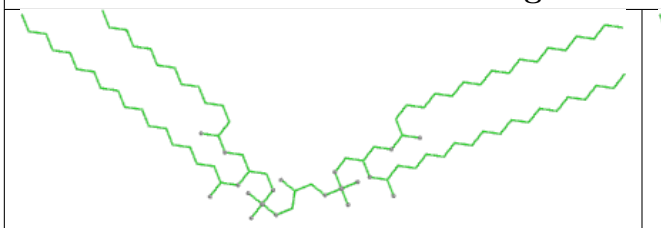


Rings

Ligand CDL V 602



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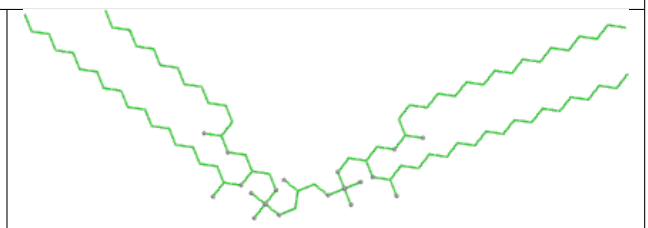
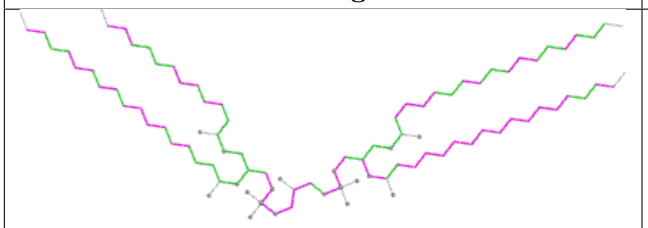


Bond angles



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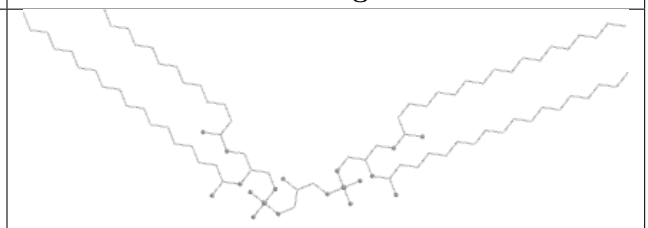
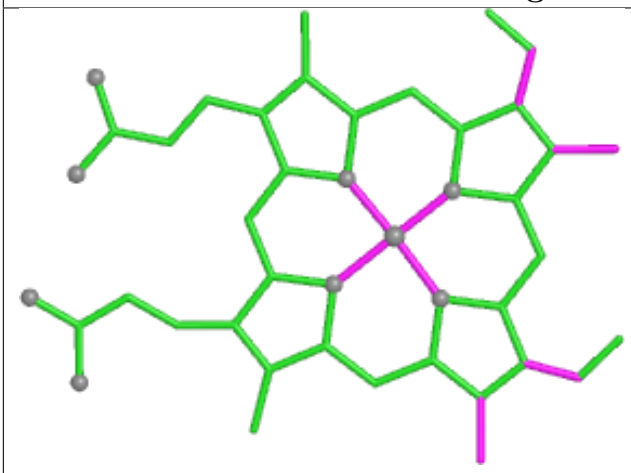
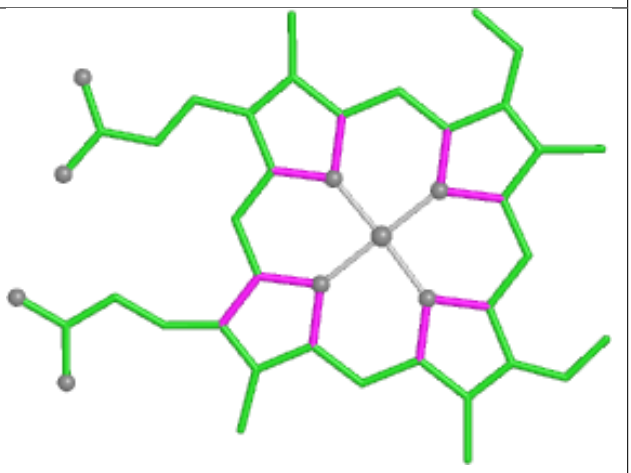
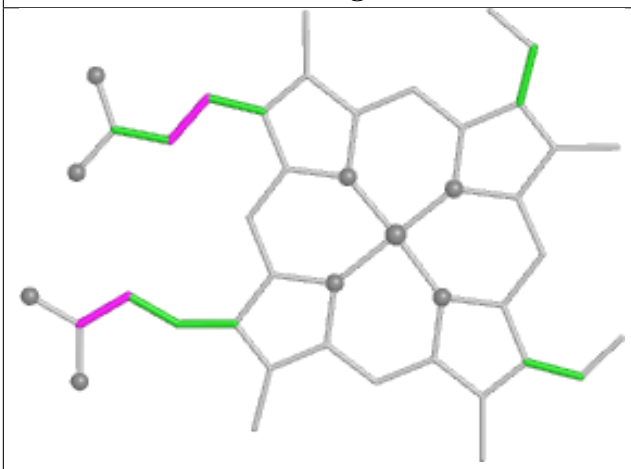
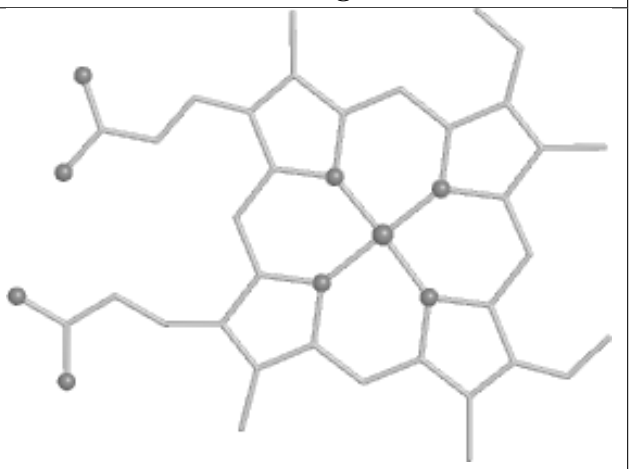
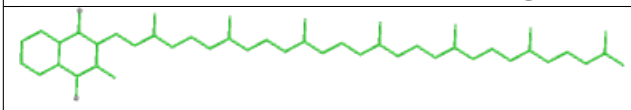
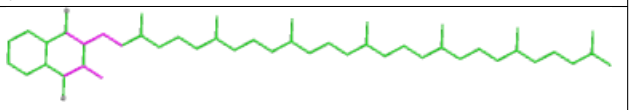
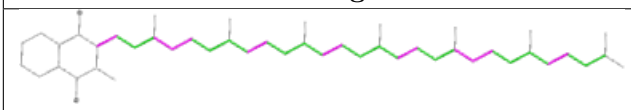
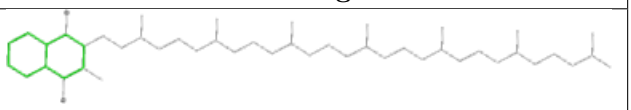
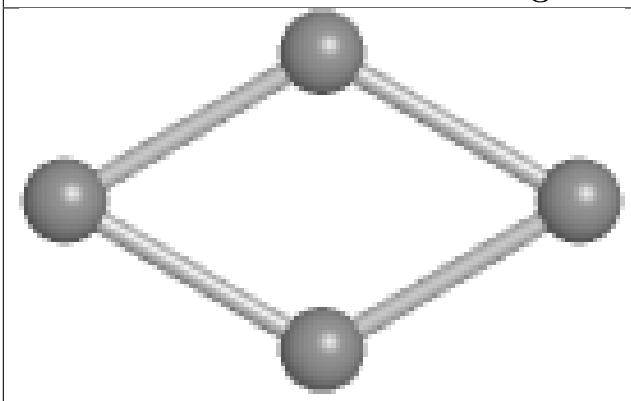


Rings

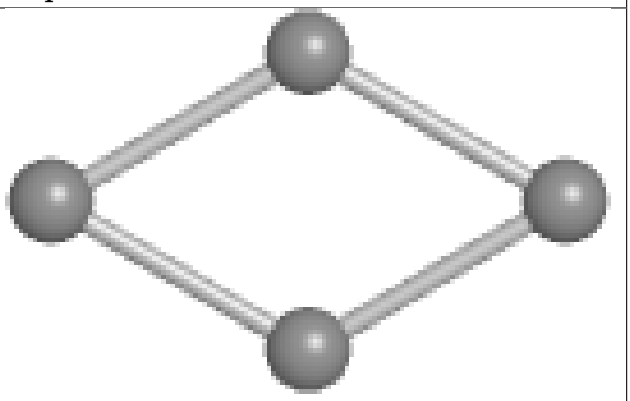
Ligand HEM i 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 m 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

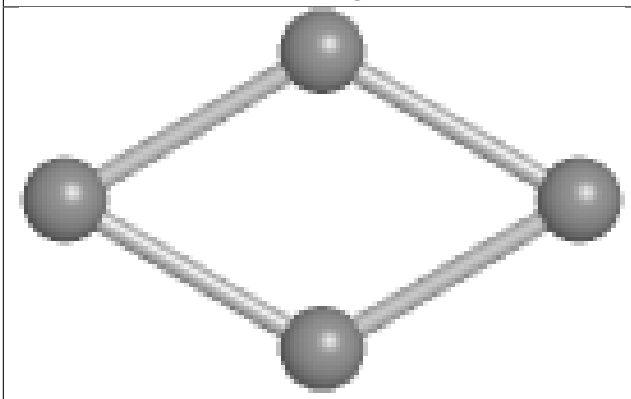
Ligand FES p 602



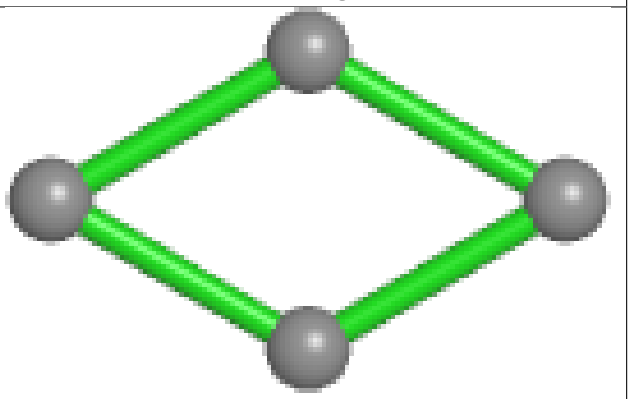
Bond lengths



Bond angles

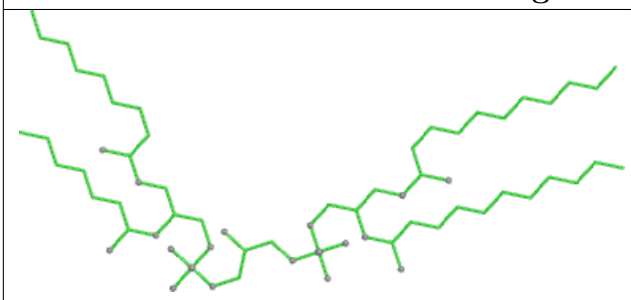


Torsions

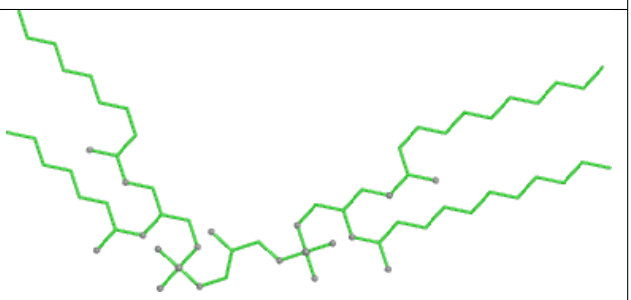


Rings

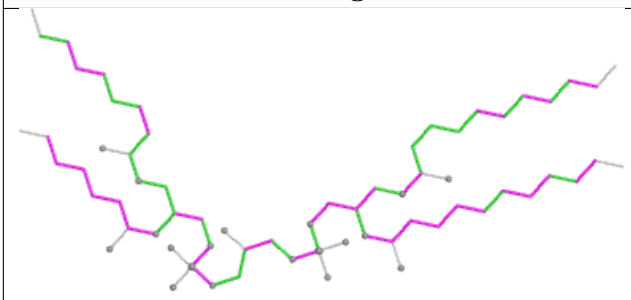
Ligand CDL i 603



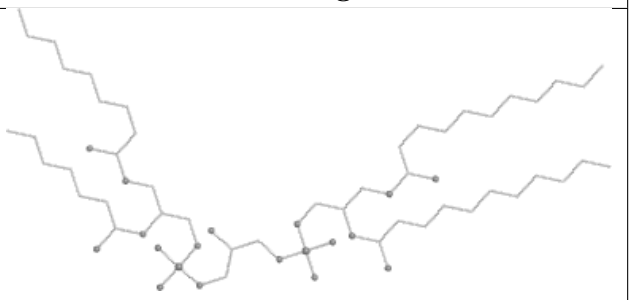
Bond lengths



Bond angles

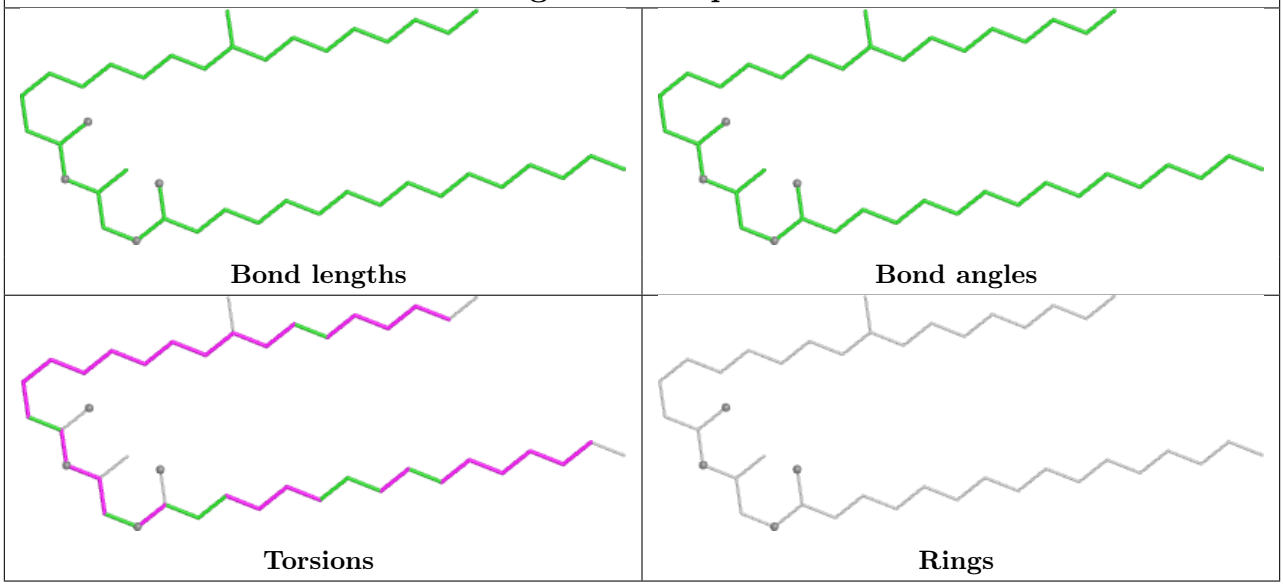


Torsions

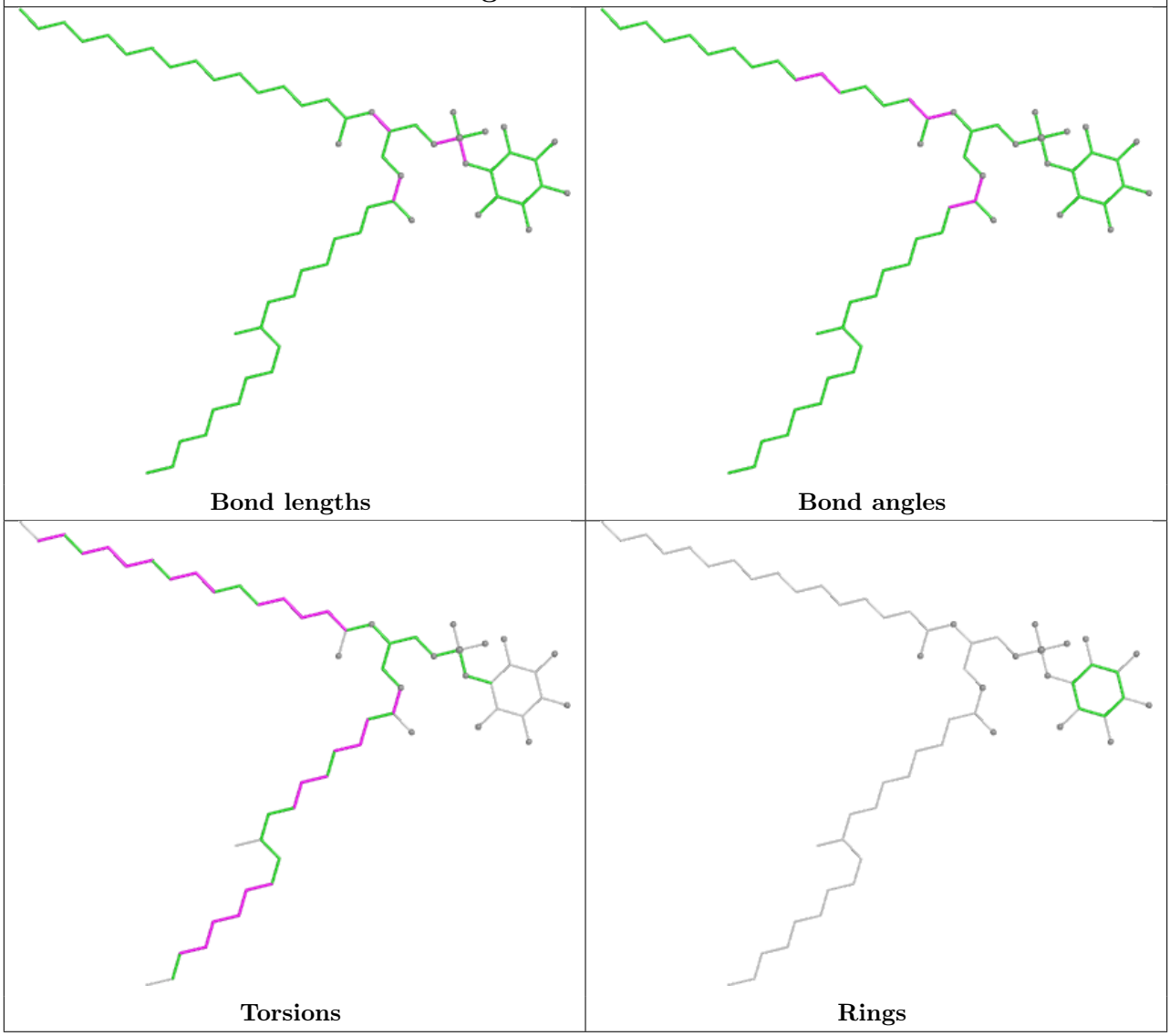


Rings

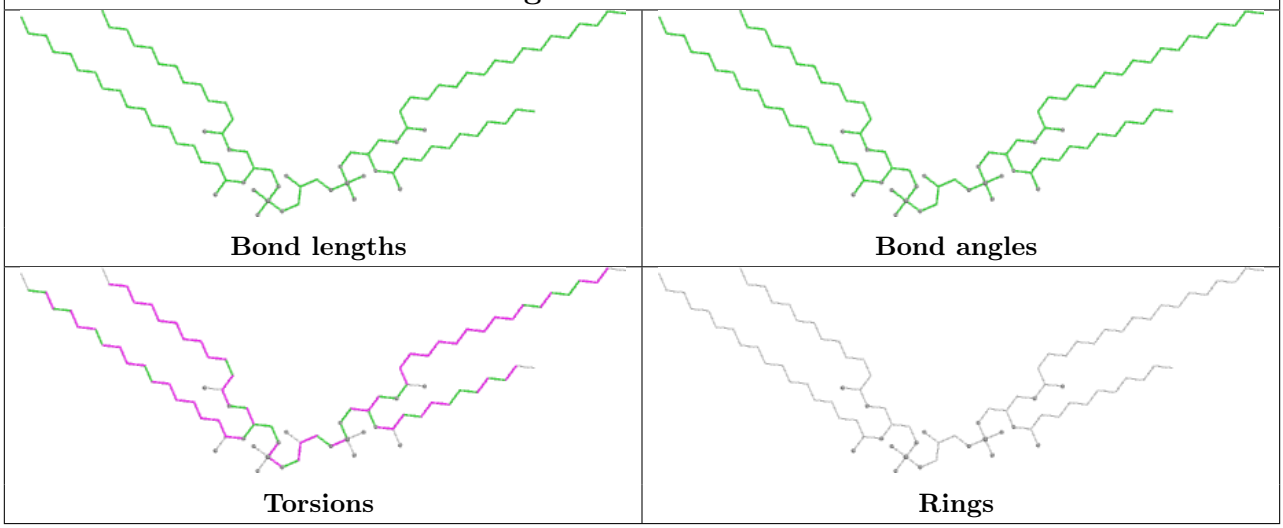
Ligand 9XX q 302



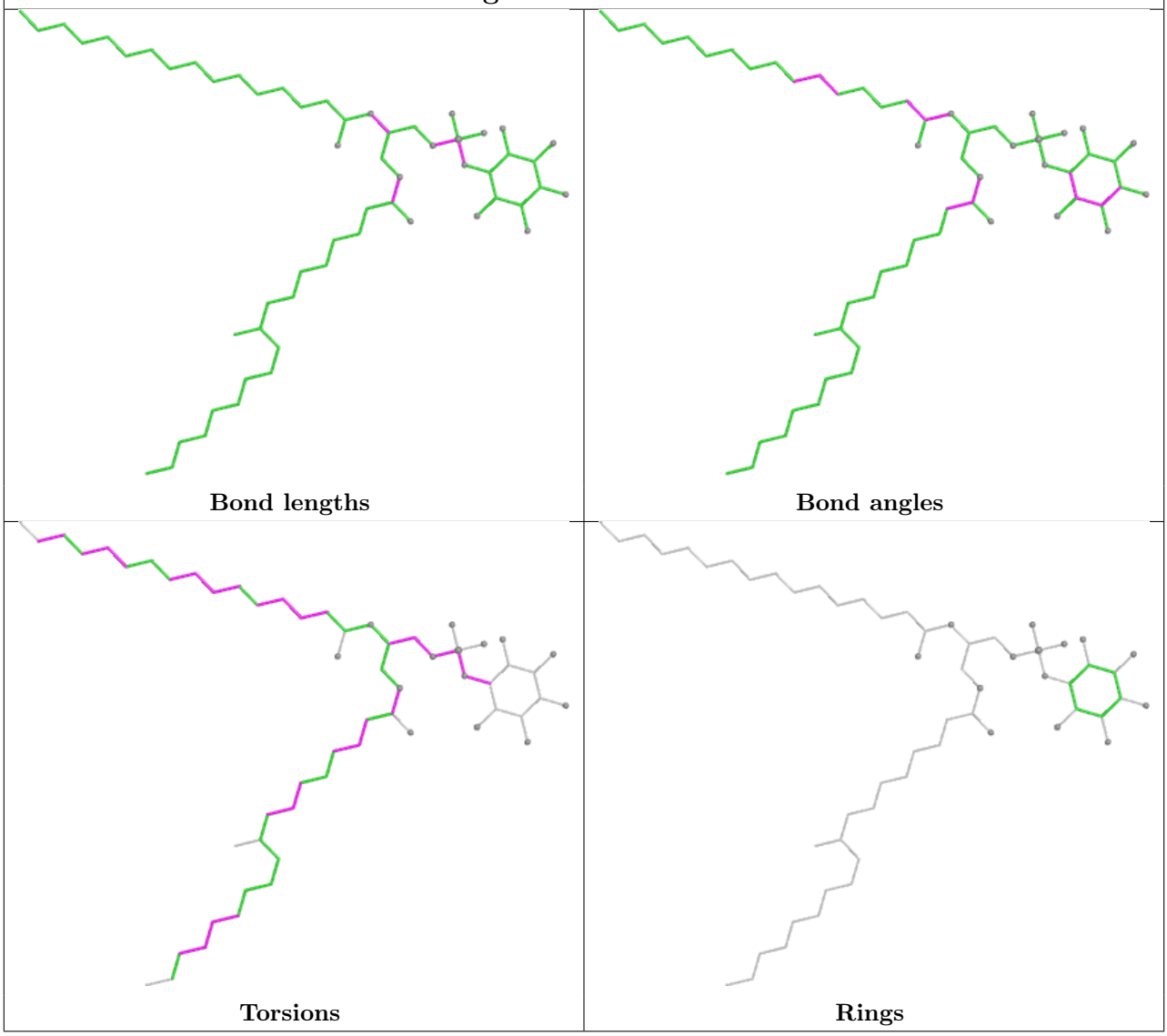
Ligand 9YF V 603



Ligand CDL G 101



Ligand 9YF L 609



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.

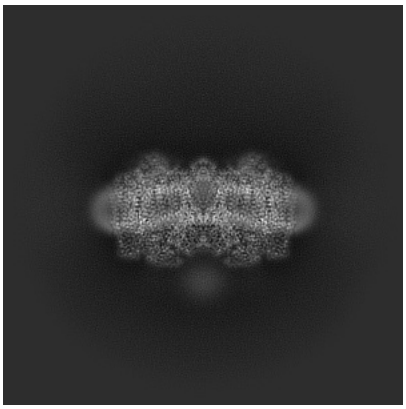
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-65879. These allow visual inspection of the internal detail of the map and identification of artifacts.

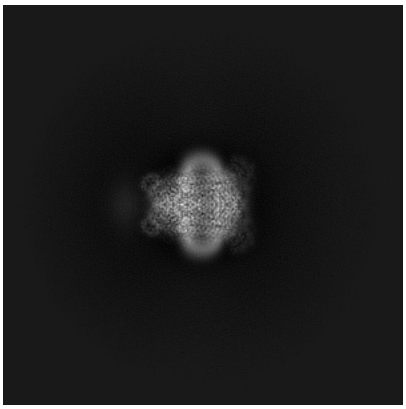
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

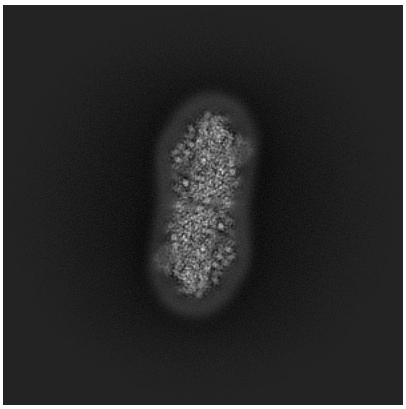
6.1.1 Primary map



X

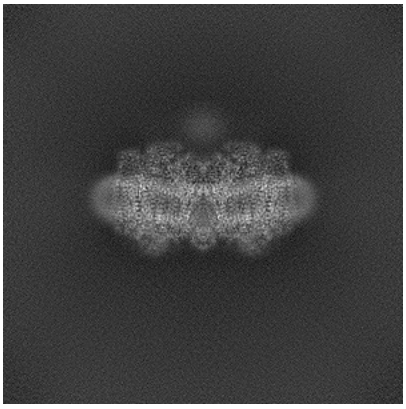


Y

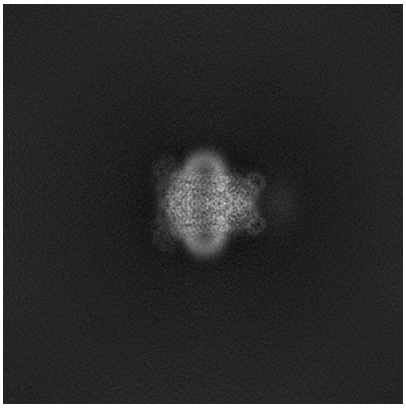


Z

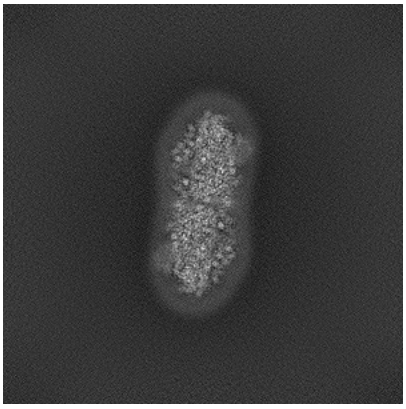
6.1.2 Raw map



X



Y

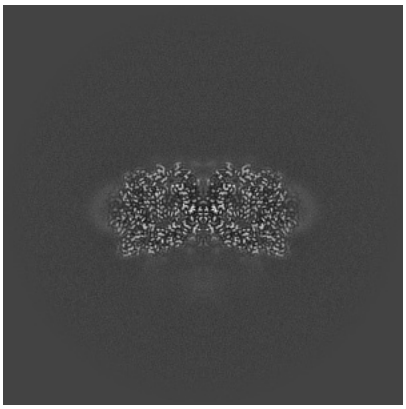


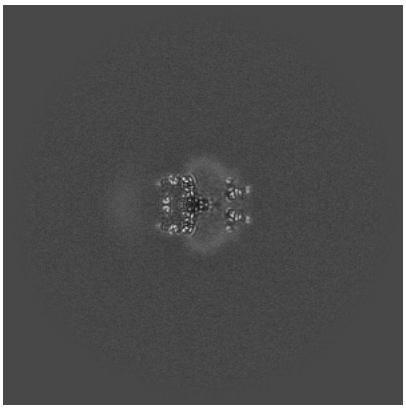
Z

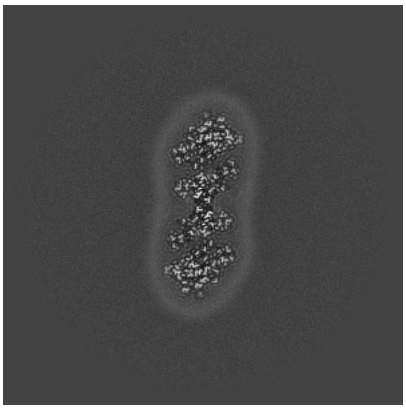
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

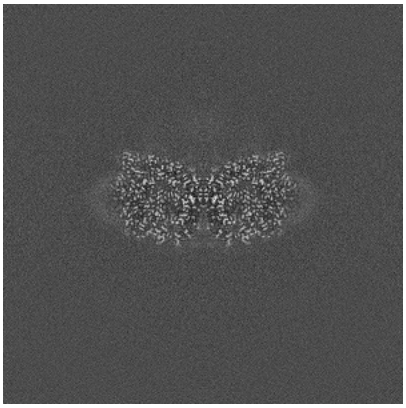
6.2.1 Primary map

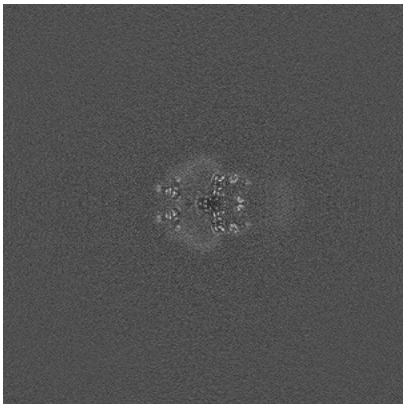

X Index: 300

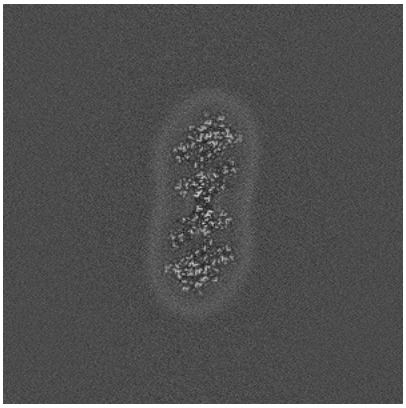

Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300

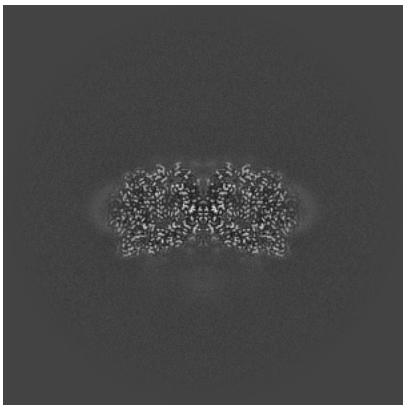

Y Index: 300


Z Index: 300

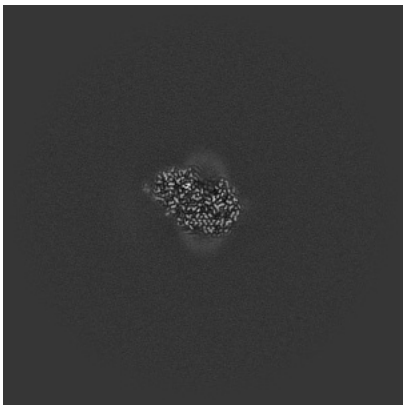
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

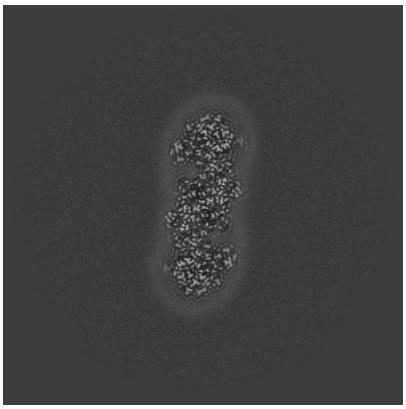
6.3.1 Primary map



X Index: 300

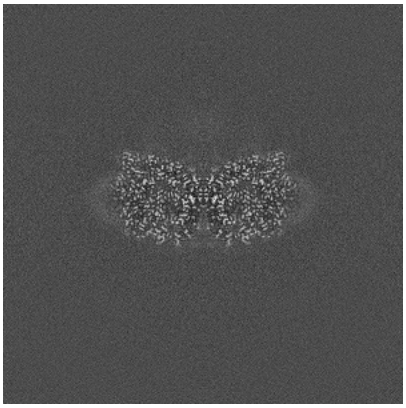


Y Index: 331

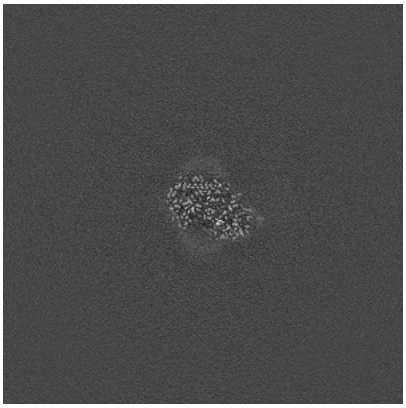


Z Index: 279

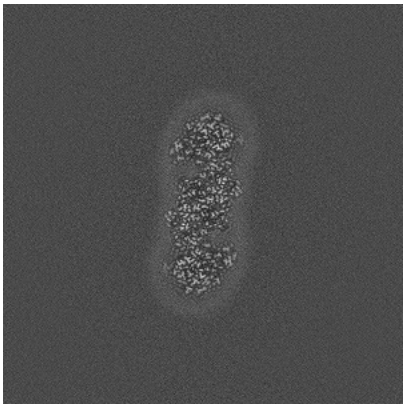
6.3.2 Raw map



X Index: 300



Y Index: 269

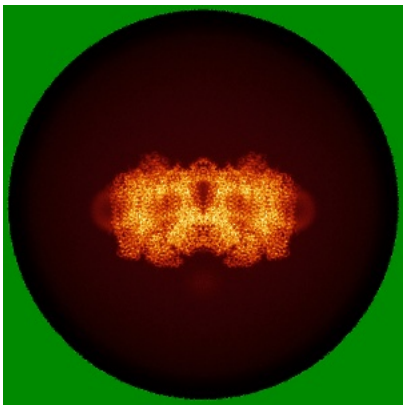


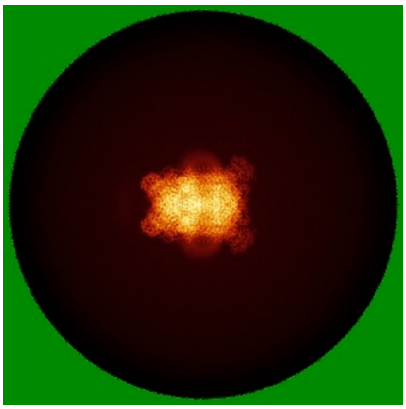
Z Index: 321

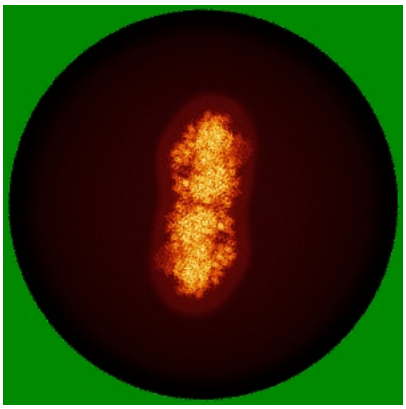
The images above show the largest variance slices of the map in three orthogonal directions.

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

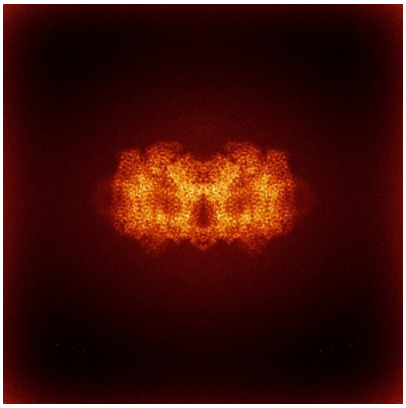
6.4.1 Primary map

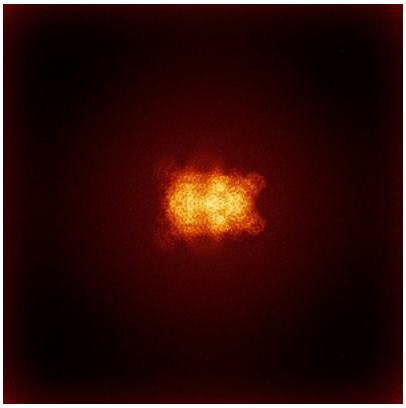

X

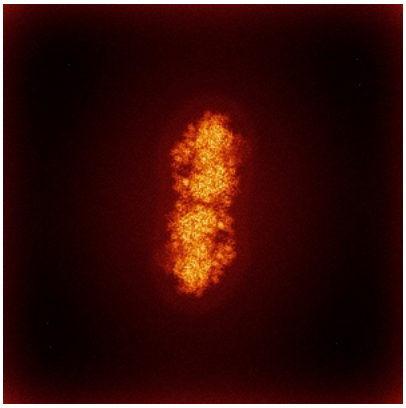

Y


Z

6.4.2 Raw map


X

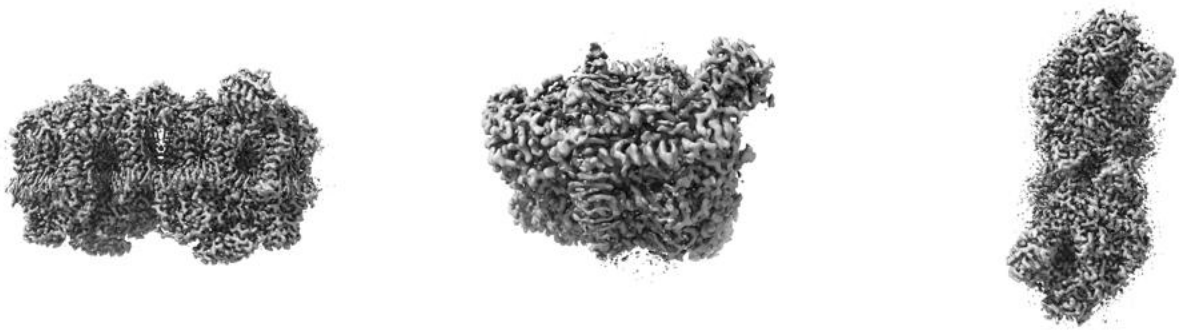

Y


Z

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

6.5 Orthogonal surface views (i)

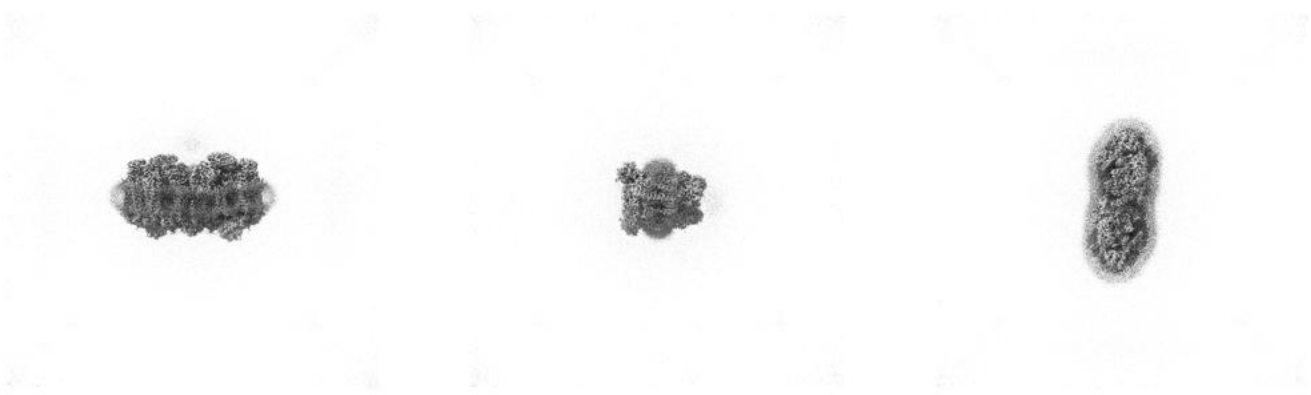
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0332. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

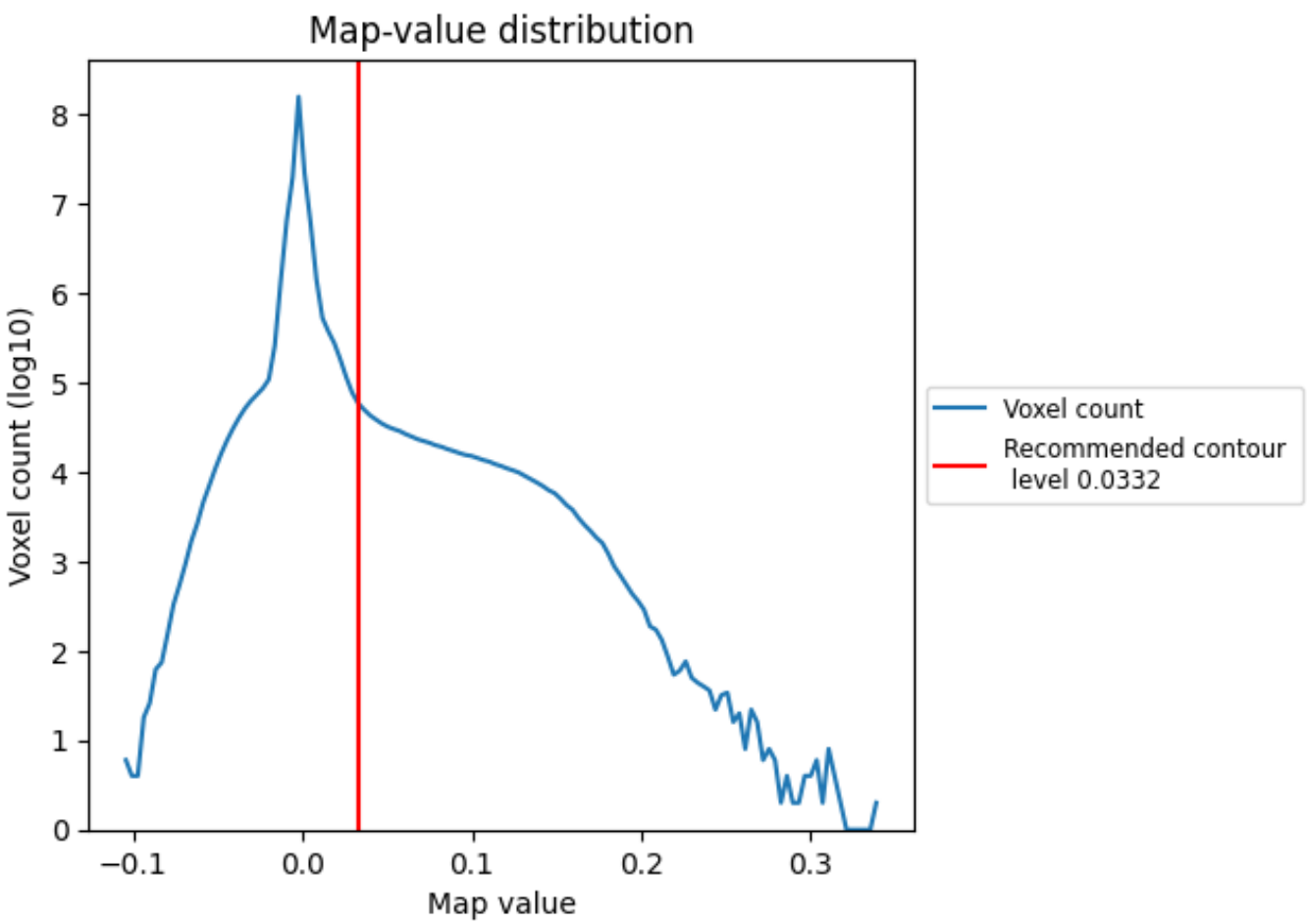
6.6 Mask visualisation (i)

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

7 Map analysis (i)

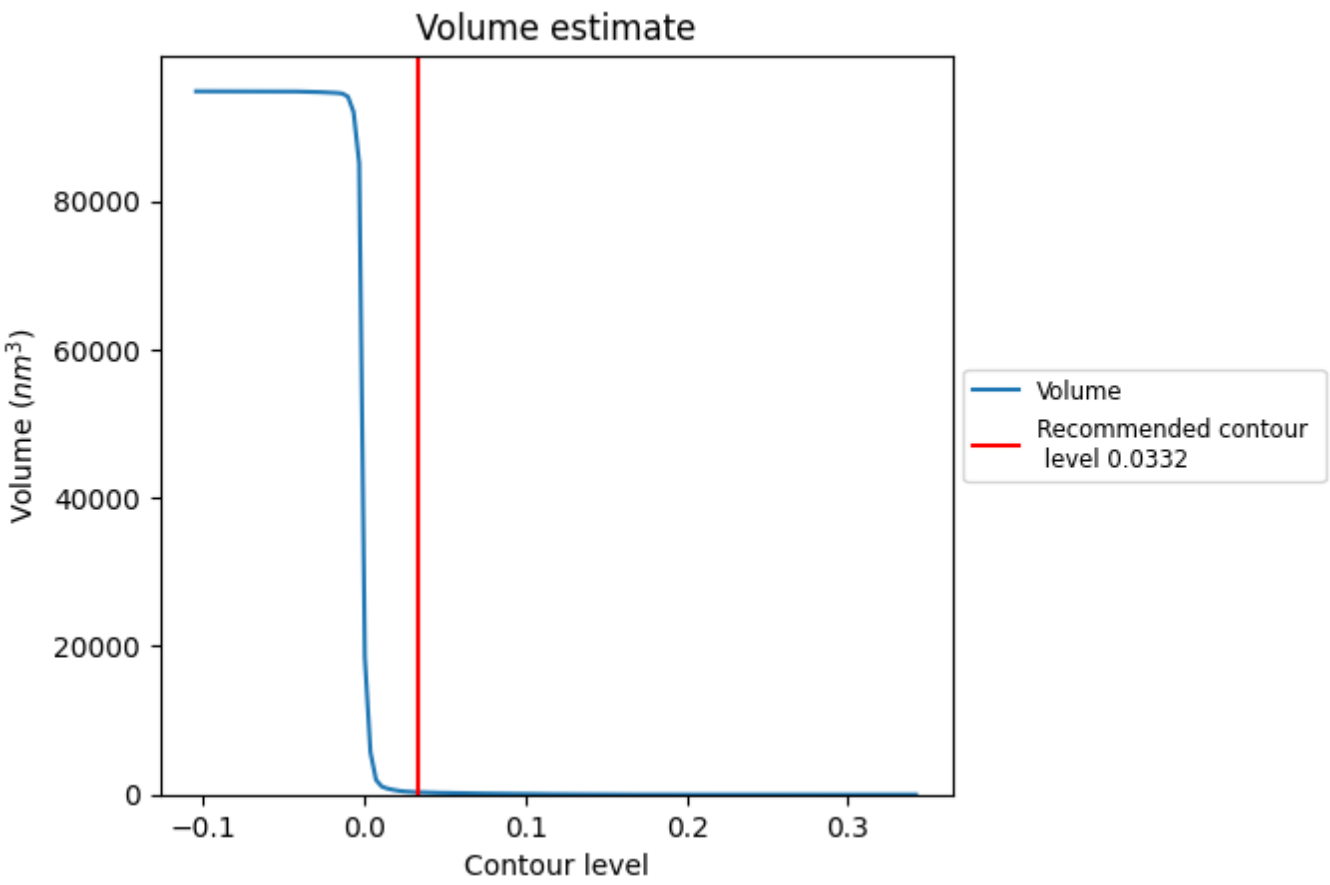
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

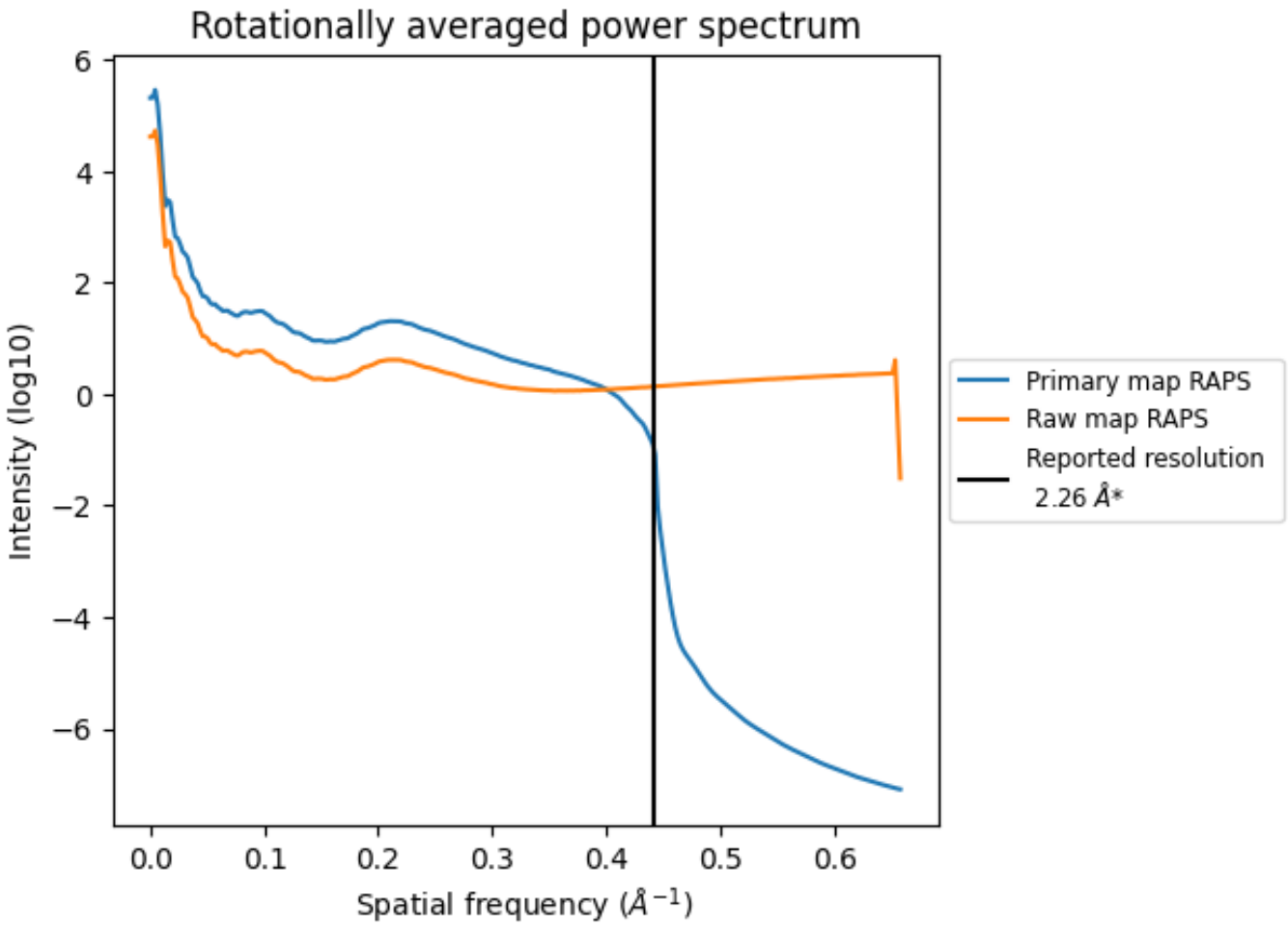
7.2 Volume estimate (i)



The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 285 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)

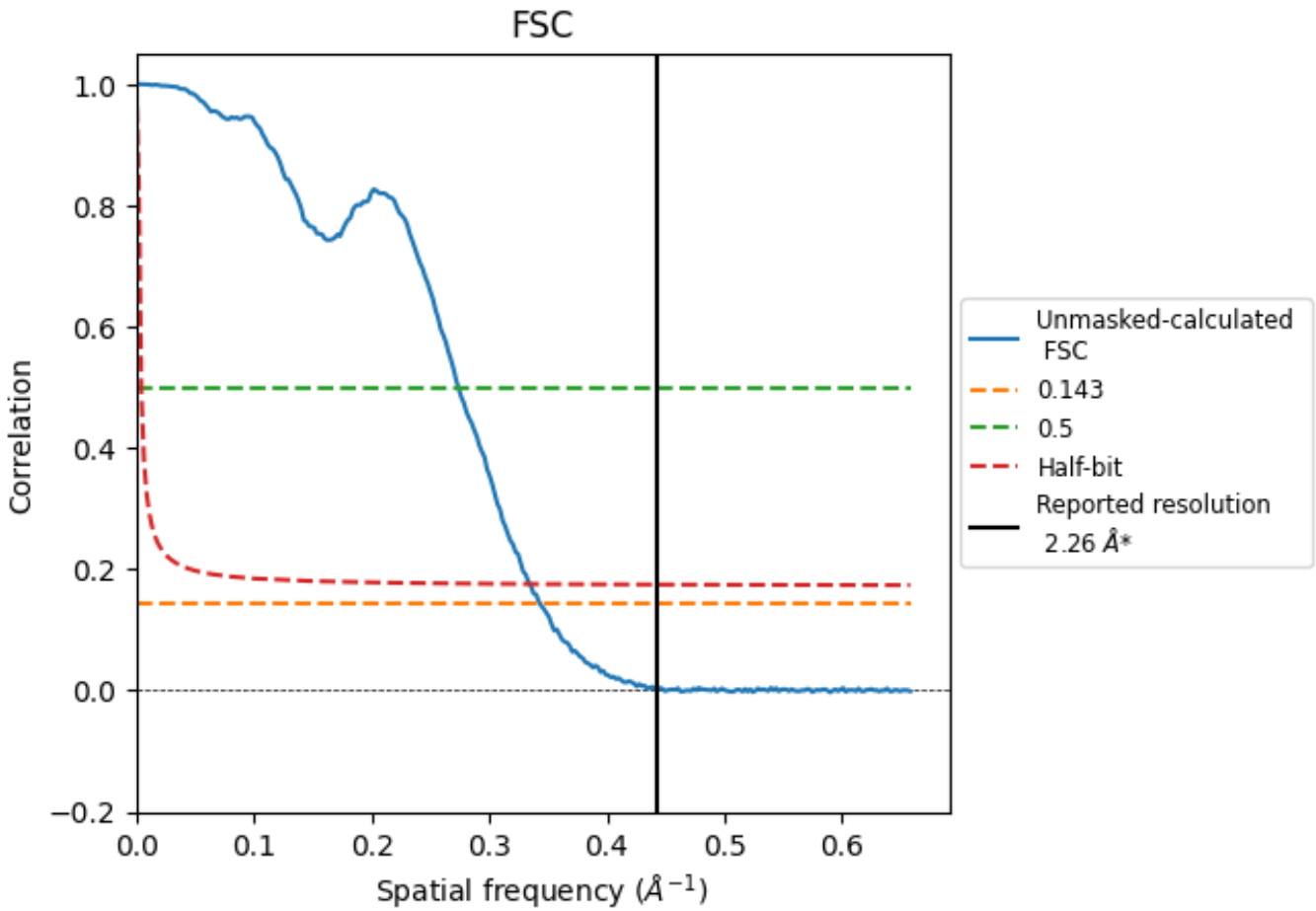


*Reported resolution corresponds to spatial frequency of 0.442 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.442 Å^{-1}

8.2 Resolution estimates (i)

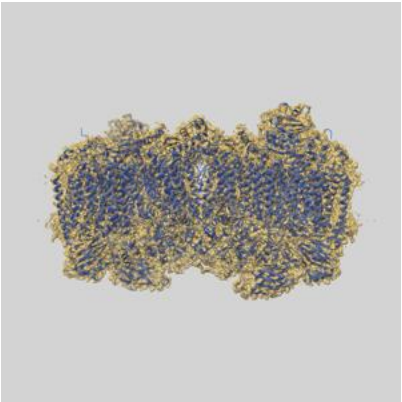
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.91	3.65	2.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.91 differs from the reported value 2.26 by more than 10 %

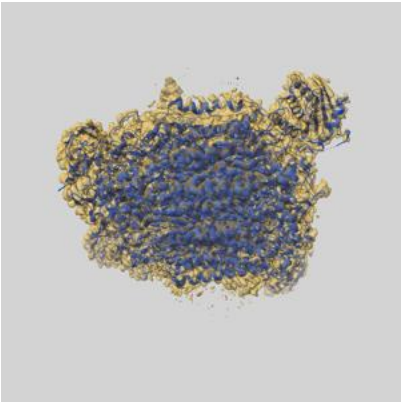
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-65879 and PDB model 9WCY. Per-residue inclusion information can be found in section 3 on page 18.

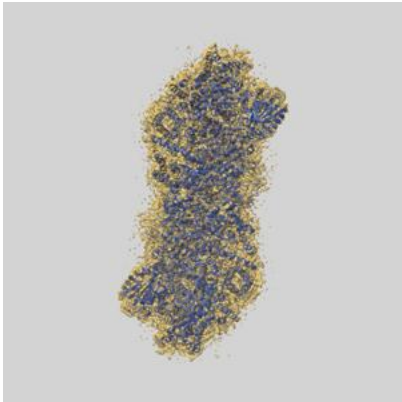
9.1 Map-model overlay (i)



X



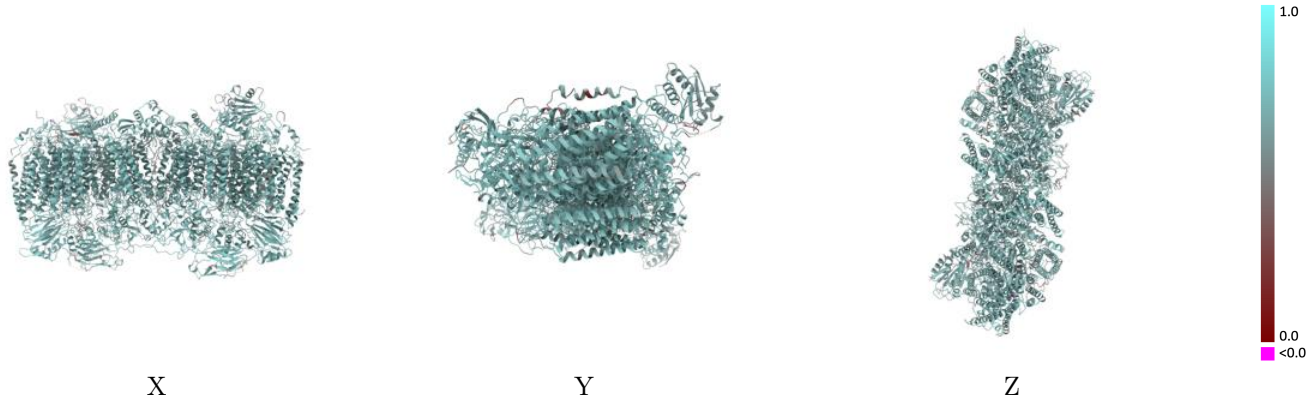
Y



Z

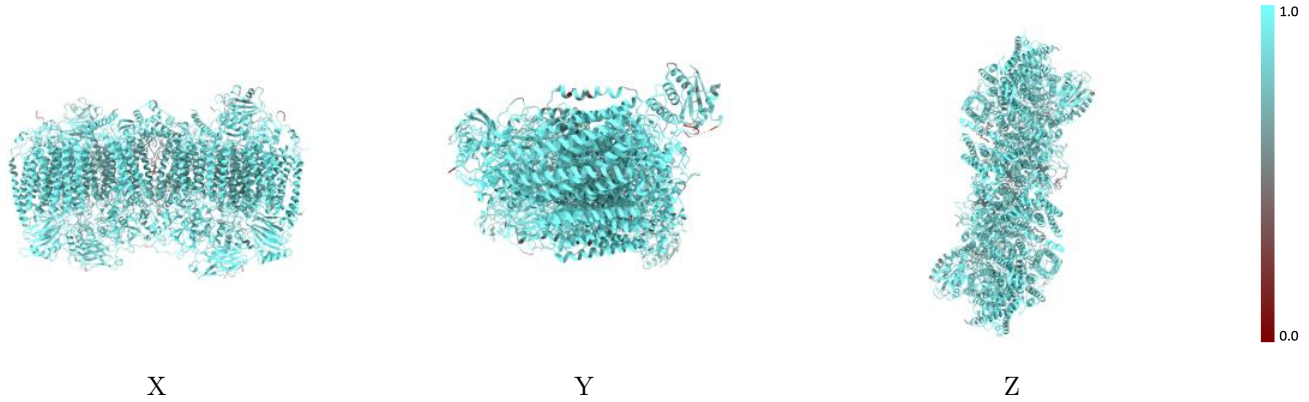
The images above show the 3D surface view of the map at the recommended contour level 0.0332 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



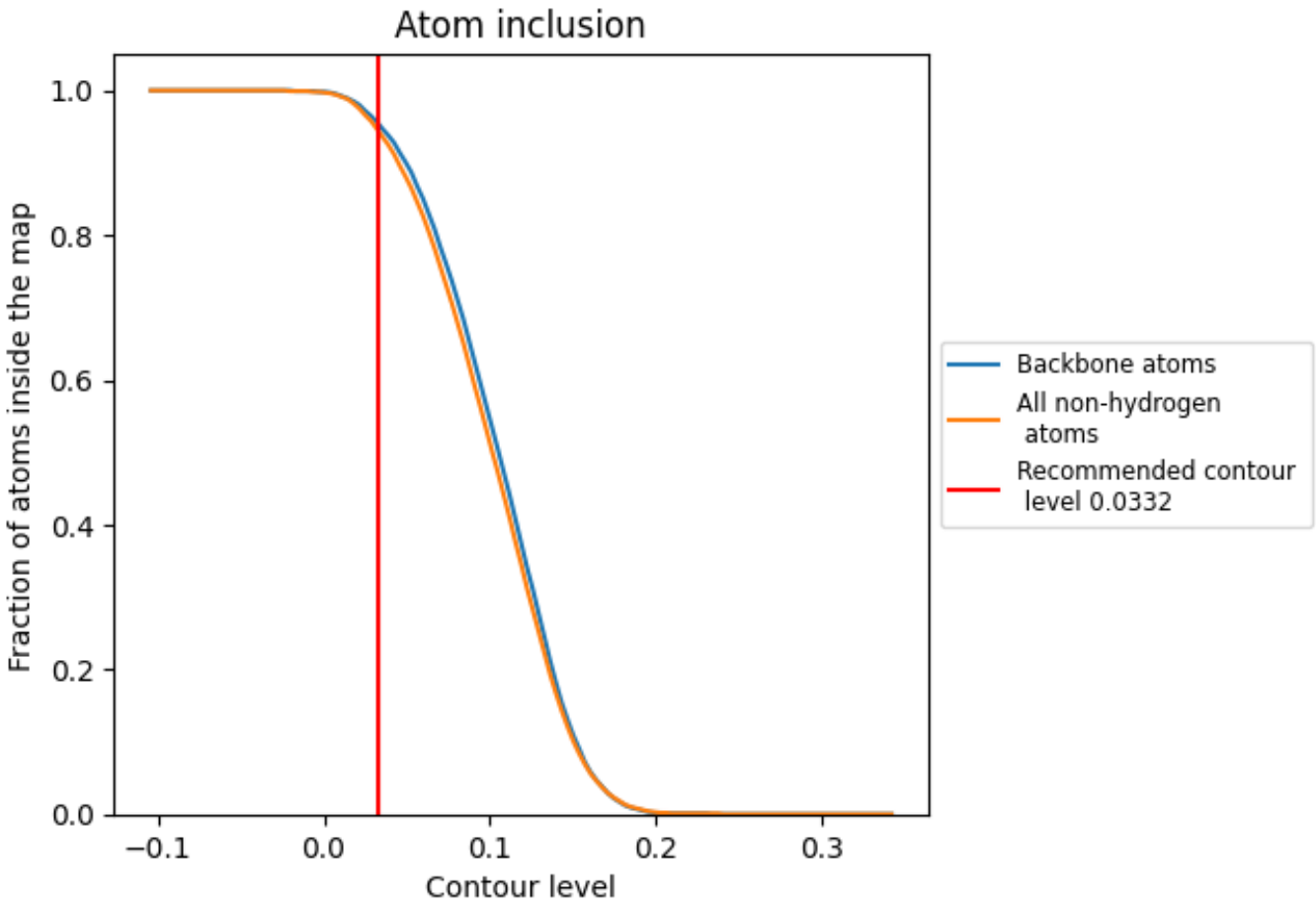
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0332).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0332) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9430	0.6610
G	0.9470	0.6630
I	0.9680	0.6730
J	0.8360	0.5880
L	0.9690	0.6720
U	0.9710	0.6830
V	0.9610	0.6780
X	0.8530	0.5900
a	0.8240	0.5880
b	0.9300	0.6490
d	0.9460	0.6560
e	0.9440	0.6590
f	0.9540	0.6410
g	0.9550	0.6420
h	0.8060	0.5750
i	0.9340	0.6660
j	0.9570	0.6740
k	0.8260	0.6020
l	0.8290	0.6050
m	0.9690	0.6630
n	0.9690	0.6610
o	0.9600	0.6800
p	0.9440	0.6700
q	0.9060	0.6440
r	0.9040	0.6310