wwPDB EM Validation Summary Report

Mar 5, 2022 – 06:47 am GMT

PDB ID	:	7Q21
EMDB ID	:	EMD-13777
Title	:	III2-IV2 respiratory supercomplex from Corynebacterium glutamicum
Authors	:	Kovalova, T.; Moe, A.; Krol, S.; Yanofsky, D.J.; Bott, M.; Sjostrand, D.; Rubinstein, J.L.; Hogbom, M.; Brzezinski, P.
Deposited on	:	2021-10-22
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

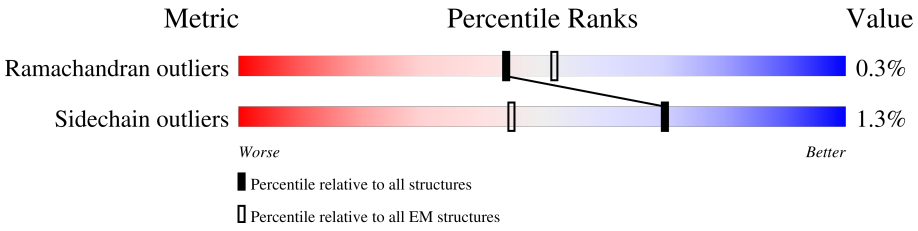
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	Y	96	100%
1	y	96	95% 5%
2	E	205	91% 8%
2	e	205	92% 8%
3	H	147	82% 15%
3	h	147	84% 14%
4	F	143	99%
4	f	143	99%
5	G	359	90% 9%

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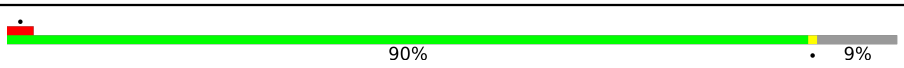
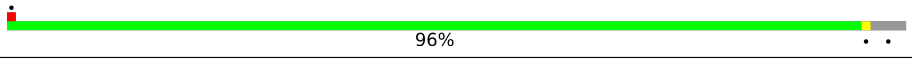
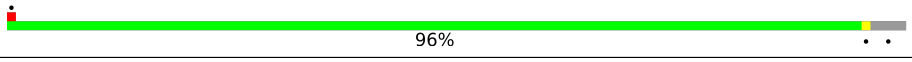
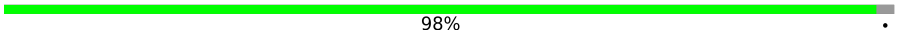
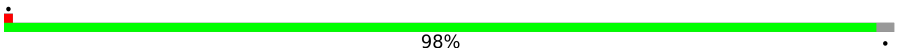
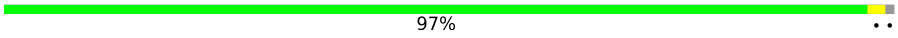
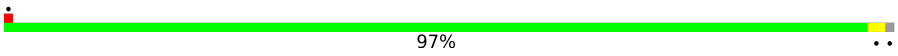
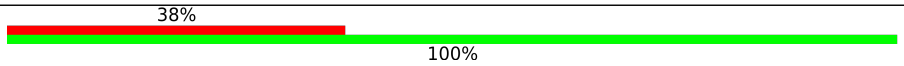
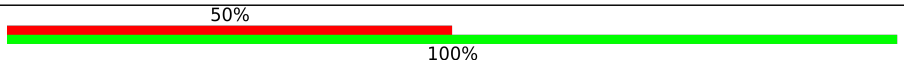
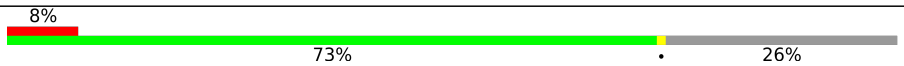
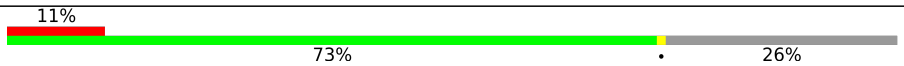
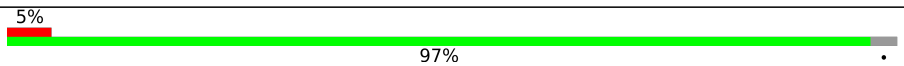
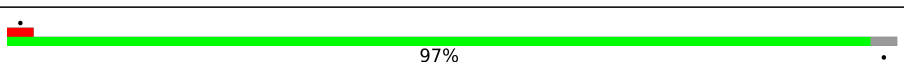
Mol	Chain	Length	Quality of chain
5	g	359	
6	D	594	
6	d	594	
7	A	408	
7	a	408	
8	L	194	
8	l	194	
9	B	539	
9	b	539	
10	C	283	
10	c	283	
11	X	21	
12	x	22	
13	V	73	
13	v	73	
14	K	65	
14	k	65	

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 47749 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 Co-purified unknown transmembrane helices built as polyALA (AscD).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Y	96	Total 480	C 288	N 96	O 96	0	0
1	y	91	Total 455	C 273	N 91	O 91	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	189	Total 1478	C 987	N 235	O 249	S 7	0	0
2	e	189	Total 1478	C 987	N 235	O 249	S 7	0	0

- Molecule 3 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	125	Total 994	C 643	N 173	O 177	S 1	0	0
3	h	126	Total 1003	C 648	N 174	O 180	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	143	Total 1094	C 728	N 167	O 190	S 9	0	0
4	f	143	Total 1094	C 728	N 167	O 190	S 9	0	0

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	325	Total	C	N	O	S	0	0
			2556	1637	422	487	10		
5	g	325	Total	C	N	O	S	0	0
			2556	1637	422	487	10		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	573	Total	C	N	O	S	0	0
			4532	3021	732	746	33		
6	d	573	Total	C	N	O	S	0	0
			4532	3021	732	746	33		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	585	ALA	-	expression tag	UNP Q79VD7
D	586	ALA	-	expression tag	UNP Q79VD7
D	587	TRP	-	expression tag	UNP Q79VD7
D	588	SER	-	expression tag	UNP Q79VD7
D	589	HIS	-	expression tag	UNP Q79VD7
D	590	PRO	-	expression tag	UNP Q79VD7
D	591	GLN	-	expression tag	UNP Q79VD7
D	592	PHE	-	expression tag	UNP Q79VD7
D	593	GLU	-	expression tag	UNP Q79VD7
D	594	LYS	-	expression tag	UNP Q79VD7
d	585	ALA	-	expression tag	UNP Q79VD7
d	586	ALA	-	expression tag	UNP Q79VD7
d	587	TRP	-	expression tag	UNP Q79VD7
d	588	SER	-	expression tag	UNP Q79VD7
d	589	HIS	-	expression tag	UNP Q79VD7
d	590	PRO	-	expression tag	UNP Q79VD7
d	591	GLN	-	expression tag	UNP Q79VD7
d	592	PHE	-	expression tag	UNP Q79VD7
d	593	GLU	-	expression tag	UNP Q79VD7
d	594	LYS	-	expression tag	UNP Q79VD7

- Molecule 7 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	400	Total	C	N	O	S	0	0
			3117	1987	532	582	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	400	Total	C	N	O	S	0	0
			3117	1987	532	582	16		

- Molecule 8 is a protein called Uncharacterized protein Cgl2664/cg2949.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	153	Total	C	N	O	S	0	0
			1120	684	184	249	3		
8	l	153	Total	C	N	O	S	0	0
			1120	684	184	249	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	534	Total	C	N	O	S	0	0
			4186	2745	704	716	21		
9	b	534	Total	C	N	O	S	0	0
			4186	2745	704	716	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	232	Total	C	N	O	S	0	0
			1729	1079	301	339	10		
10	c	232	Total	C	N	O	S	0	0
			1729	1079	301	339	10		

- Molecule 11 is a protein called Co-purified unknown peptide built as polyALA (AscE).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	21	Total	C	N	O	S	0	0
			106	63	21	21	1		

- Molecule 12 is a protein called Co-purified unknown peptide built as polyALA (AscE).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	x	22	Total	C	N	O	S	0	0
			111	66	22	22	1		

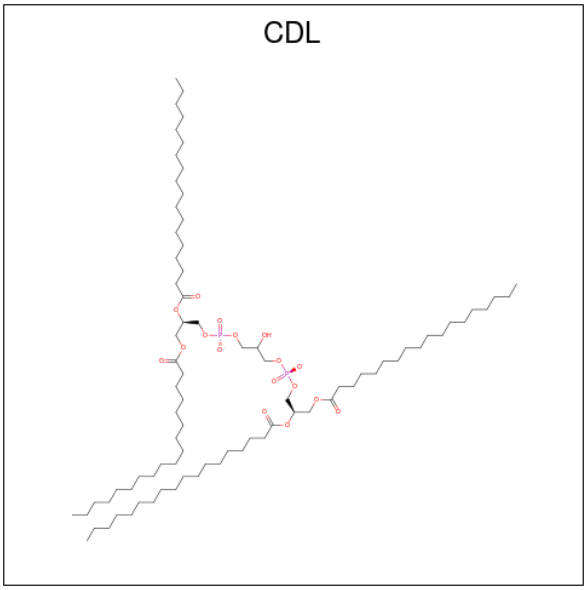
- Molecule 13 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms				AltConf	Trace
13	V	54	Total 420	C 268	N 69	O 83	0	0
13	v	54	Total 420	C 268	N 69	O 83	0	0

- Molecule 14 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	63	Total 444	C 294	N 70	O 77	S 3	0	0
14	k	63	Total 444	C 294	N 70	O 77	S 3	0	0

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



Mol	Chain	Residues	Atoms				AltConf
15	E	1	Total 66	C 47	O 17	P 2	0
15	F	1	Total 79	C 60	O 17	P 2	0
15	D	1	Total 153	C 115	O 34	P 4	0
15	D	1	Total 153	C 115	O 34	P 4	0
15	B	1	Total 151	C 113	O 34	P 4	0
15	B	1	Total 151	C 113	O 34	P 4	0

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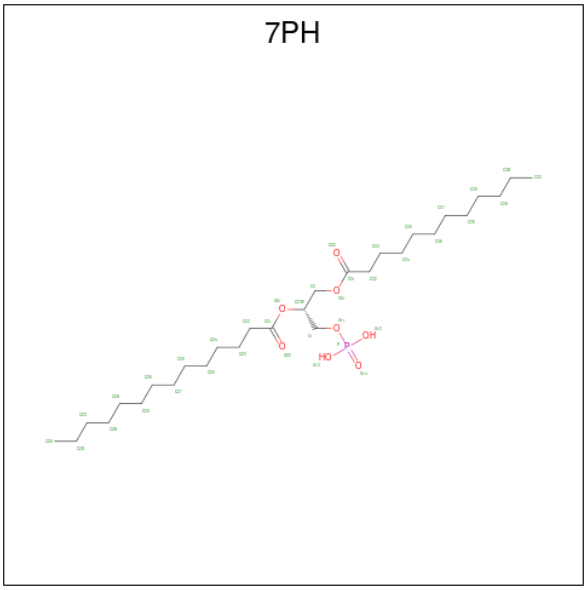
Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total	C	O	P	0
			79	60	17	2	
15	e	1	Total	C	O	P	0
			66	47	17	2	
15	f	1	Total	C	O	P	0
			79	60	17	2	
15	d	1	Total	C	O	P	0
			145	107	34	4	
15	d	1	Total	C	O	P	0
			145	107	34	4	
15	b	1	Total	C	O	P	0
			151	113	34	4	
15	b	1	Total	C	O	P	0
			151	113	34	4	
15	c	1	Total	C	O	P	0
			79	60	17	2	

- Molecule 16 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
16	E	1	Total	C	O	P	0
			38	29	8	1	
16	H	1	Total	C	O	P	0
			38	29	8	1	
16	F	1	Total	C	O	P	0
			38	29	8	1	

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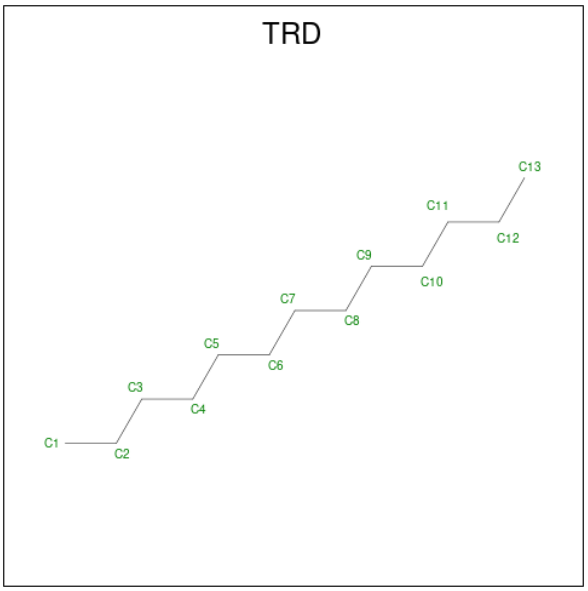
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			38	29	8	1	
16	D	1	Total	C	O	P	0
			152	116	32	4	
16	D	1	Total	C	O	P	0
			152	116	32	4	
16	D	1	Total	C	O	P	0
			152	116	32	4	
16	D	1	Total	C	O	P	0
			152	116	32	4	
16	e	1	Total	C	O	P	0
			38	29	8	1	
16	h	1	Total	C	O	P	0
			38	29	8	1	
16	f	1	Total	C	O	P	0
			38	29	8	1	
16	g	1	Total	C	O	P	0
			38	29	8	1	
16	d	1	Total	C	O	P	0
			114	87	24	3	
16	d	1	Total	C	O	P	0
			114	87	24	3	
16	d	1	Total	C	O	P	0
			114	87	24	3	
16	k	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 17 is TRIDECANE (three-letter code: TRD) (formula: $C_{13}H_{28}$).



Mol	Chain	Residues	Atoms	AltConf
17	E	1	Total C 13 13	0
17	F	1	Total C 65 65	0
17	F	1	Total C 65 65	0
17	F	1	Total C 65 65	0
17	F	1	Total C 65 65	0
17	F	1	Total C 65 65	0
17	A	1	Total C 39 39	0
17	A	1	Total C 39 39	0
17	A	1	Total C 39 39	0
17	B	1	Total C 13 13	0
17	e	1	Total C 13 13	0
17	f	1	Total C 65 65	0
17	f	1	Total C 65 65	0
17	f	1	Total C 65 65	0

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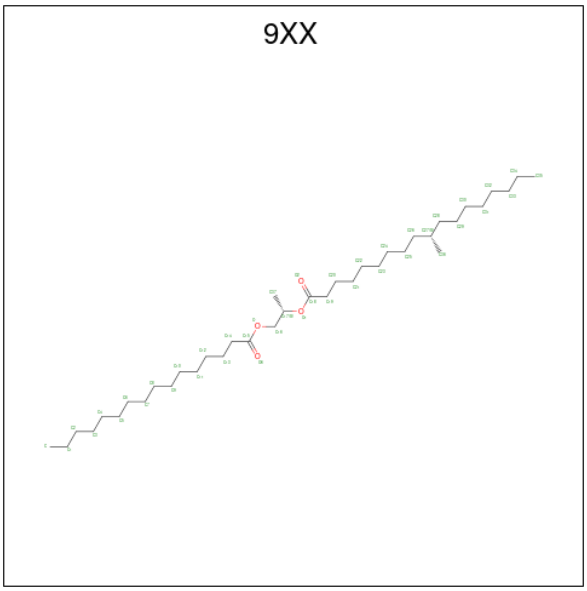
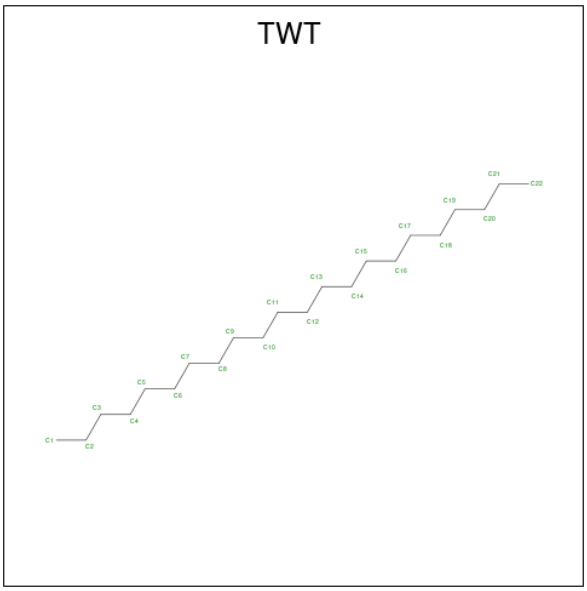
Mol	Chain	Residues	Atoms	AltConf
17	f	1	Total C 65 65	0
17	f	1	Total C 65 65	0
17	a	1	Total C 13 13	0
17	b	1	Total C 13 13	0

- Molecule 18 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (three-letter code: 9XX) (formula: $C_{38}H_{74}O_4$).



Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C O 32 28 4	0
18	B	1	Total C O 32 28 4	0
18	h	1	Total C O 64 56 8	0
18	h	1	Total C O 64 56 8	0

- Molecule 19 is DOCOSANE (three-letter code: TWT) (formula: $C_{22}H_{46}$).



Mol	Chain	Residues	Atoms	AltConf
19	H	1	Total C 22 22	0
19	h	1	Total C 22 22	0

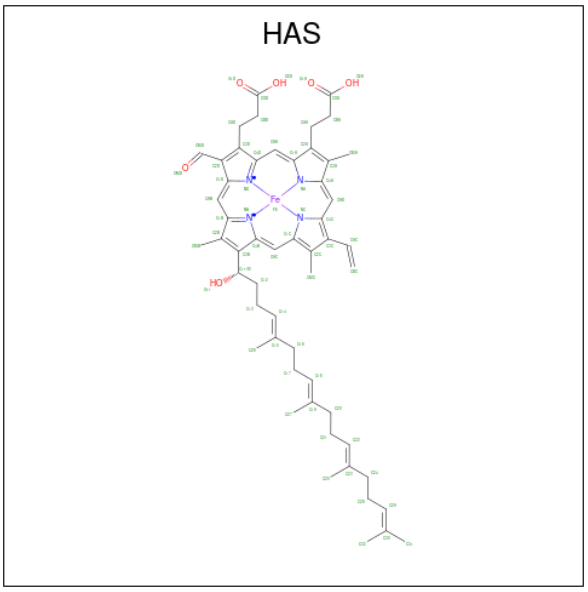
- Molecule 20 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	AltConf
20	G	2	Total Cu 2 2	0
20	D	1	Total Cu 1 1	0
20	g	2	Total Cu 2 2	0
20	d	1	Total Cu 1 1	0

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	G	1	Total Mg 1 1	0
21	d	1	Total Mg 1 1	0

- Molecule 22 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).

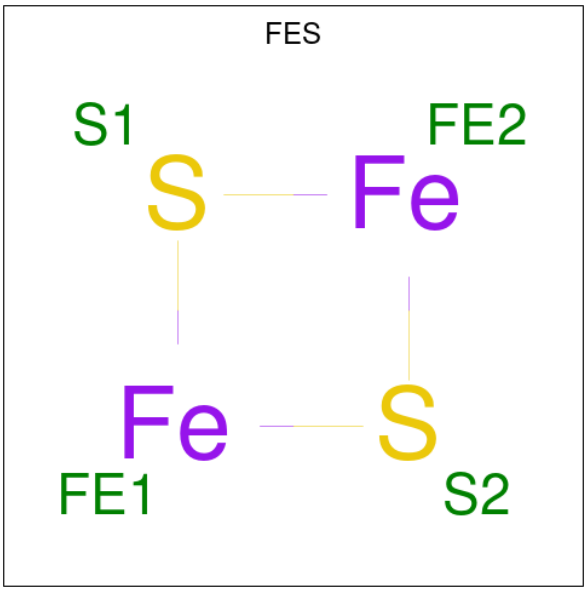


Mol	Chain	Residues	Atoms					AltConf
22	D	1	Total 130	C 108	Fe 2	N 8	O 12	0
22	D	1	Total 130	C 108	Fe 2	N 8	O 12	0
22	d	1	Total 130	C 108	Fe 2	N 8	O 12	0
22	d	1	Total 130	C 108	Fe 2	N 8	O 12	0

- Molecule 23 is CALCIUM ION (three-letter code: CA) (formula: Ca).

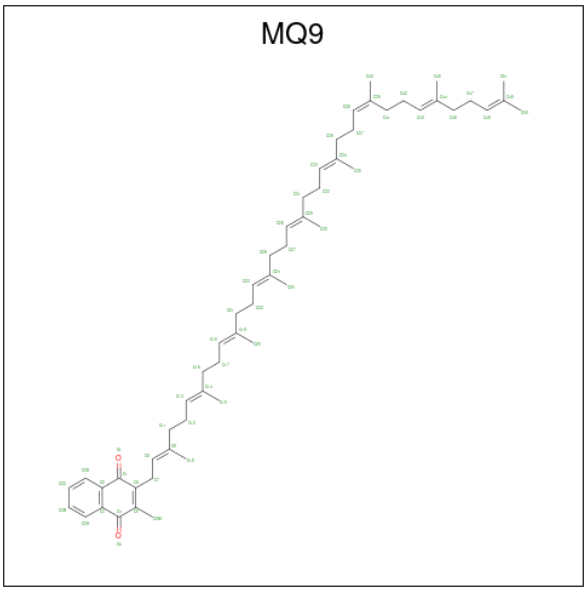
Mol	Chain	Residues	Atoms		AltConf
23	D	1	Total 1	Ca 1	0
23	d	1	Total 1	Ca 1	0

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	Fe	S	0
			4	2	2	
24	a	1	Total	Fe	S	0
			4	2	2	

- Molecule 25 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			43	41	2	

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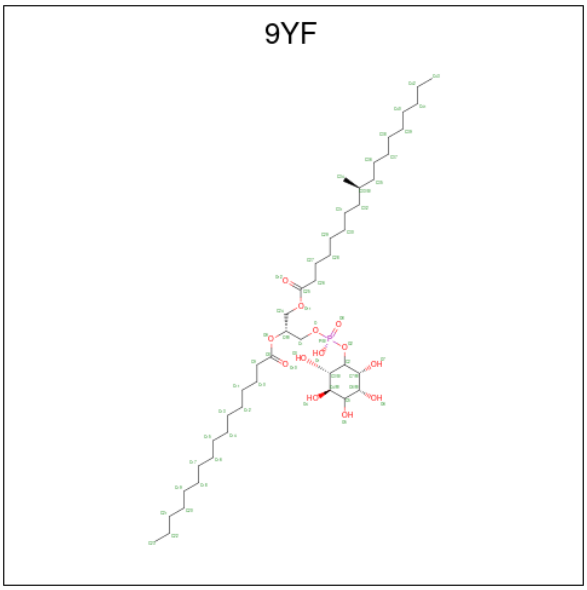
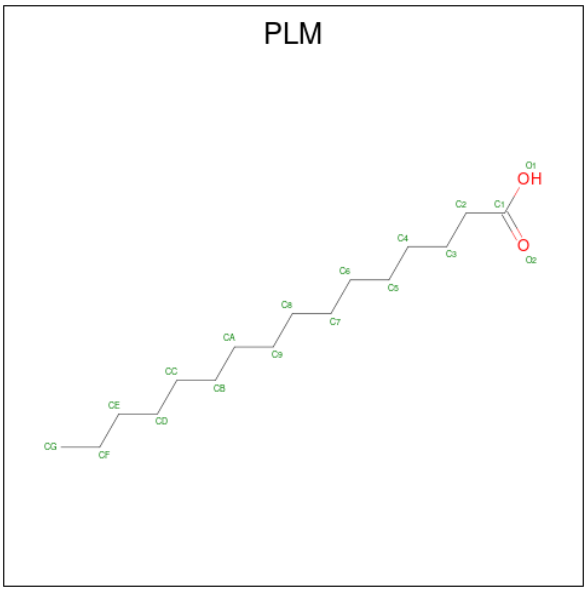
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C O 101 97 4	0
25	B	1	Total C O 101 97 4	0
25	a	1	Total C O 43 41 2	0
25	b	1	Total C O 101 97 4	0
25	b	1	Total C O 101 97 4	0

- Molecule 26 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 (three-letter code: 9YF) (formula: $C_{44}H_{85}O_{13}P$).



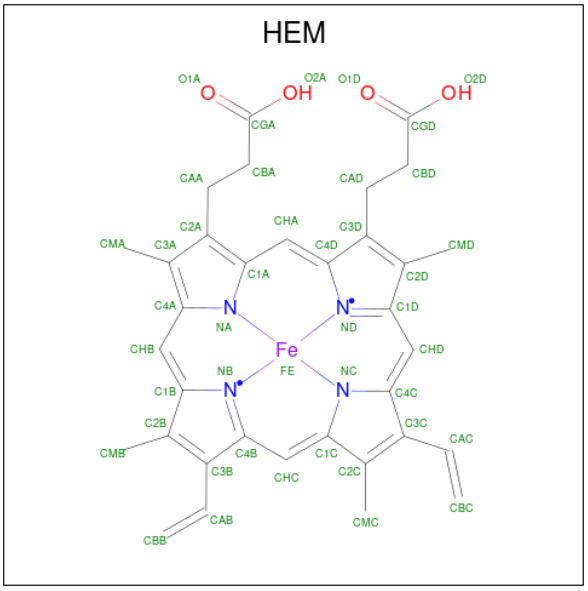
Mol	Chain	Residues	Atoms	AltConf
26	L	1	Total C O P 58 44 13 1	0
26	a	1	Total C O P 116 88 26 2	0
26	a	1	Total C O P 116 88 26 2	0
26	l	1	Total C O P 58 44 13 1	0

- Molecule 27 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



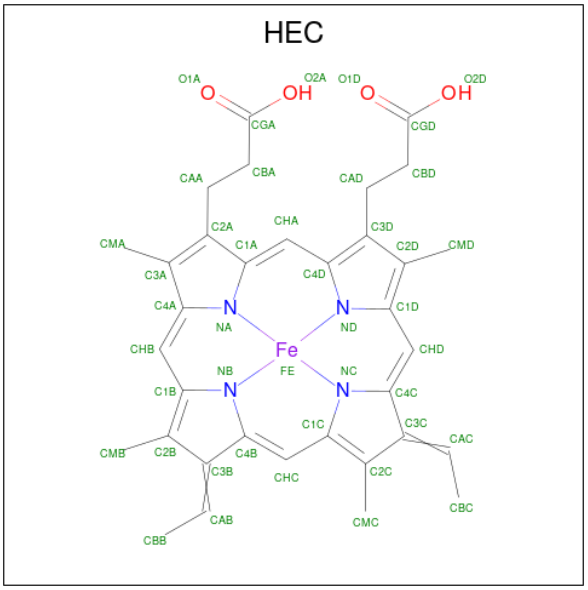
Mol	Chain	Residues	Atoms	AltConf
27	L	1	Total C O 11 10 1	0
27	d	1	Total C O 11 10 1	0
27	X	1	Total C O 11 10 1	0
27	x	1	Total C O 11 10 1	0

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
28	B	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
28	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
28	b	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

- Molecule 29 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



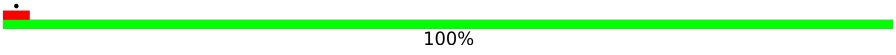
Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
29	C	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
29	c	1	Total	C	Fe	N	O	0
			86	68	2	8	8	
29	c	1	Total	C	Fe	N	O	0
			86	68	2	8	8	

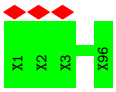
3 Residue-property plots (i)

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: Co-purified unknown transmembrane helices built as polyALA (AscD)

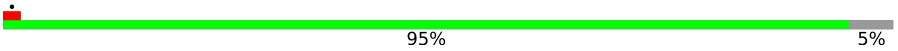
Chain Y:

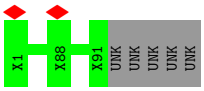




• Molecule 1: Co-purified unknown transmembrane helices built as polyALA (AscD)

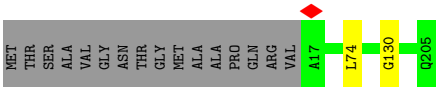
Chain y:





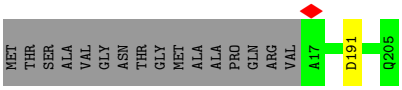
• Molecule 2: Cytochrome c oxidase subunit 3

Chain E:



• Molecule 2: Cytochrome c oxidase subunit 3

Chain e:

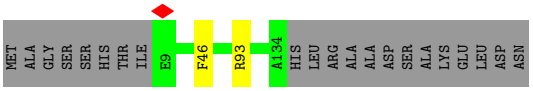


• Molecule 3: Uncharacterized membrane protein Cgl2017/cg2211

Chain H:

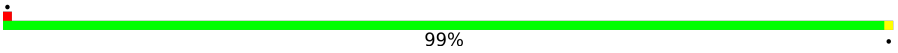
• Molecule 3: Uncharacterized membrane protein Cgl2017/cg2211

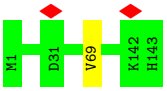
Chain h:



• Molecule 4: Cytochrome c oxidase polypeptide 4

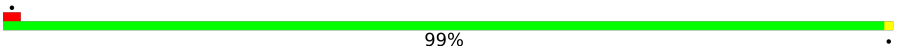
Chain F:

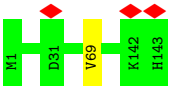




• Molecule 4: Cytochrome c oxidase polypeptide 4

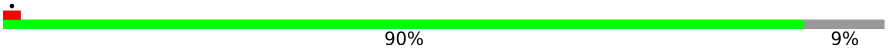
Chain f:

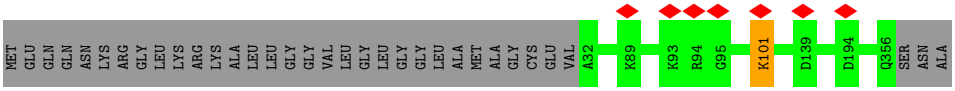




• Molecule 5: Cytochrome c oxidase subunit 2

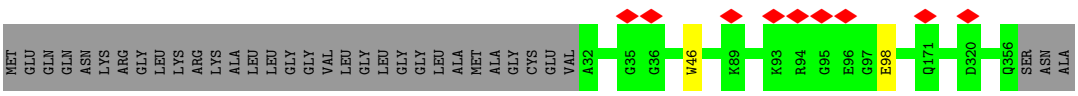
Chain G:





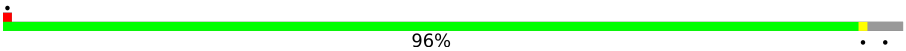
• Molecule 5: Cytochrome c oxidase subunit 2

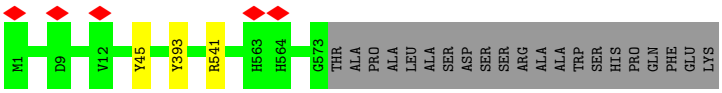
Chain g:



• Molecule 6: Cytochrome c oxidase subunit 1

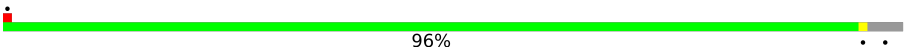
Chain D:

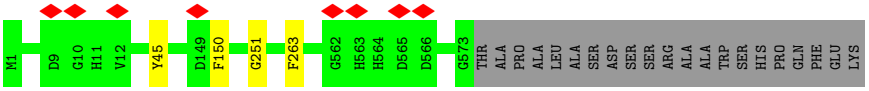




• Molecule 6: Cytochrome c oxidase subunit 1

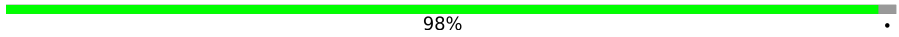
Chain d:

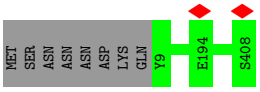




• Molecule 7: Cytochrome bc1 complex Rieske iron-sulfur subunit

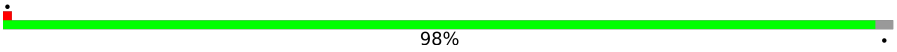
Chain A:

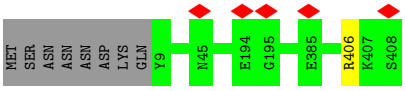




• Molecule 7: Cytochrome bc1 complex Rieske iron-sulfur subunit

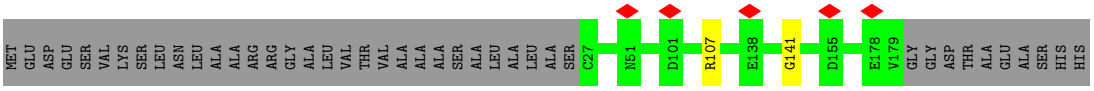
Chain a:





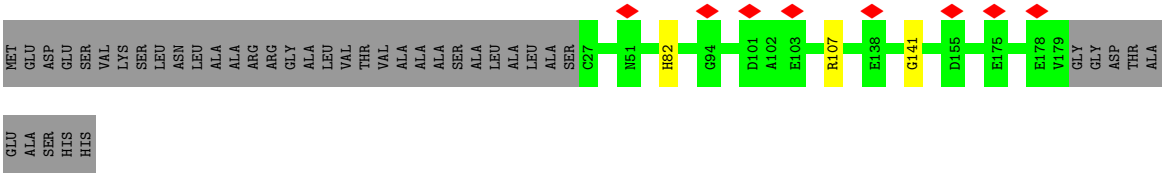
• Molecule 8: Uncharacterized protein Cgl2664/cg2949

Chain L:



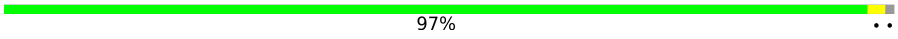
• Molecule 8: Uncharacterized protein Cgl2664/cg2949

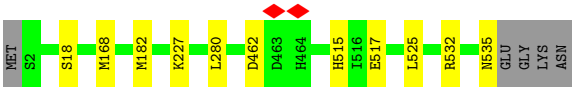
Chain l:



• Molecule 9: Cytochrome bc1 complex cytochrome b subunit

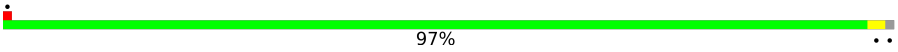
Chain B:

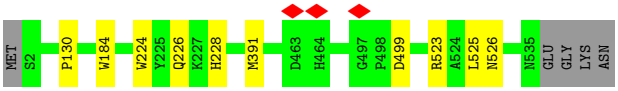




• Molecule 9: Cytochrome bc1 complex cytochrome b subunit

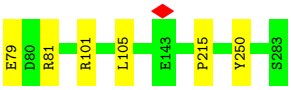
Chain b:





• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain C:

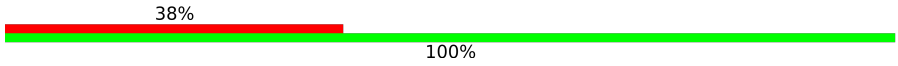


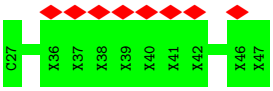
• Molecule 10: Cytochrome bc1 complex cytochrome c subunit

Chain c:

• Molecule 11: Co-purified unknown peptide built as polyALA (AscE)

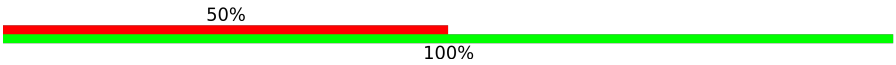
Chain X:

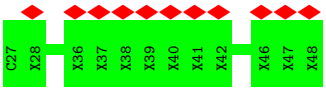




• Molecule 12: Co-purified unknown peptide built as polyALA (AscE)

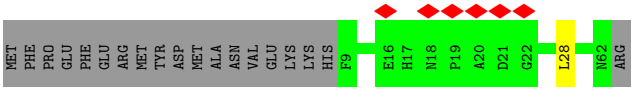
Chain x:





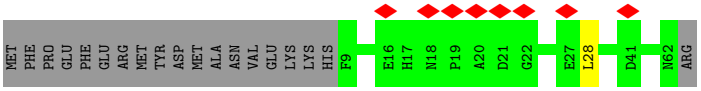
• Molecule 13: Actinobacterial supercomplex, subunit C (AscC)

Chain V:



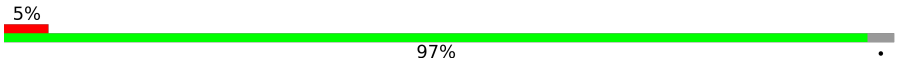
• Molecule 13: Actinobacterial supercomplex, subunit C (AscC)

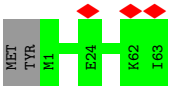
Chain v:



• Molecule 14: Hypothetical membrane protein

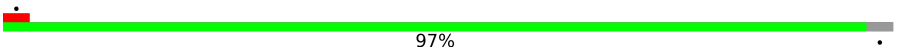
Chain K:

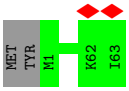




• Molecule 14: Hypothetical membrane protein

Chain k:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65391	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.331	Depositor
Minimum map value	-2.395	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.541	Depositor
Map size (Å)	328.59998, 328.59998, 328.59998	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9YF, HAS, 9XX, TWT, MG, CU, 7PH, CA, FES, HEM, TRD, MQ9, PLM, CDL, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
2	E	0.32	0/1520	0.58	0/2071
2	e	0.31	0/1520	0.58	0/2071
3	H	0.29	0/1022	0.61	0/1397
3	h	0.29	0/1031	0.59	0/1410
4	F	0.31	0/1125	0.60	0/1529
4	f	0.31	0/1125	0.57	0/1529
5	G	0.28	0/2629	0.55	0/3586
5	g	0.28	0/2629	0.54	0/3586
6	D	0.31	0/4701	0.59	0/6412
6	d	0.32	0/4701	0.58	0/6412
7	A	0.29	0/3197	0.59	0/4352
7	a	0.30	0/3197	0.60	0/4352
8	L	0.27	0/1134	0.58	0/1553
8	l	0.28	0/1134	0.57	0/1553
9	B	0.30	0/4301	0.58	0/5861
9	b	0.30	0/4301	0.58	0/5861
10	C	0.31	0/1761	0.58	0/2383
10	c	0.30	0/1761	0.58	0/2383
11	X	0.79	0/5	0.35	0/5
12	x	0.80	0/5	0.20	0/5
13	V	0.30	0/436	0.58	0/600
13	v	0.29	0/436	0.59	0/600
14	K	0.29	0/452	0.54	0/616
14	k	0.29	0/452	0.54	0/616
All	All	0.30	0/44575	0.58	0/60743

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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
2	E	187/205 (91%)	182 (97%)	4 (2%)	1 (0%)	29 68
2	e	187/205 (91%)	182 (97%)	5 (3%)	0	100 100
3	H	123/147 (84%)	109 (89%)	13 (11%)	1 (1%)	19 57
3	h	124/147 (84%)	114 (92%)	10 (8%)	0	100 100
4	F	141/143 (99%)	133 (94%)	8 (6%)	0	100 100
4	f	141/143 (99%)	138 (98%)	3 (2%)	0	100 100
5	G	323/359 (90%)	295 (91%)	27 (8%)	1 (0%)	41 76
5	g	323/359 (90%)	293 (91%)	30 (9%)	0	100 100
6	D	571/594 (96%)	543 (95%)	28 (5%)	0	100 100
6	d	571/594 (96%)	540 (95%)	30 (5%)	1 (0%)	47 82
7	A	398/408 (98%)	381 (96%)	17 (4%)	0	100 100
7	a	398/408 (98%)	372 (94%)	26 (6%)	0	100 100
8	L	151/194 (78%)	131 (87%)	19 (13%)	1 (1%)	22 60
8	l	151/194 (78%)	132 (87%)	18 (12%)	1 (1%)	22 60
9	B	532/539 (99%)	505 (95%)	25 (5%)	2 (0%)	34 72
9	b	532/539 (99%)	505 (95%)	25 (5%)	2 (0%)	34 72
10	C	230/283 (81%)	203 (88%)	24 (10%)	3 (1%)	12 45
10	c	230/283 (81%)	201 (87%)	28 (12%)	1 (0%)	34 72
13	V	52/73 (71%)	45 (86%)	7 (14%)	0	100 100
13	v	52/73 (71%)	45 (86%)	7 (14%)	0	100 100
14	K	61/65 (94%)	56 (92%)	5 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	k	61/65 (94%)	56 (92%)	5 (8%)	0	100 100
All	All	5539/6020 (92%)	5161 (93%)	364 (7%)	14 (0%)	44 76

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	141	GLY
8	l	141	GLY
2	E	130	GLY
5	G	101	LYS
3	H	111	LEU

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
2	E	155/166 (93%)	154 (99%)	1 (1%)	86 95
2	e	155/166 (93%)	154 (99%)	1 (1%)	86 95
3	H	108/125 (86%)	105 (97%)	3 (3%)	43 77
3	h	109/125 (87%)	107 (98%)	2 (2%)	59 85
4	F	114/114 (100%)	113 (99%)	1 (1%)	78 92
4	f	114/114 (100%)	113 (99%)	1 (1%)	78 92
5	G	269/292 (92%)	268 (100%)	1 (0%)	91 97
5	g	269/292 (92%)	267 (99%)	2 (1%)	84 94
6	D	472/488 (97%)	469 (99%)	3 (1%)	86 95
6	d	472/488 (97%)	469 (99%)	3 (1%)	86 95
7	A	324/332 (98%)	324 (100%)	0	100 100
7	a	324/332 (98%)	323 (100%)	1 (0%)	92 97
8	L	127/154 (82%)	126 (99%)	1 (1%)	81 93
8	l	127/154 (82%)	125 (98%)	2 (2%)	62 86
9	B	437/441 (99%)	428 (98%)	9 (2%)	53 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	b	437/441 (99%)	429 (98%)	8 (2%)	59 85
10	C	176/212 (83%)	169 (96%)	7 (4%)	31 68
10	c	176/212 (83%)	167 (95%)	9 (5%)	24 60
11	X	1/1 (100%)	1 (100%)	0	100 100
12	x	1/1 (100%)	1 (100%)	0	100 100
13	V	45/63 (71%)	44 (98%)	1 (2%)	52 81
13	v	45/63 (71%)	44 (98%)	1 (2%)	52 81
14	K	43/45 (96%)	43 (100%)	0	100 100
14	k	43/45 (96%)	43 (100%)	0	100 100
All	All	4543/4866 (93%)	4486 (99%)	57 (1%)	70 89

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	h	93	ARG
13	V	28	LEU
7	a	406	ARG
10	c	250	TYR
10	c	105	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
9	b	287	GLN
9	b	445	GLN
10	c	182	ASN
6	D	314	HIS
6	D	105	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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	$\#\|Z\|>2$
17	TRD	F	206	-	12,12,12	0.39	0	11,11,11	0.66	0
29	HEC	c	303	10	26,50,50	2.41	11 (42%)	18,82,82	2.10	4 (22%)
15	CDL	d	601	-	78,78,99	0.94	4 (5%)	84,90,111	0.69	0
15	CDL	c	301	-	78,78,99	0.86	3 (3%)	84,90,111	0.75	1 (1%)
16	7PH	d	608	-	37,37,37	0.91	2 (5%)	41,42,42	0.72	1 (2%)
17	TRD	f	203	-	12,12,12	0.38	0	11,11,11	0.60	0
17	TRD	f	201	-	12,12,12	0.38	0	11,11,11	0.69	0
26	9YF	L	201	-	58,58,58	0.91	5 (8%)	69,71,71	1.07	3 (4%)
16	7PH	d	610	-	37,37,37	0.80	1 (2%)	41,42,42	0.72	0
26	9YF	a	604	-	58,58,58	0.93	4 (6%)	69,71,71	1.00	3 (4%)
17	TRD	b	807	-	12,12,12	0.37	0	11,11,11	0.65	0
17	TRD	A	502	-	12,12,12	0.38	0	11,11,11	0.60	0
25	MQ9	b	804	-	44,44,59	1.51	6 (13%)	54,57,75	1.36	5 (9%)
17	TRD	a	605	-	12,12,12	0.38	0	11,11,11	0.62	0
16	7PH	g	403	-	37,37,37	0.87	2 (5%)	41,42,42	0.67	0
15	CDL	d	607	-	65,65,99	1.01	5 (7%)	71,77,111	0.73	2 (2%)
18	9XX	H	202	-	31,31,41	1.16	4 (12%)	34,34,44	1.30	3 (8%)
25	MQ9	A	504	-	44,44,59	1.46	5 (11%)	54,57,75	1.22	7 (12%)
22	HAS	D	603	6	56,72,72	4.72	17 (30%)	50,109,109	2.64	16 (32%)
17	TRD	f	205	-	12,12,12	0.37	0	11,11,11	0.71	0
28	HEM	B	601	9	27,50,50	1.08	2 (7%)	17,82,82	2.37	8 (47%)
17	TRD	F	205	-	12,12,12	0.37	0	11,11,11	0.64	0
25	MQ9	b	805	-	59,59,59	1.32	5 (8%)	72,75,75	1.22	9 (12%)
15	CDL	D	601	-	78,78,99	0.93	6 (7%)	84,90,111	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	7PH	D	609	-	37,37,37	0.87	2 (5%)	41,42,42	0.65	0
27	PLM	L	202	-	10,10,17	0.41	0	9,9,17	0.49	0
27	PLM	d	611	-	10,10,17	0.44	0	9,9,17	0.47	0
16	7PH	h	201	-	37,37,37	0.86	2 (5%)	41,42,42	0.71	0
19	TWT	H	203	-	21,21,21	0.35	0	20,20,20	0.81	0
17	TRD	F	203	-	12,12,12	0.39	0	11,11,11	0.62	0
16	7PH	G	403	-	37,37,37	0.87	2 (5%)	41,42,42	0.67	0
22	HAS	d	603	-	56,72,72	4.68	15 (26%)	50,109,109	2.61	19 (38%)
26	9YF	l	201	-	58,58,58	0.90	4 (6%)	69,71,71	1.08	3 (4%)
17	TRD	f	204	-	12,12,12	0.38	0	11,11,11	0.66	0
28	HEM	b	802	9	27,50,50	1.05	2 (7%)	17,82,82	2.55	8 (47%)
29	HEC	C	303	10	26,50,50	2.46	9 (34%)	18,82,82	4.46	9 (50%)
15	CDL	E	301	-	65,65,99	1.01	6 (9%)	71,77,111	0.75	0
17	TRD	A	505	-	12,12,12	0.38	0	11,11,11	0.62	0
25	MQ9	B	604	-	59,59,59	1.25	5 (8%)	72,75,75	1.24	10 (13%)
15	CDL	B	607	-	73,73,99	0.88	2 (2%)	79,85,111	0.87	4 (5%)
27	PLM	x	101	-	10,10,17	0.42	0	9,9,17	0.45	0
18	9XX	h	204	-	31,31,41	1.10	3 (9%)	34,34,44	1.24	3 (8%)
17	TRD	F	204	-	12,12,12	0.37	0	11,11,11	0.68	0
15	CDL	C	301	-	78,78,99	0.90	2 (2%)	84,90,111	0.85	2 (2%)
15	CDL	e	301	-	65,65,99	1.01	4 (6%)	71,77,111	0.80	1 (1%)
16	7PH	d	609	-	37,37,37	0.84	0	41,42,42	0.88	1 (2%)
29	HEC	c	302	10	26,50,50	1.53	6 (23%)	18,82,82	2.00	5 (27%)
15	CDL	D	606	-	73,73,99	0.98	6 (8%)	79,85,111	0.76	2 (2%)
16	7PH	E	302	-	37,37,37	0.93	2 (5%)	41,42,42	0.92	1 (2%)
15	CDL	F	202	-	78,78,99	0.99	6 (7%)	84,90,111	0.81	1 (1%)
16	7PH	D	610	-	37,37,37	0.89	2 (5%)	41,42,42	0.72	0
17	TRD	e	303	-	12,12,12	0.39	0	11,11,11	0.58	0
16	7PH	D	607	-	37,37,37	0.89	2 (5%)	41,42,42	0.77	0
16	7PH	D	608	-	37,37,37	0.95	3 (8%)	41,42,42	0.89	1 (2%)
26	9YF	a	601	-	58,58,58	0.92	3 (5%)	69,71,71	1.22	6 (8%)
17	TRD	E	303	-	12,12,12	0.40	0	11,11,11	0.56	0
28	HEM	b	803	9	27,50,50	1.18	2 (7%)	17,82,82	2.58	7 (41%)
15	CDL	b	801	-	73,73,99	0.97	5 (6%)	79,85,111	0.81	2 (2%)
16	7PH	k	101	-	37,37,37	0.83	1 (2%)	41,42,42	0.62	0
24	FES	a	603	7	0,4,4	-	-	-		
15	CDL	f	202	-	78,78,99	0.91	4 (5%)	84,90,111	0.82	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	PLM	X	101	-	10,10,17	0.41	0	9,9,17	0.45	0
25	MQ9	a	602	-	44,44,59	1.46	5 (11%)	54,57,75	1.33	9 (16%)
18	9XX	h	202	-	31,31,41	1.10	3 (9%)	34,34,44	1.34	3 (8%)
18	9XX	B	608	-	31,31,41	1.12	4 (12%)	34,34,44	1.21	4 (11%)
17	TRD	B	606	-	12,12,12	0.38	0	11,11,11	0.57	0
17	TRD	F	201	-	12,12,12	0.39	0	11,11,11	0.67	0
16	7PH	H	201	-	37,37,37	0.90	2 (5%)	41,42,42	0.90	2 (4%)
15	CDL	b	806	-	76,76,99	0.91	2 (2%)	82,88,111	0.80	1 (1%)
16	7PH	e	302	-	37,37,37	0.95	3 (8%)	41,42,42	0.68	0
16	7PH	f	207	-	37,37,37	0.87	2 (5%)	41,42,42	0.69	0
24	FES	A	501	7	0,4,4	-	-	-		
17	TRD	f	206	-	12,12,12	0.37	0	11,11,11	0.63	0
19	TWT	h	203	-	21,21,21	0.32	0	20,20,20	0.95	0
28	HEM	B	602	9	27,50,50	1.12	2 (7%)	17,82,82	2.74	7 (41%)
29	HEC	C	302	10	26,50,50	1.52	6 (23%)	18,82,82	2.06	5 (27%)
22	HAS	d	604	6	56,72,72	4.83	20 (35%)	50,109,109	3.50	19 (38%)
22	HAS	D	602	-	56,72,72	4.72	14 (25%)	50,109,109	2.60	19 (38%)
15	CDL	B	605	-	76,76,99	0.95	5 (6%)	82,88,111	0.71	0
16	7PH	F	207	-	37,37,37	0.87	2 (5%)	41,42,42	0.69	0
17	TRD	A	503	-	12,12,12	0.39	0	11,11,11	0.62	0
25	MQ9	B	603	-	44,44,59	1.44	5 (11%)	54,57,75	1.36	9 (16%)

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
17	TRD	F	206	-	-	7/10/10/10	-
29	HEC	c	303	10	-	3/6/54/54	-
15	CDL	d	601	-	-	37/89/89/110	-
15	CDL	c	301	-	-	50/89/89/110	-
16	7PH	d	608	-	-	16/39/39/39	-
17	TRD	f	203	-	-	1/10/10/10	-
17	TRD	f	201	-	-	3/10/10/10	-
26	9YF	L	201	-	-	24/54/78/78	0/1/1/1
16	7PH	d	610	-	-	23/39/39/39	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	9YF	a	604	-	-	29/54/78/78	0/1/1/1
17	TRD	b	807	-	-	2/10/10/10	-
17	TRD	A	502	-	-	7/10/10/10	-
25	MQ9	b	804	-	-	8/35/55/73	0/2/2/2
17	TRD	a	605	-	-	3/10/10/10	-
16	7PH	g	403	-	-	17/39/39/39	-
15	CDL	d	607	-	-	31/76/76/110	-
18	9XX	H	202	-	-	16/33/33/43	-
25	MQ9	A	504	-	-	12/35/55/73	0/2/2/2
22	HAS	D	603	6	-	10/35/122/122	-
17	TRD	f	205	-	-	9/10/10/10	-
28	HEM	B	601	9	-	1/6/54/54	-
17	TRD	F	205	-	-	5/10/10/10	-
25	MQ9	b	805	-	-	11/53/73/73	0/2/2/2
15	CDL	D	601	-	-	38/89/89/110	-
16	7PH	D	609	-	-	25/39/39/39	-
27	PLM	L	202	-	-	5/7/8/15	-
27	PLM	d	611	-	-	3/7/8/15	-
16	7PH	h	201	-	-	25/39/39/39	-
19	TWT	H	203	-	-	7/19/19/19	-
17	TRD	F	203	-	-	2/10/10/10	-
16	7PH	G	403	-	-	17/39/39/39	-
22	HAS	d	603	-	-	7/35/122/122	-
26	9YF	l	201	-	-	23/54/78/78	0/1/1/1
17	TRD	f	204	-	-	4/10/10/10	-
28	HEM	b	802	9	-	3/6/54/54	-
29	HEC	C	303	10	-	0/6/54/54	-
15	CDL	E	301	-	-	28/76/76/110	-
17	TRD	A	505	-	-	4/10/10/10	-
25	MQ9	B	604	-	-	21/53/73/73	0/2/2/2
15	CDL	B	607	-	-	42/84/84/110	-
27	PLM	x	101	-	-	4/7/8/15	-
18	9XX	h	204	-	-	20/33/33/43	-
17	TRD	F	204	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	C	301	-	-	48/89/89/110	-
15	CDL	e	301	-	-	40/76/76/110	-
16	7PH	d	609	-	-	22/39/39/39	-
29	HEC	c	302	10	-	2/6/54/54	-
15	CDL	D	606	-	-	41/84/84/110	-
16	7PH	E	302	-	-	14/39/39/39	-
15	CDL	F	202	-	-	45/89/89/110	-
16	7PH	D	610	-	-	23/39/39/39	-
17	TRD	e	303	-	-	7/10/10/10	-
16	7PH	D	607	-	-	23/39/39/39	-
16	7PH	D	608	-	-	18/39/39/39	-
26	9YF	a	601	-	-	35/54/78/78	0/1/1/1
17	TRD	E	303	-	-	8/10/10/10	-
28	HEM	b	803	9	-	2/6/54/54	-
15	CDL	b	801	-	-	42/84/84/110	-
16	7PH	k	101	-	-	10/39/39/39	-
24	FES	a	603	7	-	-	0/1/1/1
15	CDL	f	202	-	-	45/89/89/110	-
27	PLM	X	101	-	-	0/7/8/15	-
25	MQ9	a	602	-	-	12/35/55/73	0/2/2/2
18	9XX	h	202	-	-	14/33/33/43	-
18	9XX	B	608	-	-	15/33/33/43	-
17	TRD	B	606	-	-	7/10/10/10	-
17	TRD	F	201	-	-	3/10/10/10	-
16	7PH	H	201	-	-	19/39/39/39	-
15	CDL	b	806	-	-	44/87/87/110	-
16	7PH	e	302	-	-	21/39/39/39	-
16	7PH	f	207	-	-	19/39/39/39	-
24	FES	A	501	7	-	-	0/1/1/1
17	TRD	f	206	-	-	6/10/10/10	-
19	TWT	h	203	-	-	5/19/19/19	-
28	HEM	B	602	9	-	0/6/54/54	-
29	HEC	C	302	10	-	2/6/54/54	-
22	HAS	d	604	6	-	12/35/122/122	-
22	HAS	D	602	-	-	13/35/122/122	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	B	605	-	-	44/87/87/110	-
16	7PH	F	207	-	-	19/39/39/39	-
17	TRD	A	503	-	-	4/10/10/10	-
25	MQ9	B	603	-	-	7/35/55/73	0/2/2/2

The worst 5 of 257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	602	HAS	C2B-C3B	18.33	1.49	1.34
22	d	603	HAS	C2B-C3B	16.83	1.48	1.34
22	D	603	HAS	C2B-C3B	16.82	1.48	1.34
22	d	604	HAS	C2B-C3B	14.37	1.46	1.34
22	d	604	HAS	C1D-ND	-13.32	1.31	1.49

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	303	HEC	CBA-CAA-C2A	-11.34	91.59	112.48
22	d	604	HAS	CHB-C1B-NB	11.08	124.71	110.94
29	C	303	HEC	CMB-C2B-C3B	9.84	137.38	125.82
22	d	604	HAS	CHB-C1D-ND	9.78	123.10	110.94
28	B	602	HEM	CAD-CBD-CGD	-8.68	98.11	112.67

There are no chirality outliers.

5 of 1298 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	301	CDL	CA2-OA2-PA1-OA3
15	E	301	CDL	CB2-OB2-PB2-OB3
15	E	301	CDL	CB2-OB2-PB2-OB4
15	E	301	CDL	CB3-OB5-PB2-OB2
15	F	202	CDL	CA2-OA2-PA1-OA4

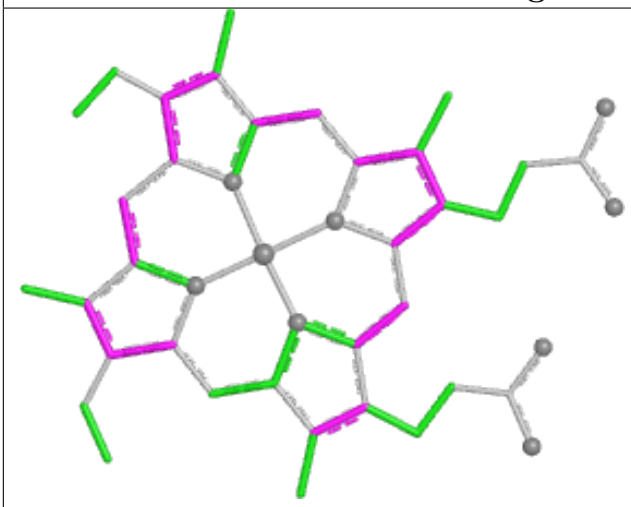
There are no ring outliers.

No monomer is involved in short contacts.

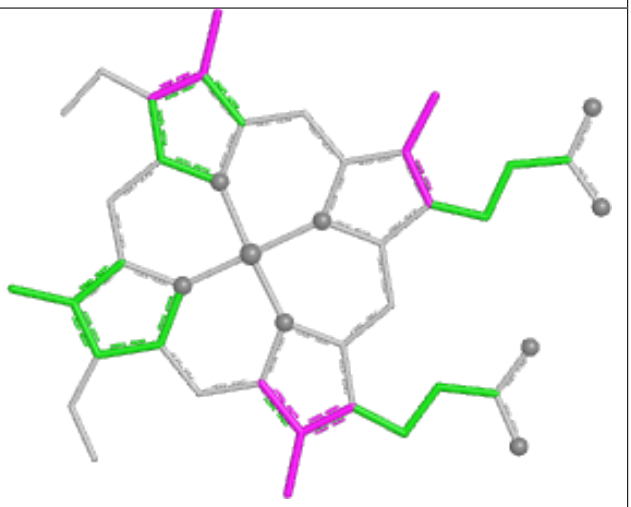
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

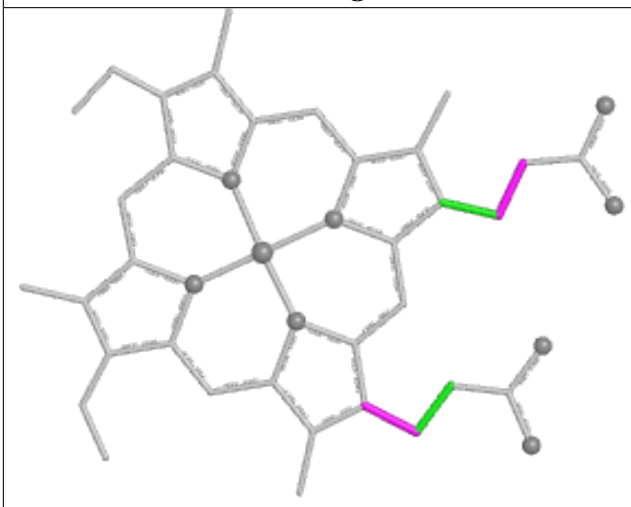
Ligand HEC c 303



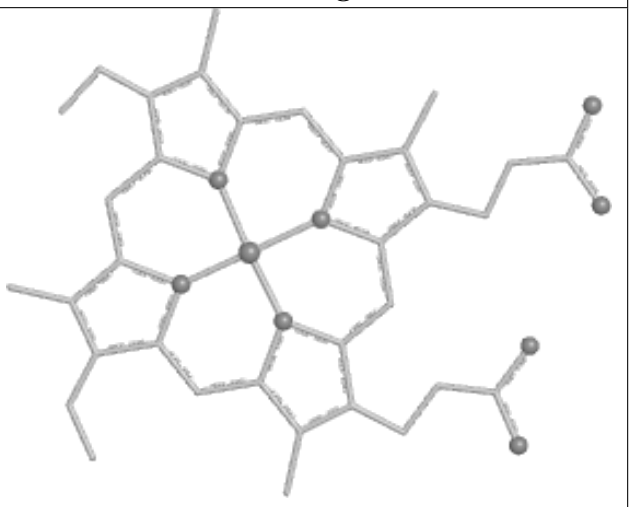
Bond lengths



Bond angles

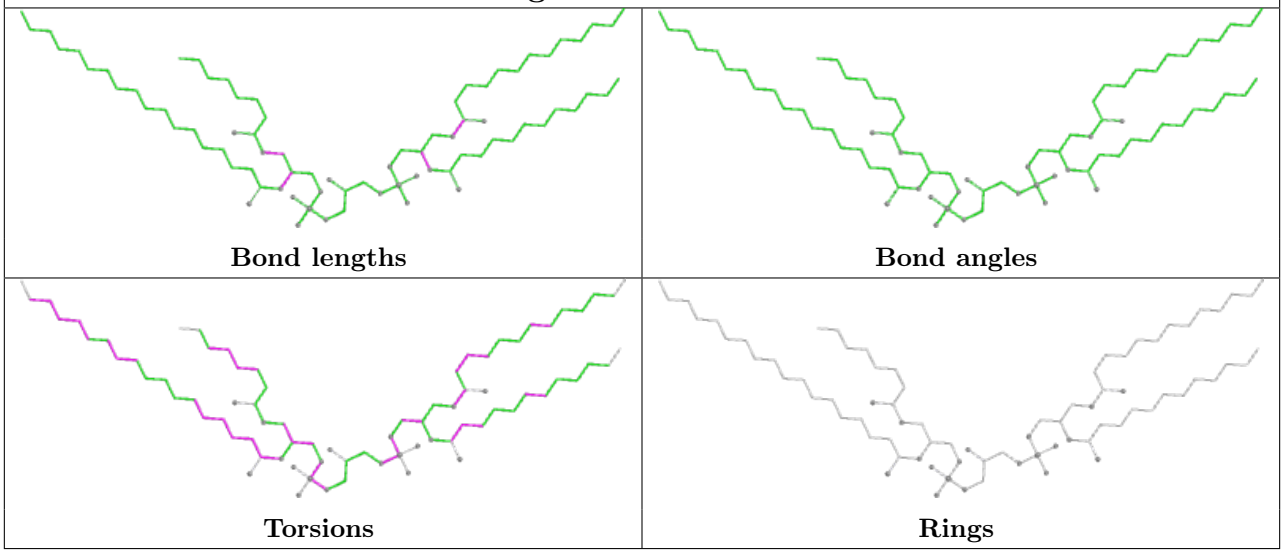


Torsions

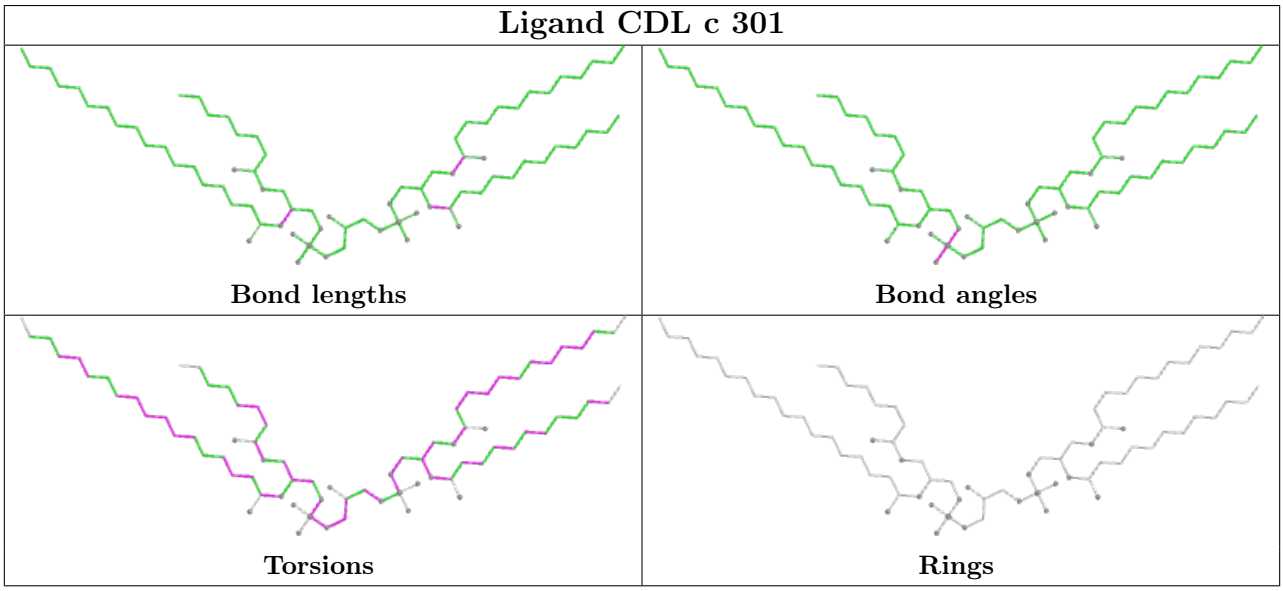


Rings

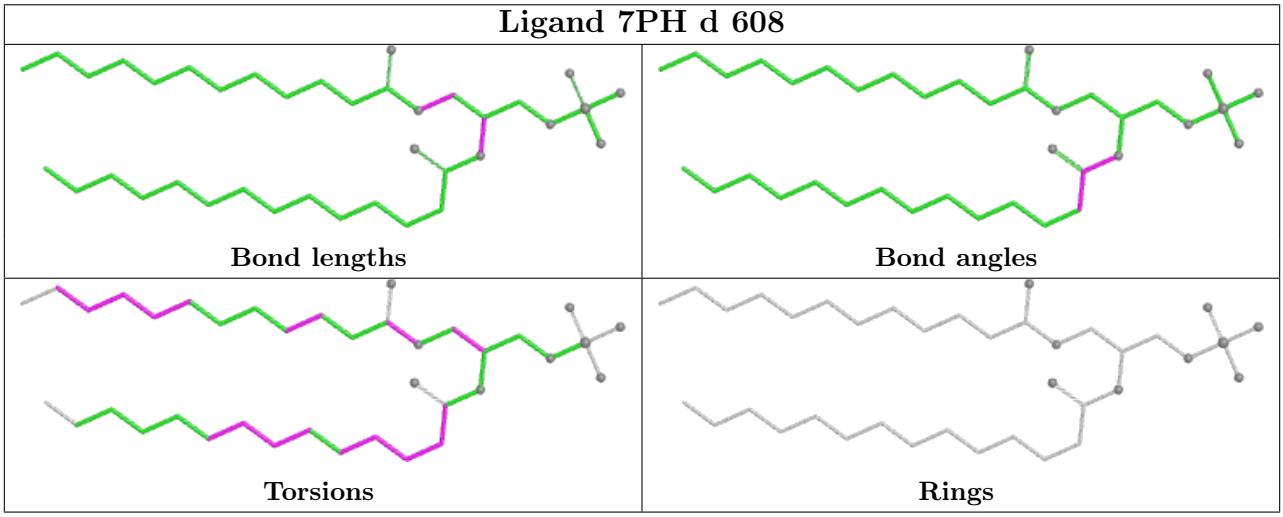
Ligand CDL d 601



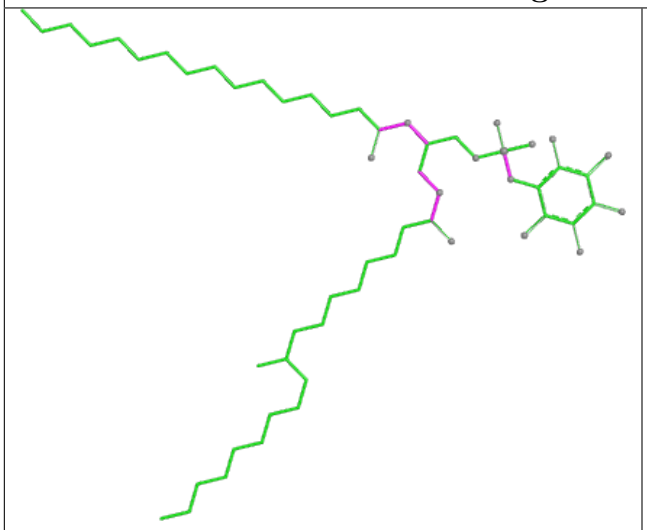
Ligand CDL c 301



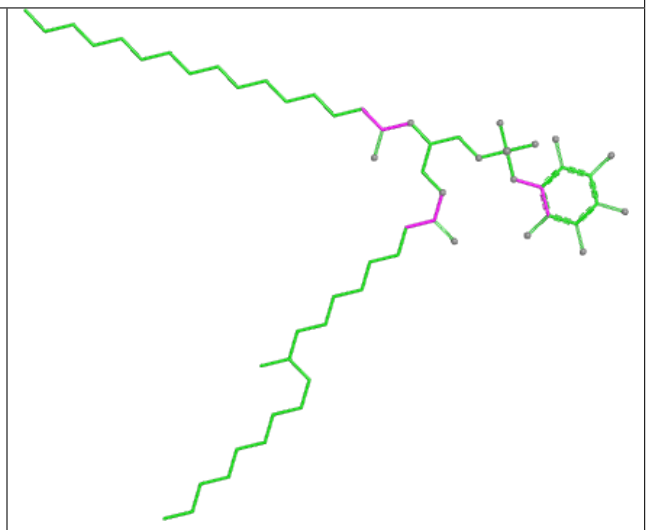
Ligand 7PH d 608



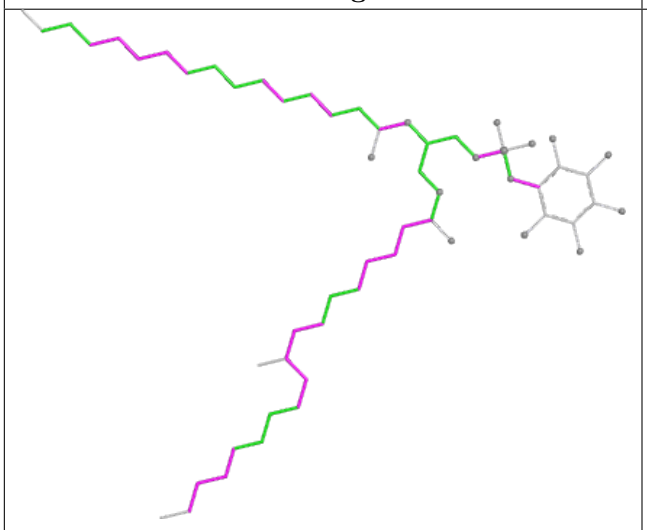
Ligand 9YF L 201



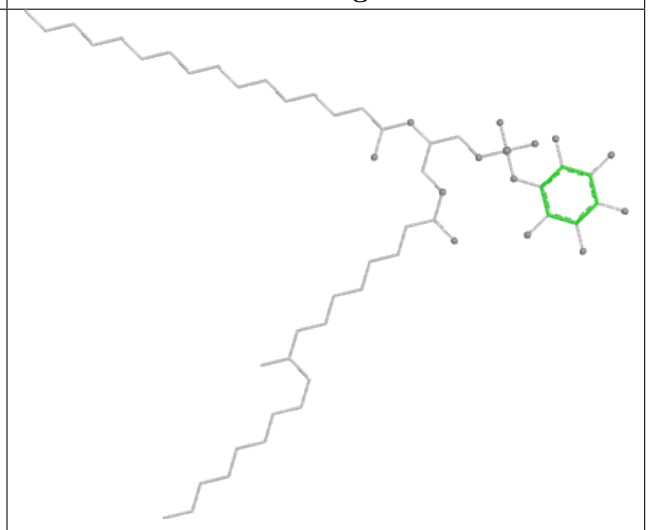
Bond lengths



Bond angles

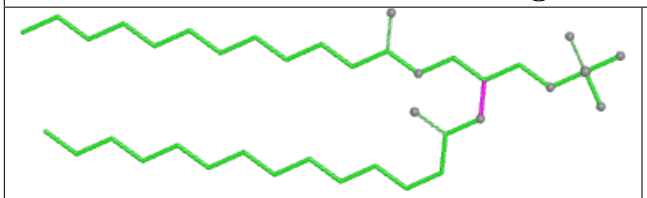


Torsions

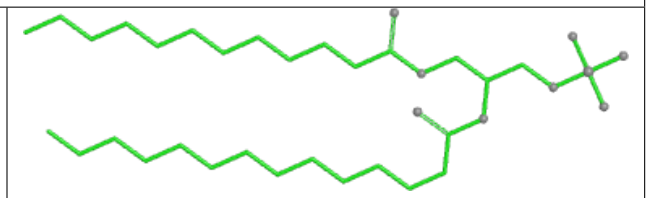


Rings

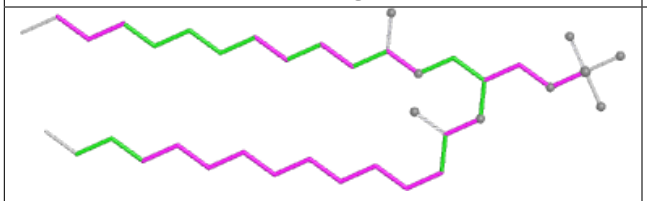
Ligand 7PH d 610



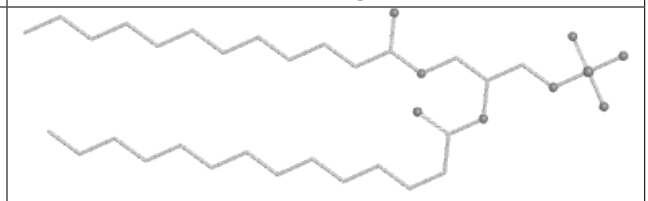
Bond lengths



Bond angles

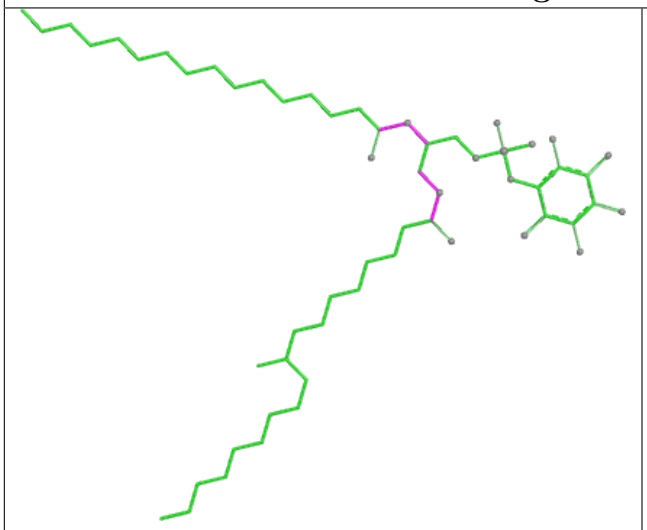


Torsions

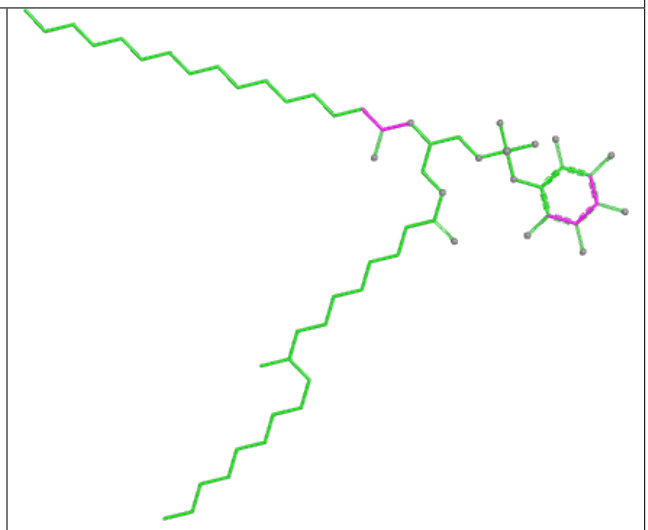


Rings

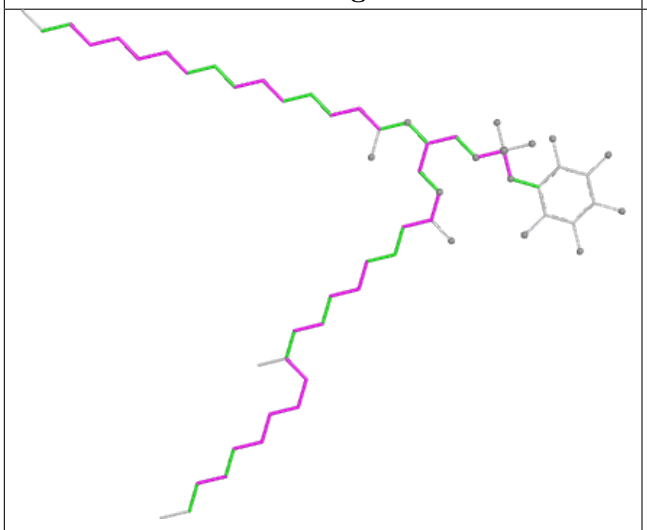
Ligand 9YF a 604



Bond lengths



Bond angles



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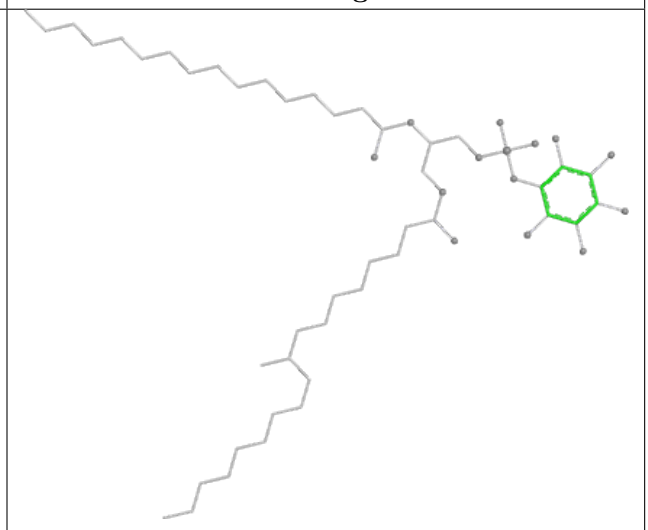
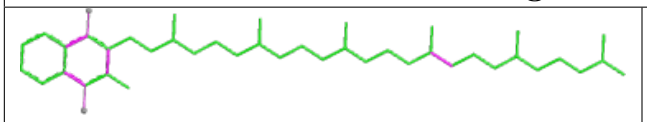


Rings

Ligand MQ9 b 804



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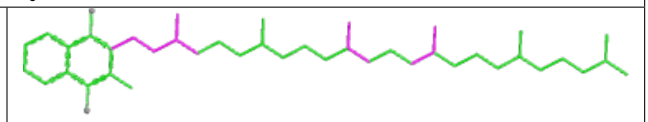
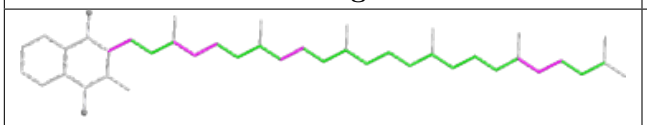


Bond angles



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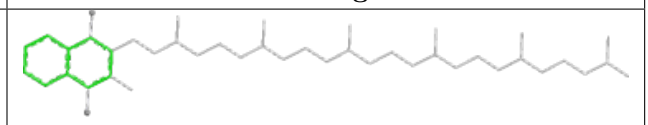
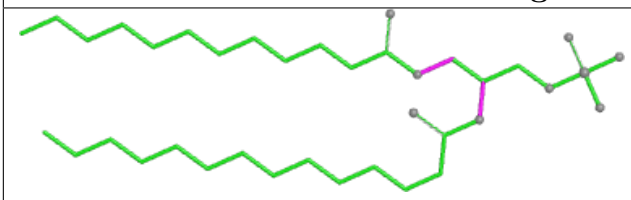
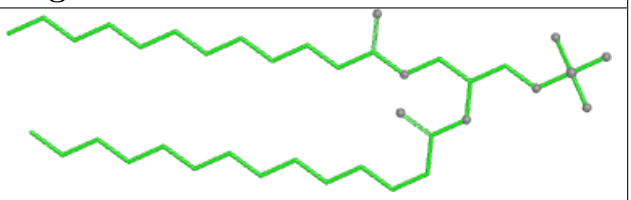


Rings

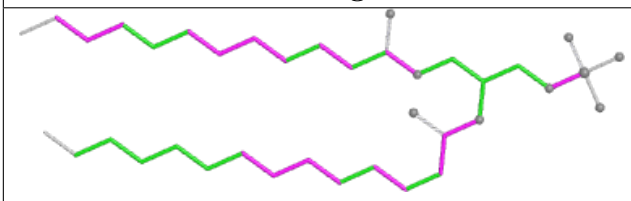
Ligand 7PH g 403



Bond lengths



Bond angles



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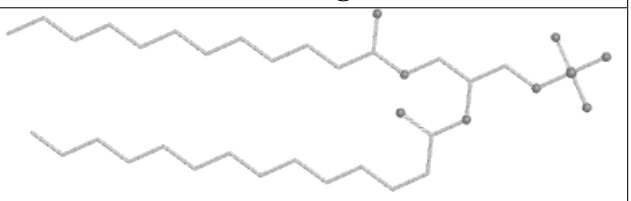
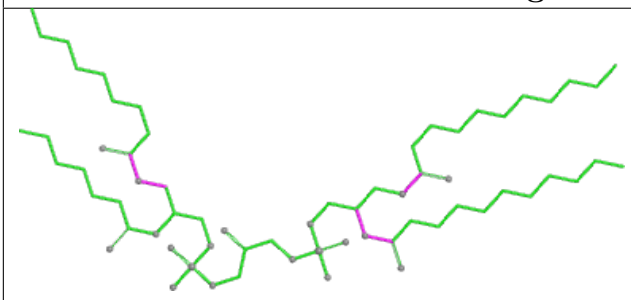
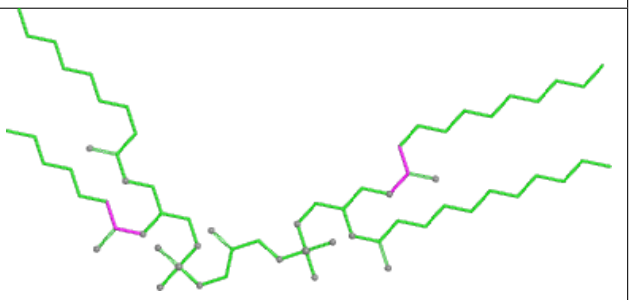


Rings

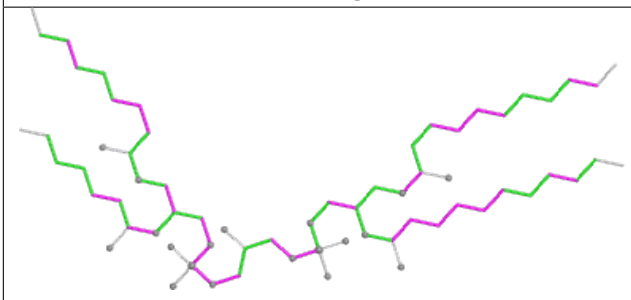
Ligand CDL d 607



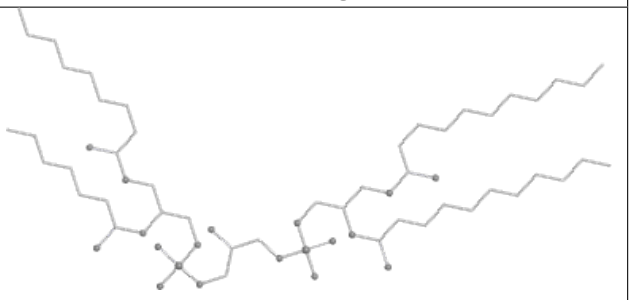
Bond lengths



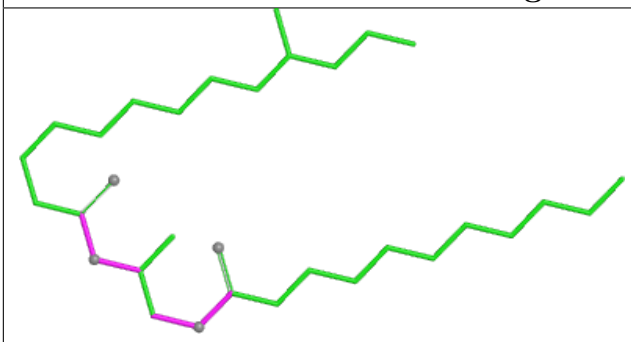
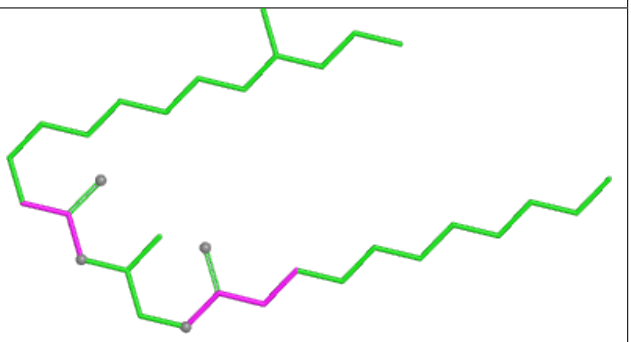
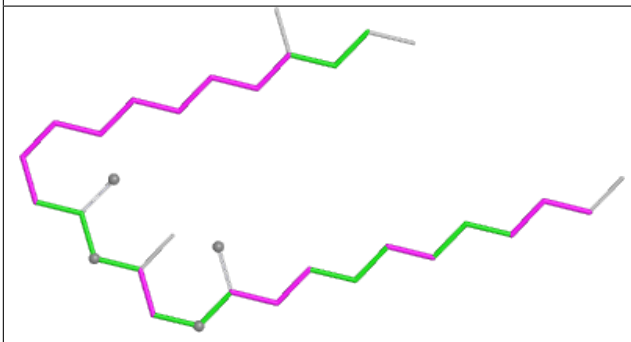
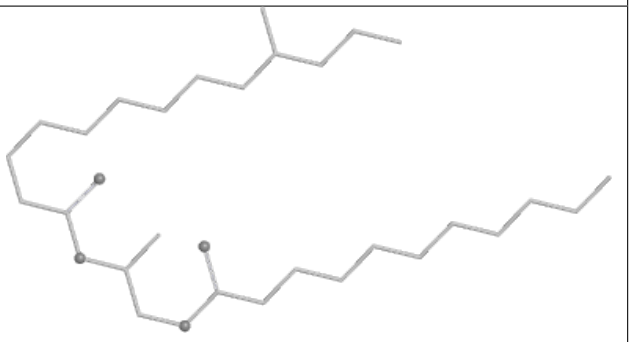
Bond angles

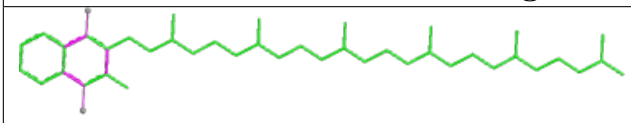
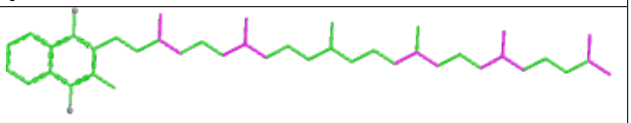
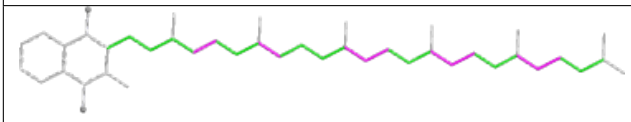
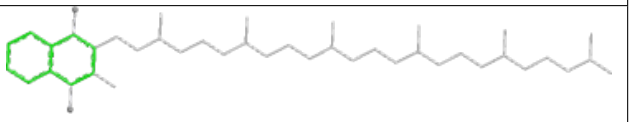


Torsions

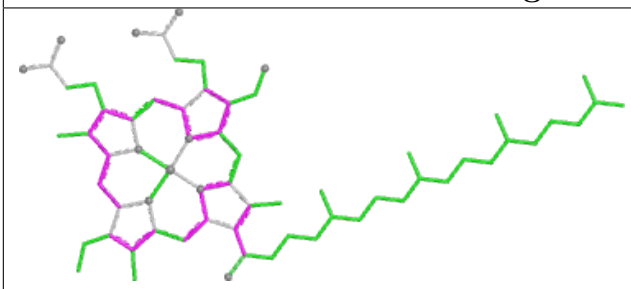


Rings

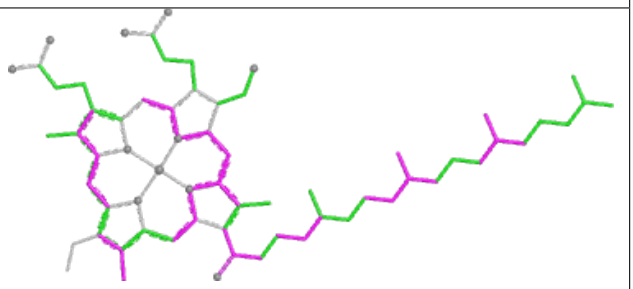
Ligand 9XX H 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 A 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

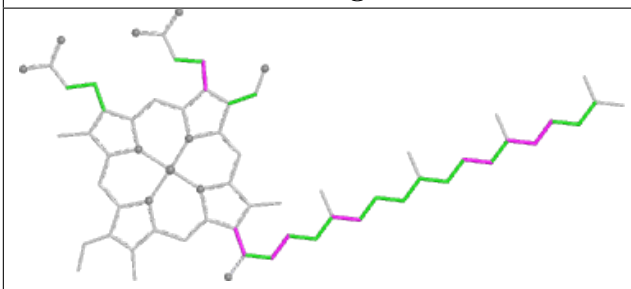
Ligand HAS D 603



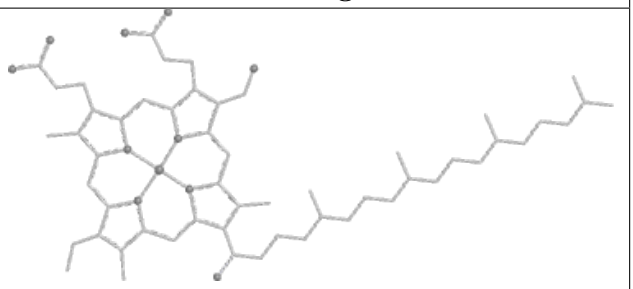
Bond lengths



Bond angles

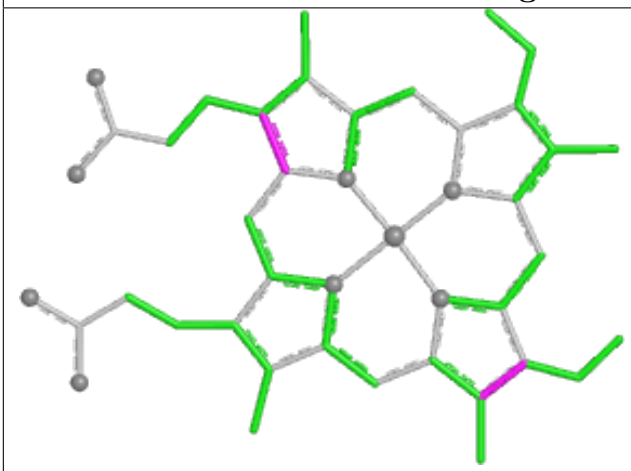


Torsions

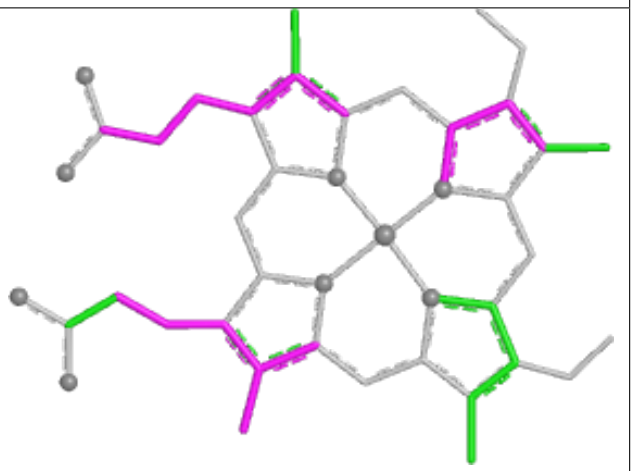


Rings

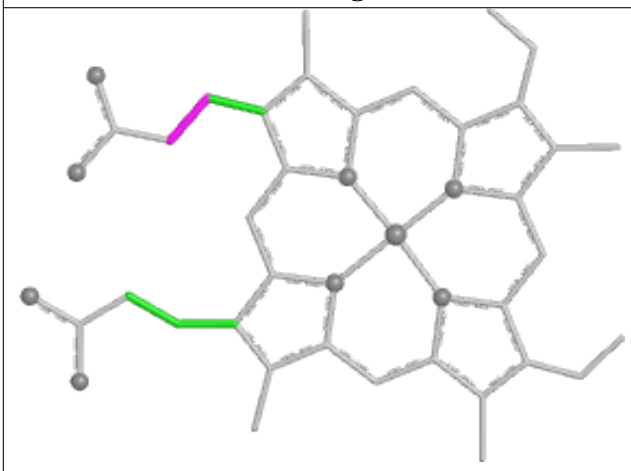
Ligand HEM B 601



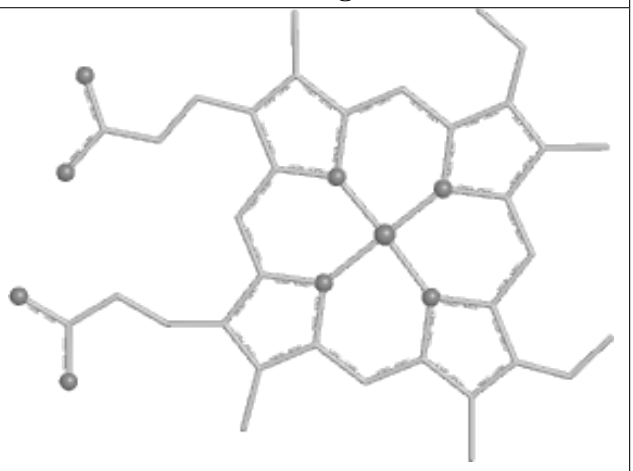
Bond lengths



Bond angles

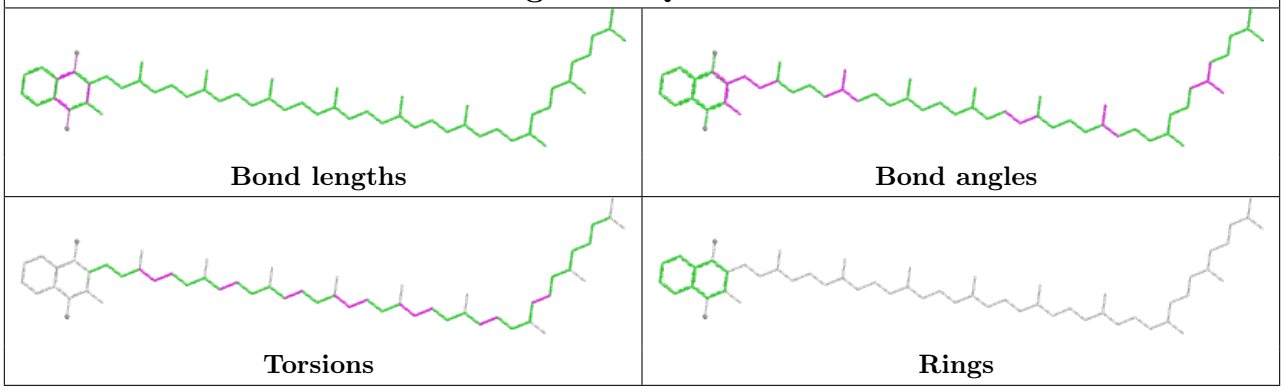


Torsions

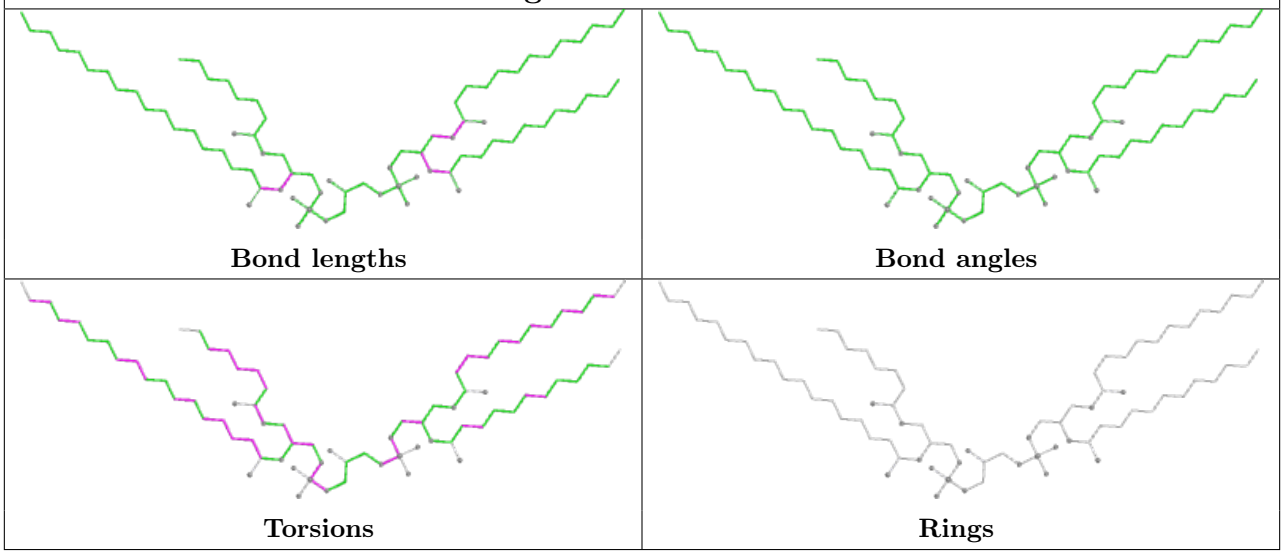


Rings

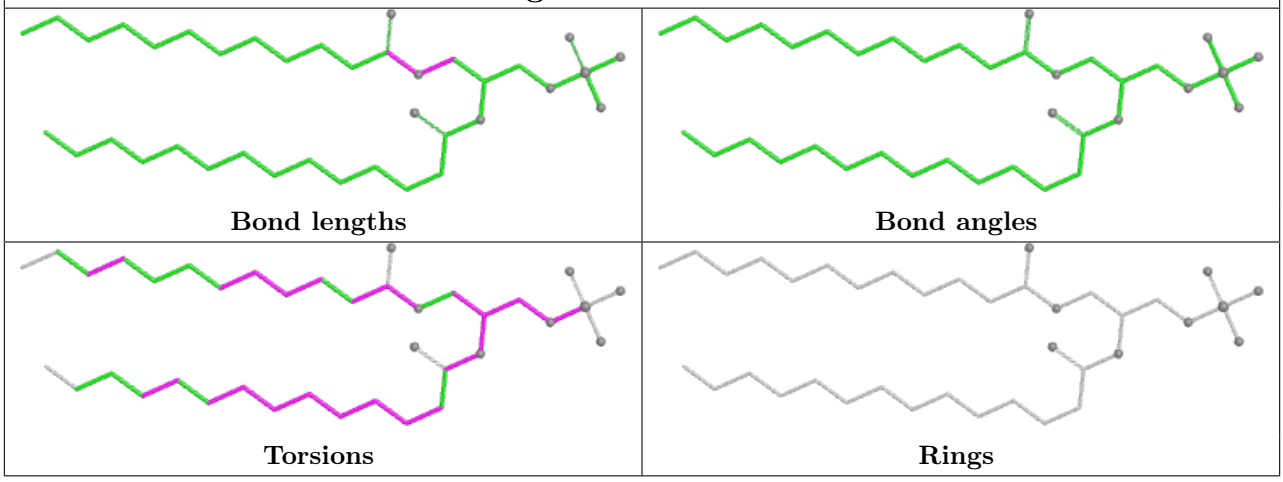
Ligand MQ9 b 805

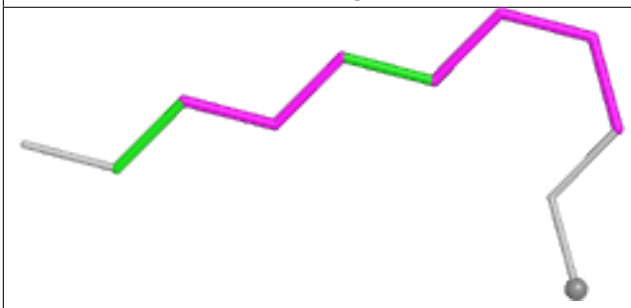
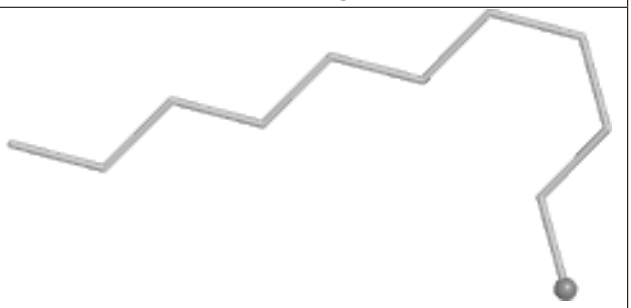


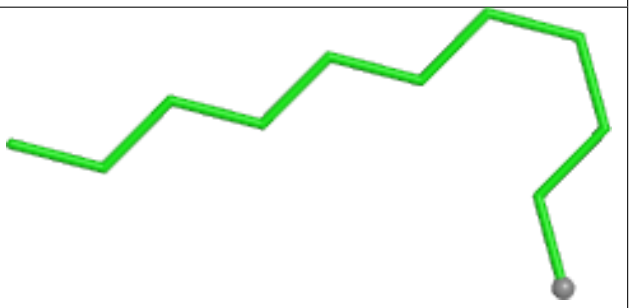
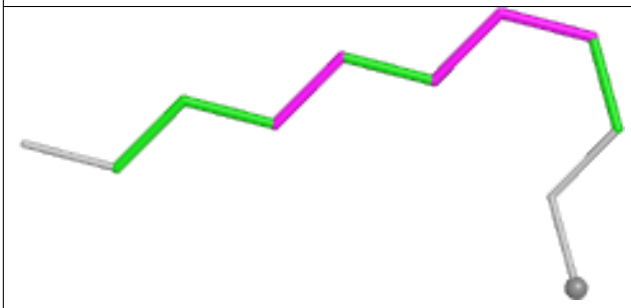
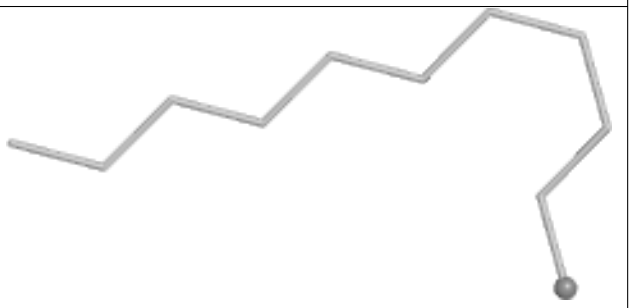
Ligand CDL D 601



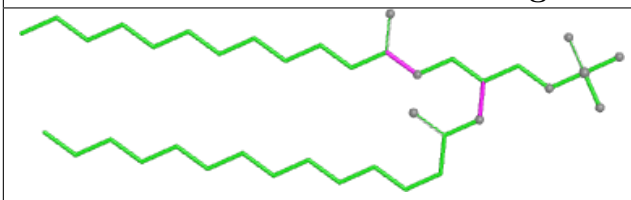
Ligand 7PH D 609



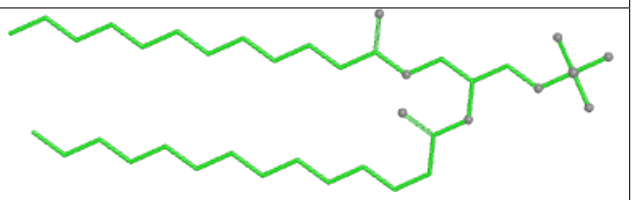
Ligand PLM L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLM d 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

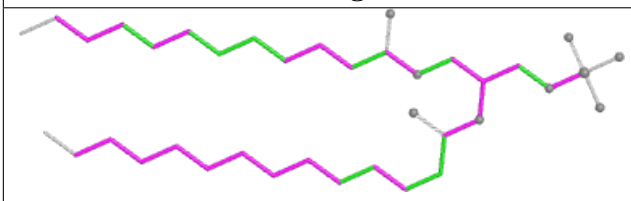
Ligand 7PH h 201



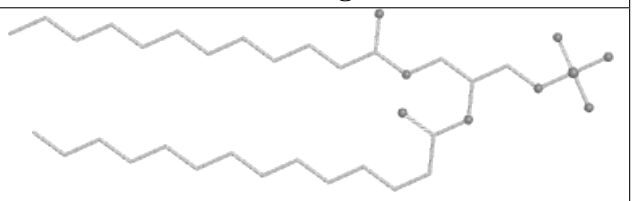
Bond lengths



Bond angles

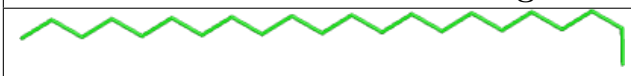


Torsions



Rings

Ligand TWT H 203



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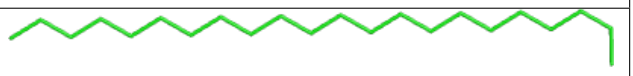

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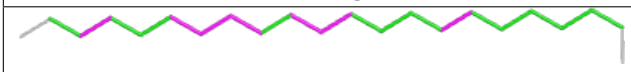
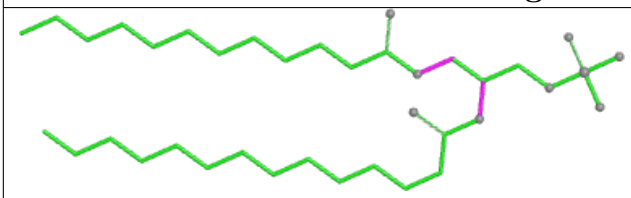


Torsions

Rings

Ligand 7PH G 403



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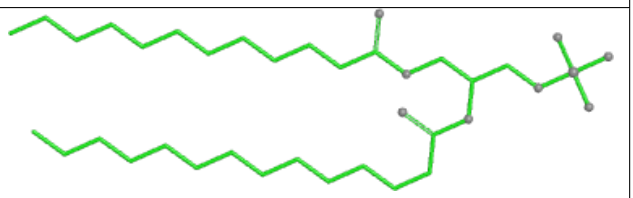
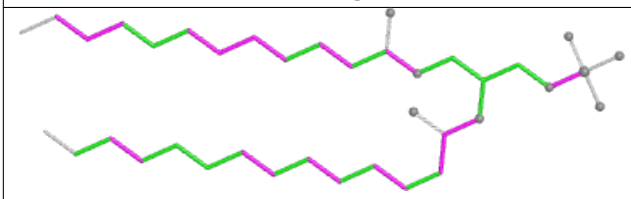
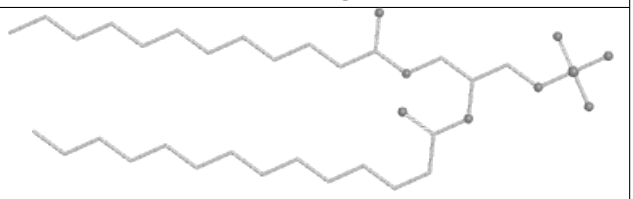


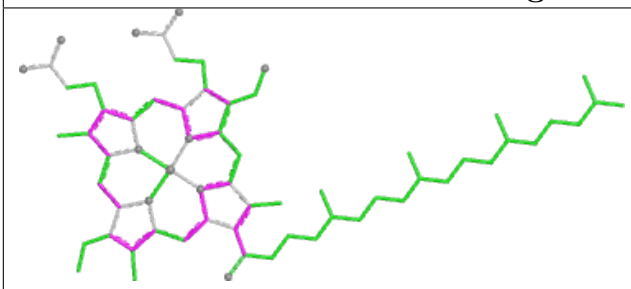
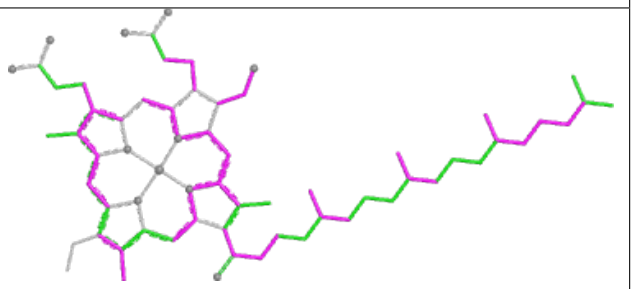
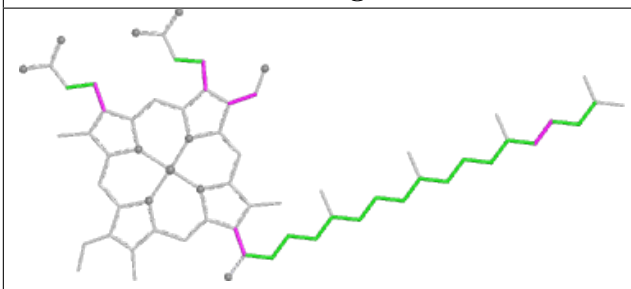
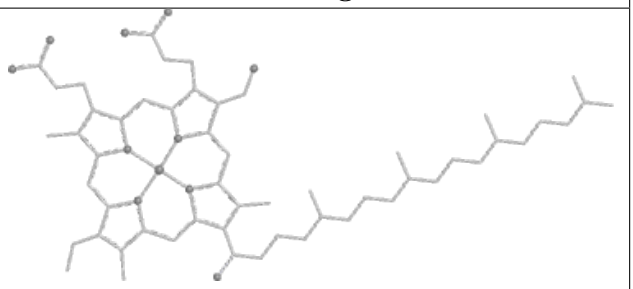
Bond angles



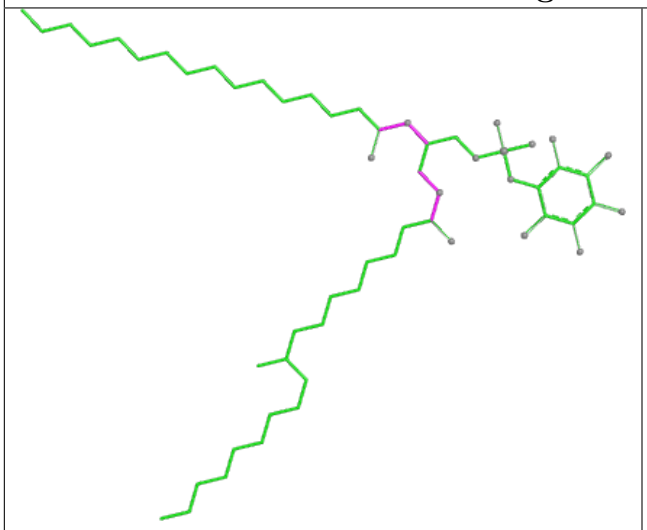
Torsions



Rings

Ligand HAS d 603	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand 9YF l 201



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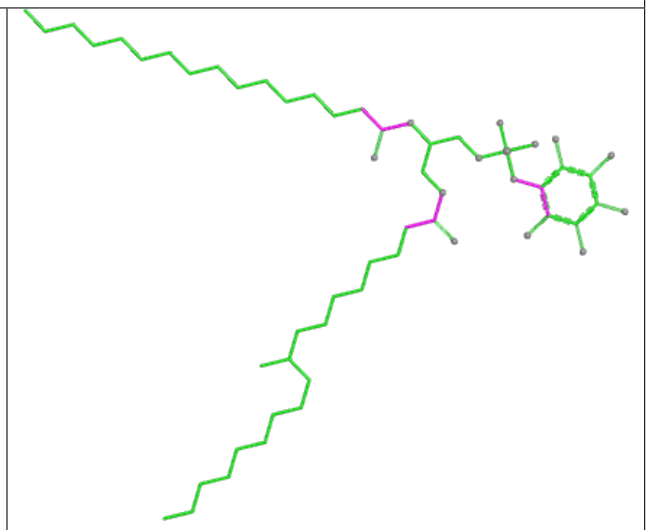
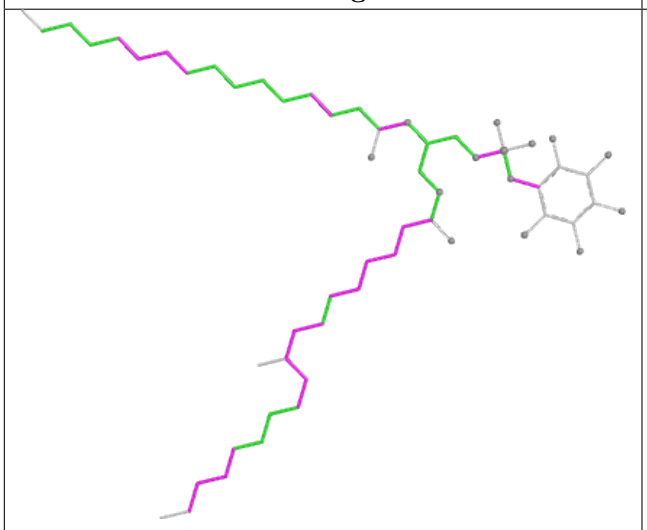


Bond angles



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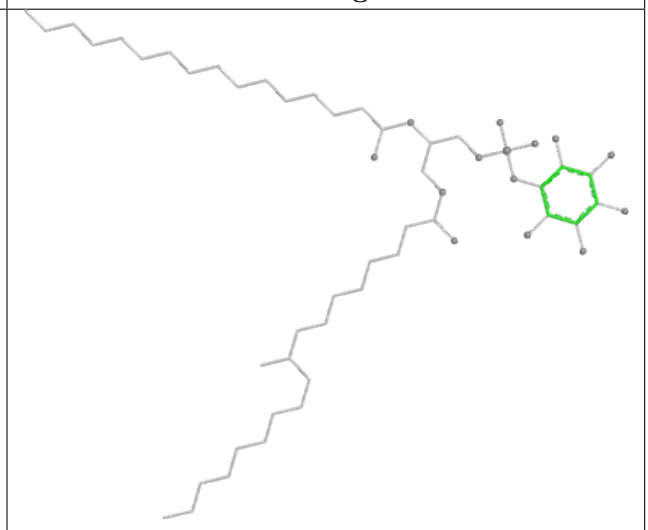
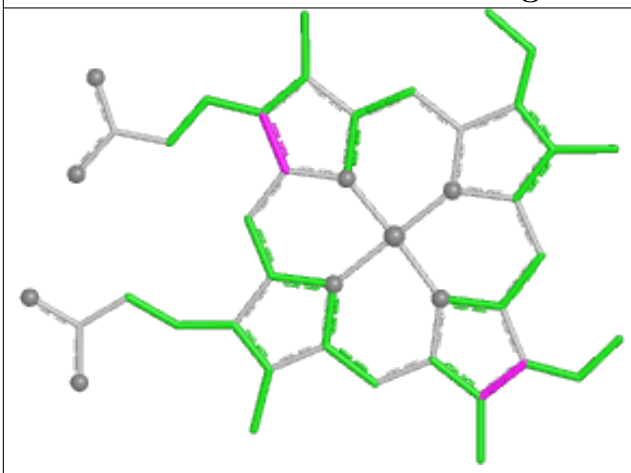
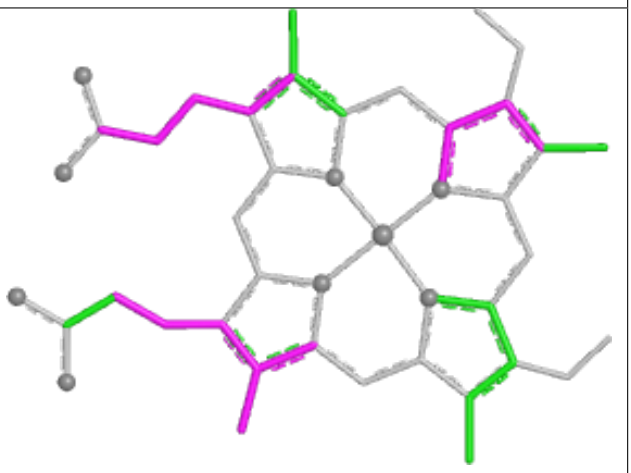


Rings

Ligand HEM b 802	
	
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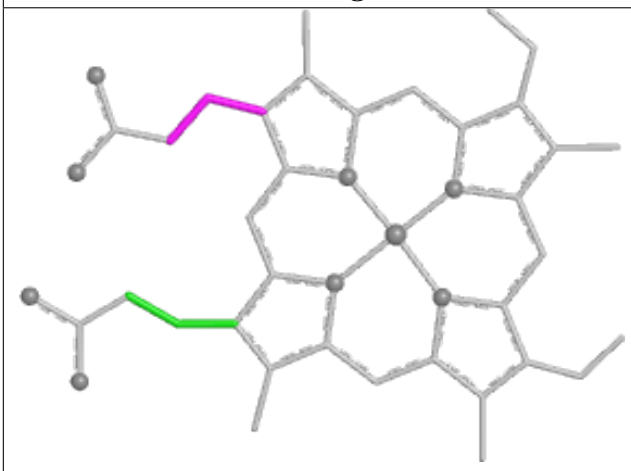
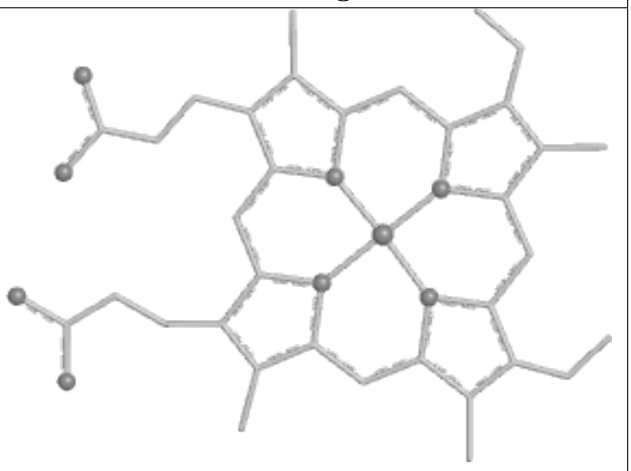
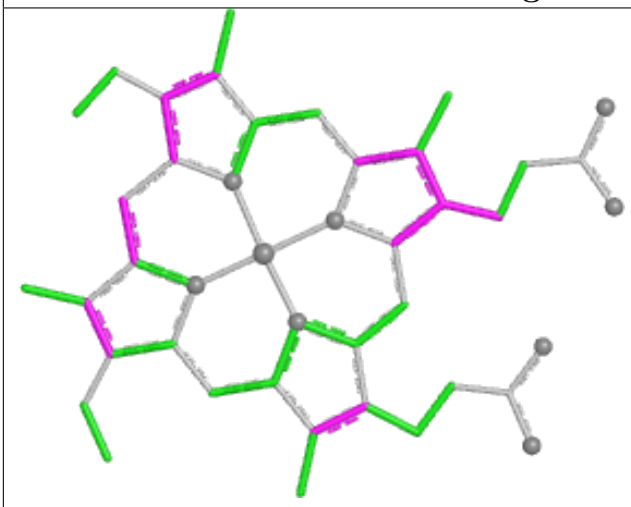
	
Torsions	**Rings**

Ligand HEC C 303



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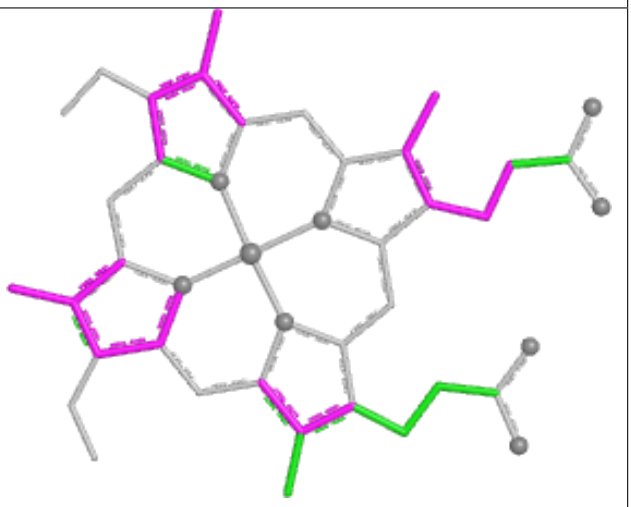
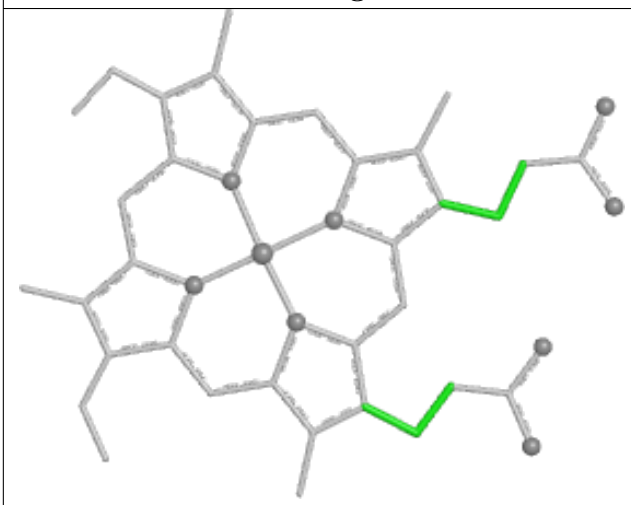
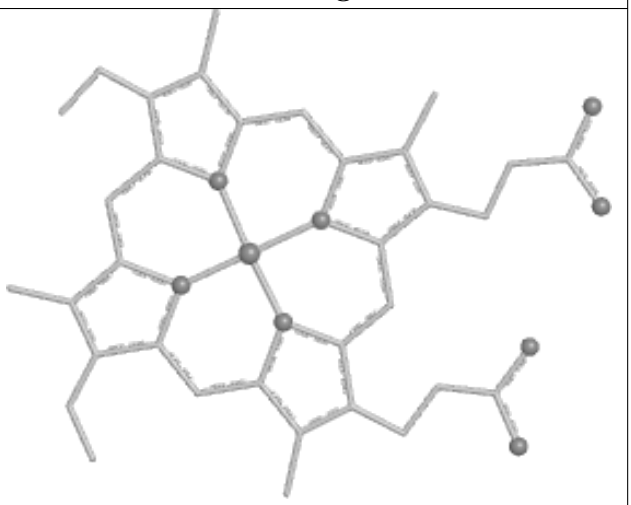


Bond angles

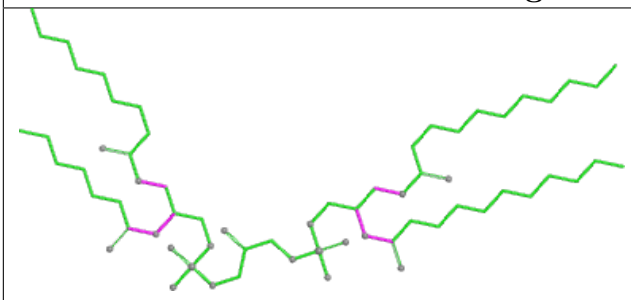


Torsions



Rings

Ligand CDL E 301



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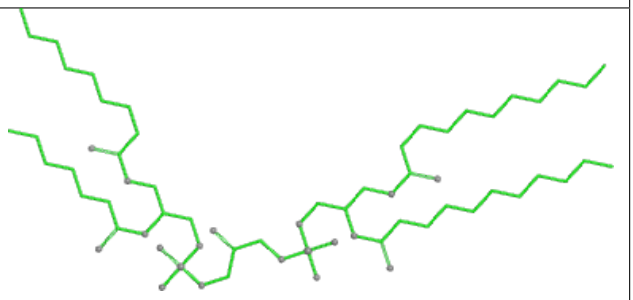
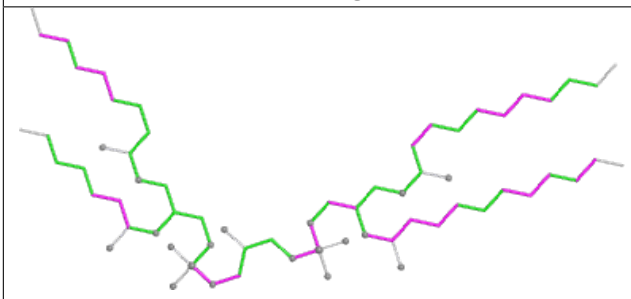


Bond angles



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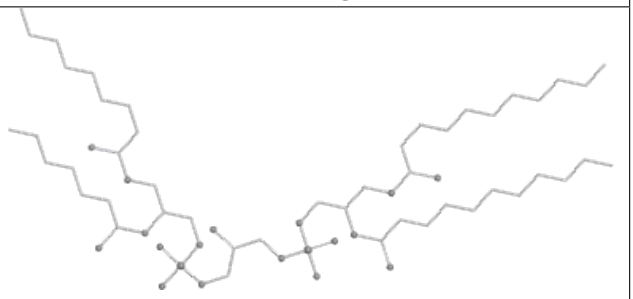
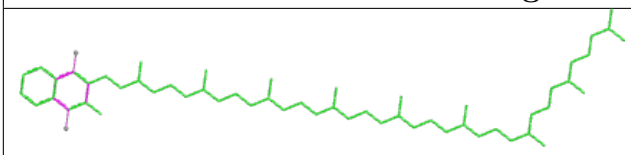
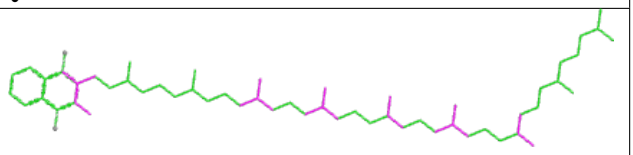


Rings

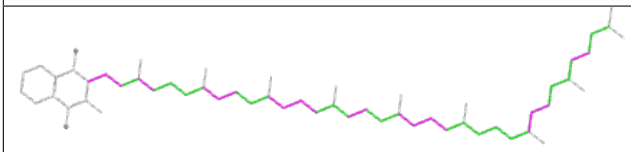
Ligand MQ9 B 604



Bond lengths



Bond angles



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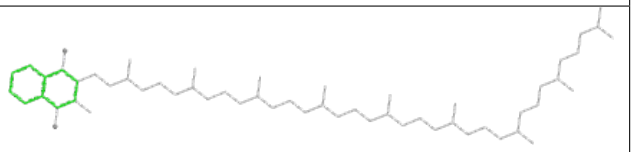
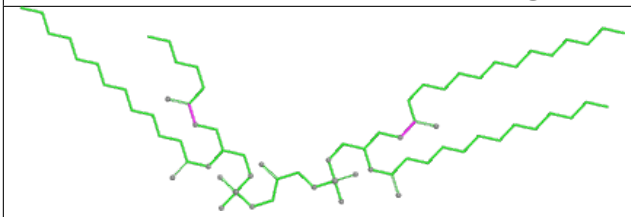


Rings

Ligand CDL B 607



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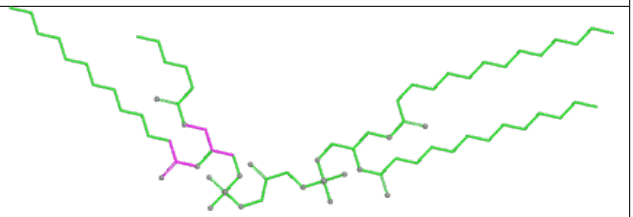

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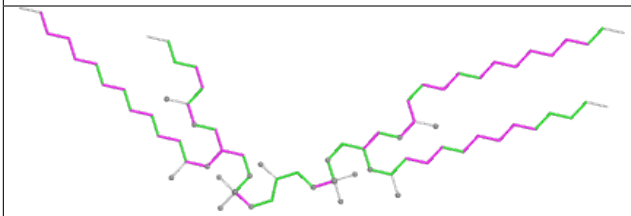

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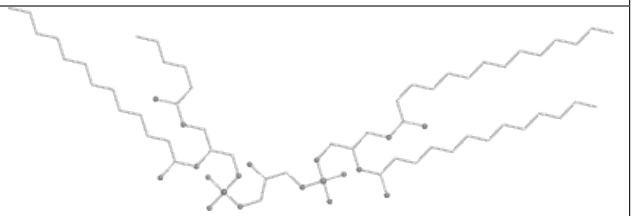
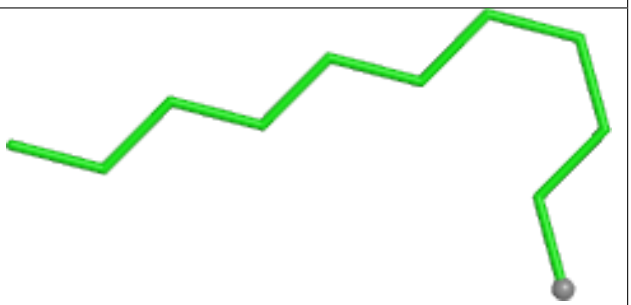


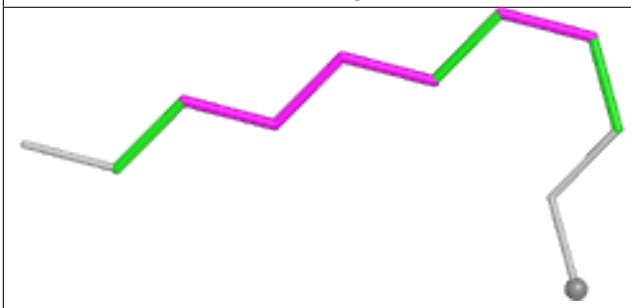
Rings

Ligand PLM x 101

Bond lengths



Bond angles



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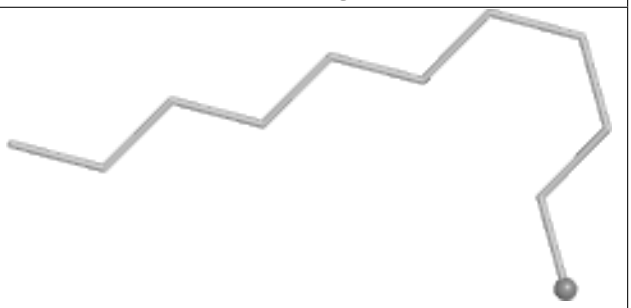
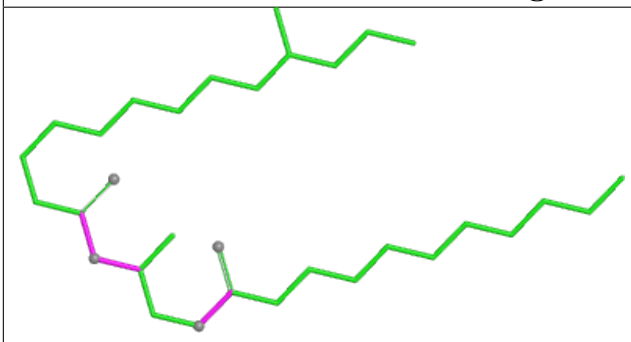


Rings

Ligand 9XX h 204



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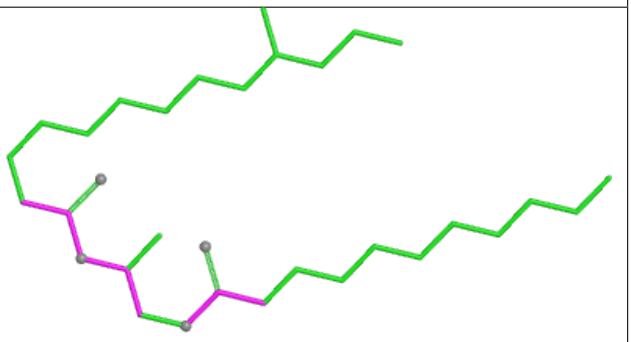
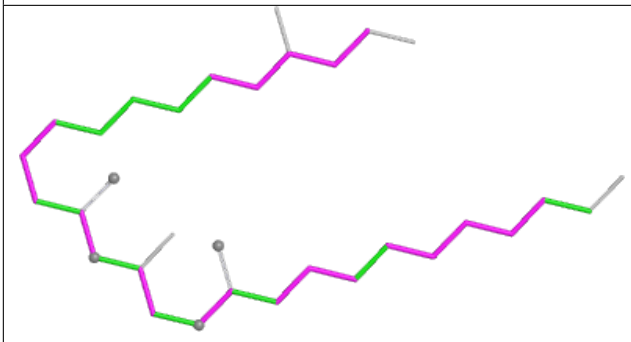


Bond angles



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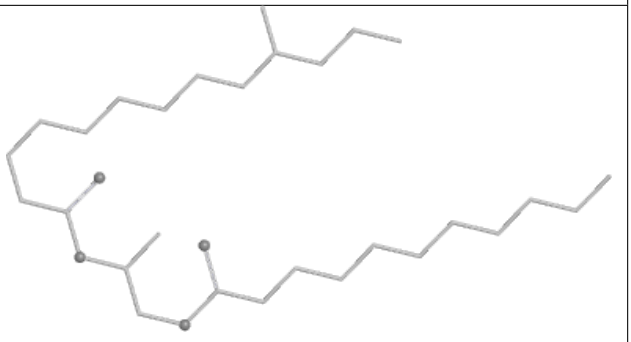
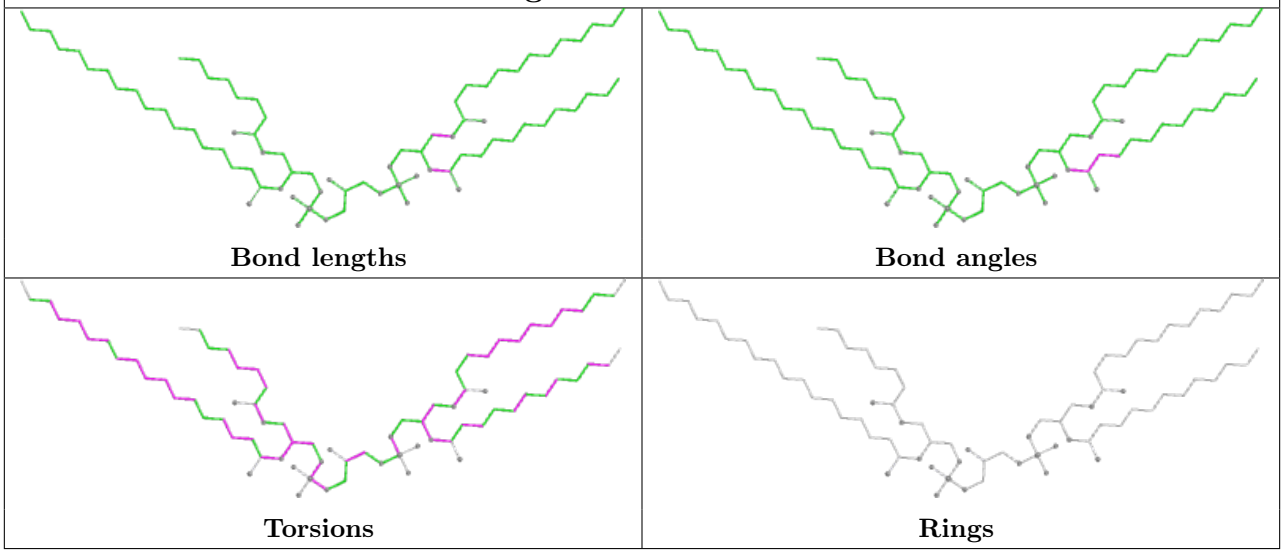
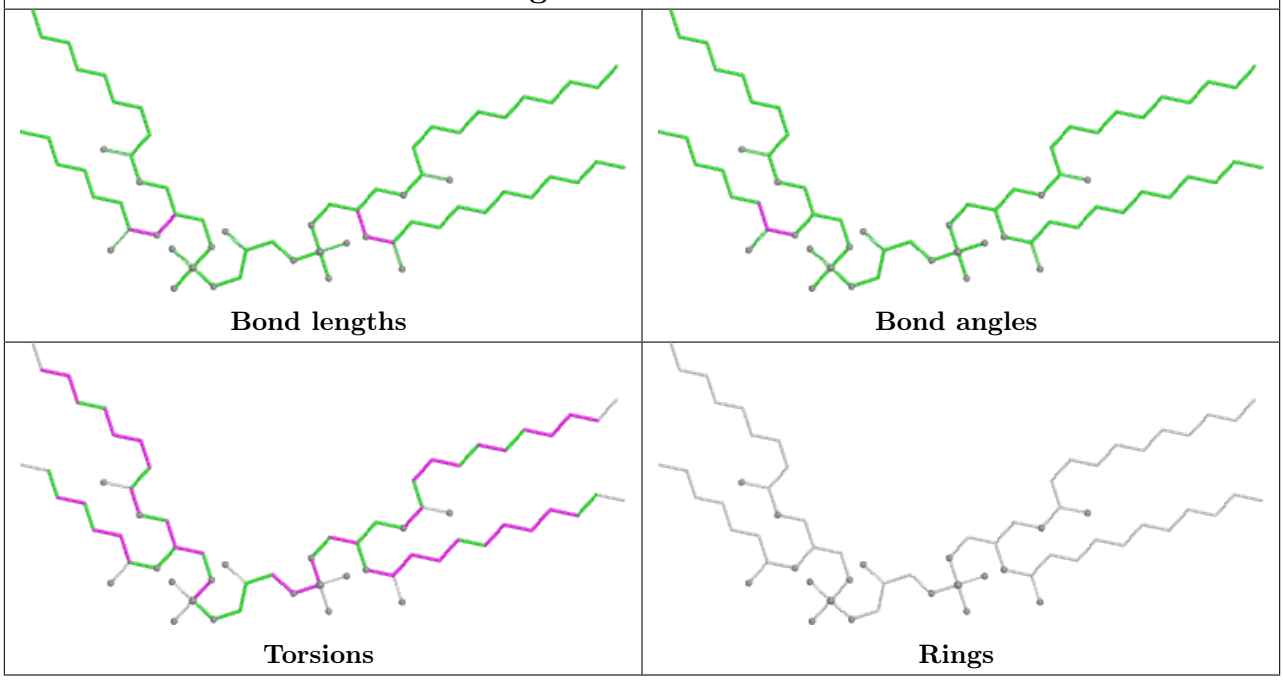


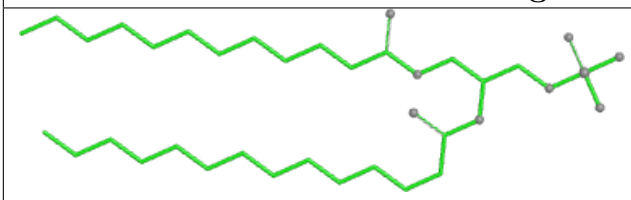
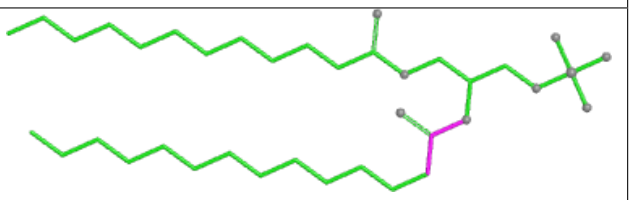
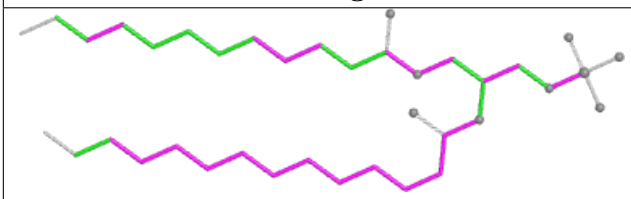
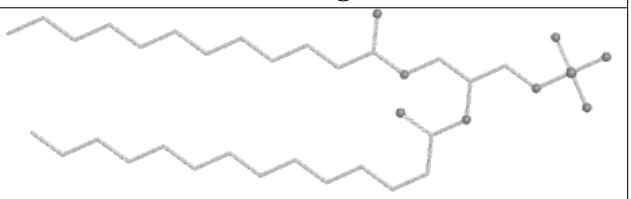
Rings

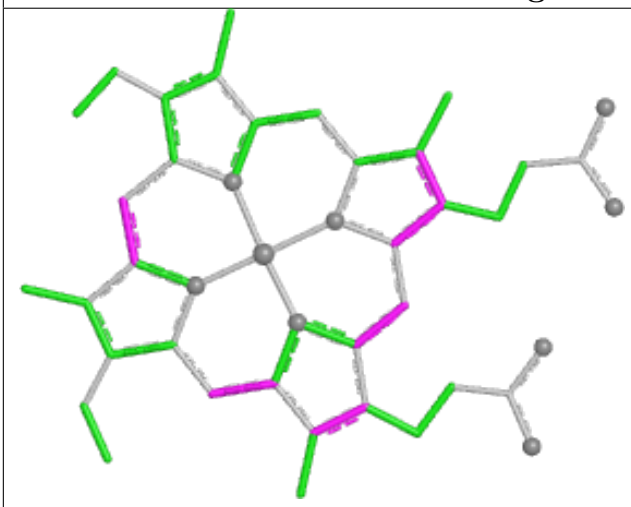
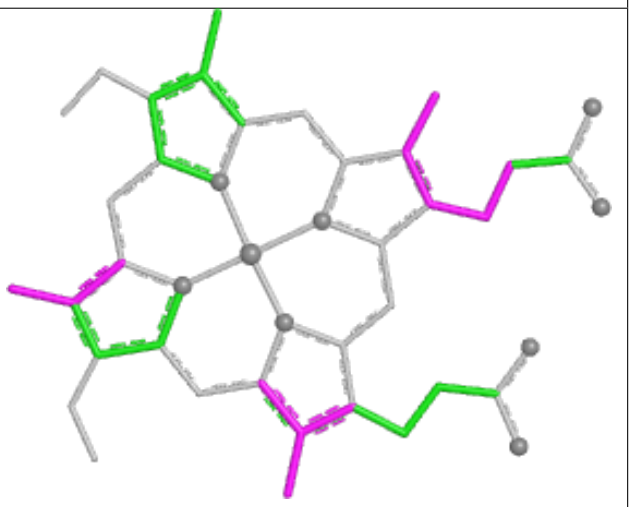
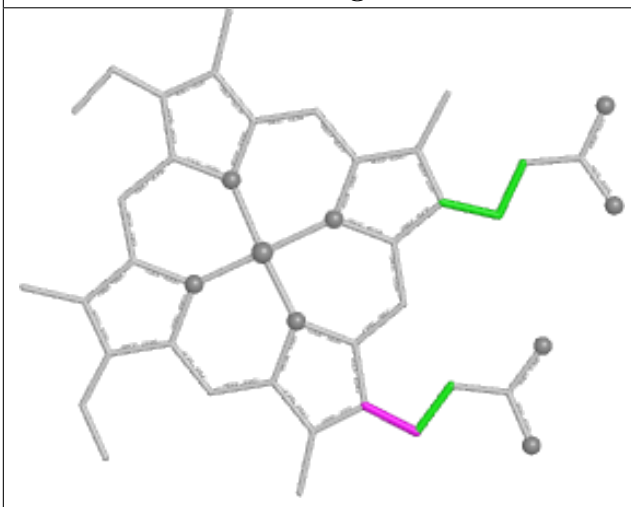
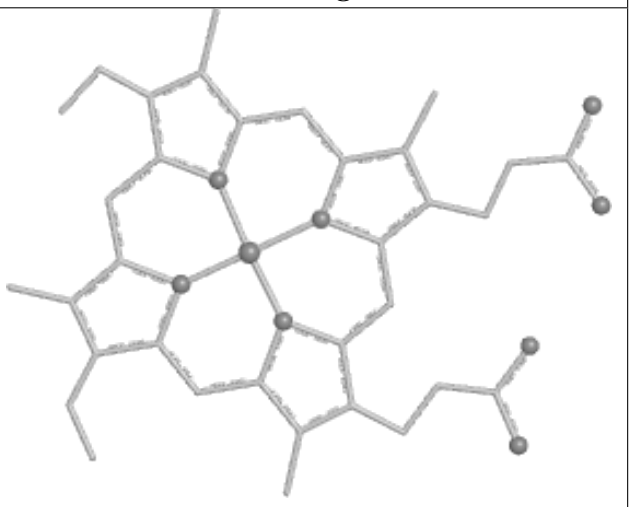
Ligand CDL C 301



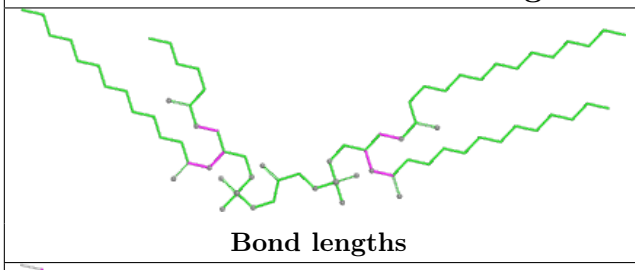
Ligand CDL e 301



Ligand 7PH d 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC c 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CDL D 606



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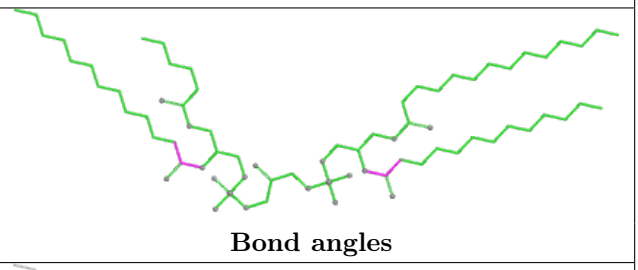
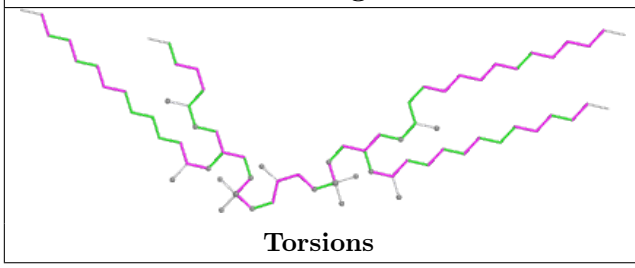
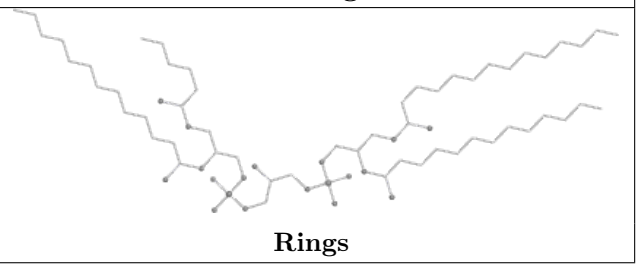


Bond angles

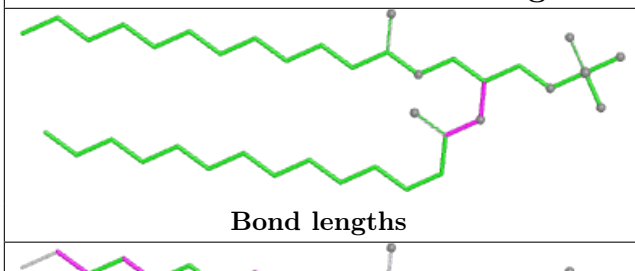


Torsions



Rings

Ligand 7PH E 302



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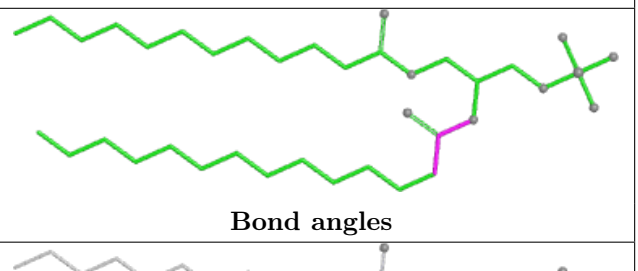

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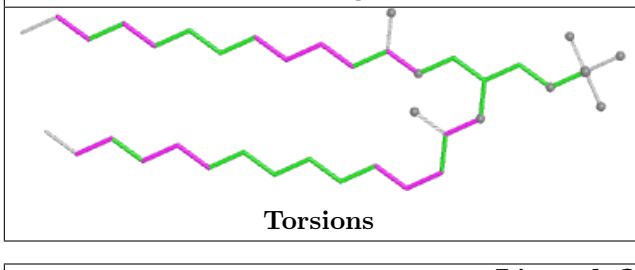

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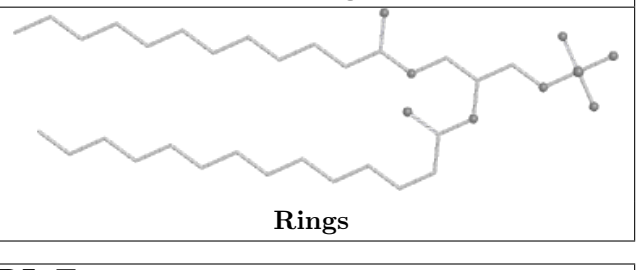
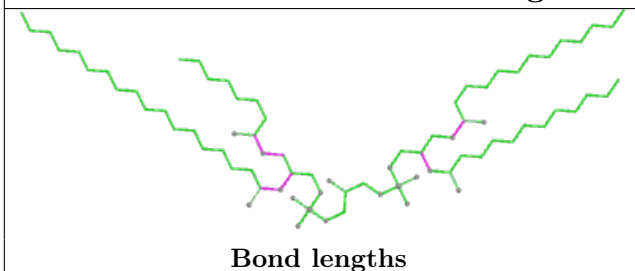


Rings

Ligand CDL F 202



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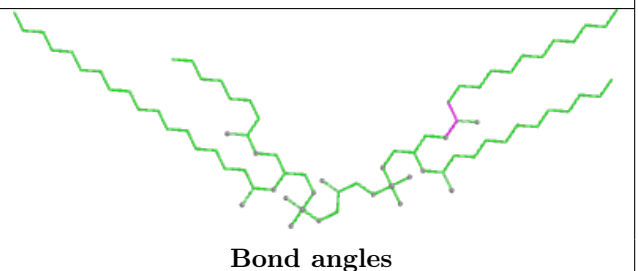

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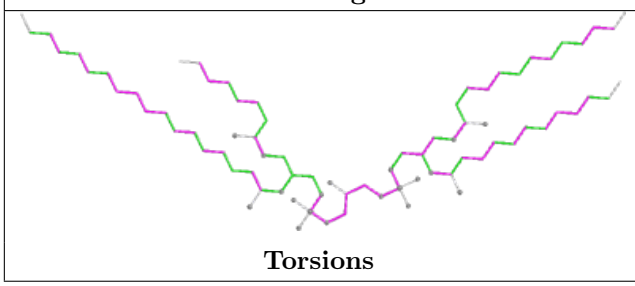

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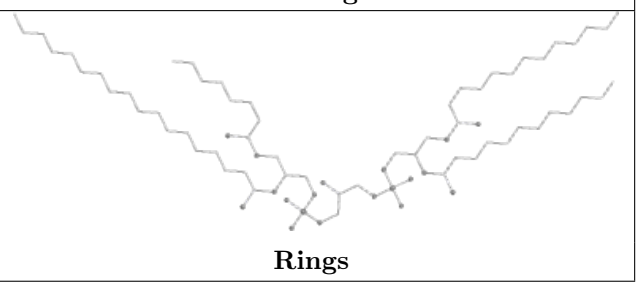
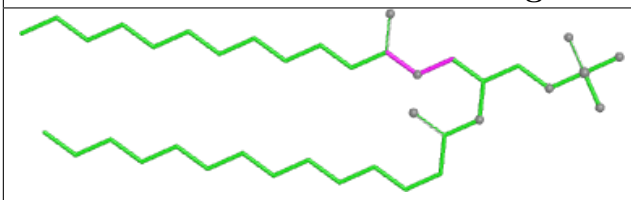


Rings

Ligand 7PH D 610



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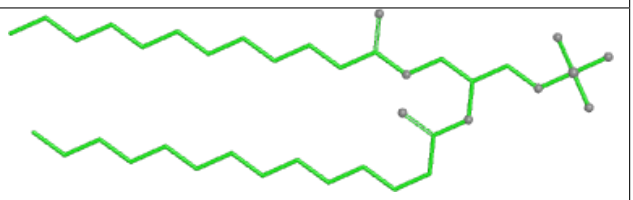
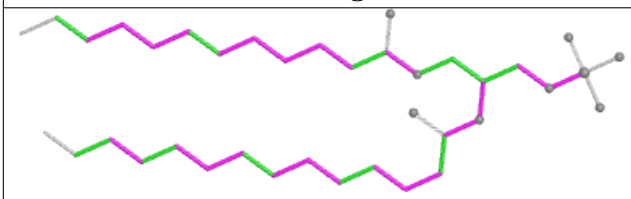
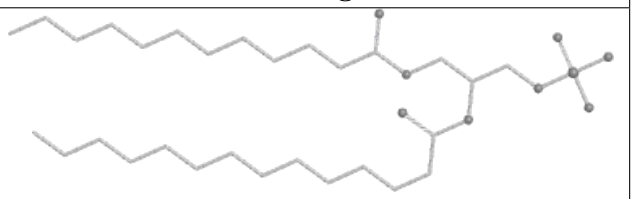


Bond angles

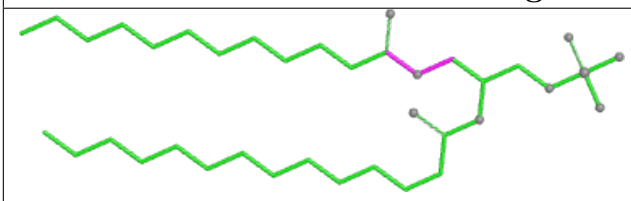


Torsions



Rings

Ligand 7PH D 607



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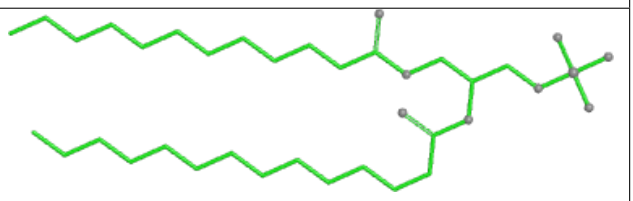

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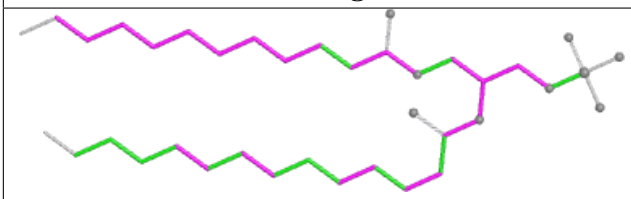

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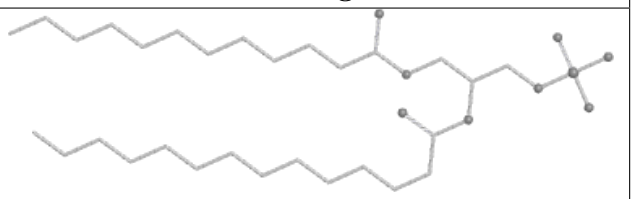
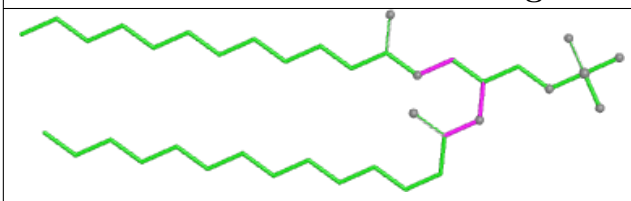


Rings

Ligand 7PH D 608



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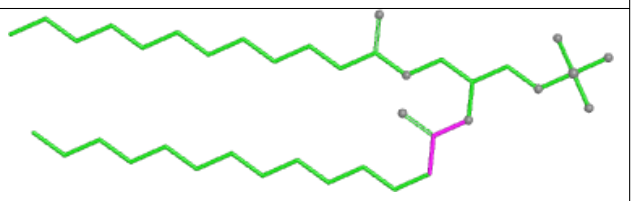

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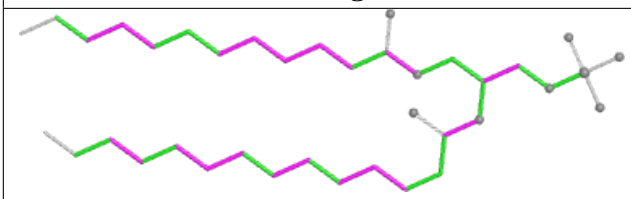

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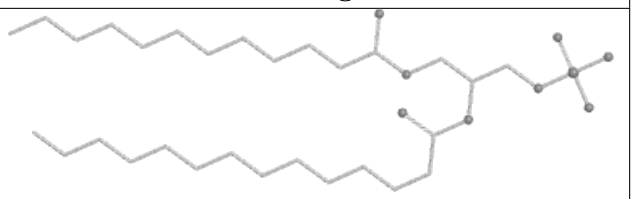
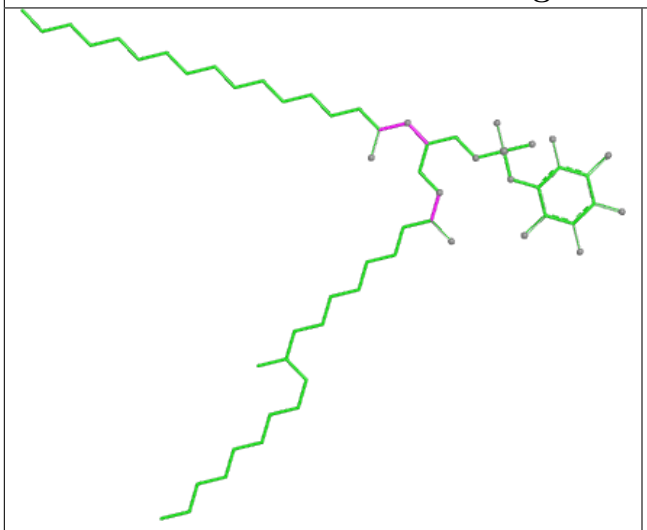


Rings

Ligand 9YF a 601



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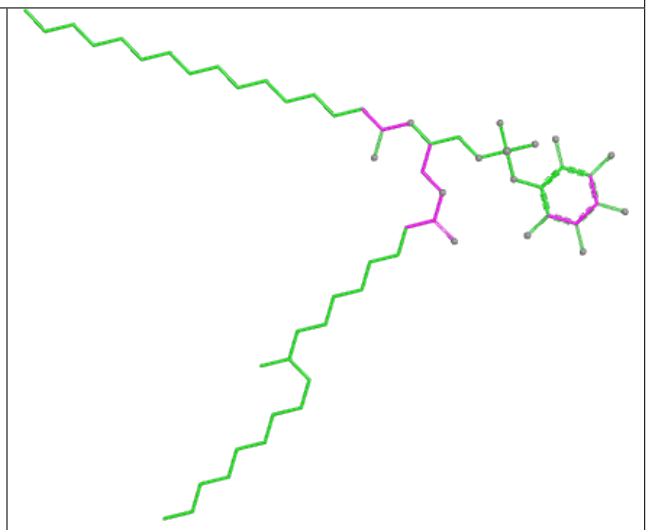

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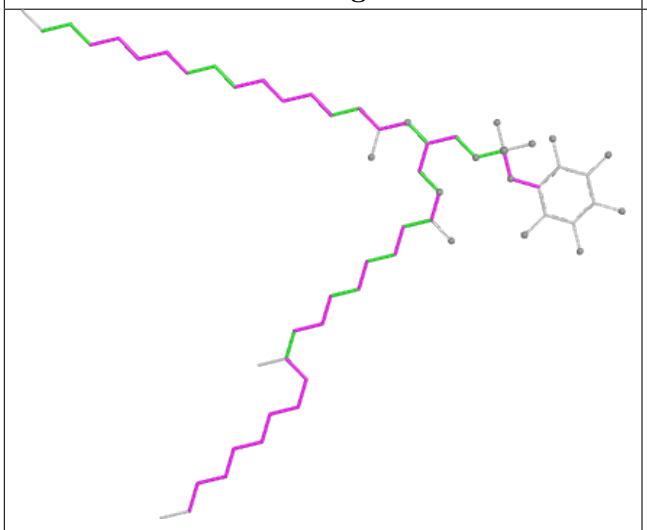

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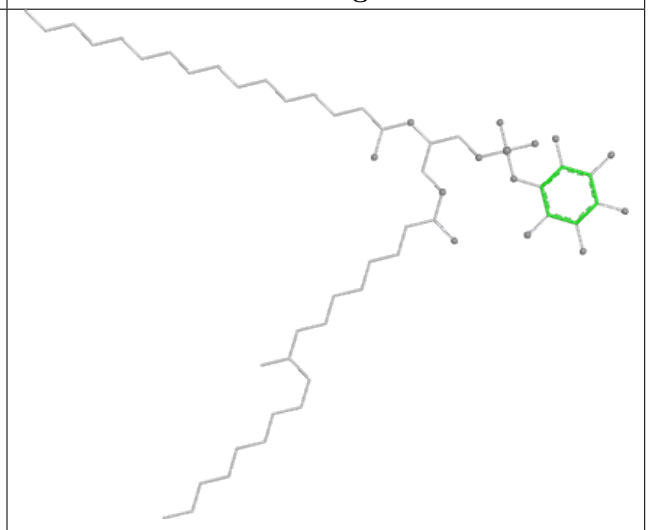
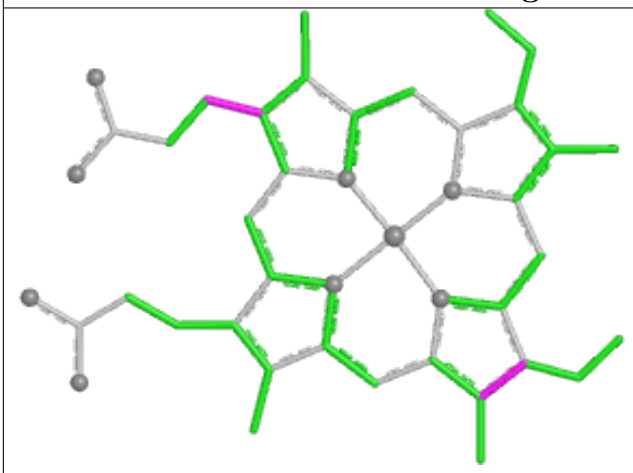


Rings

Ligand HEM b 803



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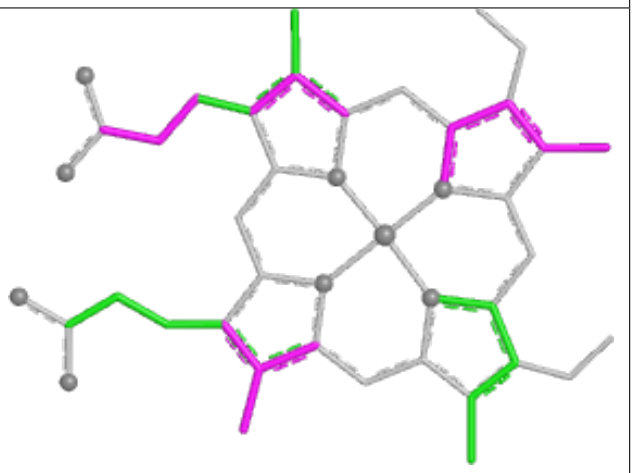

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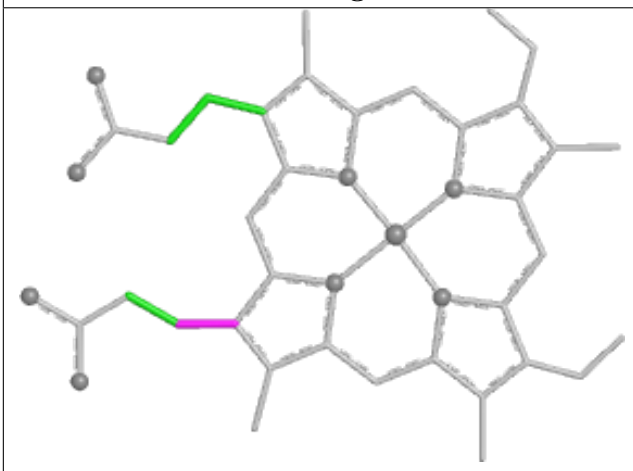

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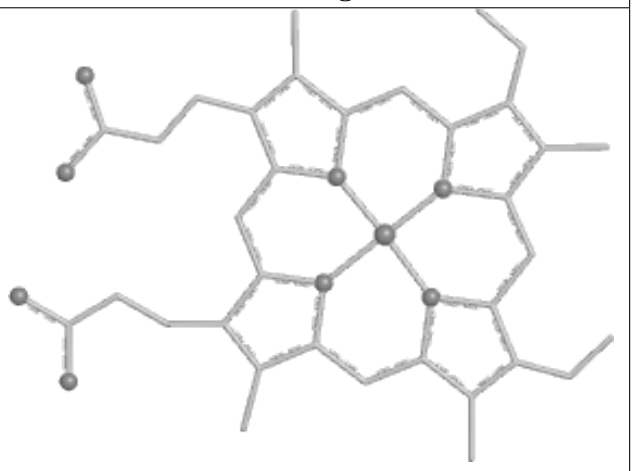
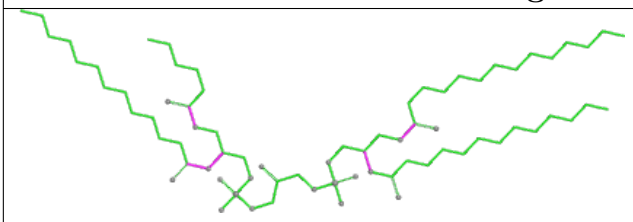
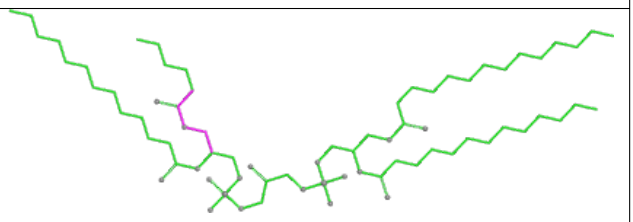


Rings

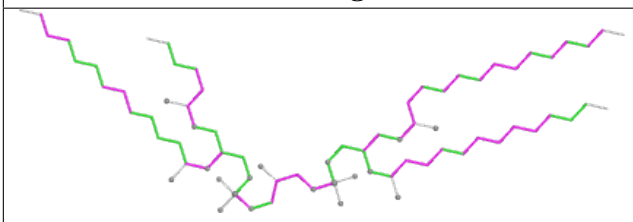
Ligand CDL b 801



Bond lengths



Bond angles



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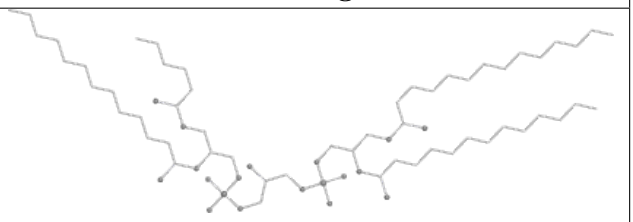
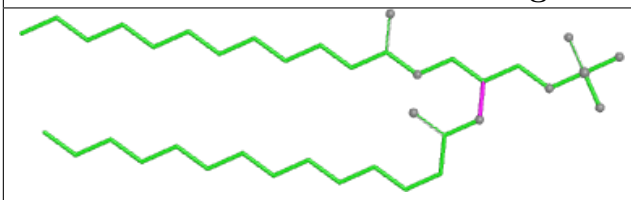
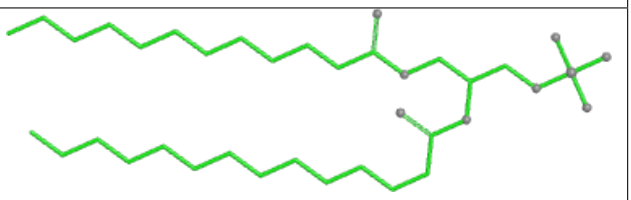
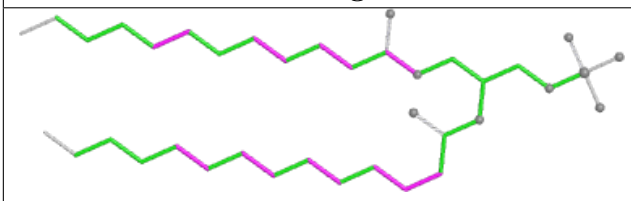
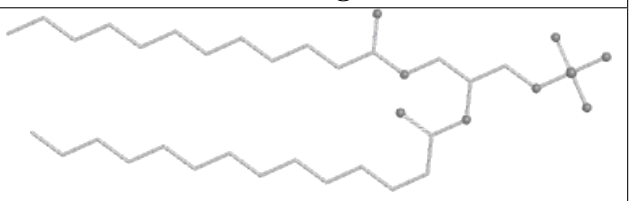
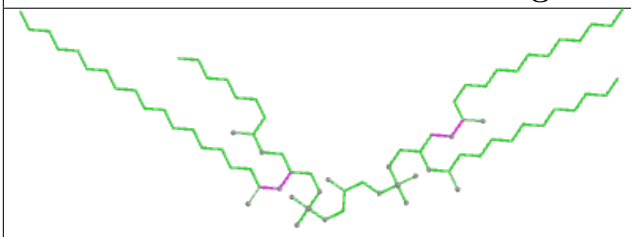
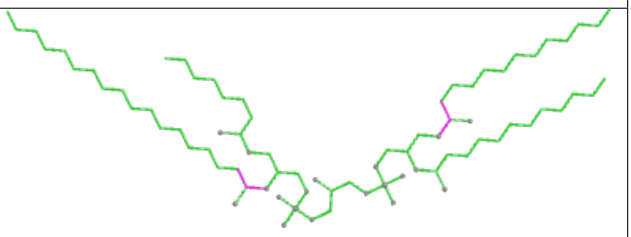
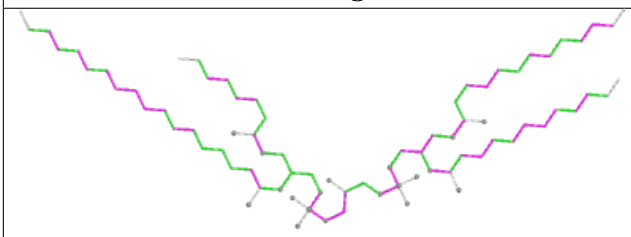
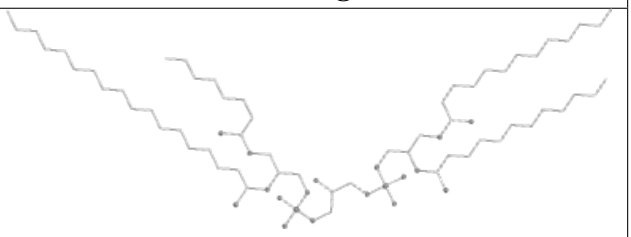
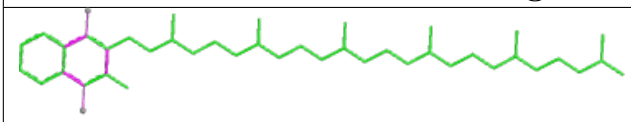
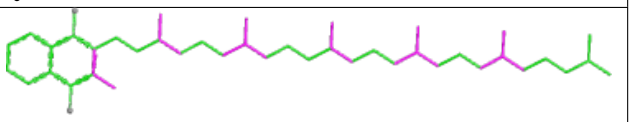
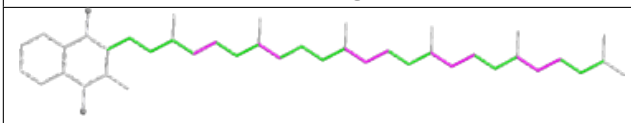
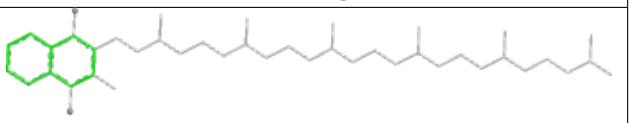
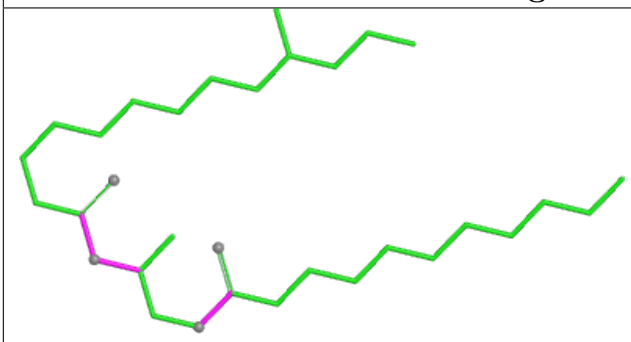
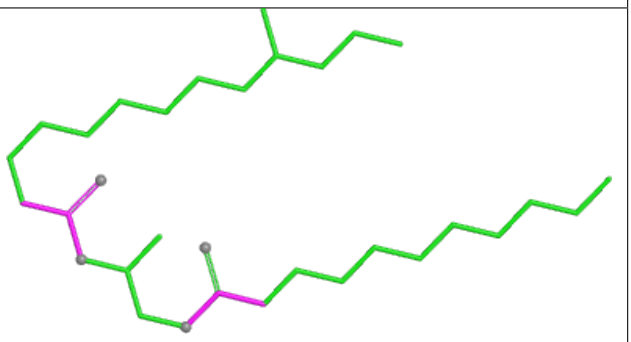
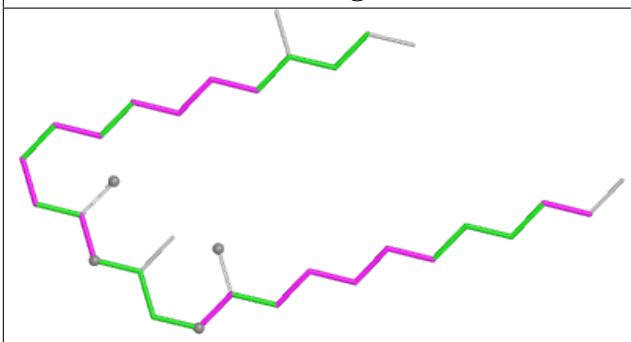
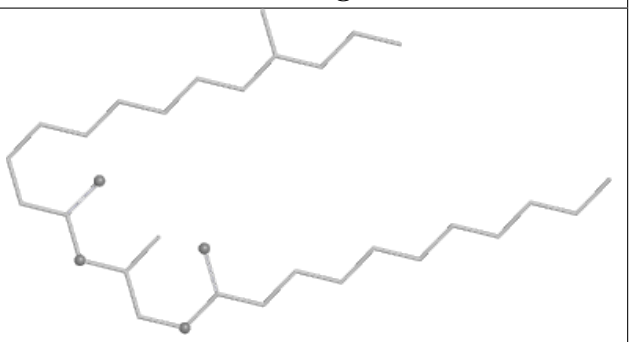


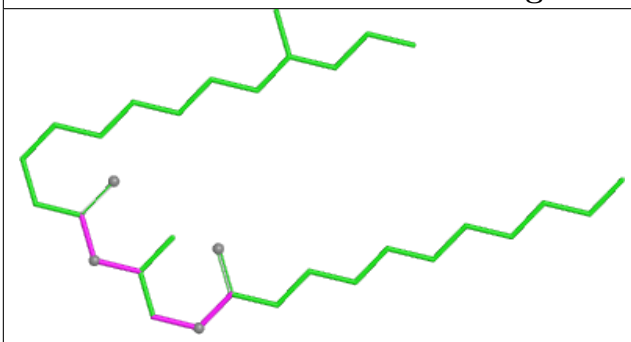
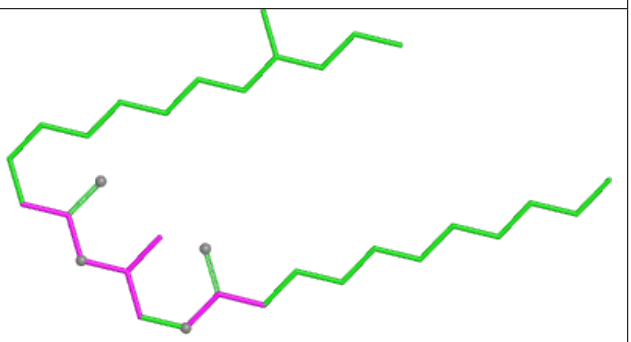
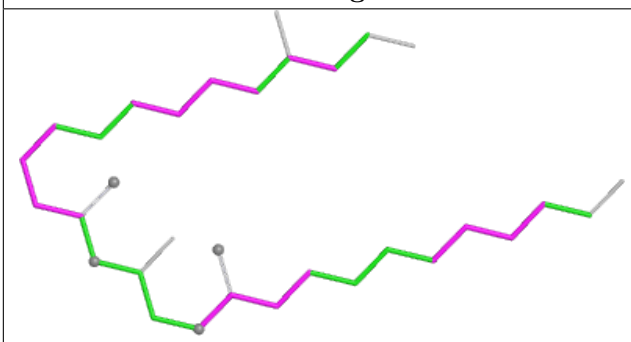
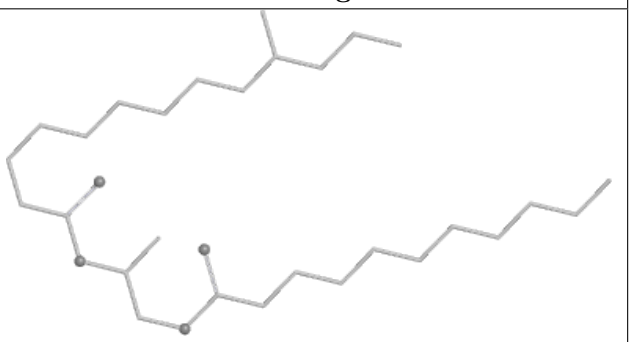
Rings

Ligand 7PH k 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

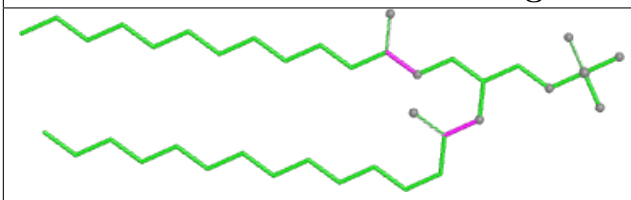
Ligand CDL f 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQ9 a 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

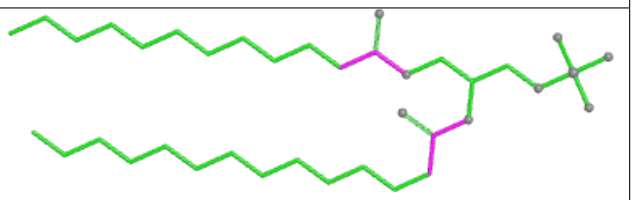
Ligand 9XX h 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 9XX B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

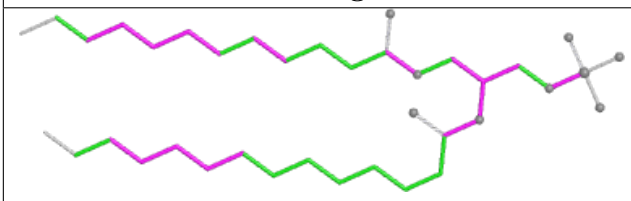
Ligand 7PH H 201



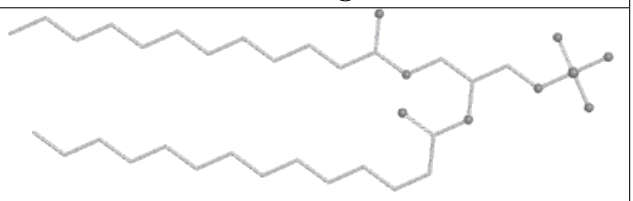
Bond lengths



Bond angles

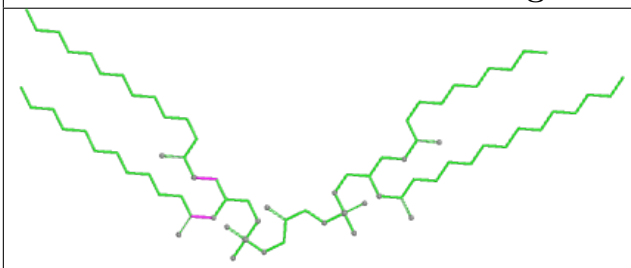


Torsions

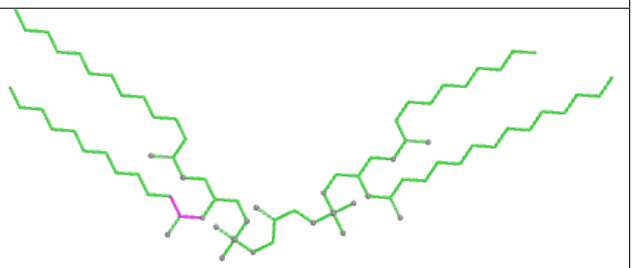


Rings

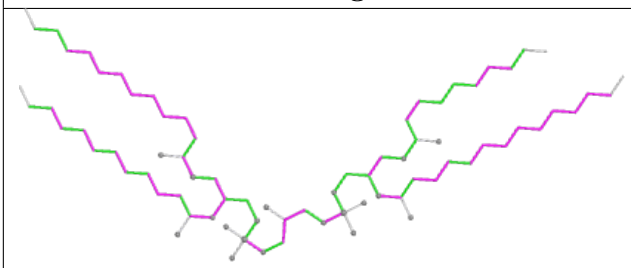
Ligand CDL b 806



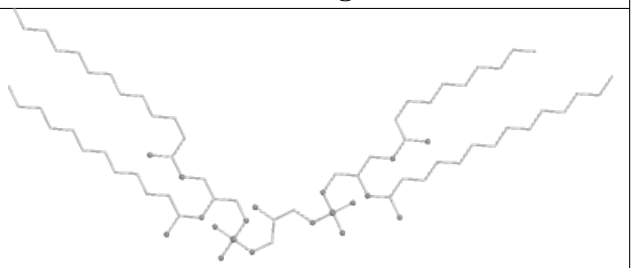
Bond lengths



Bond angles

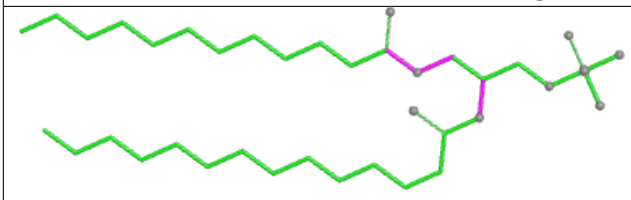


Torsions

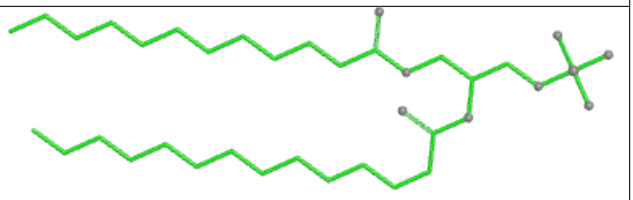


Rings

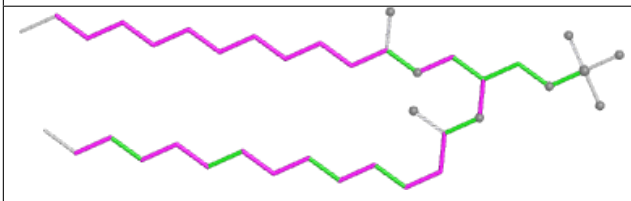
Ligand 7PH e 302



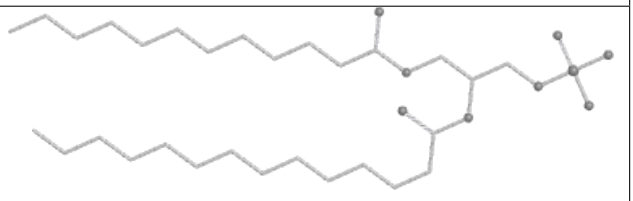
Bond lengths



Bond angles

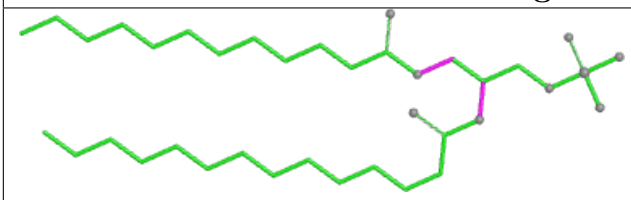


Torsions

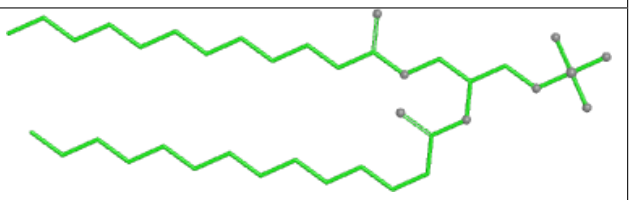


Rings

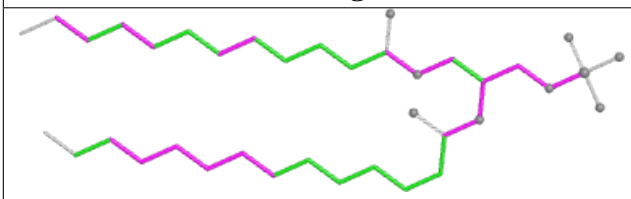
Ligand 7PH f 207



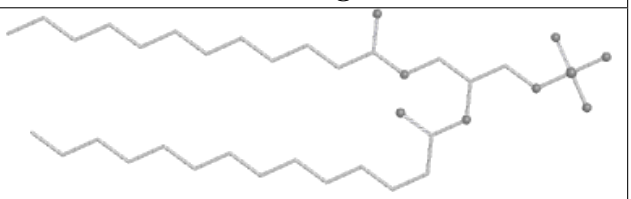
Bond lengths



Bond angles

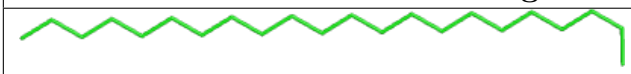


Torsions

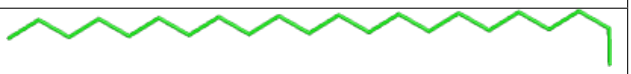


Rings

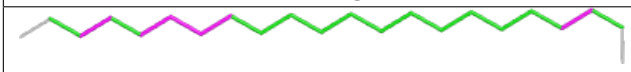
Ligand TWT h 203



Bond lengths



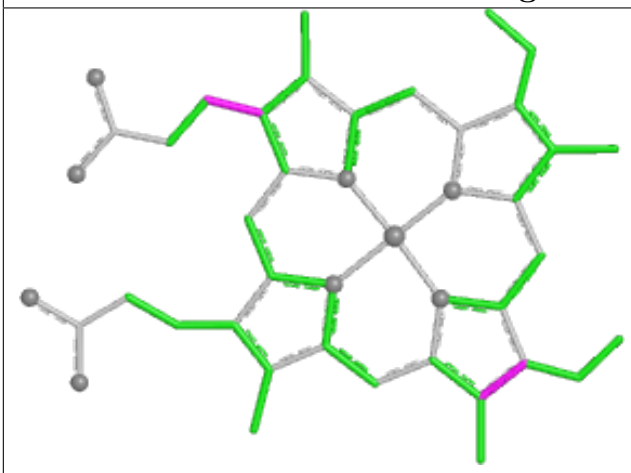
Bond angles



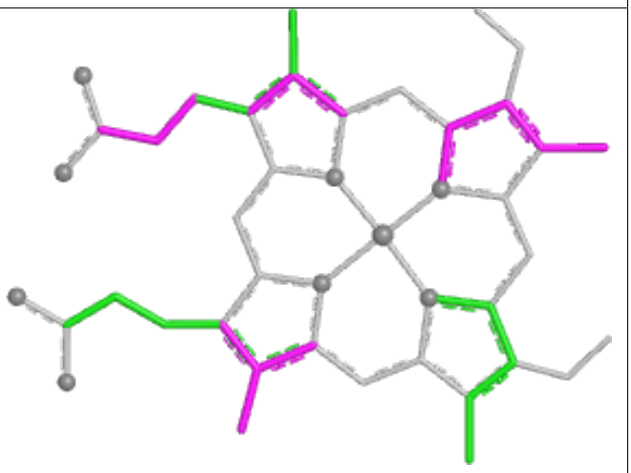
Torsions

Rings

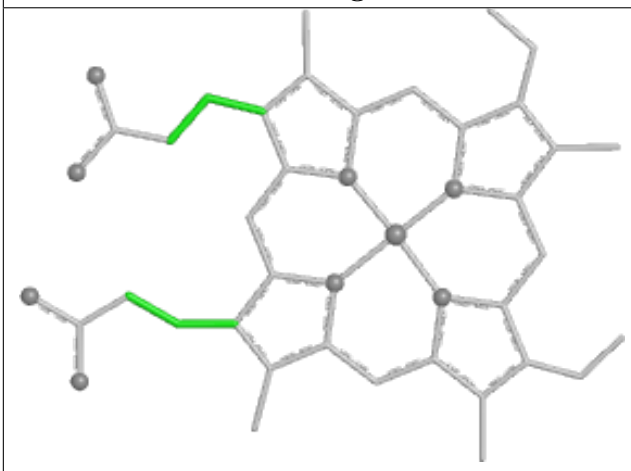
Ligand HEM B 602



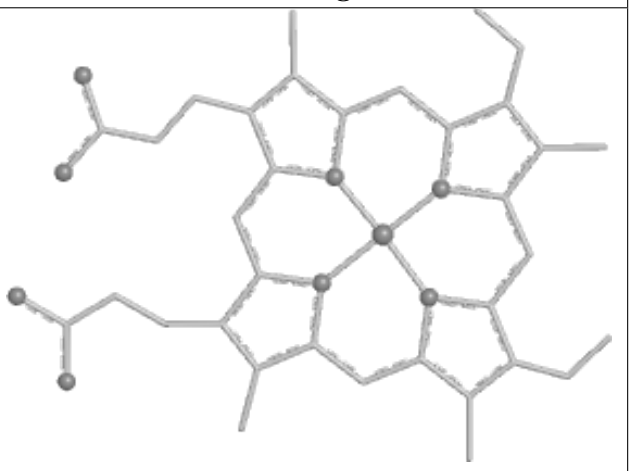
Bond lengths



Bond angles

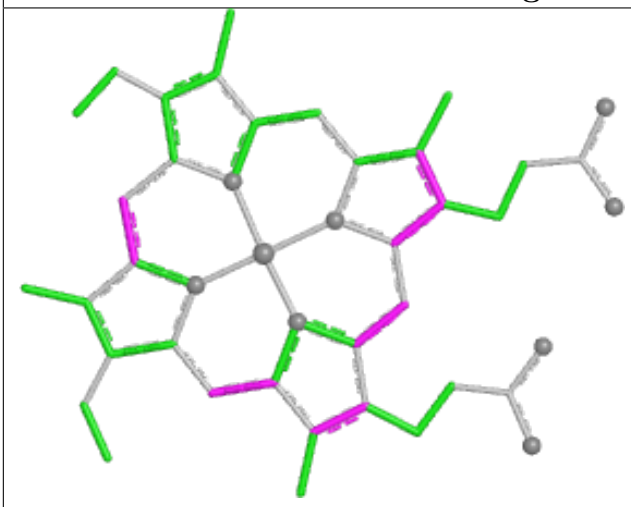


Torsions

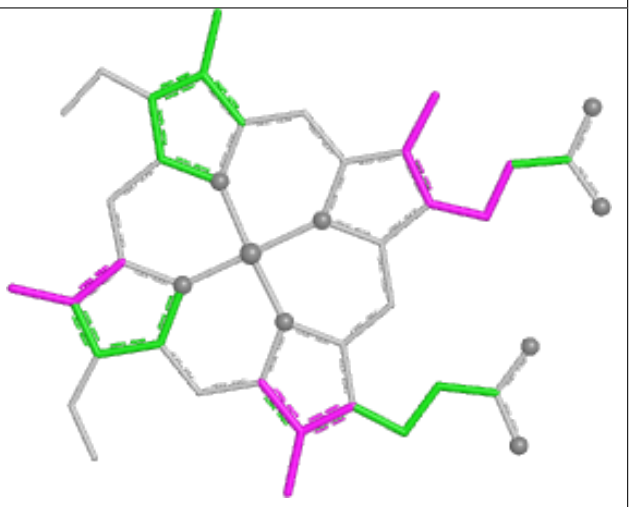


Rings

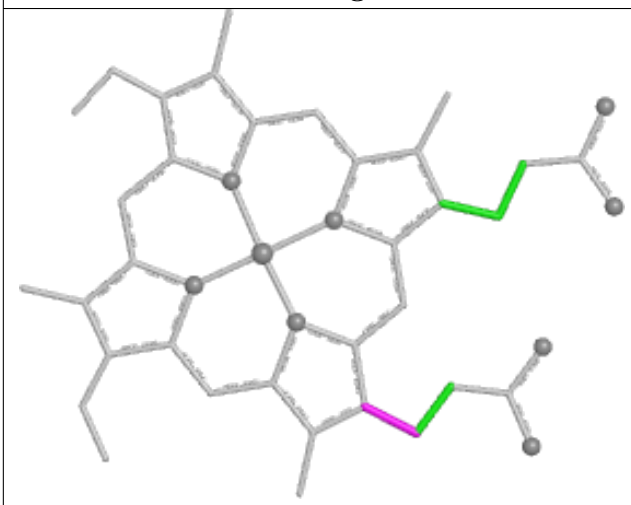
Ligand HEC C 302



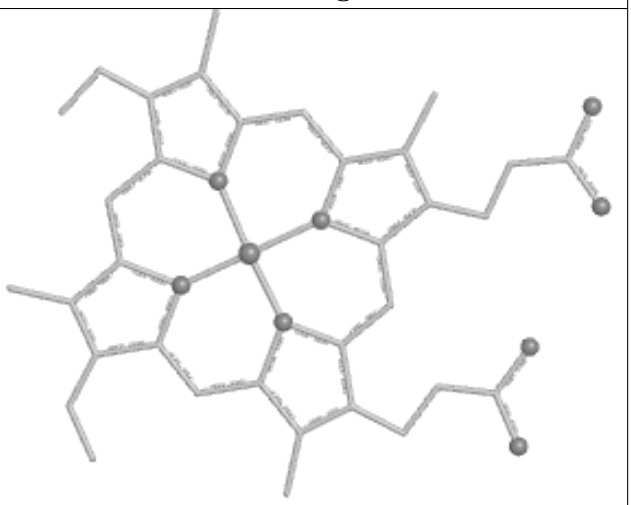
Bond lengths



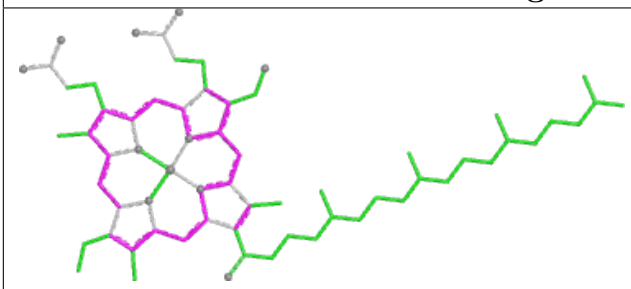
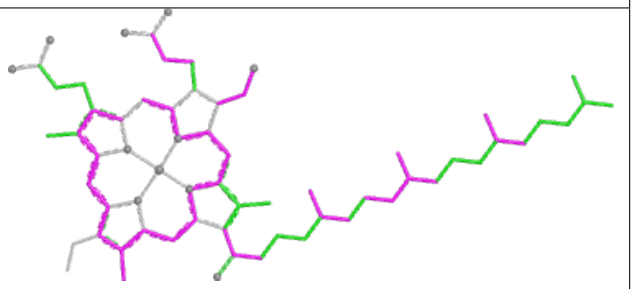
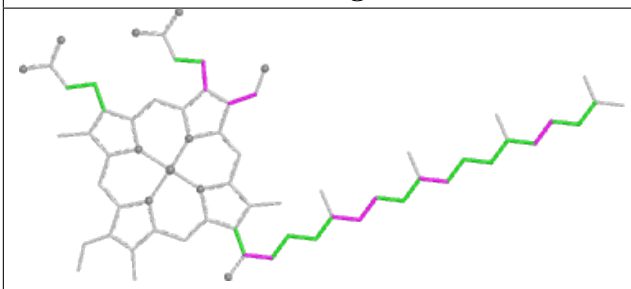
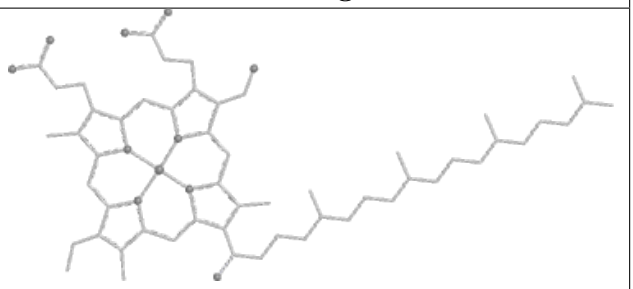
Bond angles

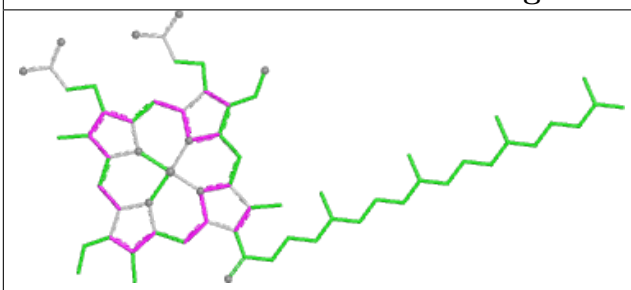
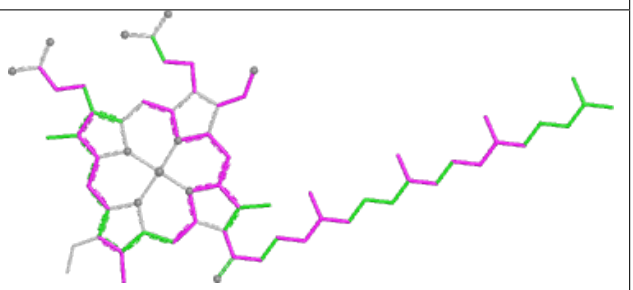
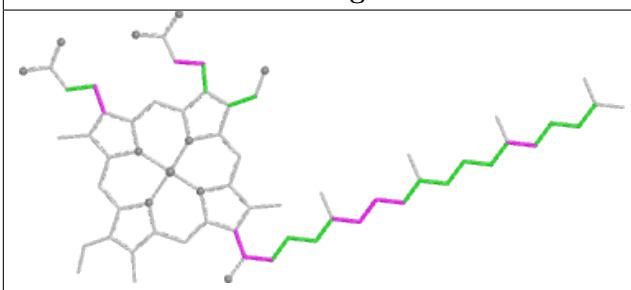
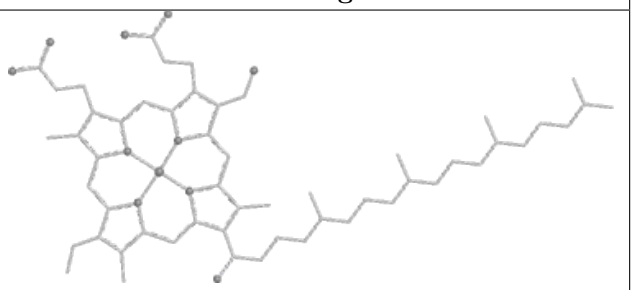


Torsions

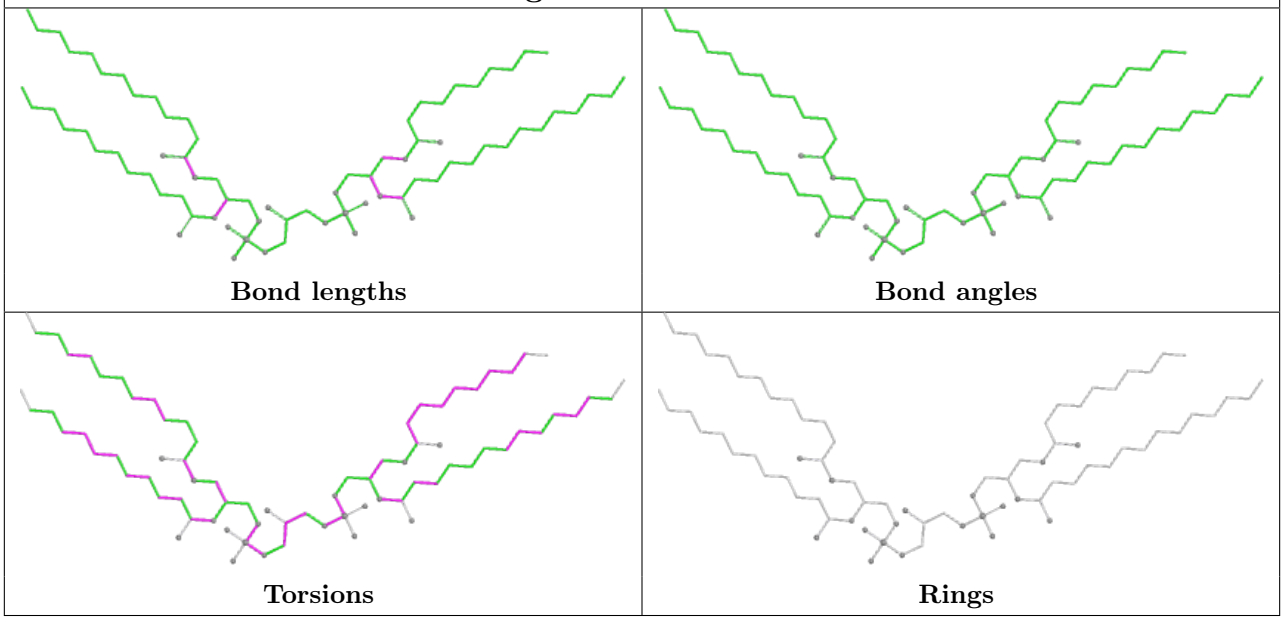


Rings

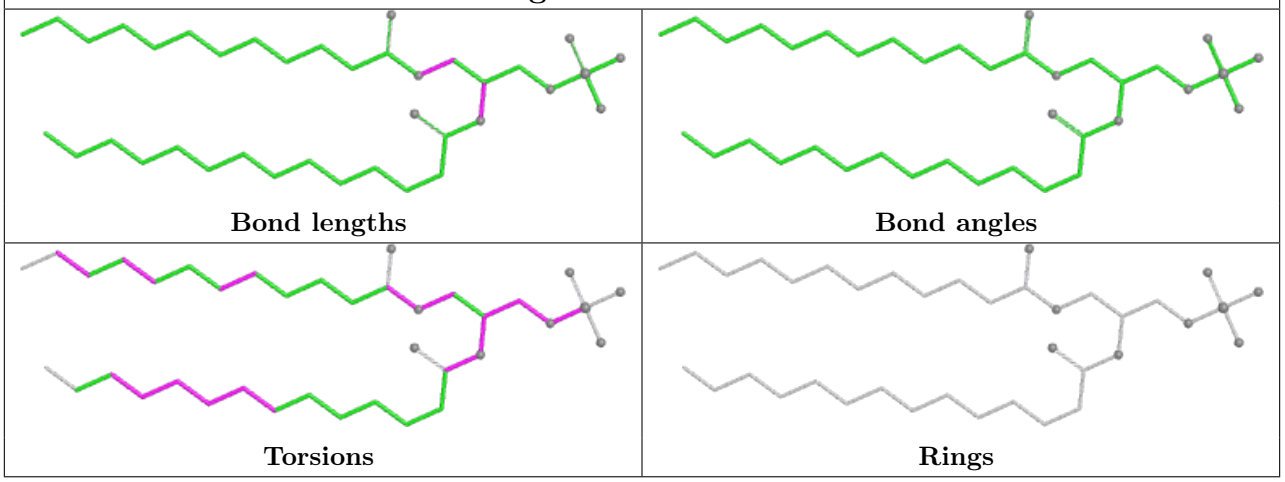
Ligand HAS d 604	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand HAS D 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

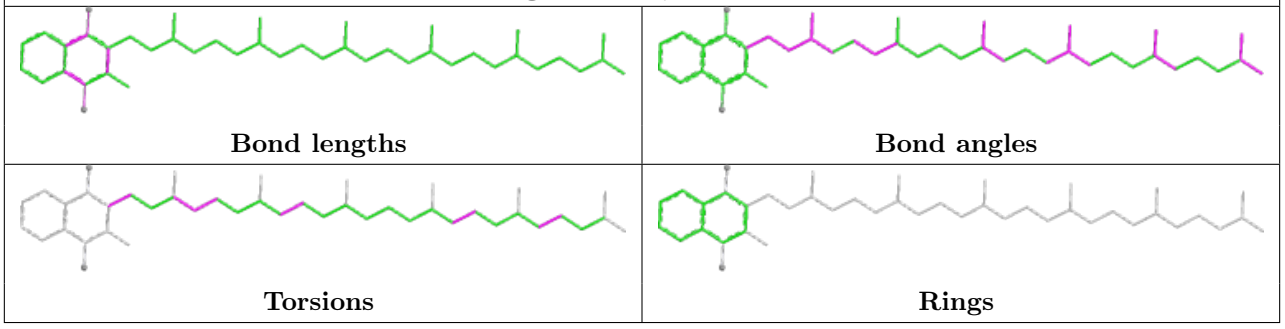
Ligand CDL B 605



Ligand 7PH F 207



Ligand MQ9 B 603



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

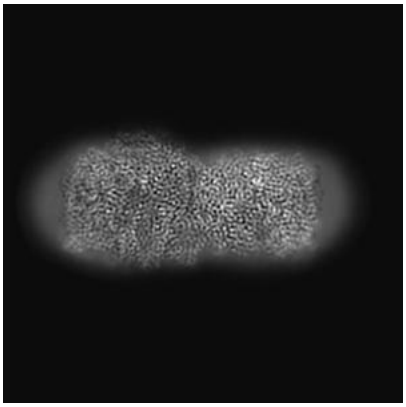
This section contains visualisations of the EMDB entry EMD-13777. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

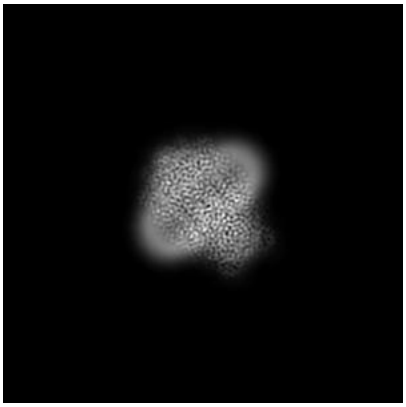
6.1 Orthogonal projections

6.1.1 Primary map

X



Y

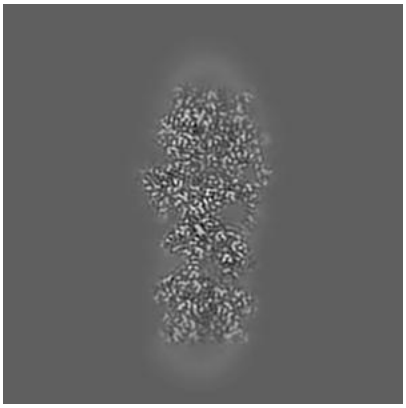


Z

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

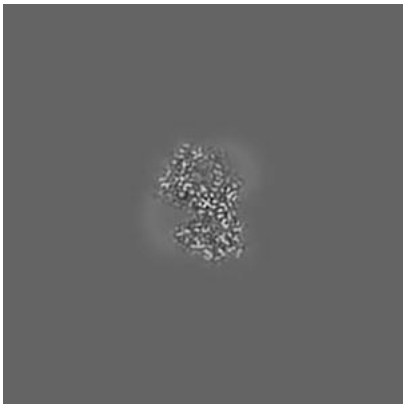
6.2 Central slices

6.2.1 Primary map



X Index: 155

Y Index: 155

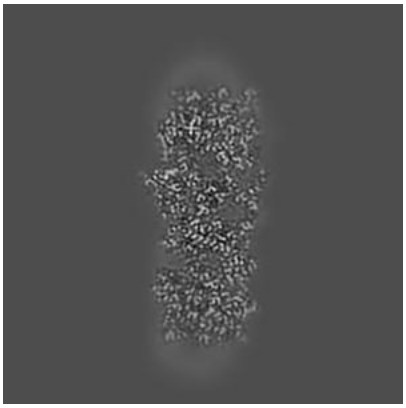


Z Index: 155

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

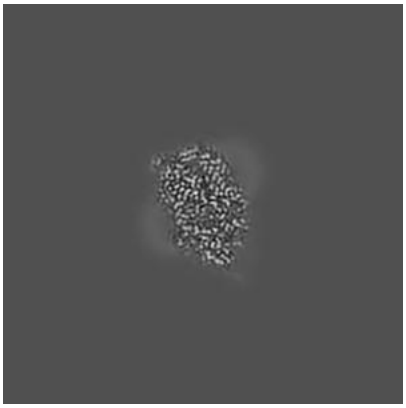
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 149

Y Index: 160



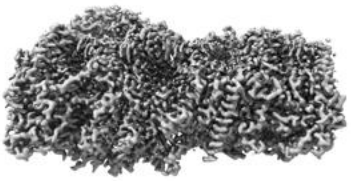
Z Index: 166

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.541. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

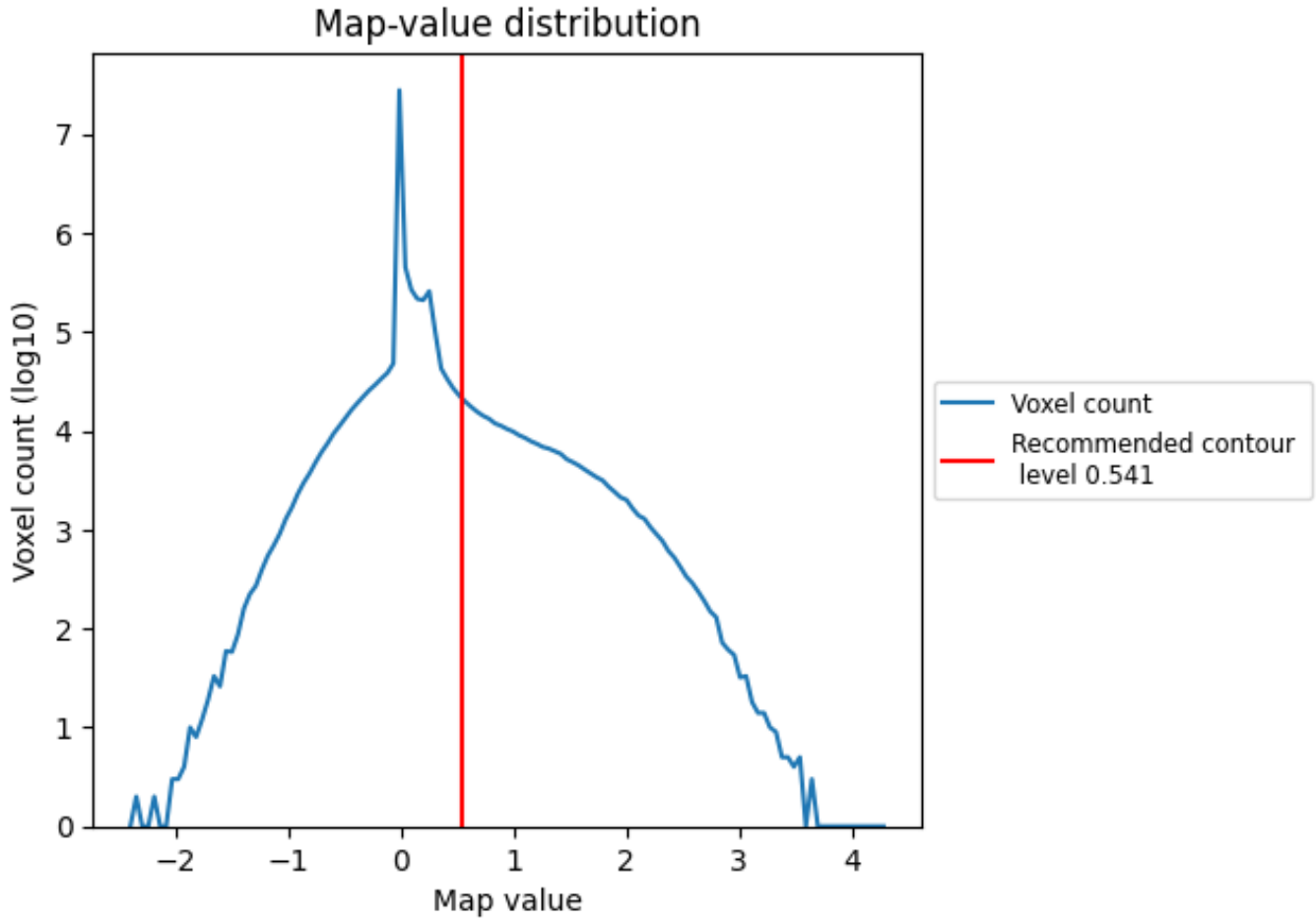
6.5 Mask visualisation (i)

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

7 Map analysis

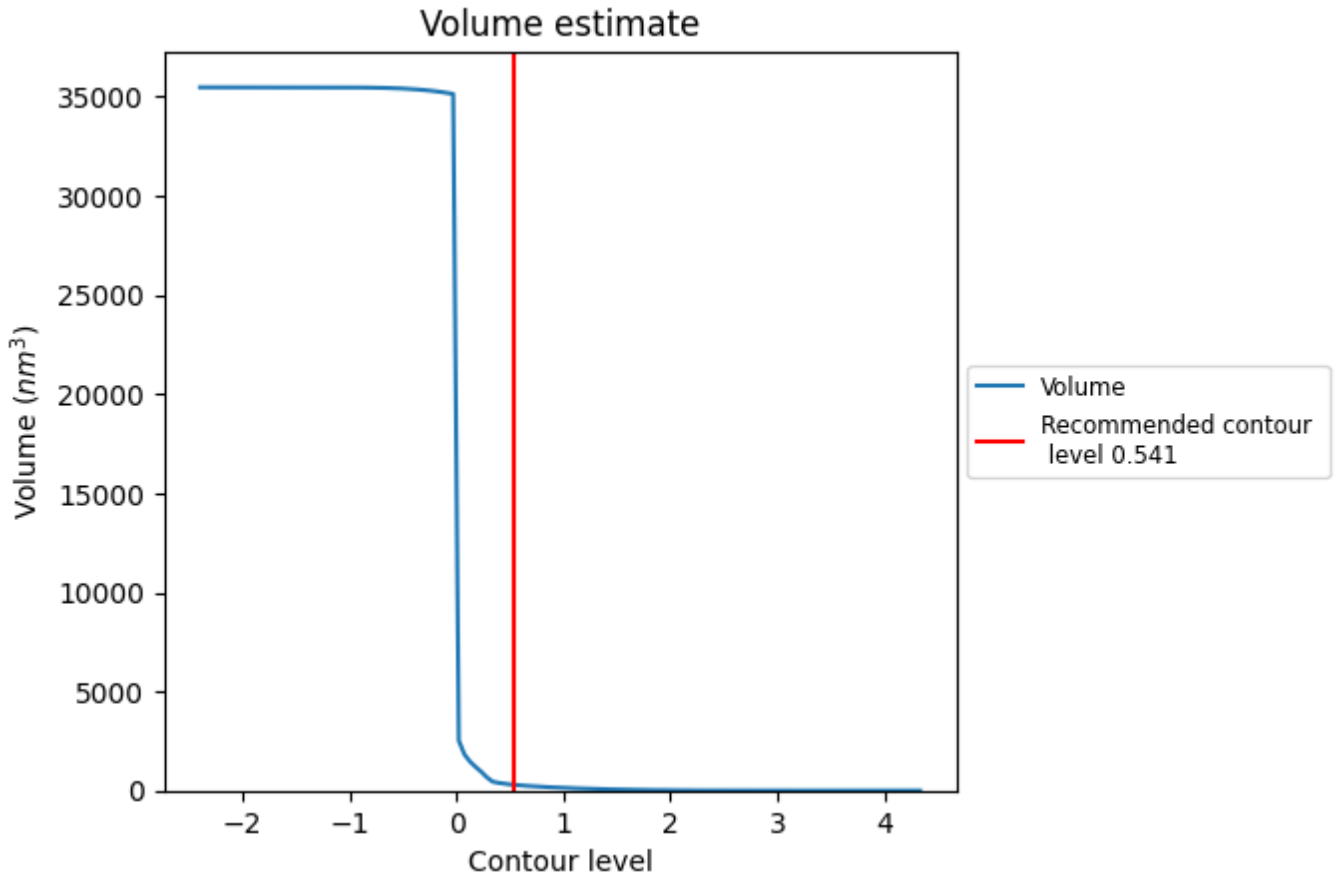
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

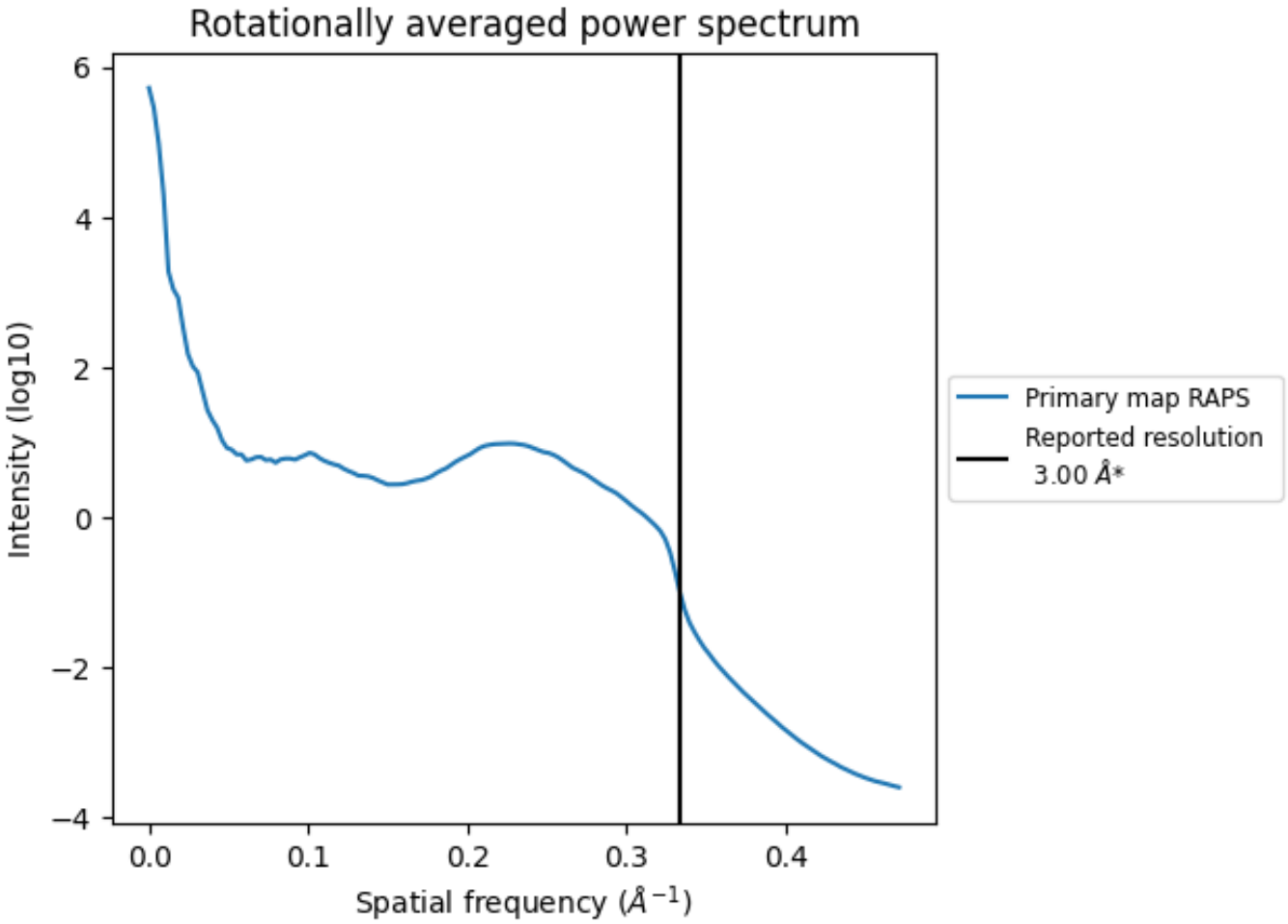
7.2 Volume estimate (i)



The volume at the recommended contour level is 288 nm^3; this corresponds to an approximate mass of 261 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

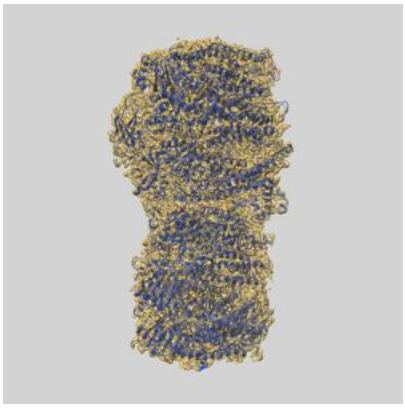
8 Fourier-Shell correlation

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

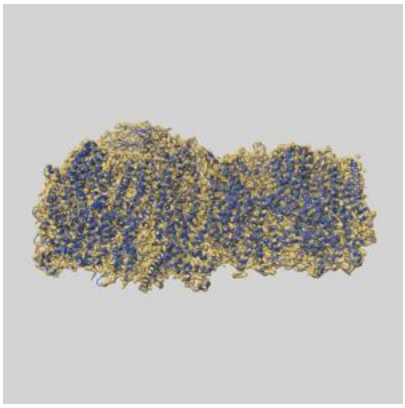
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13777 and PDB model 7Q21. Per-residue inclusion information can be found in section 3 on page 18.

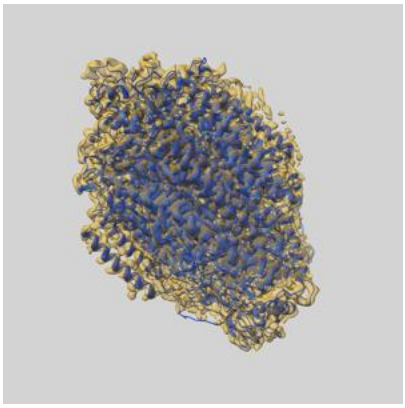
9.1 Map-model overlay



X



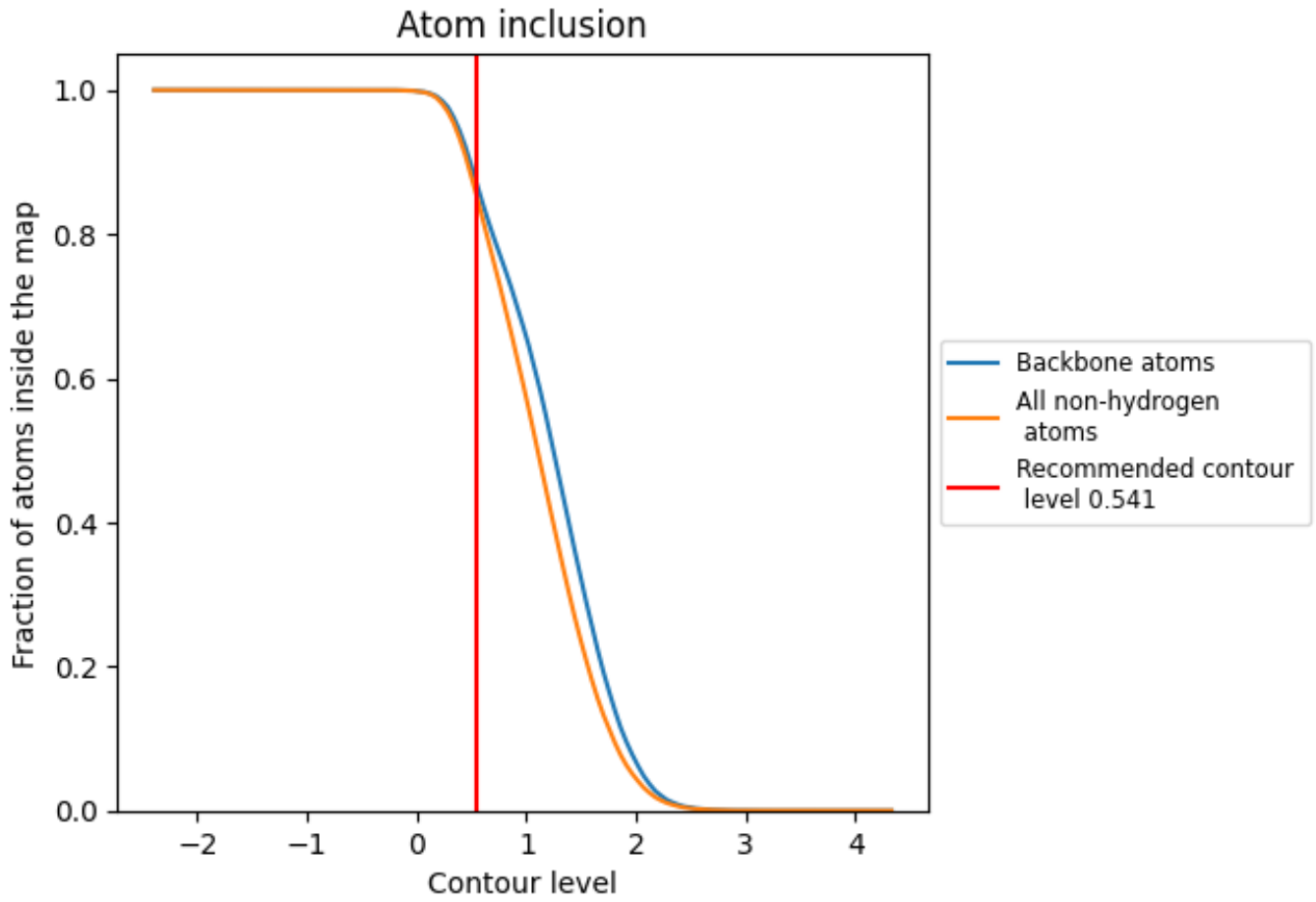
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.541 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 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.