wwPDB EM Validation Summary Report

Aug 26, 2026 – 09:17 am BST

PDB ID	:	7QHO / pdb_00007qho
EMDB ID	:	EMD-13977
Title	:	Cytochrome bcc-aa3 supercomplex (respiratory supercomplex III2/IV2) from Corynebacterium glutamicum (as isolated)
Authors	:	Kao, W.-C.; Hunte, C.
Deposited on	:	2021-12-13
Resolution	:	3.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

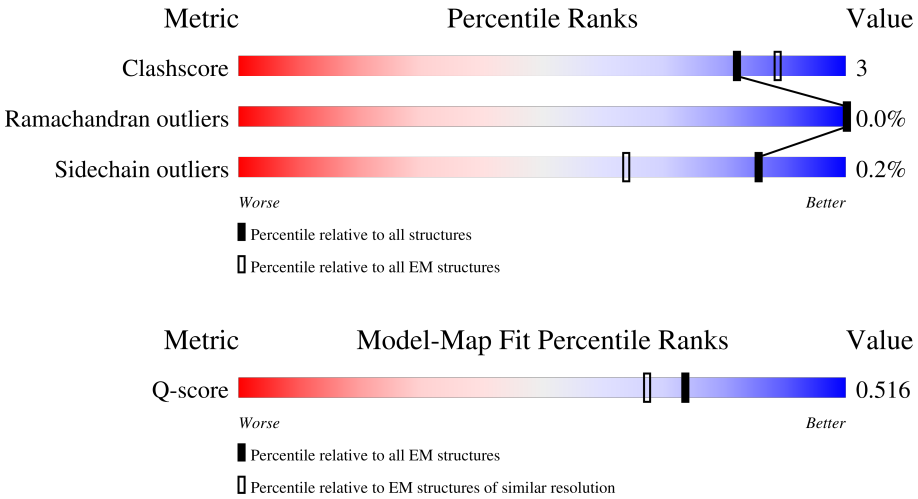
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	408	91% 7% •
1	N	408	91% 8% •
2	B	539	92% 7% •
2	O	539	91% 7% •

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Mol	Chain	Length	Quality of chain
3	C	283	78% 18%
3	P	283	78% 18%
4	D	594	91% 5%
4	Q	594	91% 6%
5	E	331	98%
5	R	331	98%
6	F	205	89% 7%
6	S	205	89% 7%
7	G	143	96%
7	T	143	92% 8%
8	H	163	91% 6%
8	U	163	91% 6%
9	I	147	86% 12%
9	V	147	86% 12%
10	J	112	87% 11%
10	W	112	86% 11%
11	K	73	74% 22%
11	X	73	73% 5% 22%
12	L	65	95%
12	Y	65	5% 95%
13	M	168	12% 85%
13	Z	168	12% 85%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	HEC	C	302	X	-	-	-
23	HEC	C	303	X	-	-	-
23	HEC	P	302	X	-	-	-
23	HEC	P	303	X	-	-	-
25	HAS	D	601	X	-	-	-
25	HAS	D	602	X	-	-	-
25	HAS	Q	601	X	-	-	-
25	HAS	Q	602	X	-	-	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 95954 atoms, of which 47460 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	402	Total	C	H	N	O	S	0	0
			6206	1998	3070	536	586	16		
1	N	402	Total	C	H	N	O	S	0	0
			6206	1998	3070	536	586	16		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	534	Total	C	H	N	O	S	5	0
			8491	2775	4268	707	719	22		
2	O	534	Total	C	H	N	O	S	5	0
			8491	2775	4268	707	719	22		

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	233	Total	C	H	N	O	S	0	0
			3418	1083	1680	302	343	10		
3	P	233	Total	C	H	N	O	S	0	0
			3418	1083	1680	302	343	10		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	574	Total	C	H	N	O	S	0	0
			8994	3023	4458	733	748	32		
4	Q	574	Total	C	H	N	O	S	0	0
			8994	3023	4458	733	748	32		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	585	ALA	-	expression tag	UNP Q79VD7

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	331	Total	C	H	N	O	S	0	0
			5066	1660	2468	429	498	11		
5	R	331	Total	C	H	N	O	S	0	0
			5066	1660	2468	429	498	11		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	190	Total	C	H	N	O	S	0	0
			2981	992	1495	236	251	7		
6	S	190	Total	C	H	N	O	S	0	0
			2981	992	1495	236	251	7		

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	143	Total	C	H	N	O	S	0	0
			2201	728	1106	167	191	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
7	T	143	Total	C	H	N	O	S	0	0
			2201	728	1106	167	191	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	154	Total	C	H	N	O	S	0	0
			2182	686	1058	185	250	3		
8	U	154	Total	C	H	N	O	S	0	0
			2182	686	1058	185	250	3		

- Molecule 9 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	129	Total	C	H	N	O	S	0	0
			2059	664	1031	182	181	1		
9	V	129	Total	C	H	N	O	S	0	0
			2059	664	1031	182	181	1		

- Molecule 10 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	100	Total	C	H	N	O	S	0	0
			1547	498	780	132	134	3		
10	W	100	Total	C	H	N	O	S	0	0
			1547	498	780	132	134	3		

- Molecule 11 is a protein called Actinobacterial supercomplex, subunit C (AscC).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	57	Total	C	H	N	O	0	0
			864	286	413	78	87		
11	X	57	Total	C	H	N	O	0	0
			864	286	413	78	87		

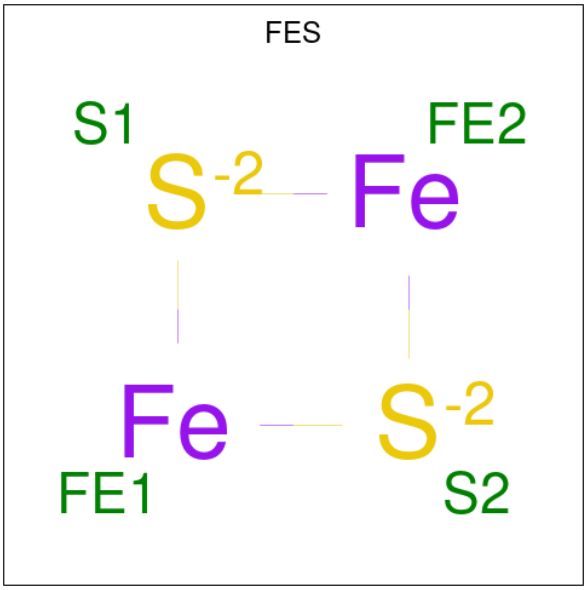
- Molecule 12 is a protein called Hypothetical membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		
12	Y	63	Total	C	H	N	O	S	0	0
			915	294	470	70	78	3		

- Molecule 13 is a protein called Thiamine biosynthesis protein X.

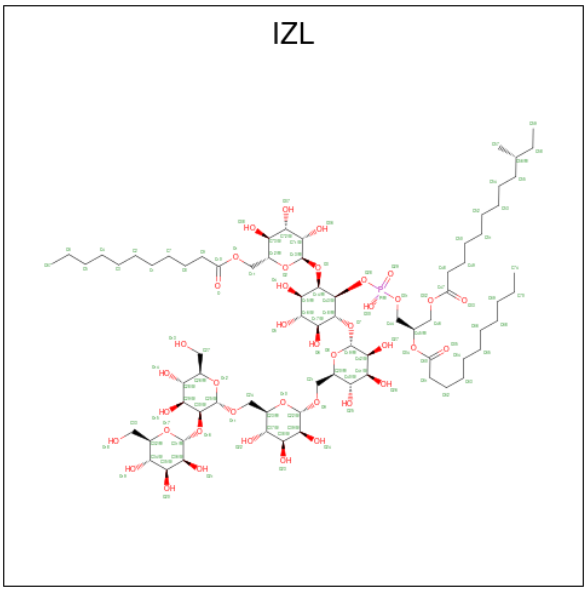
Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	25	Total	C	H	N	O	S	0	0
			372	114	179	36	42	1		
13	Z	25	Total	C	H	N	O	S	0	0
			372	114	179	36	42	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



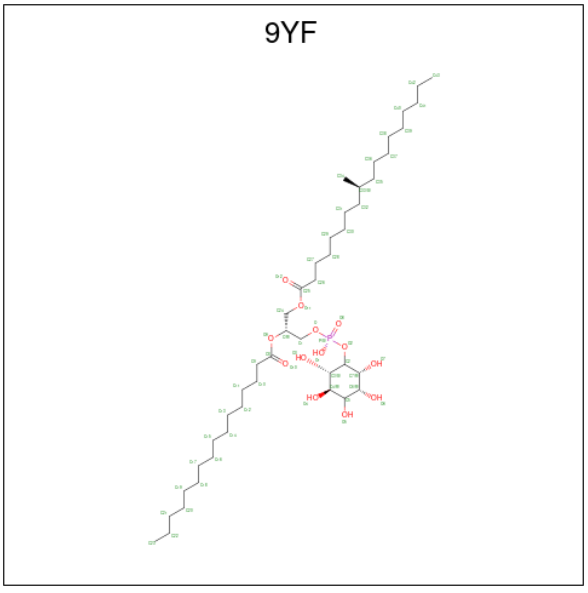
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	Fe	S		0
			4	2	2		
14	N	1	Total	Fe	S		0
			4	2	2		

- Molecule 15 is [(2 {R})-3-[[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (CCD ID: IZL) (formula: $C_{74}H_{133}O_{39}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	H	O	P	0
			212	63	109	39	1	
15	N	1	Total	C	H	O	P	0
			212	63	109	39	1	

- Molecule 16 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: $C_{44}H_{85}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	H	O	P	0
			66	22	30	13	1	

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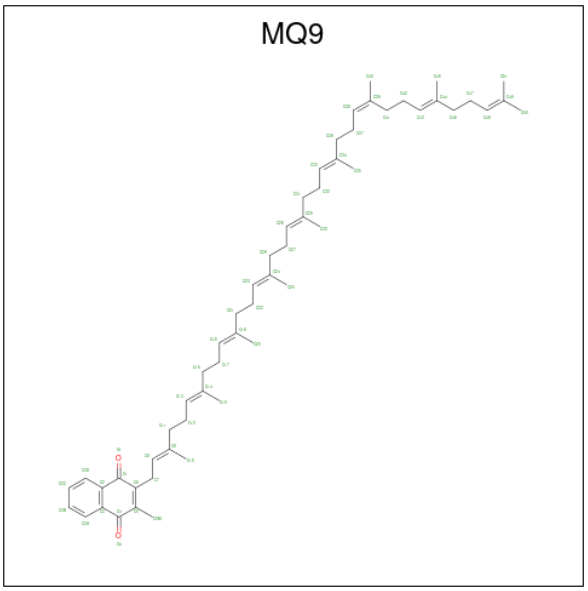
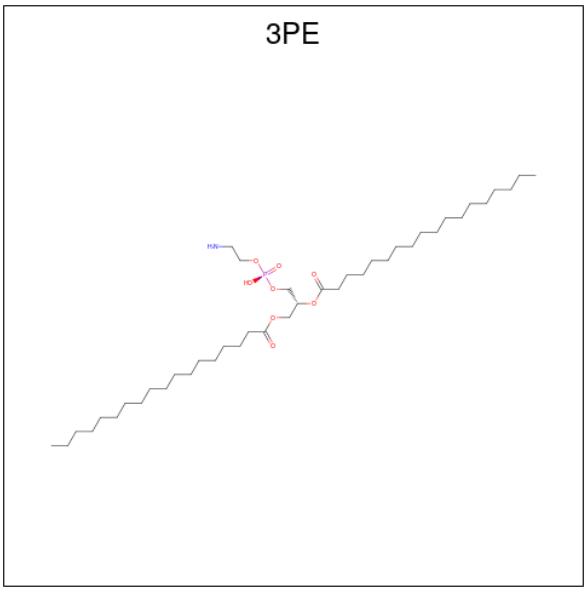
Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	H	O	P	0
			60	20	26	13	1	
16	N	1	Total	C	H	O	P	0
			66	22	30	13	1	
16	U	1	Total	C	H	O	P	0
			60	20	26	13	1	

- Molecule 17 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



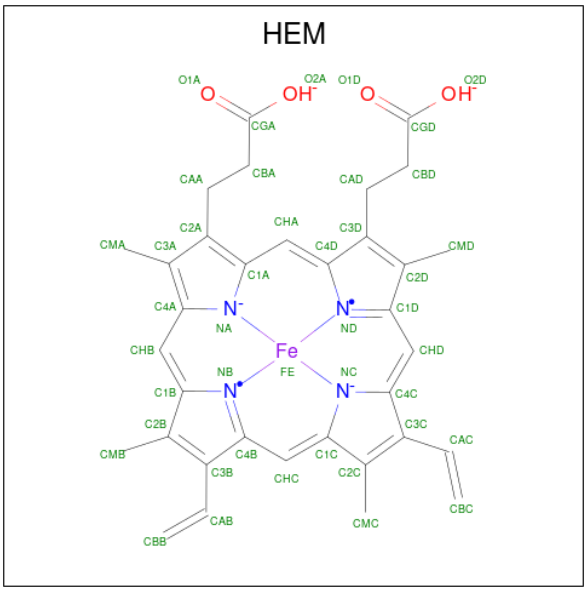
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	H	O	0
			52	24	26	2	
17	B	1	Total	C	H	O	0
			46	21	23	2	
17	B	1	Total	C	H	O	0
			46	21	23	2	
17	N	1	Total	C	H	O	0
			52	24	26	2	
17	O	1	Total	C	H	O	0
			46	21	23	2	
17	O	1	Total	C	H	O	0
			46	21	23	2	

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



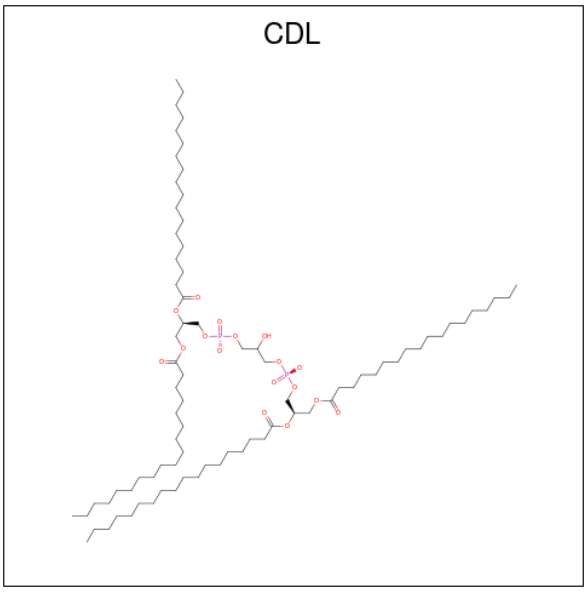
Mol	Chain	Residues	Atoms						AltConf
18	A	1	Total	C	H	N	O	P	0
			66	28	28	1	8	1	
18	D	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	E	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	F	1	Total	C	H	N	O	P	0
			54	22	22	1	8	1	
18	J	1	Total	C	H	N	O	P	0
			111	37	64	1	8	1	
18	N	1	Total	C	H	N	O	P	0
			66	28	28	1	8	1	
18	Q	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	R	1	Total	C	H	N	O	P	0
			57	21	26	1	8	1	
18	S	1	Total	C	H	N	O	P	0
			54	22	22	1	8	1	
18	W	1	Total	C	H	N	O	P	0
			111	37	64	1	8	1	

- Molecule 19 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



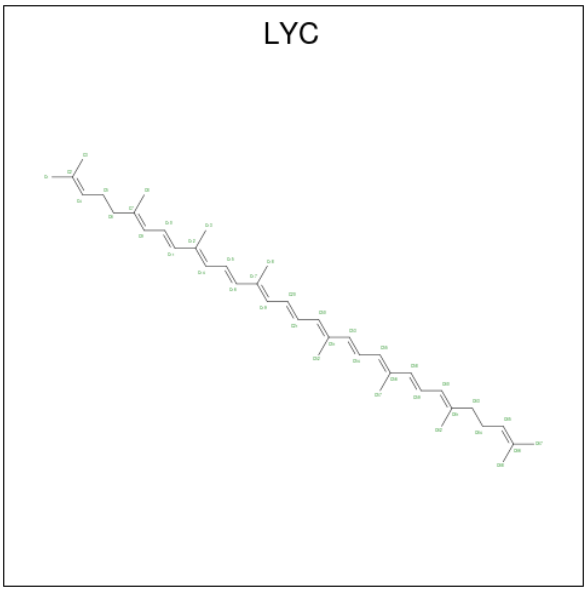
Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	B	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
19	O	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



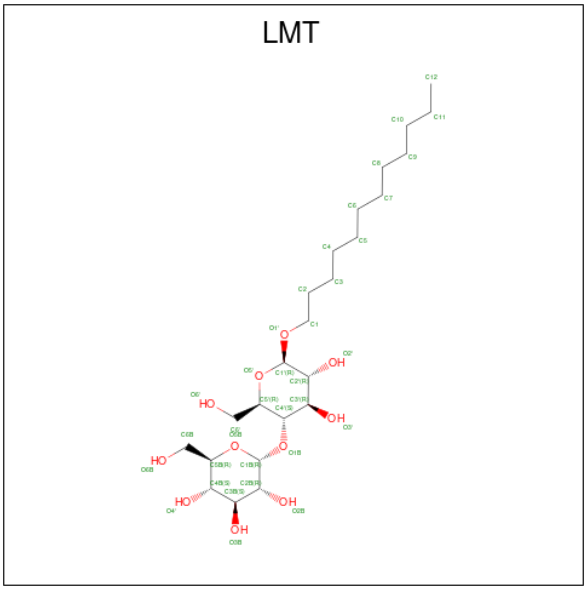
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	H	O	P	0
			72	26	27	17	2	
20	C	1	Total	C	H	O	P	0
			113	46	48	17	2	
20	D	1	Total	C	H	O	P	0
			161	58	84	17	2	
20	D	1	Total	C	H	O	P	0
			128	44	65	17	2	
20	F	1	Total	C	H	O	P	0
			94	38	37	17	2	
20	G	1	Total	C	H	O	P	0
			104	43	42	17	2	
20	I	1	Total	C	H	O	P	0
			107	38	50	17	2	
20	O	1	Total	C	H	O	P	0
			72	26	27	17	2	
20	P	1	Total	C	H	O	P	0
			113	46	48	17	2	
20	Q	1	Total	C	H	O	P	0
			161	58	84	17	2	
20	Q	1	Total	C	H	O	P	0
			128	44	65	17	2	
20	S	1	Total	C	H	O	P	0
			94	38	37	17	2	
20	S	1	Total	C	H	O	P	0
			104	43	42	17	2	
20	V	1	Total	C	H	O	P	0
			107	38	50	17	2	

- Molecule 21 is LYCOPENE (CCD ID: LYC) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



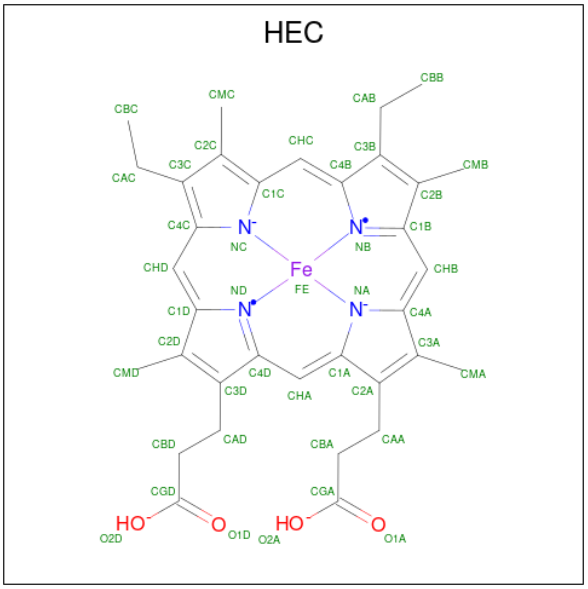
Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total 96	C 40	H 56	0
21	O	1	Total 96	C 40	H 56	0

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



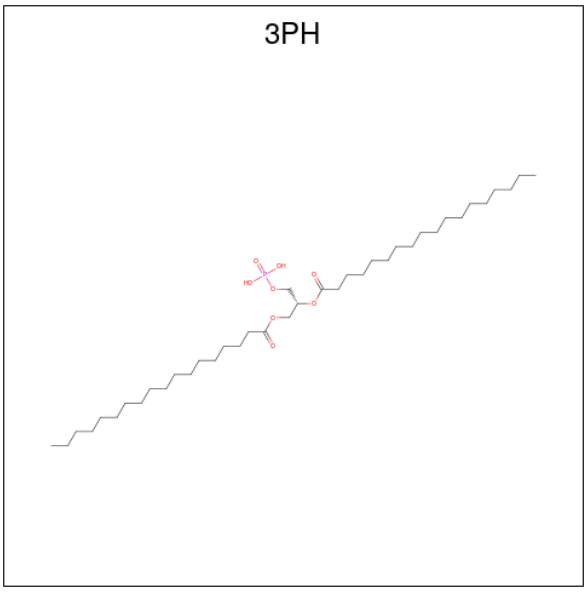
Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total 71	C 21	H 39	O 11	0
22	O	1	Total 71	C 21	H 39	O 11	0

- Molecule 23 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



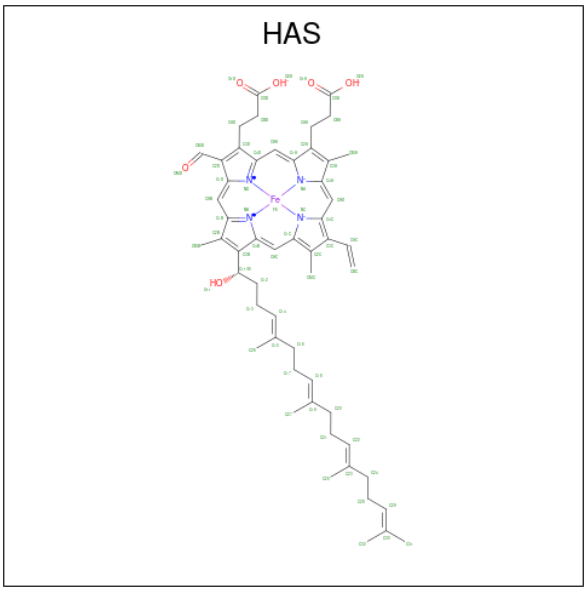
Mol	Chain	Residues	Atoms						AltConf
23	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
23	C	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
23	P	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
23	P	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 24 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	H	O	P	0
			90	29	52	8	1	
24	T	1	Total	C	H	O	P	0
			90	29	52	8	1	

- Molecule 25 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
25	D	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	
25	Q	1	Total	C	Fe	H	N	O	0
			127	54	1	62	4	6	

- Molecule 26 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Cu	0
			1	1	
26	Q	1	Total	Cu	0
			1	1	

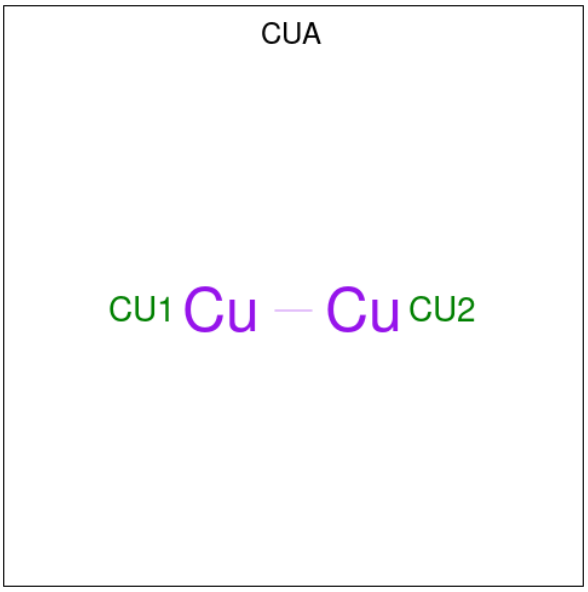
- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	D	1	Total	Ca	0
			1	1	
27	Q	1	Total	Ca	0
			1	1	

- Molecule 28 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

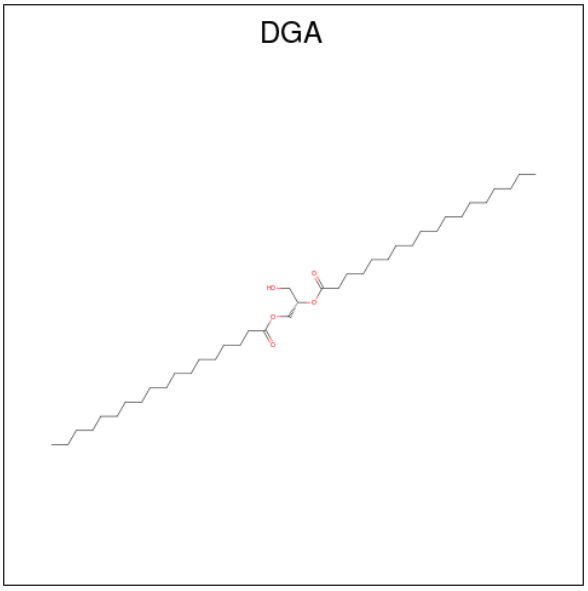
Mol	Chain	Residues	Atoms		AltConf
28	E	1	Total	Mn	0
			1	1	
28	R	1	Total	Mn	0
			1	1	

- Molecule 29 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).



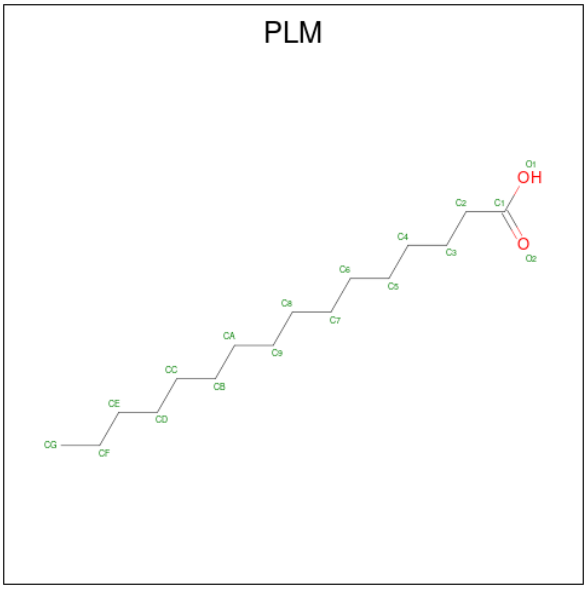
Mol	Chain	Residues	Atoms	AltConf
29	E	1	Total Cu 1 1	0
29	E	1	Total Cu 1 1	0
29	R	1	Total Cu 1 1	0
29	R	1	Total Cu 1 1	0

- Molecule 30 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
30	E	1	Total C O 20 16 4	0
30	H	1	Total C O 17 13 4	0
30	M	1	Total C O 22 18 4	0
30	R	1	Total C O 20 16 4	0
30	U	1	Total C O 17 13 4	0
30	Z	1	Total C O 22 18 4	0

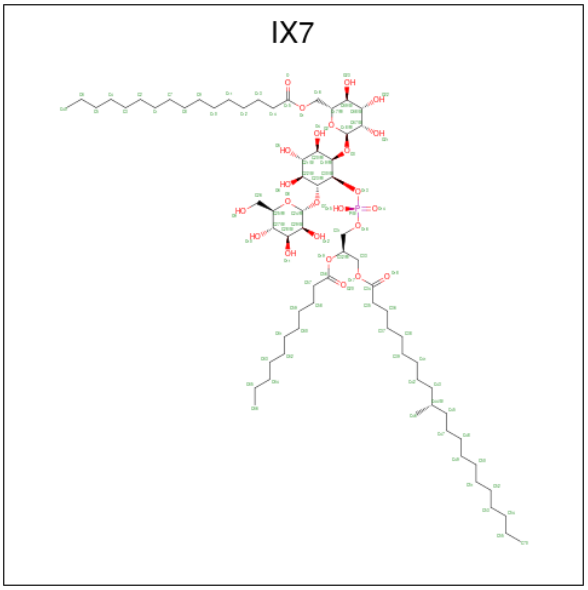
- Molecule 31 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
31	H	1	Total C H O 35 14 20 1	0
31	M	1	Total C H O 9 4 4 1	0
31	U	1	Total C H O 35 14 20 1	0
31	Z	1	Total C H O 9 4 4 1	0

- Molecule 32 is [(2 {R})-3-[[(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {

S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {S})-10-methylhenicosanoate (CCD ID: IX7) (formula: $C_{70}H_{131}O_{24}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	I	1	Total	C	H	O	P	0
			155	47	83	24	1	
32	R	1	Total	C	H	O	P	0
			155	47	83	24	1	

- Molecule 33 is water.

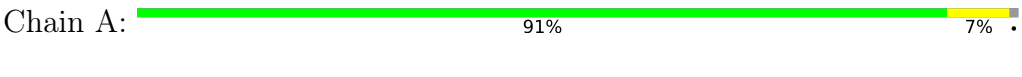
Mol	Chain	Residues	Atoms		AltConf
33	B	2	Total	O	0
			2	2	
33	D	2	Total	O	0
			2	2	
33	E	1	Total	O	0
			1	1	
33	O	2	Total	O	0
			2	2	
33	Q	2	Total	O	0
			2	2	
33	R	1	Total	O	0
			1	1	

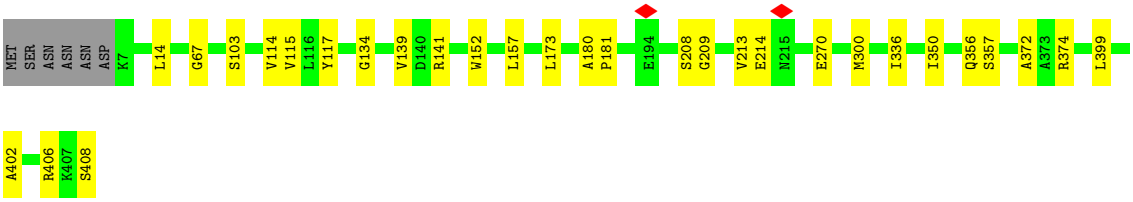
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

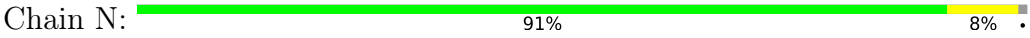
Chain A:

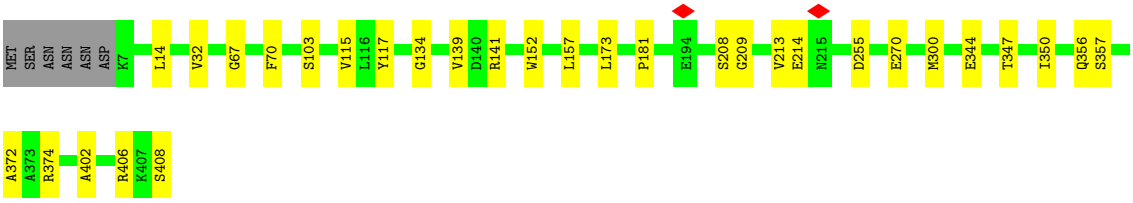




• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

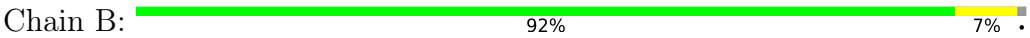
Chain N:

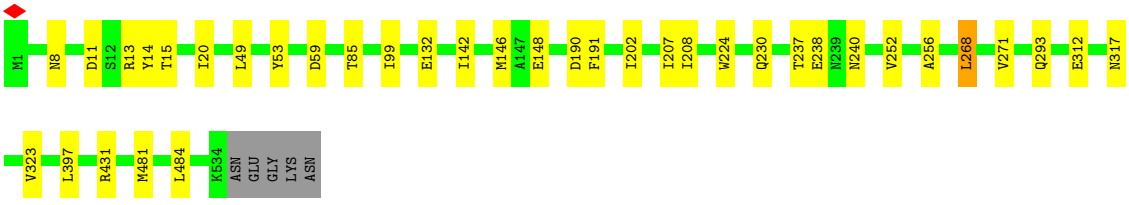




• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain B:

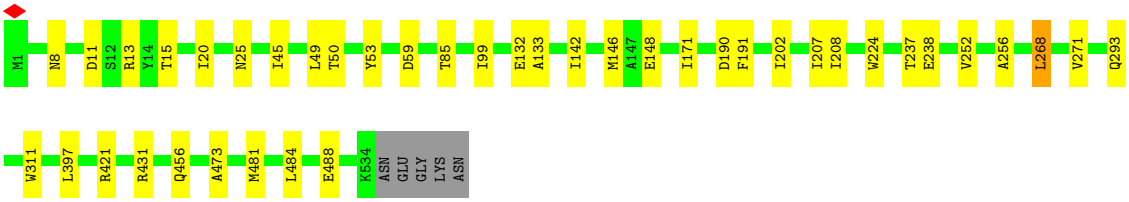




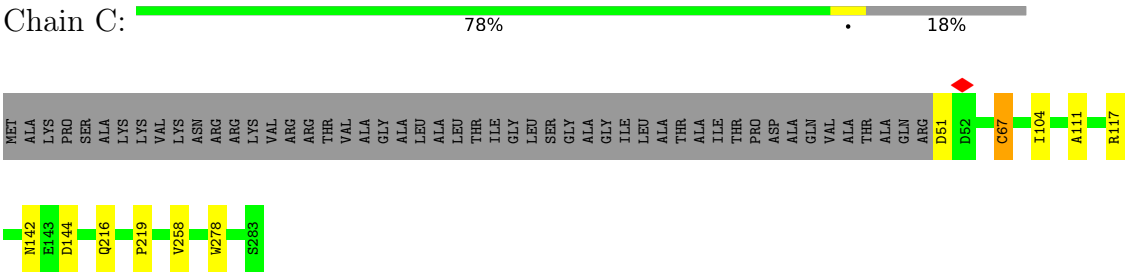
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain O:

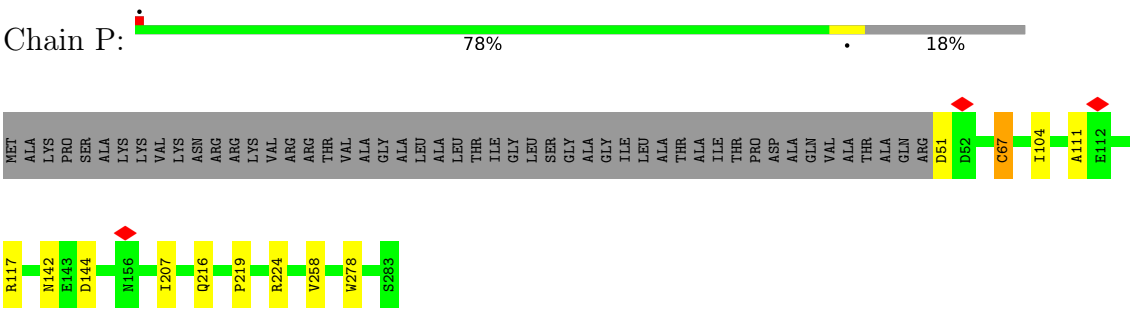




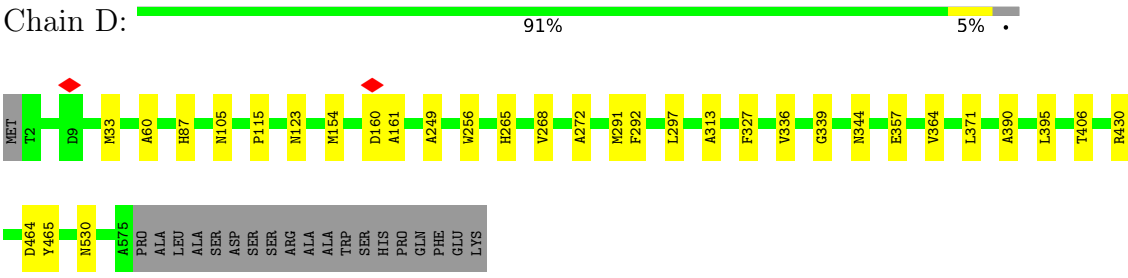
• Molecule 3: Cytochrome bc1 complex cytochrome c subunit



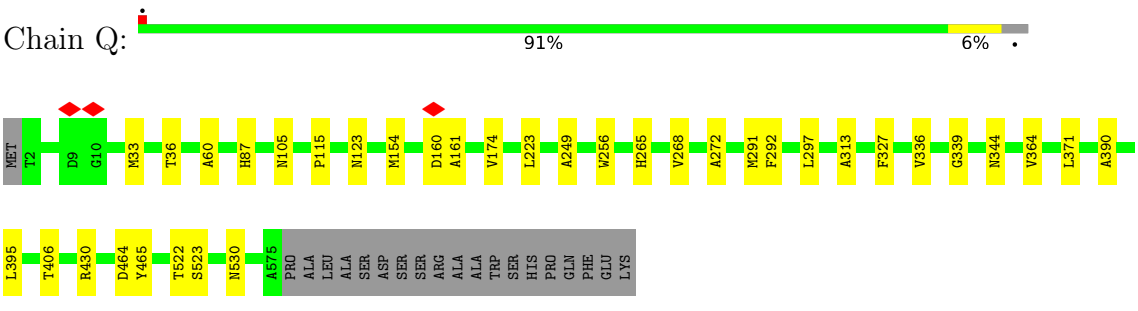
• Molecule 3: Cytochrome bc1 complex cytochrome c subunit



• Molecule 4: Cytochrome c oxidase subunit 1

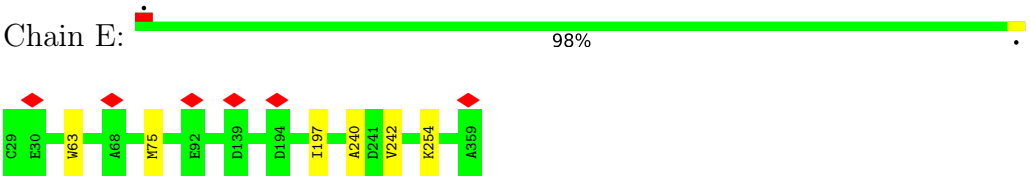


• Molecule 4: Cytochrome c oxidase subunit 1



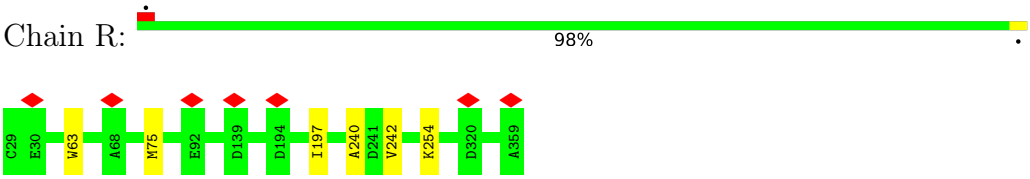
• Molecule 5: Cytochrome c oxidase subunit 2

Chain E:



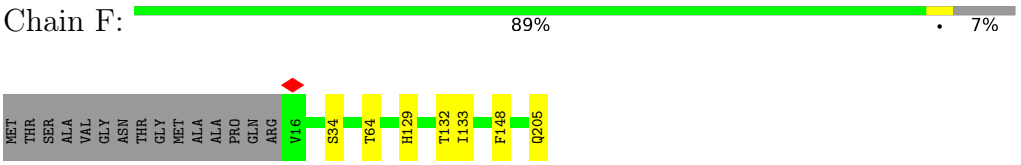
• Molecule 5: Cytochrome c oxidase subunit 2

Chain R:



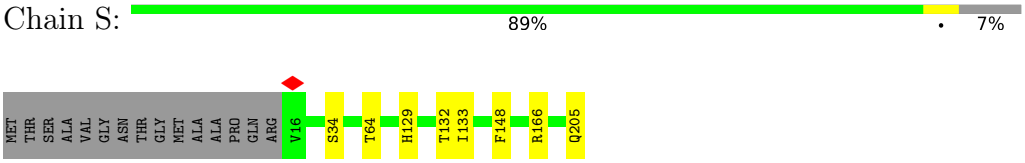
• Molecule 6: Cytochrome c oxidase subunit 3

Chain F:



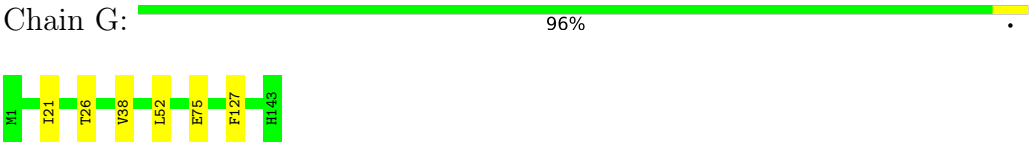
• Molecule 6: Cytochrome c oxidase subunit 3

Chain S:



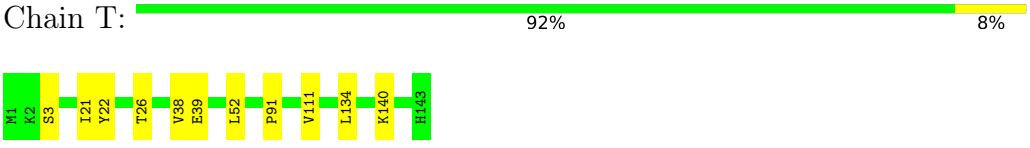
• Molecule 7: Cytochrome c oxidase polypeptide 4

Chain G:



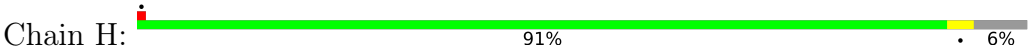
• Molecule 7: Cytochrome c oxidase polypeptide 4

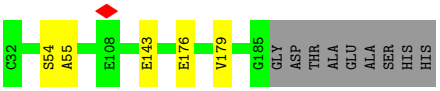
Chain T:



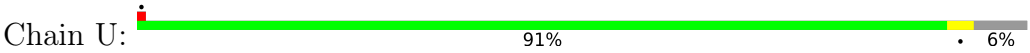
• Molecule 8: Uncharacterized protein Cgl2664/cg2949

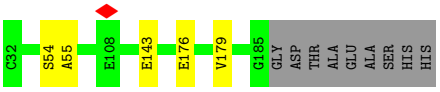
Chain H:



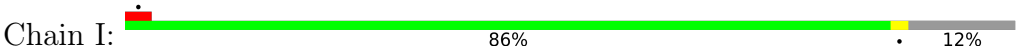


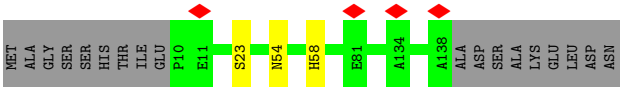
• Molecule 8: Uncharacterized protein Cgl2664/cg2949



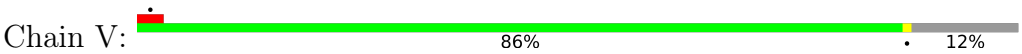


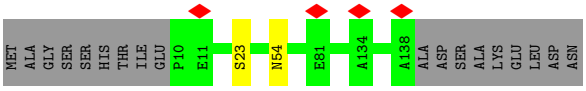
• Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211



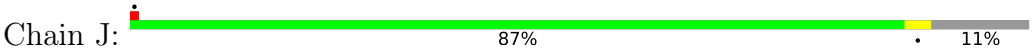


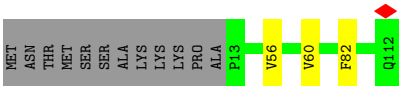
• Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211



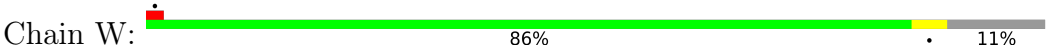


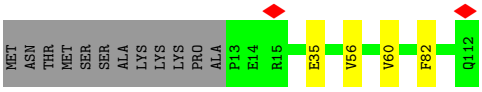
• Molecule 10: Hypothetical membrane protein





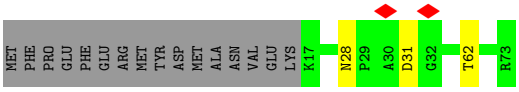
• Molecule 10: Hypothetical membrane protein





• Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

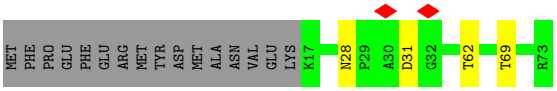




• Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

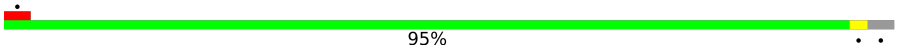
Chain X:

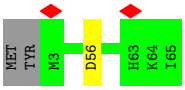




• Molecule 12: Hypothetical membrane protein

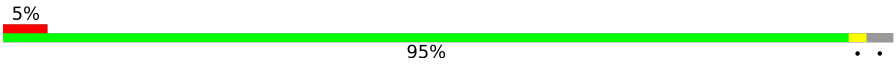
Chain L:

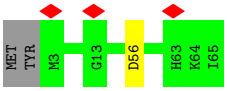




• Molecule 12: Hypothetical membrane protein

Chain Y:

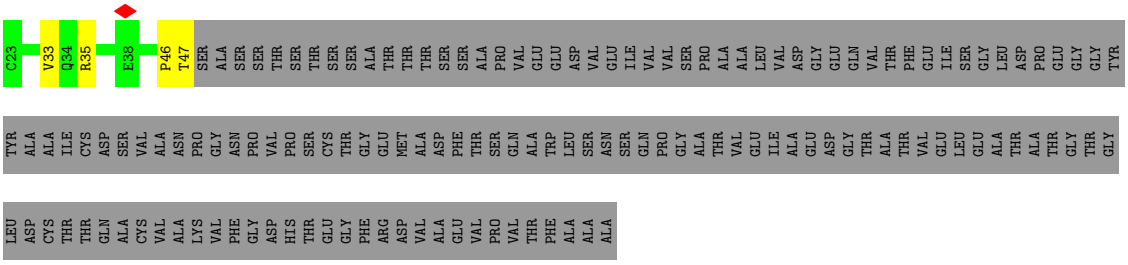




• Molecule 13: Thiamine biosynthesis protein X

Chain M:

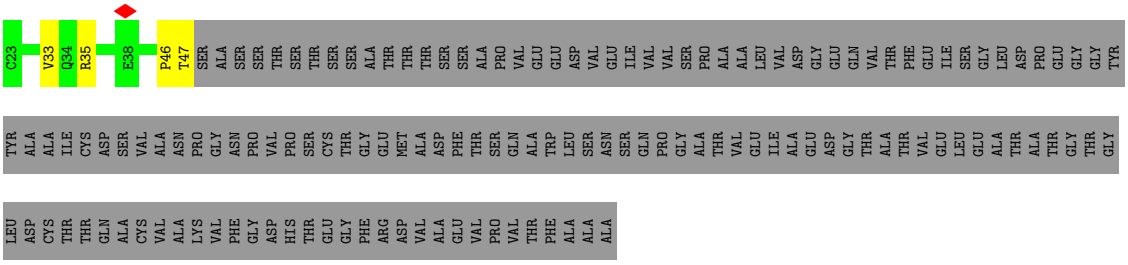




• Molecule 13: Thiamine biosynthesis protein X

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	51060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.95	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.056	Depositor
Minimum map value	-0.798	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	232.20001, 249.48001, 162.0	wwPDB
Map dimensions	150, 231, 215	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, DGA, IZL, IX7, CUA, MN, CDL, HEC, PLM, LYC, CA, MQ9, 3PE, FES, 9YF, CU, 3PH, HAS, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/3216	0.50	0/4375
1	N	0.29	0/3216	0.50	0/4375
2	B	0.36	1/4361 (0.0%)	0.49	0/5944
2	O	0.36	1/4361 (0.0%)	0.49	0/5944
3	C	0.19	0/1770	0.41	0/2394
3	P	0.20	0/1770	0.41	0/2394
4	D	0.22	0/4705	0.44	0/6419
4	Q	0.22	0/4705	0.44	0/6419
5	E	0.22	0/2671	0.43	0/3642
5	R	0.22	0/2671	0.43	0/3642
6	F	0.19	0/1528	0.41	0/2081
6	S	0.19	0/1528	0.41	0/2081
7	G	0.21	0/1126	0.42	0/1529
7	T	0.21	0/1126	0.42	0/1529
8	H	0.22	0/1138	0.43	0/1558
8	U	0.22	0/1138	0.43	0/1558
9	I	0.18	0/1057	0.40	0/1444
9	V	0.18	0/1057	0.40	0/1444
10	J	0.17	0/786	0.38	0/1068
10	W	0.17	0/786	0.38	0/1068
11	K	0.22	0/468	0.40	0/640
11	X	0.22	0/468	0.40	0/640
12	L	0.17	0/453	0.44	0/616
12	Y	0.17	0/453	0.44	0/616
13	M	0.21	0/197	0.46	0/271
13	Z	0.21	0/197	0.46	0/271
All	All	0.25	2/46952 (0.0%)	0.45	0/63962

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	ILE	CG1-CD1	-9.16	1.16	1.51
2	O	202	ILE	CG1-CD1	-9.16	1.16	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3136	3070	3070	37	0
1	N	3136	3070	3070	32	0
2	B	4223	4268	4252	32	0
2	O	4223	4268	4252	37	0
3	C	1738	1680	1680	10	0
3	P	1738	1680	1680	12	0
4	D	4536	4458	4459	22	0
4	Q	4536	4458	4459	25	0
5	E	2598	2468	2468	7	0
5	R	2598	2468	2468	7	0
6	F	1486	1495	1494	5	0
6	S	1486	1495	1494	6	0
7	G	1095	1106	1106	5	0
7	T	1095	1106	1106	11	0
8	H	1124	1058	1057	3	0
8	U	1124	1058	1057	3	0
9	I	1028	1031	1031	3	0
9	V	1028	1031	1031	2	0
10	J	767	780	780	2	0
10	W	767	780	780	4	0
11	K	451	413	413	3	0
11	X	451	413	413	5	0
12	L	445	470	469	1	0
12	Y	445	470	469	1	0
13	M	193	179	179	2	0
13	Z	193	179	179	2	0
14	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	4	0	0	1	0
15	A	103	109	0	4	0
15	N	103	109	0	3	0
16	A	36	30	0	0	0
16	B	34	26	0	0	0
16	N	36	30	0	0	0
16	U	34	26	0	0	0
17	A	26	26	26	6	0
17	B	46	46	42	0	0
17	N	26	26	26	2	0
17	O	46	46	42	2	0
18	A	38	28	53	8	0
18	D	31	26	36	1	0
18	E	31	26	36	0	0
18	F	32	22	38	1	0
18	J	47	64	71	1	0
18	N	38	28	53	9	0
18	Q	31	26	36	1	0
18	R	31	26	36	0	0
18	S	32	22	38	1	0
18	W	47	64	71	1	0
19	B	86	60	60	1	0
19	O	86	60	60	1	0
20	B	45	27	34	1	0
20	C	65	48	74	4	0
20	D	140	149	171	0	0
20	F	57	37	58	0	0
20	G	62	42	68	3	0
20	I	57	50	61	0	0
20	O	45	27	34	1	0
20	P	65	48	74	4	0
20	Q	140	149	171	1	0
20	S	119	79	126	2	0
20	V	57	50	61	0	0
21	B	40	56	56	2	0
21	O	40	56	56	2	0
22	B	32	39	37	3	0
22	O	32	39	37	3	0
23	C	86	60	60	5	0
23	P	86	60	60	6	0
24	C	38	52	48	0	0
24	T	38	52	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D	130	124	124	5	0
25	Q	130	124	124	5	0
26	D	1	0	0	0	0
26	Q	1	0	0	0	0
27	D	1	0	0	0	0
27	Q	1	0	0	0	0
28	E	1	0	0	0	0
28	R	1	0	0	0	0
29	E	2	0	0	0	0
29	R	2	0	0	0	0
30	E	20	0	21	1	0
30	H	17	0	15	0	0
30	M	22	0	25	0	0
30	R	20	0	21	1	0
30	U	17	0	15	0	0
30	Z	22	0	25	1	0
31	H	15	20	20	0	0
31	M	5	4	4	0	0
31	U	15	20	20	0	0
31	Z	5	4	4	0	0
32	I	72	83	0	2	0
32	R	72	83	0	1	0
33	B	2	0	0	0	0
33	D	2	0	0	0	0
33	E	1	0	0	0	0
33	O	2	0	0	0	0
33	Q	2	0	0	0	0
33	R	1	0	0	0	0
All	All	48494	47460	47392	244	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 244 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:504:IZL:O30	15:N:504:IZL:O33	2.07	0.72
15:A:502:IZL:O30	15:A:502:IZL:O33	2.07	0.71
1:A:134:GLY:O	2:O:15:THR:HG22	1.91	0.71
2:B:13:ARG:NH1	2:O:132:GLU:OE1	2.25	0.69
2:B:15:THR:HG22	1:N:134:GLY:O	1.93	0.69

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/408 (98%)	376 (94%)	24 (6%)	0	100	100
1	N	400/408 (98%)	376 (94%)	24 (6%)	0	100	100
2	B	537/539 (100%)	525 (98%)	12 (2%)	0	100	100
2	O	537/539 (100%)	524 (98%)	13 (2%)	0	100	100
3	C	231/283 (82%)	219 (95%)	12 (5%)	0	100	100
3	P	231/283 (82%)	219 (95%)	12 (5%)	0	100	100
4	D	572/594 (96%)	556 (97%)	16 (3%)	0	100	100
4	Q	572/594 (96%)	556 (97%)	16 (3%)	0	100	100
5	E	329/331 (99%)	311 (94%)	17 (5%)	1 (0%)	36	67
5	R	329/331 (99%)	311 (94%)	17 (5%)	1 (0%)	36	67
6	F	188/205 (92%)	187 (100%)	1 (0%)	0	100	100
6	S	188/205 (92%)	187 (100%)	1 (0%)	0	100	100
7	G	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
7	T	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
8	H	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
8	U	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
9	I	127/147 (86%)	120 (94%)	7 (6%)	0	100	100
9	V	127/147 (86%)	120 (94%)	7 (6%)	0	100	100
10	J	98/112 (88%)	96 (98%)	2 (2%)	0	100	100
10	W	98/112 (88%)	96 (98%)	2 (2%)	0	100	100
11	K	55/73 (75%)	54 (98%)	1 (2%)	0	100	100
11	X	55/73 (75%)	54 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
12	Y	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
13	M	23/168 (14%)	23 (100%)	0	0	100	100
13	Z	23/168 (14%)	23 (100%)	0	0	100	100
All	All	5828/6462 (90%)	5623 (96%)	203 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	242	VAL
5	R	242	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/332 (98%)	325 (100%)	1 (0%)	86	87
1	N	326/332 (98%)	325 (100%)	1 (0%)	86	87
2	B	442/441 (100%)	438 (99%)	4 (1%)	70	80
2	O	442/441 (100%)	438 (99%)	4 (1%)	70	80
3	C	177/212 (84%)	176 (99%)	1 (1%)	78	83
3	P	177/212 (84%)	176 (99%)	1 (1%)	78	83
4	D	472/488 (97%)	472 (100%)	0	100	100
4	Q	472/488 (97%)	472 (100%)	0	100	100
5	E	274/274 (100%)	274 (100%)	0	100	100
5	R	274/274 (100%)	274 (100%)	0	100	100
6	F	156/166 (94%)	156 (100%)	0	100	100
6	S	156/166 (94%)	156 (100%)	0	100	100
7	G	114/114 (100%)	114 (100%)	0	100	100
7	T	114/114 (100%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	127/133 (96%)	127 (100%)	0	100	100
8	U	127/133 (96%)	127 (100%)	0	100	100
9	I	111/125 (89%)	111 (100%)	0	100	100
9	V	111/125 (89%)	111 (100%)	0	100	100
10	J	80/90 (89%)	80 (100%)	0	100	100
10	W	80/90 (89%)	80 (100%)	0	100	100
11	K	48/63 (76%)	48 (100%)	0	100	100
11	X	48/63 (76%)	48 (100%)	0	100	100
12	L	43/45 (96%)	43 (100%)	0	100	100
12	Y	43/45 (96%)	43 (100%)	0	100	100
13	M	25/135 (18%)	25 (100%)	0	100	100
13	Z	25/135 (18%)	25 (100%)	0	100	100
All	All	4790/5236 (92%)	4778 (100%)	12 (0%)	85	87

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	207	ILE
2	O	224[A]	TRP
3	P	67	CYS
2	O	224[B]	TRP
2	B	224[B]	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	244	HIS
9	V	55	HIS
4	Q	257	GLN
6	S	134	GLN
6	F	63	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 78 ligands modelled in this entry, 6 are monoatomic and 4 are modelled with single atom - leaving 68 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	$\#\|Z\| > 2$
19	HEM	O	604	2	50,50,50	1.20	4 (8%)	66,82,82	0.93	2 (3%)
19	HEM	O	603	2	50,50,50	1.15	4 (8%)	66,82,82	0.96	2 (3%)
18	3PE	E	405	-	30,30,50	0.38	0	33,35,55	0.35	0
18	3PE	J	201	-	46,46,50	0.32	0	49,51,55	0.31	0
20	CDL	F	302	-	56,56,99	0.38	0	62,68,111	0.33	0
16	9YF	U	203	-	34,34,58	0.38	0	44,46,71	0.37	0
17	MQ9	N	501	-	27,27,59	0.96	1 (3%)	33,36,75	1.72	2 (6%)
30	DGA	H	201	-	16,16,43	0.29	0	18,18,45	0.20	0
17	MQ9	B	604	-	24,24,59	0.40	0	30,33,75	0.67	1 (3%)
31	PLM	Z	202	13	4,4,17	0.33	0	3,3,17	0.46	0
24	3PH	T	201	-	36,36,47	0.28	0	39,40,52	0.55	1 (2%)
25	HAS	Q	601	4	71,72,72	1.20	7 (9%)	84,109,109	1.34	10 (11%)
17	MQ9	B	601	-	24,24,59	0.44	0	30,33,75	0.61	1 (3%)
25	HAS	D	601	4	71,72,72	1.20	7 (9%)	84,109,109	1.34	10 (11%)
30	DGA	U	201	-	16,16,43	0.29	0	18,18,45	0.20	0
32	IX7	I	202	-	74,74,97	0.30	0	97,99,123	0.83	6 (6%)
18	3PE	D	607	-	30,30,50	0.38	0	33,35,55	0.33	0
24	3PH	C	304	-	36,36,47	0.28	0	39,40,52	0.55	1 (2%)
25	HAS	D	602	4	71,72,72	1.20	7 (9%)	84,109,109	1.46	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	HEM	B	602	2	50,50,50	1.15	4 (8%)	66,82,82	0.96	2 (3%)
22	LMT	B	608	-	33,33,36	0.40	0	44,44,47	0.74	1 (2%)
17	MQ9	A	504	-	27,27,59	0.96	1 (3%)	33,36,75	1.72	2 (6%)
15	IZL	N	504	-	108,108,119	0.40	0	150,152,163	1.04	11 (7%)
14	FES	A	501	1	0,4,4	-	-	-		
20	CDL	G	201	-	61,61,99	0.38	0	67,73,111	0.39	0
18	3PE	R	405	-	30,30,50	0.38	0	33,35,55	0.35	0
20	CDL	O	606	-	44,44,99	0.42	0	50,56,111	0.43	0
19	HEM	B	603	2	50,50,50	1.20	4 (8%)	66,82,82	0.93	2 (3%)
20	CDL	Q	605	-	76,76,99	0.35	0	82,88,111	0.50	1 (1%)
21	LYC	B	606	-	39,39,39	0.19	0	44,46,46	0.39	0
18	3PE	A	505	-	37,37,50	0.39	0	40,42,55	0.72	1 (2%)
20	CDL	C	301	-	64,64,99	0.37	0	70,76,111	0.36	0
20	CDL	S	302	-	56,56,99	0.38	0	62,68,111	0.33	0
31	PLM	M	202	13	4,4,17	0.33	0	3,3,17	0.46	0
15	IZL	A	502	-	108,108,119	0.40	0	150,152,163	1.04	11 (7%)
18	3PE	W	201	-	46,46,50	0.32	0	49,51,55	0.31	0
17	MQ9	O	602	-	24,24,59	0.44	0	30,33,75	0.61	1 (3%)
18	3PE	F	301	-	31,31,50	0.40	0	34,36,55	0.68	1 (2%)
18	3PE	S	301	-	31,31,50	0.40	0	34,36,55	0.68	1 (2%)
20	CDL	P	301	-	64,64,99	0.37	0	70,76,111	0.36	0
22	LMT	O	601	-	33,33,36	0.40	0	44,44,47	0.74	1 (2%)
30	DGA	R	404	-	19,19,43	0.27	0	21,21,45	0.26	0
20	CDL	S	303	-	61,61,99	0.38	0	67,73,111	0.39	0
31	PLM	H	202	8	13,13,17	0.25	0	11,11,17	0.18	0
31	PLM	U	202	8	13,13,17	0.25	0	11,11,17	0.18	0
16	9YF	N	505	-	36,36,58	0.35	0	46,48,71	0.51	0
20	CDL	I	201	-	56,56,99	0.38	0	62,68,111	0.34	0
30	DGA	M	201	-	21,21,43	0.27	0	23,23,45	0.23	0
32	IX7	R	406	-	74,74,97	0.30	0	97,99,123	0.83	6 (6%)
17	MQ9	O	605	-	24,24,59	0.40	0	30,33,75	0.66	1 (3%)
20	CDL	Q	606	-	62,62,99	0.38	0	68,74,111	0.36	0
23	HEC	P	302	3	50,50,50	1.04	4 (8%)	68,82,82	1.18	7 (10%)
20	CDL	D	605	-	76,76,99	0.35	0	82,88,111	0.50	1 (1%)
16	9YF	A	503	-	36,36,58	0.35	0	46,48,71	0.51	0
18	3PE	N	502	-	37,37,50	0.39	0	40,42,55	0.72	1 (2%)
30	DGA	Z	201	-	21,21,43	0.27	0	23,23,45	0.23	0
23	HEC	C	303	3	50,50,50	1.02	4 (8%)	68,82,82	1.11	4 (5%)
20	CDL	B	605	-	44,44,99	0.42	0	50,56,111	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	LYC	O	607	-	39,39,39	0.20	0	44,46,46	0.39	0
30	DGA	E	404	-	19,19,43	0.27	0	21,21,45	0.26	0
18	3PE	Q	607	-	30,30,50	0.38	0	33,35,55	0.33	0
16	9YF	B	607	-	34,34,58	0.38	0	44,46,71	0.36	0
14	FES	N	503	1	0,4,4	-	-	-		
23	HEC	P	303	3	50,50,50	1.02	4 (8%)	68,82,82	1.12	4 (5%)
23	HEC	C	302	3	50,50,50	1.04	4 (8%)	68,82,82	1.18	7 (10%)
25	HAS	Q	602	4	71,72,72	1.20	7 (9%)	84,109,109	1.46	13 (15%)
20	CDL	D	606	-	62,62,99	0.38	0	68,74,111	0.36	0
20	CDL	V	201	-	56,56,99	0.38	0	62,68,111	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	HEM	O	604	2	-	2/14/54/54	-
19	HEM	O	603	2	-	3/14/54/54	-
18	3PE	E	405	-	-	1/34/34/54	-
18	3PE	J	201	-	-	7/50/50/54	-
20	CDL	F	302	-	-	19/67/67/110	-
16	9YF	U	203	-	-	5/29/53/78	0/1/1/1
17	MQ9	N	501	-	-	6/15/35/73	0/2/2/2
30	DGA	H	201	-	-	1/17/17/45	-
17	MQ9	B	604	-	-	0/11/31/73	0/2/2/2
31	PLM	Z	202	13	-	0/1/2/15	-
25	HAS	Q	601	4	1/1/18/18	9/42/82/82	-
24	3PH	T	201	-	-	8/37/37/49	-
17	MQ9	B	601	-	-	3/11/31/73	0/2/2/2
25	HAS	D	601	4	1/1/18/18	9/42/82/82	-
30	DGA	U	201	-	-	1/17/17/45	-
32	IX7	I	202	-	-	29/58/122/146	0/3/3/3
18	3PE	D	607	-	-	5/34/34/54	-
24	3PH	C	304	-	-	8/37/37/49	-
25	HAS	D	602	4	1/1/18/18	12/42/82/82	-
19	HEM	B	602	2	-	3/14/54/54	-
22	LMT	B	608	-	-	3/18/58/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MQ9	A	504	-	-	6/15/35/73	0/2/2/2
15	IZL	N	504	-	-	34/73/197/208	0/6/6/6
20	CDL	G	201	-	-	19/72/72/110	-
14	FES	A	501	1	-	-	0/1/1/1
18	3PE	R	405	-	-	1/34/34/54	-
20	CDL	O	606	-	-	7/54/54/110	-
19	HEM	B	603	2	-	2/14/54/54	-
20	CDL	Q	605	-	-	27/87/87/110	-
21	LYC	B	606	-	-	3/43/43/43	-
18	3PE	A	505	-	-	25/41/41/54	-
20	CDL	C	301	-	-	16/75/75/110	-
20	CDL	S	302	-	-	19/67/67/110	-
31	PLM	M	202	13	-	0/1/2/15	-
15	IZL	A	502	-	-	34/73/197/208	0/6/6/6
18	3PE	W	201	-	-	8/50/50/54	-
17	MQ9	O	602	-	-	3/11/31/73	0/2/2/2
18	3PE	F	301	-	-	16/35/35/54	-
18	3PE	S	301	-	-	16/35/35/54	-
20	CDL	P	301	-	-	16/75/75/110	-
22	LMT	O	601	-	-	3/18/58/61	0/2/2/2
30	DGA	R	404	-	-	0/20/20/45	-
20	CDL	S	303	-	-	19/72/72/110	-
31	PLM	H	202	8	-	0/8/9/15	-
31	PLM	U	202	8	-	0/8/9/15	-
16	9YF	N	505	-	-	6/31/55/78	0/1/1/1
20	CDL	I	201	-	-	19/67/67/110	-
30	DGA	M	201	-	-	3/22/22/45	-
32	IX7	R	406	-	-	29/58/122/146	0/3/3/3
17	MQ9	O	605	-	-	0/11/31/73	0/2/2/2
20	CDL	Q	606	-	-	21/73/73/110	-
23	HEC	P	302	3	1/1/7/7	7/14/54/54	-
20	CDL	D	605	-	-	27/87/87/110	-
16	9YF	A	503	-	-	6/31/55/78	0/1/1/1
18	3PE	N	502	-	-	25/41/41/54	-
30	DGA	Z	201	-	-	3/22/22/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	HEC	C	303	3	1/1/7/7	4/14/54/54	-
20	CDL	B	605	-	-	7/54/54/110	-
21	LYC	O	607	-	-	3/43/43/43	-
30	DGA	E	404	-	-	0/20/20/45	-
18	3PE	Q	607	-	-	5/34/34/54	-
16	9YF	B	607	-	-	5/29/53/78	0/1/1/1
14	FES	N	503	1	-	-	0/1/1/1
23	HEC	P	303	3	1/1/7/7	4/14/54/54	-
23	HEC	C	302	3	1/1/7/7	7/14/54/54	-
25	HAS	Q	602	4	1/1/18/18	12/42/82/82	-
20	CDL	D	606	-	-	21/73/73/110	-
20	CDL	V	201	-	-	19/67/67/110	-

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	602	HAS	OMD-CMD	4.95	1.33	1.22
25	Q	602	HAS	OMD-CMD	4.93	1.33	1.22
25	D	601	HAS	OMD-CMD	4.91	1.33	1.22
25	Q	601	HAS	OMD-CMD	4.89	1.33	1.22
17	A	504	MQ9	C6-C5	3.91	1.42	1.35

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	504	MQ9	C8-C7-C6	8.57	135.14	112.05
17	N	501	MQ9	C8-C7-C6	8.56	135.12	112.05
25	Q	602	HAS	C26-C15-C16	4.49	122.83	115.27
25	D	602	HAS	C26-C15-C16	4.46	122.78	115.27
25	Q	601	HAS	C25-C23-C24	3.83	121.71	115.27

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	302	HEC	NA
23	C	303	HEC	NA
23	P	302	HEC	NA
23	P	303	HEC	NA
25	D	601	HAS	NA

5 of 641 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	502	IZL	O34-C45-C46-O32
15	A	502	IZL	C61-C60-O34-C45
15	A	502	IZL	O35-C60-O34-C45
15	A	502	IZL	C44-O31-P-O28
15	N	504	IZL	O34-C45-C46-O32

There are no ring outliers.

41 monomers are involved in 95 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	O	604	HEM	1	0
18	J	201	3PE	1	0
17	N	501	MQ9	2	0
25	Q	601	HAS	1	0
25	D	601	HAS	1	0
32	I	202	IX7	2	0
18	D	607	3PE	1	0
25	D	602	HAS	4	0
22	B	608	LMT	3	0
17	A	504	MQ9	6	0
15	N	504	IZL	3	0
14	A	501	FES	1	0
20	G	201	CDL	3	0
20	O	606	CDL	1	0
19	B	603	HEM	1	0
21	B	606	LYC	2	0
18	A	505	3PE	8	0
20	C	301	CDL	4	0
15	A	502	IZL	4	0
18	W	201	3PE	1	0
17	O	602	MQ9	2	0
18	F	301	3PE	1	0
18	S	301	3PE	1	0
20	P	301	CDL	4	0
22	O	601	LMT	3	0
30	R	404	DGA	1	0
20	S	303	CDL	2	0
32	R	406	IX7	1	0
20	Q	606	CDL	1	0
23	P	302	HEC	3	0
18	N	502	3PE	9	0

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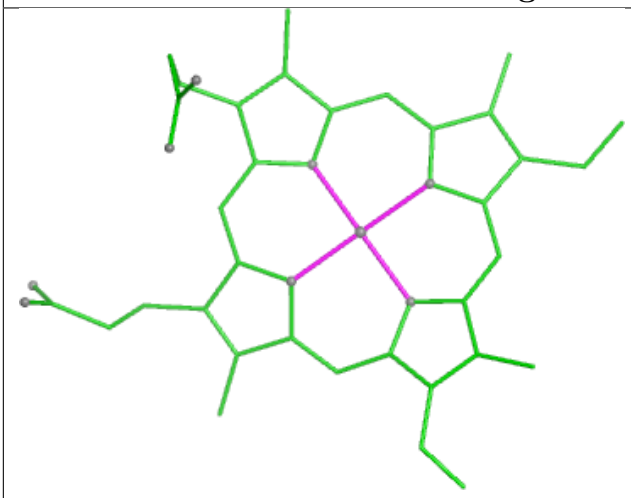
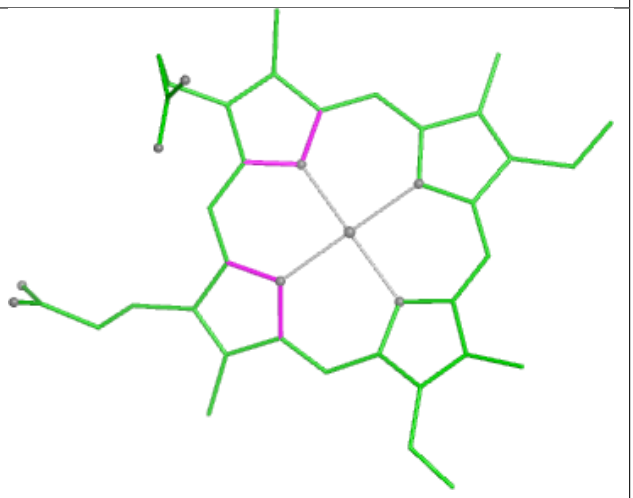
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	Z	201	DGA	1	0
23	C	303	HEC	2	0
20	B	605	CDL	1	0
21	O	607	LYC	2	0
30	E	404	DGA	1	0
18	Q	607	3PE	1	0
14	N	503	FES	1	0
23	P	303	HEC	3	0
23	C	302	HEC	3	0
25	Q	602	HAS	4	0

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

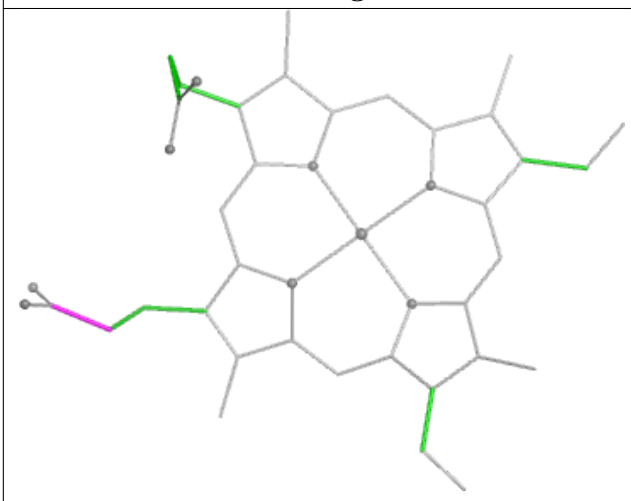
Ligand HEM O 604



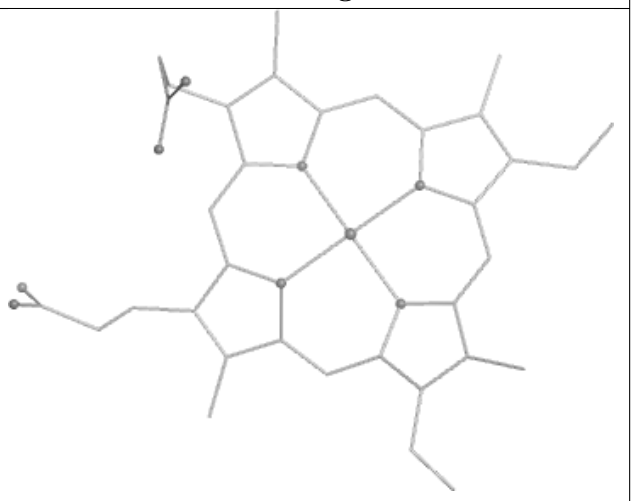
Bond lengths



Bond angles

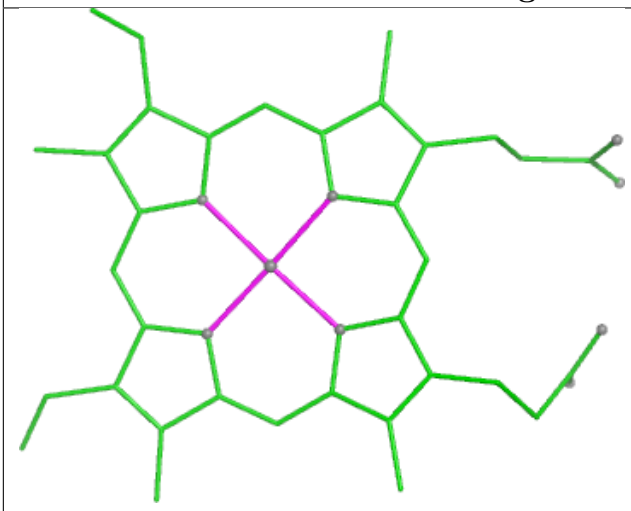


Torsions

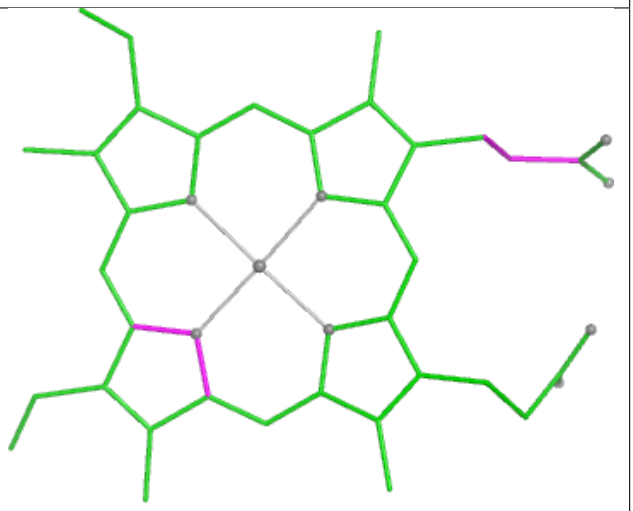


Rings

Ligand HEM O 603



Bond lengths



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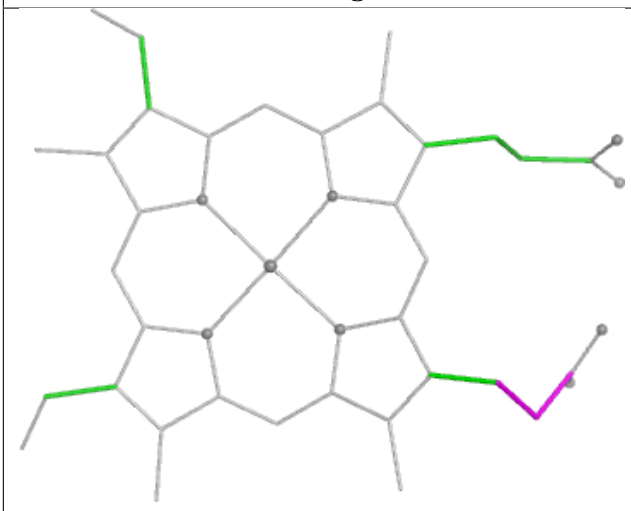

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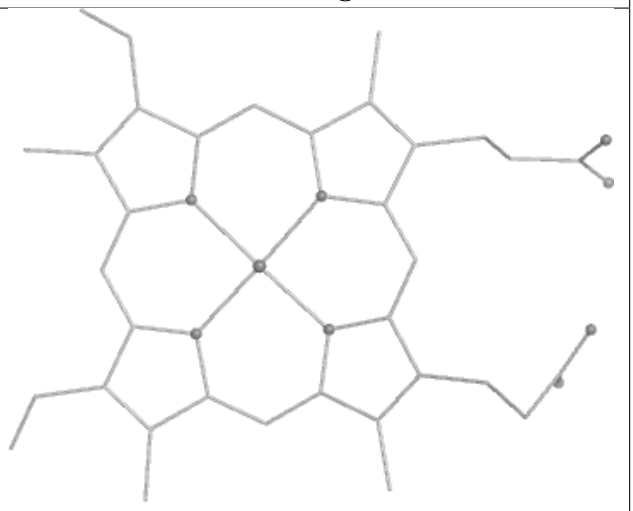
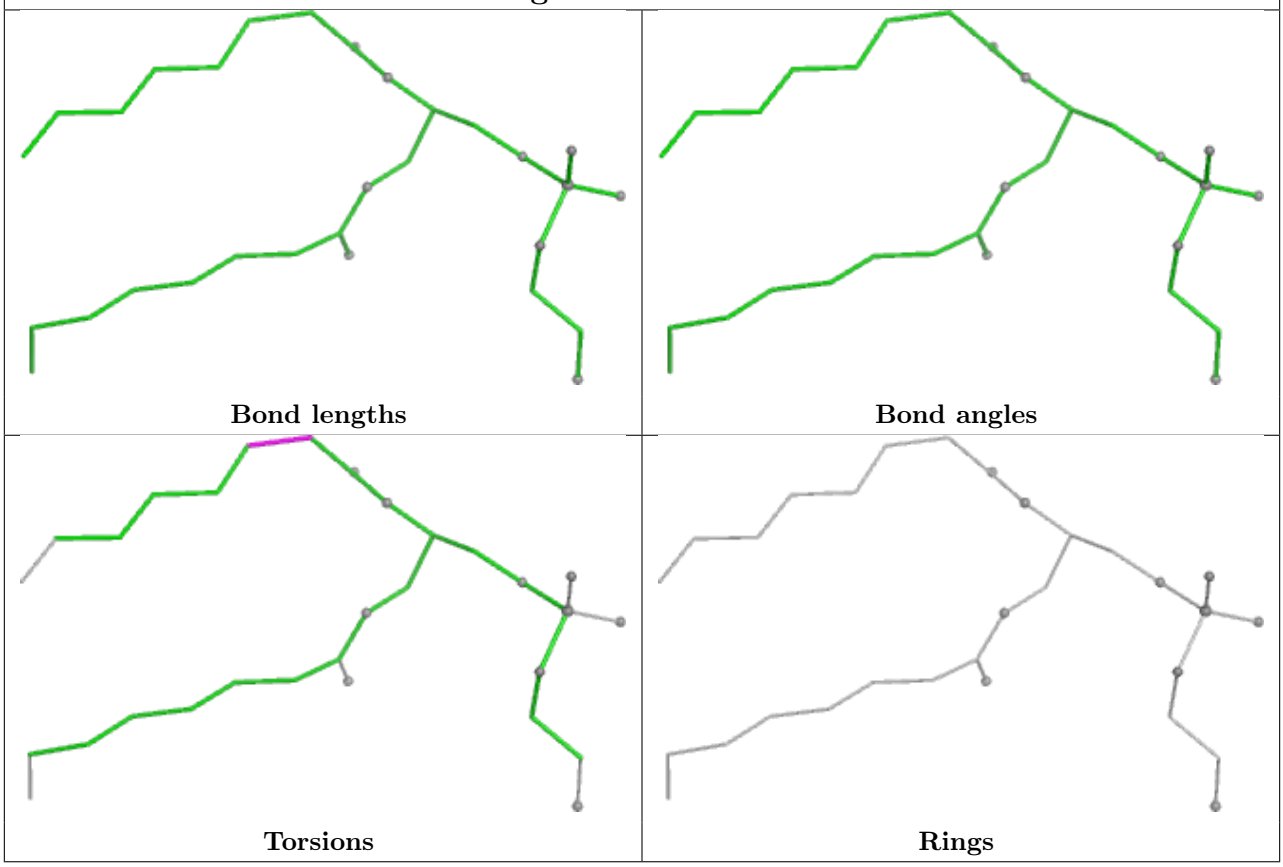


Rings

Ligand 3PE E 405



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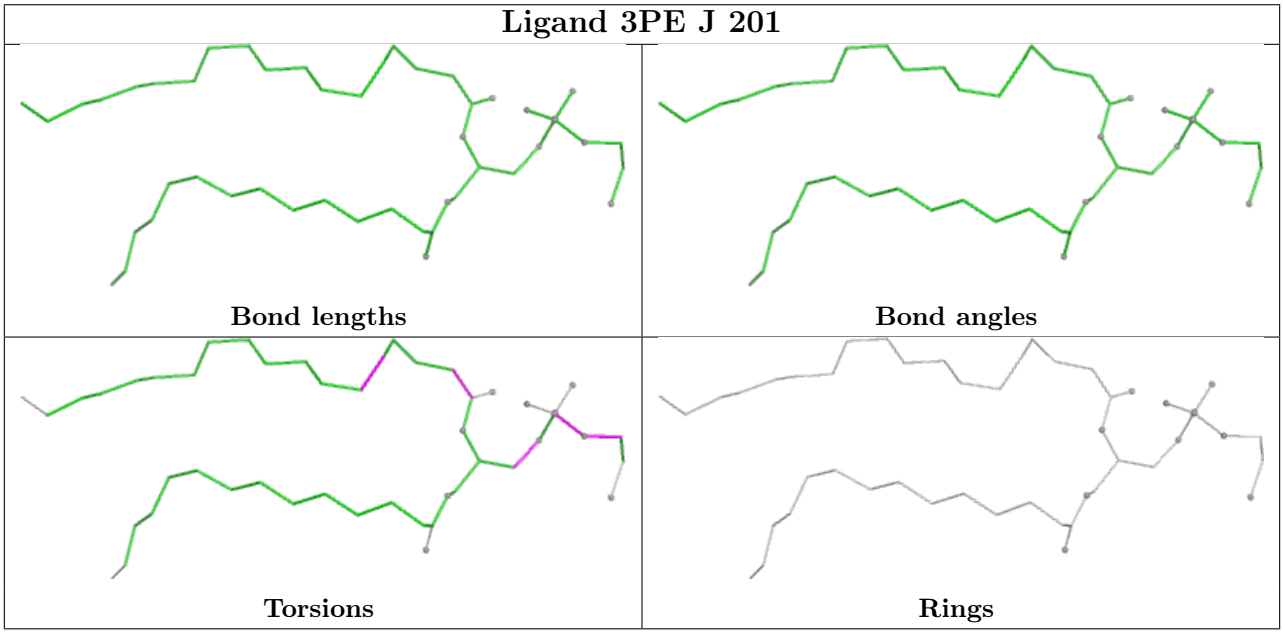

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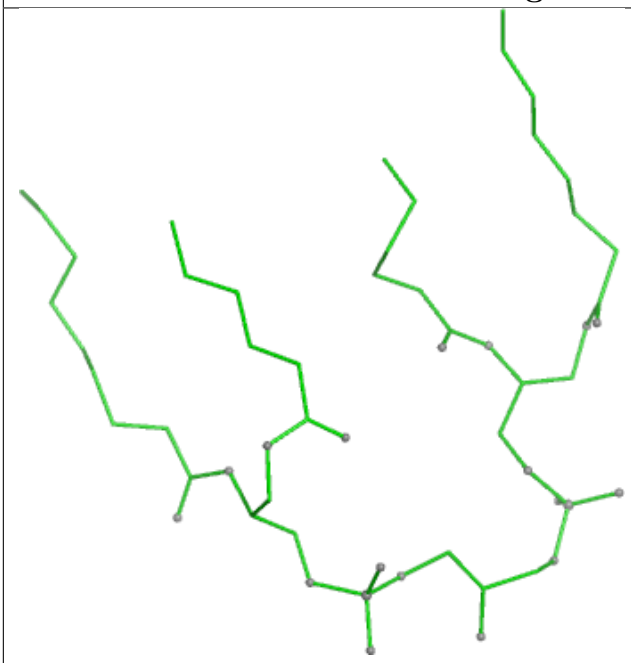

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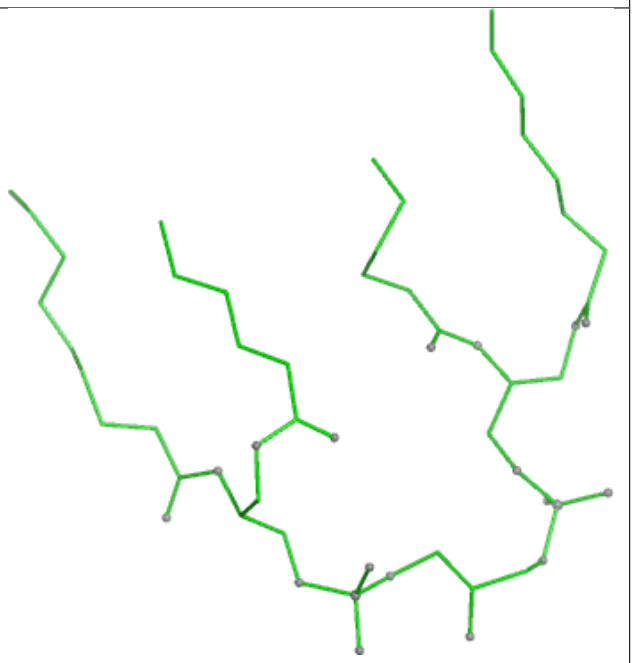

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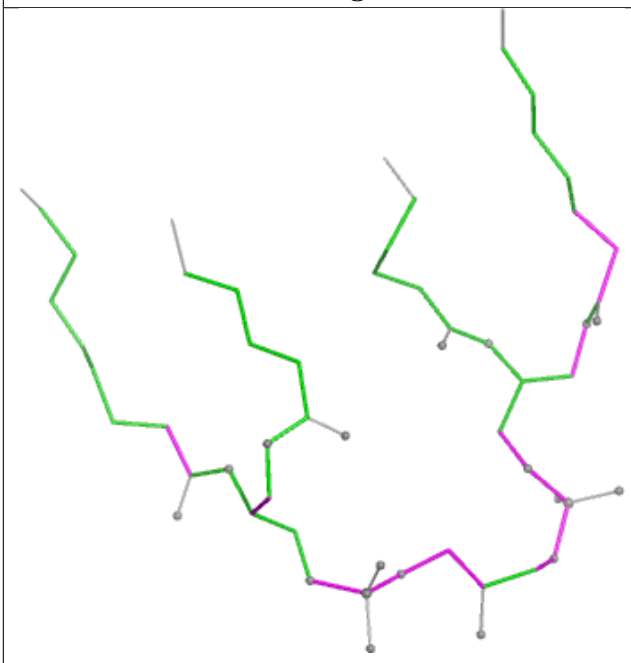

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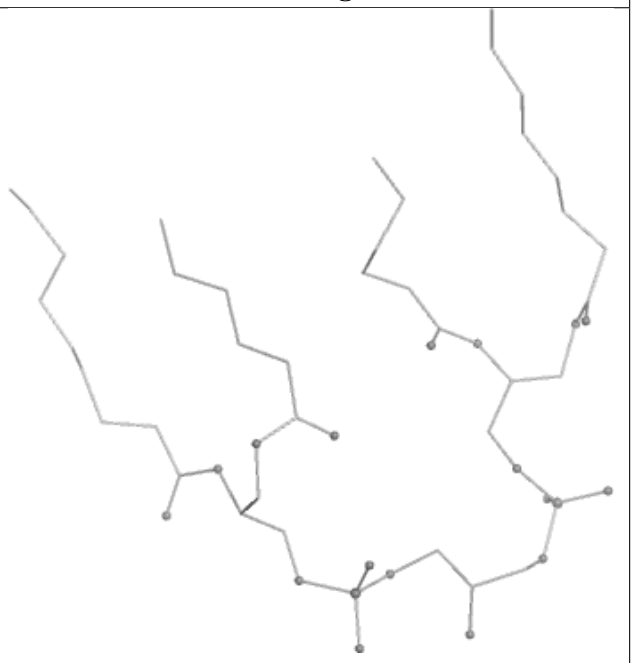
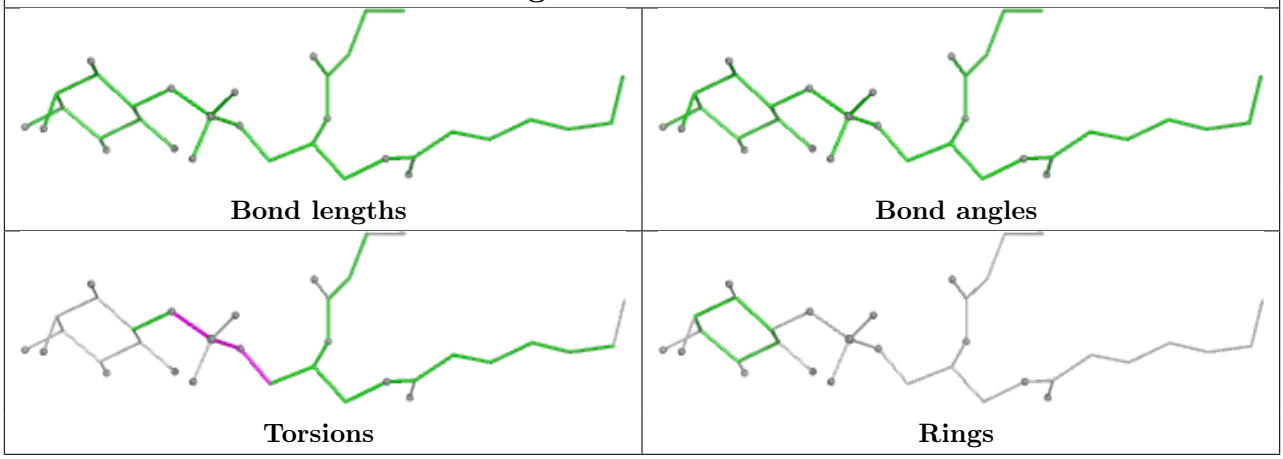
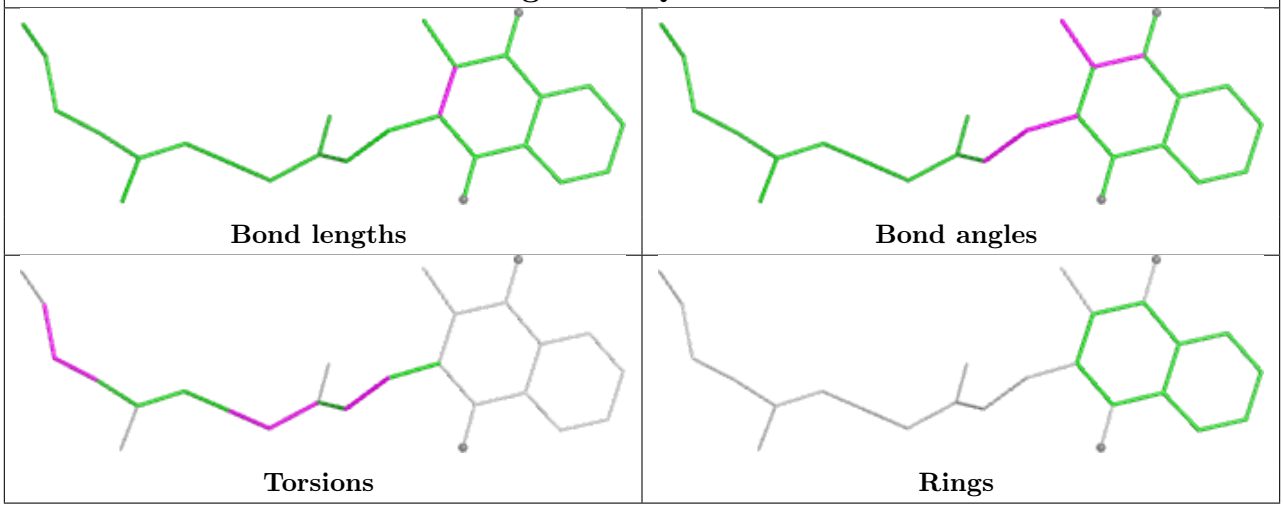


Rings

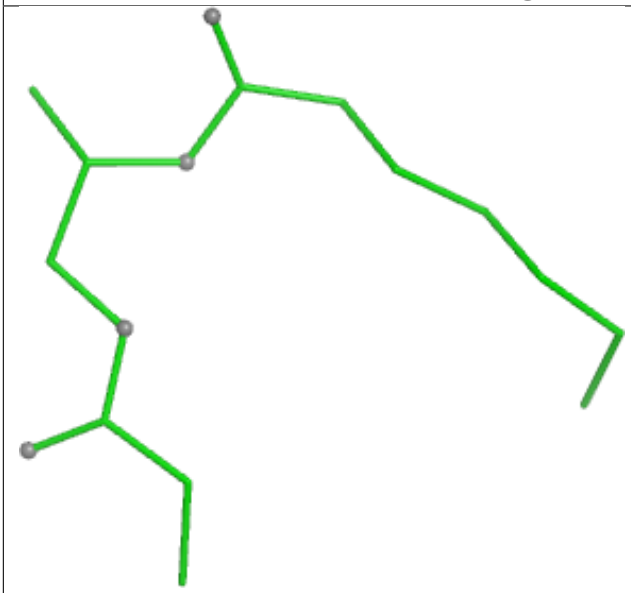
Ligand 9YF U 203



Ligand MQ9 N 501



Ligand DGA H 201



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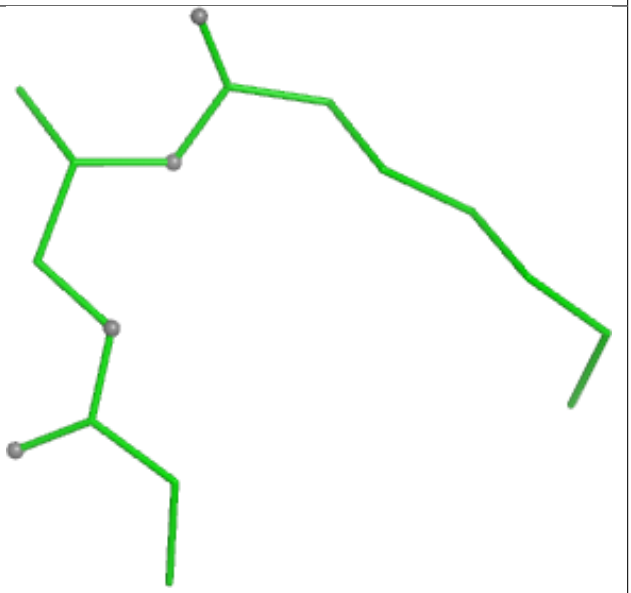

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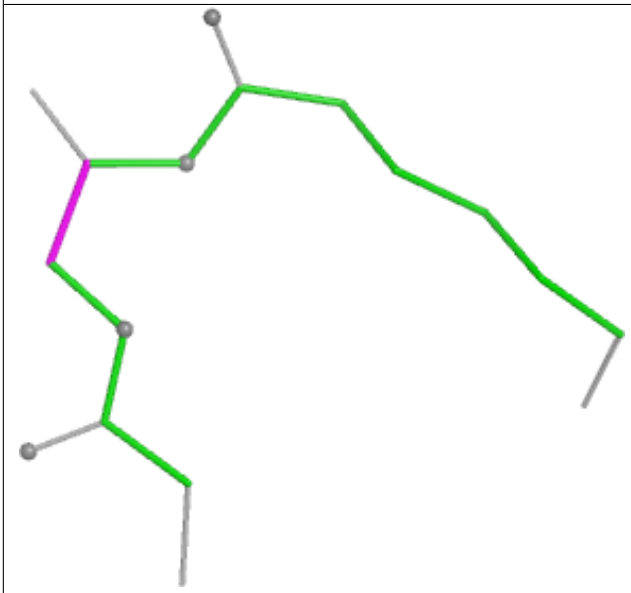

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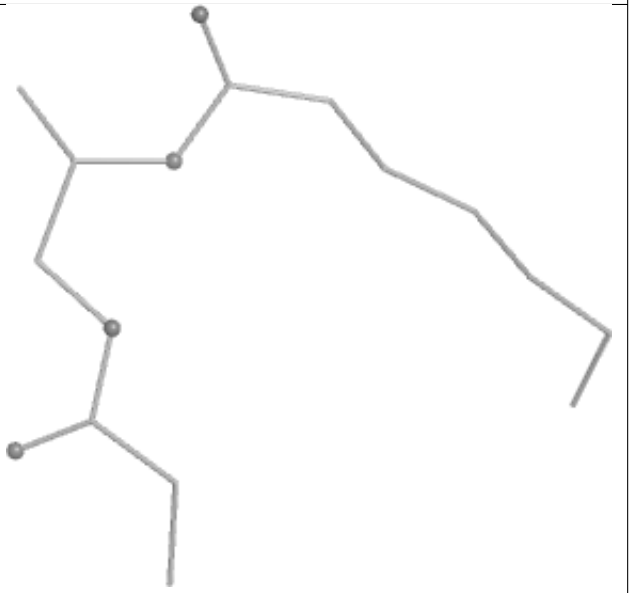
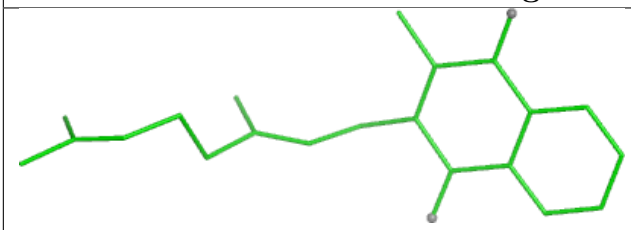


Rings

Ligand MQ9 B 604



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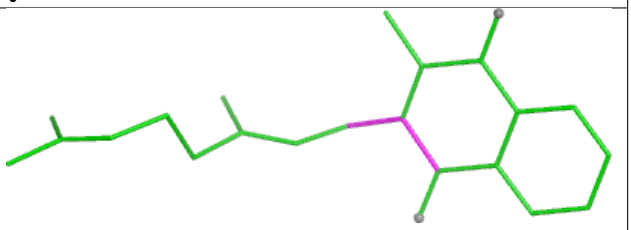
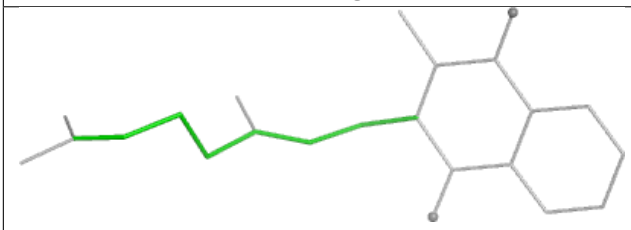


Bond angles



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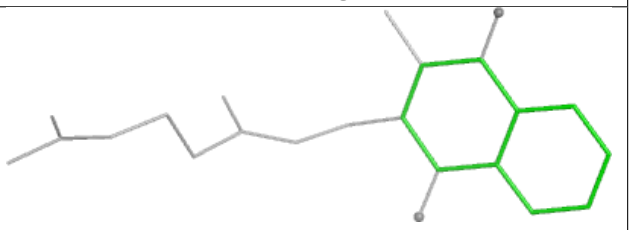
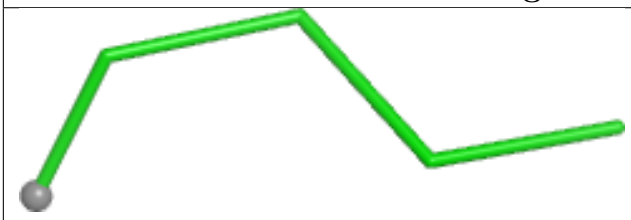


Rings

Ligand PLM Z 202



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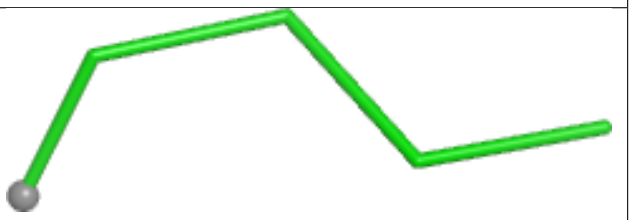

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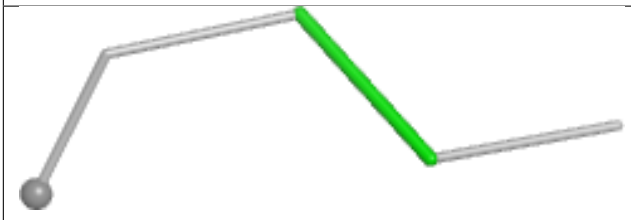
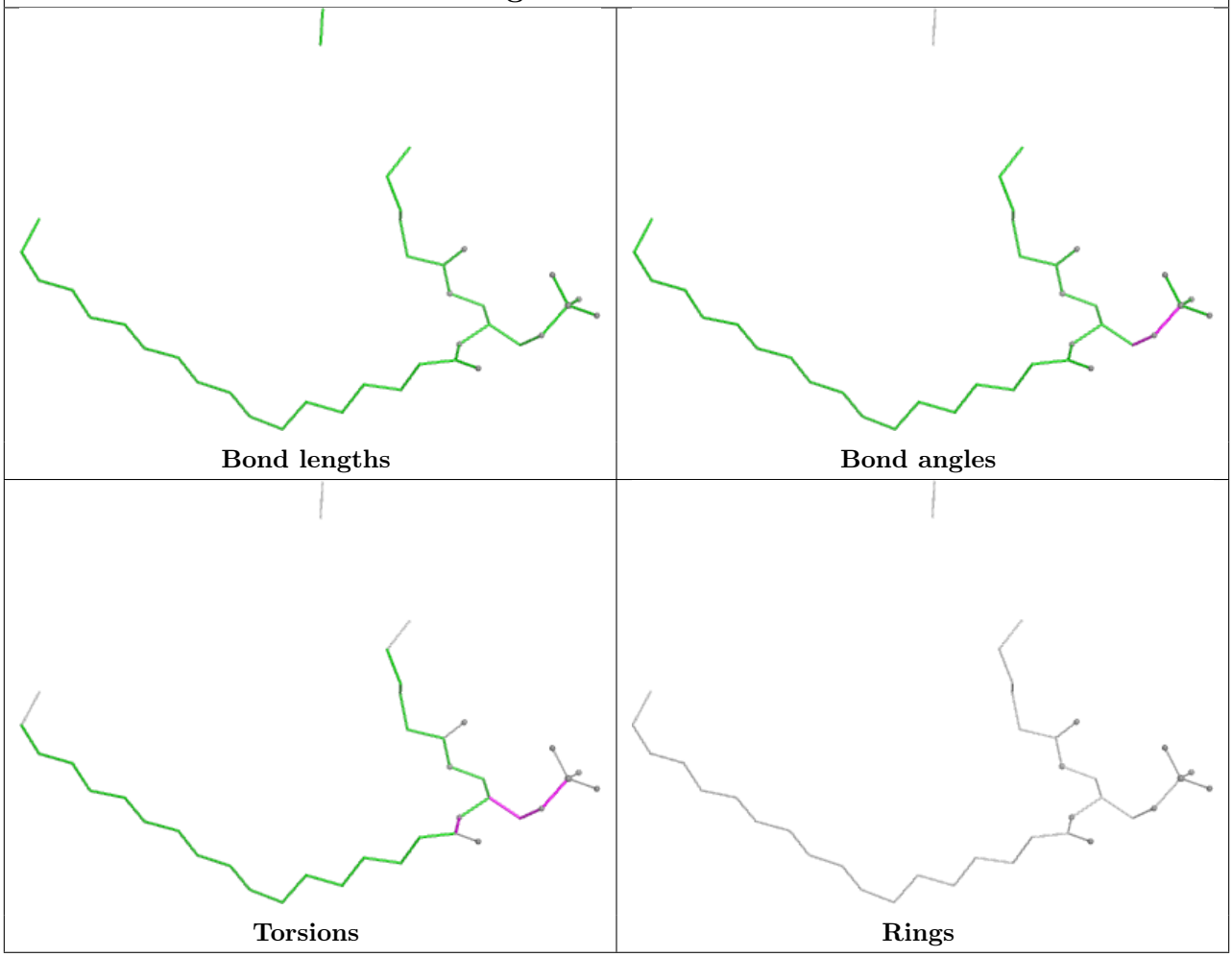


Torsions



Rings

Ligand 3PH T 201



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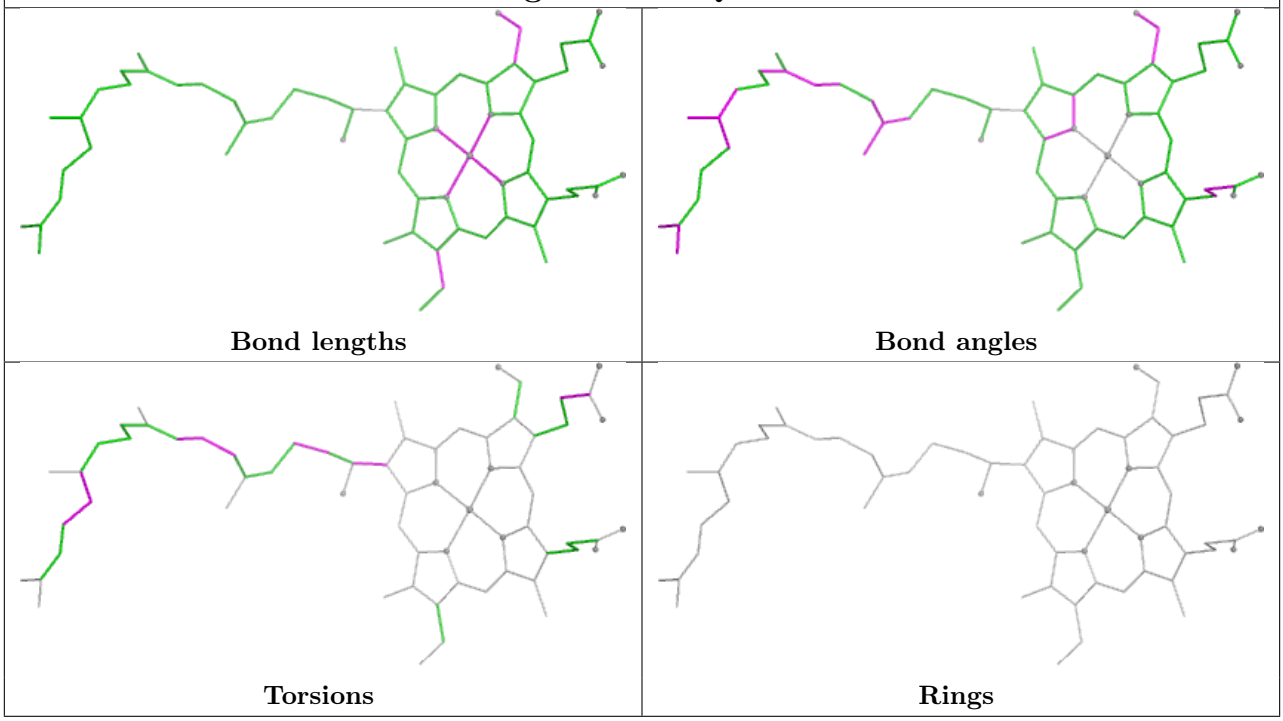

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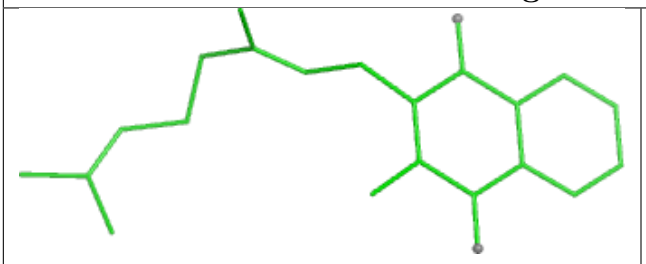

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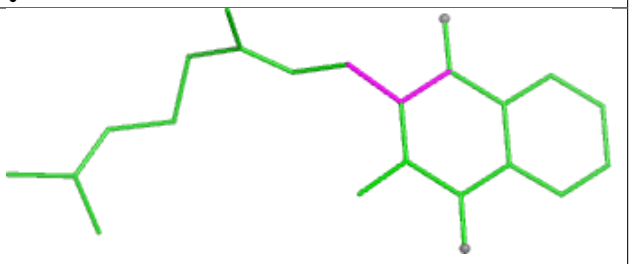

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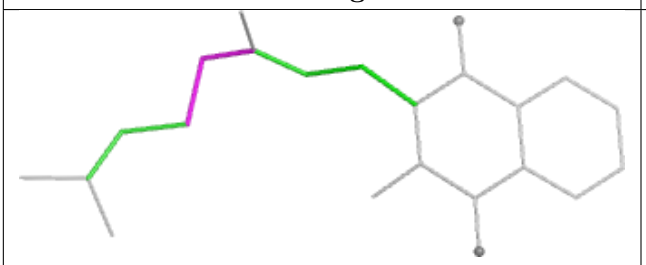

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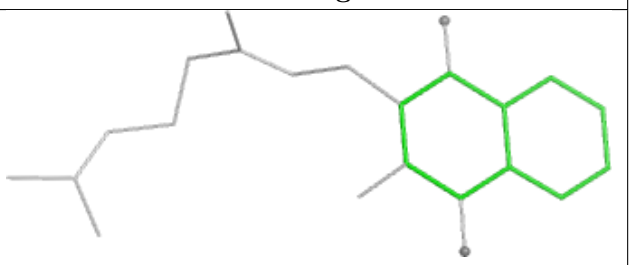
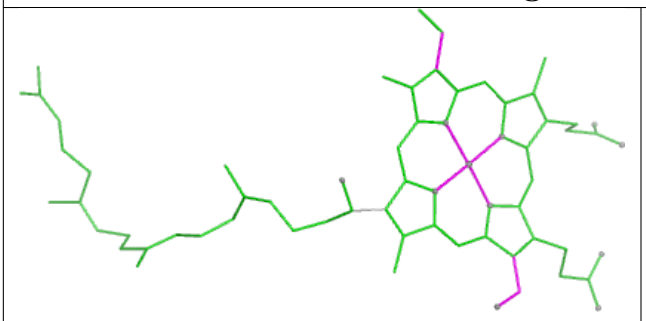


Rings

Ligand HAS D 601



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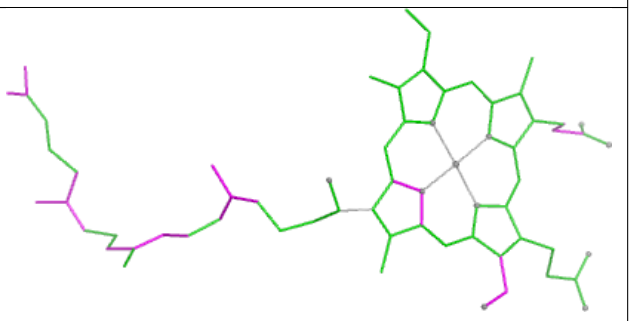
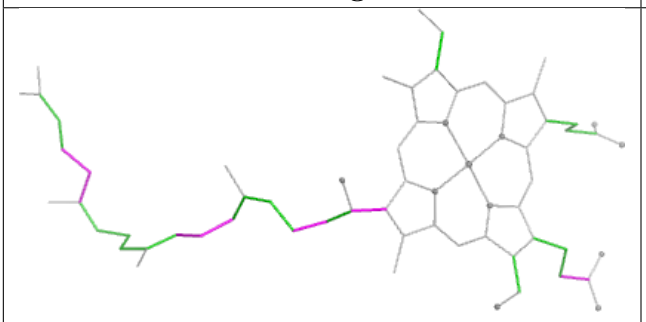
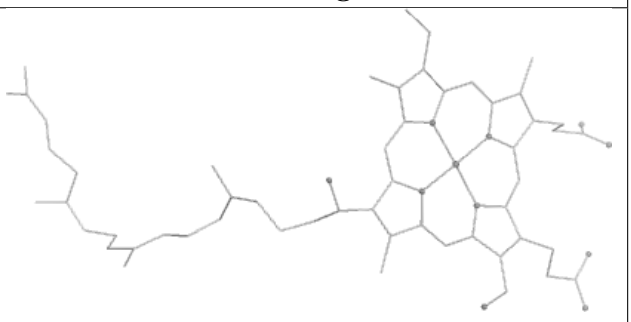


Bond angles

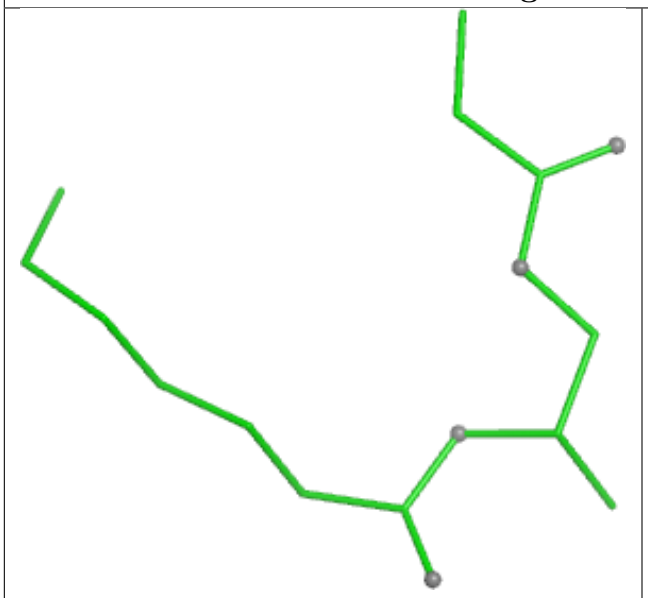


Torsions

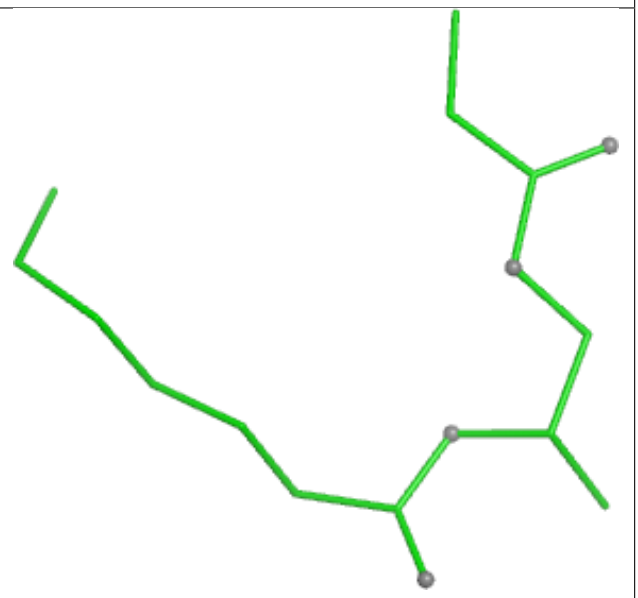


Rings

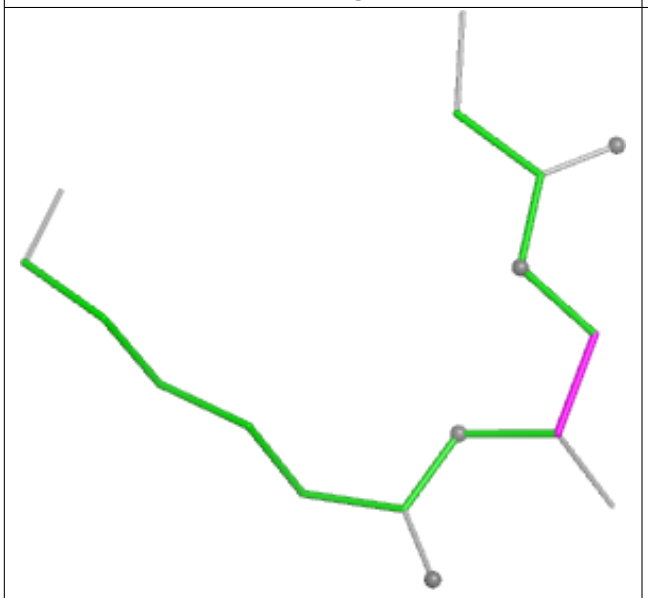
Ligand DGA U 201



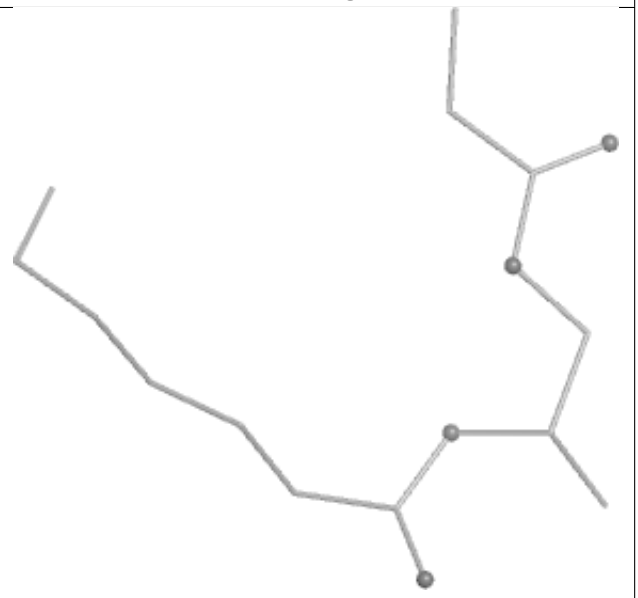
Bond lengths



Bond angles

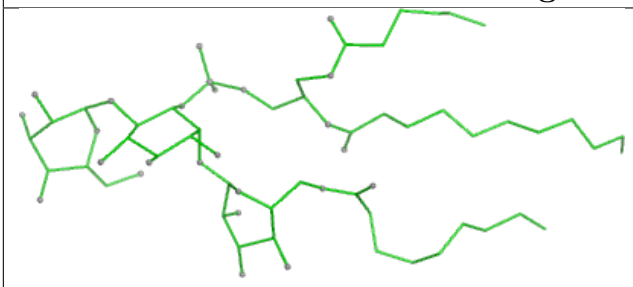


Torsions



Rings

Ligand IX7 I 202



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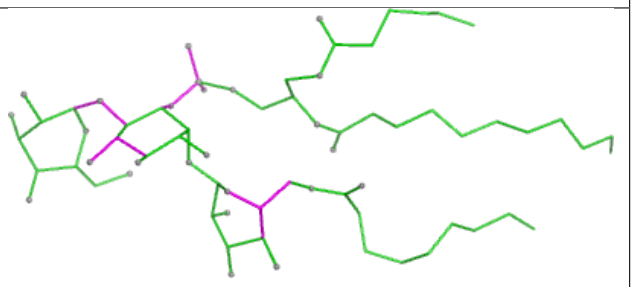

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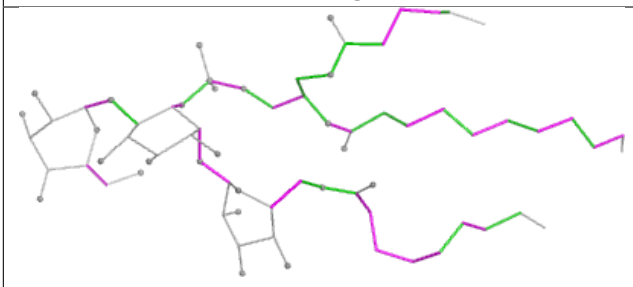

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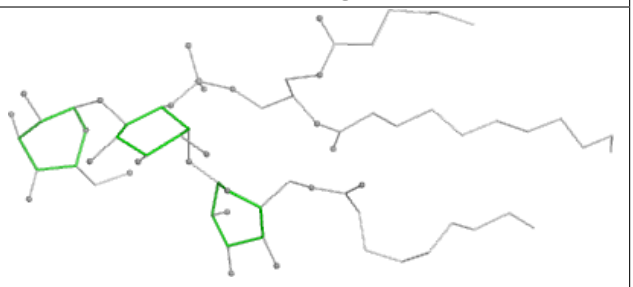
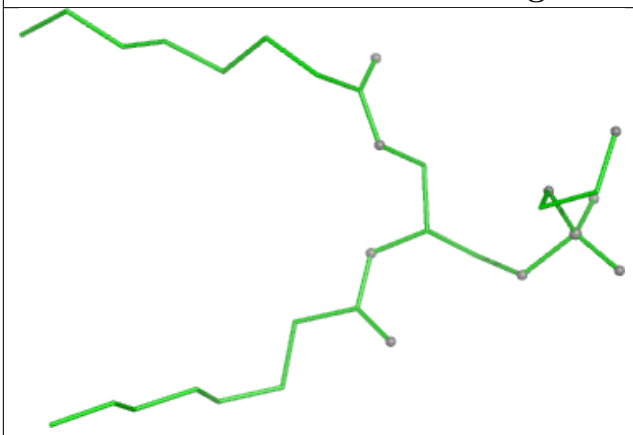


Rings

Ligand 3PE D 607



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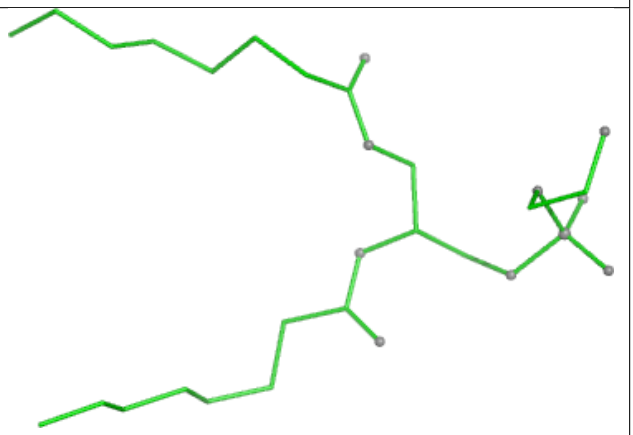

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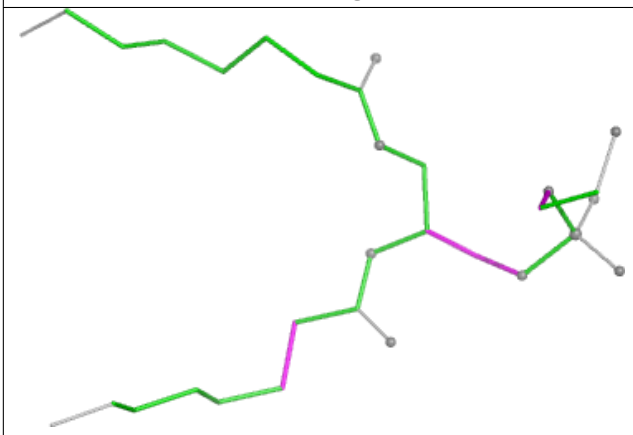

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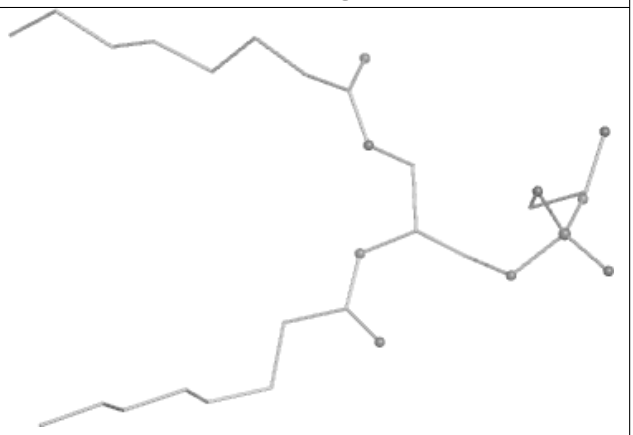
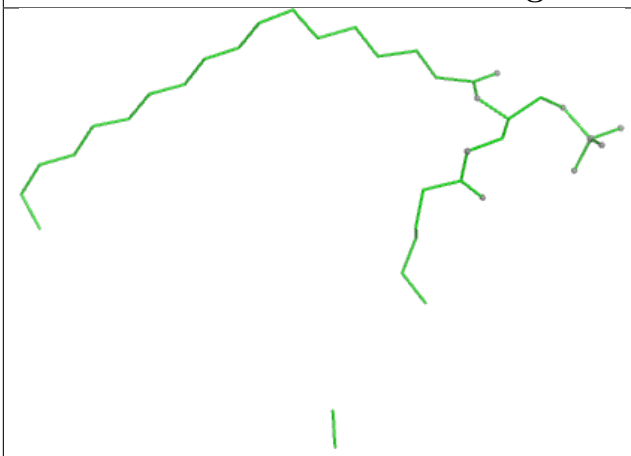


Rings

Ligand 3PH C 304



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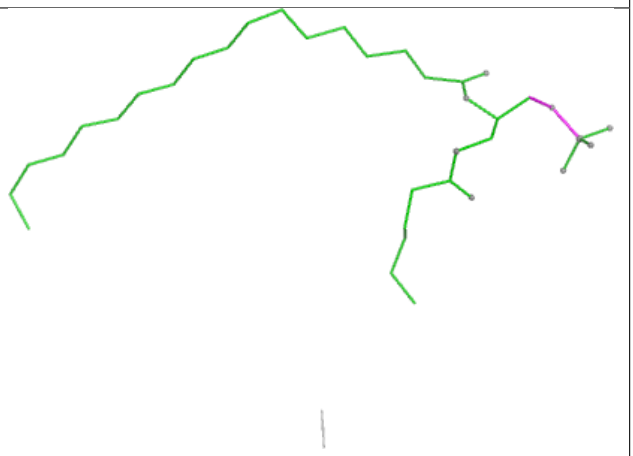

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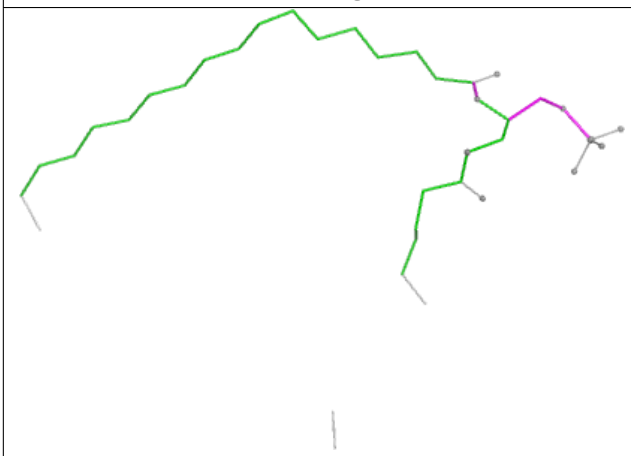
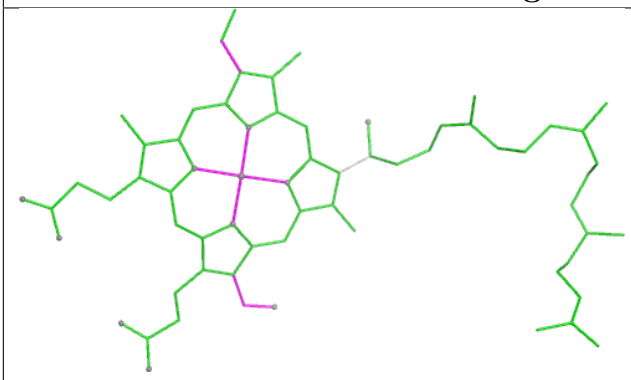


Torsions



Rings

Ligand HAS D 602



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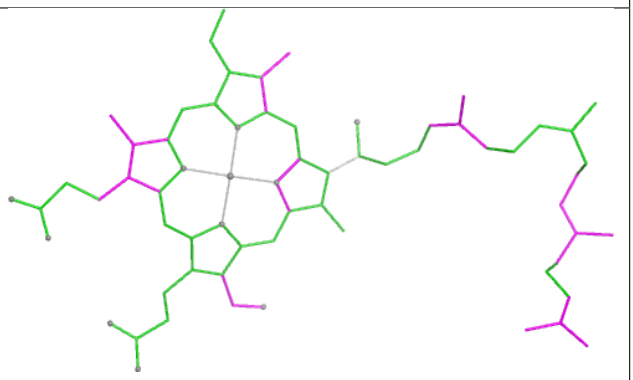
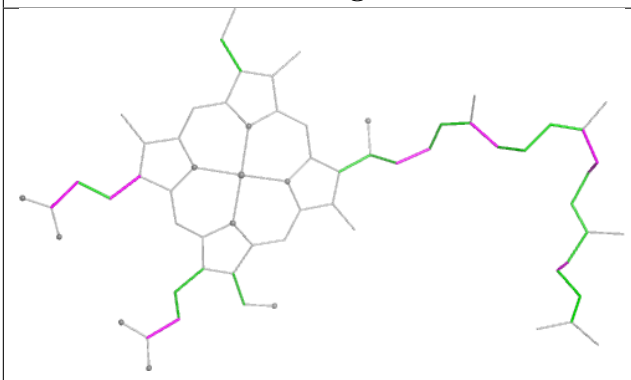


Bond angles



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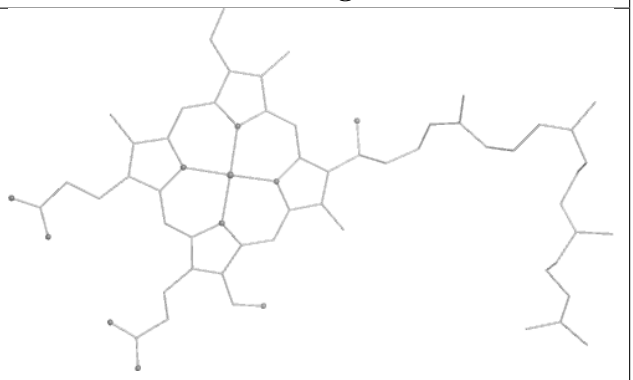
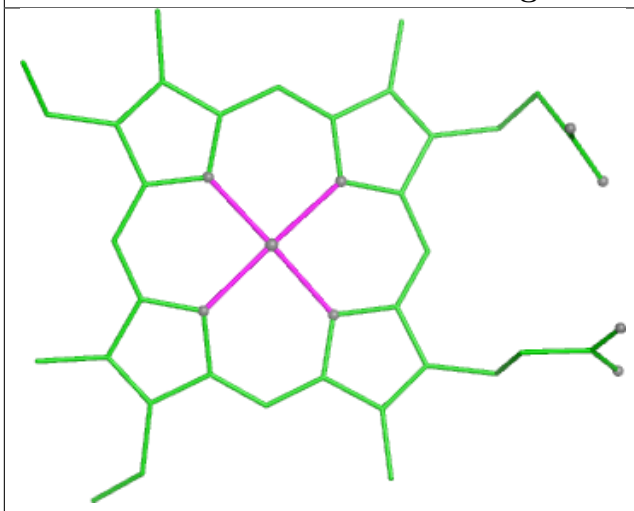


Rings

Ligand HEM B 602



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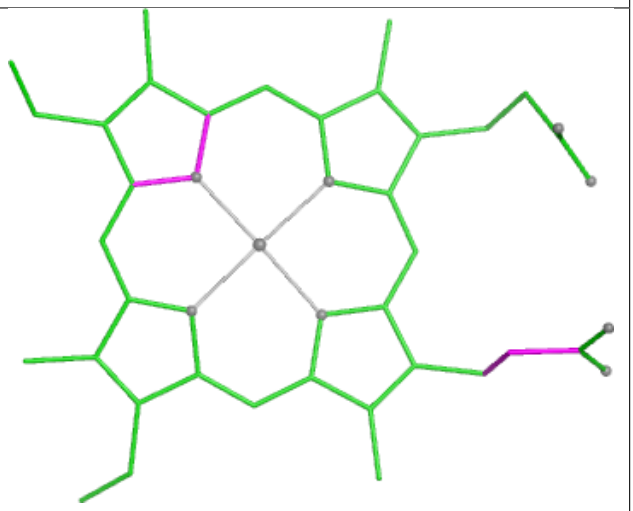
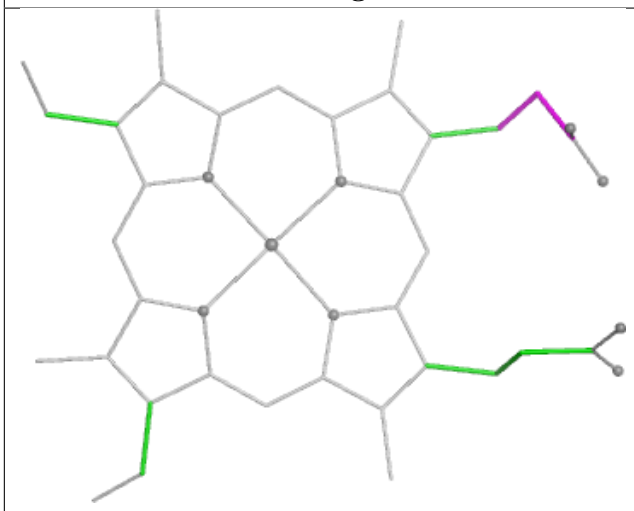


Bond angles



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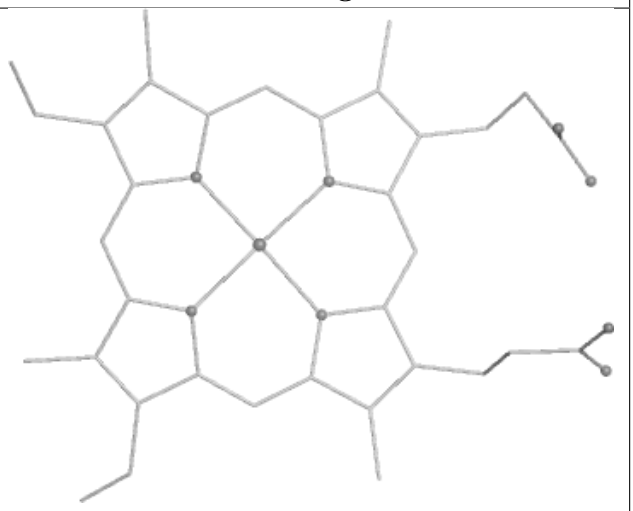
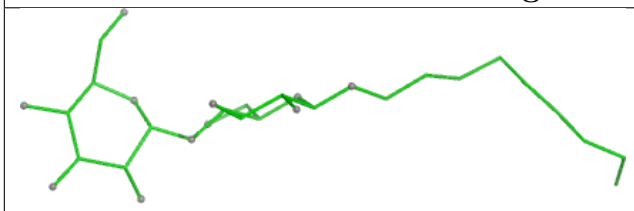


Rings

Ligand LMT B 608



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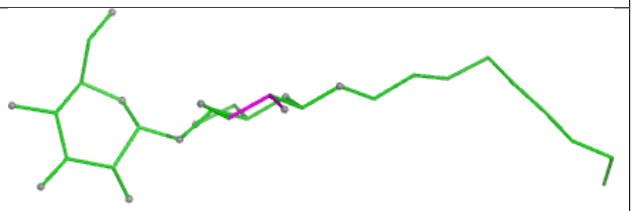
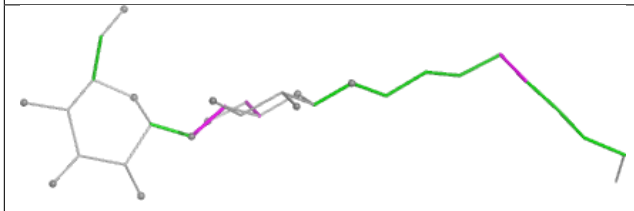


Bond angles



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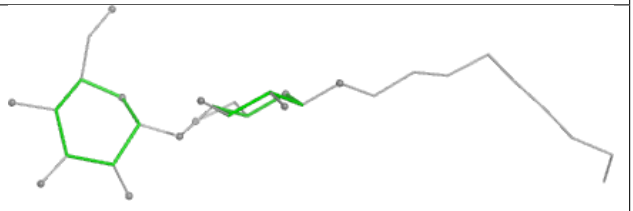
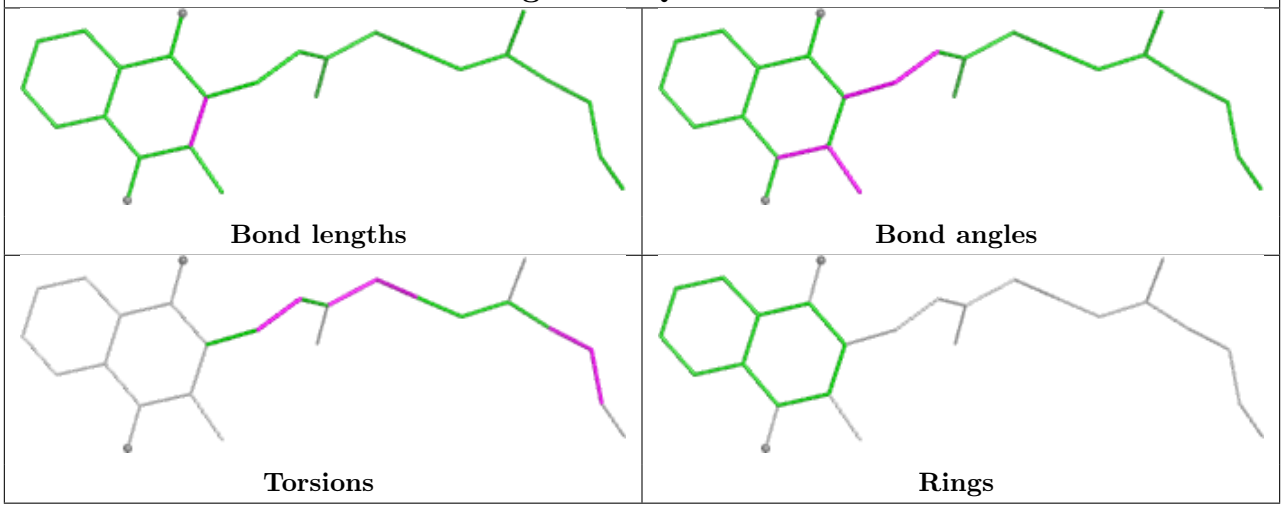


Rings

Ligand MQ9 A 504



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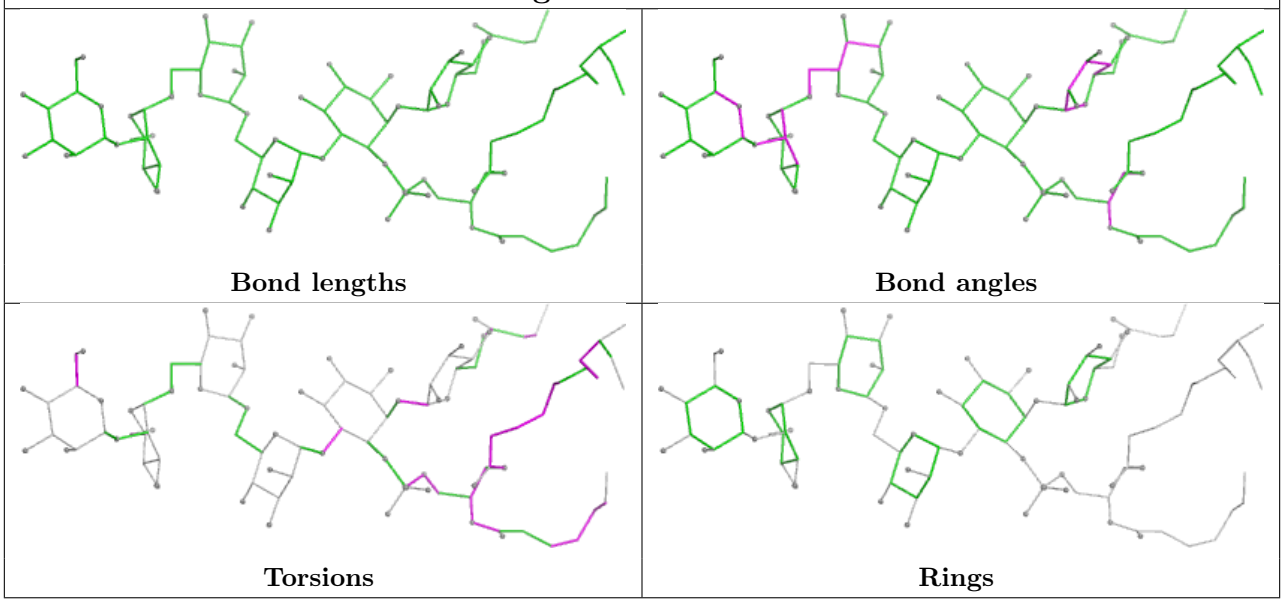

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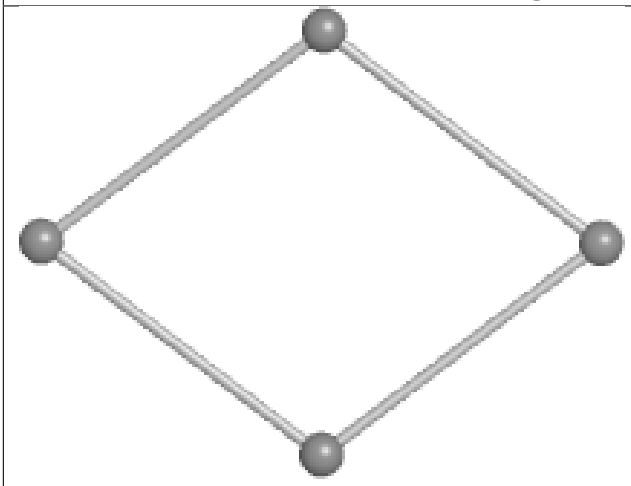

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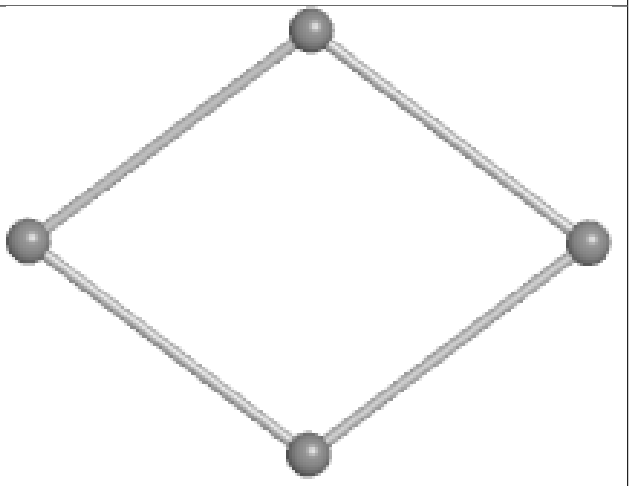
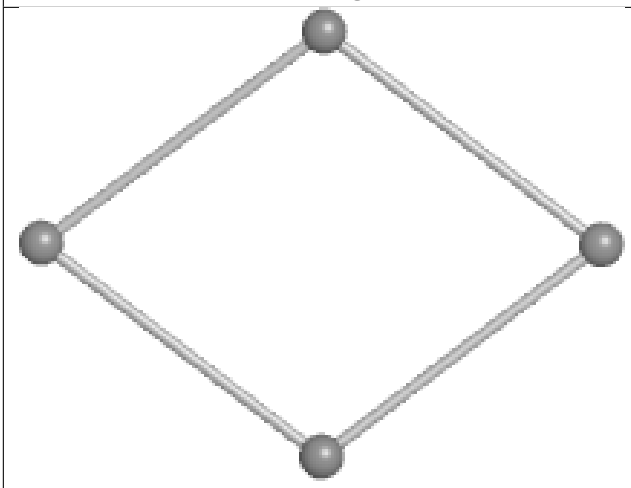


Bond angles



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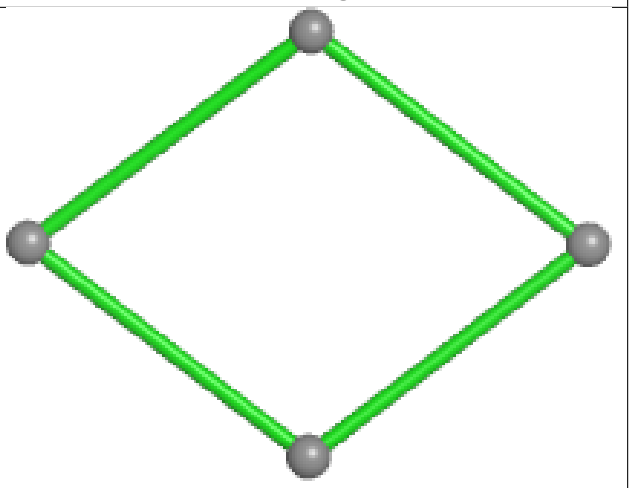
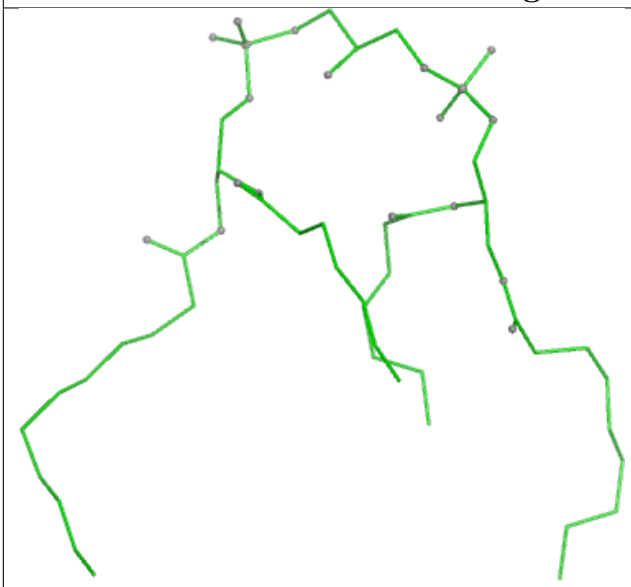


Rings

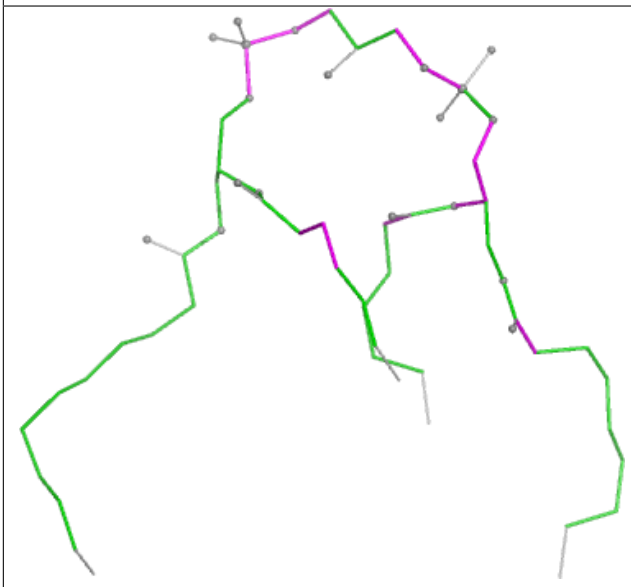
Ligand CDL G 201



Bond lengths



Bond angles

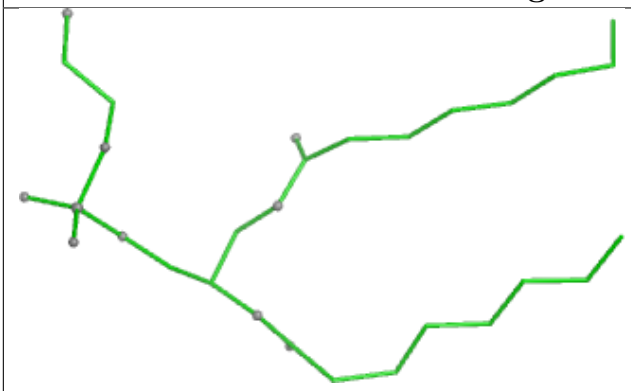


Torsions



Rings

Ligand 3PE R 405



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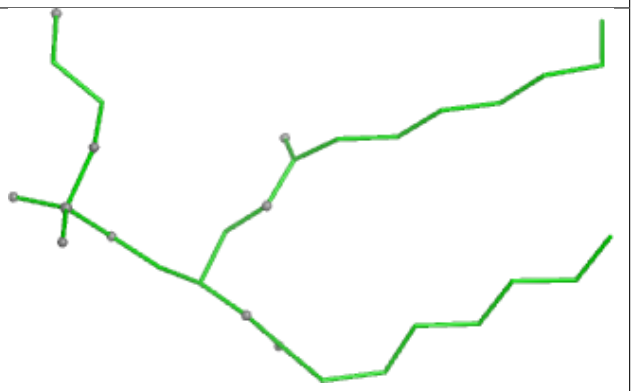
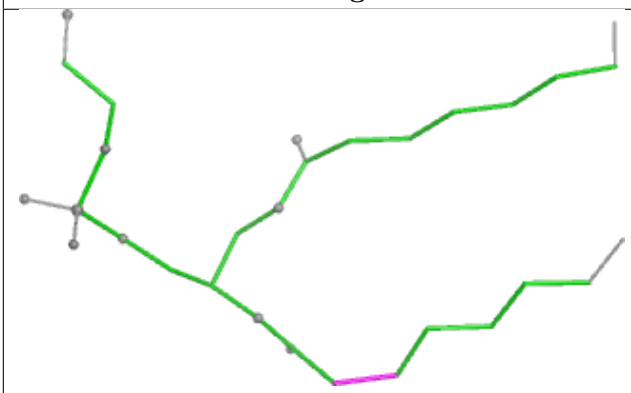


Bond angles



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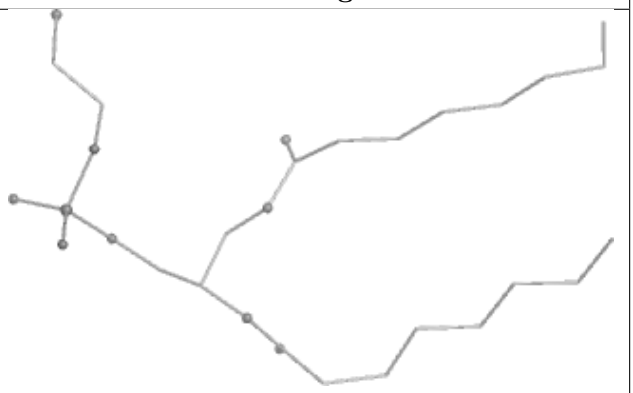
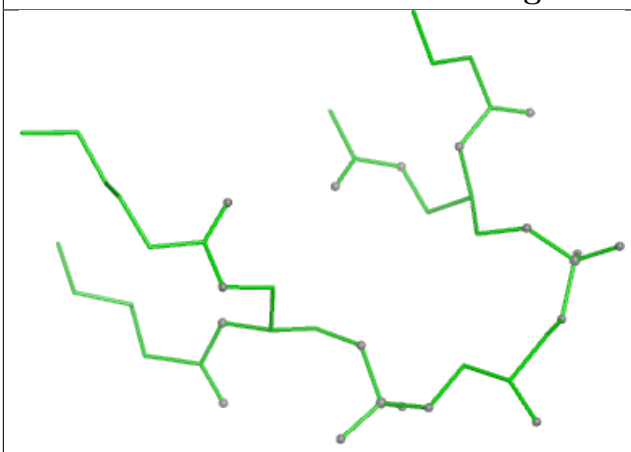


Rings

Ligand CDL O 606



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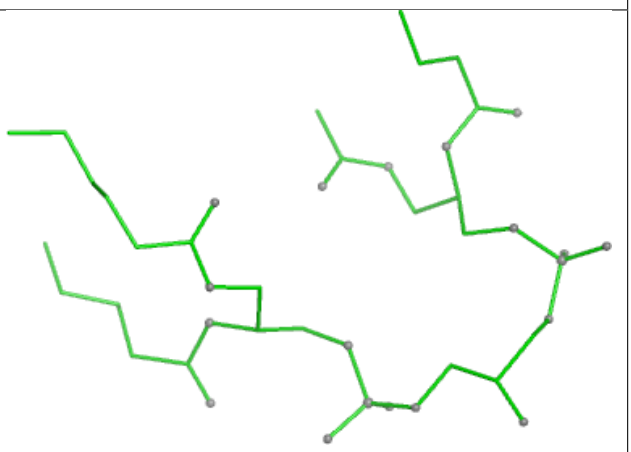
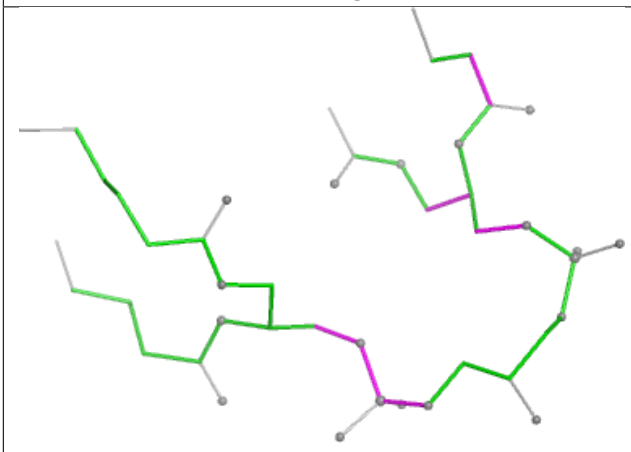


Bond angles



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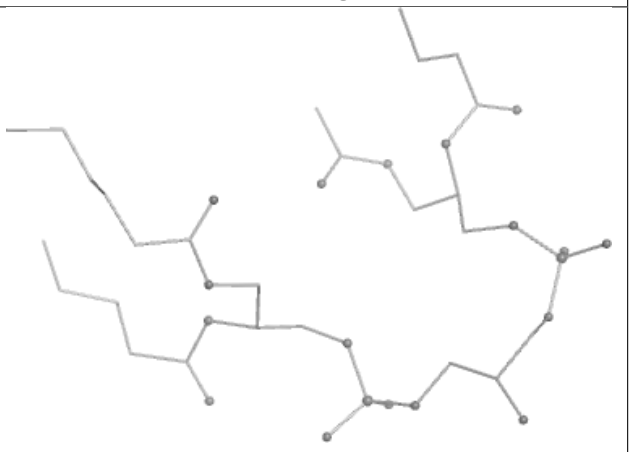
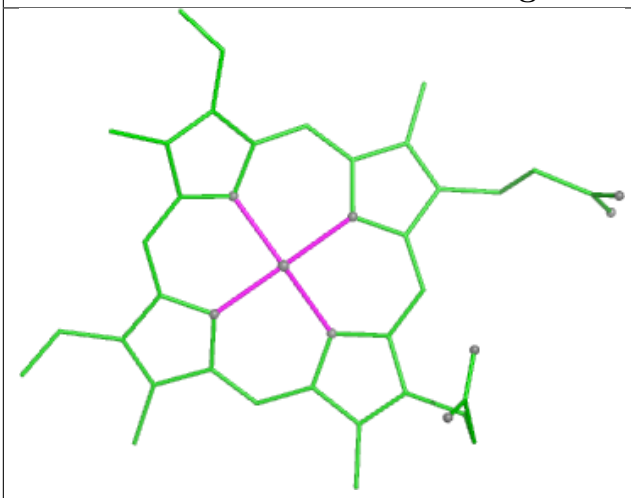


Rings

Ligand HEM B 603



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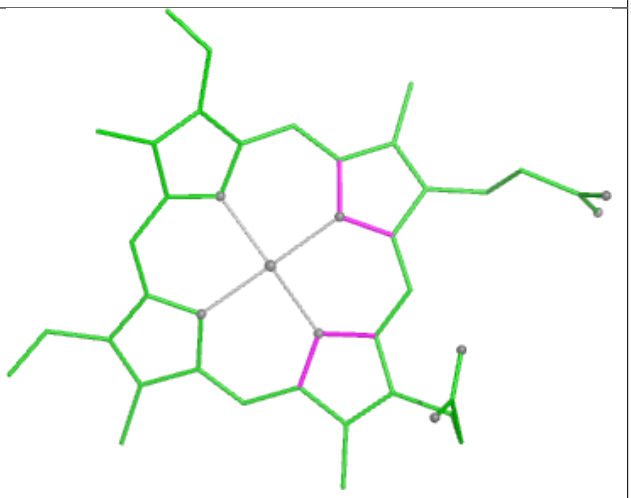
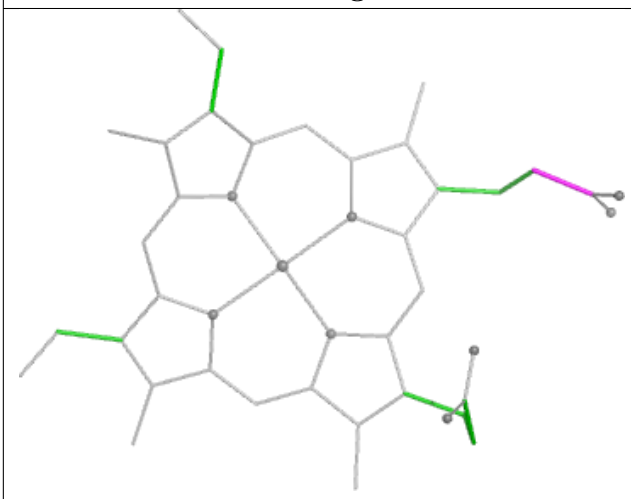


Bond angles



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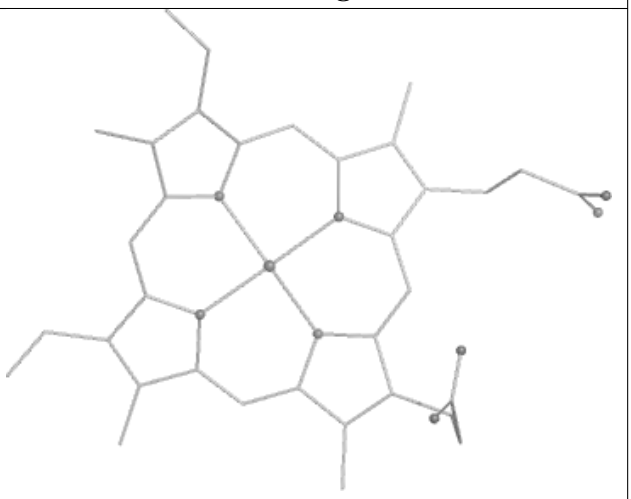
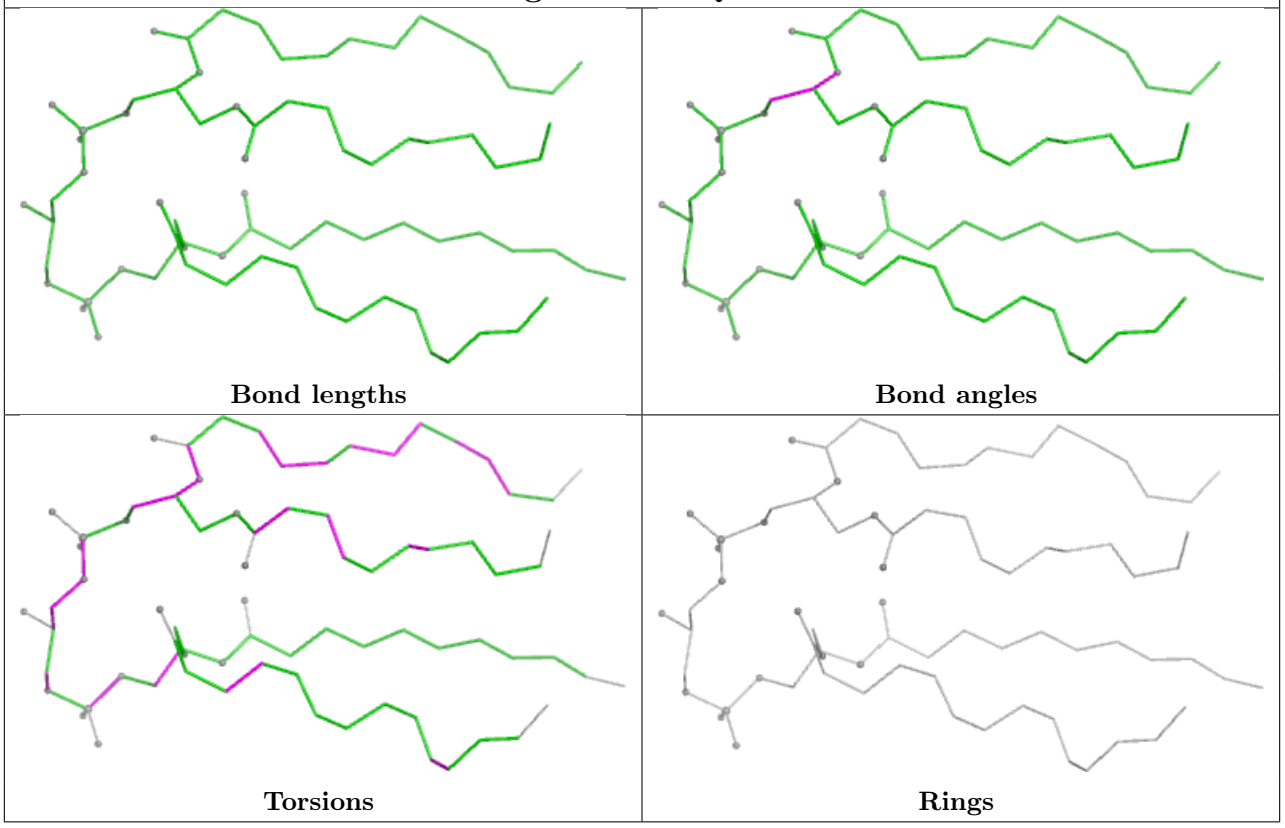
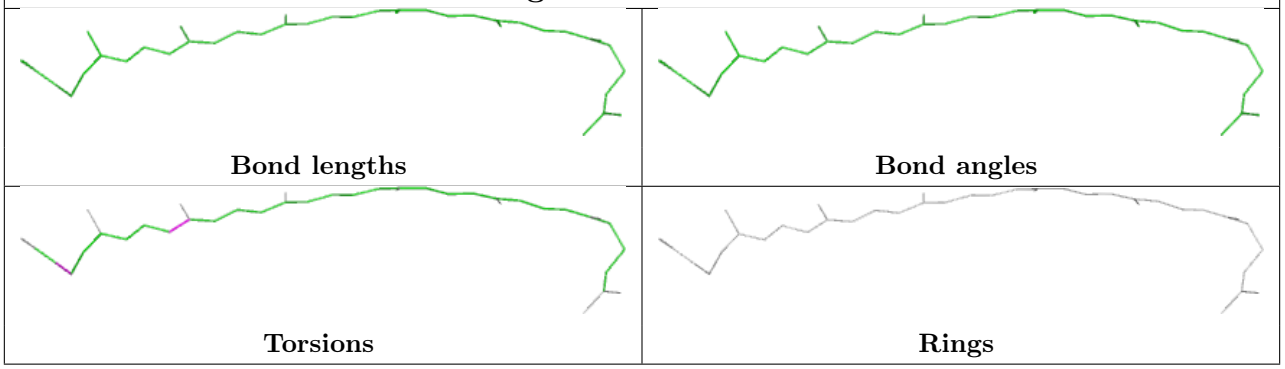


Rings

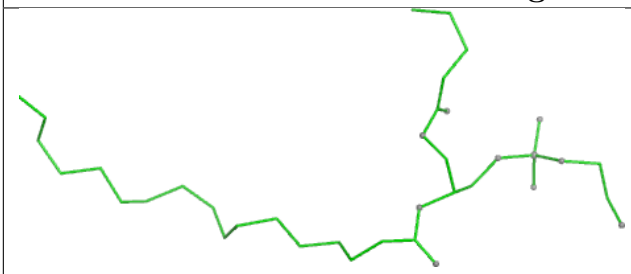
Ligand CDL Q 605



Ligand LYC B 606



Ligand 3PE A 505



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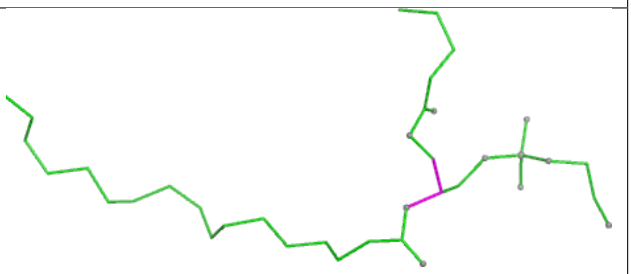
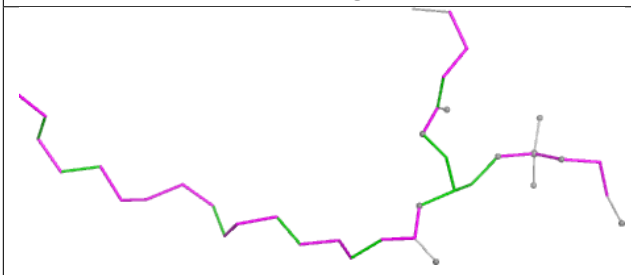


Bond angles



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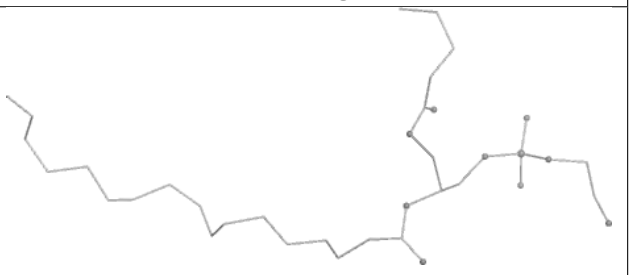
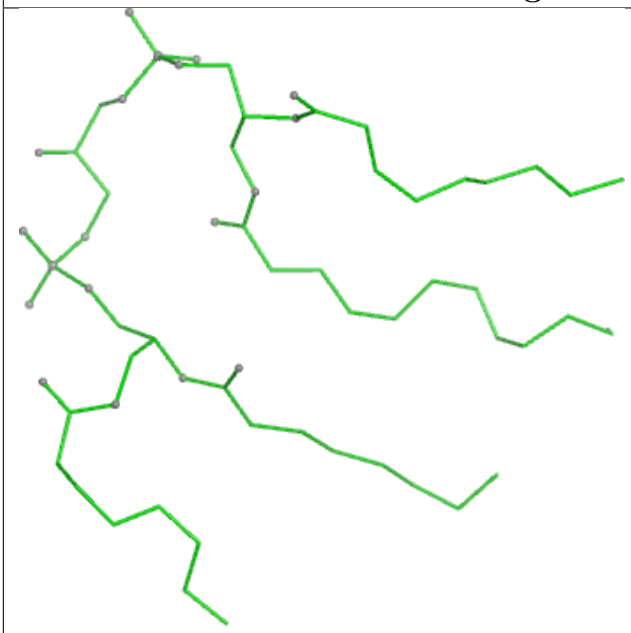
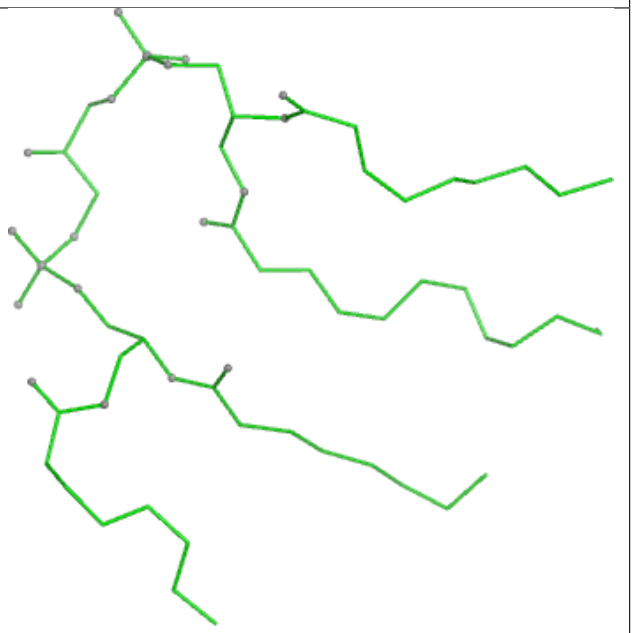


Rings

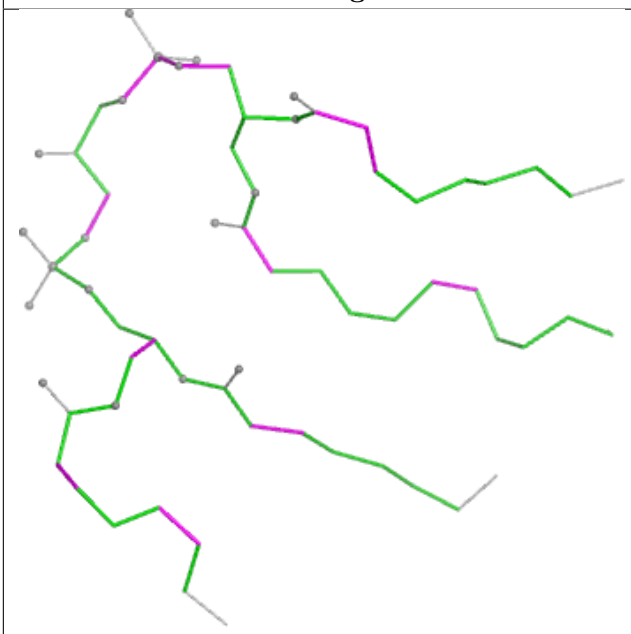
Ligand CDL C 301



Bond lengths



Bond angles



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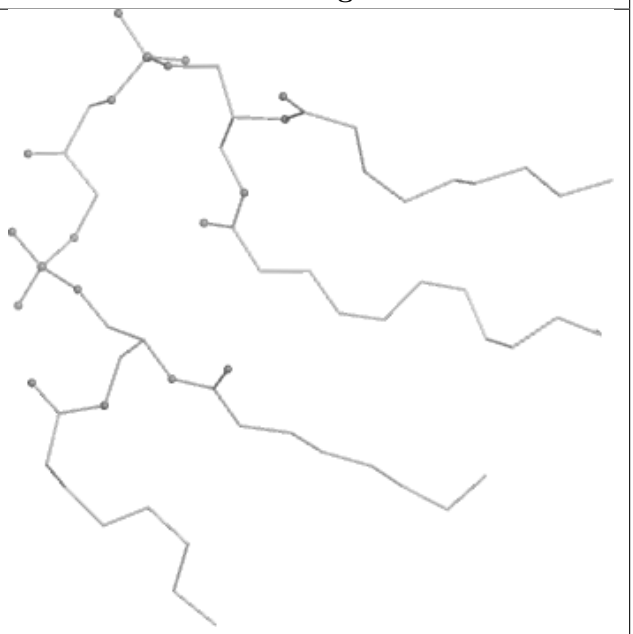
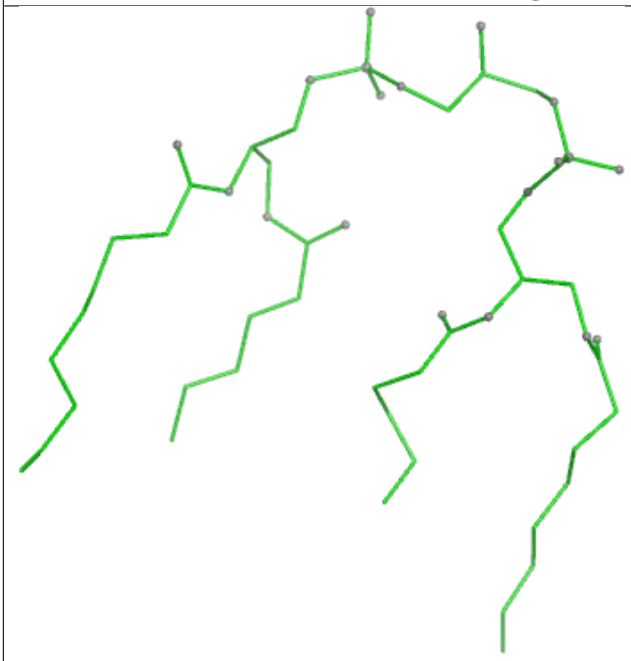
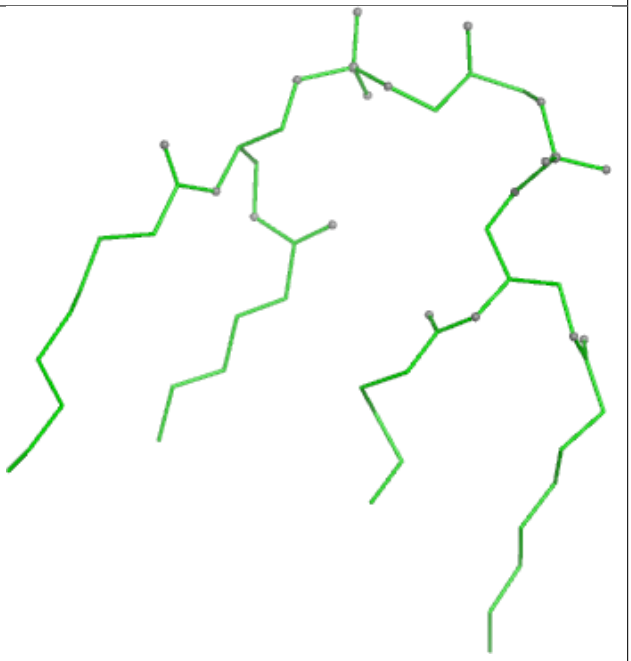


Rings

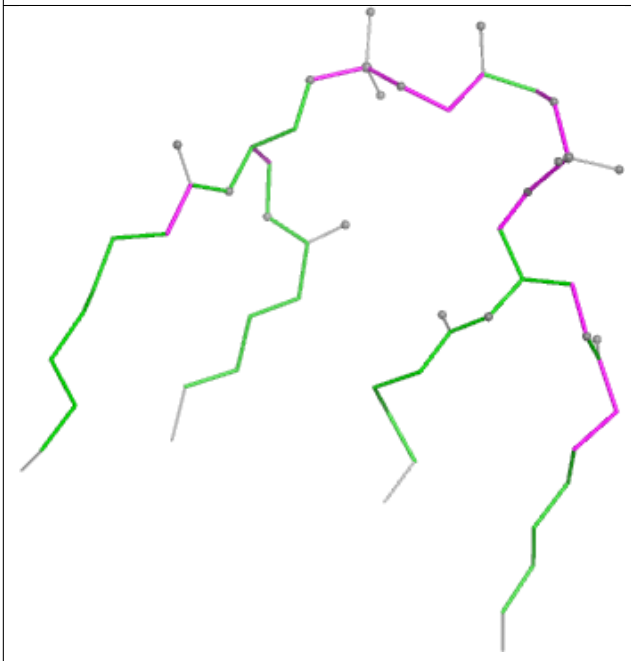
Ligand CDL S 302



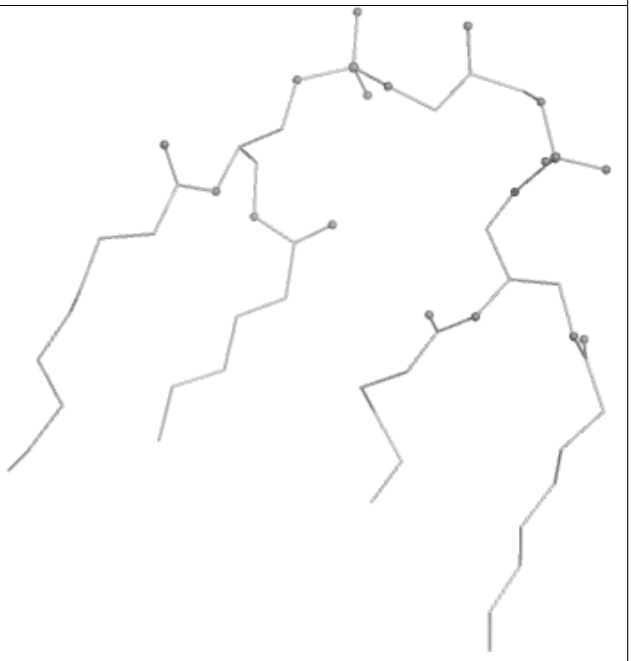
Bond lengths



Bond angles

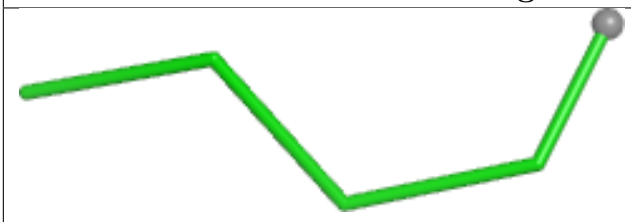


Torsions

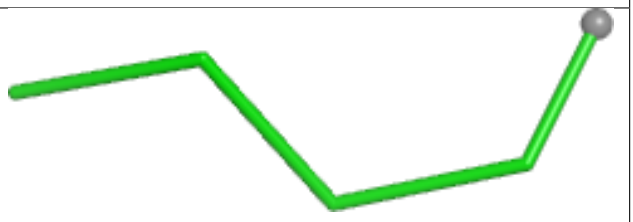


Rings

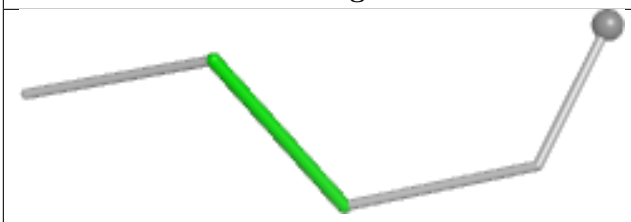
Ligand PLM M 202



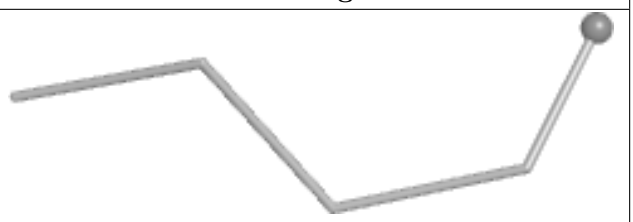
Bond lengths



Bond angles

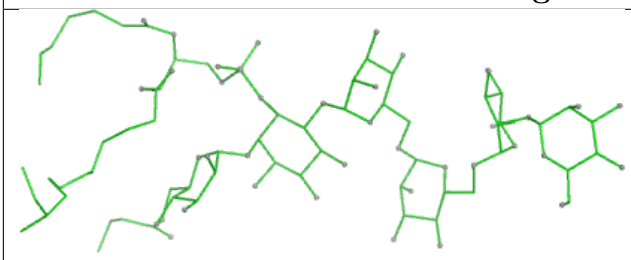


Torsions



Rings

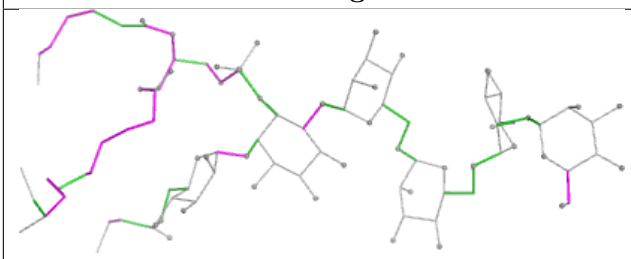
Ligand IZL A 502



Bond lengths



Bond angles



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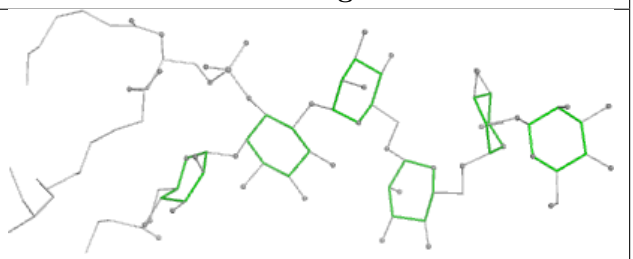
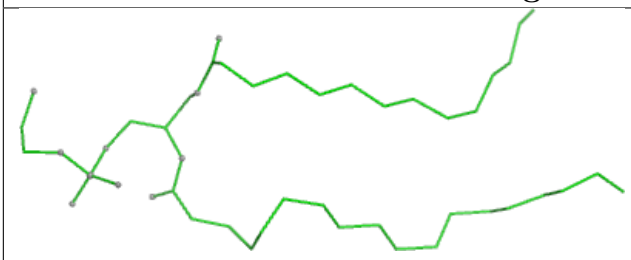
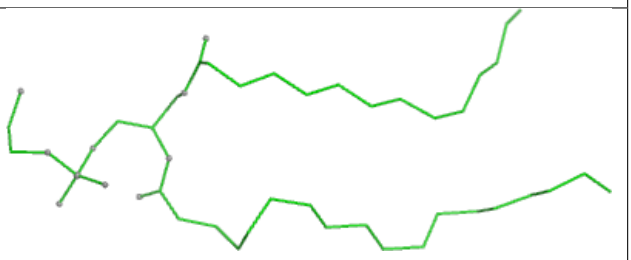


Rings

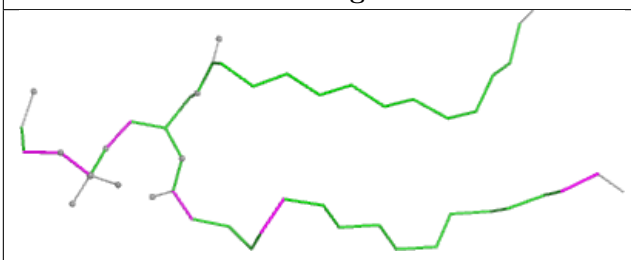
Ligand 3PE W 201



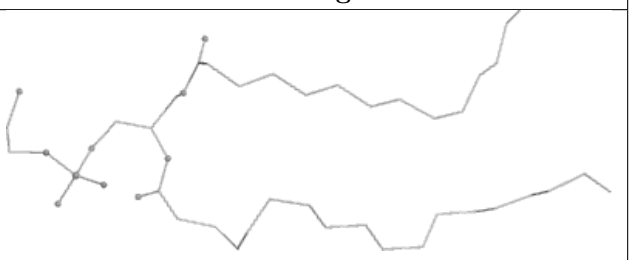
Bond lengths



Bond angles

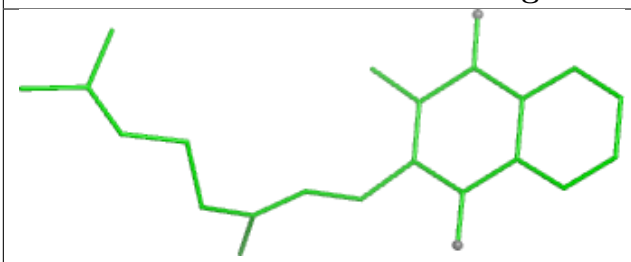


Torsions



Rings

Ligand MQ9 O 602



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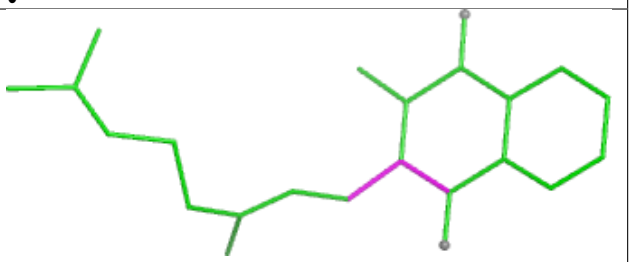
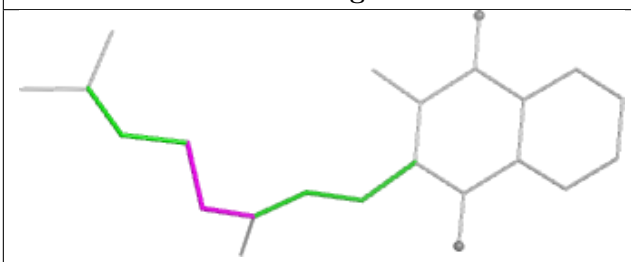


Bond angles



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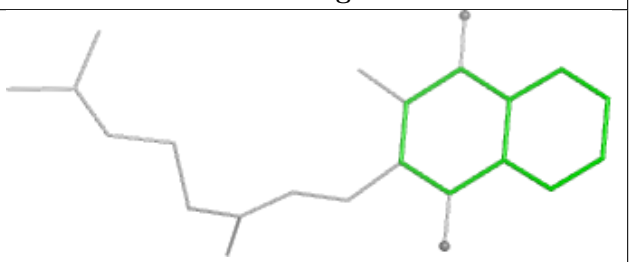
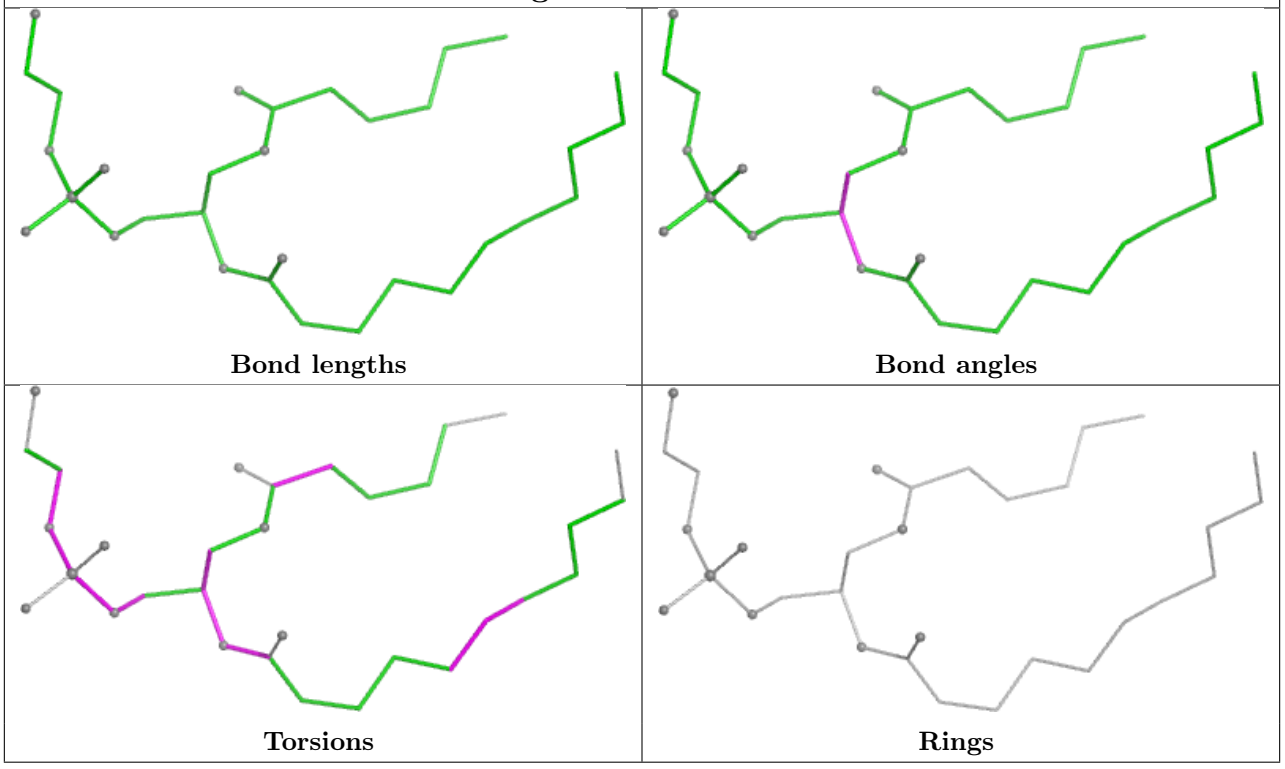
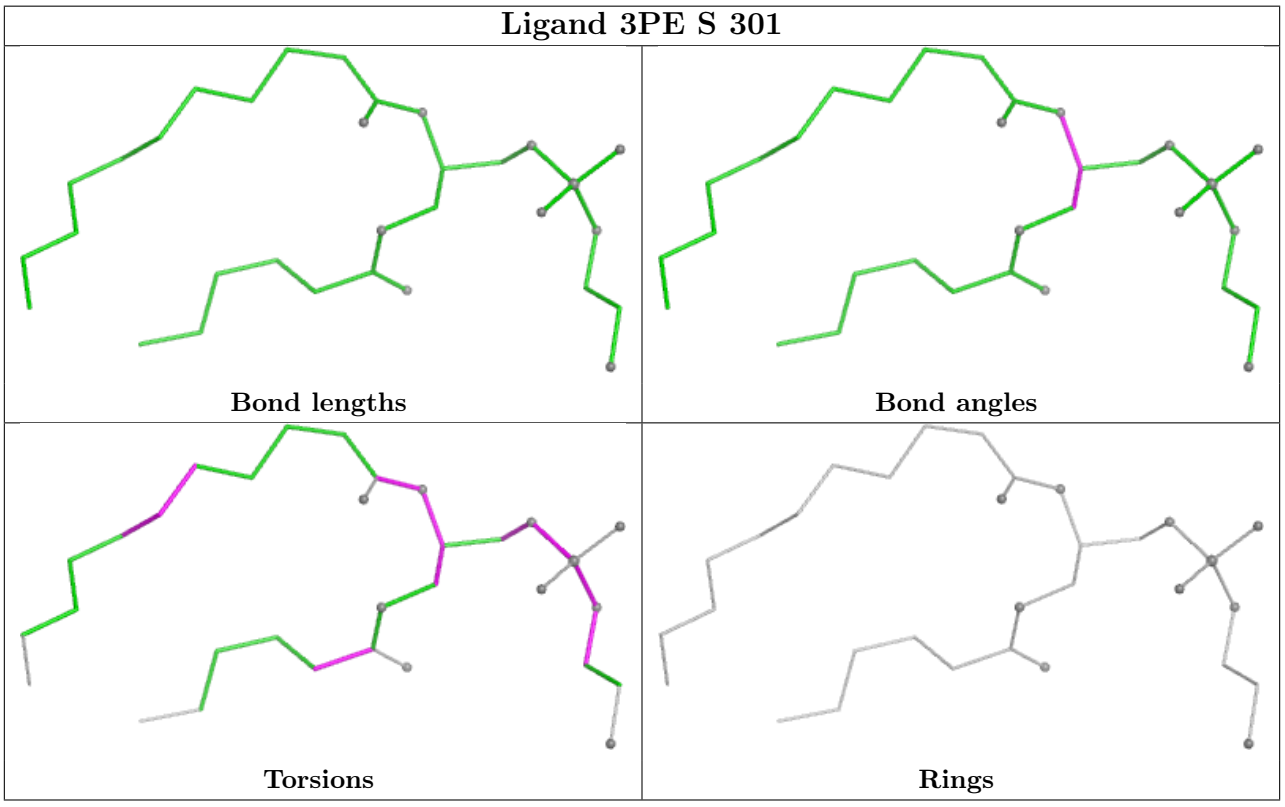


Rings

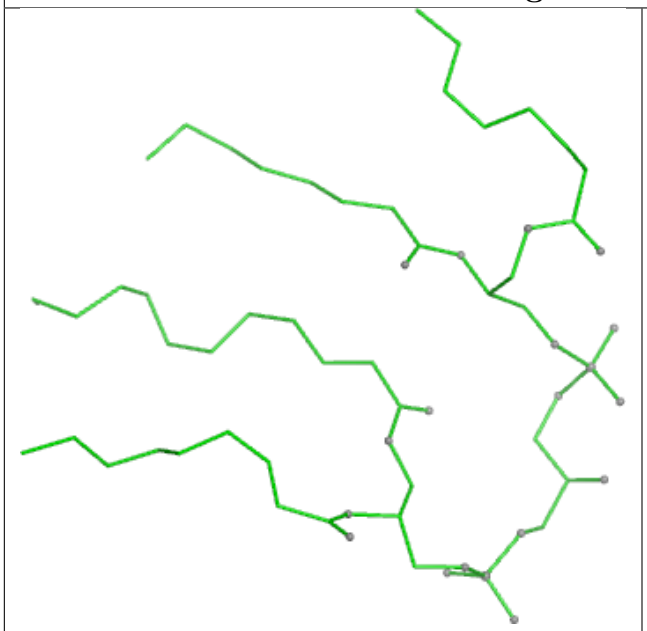
Ligand 3PE F 301



Ligand 3PE S 301



Ligand CDL P 301



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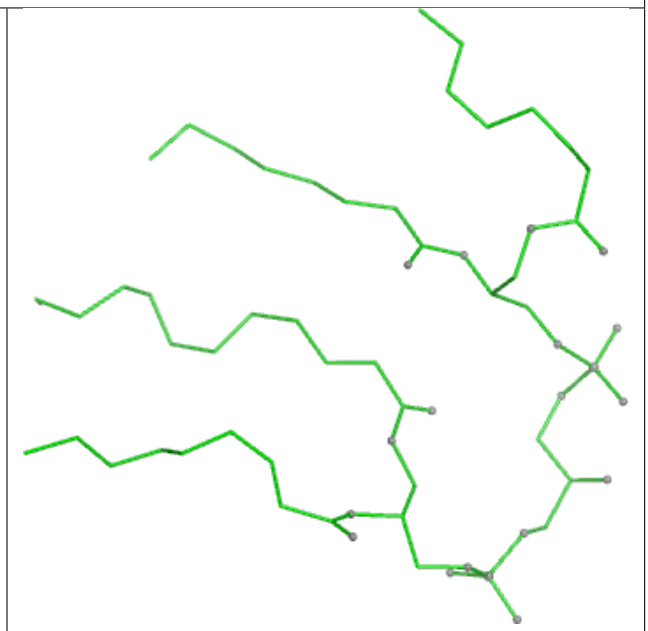
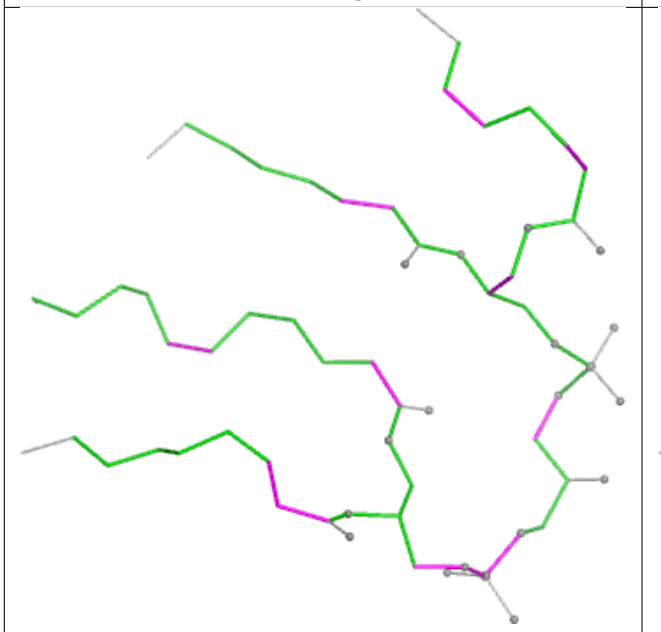


Bond angles



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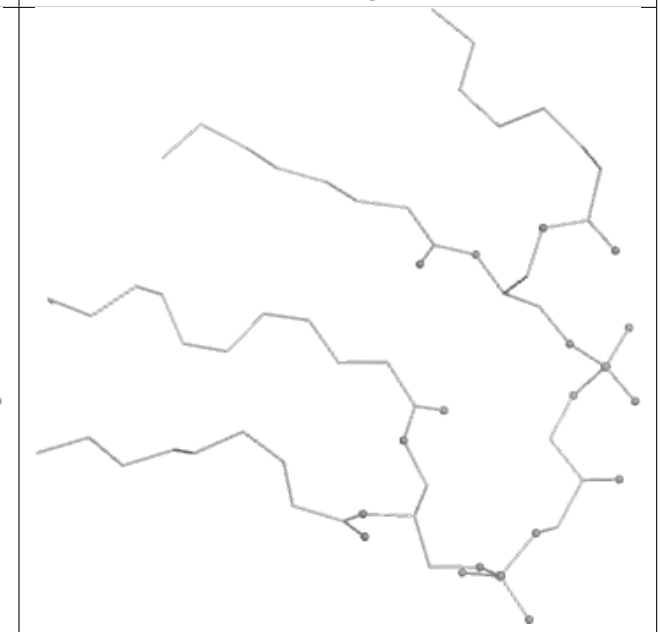
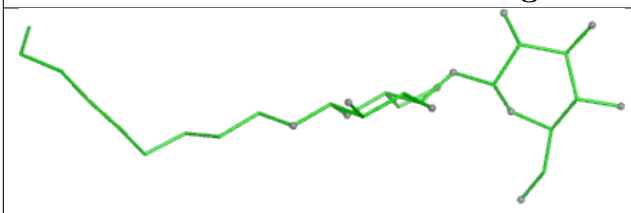
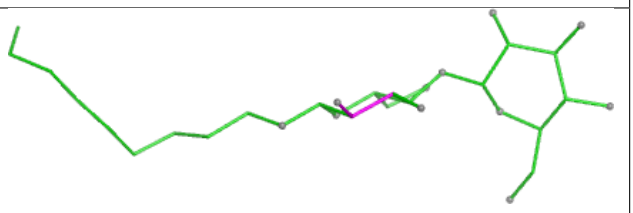


Rings

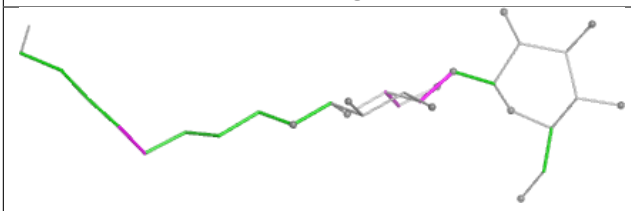
Ligand LMT O 601



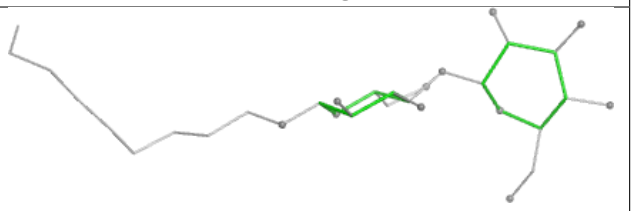
Bond lengths



Bond angles

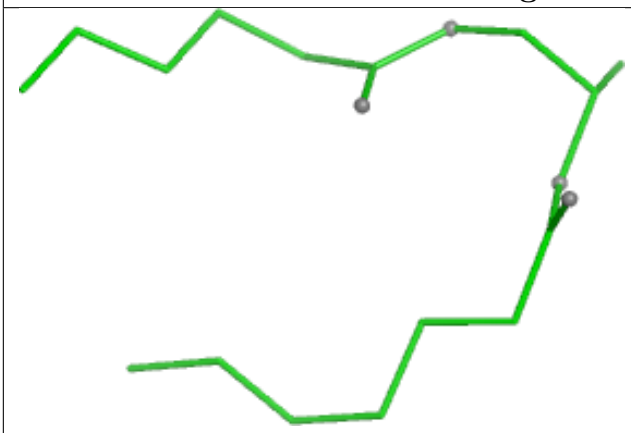


Torsions

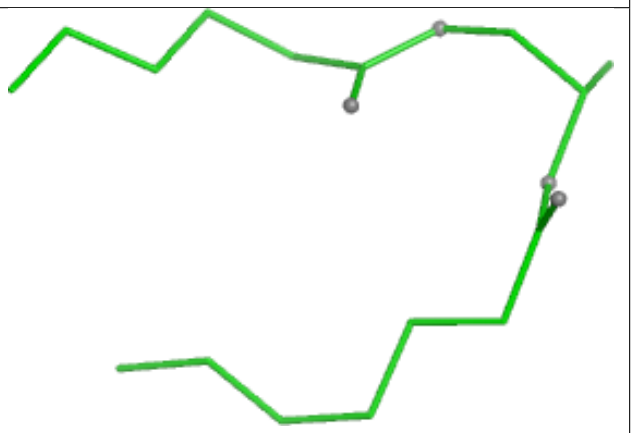


Rings

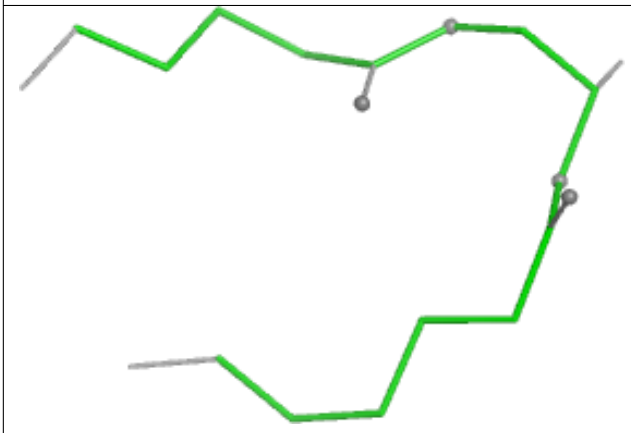
Ligand DGA R 404



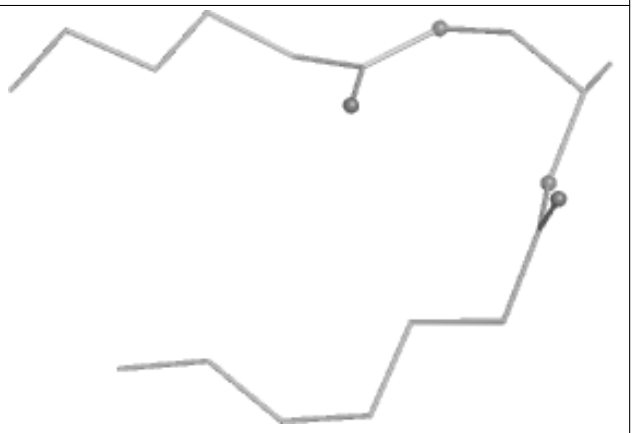
Bond lengths



Bond angles



Torsions

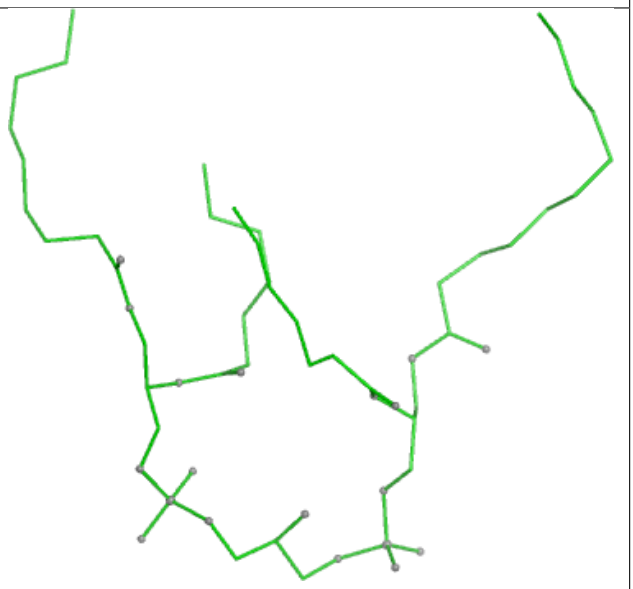


Rings

Ligand CDL S 303



Bond lengths



Bond angles

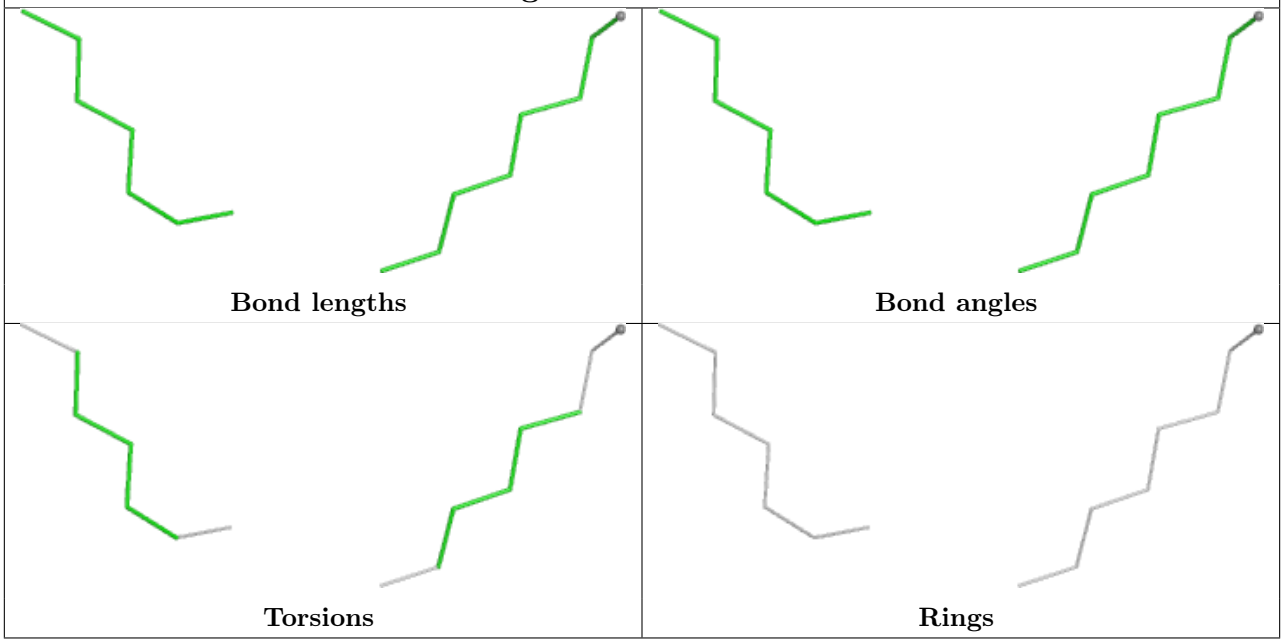


Torsions

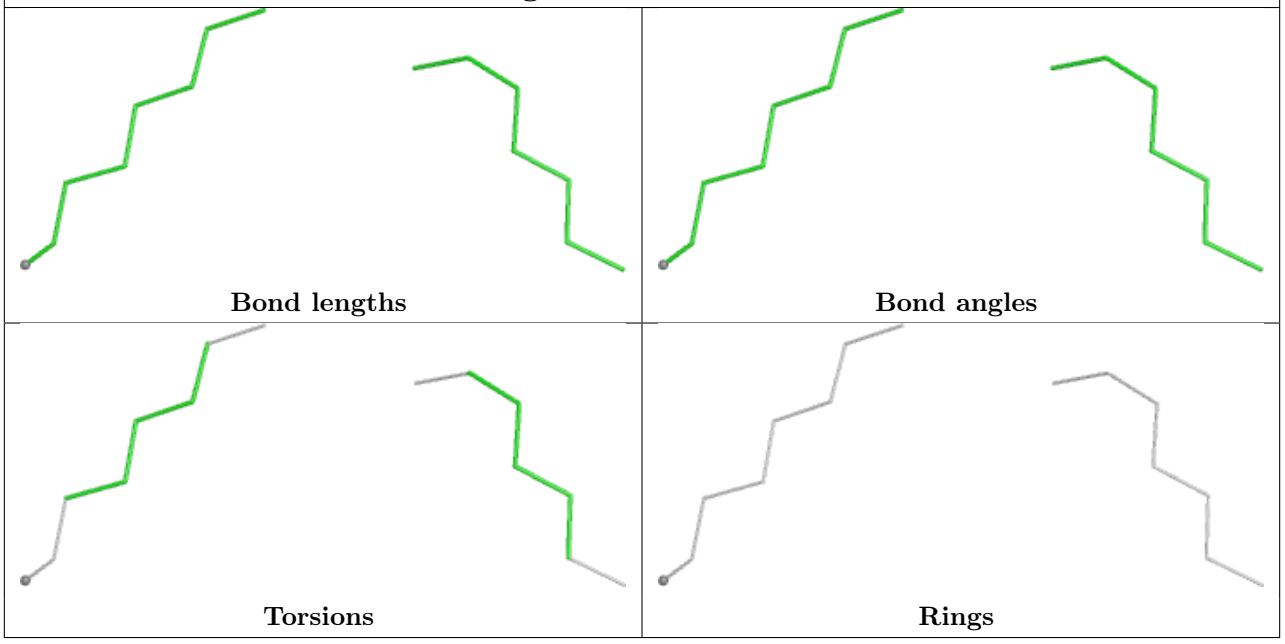


Rings

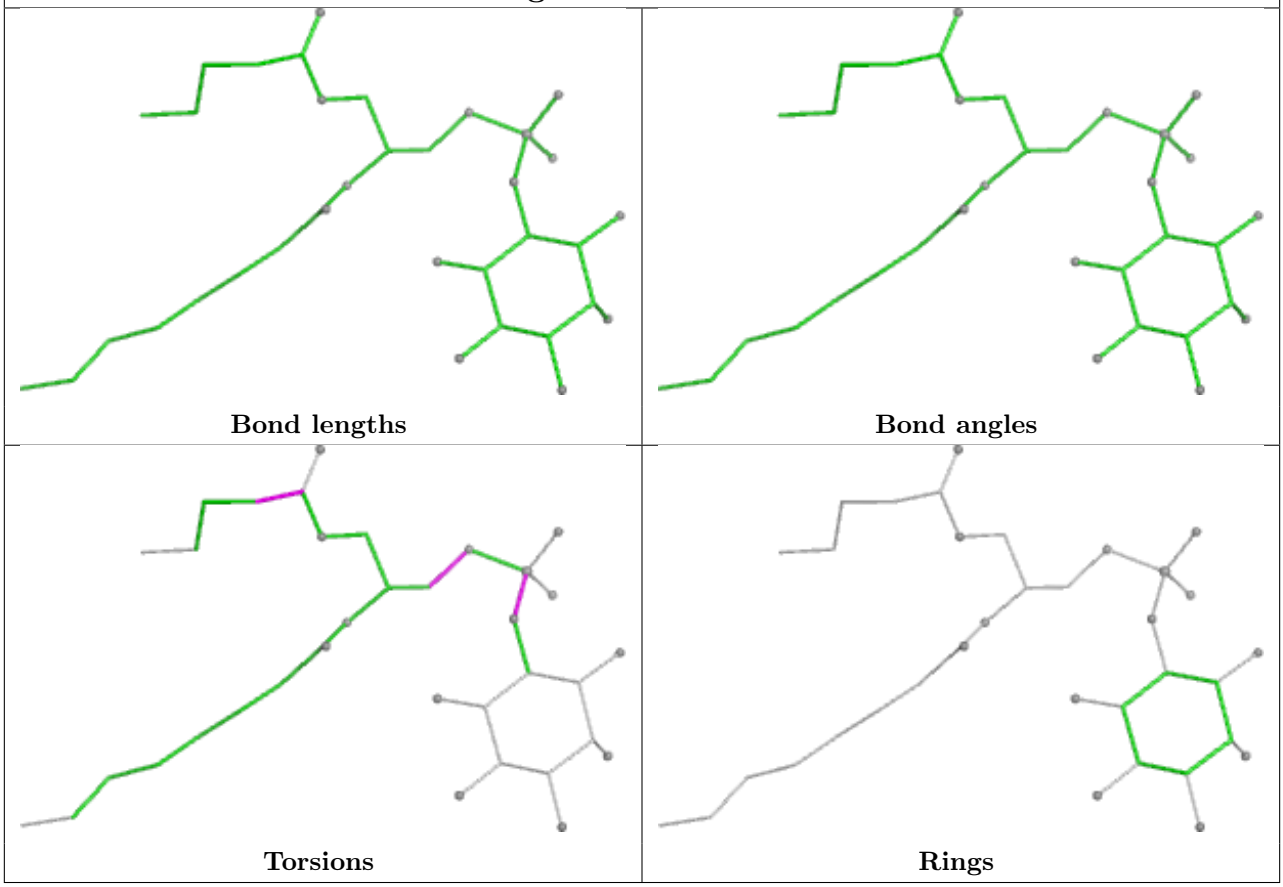
Ligand PLM H 202



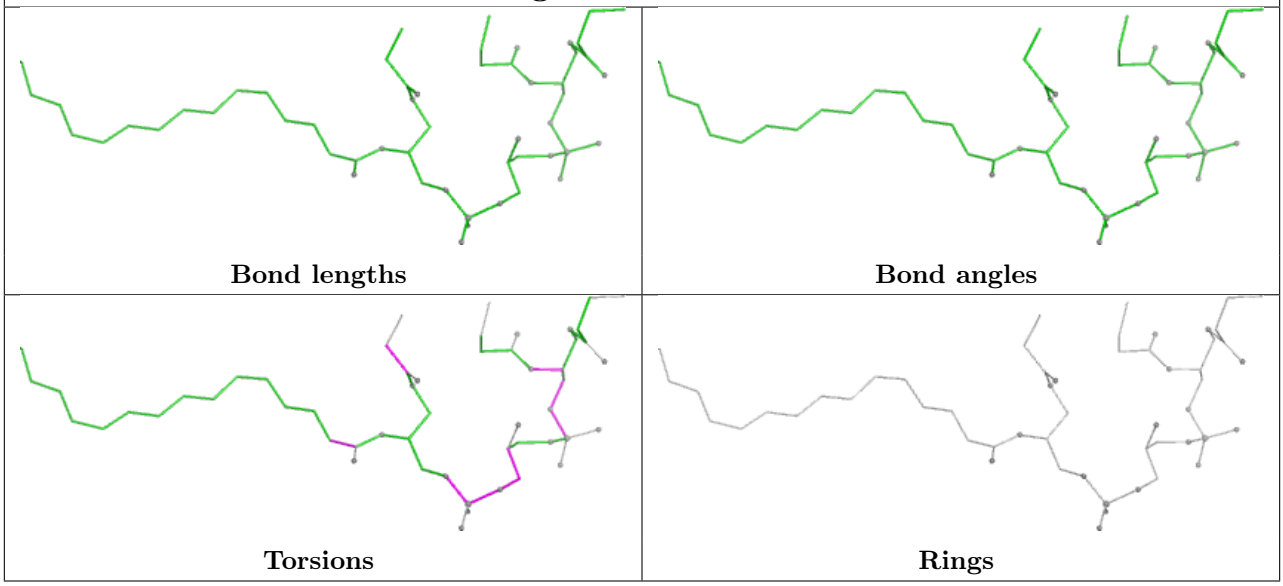
Ligand PLM U 202



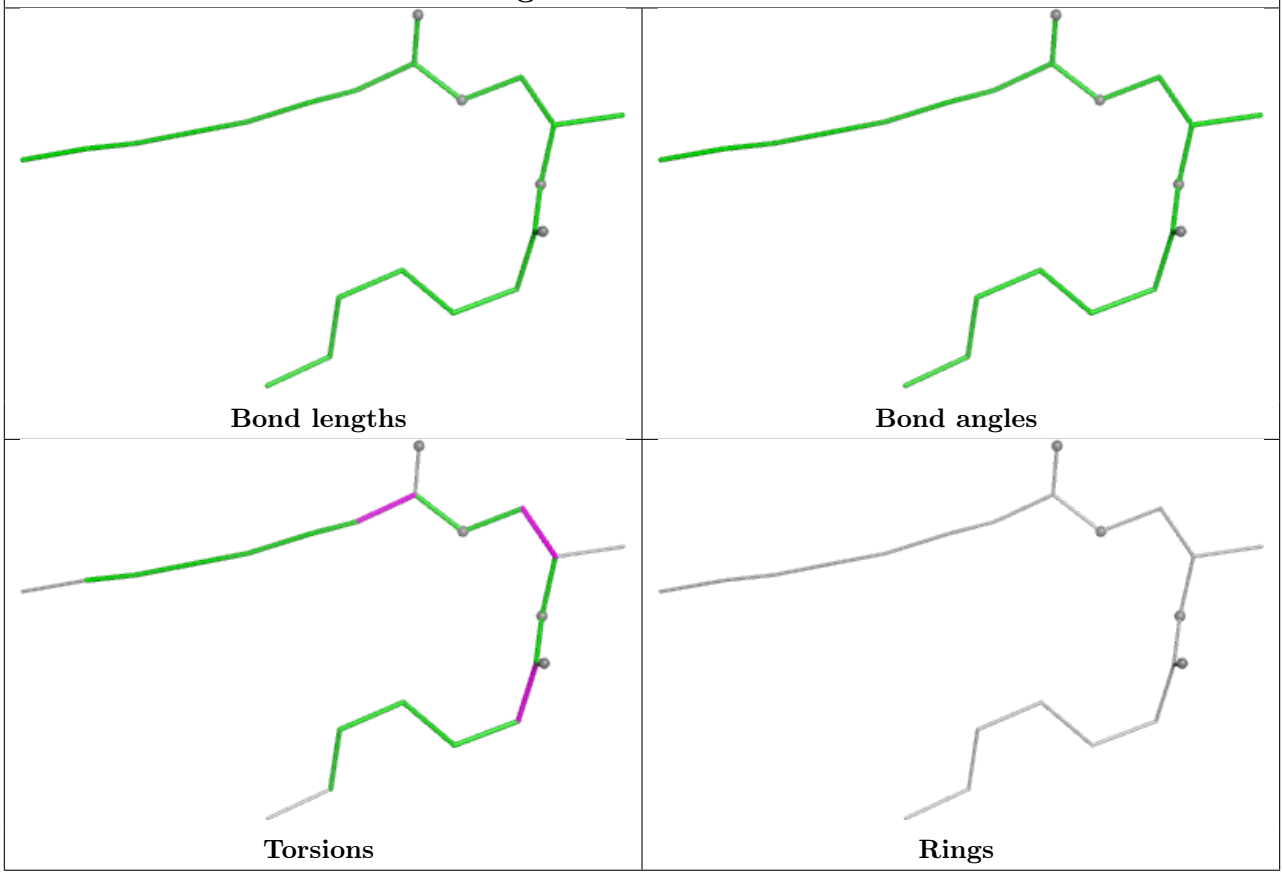
Ligand 9YF N 505



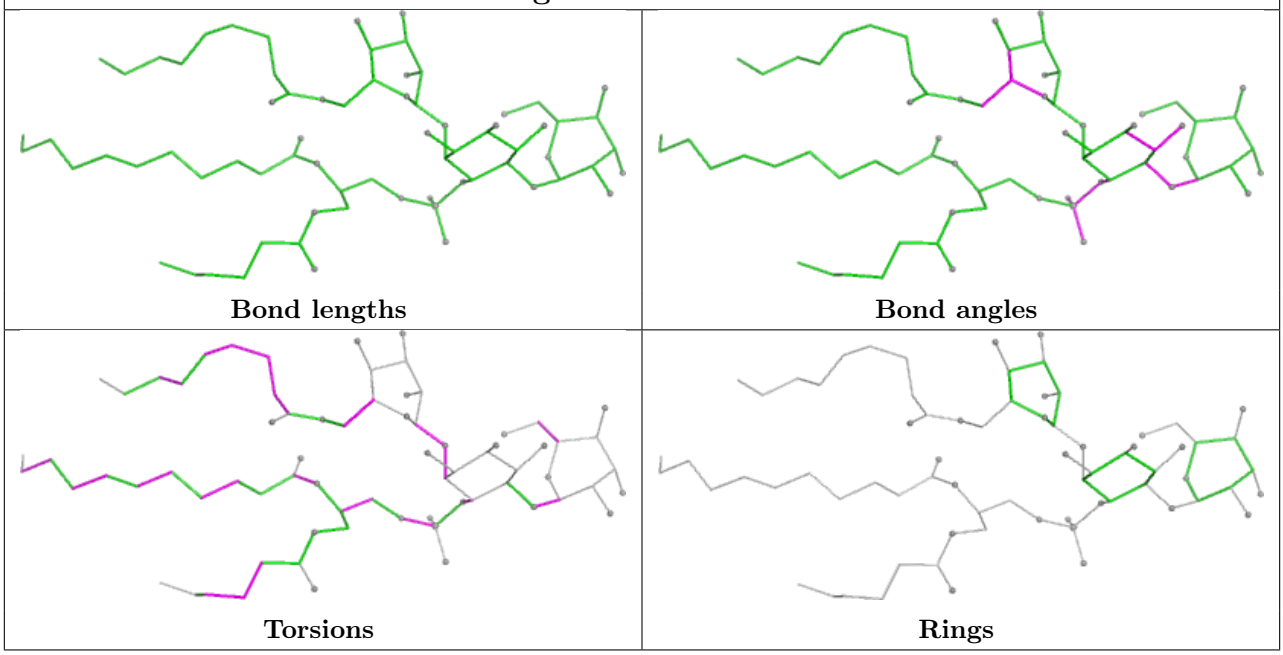
Ligand CDL I 201



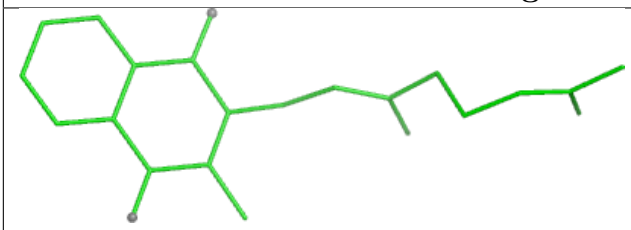
Ligand DGA M 201



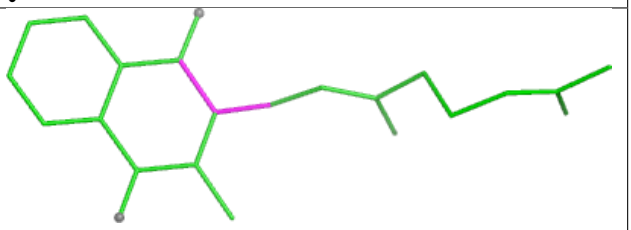
Ligand IX7 R 406



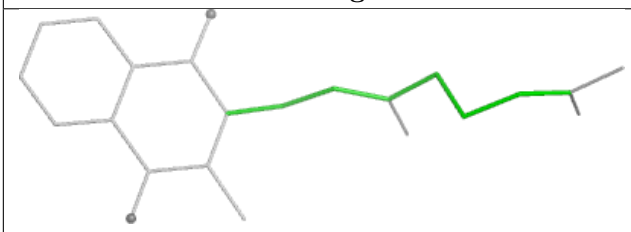
Ligand MQ9 O 605



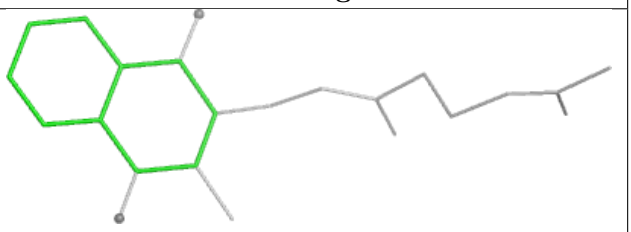
Bond lengths



Bond angles

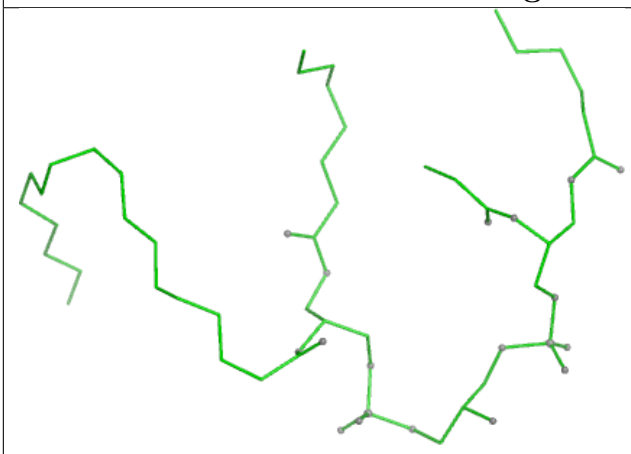


Torsions



Rings

Ligand CDL Q 606



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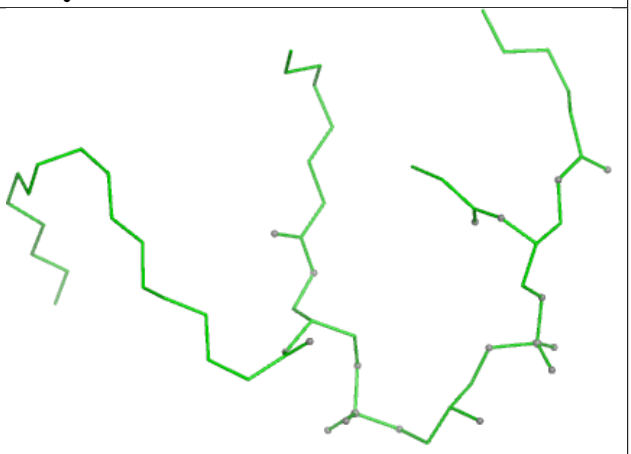
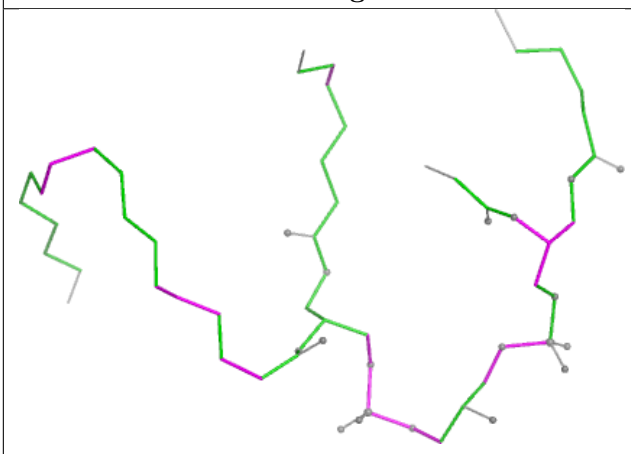


Bond angles



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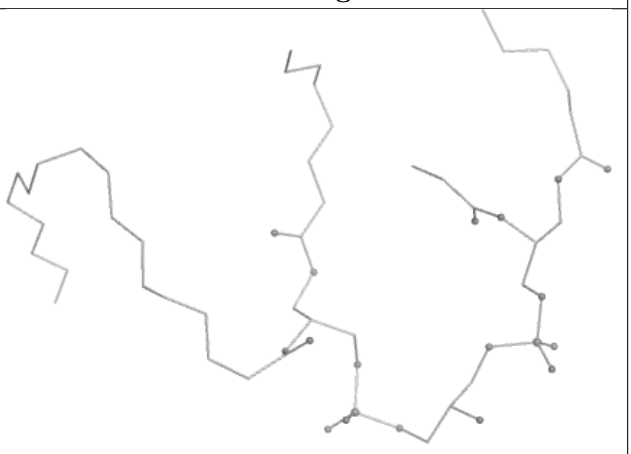
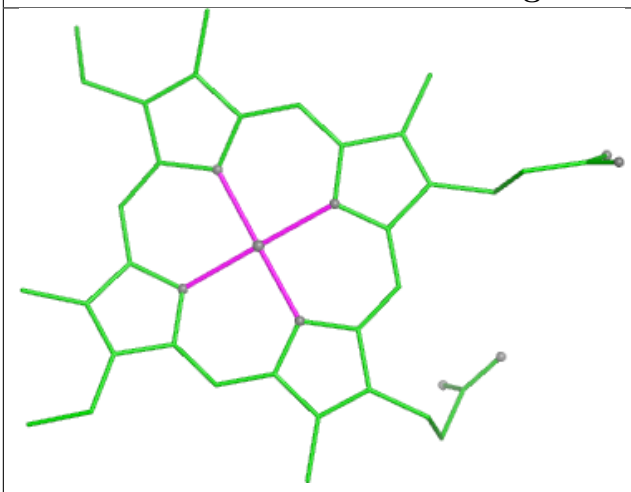
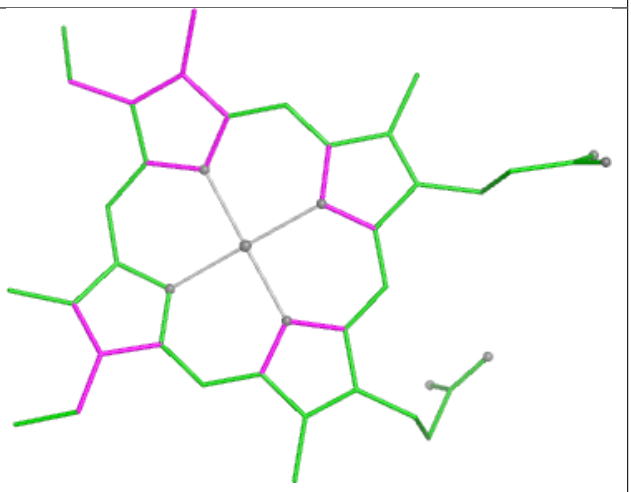


Rings

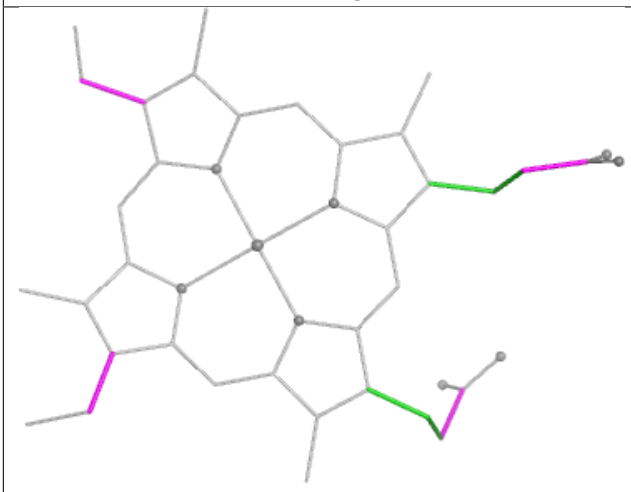
Ligand HEC P 302



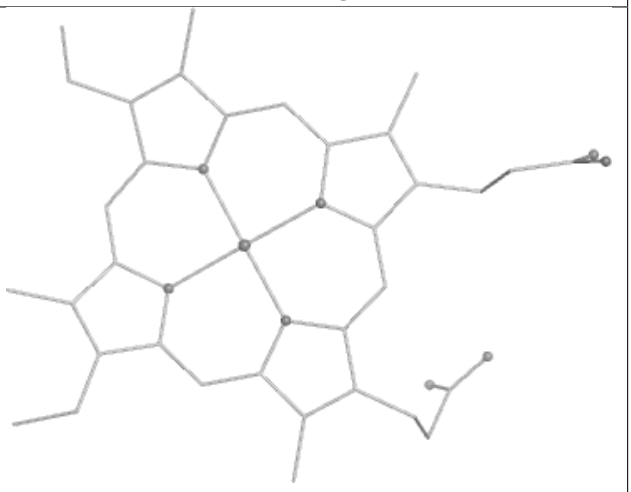
Bond lengths



Bond angles

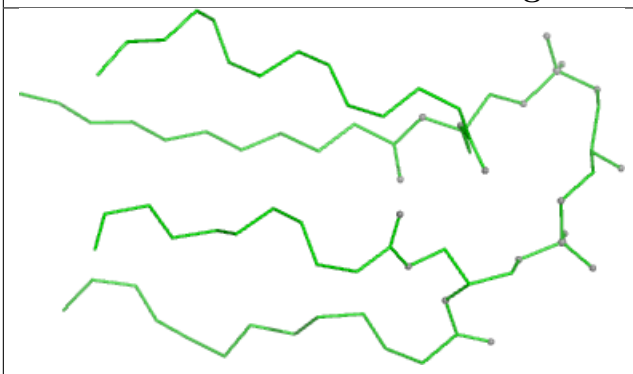


Torsions

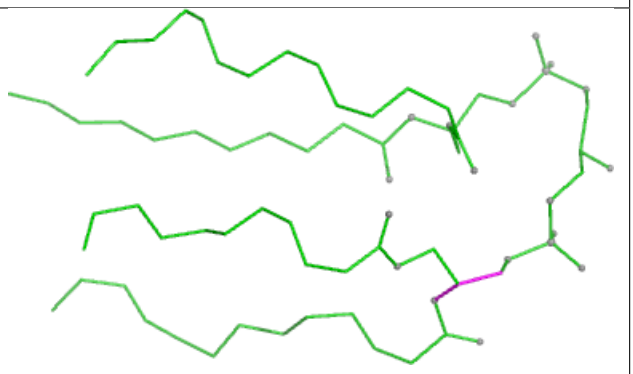


Rings

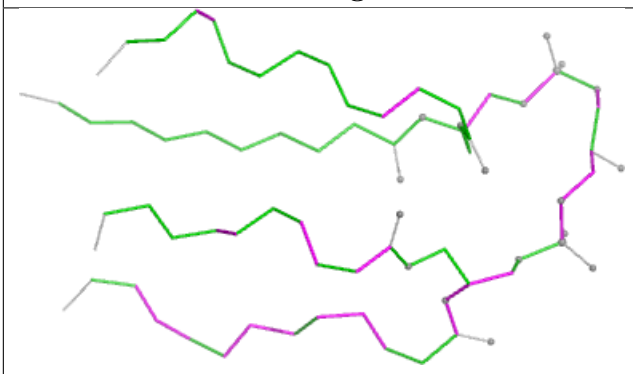
Ligand CDL D 605



Bond lengths



Bond angles



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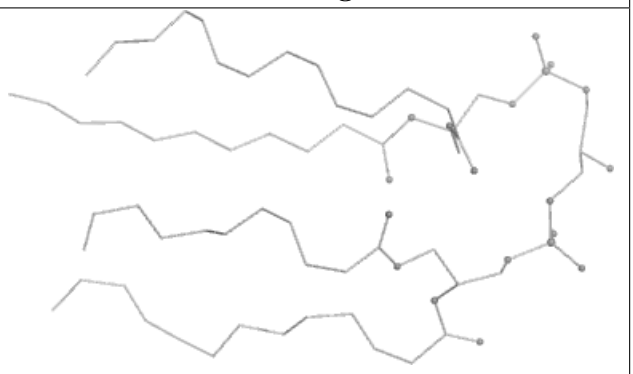
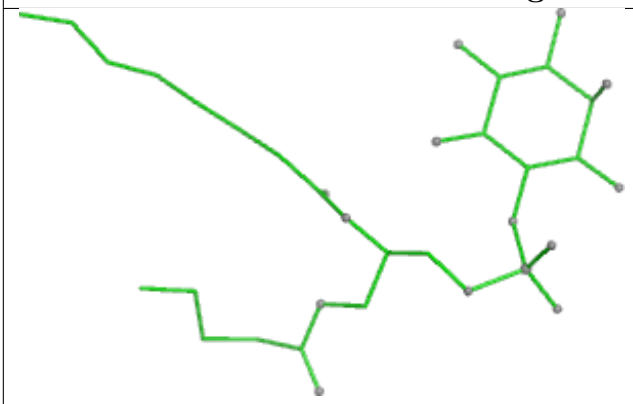
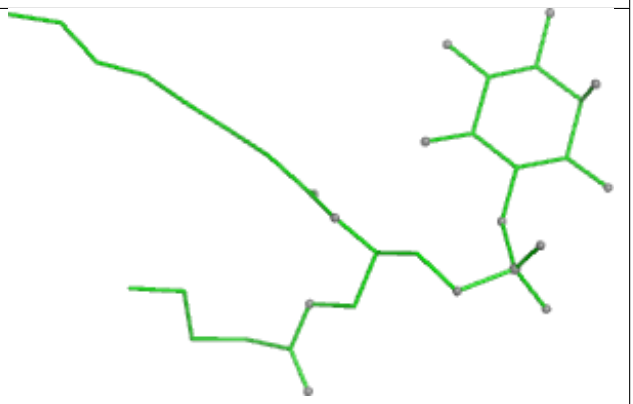


Rings

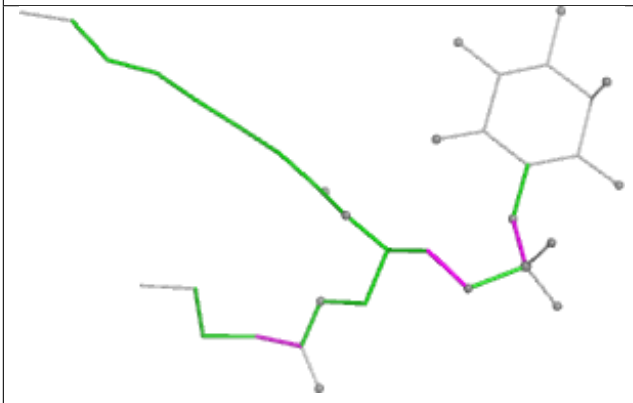
Ligand 9YF A 503



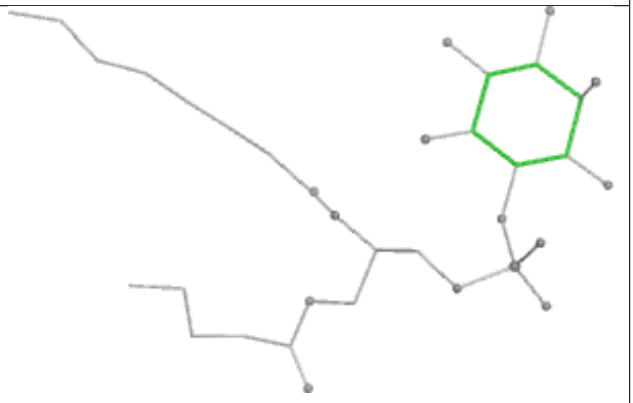
Bond lengths



Bond angles

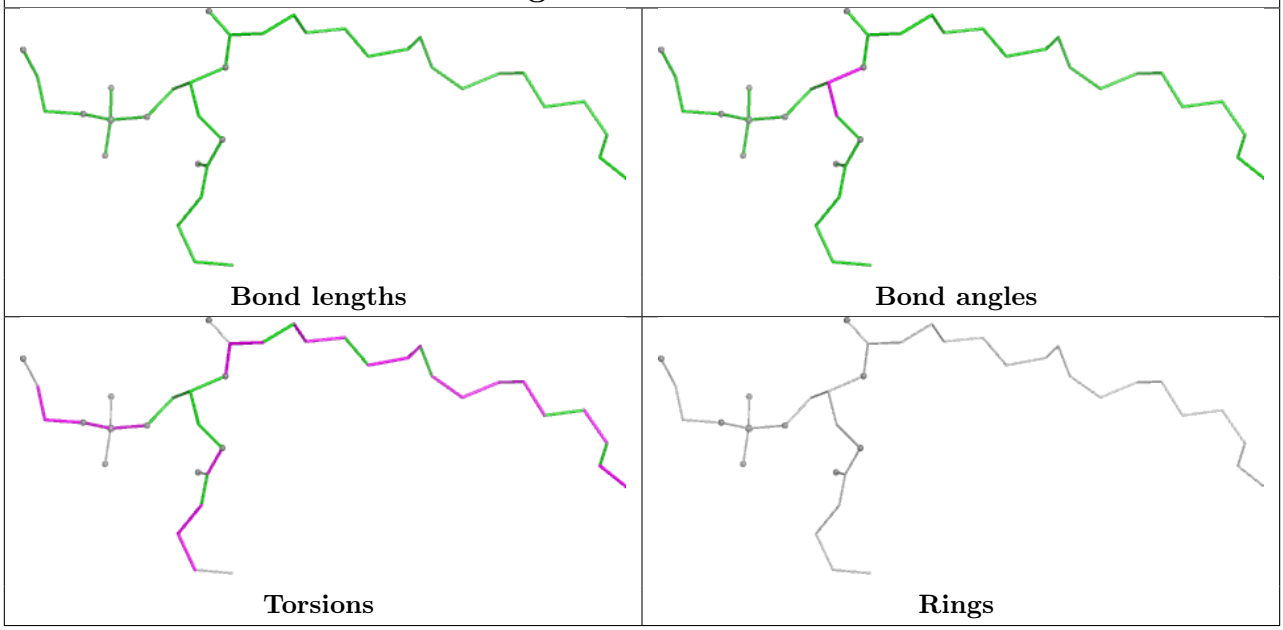


Torsions

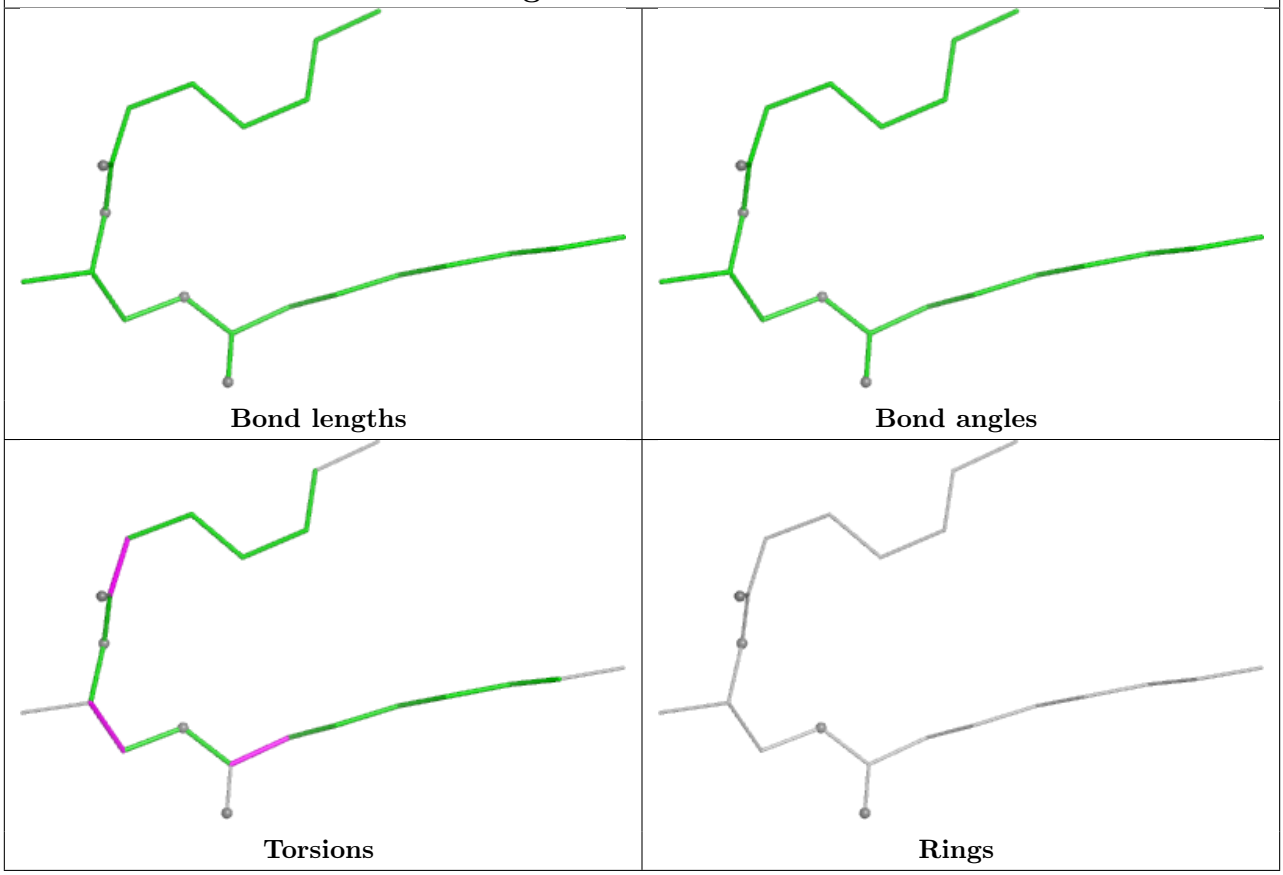


Rings

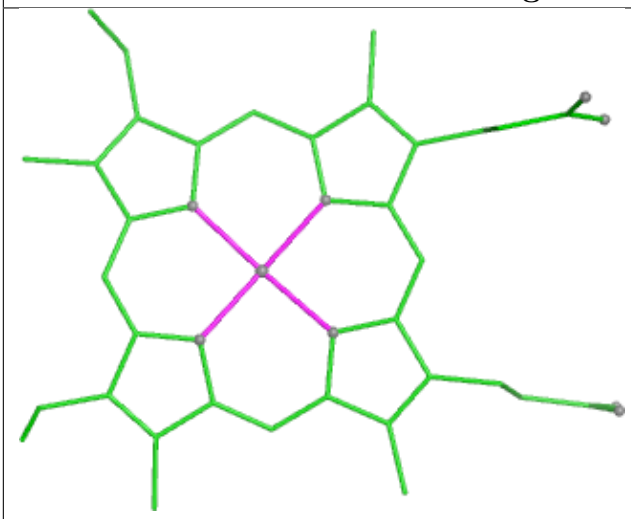
Ligand 3PE N 502



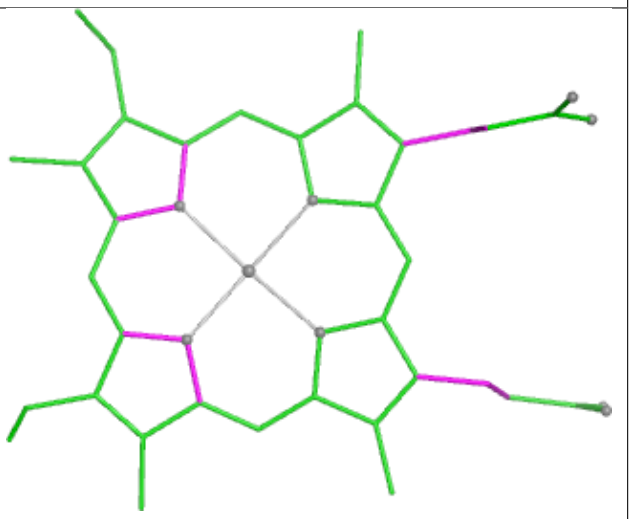
Ligand DGA Z 201



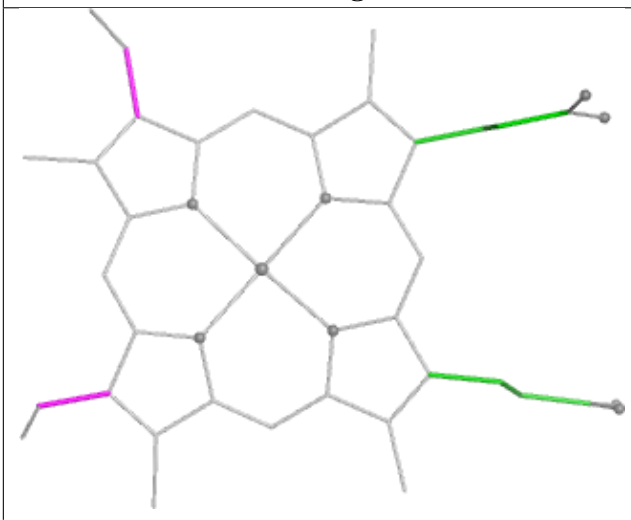
Ligand HEC C 303



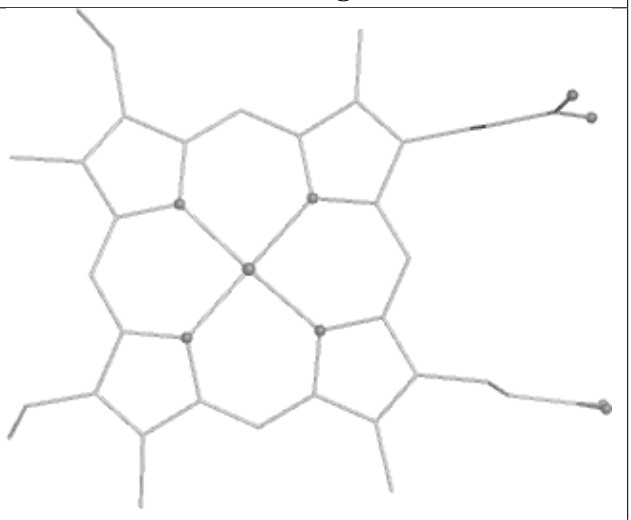
Bond lengths



Bond angles

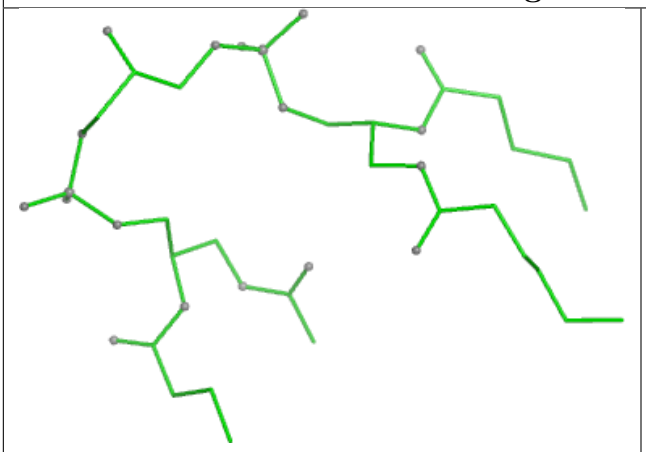


Torsions

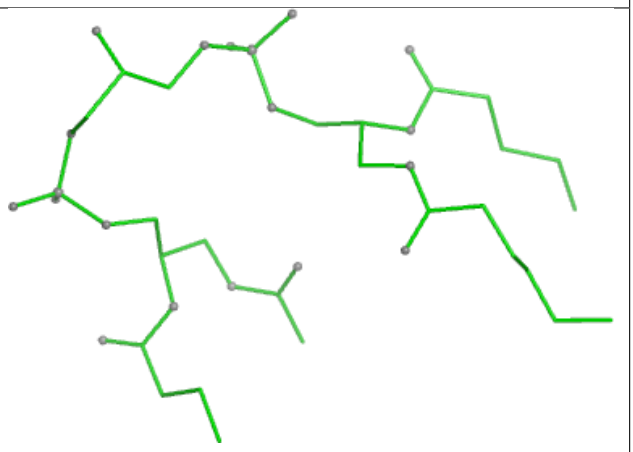


Rings

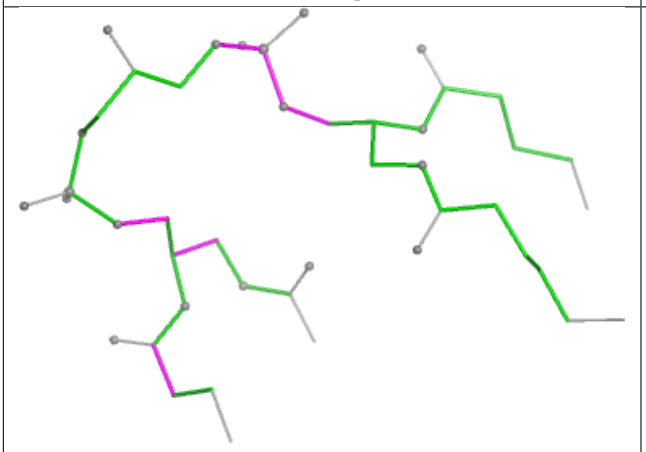
Ligand CDL B 605



Bond lengths



Bond angles



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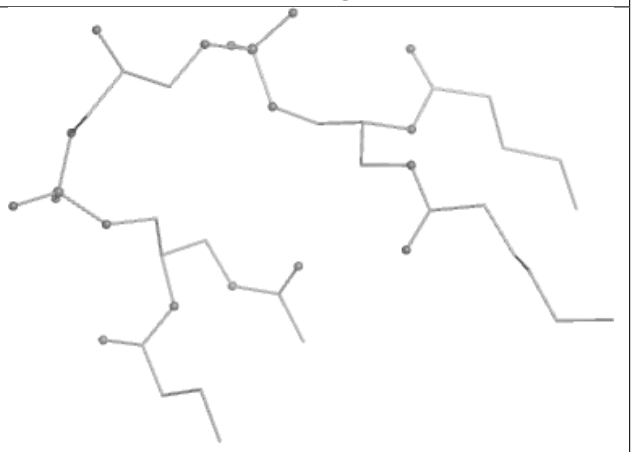
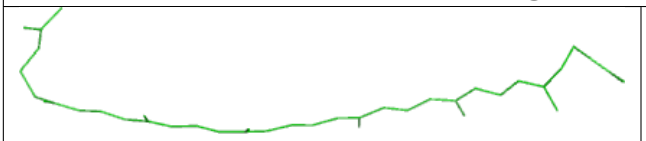
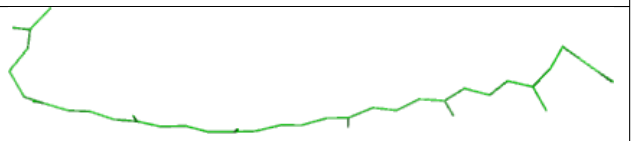


Rings

Ligand LYC O 607



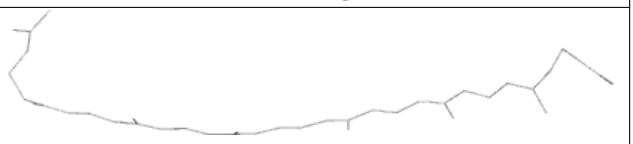
Bond lengths



Bond angles

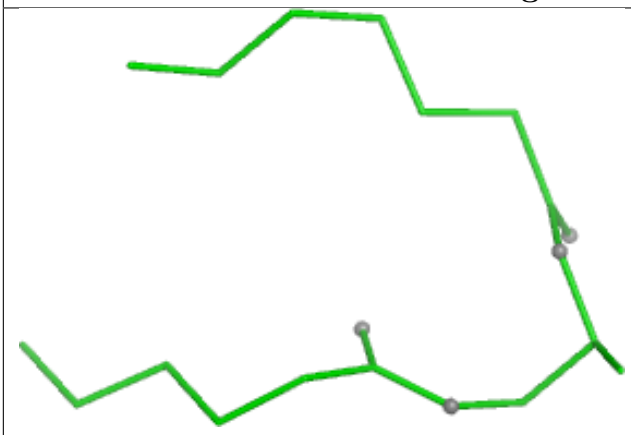


Torsions

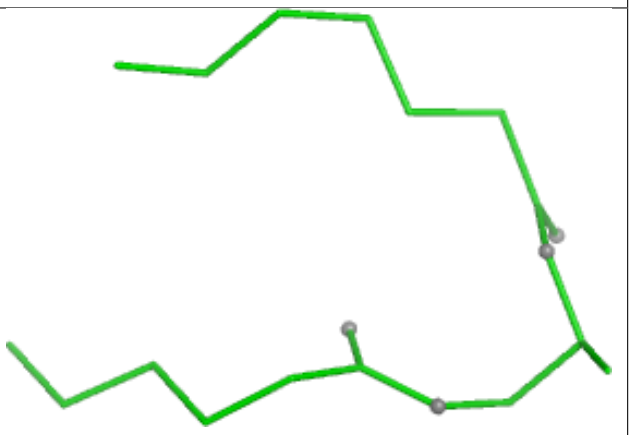


Rings

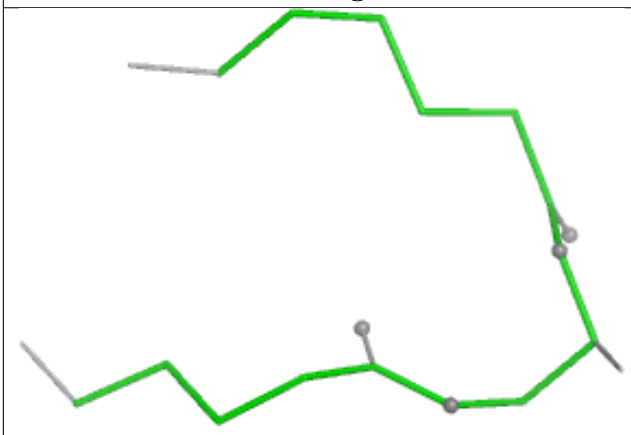
Ligand DGA E 404



Bond lengths



Bond angles

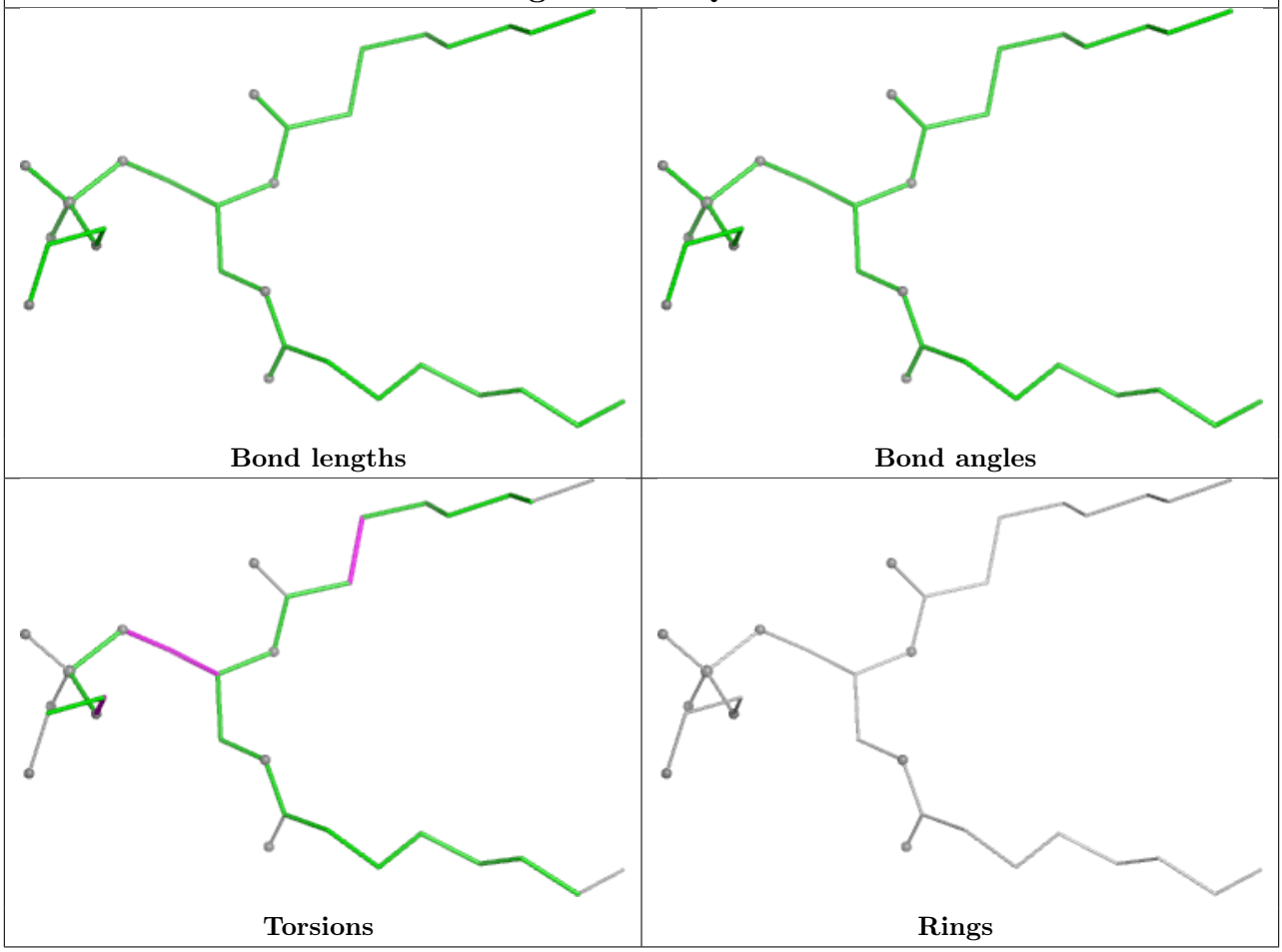


Torsions

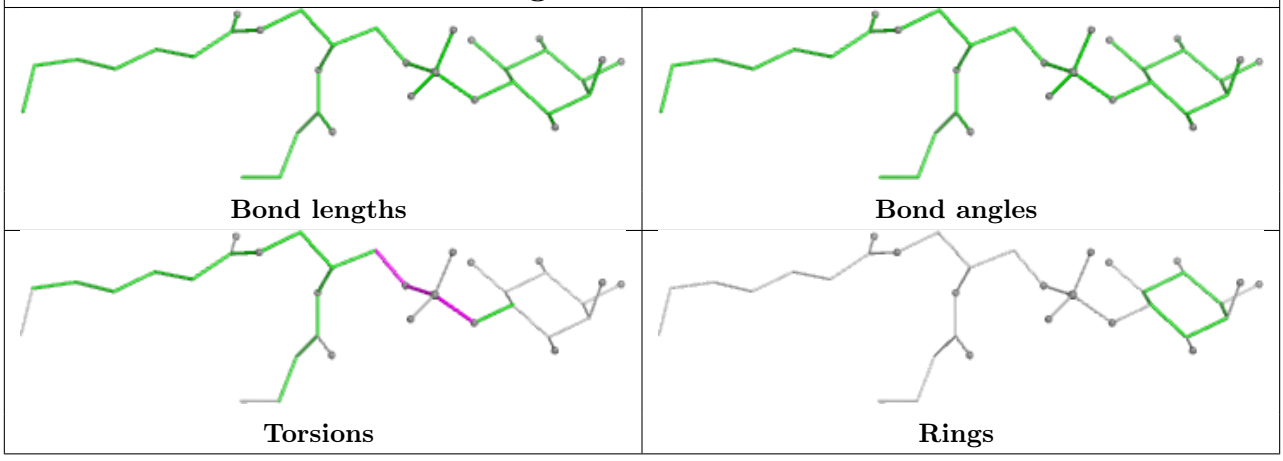


Rings

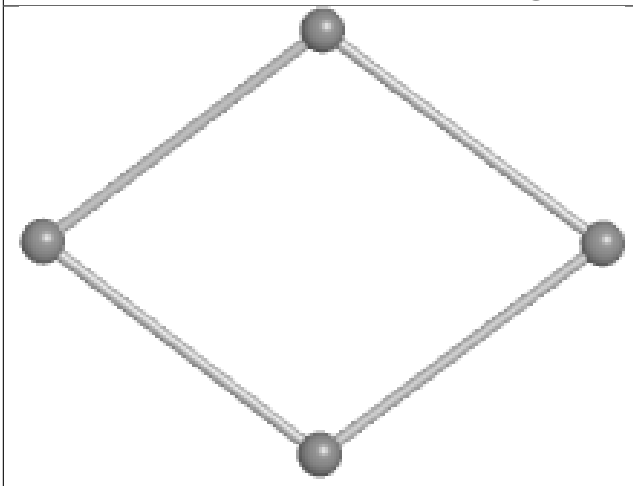
Ligand 3PE Q 607



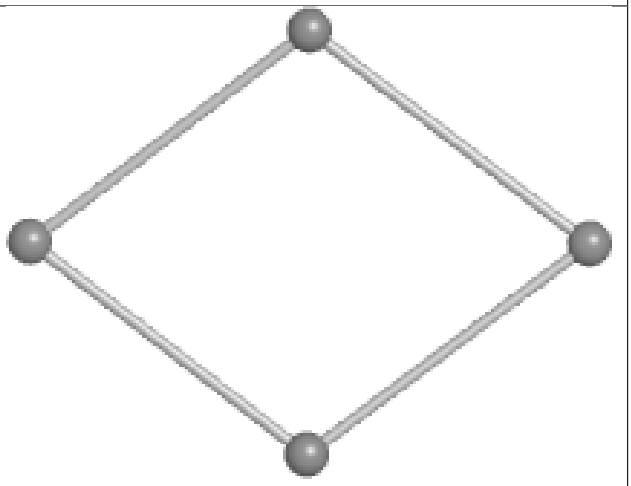
Ligand 9YF B 607



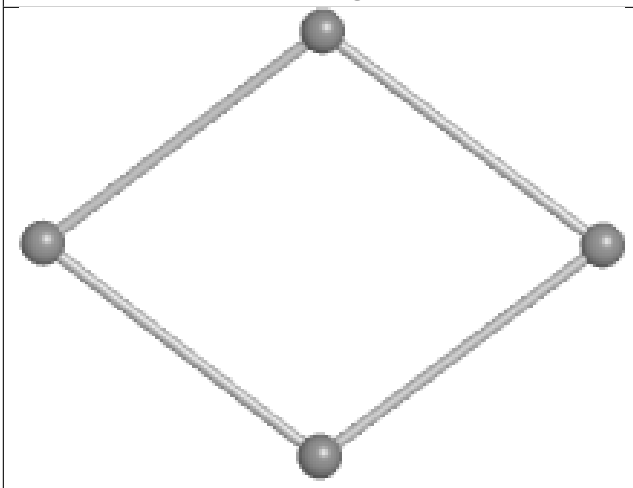
Ligand FES N 503



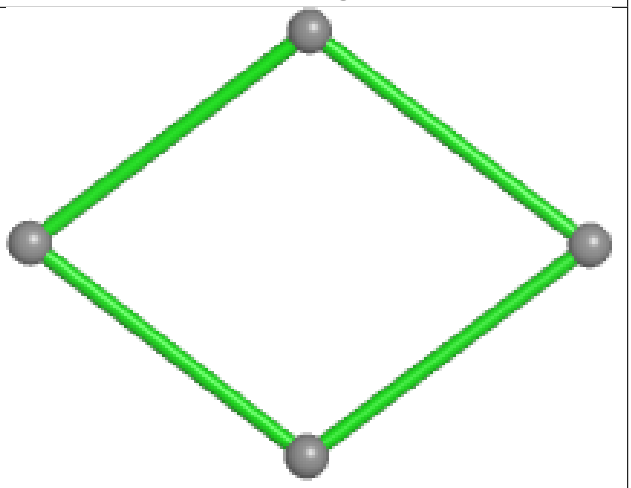
Bond lengths



Bond angles

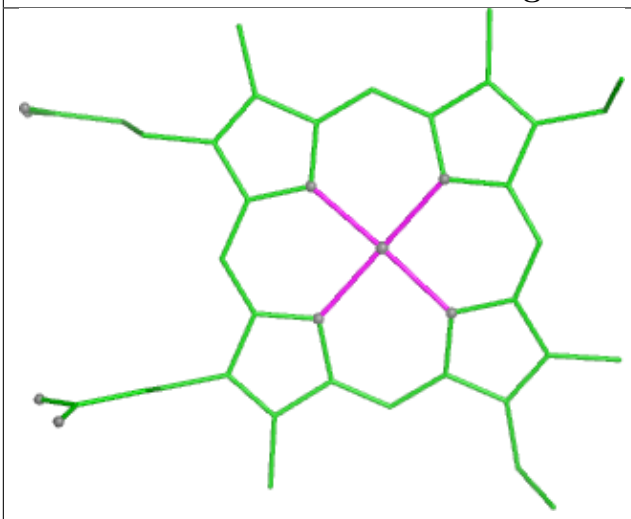


Torsions

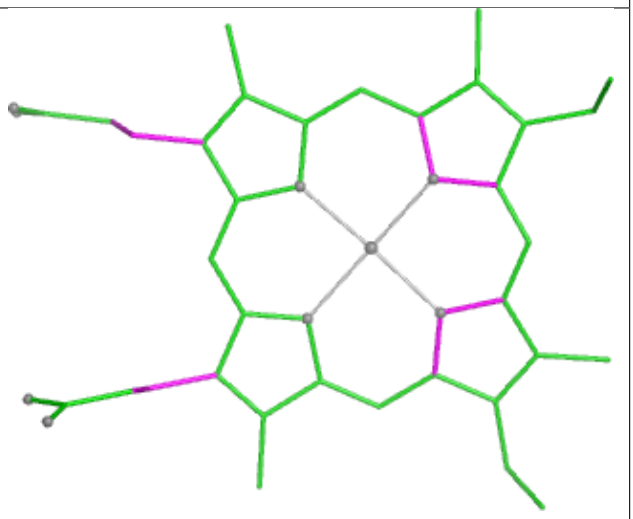


Rings

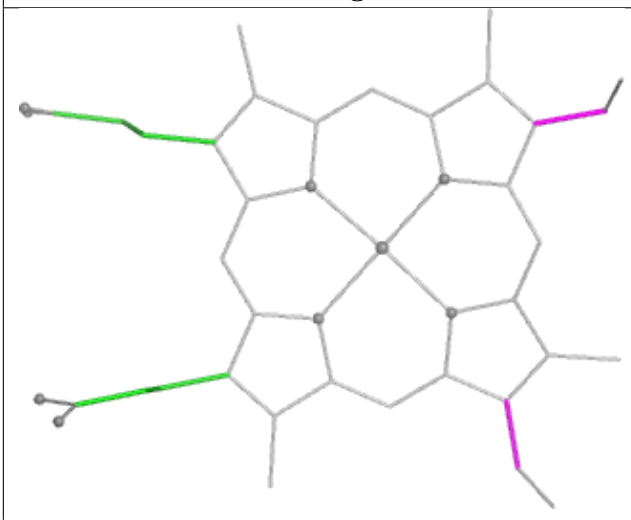
Ligand HEC P 303



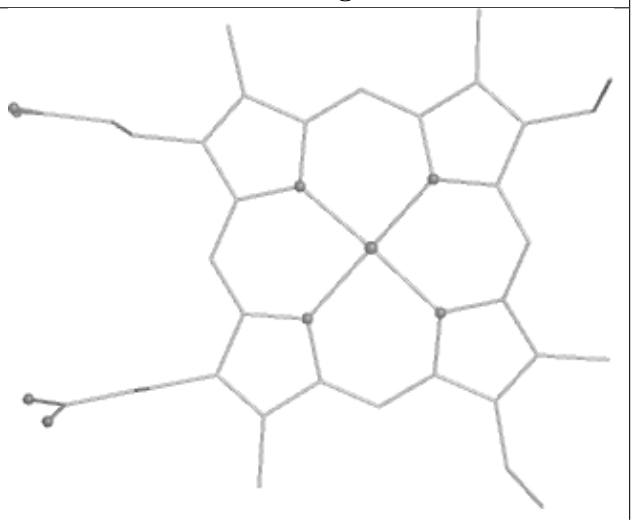
Bond lengths



Bond angles

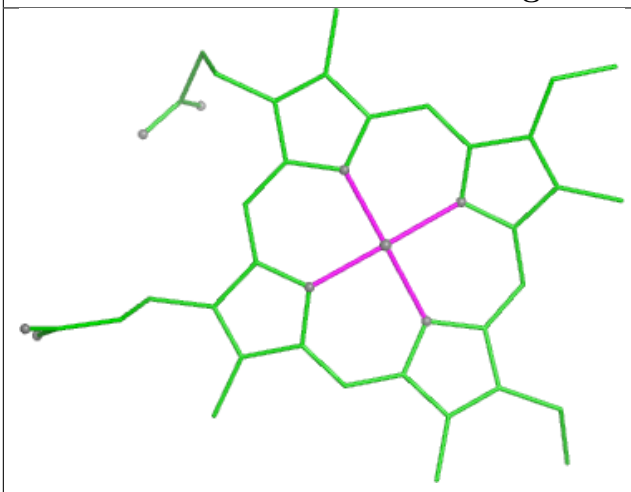


Torsions

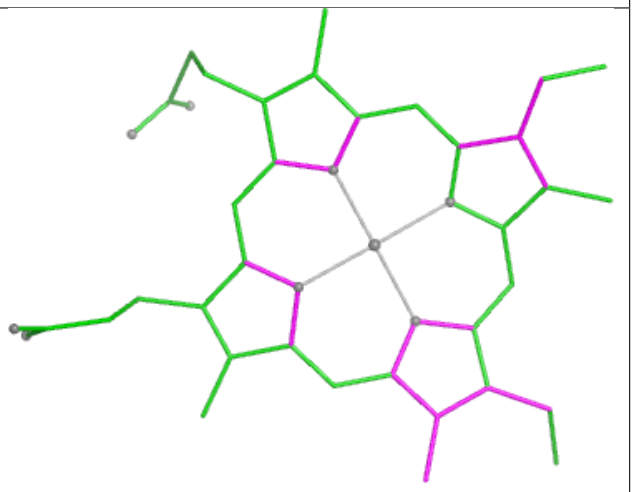


Rings

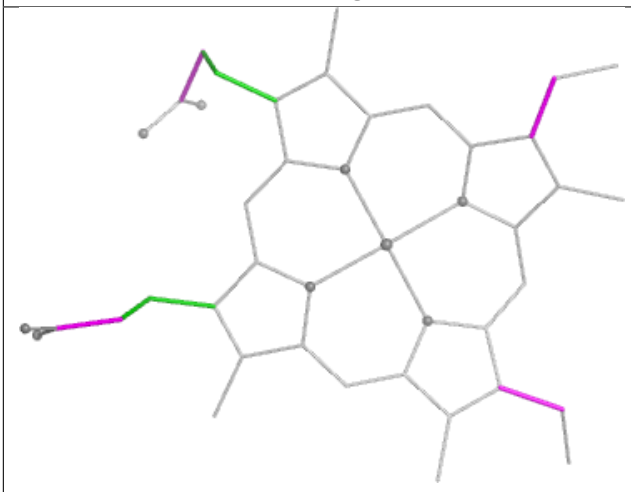
Ligand HEC C 302



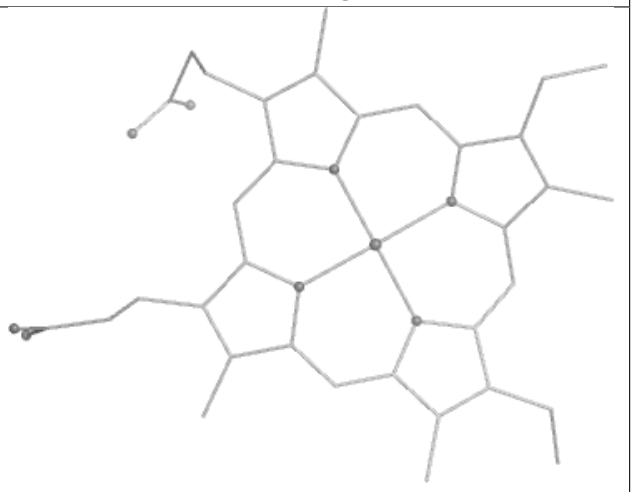
Bond lengths



Bond angles

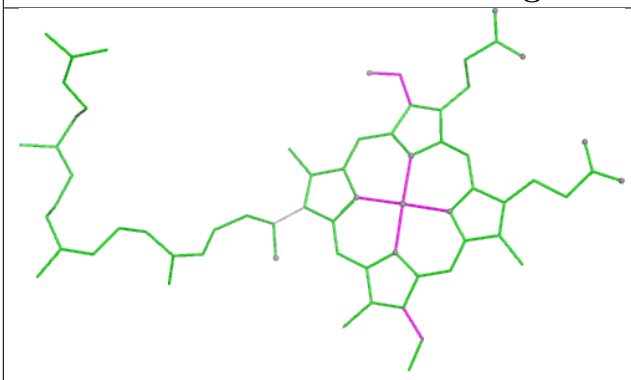


Torsions

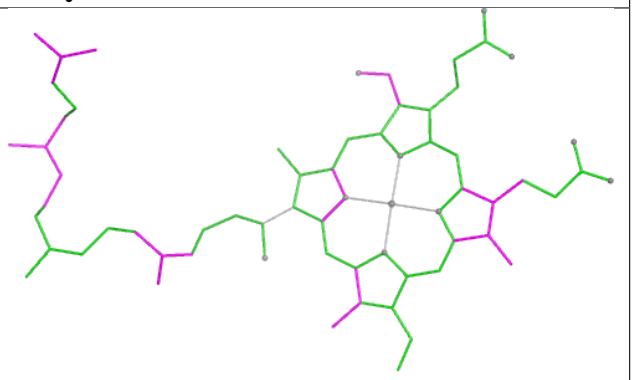


Rings

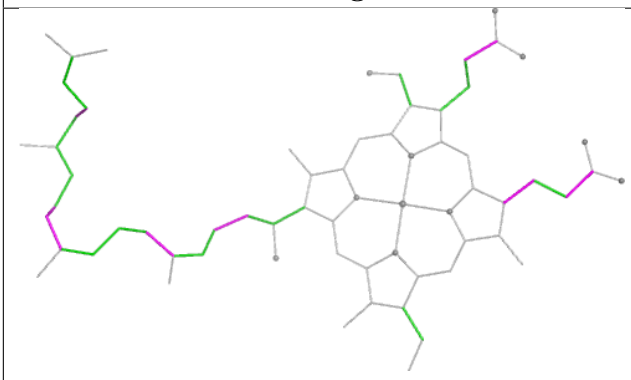
Ligand HAS Q 602



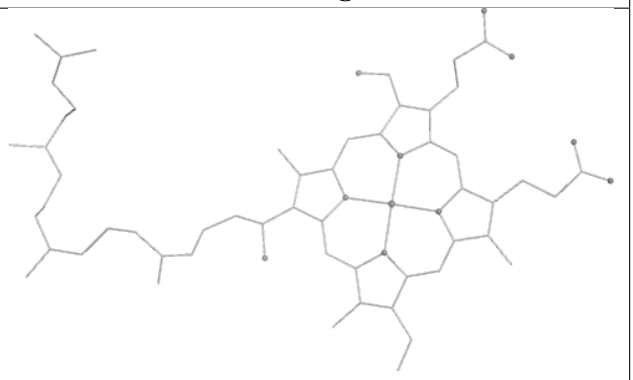
Bond lengths



Bond angles

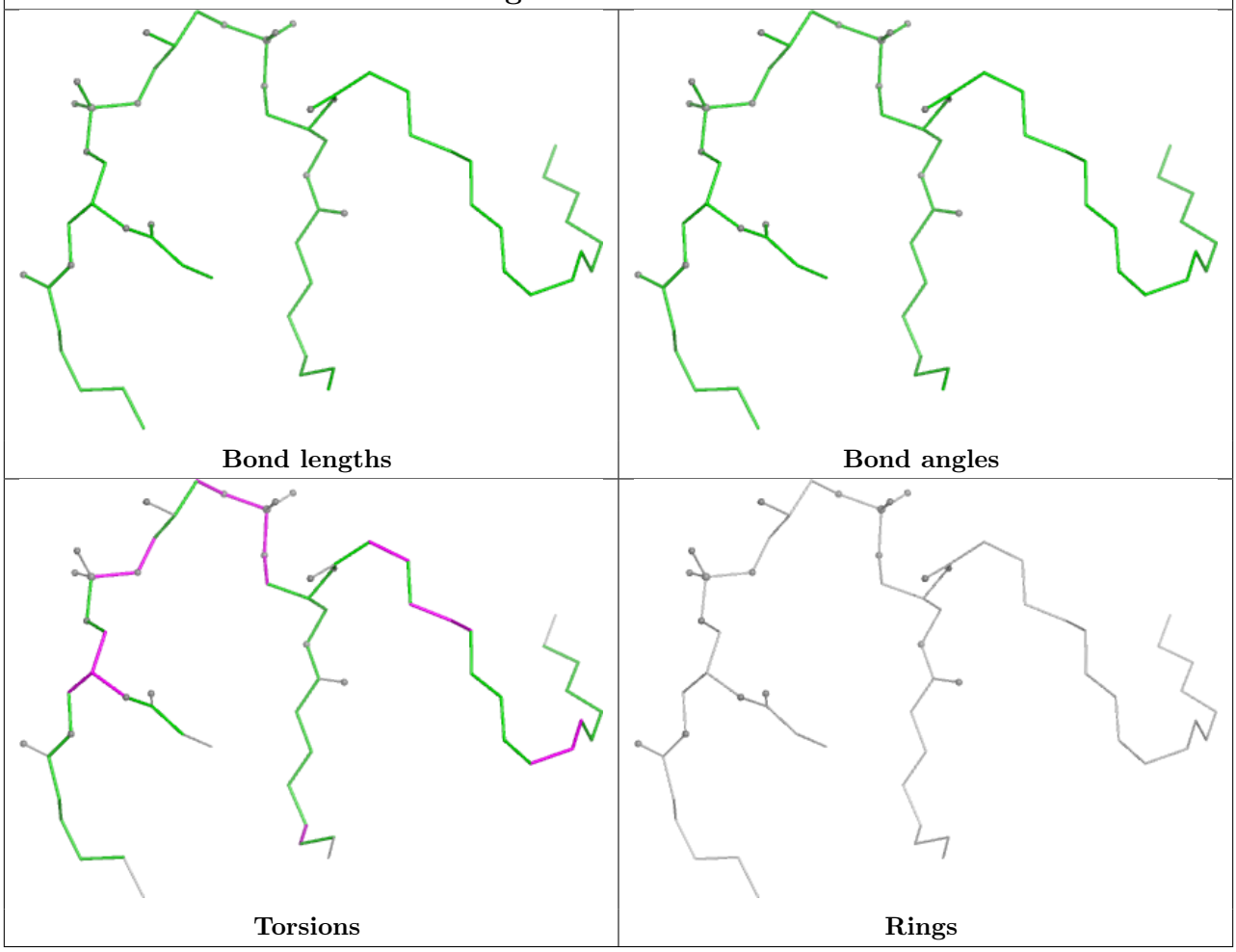


Torsions

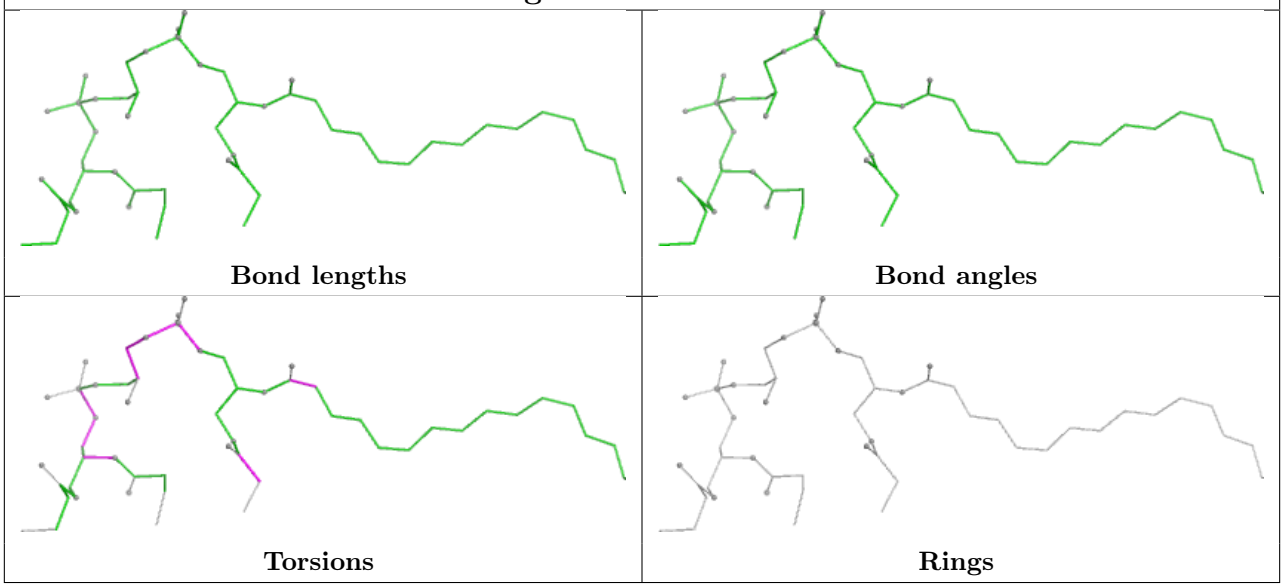


Rings

Ligand CDL D 606



Ligand CDL V 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

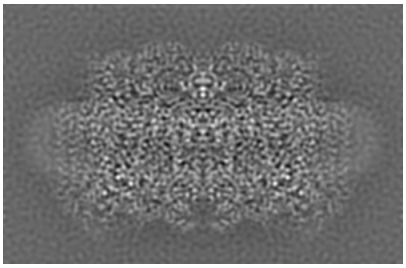
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13977. These allow visual inspection of the internal detail of the map and identification of artifacts.

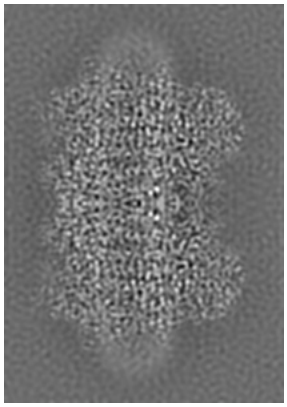
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

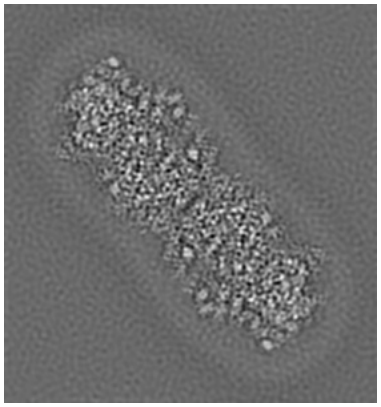
6.1.1 Primary map



X



Y

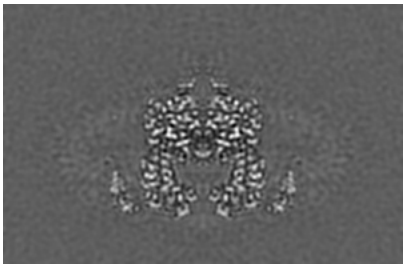


Z

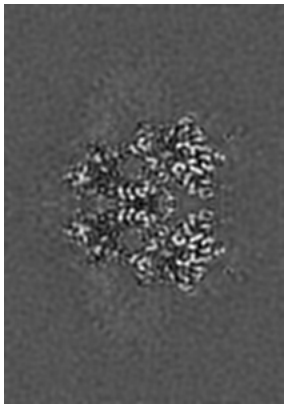
The images above show the map projected in three orthogonal directions.

6.2 Central slices

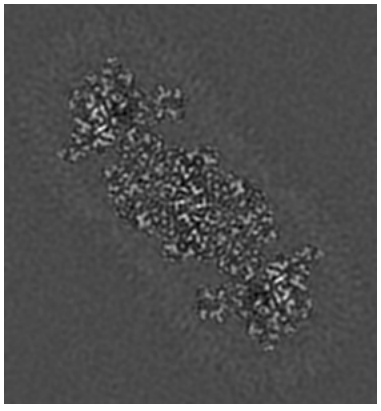
6.2.1 Primary map



X Index: 107



Y Index: 115

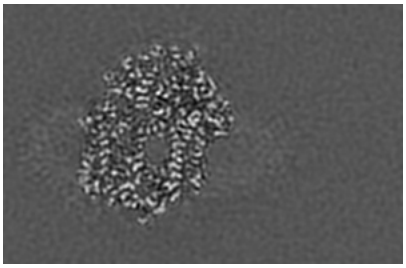


Z Index: 75

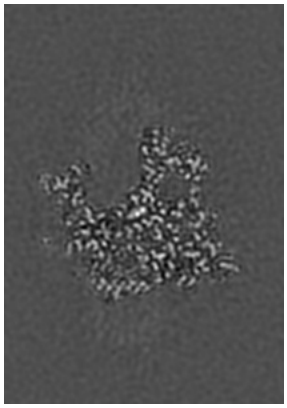
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

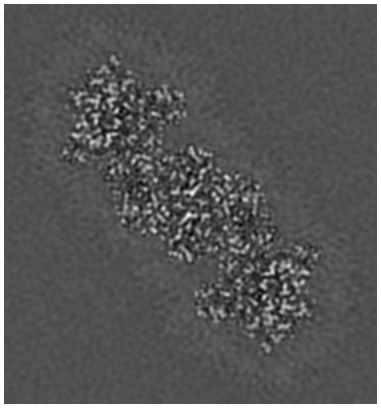
6.3.1 Primary map



X Index: 136



Y Index: 123

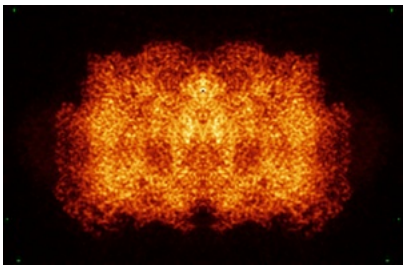


Z Index: 79

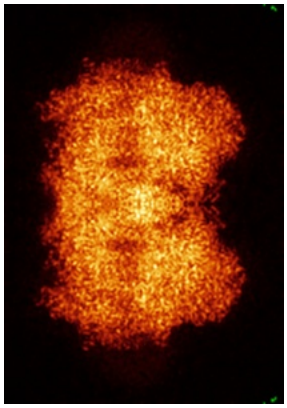
The images above show the largest variance slices of the map in three orthogonal directions.

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

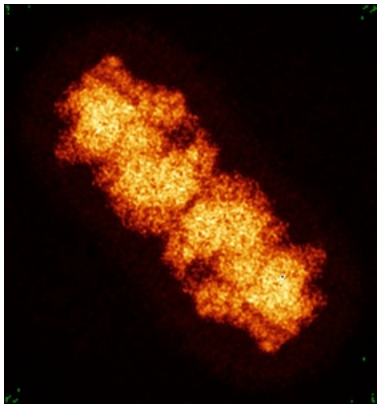
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

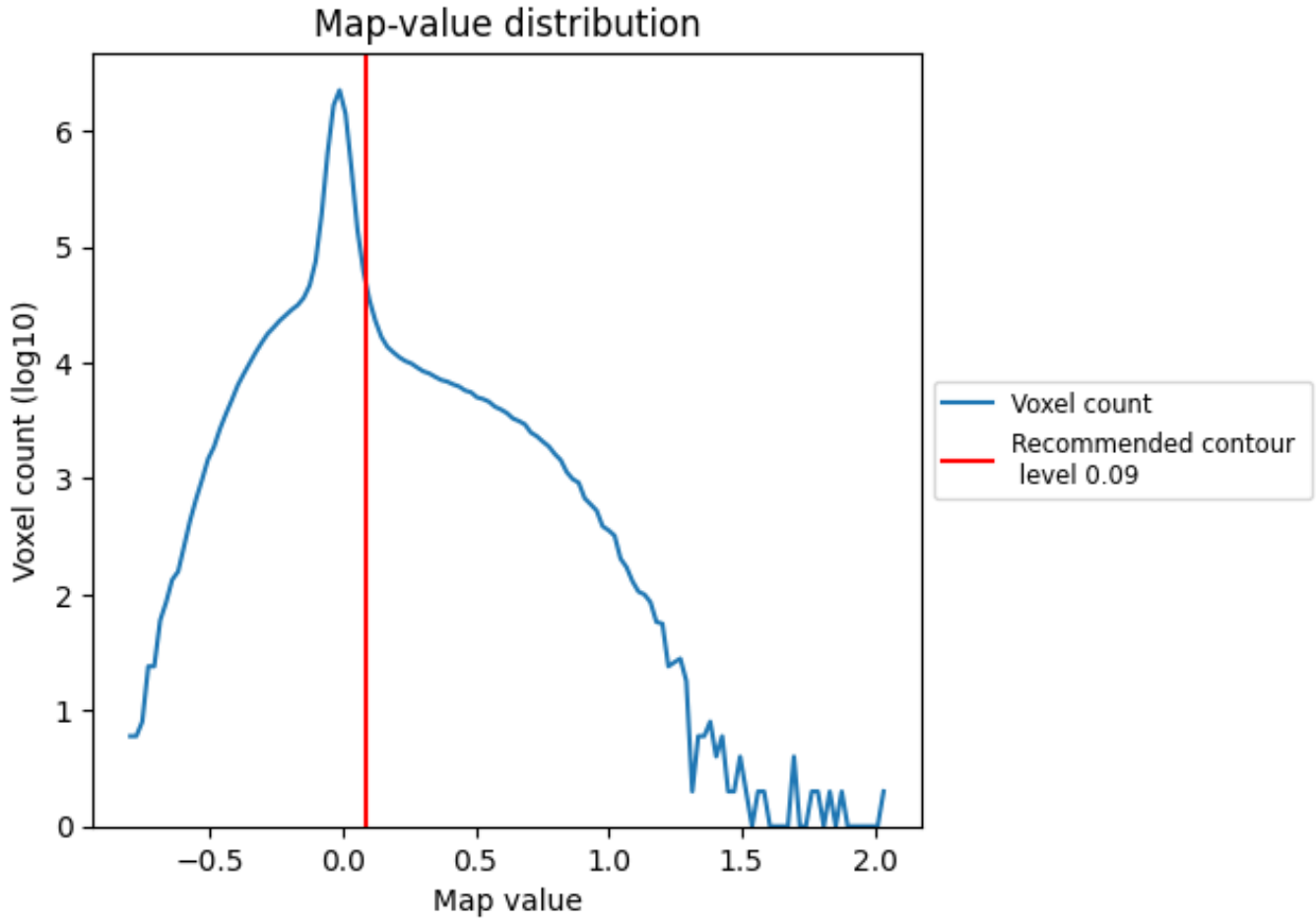
6.6 Mask visualisation (i)

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

7 Map analysis

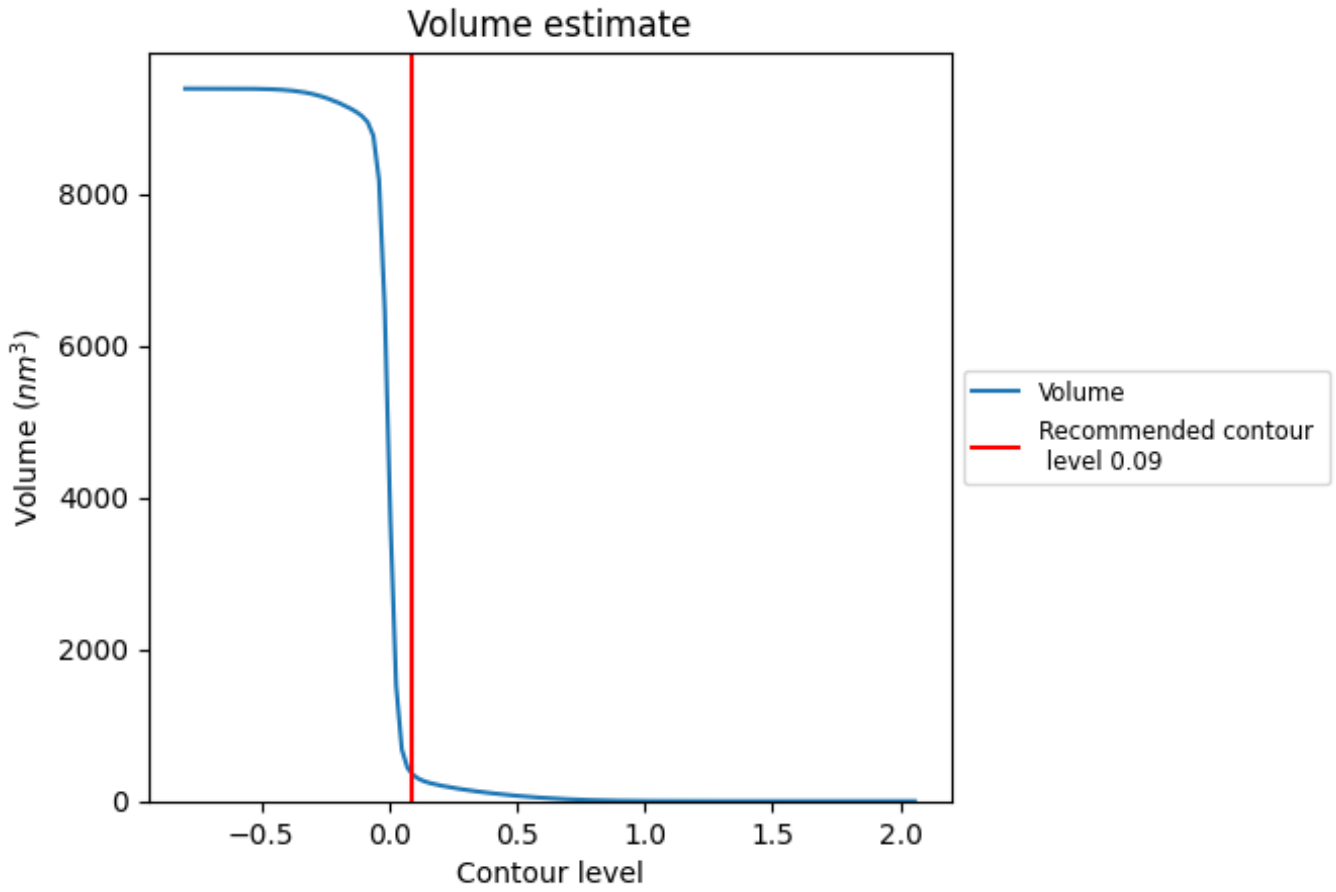
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate (i)



The volume at the recommended contour level is 359 nm^3; this corresponds to an approximate mass of 325 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

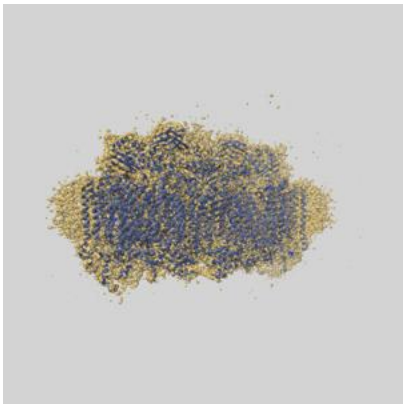
8 Fourier-Shell correlation

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

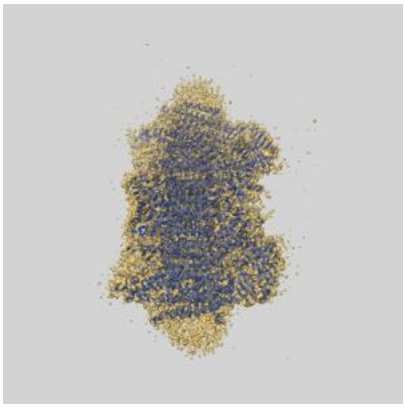
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13977 and PDB model 7QHO. Per-residue inclusion information can be found in section 3 on page 21.

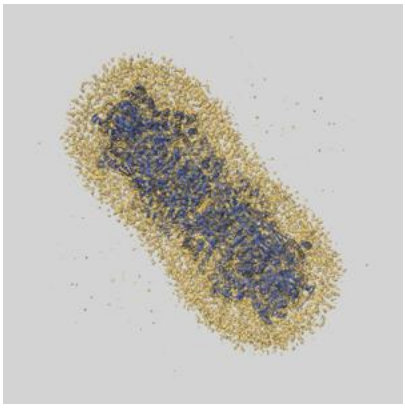
9.1 Map-model overlay



X



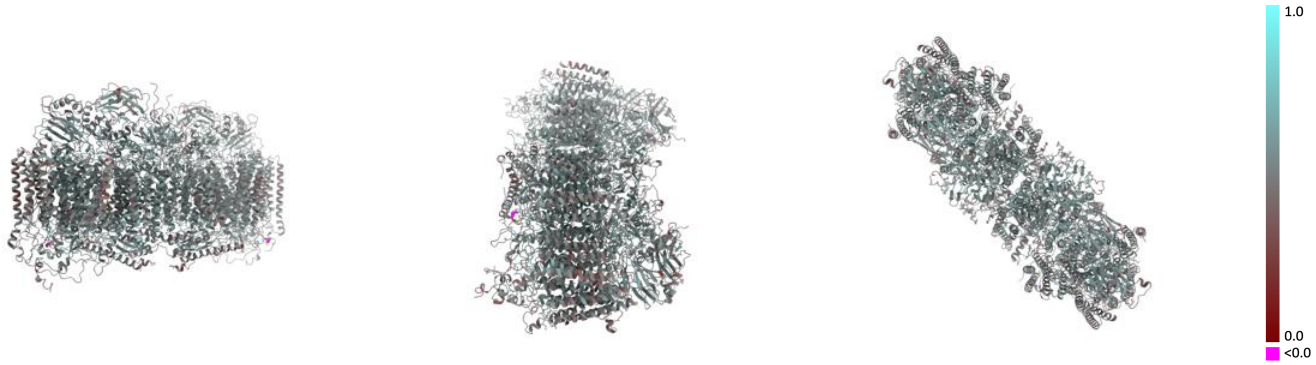
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

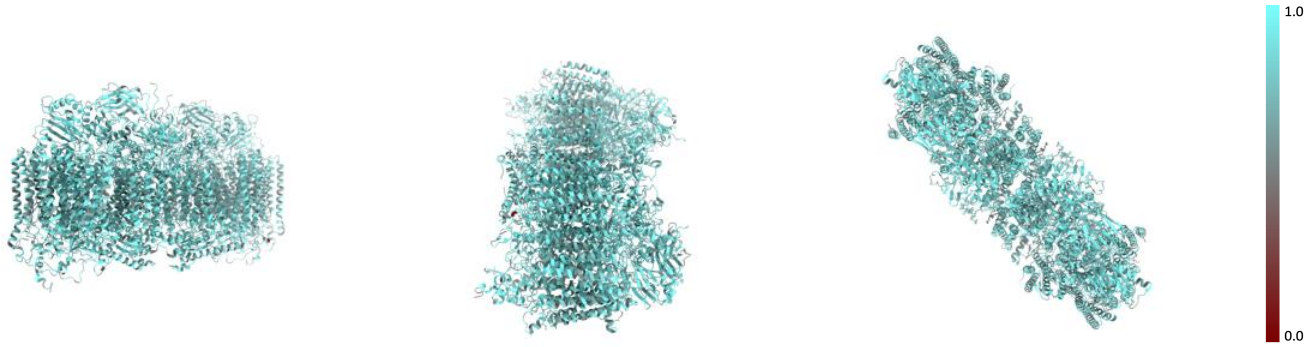
9.2 Q-score mapped to coordinate model



X Y Z

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

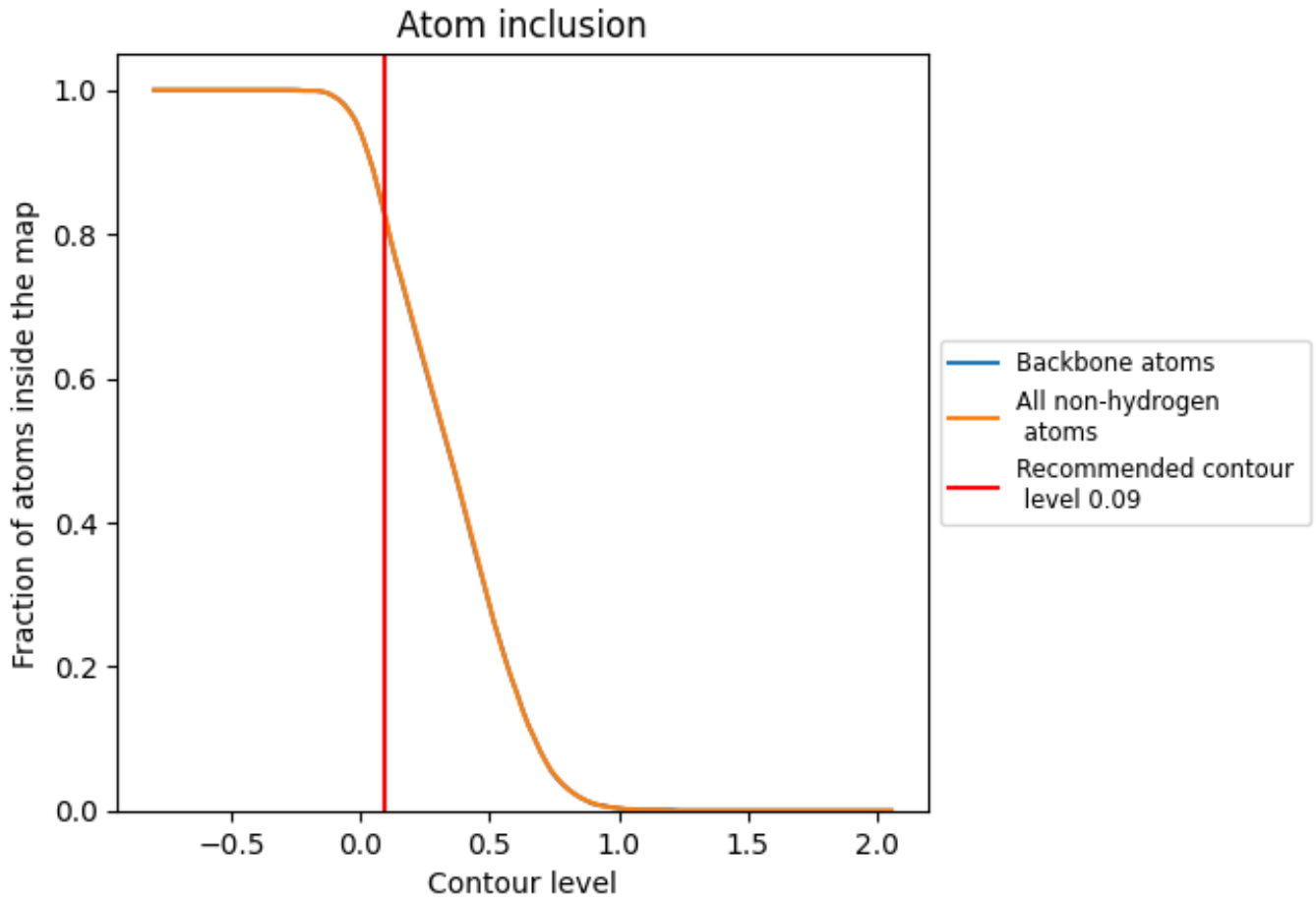
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5160
A	0.8510	0.5230
B	0.8770	0.5420
C	0.8580	0.5370
D	0.8600	0.5360
E	0.8160	0.5020
F	0.8270	0.5120
G	0.8110	0.5000
H	0.7850	0.4870
I	0.7920	0.4870
J	0.7520	0.4580
K	0.8060	0.4840
L	0.7480	0.4400
M	0.7340	0.4390
N	0.8450	0.5200
O	0.8750	0.5390
P	0.8520	0.5340
Q	0.8610	0.5350
R	0.8120	0.5010
S	0.8300	0.5090
T	0.8120	0.5000
U	0.7900	0.4860
V	0.7950	0.4850
W	0.7560	0.4590
X	0.7920	0.4770
Y	0.7460	0.4370
Z	0.7250	0.4350

