wwPDB EM Validation Summary Report (i)

Nov 27, 2023 – 02:25 PM JST

PDB ID	:	8IUG
EMDB ID	:	EMD-35721
Title	:	Cryo-EM structure of the RC-LH core complex from roseiflexus castenholzii
Authors	:	Wang, G.-L.; Qi, C.-H.; Yu, L.-J.
Deposited on	:	2023-03-24
Resolution	:	2.86 Å(reported)

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

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

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

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

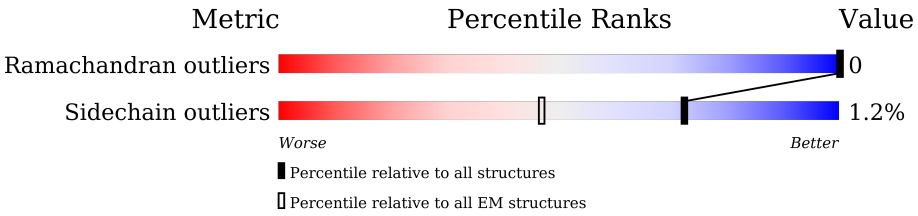
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.86 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	91% 9%
1	2	55	5% 85% 5% 9%
1	4	55	89% 9%
1	6	55	91% 9%
1	8	55	91% 9%
1	B	55	91% 9%
1	E	55	91% 9%
1	G	55	89% 9%
1	I	55	91% 9%

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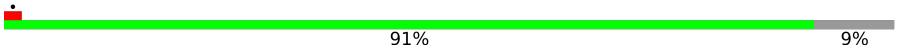
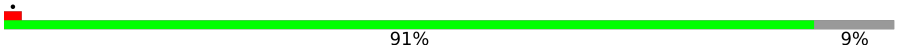
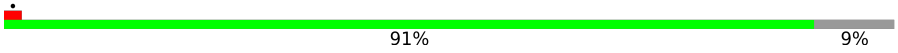
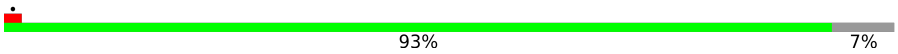
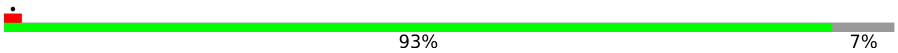
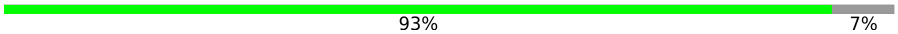
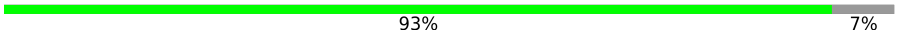
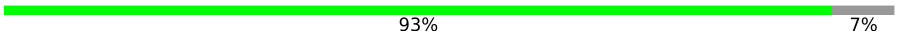
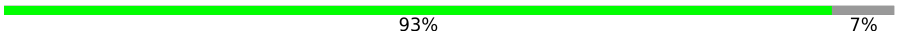
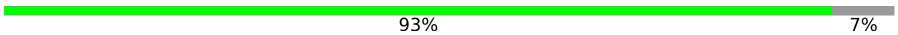
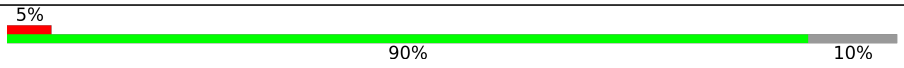
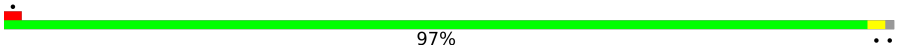
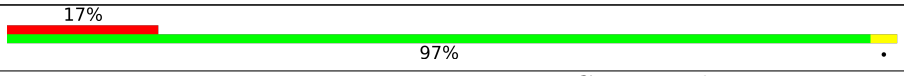
Mol	Chain	Length	Quality of chain
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	1	42	
2	3	42	
2	5	42	
2	7	42	
2	9	42	
2	A	42	
2	D	42	
2	F	42	
2	H	42	
2	J	42	
2	N	42	
2	P	42	
2	R	42	
2	T	42	
2	V	42	
3	C	320	
4	L	641	
4	M	641	
5	X	30	

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Mol	Chain	Length	Quality of chain
6	Y	39	82% 18%
7	Z	10	100%
8	h	63	73% 25%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 25238 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	2	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	4	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	6	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	8	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	B	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	E	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	G	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	I	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	K	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	O	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	Q	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	S	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	U	50	Total	C	N	O	S	0	0
			416	280	69	66	1		
1	W	50	Total	C	N	O	S	0	0
			416	280	69	66	1		

- Molecule 2 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	3	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	5	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	7	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	D	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	H	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	J	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	N	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	P	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	R	39	Total	C	N	O	S	0	0
			308	205	52	50	1		
2	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	V	38	Total	C	N	O	S	0	0
			300	201	51	47	1		

- Molecule 3 is a protein called Cytochrome subunit of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	316	Total	C	N	O	S	0	0
			2411	1537	408	444	22		

- Molecule 4 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	286	Total	C	N	O	S	0	0
			2278	1527	367	376	8		
4	M	306	Total	C	N	O	S	0	0
			2488	1673	399	409	7		

- Molecule 5 is a protein called TMx polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	30	Total	C	N	O	S	1	0
			246	172	32	38	4		

- Molecule 6 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	32	Total	C	N	O	S	0	0
			259	181	36	39	3		

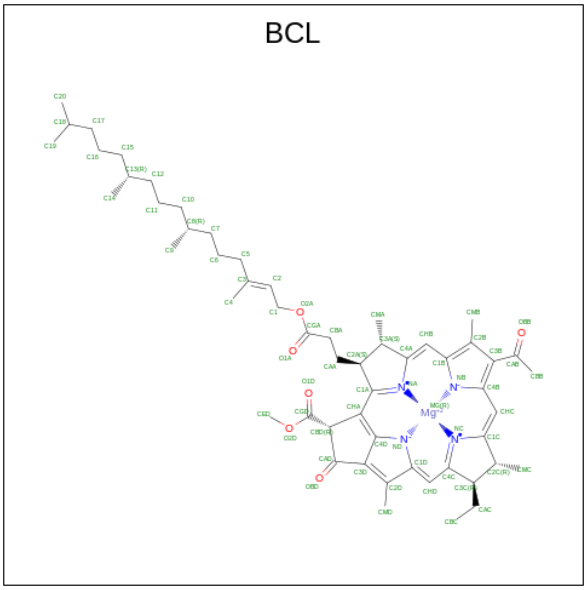
- Molecule 7 is a protein called reaction center unknown polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Z	10	Total	C	N	O	0	0
			51	31	10	10		

- Molecule 8 is a protein called reaction center small polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	47	Total	C	N	O	S	0	0
			362	242	59	60	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
9	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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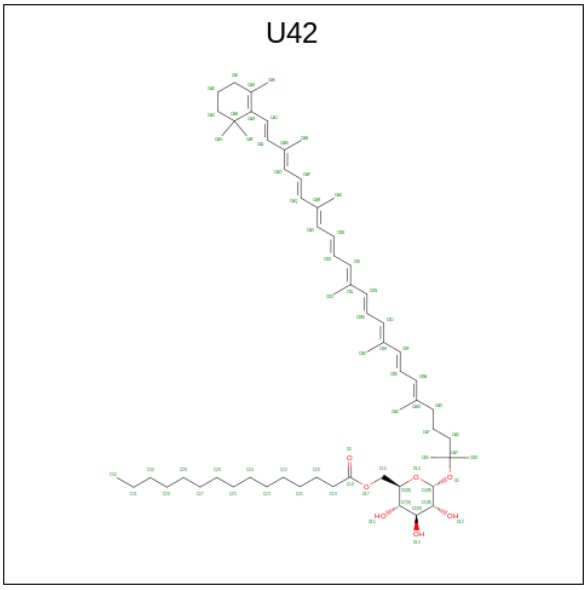
Mol	Chain	Residues	Atoms					AltConf
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is [(2 {R},3 {S},4 {S},5 {R},6 {R})-6-[(6 {E},8 {E},10 {E},12 {E},14 {E},16 {E},18 {E},20 {E},22 {E},24 {E})-2,6,10,14,19,23-hexamethyl-25-(2,6,6-trimethylcyclohexen-1-yl)pentacosa-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl pentadecanoate (three-letter code: U42) (formula: $C_{61}H_{96}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
10	0	1	Total	C	O	0
			68	61	7	
10	4	1	Total	C	O	0
			68	61	7	
10	4	1	Total	C	O	0
			68	61	7	
10	8	1	Total	C	O	0
			68	61	7	

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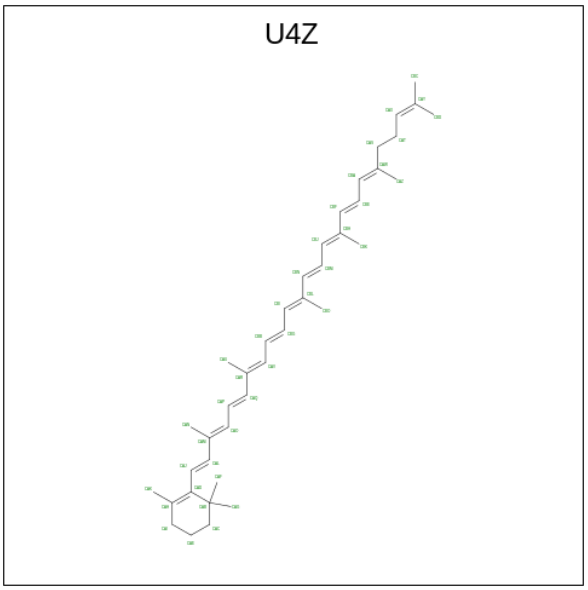
Mol	Chain	Residues	Atoms	AltConf
10	B	1	Total C O 68 61 7	0
10	E	1	Total C O 68 61 7	0
10	G	1	Total C O 68 61 7	0
10	I	1	Total C O 68 61 7	0
10	I	1	Total C O 68 61 7	0
10	O	1	Total C O 68 61 7	0
10	Q	1	Total C O 68 61 7	0
10	S	1	Total C O 68 61 7	0
10	U	1	Total C O 68 61 7	0
10	U	1	Total C O 68 61 7	0

- Molecule 11 is gamma-Carotene (three-letter code: U4Z) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
11	1	1	Total C 40 40	0

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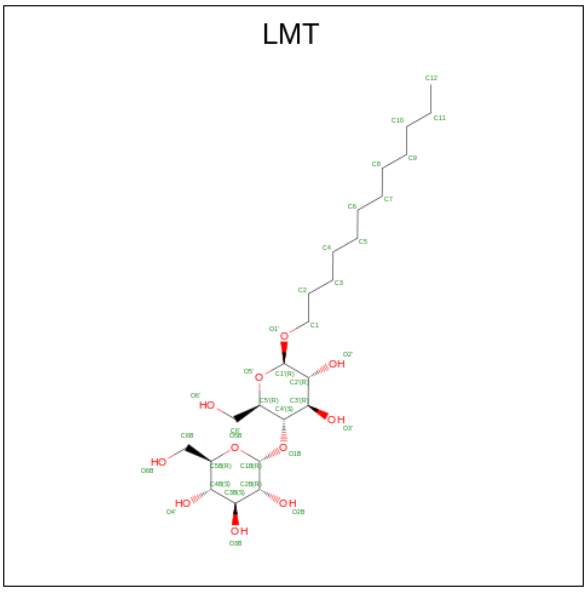
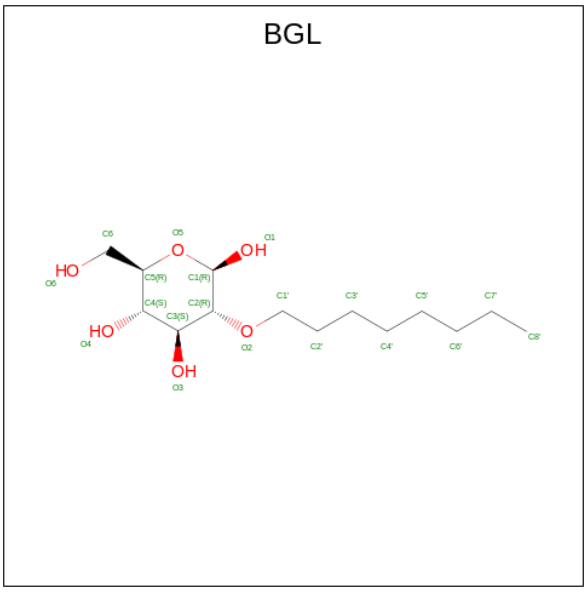
Mol	Chain	Residues	Atoms	AltConf
11	3	1	Total C 40 40	0
11	5	1	Total C 40 40	0
11	7	1	Total C 40 40	0
11	9	1	Total C 40 40	0
11	A	1	Total C 40 40	0
11	C	1	Total C 40 40	0
11	D	1	Total C 40 40	0
11	F	1	Total C 40 40	0
11	H	1	Total C 40 40	0
11	J	1	Total C 40 40	0
11	N	1	Total C 40 40	0
11	P	1	Total C 40 40	0
11	S	1	Total C 40 40	0
11	T	1	Total C 40 40	0
11	V	1	Total C 40 40	0

- Molecule 12 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



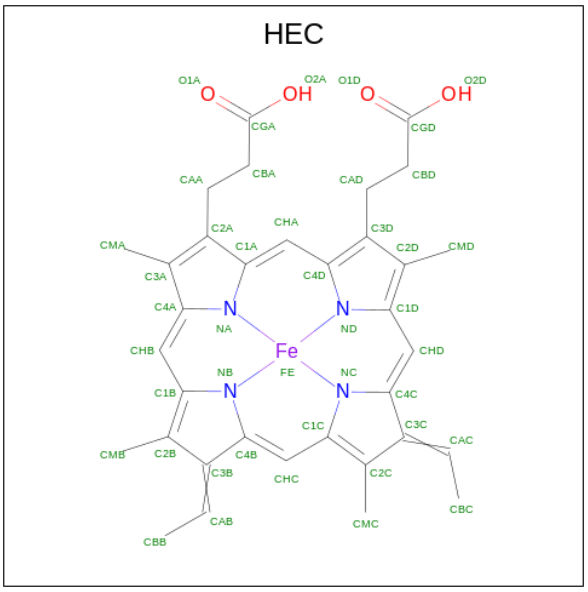
Mol	Chain	Residues	Atoms			AltConf
12	1	1	Total	C	O	0
			35	24	11	
12	D	1	Total	C	O	0
			35	24	11	
12	T	1	Total	C	O	0
			35	24	11	

- Molecule 13 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			AltConf
13	3	1	Total	C	O	0
			20	14	6	
13	C	1	Total	C	O	0
			20	14	6	
13	C	1	Total	C	O	0
			20	14	6	
13	D	1	Total	C	O	0
			20	14	6	
13	F	1	Total	C	O	0
			20	14	6	
13	H	1	Total	C	O	0
			20	14	6	
13	H	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	L	1	Total	C	O	0
			20	14	6	
13	N	1	Total	C	O	0
			20	14	6	
13	Y	1	Total	C	O	0
			20	14	6	

- Molecule 14 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

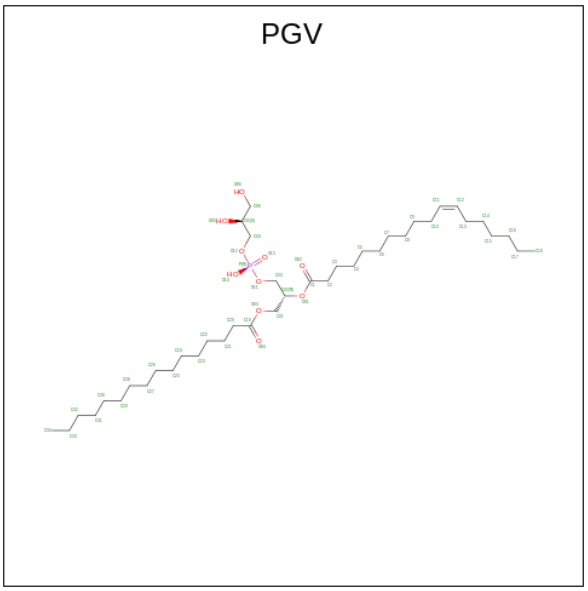


Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
15	C	1	Total	Ca	0
			1	1	

- Molecule 16 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
16	C	1	Total 41	C 30	O 10	P 1	0
16	C	1	Total 51	C 40	O 10	P 1	0
16	L	1	Total 51	C 40	O 10	P 1	0
16	L	1	Total 51	C 40	O 10	P 1	0
16	L	1	Total 51	C 40	O 10	P 1	0
16	M	1	Total 51	C 40	O 10	P 1	0
16	M	1	Total 51	C 40	O 10	P 1	0
16	P	1	Total 43	C 32	O 10	P 1	0
16	P	1	Total 51	C 40	O 10	P 1	0

- Molecule 17 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		AltConf
17	C	2	Total 34	C 34	0
17	H	4	Total 52	C 52	0
17	L	4	Total 48	C 48	0

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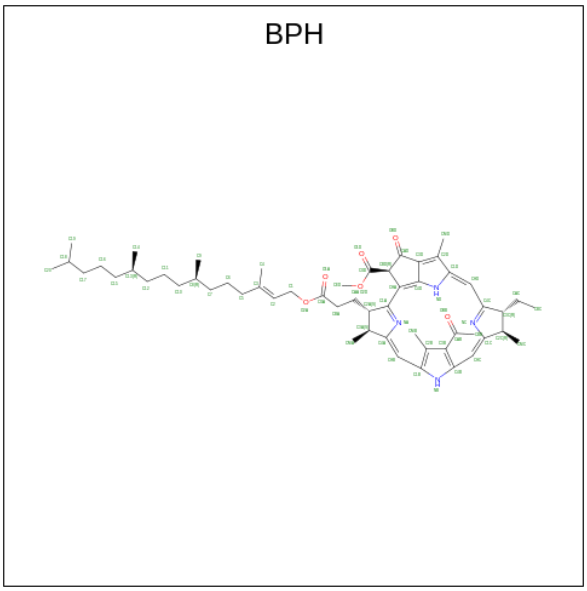
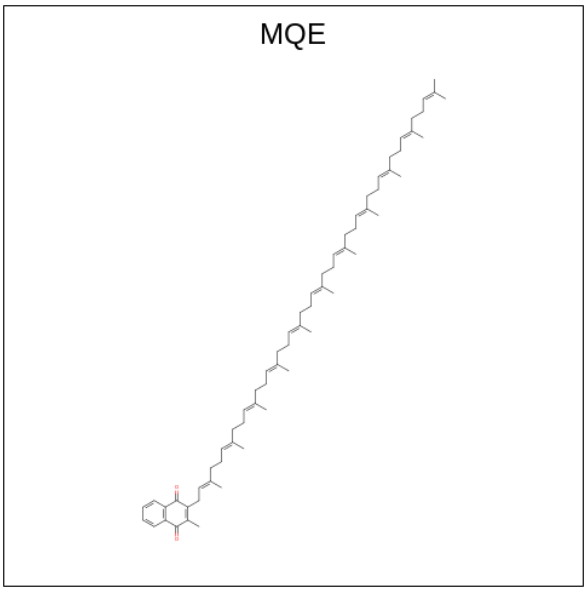
Mol	Chain	Residues	Atoms	AltConf
17	M	1	Total C 12 12	0
17	V	3	Total C 33 33	0
17	Y	1	Total C 14 14	0
17	h	2	Total C 24 24	0

- Molecule 18 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



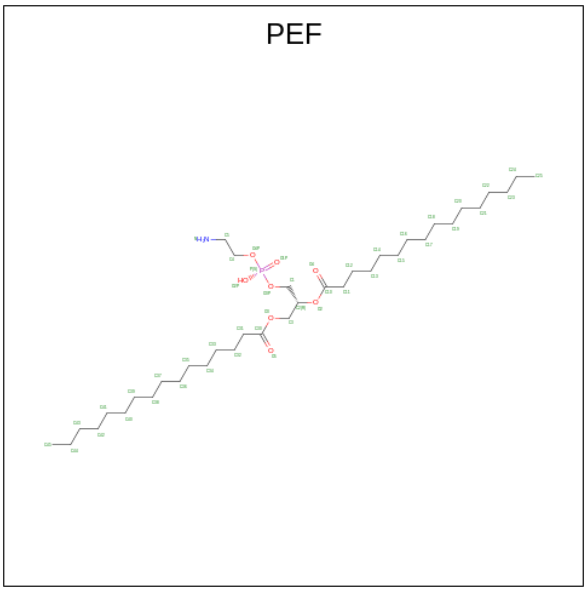
Mol	Chain	Residues	Atoms	AltConf
18	L	1	Total C N O 65 55 4 6	0
18	L	1	Total C N O 65 55 4 6	0
18	M	1	Total C N O 65 55 4 6	0

- Molecule 19 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetratetraconta-2,6,10,1 4,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (three-letter code: MQE) (formula: $C_{66}H_{96}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	L	1	Total 53	C 51	O 2	0
19	M	1	Total 68	C 66	O 2	0

- Molecule 20 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).

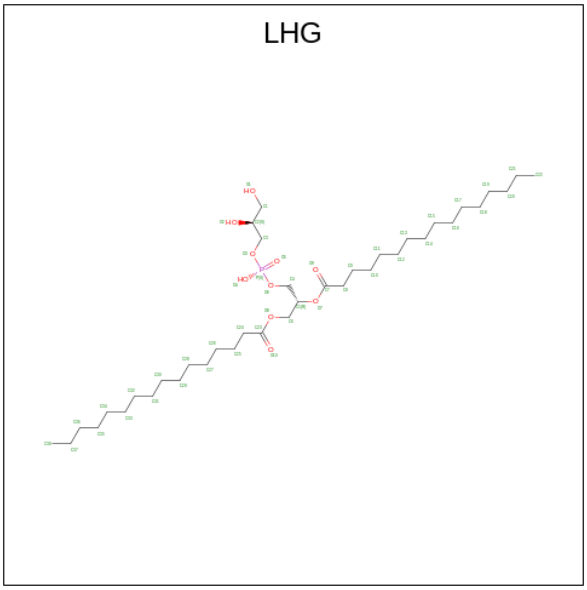


Mol	Chain	Residues	Atoms					AltConf
20	L	1	Total 41	C 31	N 1	O 8	P 1	0

- Molecule 21 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
21	M	1	1	1	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



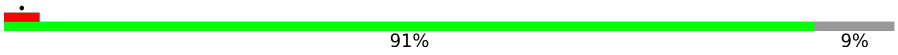
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
22	h	1	17	16	1	0

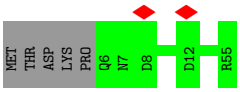
3 Residue-property plots (i)

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

• Molecule 1: Antenna complex alpha/beta subunit

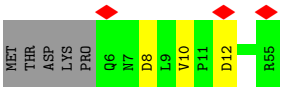
Chain 0:





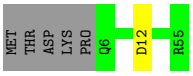
• Molecule 1: Antenna complex alpha/beta subunit

Chain 2:



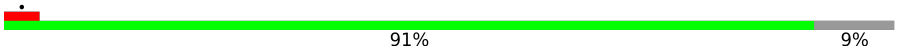
• Molecule 1: Antenna complex alpha/beta subunit

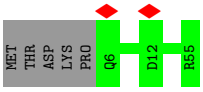
Chain 4:



• Molecule 1: Antenna complex alpha/beta subunit

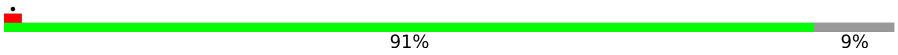
Chain 6:

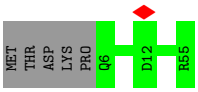




• Molecule 1: Antenna complex alpha/beta subunit

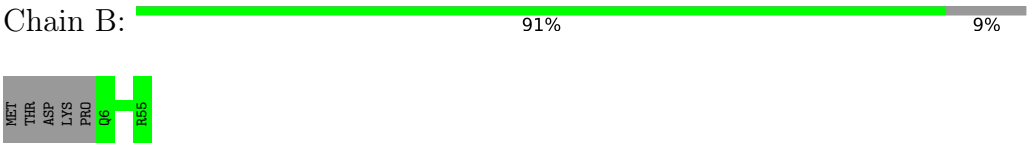
Chain 8:





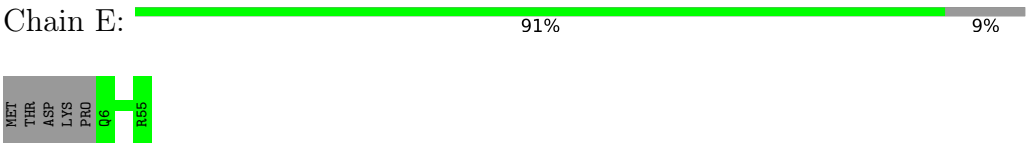
• Molecule 1: Antenna complex alpha/beta subunit

Chain B:



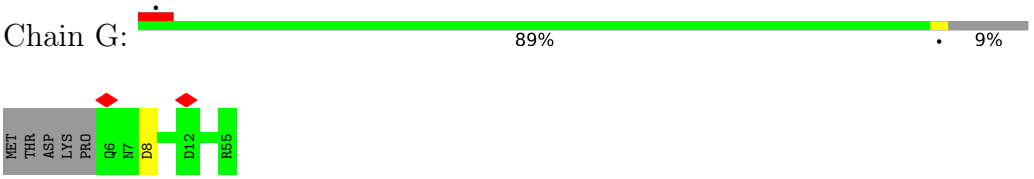
• Molecule 1: Antenna complex alpha/beta subunit

Chain E:



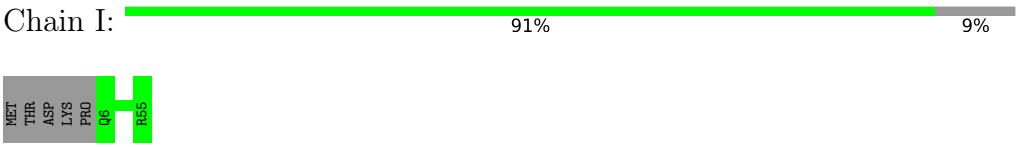
• Molecule 1: Antenna complex alpha/beta subunit

Chain G:



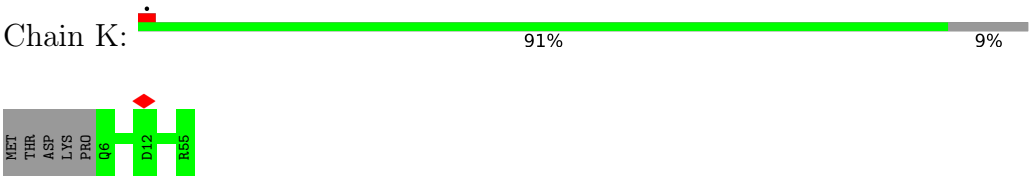
• Molecule 1: Antenna complex alpha/beta subunit

Chain I:



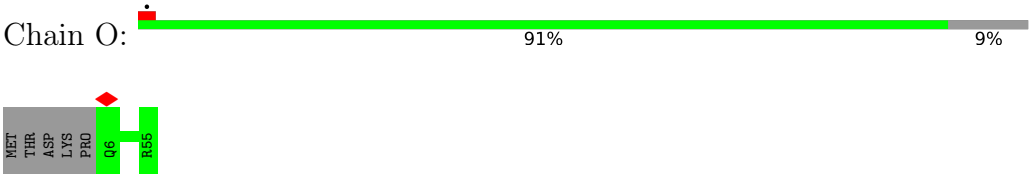
• Molecule 1: Antenna complex alpha/beta subunit

Chain K:



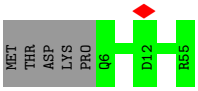
• Molecule 1: Antenna complex alpha/beta subunit

Chain O:



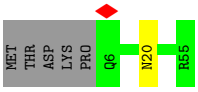
• Molecule 1: Antenna complex alpha/beta subunit

Chain Q:



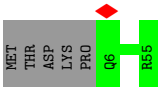
• Molecule 1: Antenna complex alpha/beta subunit

Chain S:



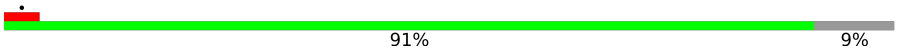
• Molecule 1: Antenna complex alpha/beta subunit

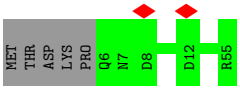
Chain U:



• Molecule 1: Antenna complex alpha/beta subunit

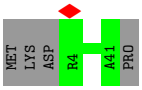
Chain W:





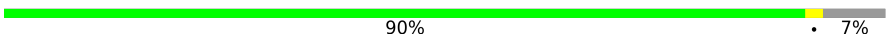
• Molecule 2: Alpha subunit of light-harvesting 1

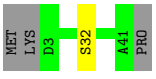
Chain 1:



• Molecule 2: Alpha subunit of light-harvesting 1

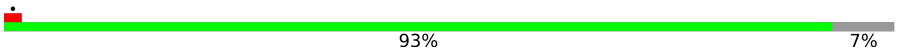
Chain 3:

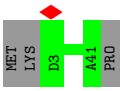




• Molecule 2: Alpha subunit of light-harvesting 1

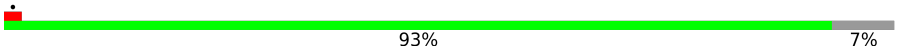
Chain 5:

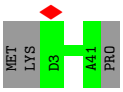




• Molecule 2: Alpha subunit of light-harvesting 1

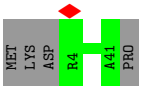
Chain 7:





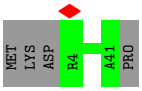
• Molecule 2: Alpha subunit of light-harvesting 1

Chain 9:



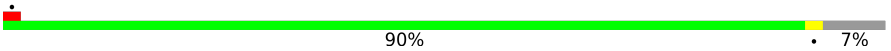
• Molecule 2: Alpha subunit of light-harvesting 1

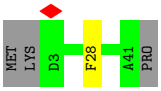
Chain A:



• Molecule 2: Alpha subunit of light-harvesting 1

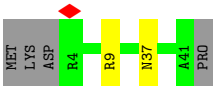
Chain D:





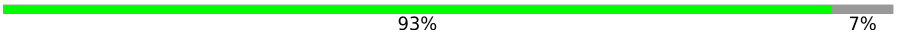
• Molecule 2: Alpha subunit of light-harvesting 1

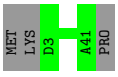
Chain F:



• Molecule 2: Alpha subunit of light-harvesting 1

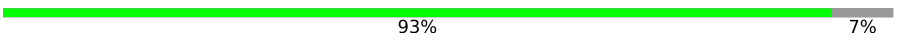
Chain H:

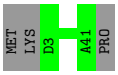




• Molecule 2: Alpha subunit of light-harvesting 1

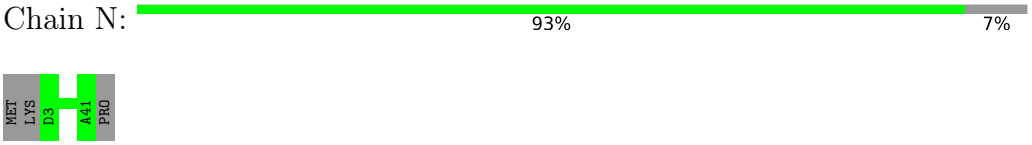
Chain J:





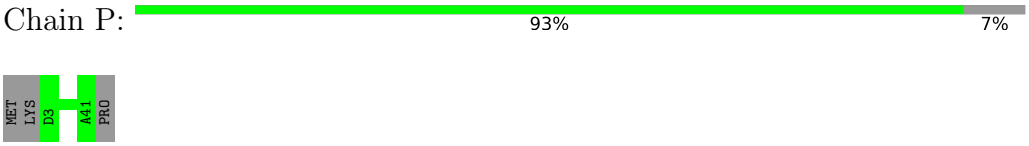
• Molecule 2: Alpha subunit of light-harvesting 1

Chain N:



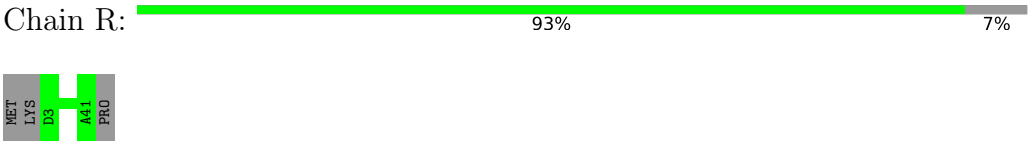
• Molecule 2: Alpha subunit of light-harvesting 1

Chain P:



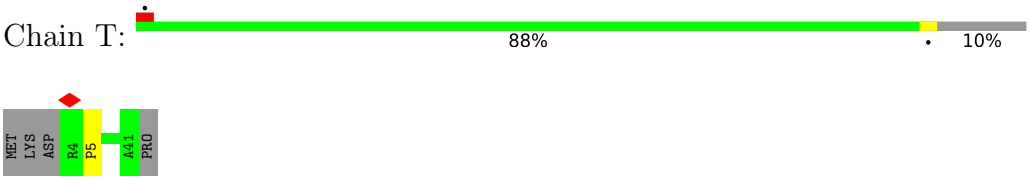
• Molecule 2: Alpha subunit of light-harvesting 1

Chain R:



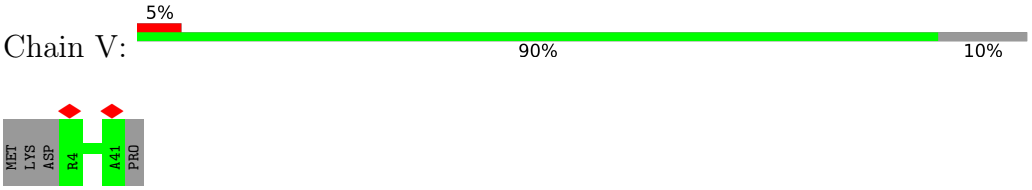
• Molecule 2: Alpha subunit of light-harvesting 1

Chain T:



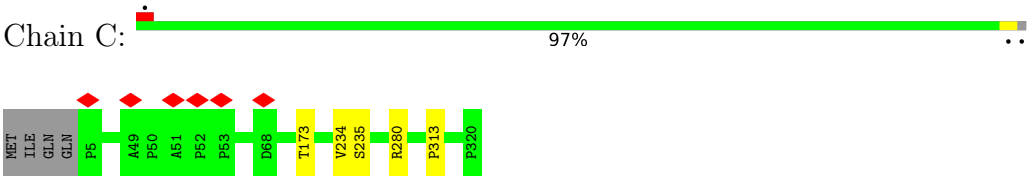
• Molecule 2: Alpha subunit of light-harvesting 1

Chain V:



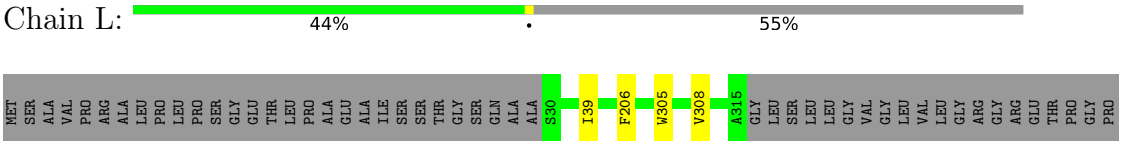
• Molecule 3: Cytochrome subunit of photosynthetic reaction center

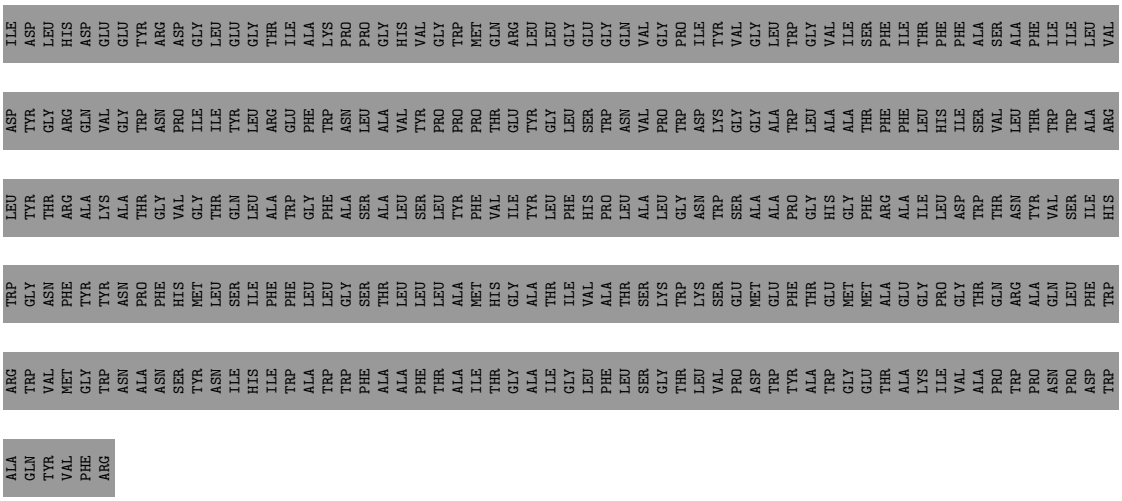
Chain C:



• Molecule 4: Reaction center protein L chain

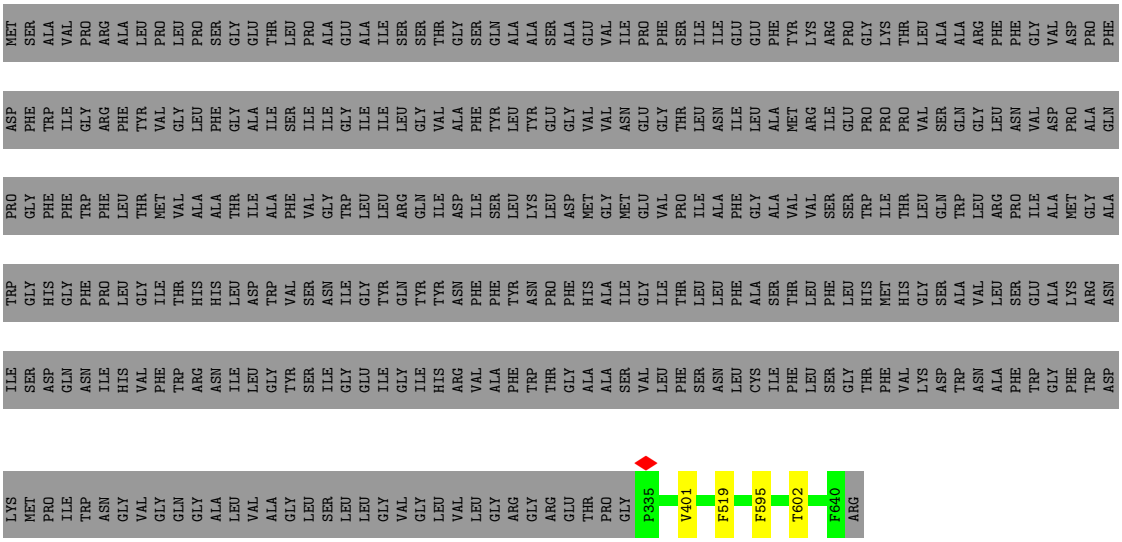
Chain L:





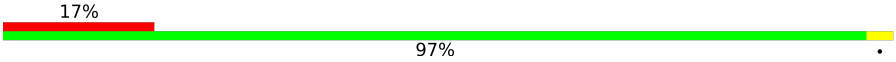
• Molecule 4: Reaction center protein L chain

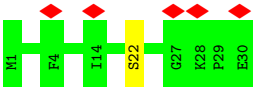
Chain M:



• Molecule 5: TMx polypeptide

Chain X:





• Molecule 6: reaction center small polypeptide

Chain Y:

• Molecule 7: reaction center unknown polypeptide

Chain Z:

There are no outlier residues recorded for this chain.

• Molecule 8: reaction center small polypeptide

Chain h:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	639374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.066	Depositor
Minimum map value	-1.238	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.226	Depositor
Map size (Å)	320.4, 320.4, 320.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89, 0.89, 0.89	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: PEF, U4Z, U42, UNL, MN, MQE, LMT, BPH, HEC, BGL, CA, LHG, PGV, BCL

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	0	0.29	0/432	0.42	0/597
1	2	0.30	0/432	0.43	0/597
1	4	0.31	0/432	0.45	0/597
1	6	0.31	0/432	0.44	0/597
1	8	0.31	0/432	0.45	0/597
1	B	0.28	0/432	0.42	0/597
1	E	0.29	0/432	0.43	0/597
1	G	0.30	0/432	0.43	0/597
1	I	0.30	0/432	0.42	0/597
1	K	0.30	0/432	0.43	0/597
1	O	0.29	0/432	0.42	0/597
1	Q	0.30	0/432	0.43	0/597
1	S	0.31	0/432	0.42	0/597
1	U	0.29	0/432	0.42	0/597
1	W	0.28	0/432	0.40	0/597
2	1	0.28	0/307	0.52	0/417
2	3	0.29	0/315	0.51	0/428
2	5	0.33	0/315	0.54	0/428
2	7	0.30	0/315	0.52	0/428
2	9	0.29	0/307	0.50	0/417
2	A	0.29	0/307	0.52	0/417
2	D	0.28	0/315	0.49	0/428
2	F	0.29	0/307	0.53	0/417
2	H	0.40	0/315	0.53	0/428
2	J	0.35	0/315	0.56	0/428
2	N	0.28	0/315	0.48	0/428
2	P	0.30	0/315	0.52	0/428
2	R	0.34	0/315	0.51	0/428
2	T	0.78	1/307 (0.3%)	0.56	0/417
2	V	0.28	0/307	0.50	0/417
3	C	0.63	1/2477 (0.0%)	0.52	1/3383 (0.0%)
4	L	0.35	0/2360	0.54	0/3220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	M	0.32	0/2597	0.49	0/3566
5	X	0.29	0/253	0.37	0/341
6	Y	0.29	0/268	0.43	0/370
7	Z	0.67	0/51	0.94	0/70
8	h	0.30	0/374	0.48	0/513
All	All	0.38	2/19537 (0.0%)	0.49	1/26772 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	313	PRO	N-CD	-26.93	1.10	1.47
2	T	5	PRO	N-CD	-12.60	1.30	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	313	PRO	CA-N-CD	5.91	119.98	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	2	48/55 (87%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	6	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	8	48/55 (87%)	44 (92%)	4 (8%)	0	100	100
1	B	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	E	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	G	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	I	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	K	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	O	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	Q	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
1	S	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	U	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
1	W	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
2	1	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	3	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
2	5	37/42 (88%)	35 (95%)	2 (5%)	0	100	100
2	7	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
2	9	36/42 (86%)	36 (100%)	0	0	100	100
2	A	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	D	37/42 (88%)	37 (100%)	0	0	100	100
2	F	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	H	37/42 (88%)	37 (100%)	0	0	100	100
2	J	37/42 (88%)	37 (100%)	0	0	100	100
2	N	37/42 (88%)	34 (92%)	3 (8%)	0	100	100
2	P	37/42 (88%)	35 (95%)	2 (5%)	0	100	100
2	R	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
2	T	36/42 (86%)	36 (100%)	0	0	100	100
2	V	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
3	C	314/320 (98%)	302 (96%)	12 (4%)	0	100	100
4	L	284/641 (44%)	269 (95%)	15 (5%)	0	100	100
4	M	304/641 (47%)	293 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	X	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
6	Y	30/39 (77%)	29 (97%)	1 (3%)	0	100	100
7	Z	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
8	h	45/63 (71%)	45 (100%)	0	0	100	100
All	All	2283/3199 (71%)	2197 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	0	44/49 (90%)	44 (100%)	0	100	100
1	2	44/49 (90%)	41 (93%)	3 (7%)	16	38
1	4	44/49 (90%)	43 (98%)	1 (2%)	50	78
1	6	44/49 (90%)	44 (100%)	0	100	100
1	8	44/49 (90%)	44 (100%)	0	100	100
1	B	44/49 (90%)	44 (100%)	0	100	100
1	E	44/49 (90%)	44 (100%)	0	100	100
1	G	44/49 (90%)	43 (98%)	1 (2%)	50	78
1	I	44/49 (90%)	44 (100%)	0	100	100
1	K	44/49 (90%)	44 (100%)	0	100	100
1	O	44/49 (90%)	44 (100%)	0	100	100
1	Q	44/49 (90%)	44 (100%)	0	100	100
1	S	44/49 (90%)	43 (98%)	1 (2%)	50	78
1	U	44/49 (90%)	44 (100%)	0	100	100
1	W	44/49 (90%)	44 (100%)	0	100	100
2	1	33/37 (89%)	33 (100%)	0	100	100
2	3	34/37 (92%)	33 (97%)	1 (3%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5	34/37 (92%)	34 (100%)	0	100	100
2	7	34/37 (92%)	34 (100%)	0	100	100
2	9	33/37 (89%)	33 (100%)	0	100	100
2	A	33/37 (89%)	33 (100%)	0	100	100
2	D	34/37 (92%)	33 (97%)	1 (3%)	42	72
2	F	33/37 (89%)	31 (94%)	2 (6%)	18	43
2	H	34/37 (92%)	34 (100%)	0	100	100
2	J	34/37 (92%)	34 (100%)	0	100	100
2	N	34/37 (92%)	34 (100%)	0	100	100
2	P	34/37 (92%)	34 (100%)	0	100	100
2	R	34/37 (92%)	34 (100%)	0	100	100
2	T	33/37 (89%)	33 (100%)	0	100	100
2	V	33/37 (89%)	33 (100%)	0	100	100
3	C	258/262 (98%)	254 (98%)	4 (2%)	62	84
4	L	232/511 (45%)	228 (98%)	4 (2%)	60	83
4	M	244/511 (48%)	240 (98%)	4 (2%)	62	84
5	X	27/26 (104%)	26 (96%)	1 (4%)	34	65
6	Y	29/36 (81%)	29 (100%)	0	100	100
7	Z	1/1 (100%)	1 (100%)	0	100	100
8	h	36/50 (72%)	35 (97%)	1 (3%)	43	73
All	All	1991/2687 (74%)	1967 (99%)	24 (1%)	72	89

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	206	PHE
4	M	401	VAL
4	L	308	VAL
4	M	519	PHE
3	C	234	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	7	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 133 ligands modelled in this entry, 2 are monoatomic and 17 are unknown - leaving 114 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	$\#\|Z\| > 2$
10	U42	0	103	-	69,69,69	2.39	16 (23%)	86,89,89	2.48	29 (33%)
16	PGV	P	104	-	50,50,50	0.49	0	53,56,56	0.48	0
18	BPH	M	702	-	51,70,70	0.54	0	52,101,101	0.79	1 (1%)
9	BCL	W	101	-	64,74,74	1.74	14 (21%)	78,115,115	2.16	21 (26%)
9	BCL	K	102	-	64,74,74	1.76	16 (25%)	78,115,115	2.50	25 (32%)
11	U4Z	P	102	-	40,40,40	1.78	9 (22%)	50,51,51	1.68	12 (24%)
12	LMT	T	103	-	36,36,36	0.47	0	47,47,47	0.96	2 (4%)
9	BCL	Q	102	-	64,74,74	1.71	13 (20%)	78,115,115	2.16	21 (26%)
11	U4Z	5	102	-	40,40,40	1.80	9 (22%)	50,51,51	1.70	12 (24%)
11	U4Z	1	102	-	40,40,40	1.77	9 (22%)	50,51,51	1.68	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	U4Z	S	104	-	40,40,40	1.83	9 (22%)	50,51,51	1.74	12 (24%)
9	BCL	M	701	-	64,74,74	1.74	14 (21%)	78,115,115	2.39	23 (29%)
9	BCL	F	102	-	64,74,74	1.71	12 (18%)	78,115,115	2.10	21 (26%)
9	BCL	G	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.40	25 (32%)
9	BCL	A	101	-	64,74,74	1.74	14 (21%)	78,115,115	2.27	20 (25%)
10	U42	I	101	-	69,69,69	2.31	24 (34%)	86,89,89	2.55	19 (22%)
13	BGL	L	1012	-	20,20,20	1.03	1 (5%)	24,25,25	0.76	0
13	BGL	L	1011	-	20,20,20	1.08	1 (5%)	24,25,25	0.92	1 (4%)
9	BCL	8	103	-	64,74,74	1.70	14 (21%)	78,115,115	2.28	23 (29%)
9	BCL	T	101	-	64,74,74	1.66	12 (18%)	78,115,115	2.25	21 (26%)
14	HEC	C	405	3	32,50,50	2.12	3 (9%)	24,82,82	1.55	2 (8%)
18	BPH	L	1003	-	51,70,70	1.81	7 (13%)	52,101,101	2.11	11 (21%)
11	U4Z	7	102	-	40,40,40	1.79	10 (25%)	50,51,51	1.70	12 (24%)
9	BCL	D	102	-	64,74,74	1.70	12 (18%)	78,115,115	2.14	22 (28%)
9	BCL	I	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.28	19 (24%)
10	U42	Q	101	-	69,69,69	2.14	20 (28%)	86,89,89	2.03	25 (29%)
11	U4Z	A	102	-	40,40,40	1.80	9 (22%)	50,51,51	1.74	12 (24%)
10	U42	S	101	-	69,69,69	2.20	19 (27%)	86,89,89	2.15	22 (25%)
11	U4Z	D	103	-	40,40,40	1.83	9 (22%)	50,51,51	1.71	13 (26%)
9	BCL	N	101	-	64,74,74	1.67	10 (15%)	78,115,115	2.20	20 (25%)
9	BCL	B	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.14	19 (24%)
13	BGL	C	409	-	20,20,20	1.01	1 (5%)	24,25,25	0.89	0
9	BCL	0	101	-	64,74,74	1.72	13 (20%)	78,115,115	2.16	19 (24%)
16	PGV	M	706	-	50,50,50	0.49	0	53,56,56	0.53	0
9	BCL	7	101	-	64,74,74	1.69	12 (18%)	78,115,115	2.19	18 (23%)
10	U42	O	101	-	69,69,69	2.40	17 (24%)	86,89,89	2.03	20 (23%)
16	PGV	P	103	-	42,42,50	0.55	0	45,48,56	0.53	0
10	U42	4	101	-	69,69,69	2.08	21 (30%)	86,89,89	1.82	21 (24%)
18	BPH	L	1005	-	51,70,70	0.61	1 (1%)	52,101,101	0.75	1 (1%)
9	BCL	S	102	-	64,74,74	1.71	13 (20%)	78,115,115	2.26	24 (30%)
16	PGV	C	408	15	50,50,50	0.54	0	53,56,56	0.51	0
9	BCL	R	101	-	64,74,74	1.68	11 (17%)	78,115,115	2.23	21 (26%)
9	BCL	4	102	-	64,74,74	1.72	13 (20%)	78,115,115	2.15	21 (26%)
13	BGL	F	104	-	20,20,20	0.99	1 (5%)	24,25,25	0.94	0
13	BGL	L	1013	-	20,20,20	0.96	1 (5%)	24,25,25	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	U42	U	104	-	69,69,69	2.06	13 (18%)	86,89,89	2.29	27 (31%)
9	BCL	B	103	-	64,74,74	1.69	14 (21%)	78,115,115	2.41	22 (28%)
11	U4Z	V	102	-	40,40,40	1.84	9 (22%)	50,51,51	1.77	13 (26%)
9	BCL	1	101	-	64,74,74	1.65	11 (17%)	78,115,115	2.38	20 (25%)
9	BCL	Q	103	-	64,74,74	1.68	13 (20%)	78,115,115	2.45	21 (26%)
13	BGL	Y	101	-	20,20,20	1.01	1 (5%)	24,25,25	0.77	0
9	BCL	2	102	-	64,74,74	1.74	17 (26%)	78,115,115	2.30	21 (26%)
9	BCL	2	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.22	22 (28%)
9	BCL	O	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.25	23 (29%)
13	BGL	3	103	-	20,20,20	1.04	1 (5%)	24,25,25	0.80	0
16	PGV	C	407	-	40,40,50	0.55	0	42,46,56	0.52	0
9	BCL	P	101	-	64,74,74	1.74	14 (21%)	78,115,115	2.23	22 (28%)
9	BCL	U	102	-	64,74,74	1.69	12 (18%)	78,115,115	2.13	21 (26%)
9	BCL	9	102	-	64,74,74	1.66	11 (17%)	78,115,115	2.29	22 (28%)
12	LMT	1	103	-	36,36,36	0.39	0	47,47,47	0.72	1 (2%)
14	HEC	C	404	3	32,50,50	2.12	3 (9%)	24,82,82	1.63	3 (12%)
14	HEC	C	403	3	32,50,50	2.12	3 (9%)	24,82,82	1.65	4 (16%)
16	PGV	L	1007	-	50,50,50	0.49	0	53,56,56	0.48	0
13	BGL	C	410	-	20,20,20	0.99	1 (5%)	24,25,25	0.91	0
11	U4Z	T	102	-	40,40,40	1.78	9 (22%)	50,51,51	1.70	12 (24%)
22	LHG	h	101	-	16,16,48	1.05	1 (6%)	15,15,54	0.34	0
9	BCL	D	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.37	23 (29%)
9	BCL	O	103	-	64,74,74	1.67	12 (18%)	78,115,115	2.43	19 (24%)
12	LMT	D	105	-	36,36,36	0.41	0	47,47,47	0.78	1 (2%)
9	BCL	U	103	-	64,74,74	1.66	13 (20%)	78,115,115	2.40	18 (23%)
11	U4Z	F	103	-	40,40,40	1.83	9 (22%)	50,51,51	1.72	12 (24%)
13	BGL	H	107	-	20,20,20	1.04	1 (5%)	24,25,25	0.81	0
9	BCL	L	1002	-	64,74,74	1.71	13 (20%)	78,115,115	2.28	21 (26%)
9	BCL	0	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.44	22 (28%)
10	U42	4	104	-	69,69,69	1.81	18 (26%)	86,89,89	2.29	26 (30%)
13	BGL	L	1015	-	20,20,20	1.06	2 (10%)	24,25,25	1.09	2 (8%)
9	BCL	E	102	-	64,74,74	1.72	14 (21%)	78,115,115	2.42	21 (26%)
10	U42	U	101	-	69,69,69	2.02	16 (23%)	86,89,89	2.22	22 (25%)
9	BCL	K	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.13	21 (26%)
9	BCL	S	103	-	64,74,74	1.68	14 (21%)	78,115,115	2.48	26 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	U42	B	101	-	69,69,69	2.11	20 (28%)	86,89,89	2.13	21 (24%)
19	MQE	M	704	-	69,69,69	0.33	0	84,87,87	0.74	2 (2%)
14	HEC	C	402	3	32,50,50	2.17	3 (9%)	24,82,82	1.43	3 (12%)
9	BCL	5	101	-	64,74,74	1.69	11 (17%)	78,115,115	2.25	23 (29%)
11	U4Z	H	102	-	40,40,40	1.81	9 (22%)	50,51,51	1.69	12 (24%)
10	U42	8	101	-	69,69,69	2.13	13 (18%)	86,89,89	2.31	21 (24%)
13	BGL	D	104	-	20,20,20	1.03	1 (5%)	24,25,25	0.78	0
16	PGV	L	1008	-	50,50,50	0.49	0	53,56,56	0.45	0
9	BCL	W	102	-	64,74,74	1.67	13 (20%)	78,115,115	2.43	21 (26%)
9	BCL	F	101	-	64,74,74	1.68	11 (17%)	78,115,115	2.25	23 (29%)
9	BCL	V	101	-	64,74,74	1.65	12 (18%)	78,115,115	2.09	21 (26%)
11	U4Z	J	102	-	40,40,40	1.83	9 (22%)	50,51,51	1.74	13 (26%)
9	BCL	J	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.32	22 (28%)
9	BCL	8	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.05	20 (25%)
9	BCL	4	103	-	64,74,74	1.71	14 (21%)	78,115,115	2.56	26 (33%)
10	U42	E	101	-	69,69,69	2.28	19 (27%)	86,89,89	1.90	20 (23%)
10	U42	G	101	-	69,69,69	2.02	25 (36%)	86,89,89	2.29	13 (15%)
9	BCL	I	103	-	64,74,74	1.70	14 (21%)	78,115,115	2.41	21 (26%)
13	BGL	H	103	-	20,20,20	1.00	1 (5%)	24,25,25	0.80	0
11	U4Z	3	102	-	40,40,40	1.80	9 (22%)	50,51,51	1.71	13 (26%)
11	U4Z	C	401	-	40,40,40	1.76	12 (30%)	50,51,51	2.31	17 (34%)
10	U42	I	104	-	69,69,69	2.05	20 (28%)	86,89,89	2.29	20 (23%)
19	MQE	L	1004	-	54,54,69	0.38	0	66,69,87	0.81	3 (4%)
13	BGL	N	103	-	20,20,20	1.00	1 (5%)	24,25,25	0.86	0
11	U4Z	N	102	-	40,40,40	1.86	9 (22%)	50,51,51	1.72	12 (24%)
20	PEF	L	1017	-	40,40,46	1.03	2 (5%)	43,45,51	1.06	2 (4%)
9	BCL	L	1001	-	64,74,74	1.70	13 (20%)	78,115,115	2.36	20 (25%)
11	U4Z	9	101	-	40,40,40	1.80	9 (22%)	50,51,51	1.71	13 (26%)
9	BCL	6	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.44	19 (24%)
9	BCL	6	101	-	64,74,74	1.70	13 (20%)	78,115,115	2.14	21 (26%)
9	BCL	H	101	-	64,74,74	1.67	12 (18%)	78,115,115	2.39	22 (28%)
16	PGV	M	705	-	50,50,50	0.49	0	53,56,56	0.48	0
16	PGV	L	1006	-	50,50,50	0.51	0	53,56,56	0.44	0
9	BCL	3	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.22	22 (28%)

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
10	U42	0	103	-	-	13/61/98/98	0/2/2/2
16	PGV	P	104	-	-	21/55/55/55	-
18	BPH	M	702	-	-	18/37/105/105	0/5/6/6
9	BCL	W	101	-	-	15/37/137/137	-
9	BCL	K	102	-	-	14/37/137/137	-
11	U4Z	P	102	-	-	4/36/53/53	0/1/1/1
12	LMT	T	103	-	-	11/21/61/61	0/2/2/2
9	BCL	Q	102	-	-	12/37/137/137	-
11	U4Z	5	102	-	-	4/36/53/53	0/1/1/1
11	U4Z	1	102	-	-	4/36/53/53	0/1/1/1
11	U4Z	S	104	-	-	3/36/53/53	0/1/1/1
9	BCL	M	701	-	-	24/37/137/137	-
9	BCL	F	102	-	-	19/37/137/137	-
9	BCL	G	102	-	-	22/37/137/137	-
9	BCL	A	101	-	-	12/37/137/137	-
10	U42	I	101	-	-	19/61/98/98	0/2/2/2
13	BGL	L	1012	-	-	4/11/31/31	0/1/1/1
13	BGL	L	1011	-	-	4/11/31/31	0/1/1/1
9	BCL	8	103	-	-	18/37/137/137	-
9	BCL	T	101	-	-	12/37/137/137	-
14	HEC	C	405	3	-	0/10/54/54	-
18	BPH	L	1003	-	-	12/37/105/105	0/5/6/6
11	U4Z	7	102	-	-	2/36/53/53	0/1/1/1
9	BCL	D	102	-	-	18/37/137/137	-
9	BCL	I	102	-	-	13/37/137/137	-
10	U42	Q	101	-	-	18/61/98/98	0/2/2/2
11	U4Z	A	102	-	-	4/36/53/53	0/1/1/1
10	U42	S	101	-	-	23/61/98/98	0/2/2/2
11	U4Z	D	103	-	-	4/36/53/53	0/1/1/1
9	BCL	N	101	-	-	20/37/137/137	-
9	BCL	B	102	-	-	9/37/137/137	-
13	BGL	C	409	-	-	3/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	0	101	-	-	11/37/137/137	-
16	PGV	M	706	-	-	21/55/55/55	-
9	BCL	7	101	-	-	19/37/137/137	-
10	U42	O	101	-	-	23/61/98/98	0/2/2/2
16	PGV	P	103	-	-	17/47/47/55	-
10	U42	4	101	-	-	12/61/98/98	0/2/2/2
18	BPH	L	1005	-	-	18/37/105/105	0/5/6/6
9	BCL	S	102	-	-	17/37/137/137	-
16	PGV	C	408	15	-	25/55/55/55	-
9	BCL	R	101	-	-	17/37/137/137	-
9	BCL	4	102	-	-	13/37/137/137	-
13	BGL	F	104	-	-	4/11/31/31	0/1/1/1
13	BGL	L	1013	-	-	4/11/31/31	0/1/1/1
10	U42	U	104	-	-	24/61/98/98	0/2/2/2
9	BCL	B	103	-	-	22/37/137/137	-
11	U4Z	V	102	-	-	4/36/53/53	0/1/1/1
9	BCL	1	101	-	-	15/37/137/137	-
9	BCL	Q	103	-	-	19/37/137/137	-
13	BGL	Y	101	-	-	6/11/31/31	0/1/1/1
9	BCL	2	102	-	-	21/37/137/137	-
9	BCL	2	101	-	-	17/37/137/137	-
9	BCL	O	102	-	-	12/37/137/137	-
13	BGL	3	103	-	-	4/11/31/31	0/1/1/1
16	PGV	C	407	-	-	17/45/45/55	-
9	BCL	P	101	-	-	16/37/137/137	-
9	BCL	U	102	-	-	10/37/137/137	-
9	BCL	9	102	-	-	13/37/137/137	-
12	LMT	1	103	-	-	4/21/61/61	0/2/2/2
14	HEC	C	404	3	-	2/10/54/54	-
14	HEC	C	403	3	-	0/10/54/54	-
16	PGV	L	1007	-	-	19/55/55/55	-
13	BGL	C	410	-	-	3/11/31/31	0/1/1/1
11	U4Z	T	102	-	-	4/36/53/53	0/1/1/1
22	LHG	h	101	-	-	11/14/14/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	D	101	-	-	15/37/137/137	-
9	BCL	O	103	-	-	16/37/137/137	-
12	LMT	D	105	-	-	4/21/61/61	0/2/2/2
9	BCL	U	103	-	-	21/37/137/137	-
11	U4Z	F	103	-	-	4/36/53/53	0/1/1/1
13	BGL	H	107	-	-	5/11/31/31	0/1/1/1
9	BCL	L	1002	-	-	12/37/137/137	-
9	BCL	0	102	-	-	14/37/137/137	-
10	U42	4	104	-	-	14/61/98/98	0/2/2/2
13	BGL	L	1015	-	-	8/11/31/31	0/1/1/1
9	BCL	E	102	-	-	22/37/137/137	-
10	U42	U	101	-	-	22/61/98/98	0/2/2/2
9	BCL	K	101	-	-	12/37/137/137	-
9	BCL	S	103	-	-	24/37/137/137	-
10	U42	B	101	-	-	15/61/98/98	0/2/2/2
19	MQE	M	704	-	-	7/65/85/85	0/2/2/2
14	HEC	C	402	3	-	5/10/54/54	-
9	BCL	5	101	-	-	15/37/137/137	-
11	U4Z	H	102	-	-	3/36/53/53	0/1/1/1
10	U42	8	101	-	-	14/61/98/98	0/2/2/2
13	BGL	D	104	-	-	2/11/31/31	0/1/1/1
16	PGV	L	1008	-	-	24/55/55/55	-
9	BCL	W	102	-	-	18/37/137/137	-
9	BCL	F	101	-	-	19/37/137/137	-
9	BCL	V	101	-	-	16/37/137/137	-
11	U4Z	J	102	-	-	4/36/53/53	0/1/1/1
9	BCL	J	101	-	-	15/37/137/137	-
9	BCL	8	102	-	-	14/37/137/137	-
9	BCL	4	103	-	-	15/37/137/137	-
10	U42	E	101	-	-	23/61/98/98	0/2/2/2
10	U42	G	101	-	-	14/61/98/98	0/2/2/2
9	BCL	I	103	-	-	24/37/137/137	-
13	BGL	H	103	-	-	0/11/31/31	0/1/1/1
11	U4Z	3	102	-	-	4/36/53/53	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	U4Z	C	401	-	-	15/36/53/53	0/1/1/1
10	U42	I	104	-	-	12/61/98/98	0/2/2/2
19	MQE	L	1004	-	-	18/47/67/85	0/2/2/2
13	BGL	N	103	-	-	5/11/31/31	0/1/1/1
11	U4Z	N	102	-	-	2/36/53/53	0/1/1/1
20	PEF	L	1017	-	-	8/44/44/50	-
9	BCL	L	1001	-	-	15/37/137/137	-
11	U4Z	9	101	-	-	2/36/53/53	0/1/1/1
9	BCL	6	102	-	-	19/37/137/137	-
9	BCL	6	101	-	-	10/37/137/137	-
9	BCL	H	101	-	-	16/37/137/137	-
16	PGV	M	705	-	-	31/55/55/55	-
16	PGV	L	1006	-	-	22/55/55/55	-
9	BCL	3	101	-	-	17/37/137/137	-

The worst 5 of 1055 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	101	U42	CAV-CAR	8.55	1.47	1.35
10	E	101	U42	CAV-CAR	8.03	1.46	1.35
10	E	101	U42	CBI-CBL	7.82	1.46	1.35
10	0	103	U42	CBO-CBL	-7.73	1.34	1.50
10	O	101	U42	CBF-CBH	-7.15	1.30	1.45

The worst 5 of 1578 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	101	U42	CAL-CAM-CAO	12.51	138.14	118.94
10	I	101	U42	CAL-CAM-CAO	10.77	135.47	118.94
10	4	104	U42	CAL-CAM-CAO	10.53	135.10	118.94
10	8	101	U42	CAL-CAM-CAO	9.84	134.04	118.94
10	U	101	U42	CAL-CAM-CAO	9.38	133.33	118.94

There are no chirality outliers.

5 of 1459 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	102	BCL	C4C-C3C-CAC-CBC

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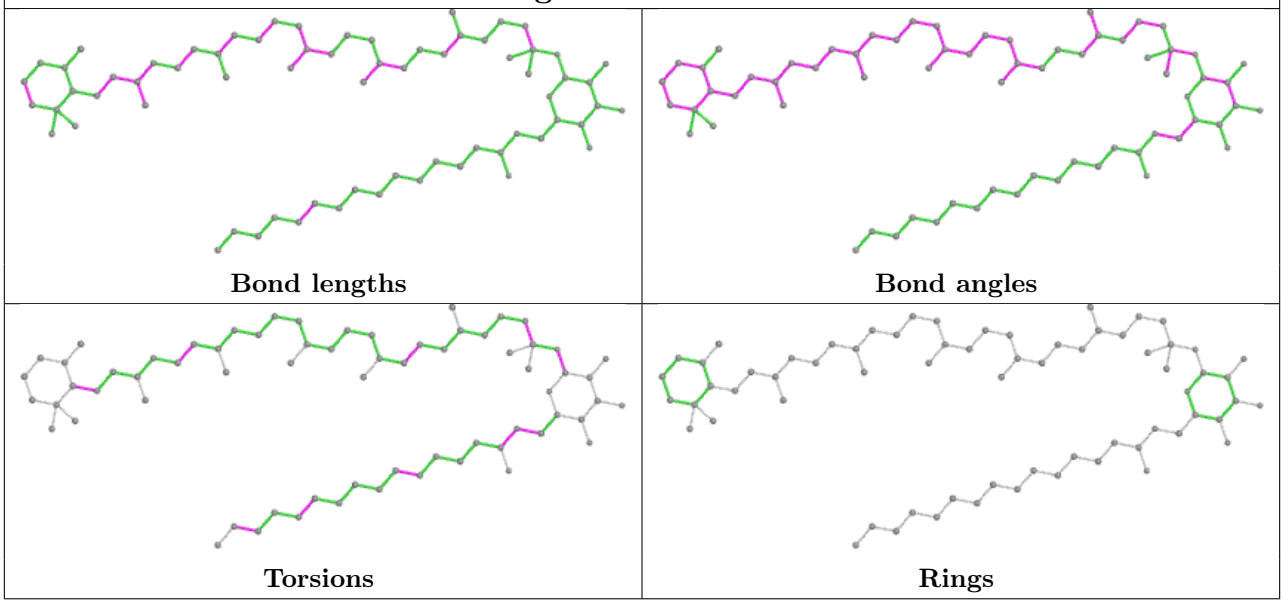
Mol	Chain	Res	Type	Atoms
9	1	101	BCL	C1A-C2A-CAA-CBA
9	1	101	BCL	C3A-C2A-CAA-CBA
9	1	101	BCL	C2C-C3C-CAC-CBC
9	1	101	BCL	C4C-C3C-CAC-CBC

There are no ring outliers.

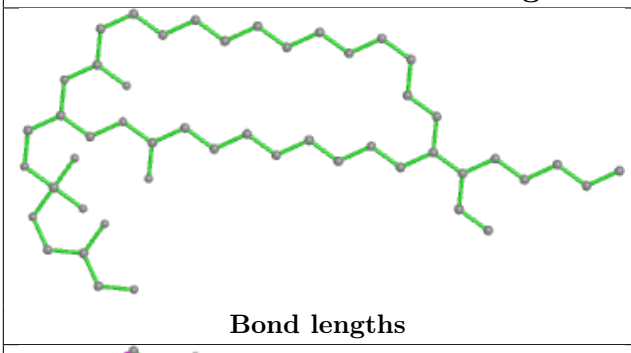
No monomer is involved in short contacts.

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

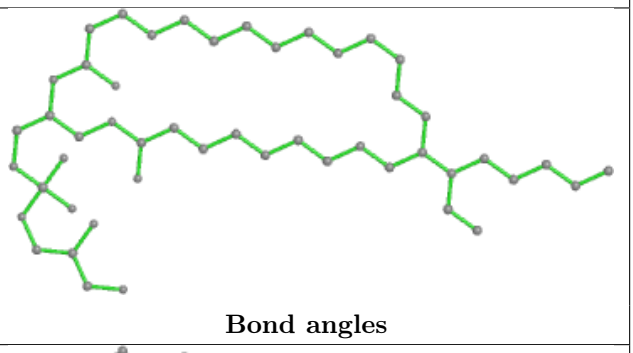
Ligand U42 0 103



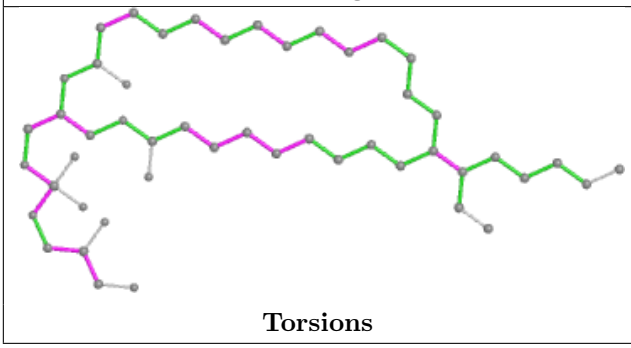
Ligand PGV P 104



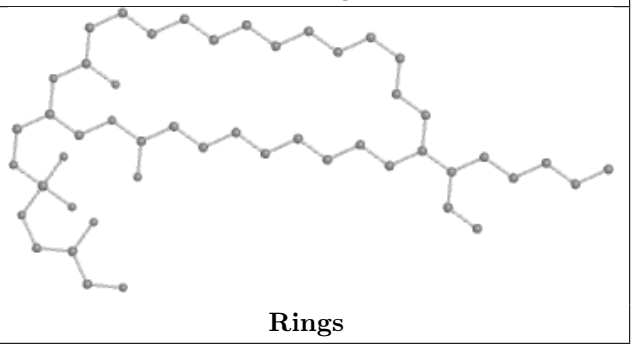
Bond lengths



Bond angles

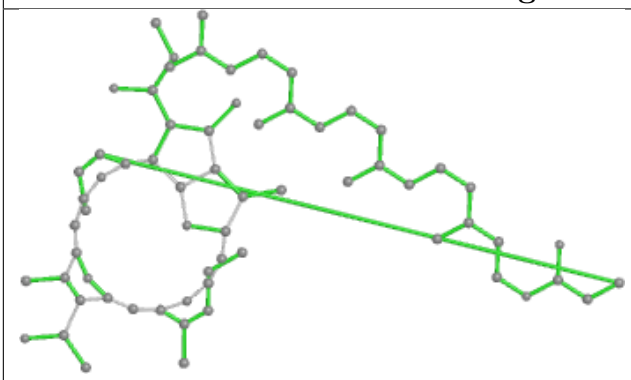


Torsions

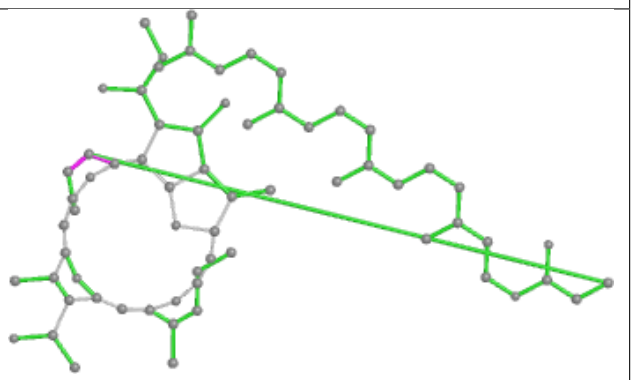


Rings

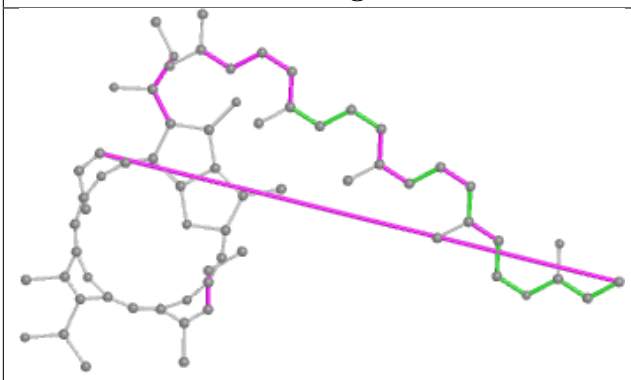
Ligand BPH M 702



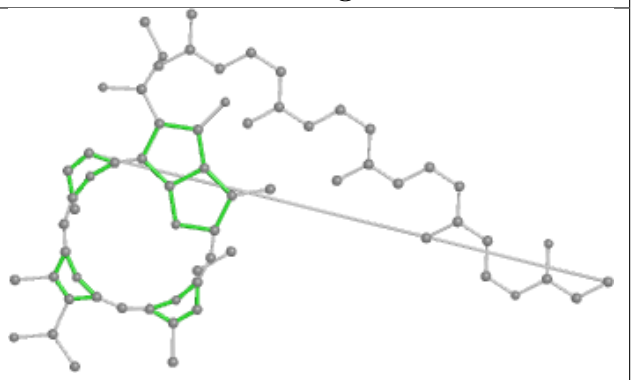
Bond lengths



Bond angles

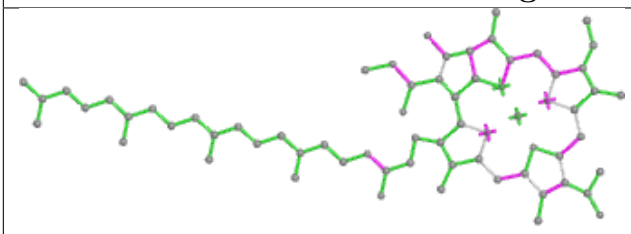


Torsions

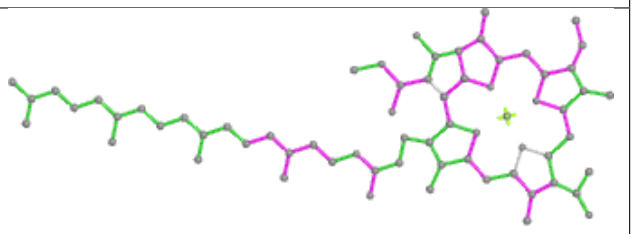


Rings

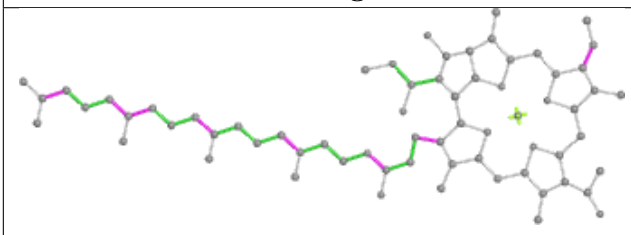
Ligand BCL W 101



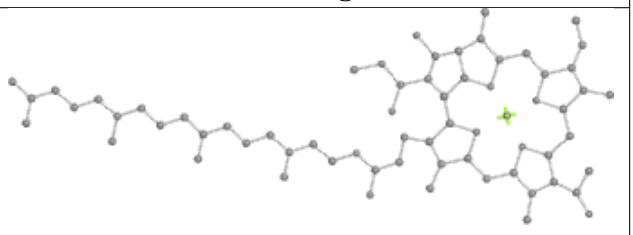
Bond lengths



Bond angles

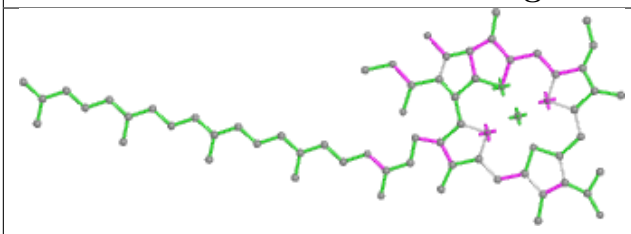


Torsions

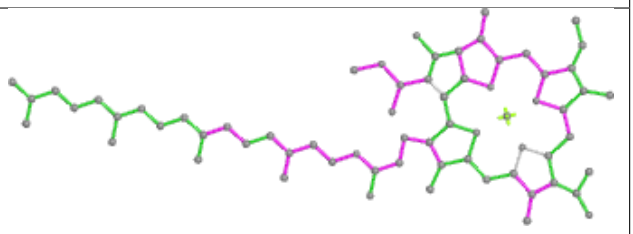


Rings

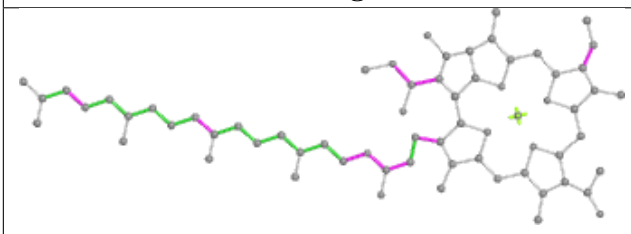
Ligand BCL K 102



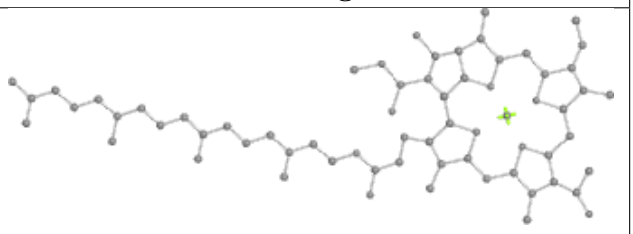
Bond lengths



Bond angles

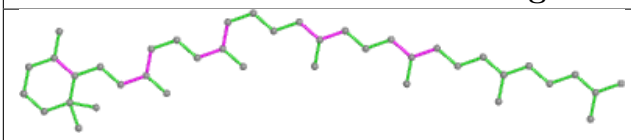


Torsions

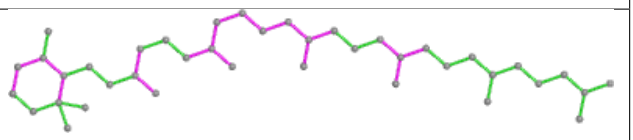


Rings

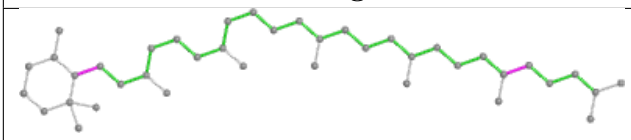
Ligand U4Z P 102



Bond lengths



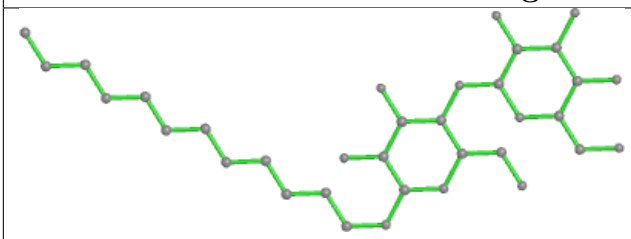
Bond angles



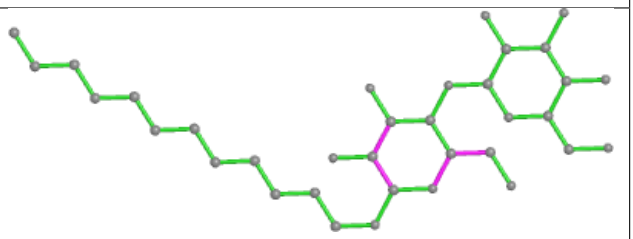
Torsions

Rings

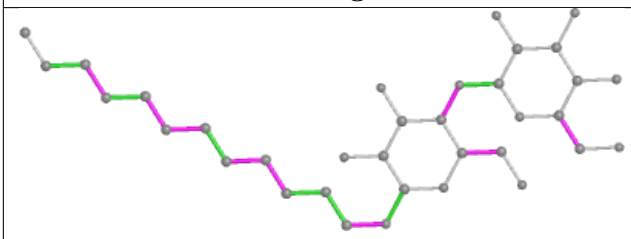
Ligand LMT T 103



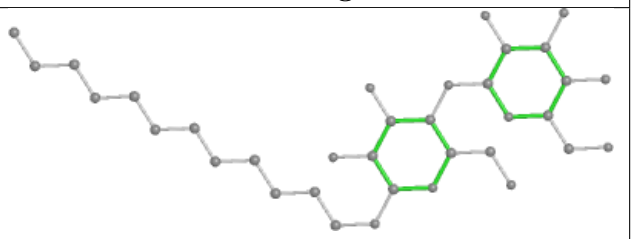
Bond lengths



Bond angles

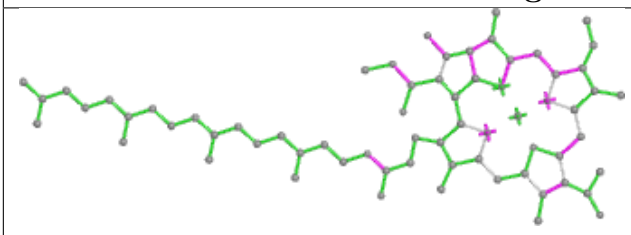


Torsions

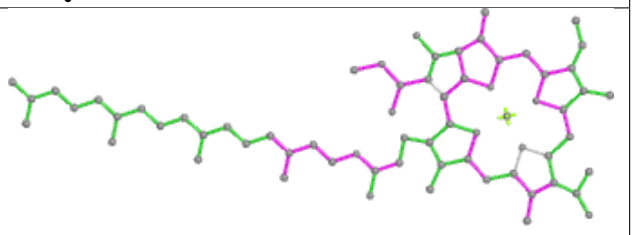


Rings

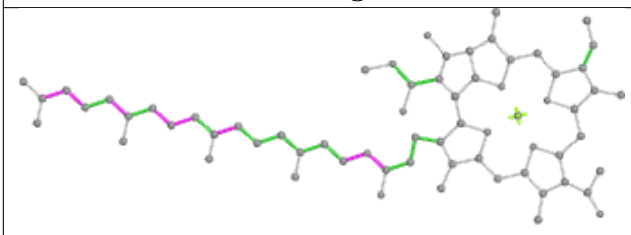
Ligand BCL Q 102



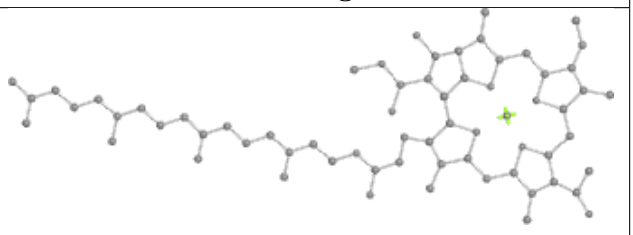
Bond lengths



Bond angles

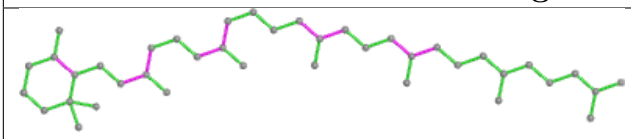


Torsions

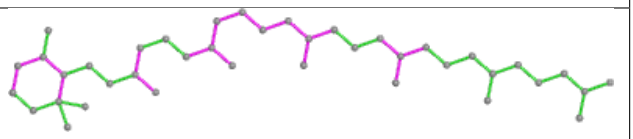


Rings

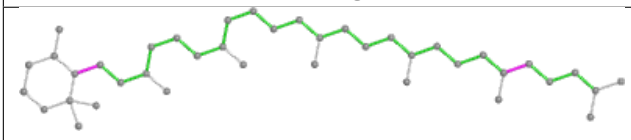
Ligand U4Z 5 102



Bond lengths



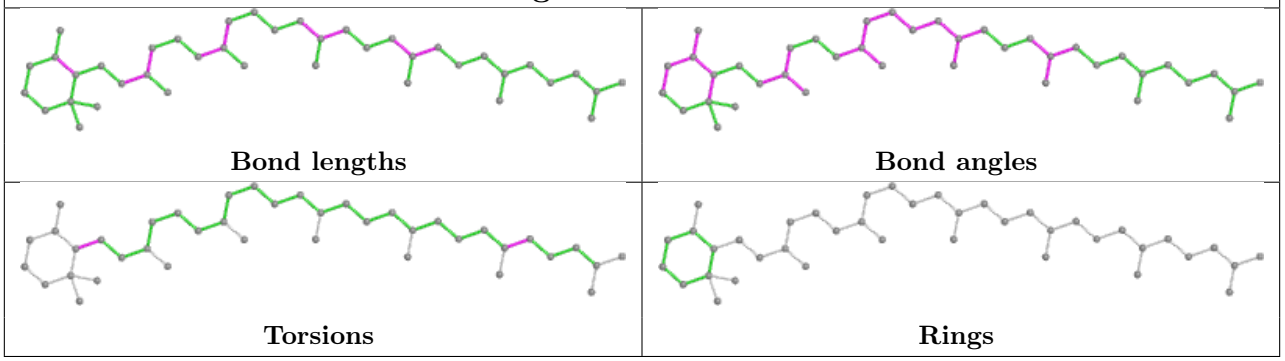
Bond angles



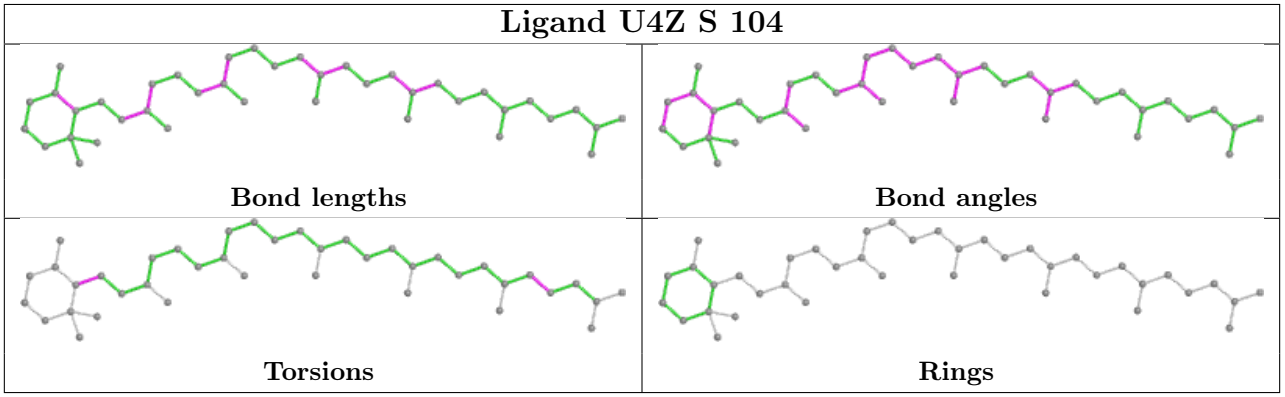
Torsions

Rings

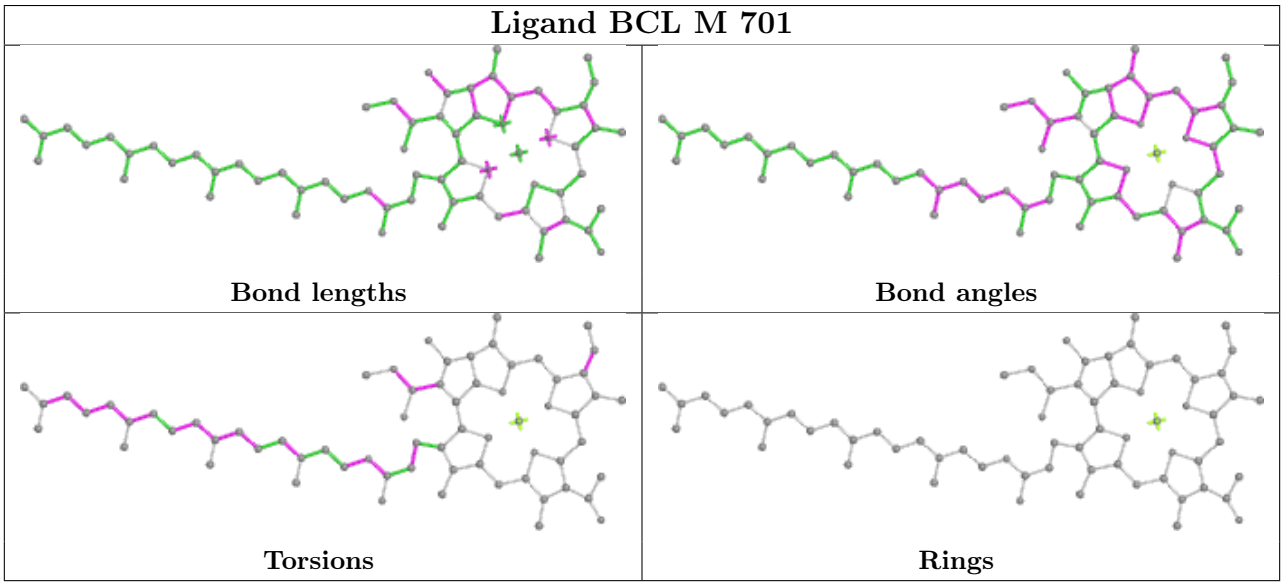
Ligand U4Z 1 102



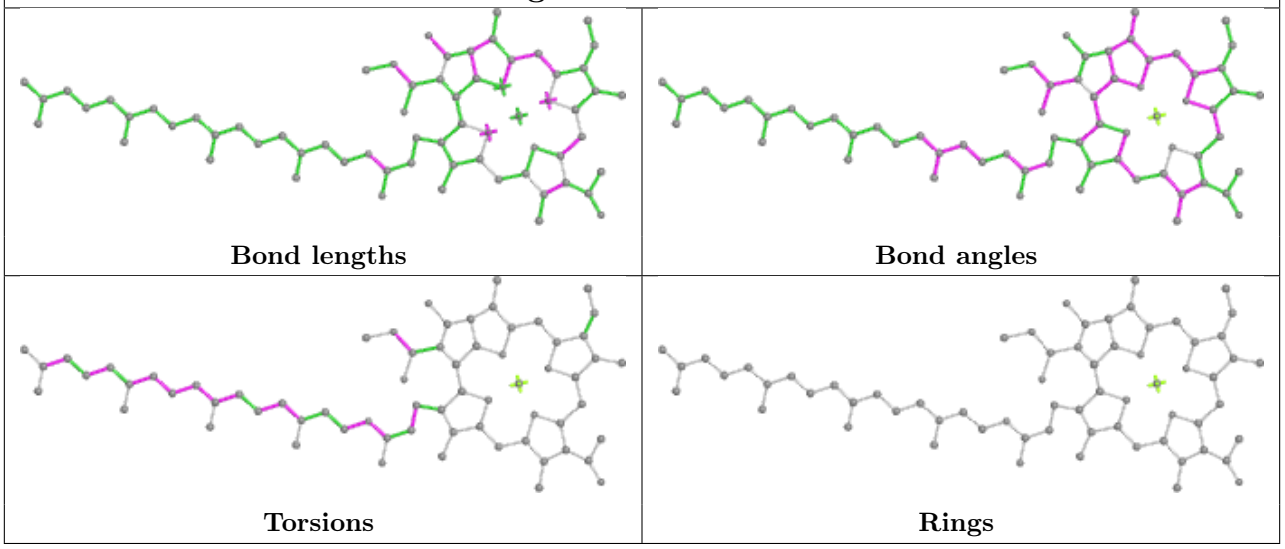
Ligand U4Z S 104



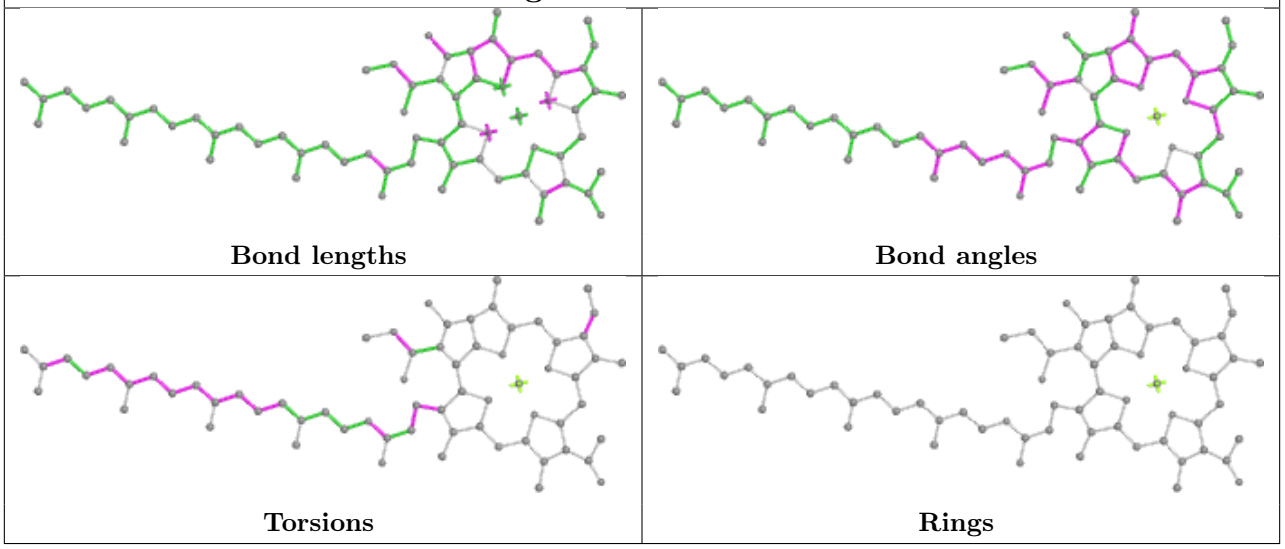
Ligand BCL M 701



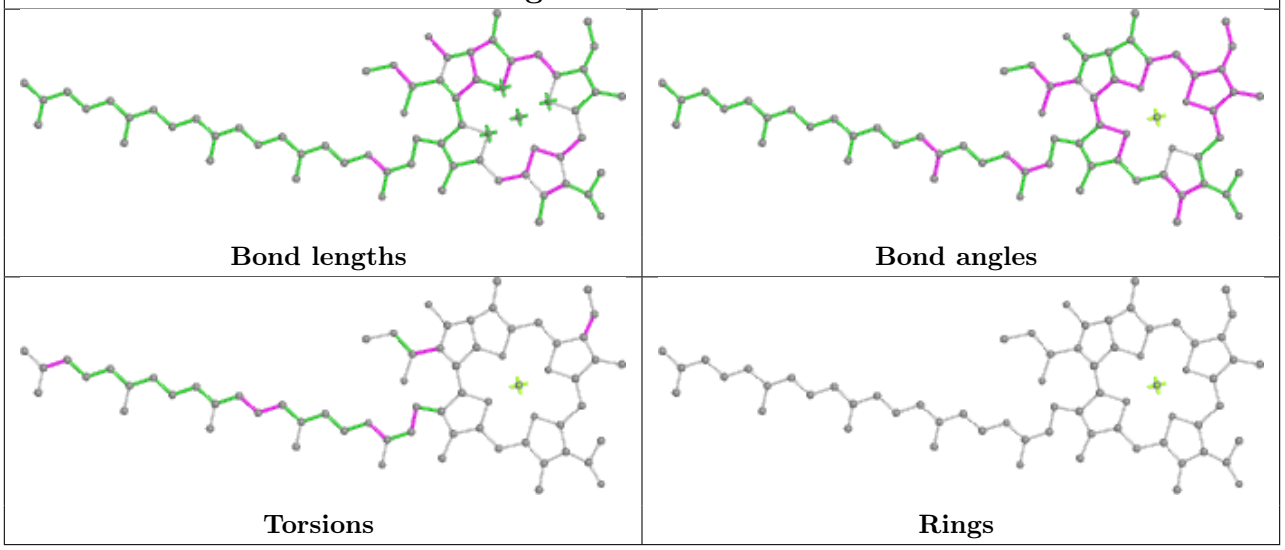
Ligand BCL F 102



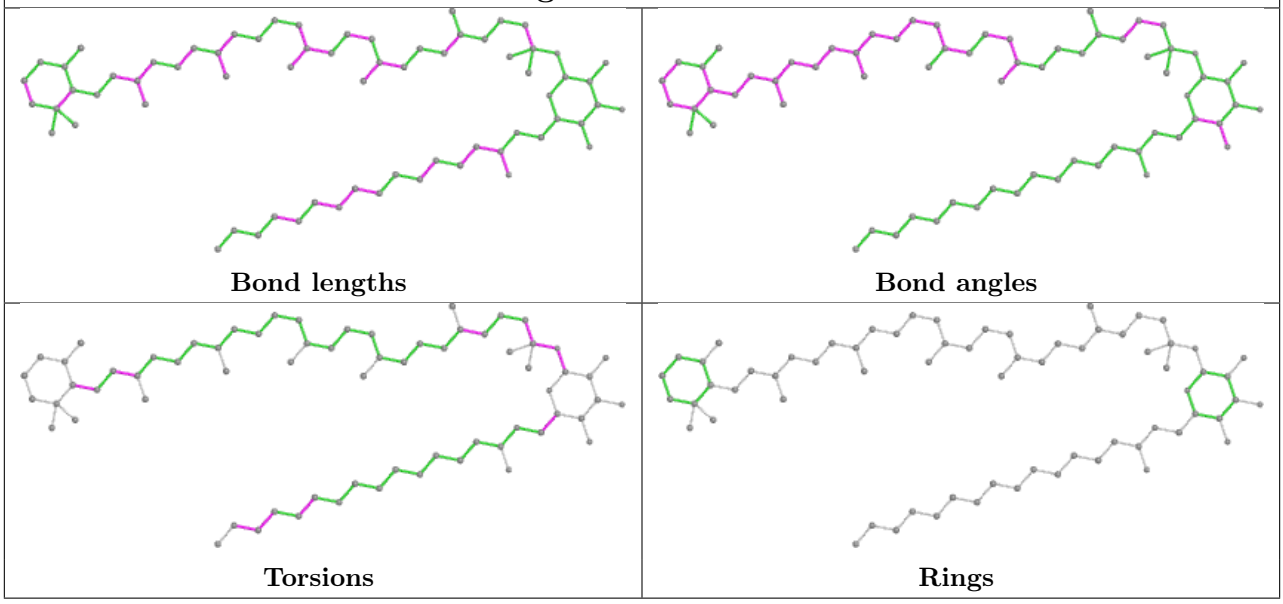
Ligand BCL G 102



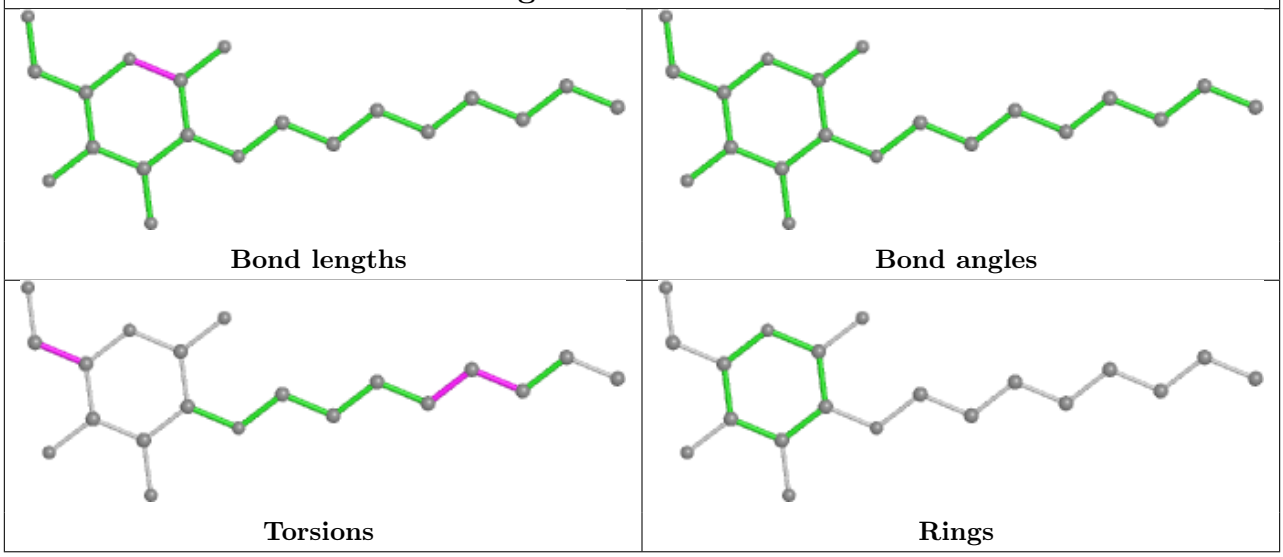
Ligand BCL A 101



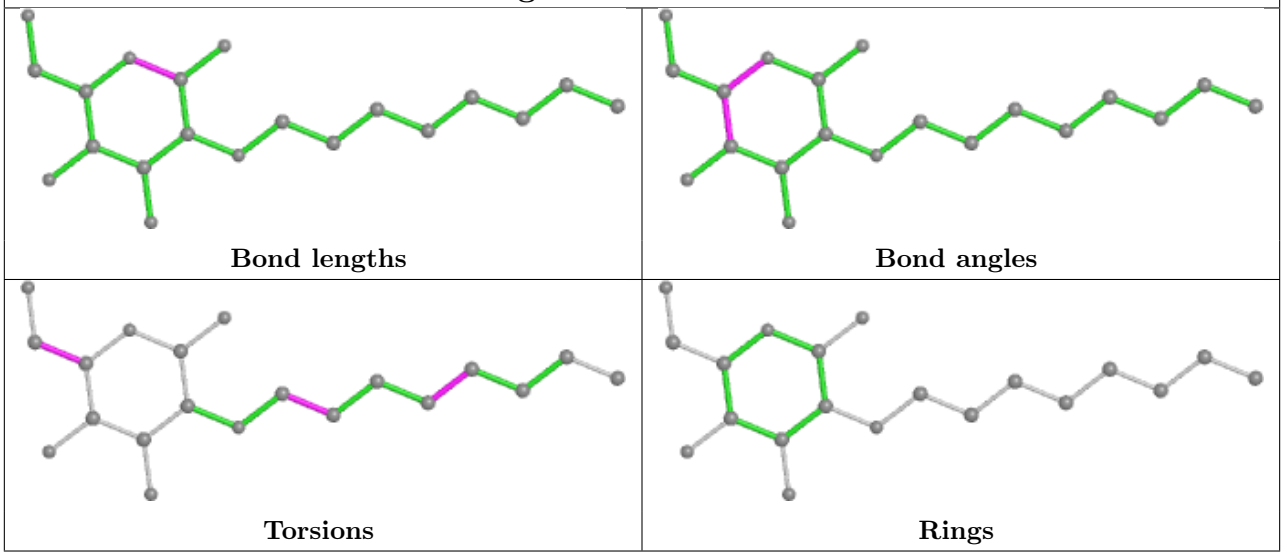
Ligand U42 I 101



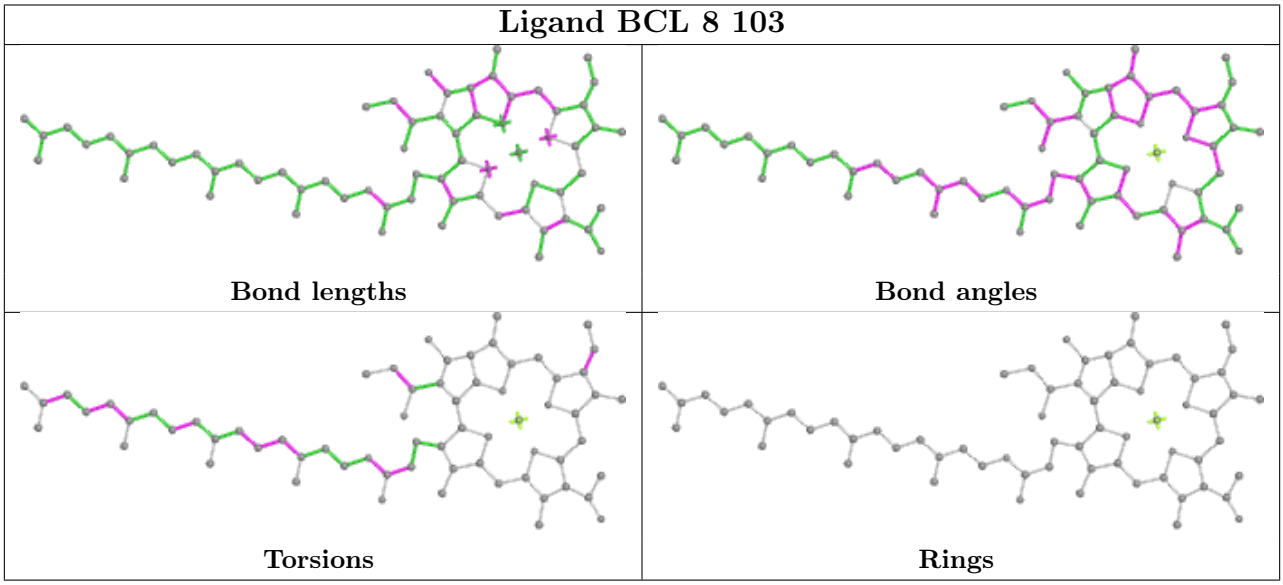
Ligand BGL L 1012



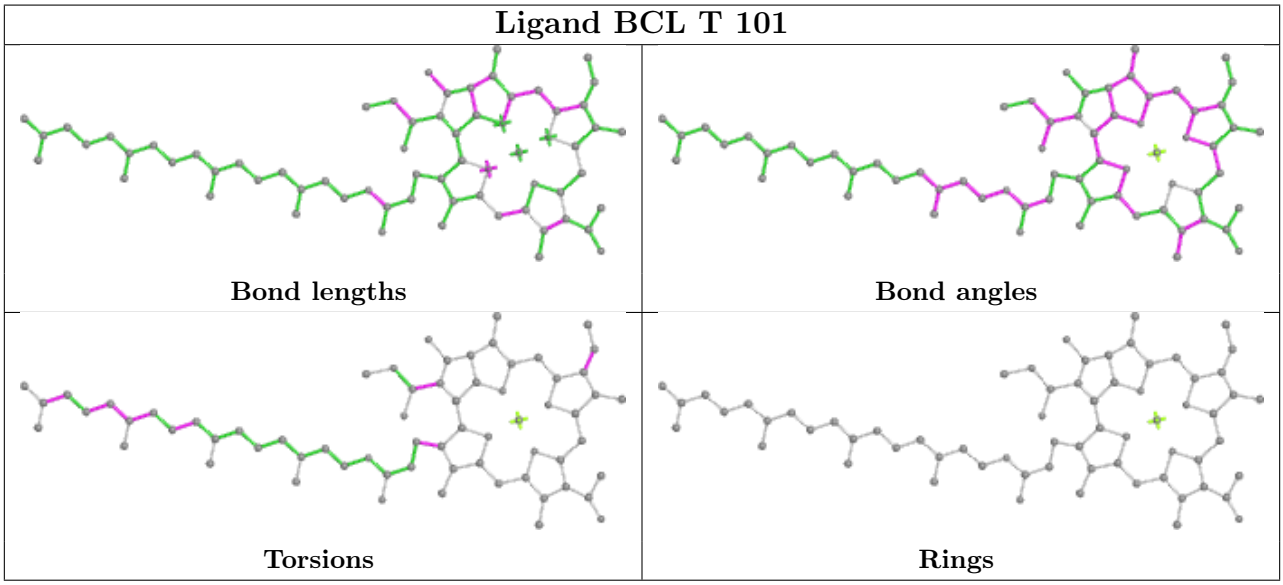
Ligand BGL L 1011



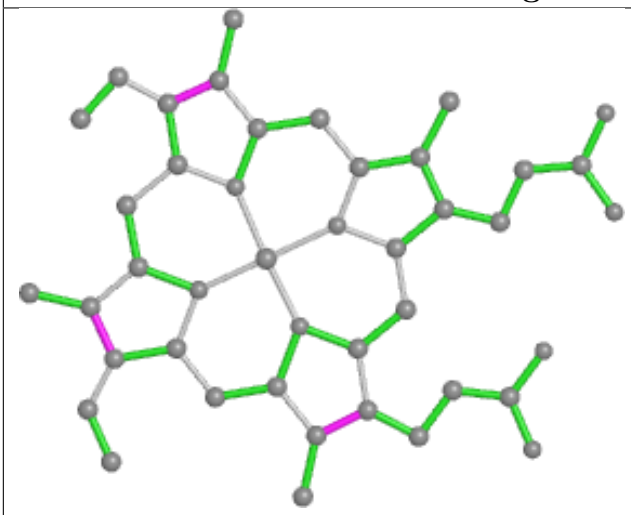
Ligand BCL 8 103



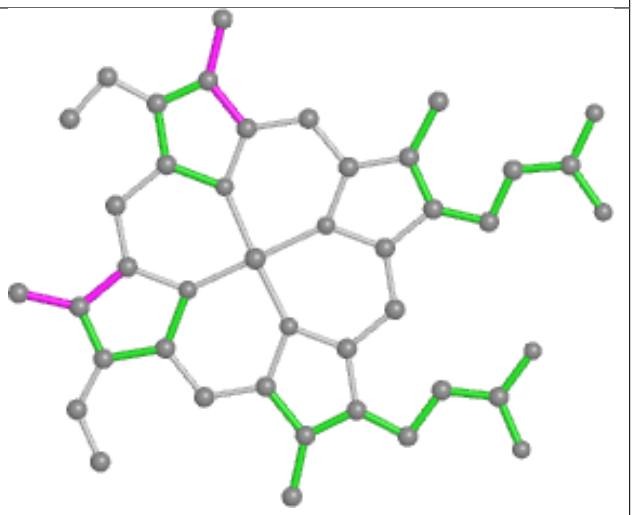
Ligand BCL T 101



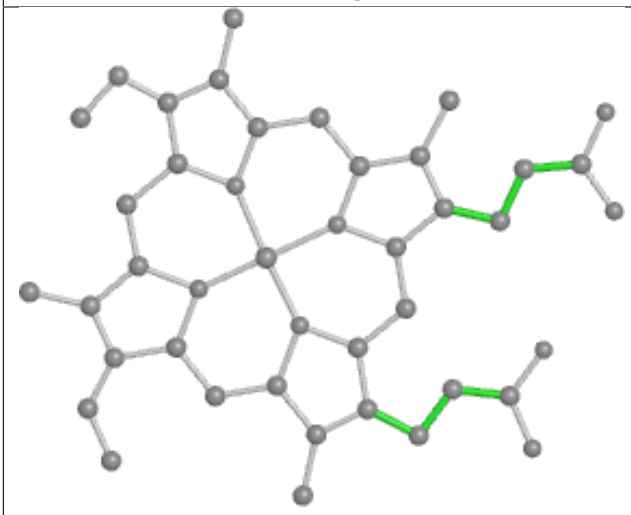
Ligand HEC C 405



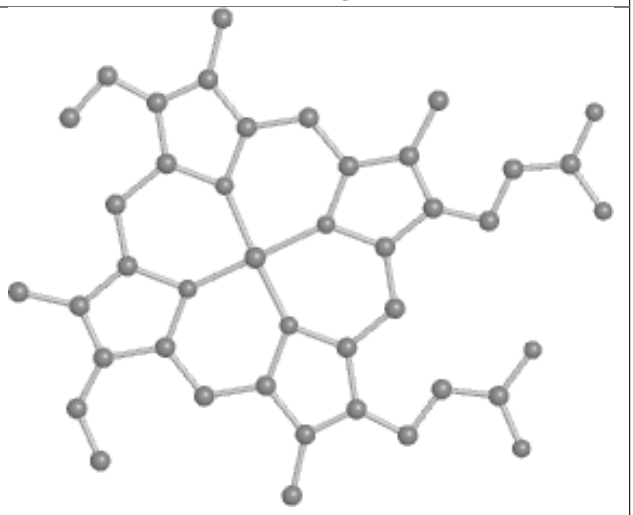
Bond lengths



Bond angles

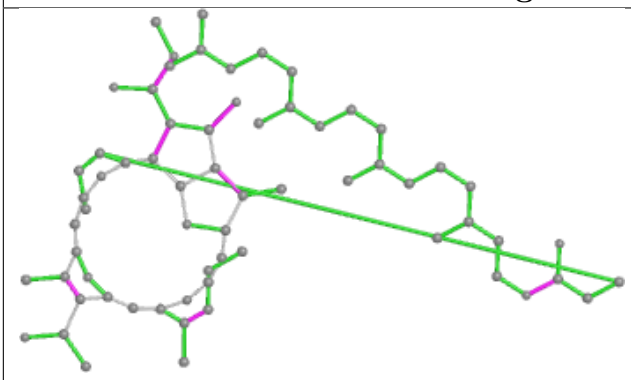


Torsions

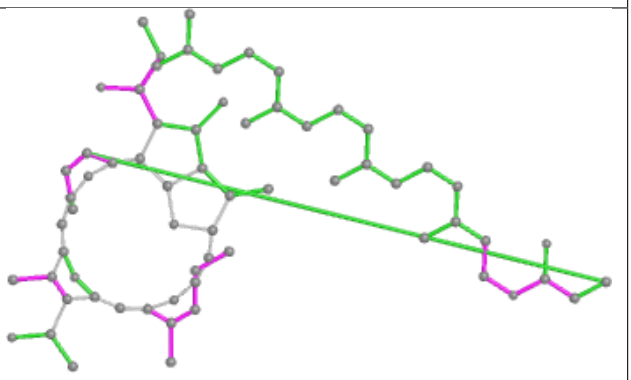


Rings

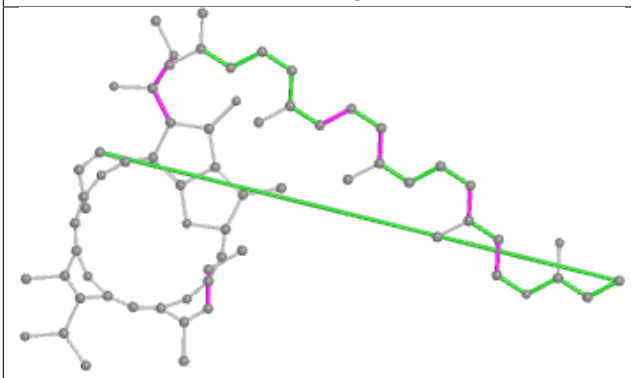
Ligand BPH L 1003



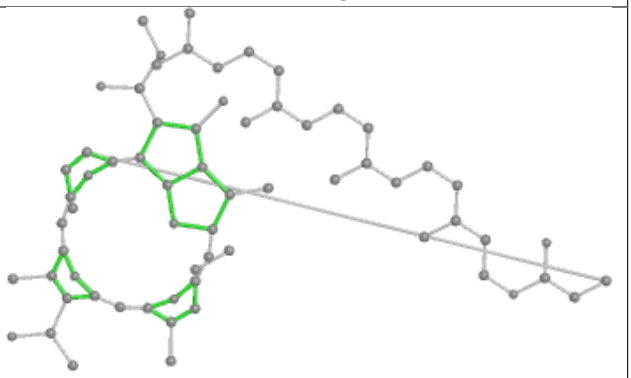
Bond lengths



Bond angles

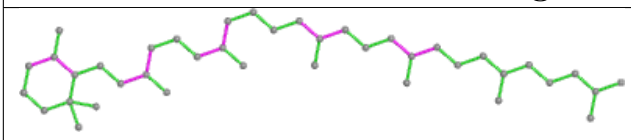


Torsions

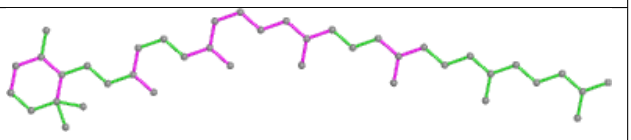


Rings

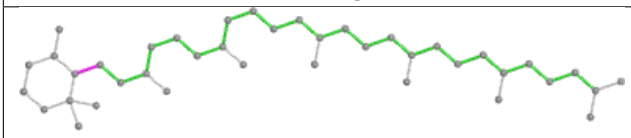
Ligand U4Z 7 102



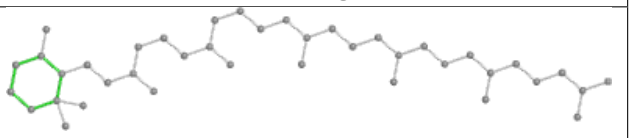
Bond lengths



Bond angles

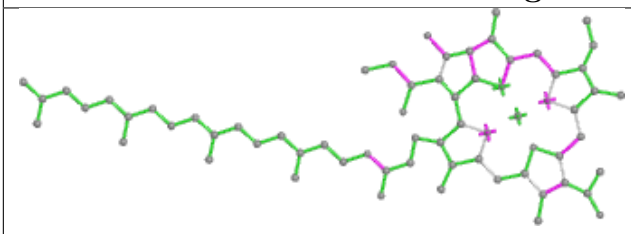


Torsions

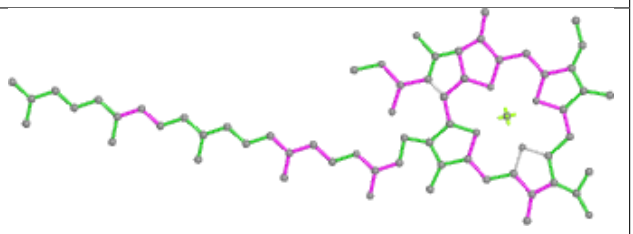


Rings

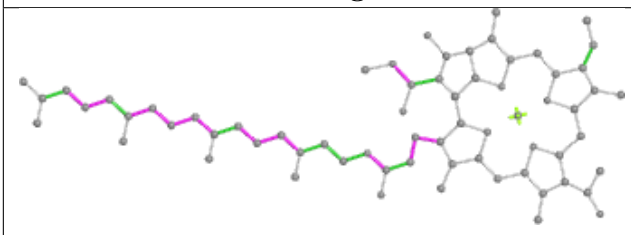
Ligand BCL D 102



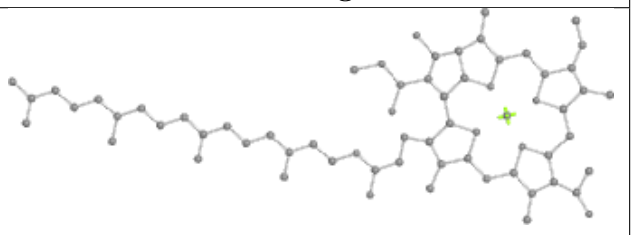
Bond lengths



Bond angles

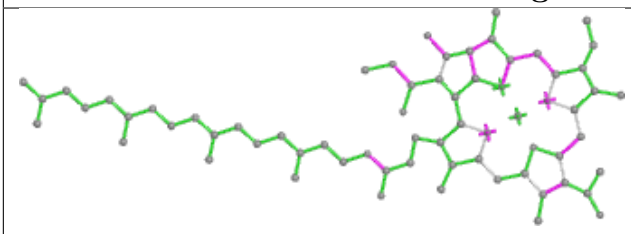


Torsions

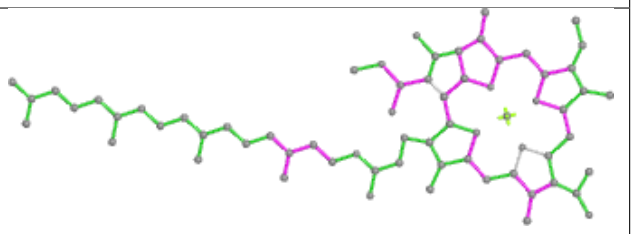


Rings

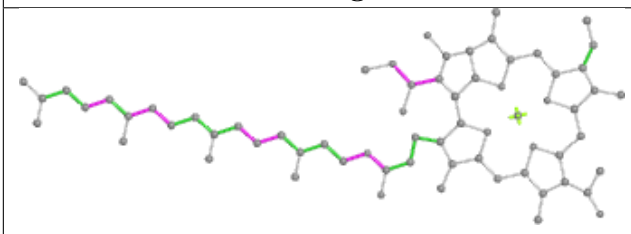
Ligand BCL I 102



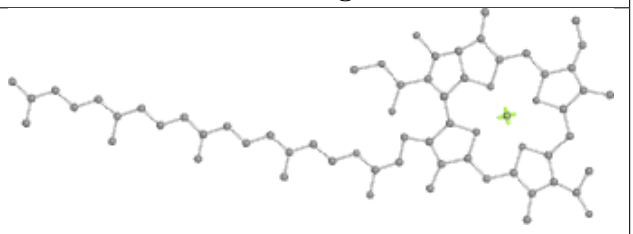
Bond lengths



Bond angles

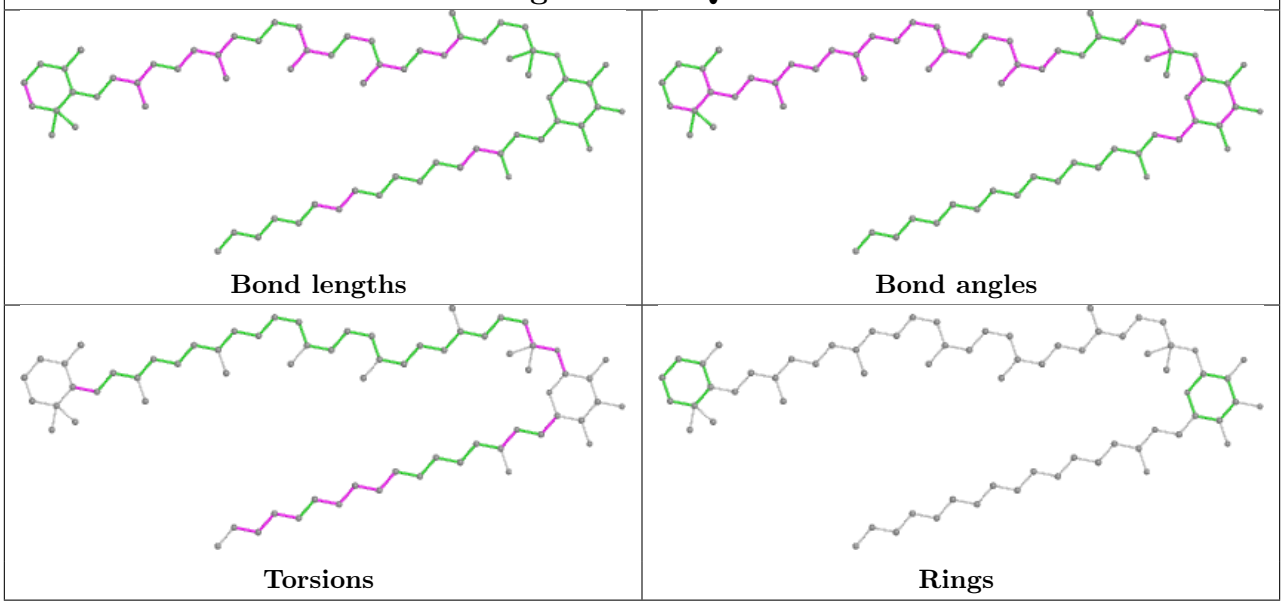


Torsions

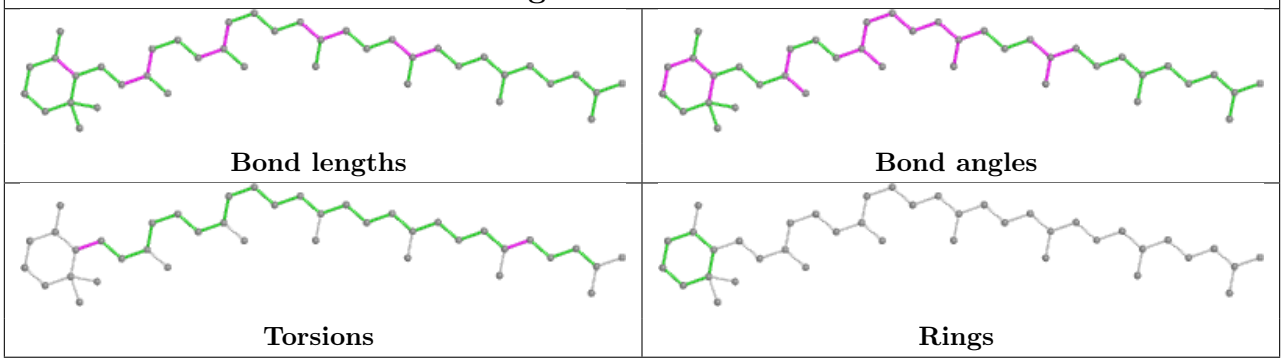


Rings

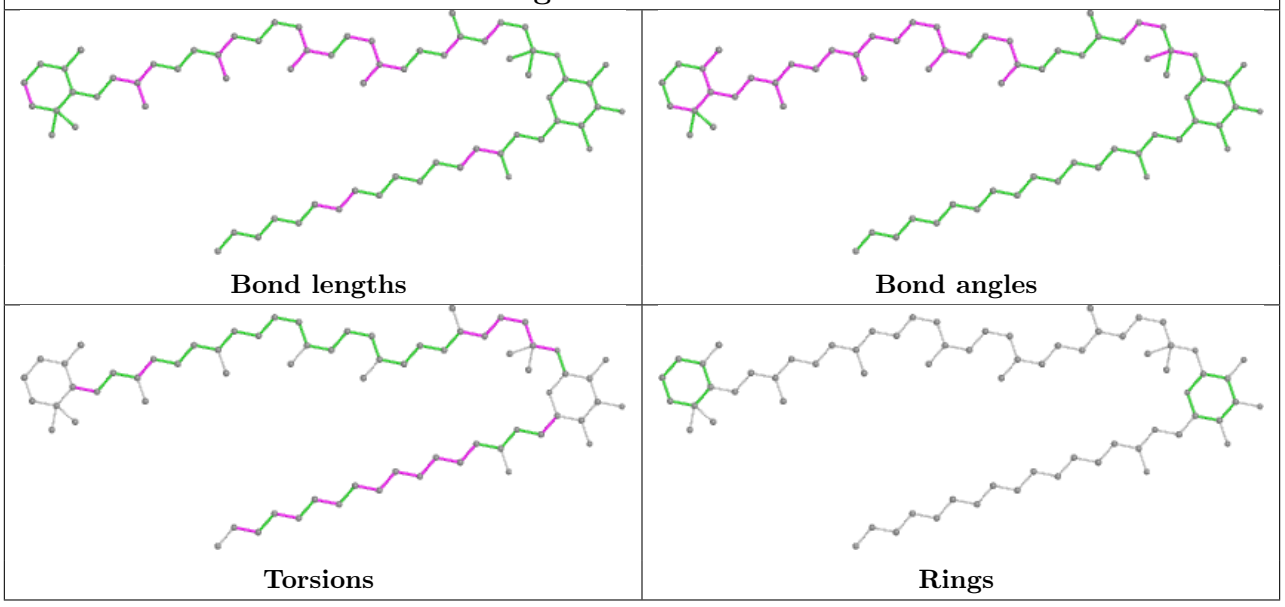
Ligand U42 Q 101



Ligand U4Z A 102

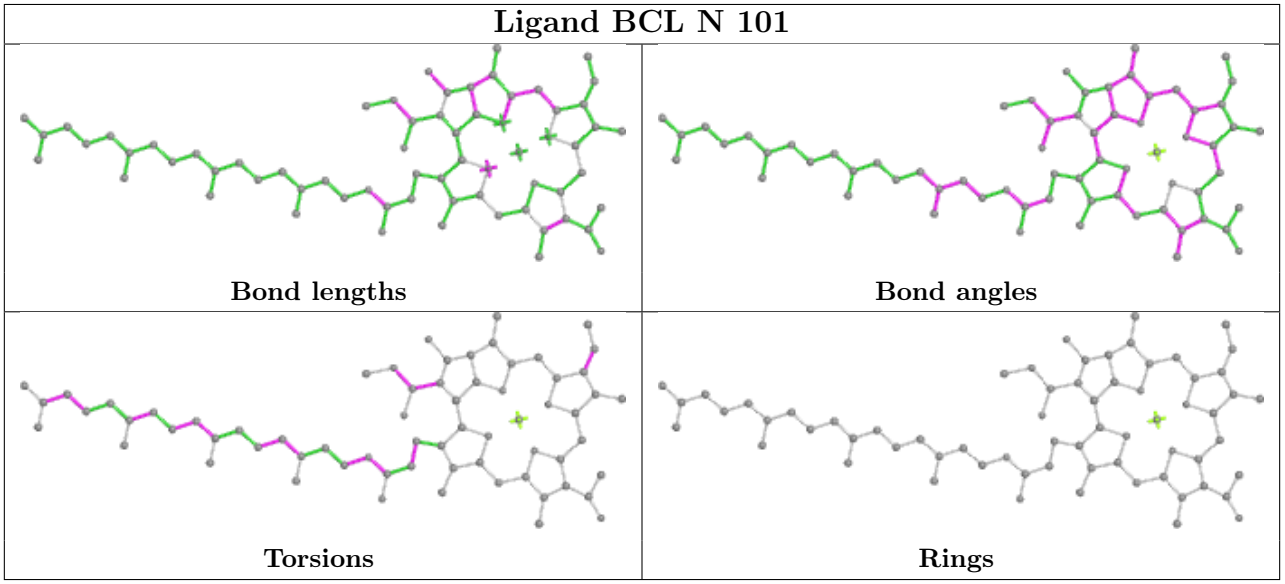


Ligand U42 S 101

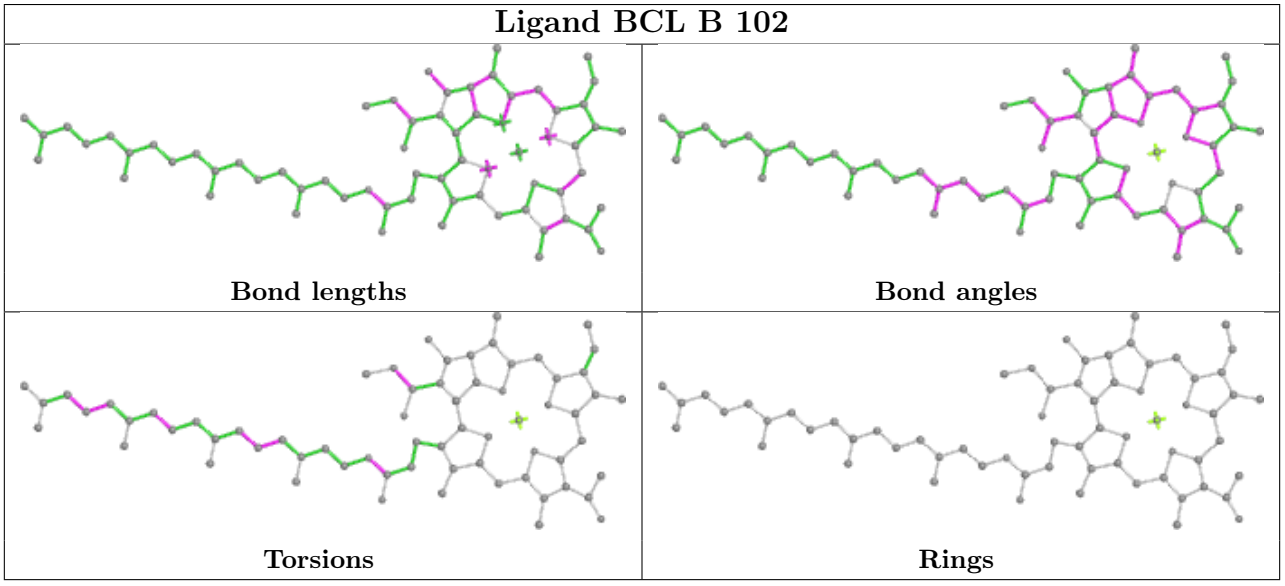


Ligand U4Z D 103

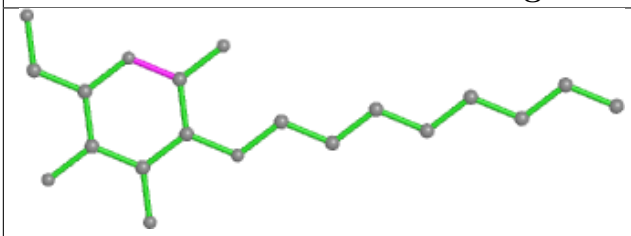
Ligand BCL N 101



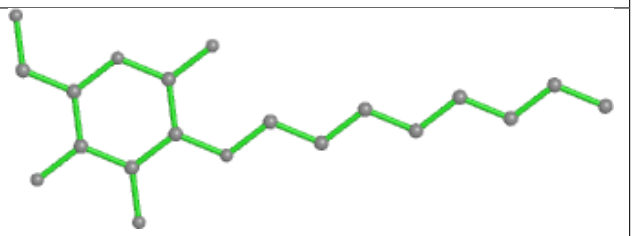
Ligand BCL B 102



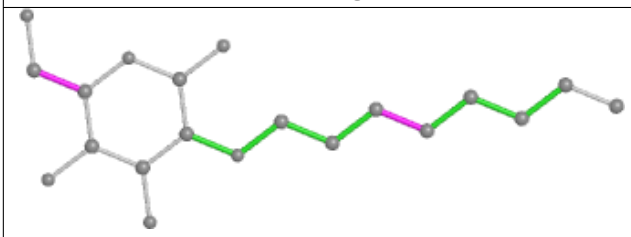
Ligand BGL C 409



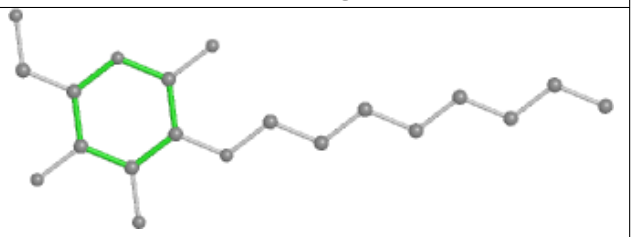
Bond lengths



Bond angles

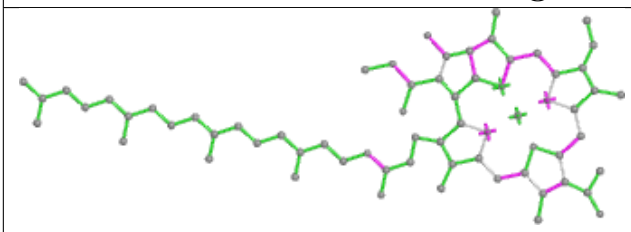


Torsions

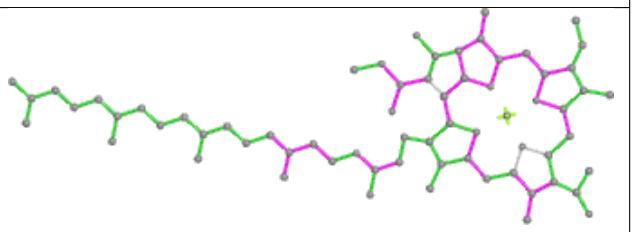


Rings

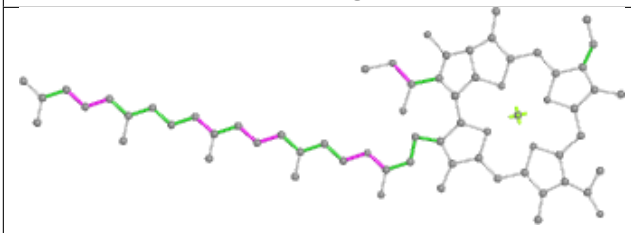
Ligand BCL 0 101



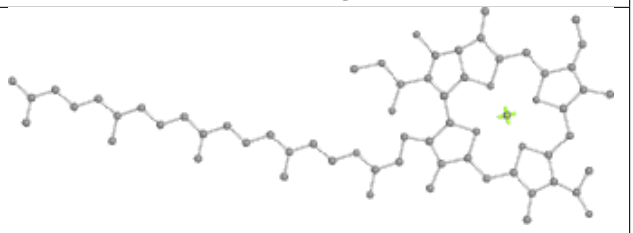
Bond lengths



Bond angles

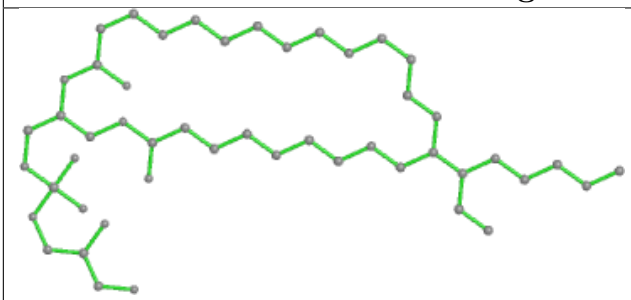


Torsions

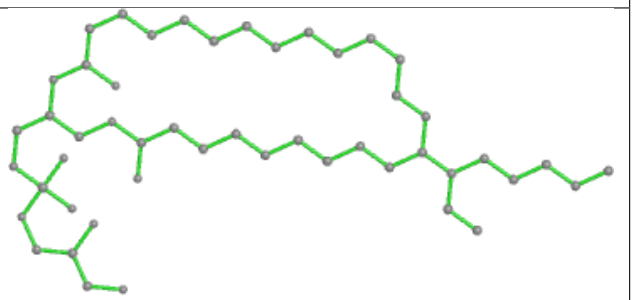


Rings

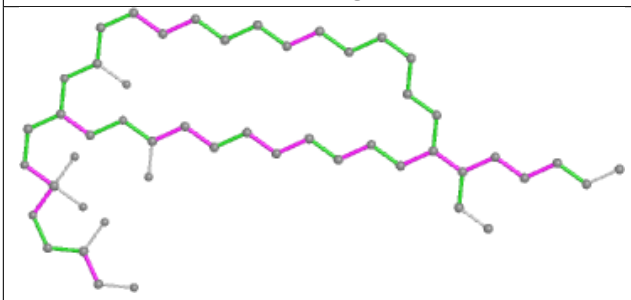
Ligand PGV M 706



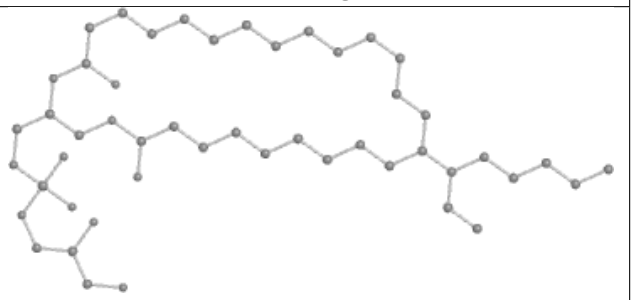
Bond lengths



Bond angles

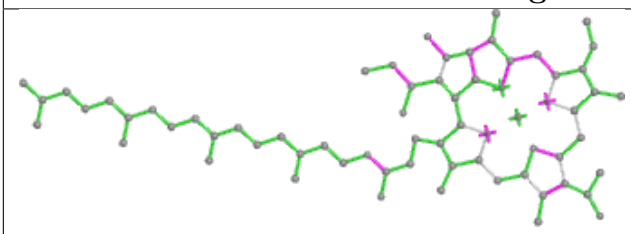


Torsions

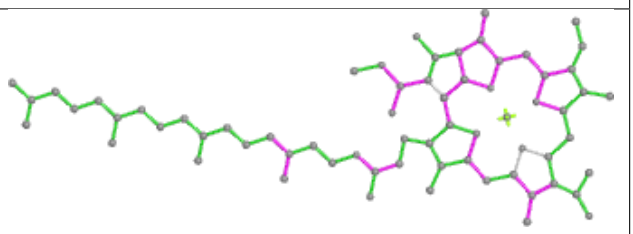


Rings

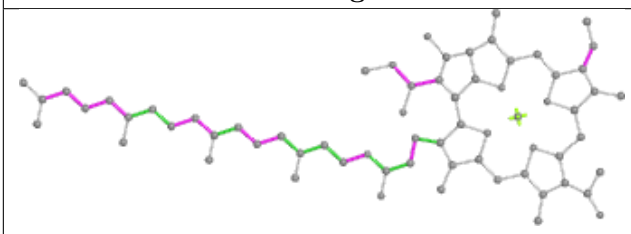
Ligand BCL 7 101



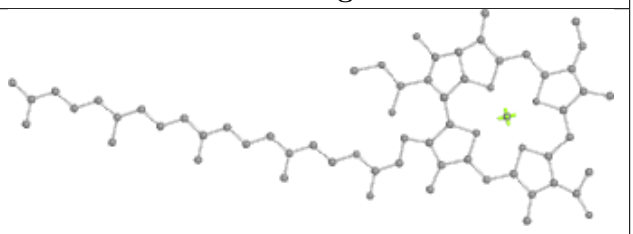
Bond lengths



Bond angles

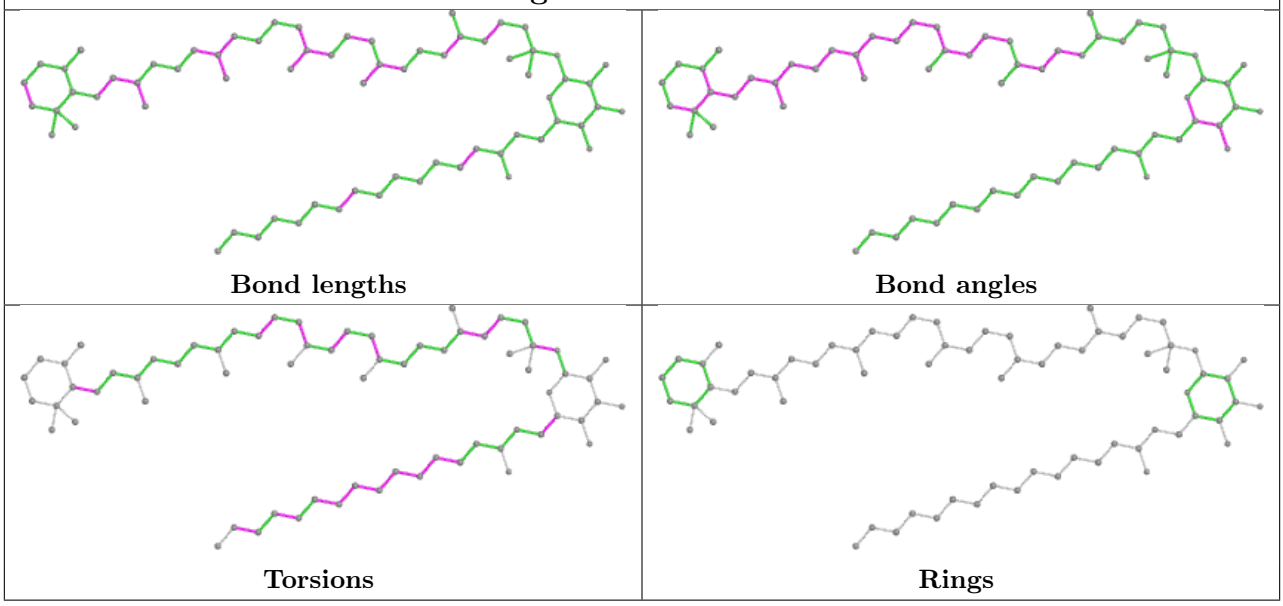


Torsions

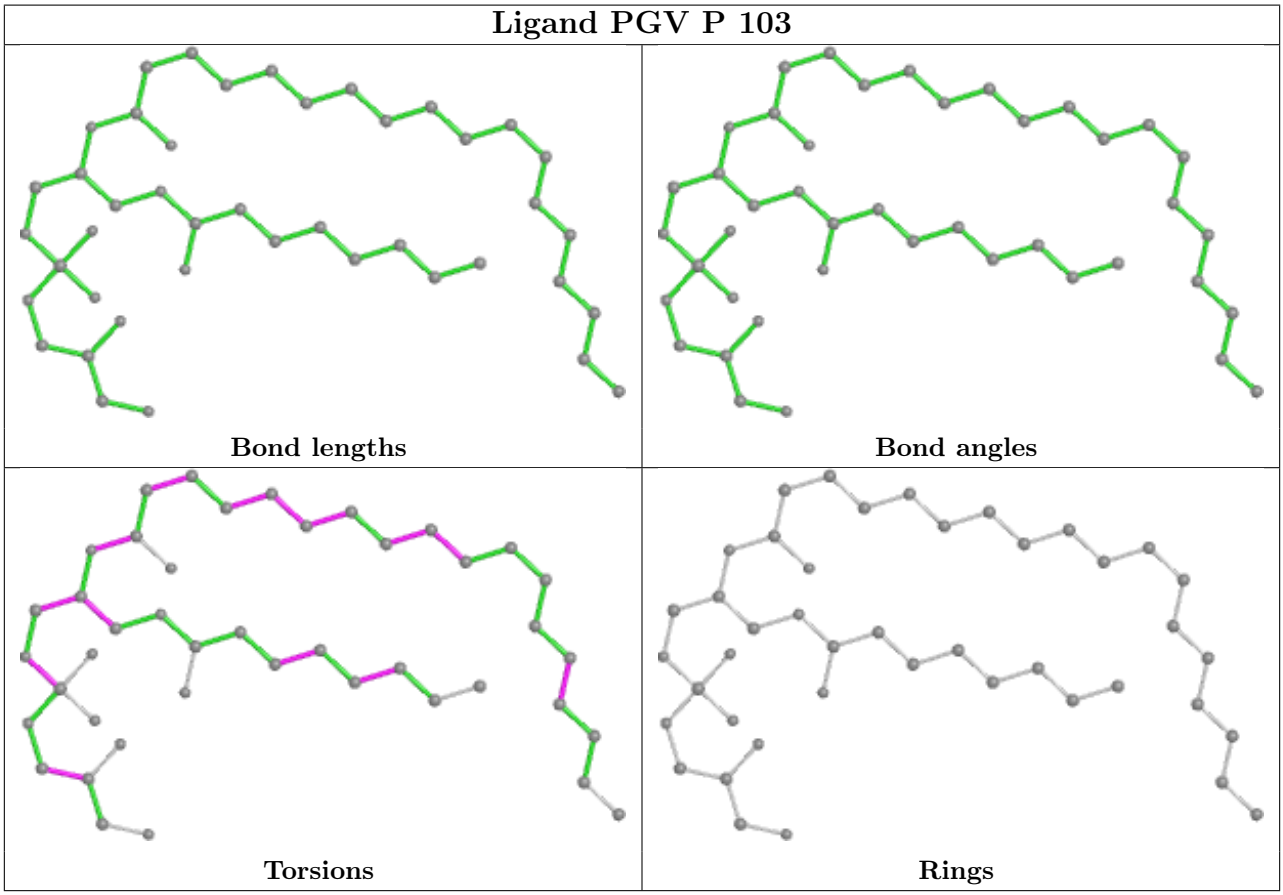


Rings

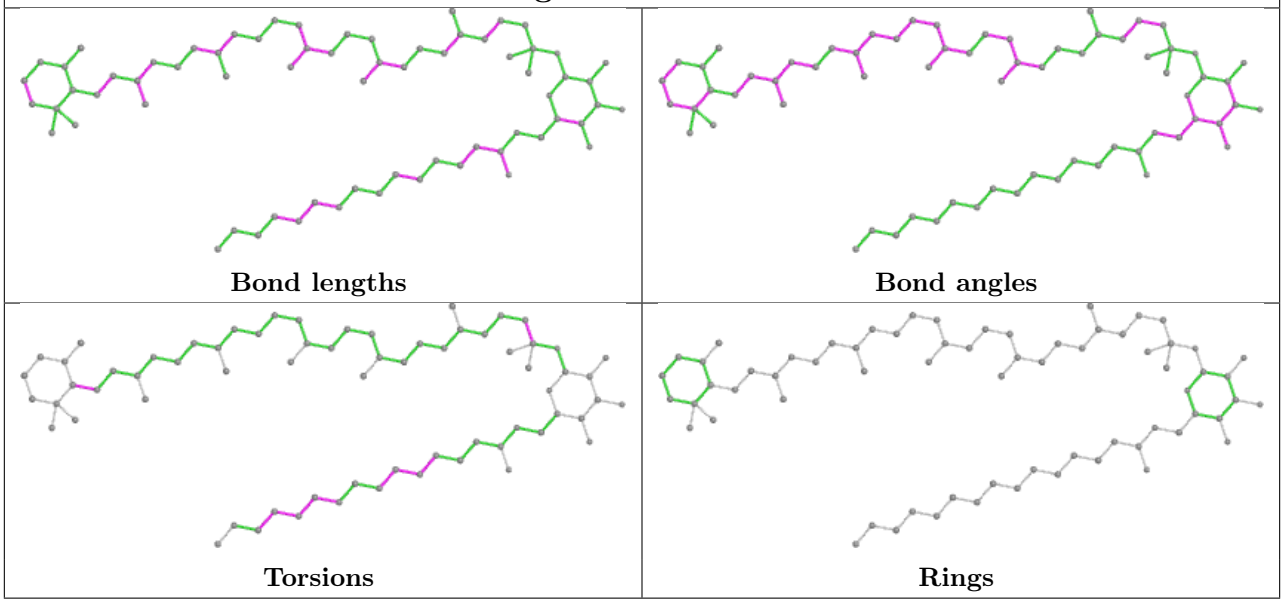
Ligand U42 O 101



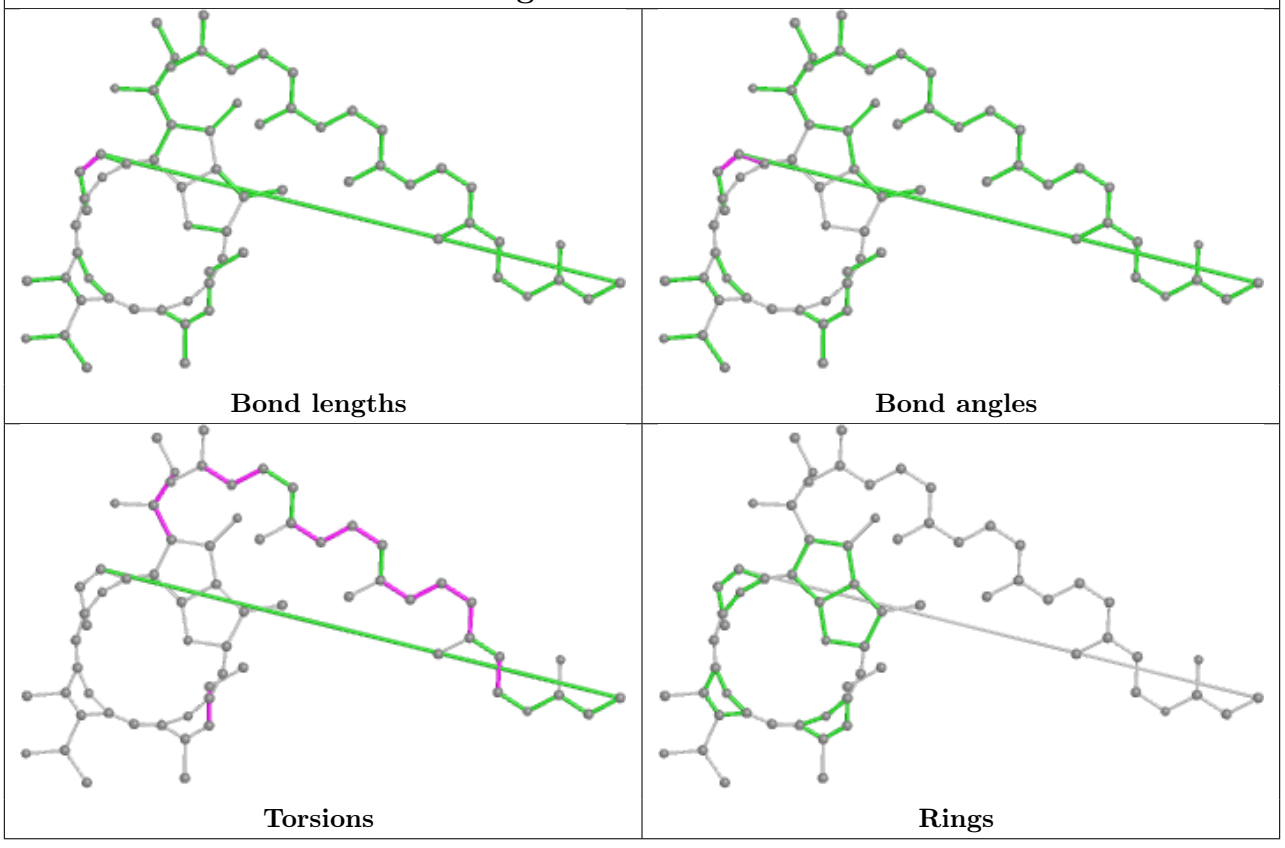
Ligand PGV P 103



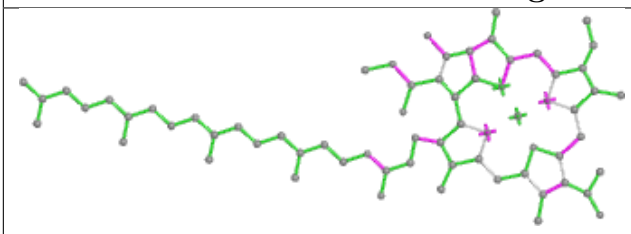
Ligand U42 4 101



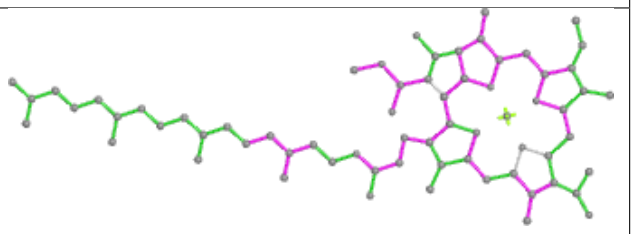
Ligand BPH L 1005



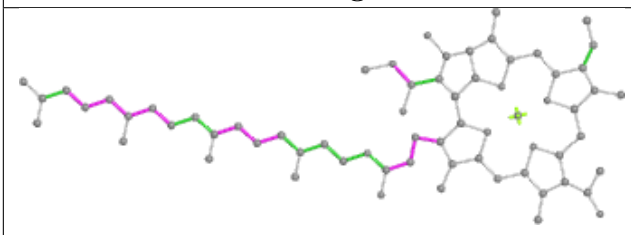
Ligand BCL S 102



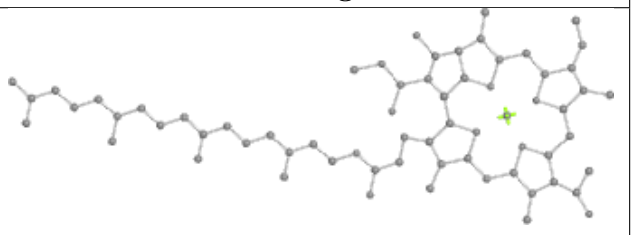
Bond lengths



Bond angles

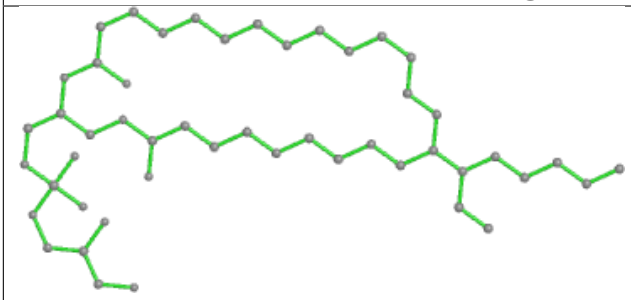


Torsions

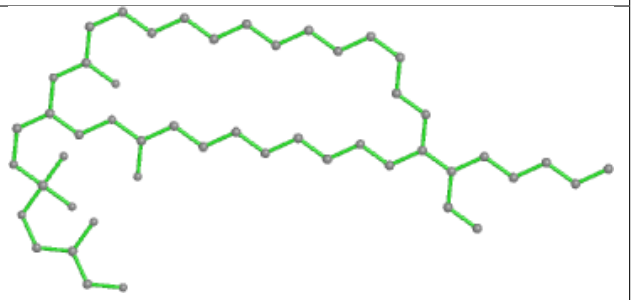


Rings

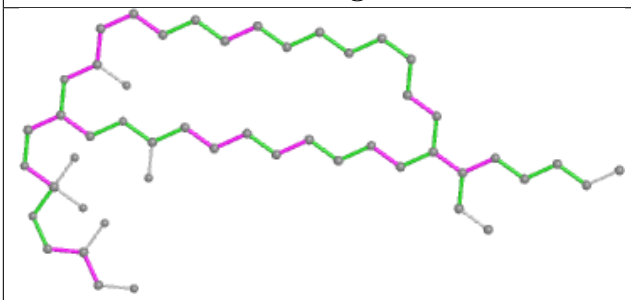
Ligand PGV C 408



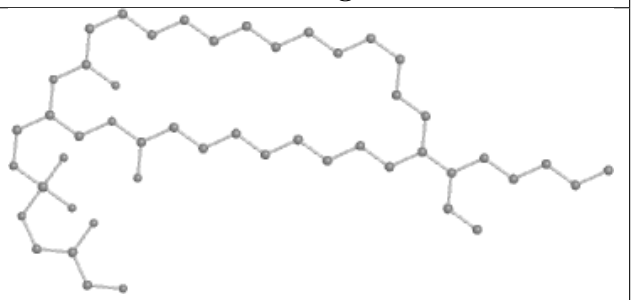
Bond lengths



Bond angles

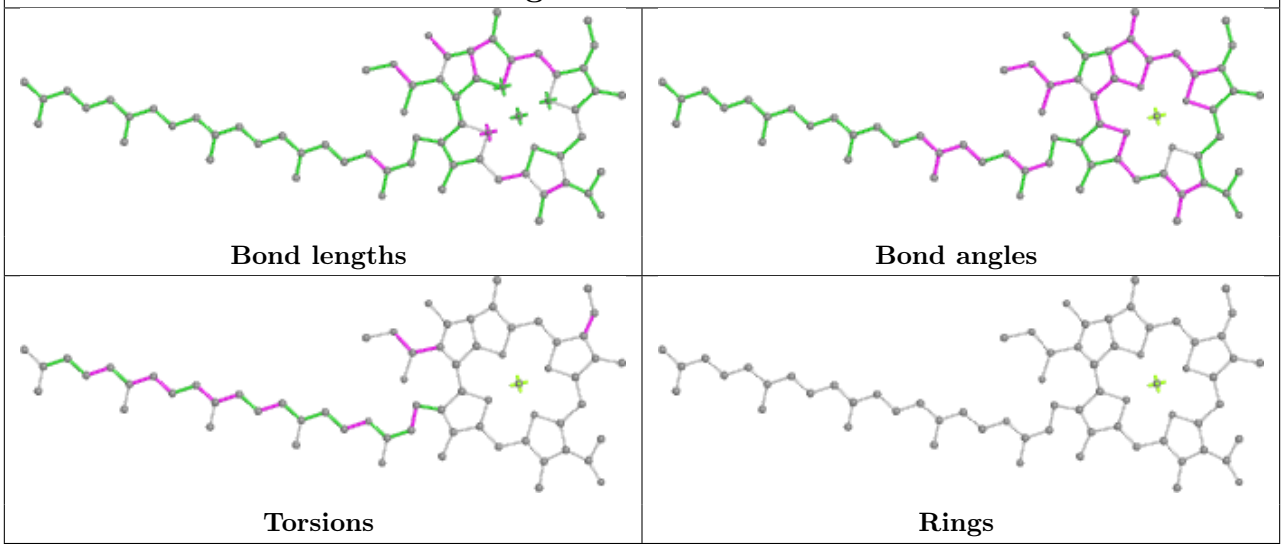


Torsions

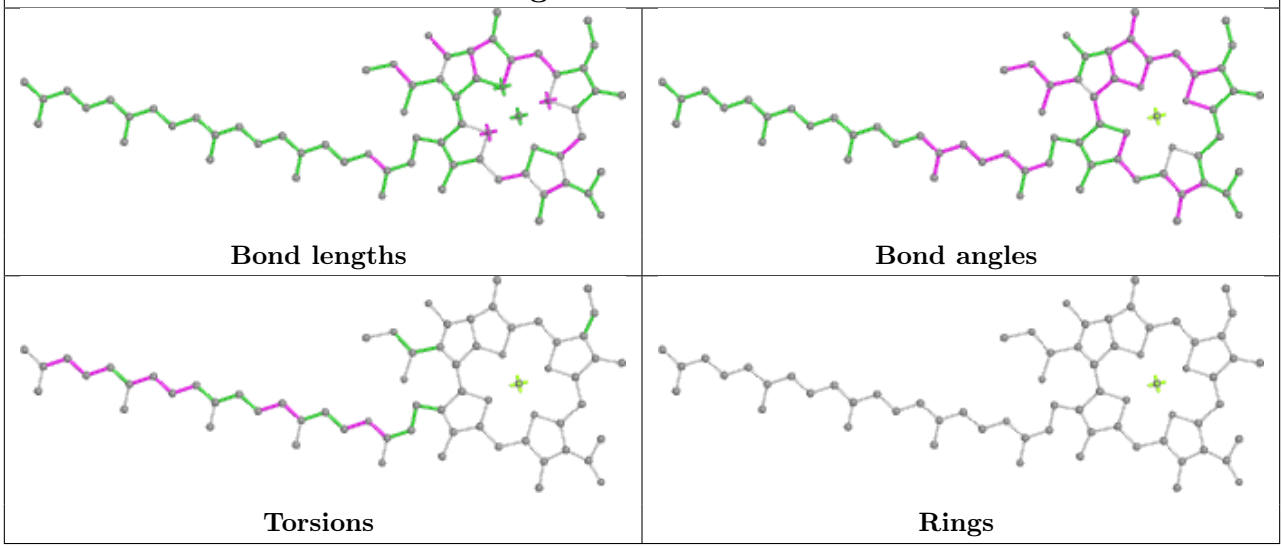


Rings

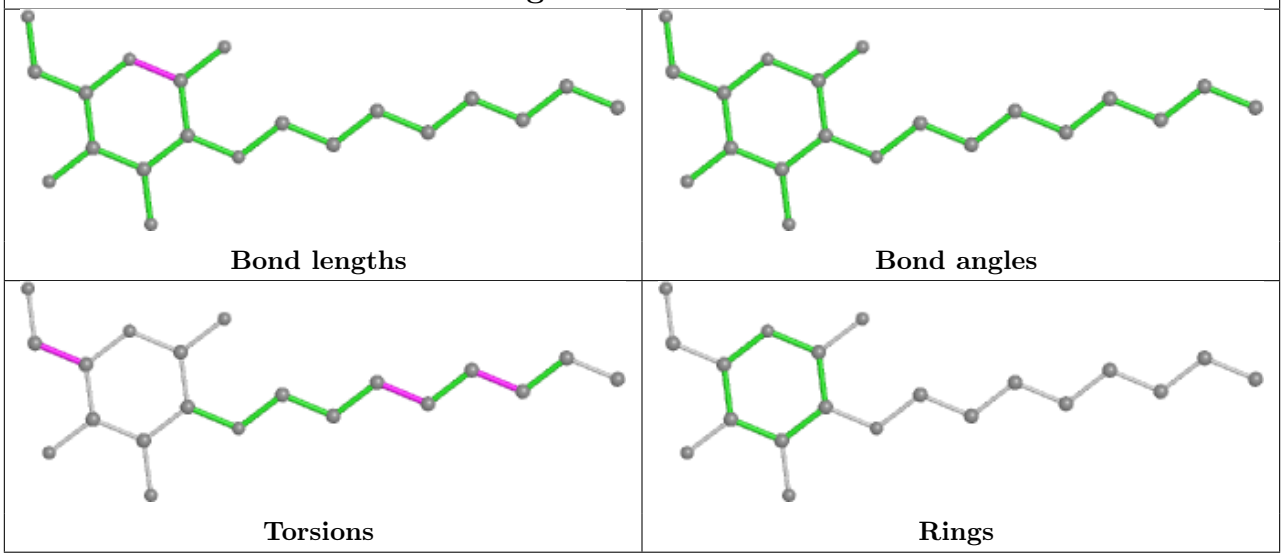
Ligand BCL R 101



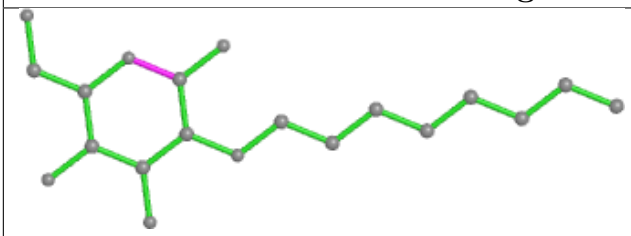
Ligand BCL 4 102



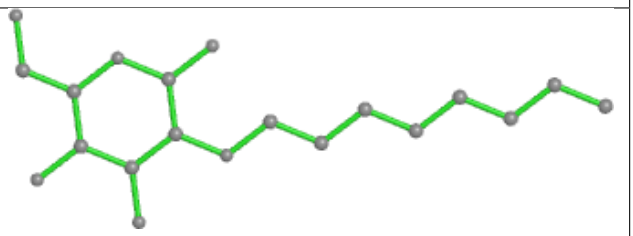
Ligand BGL F 104



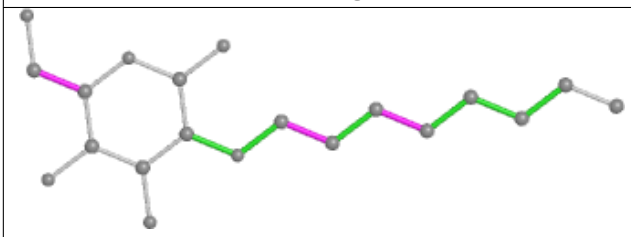
Ligand BGL L 1013



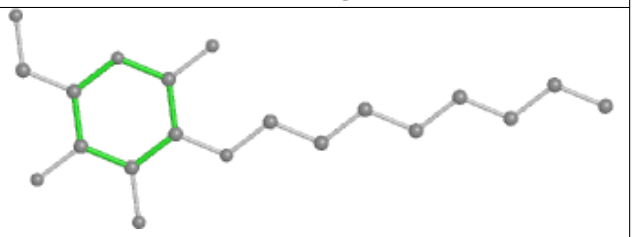
Bond lengths



Bond angles

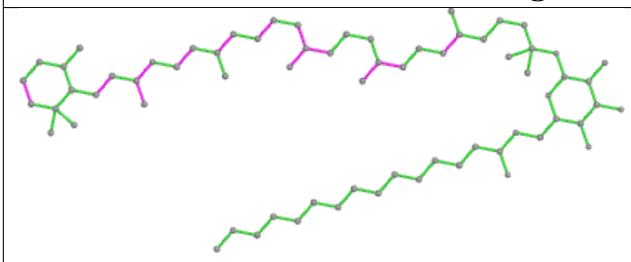


Torsions

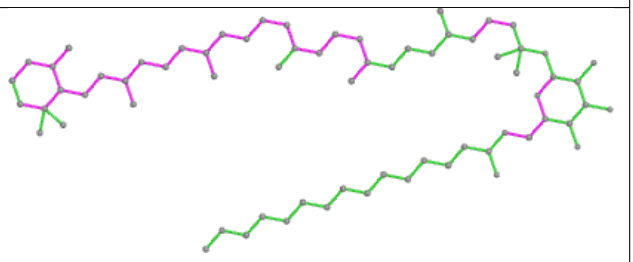


Rings

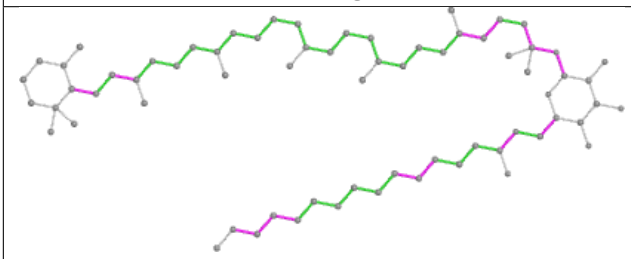
Ligand U42 U 104



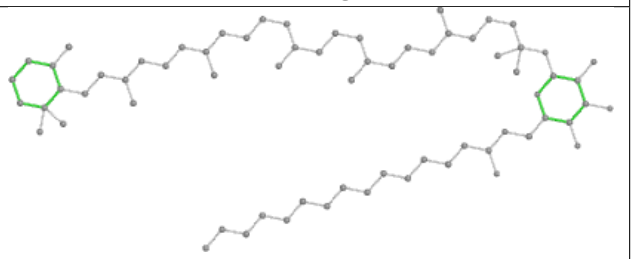
Bond lengths



Bond angles

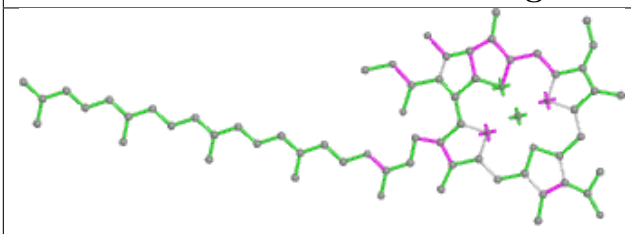


Torsions

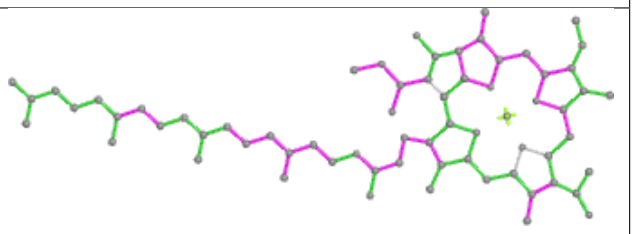


Rings

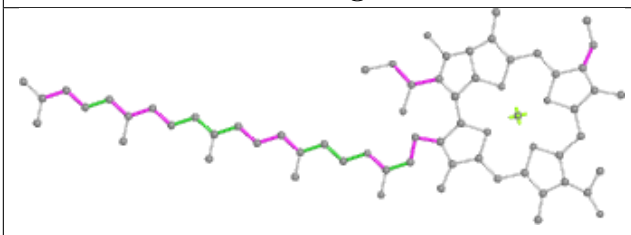
Ligand BCL B 103



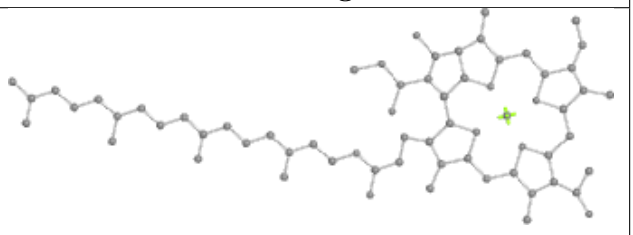
Bond lengths



Bond angles

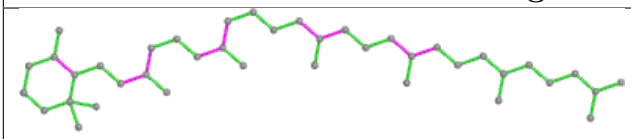


Torsions

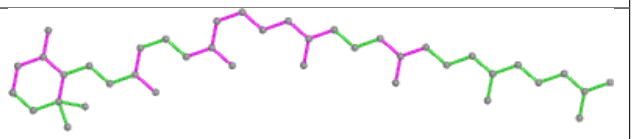


Rings

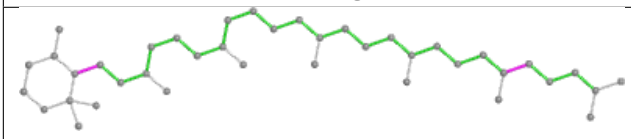
Ligand U4Z V 102



Bond lengths



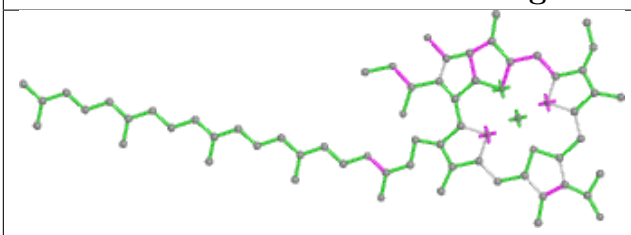
Bond angles



Torsions

Rings

Ligand BCL 1 101



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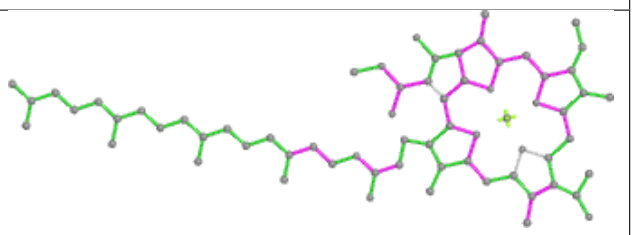
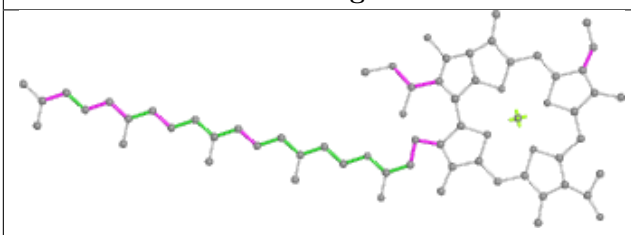
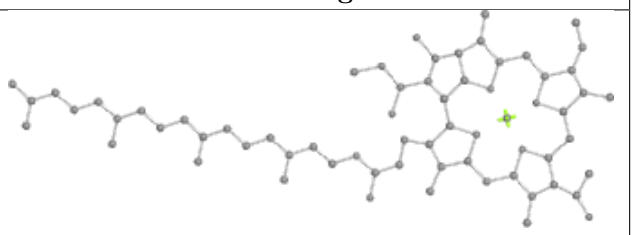


Bond angles

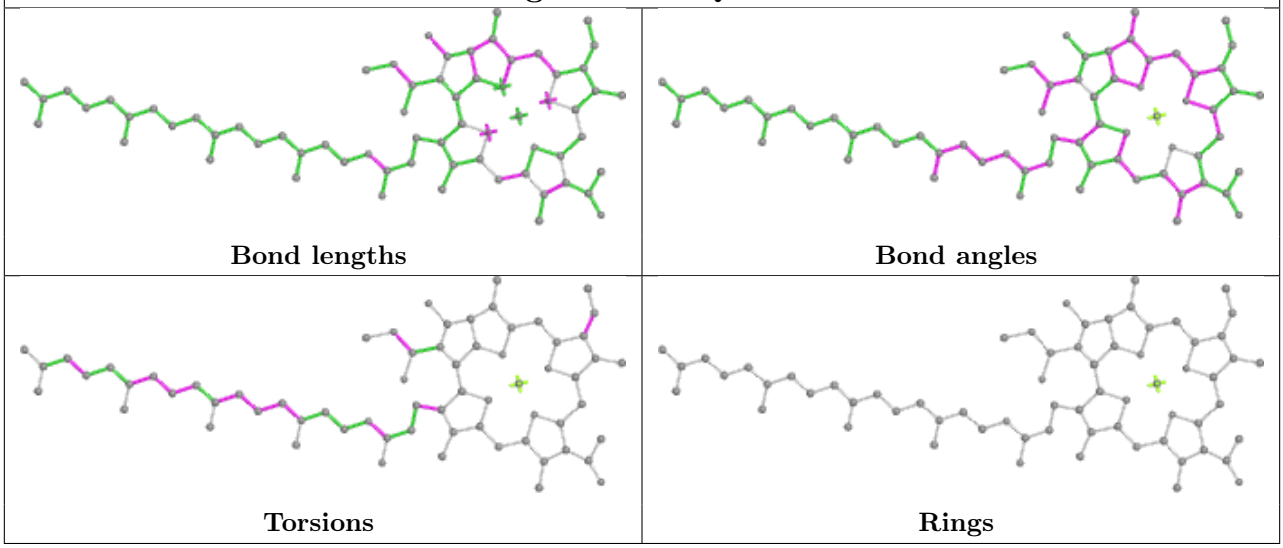


Torsions

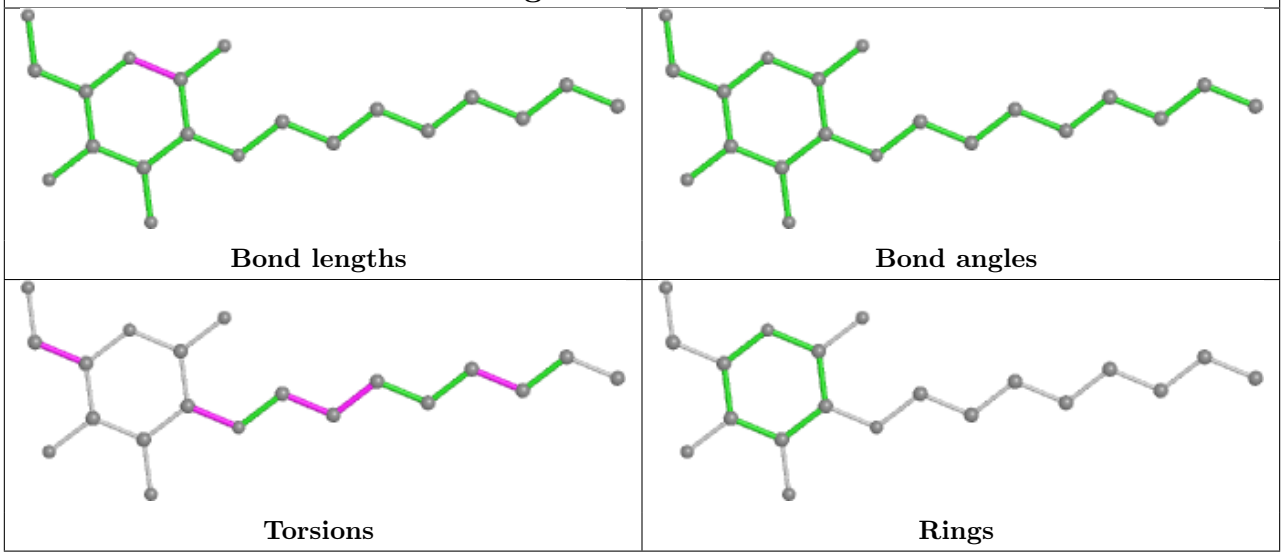


Rings

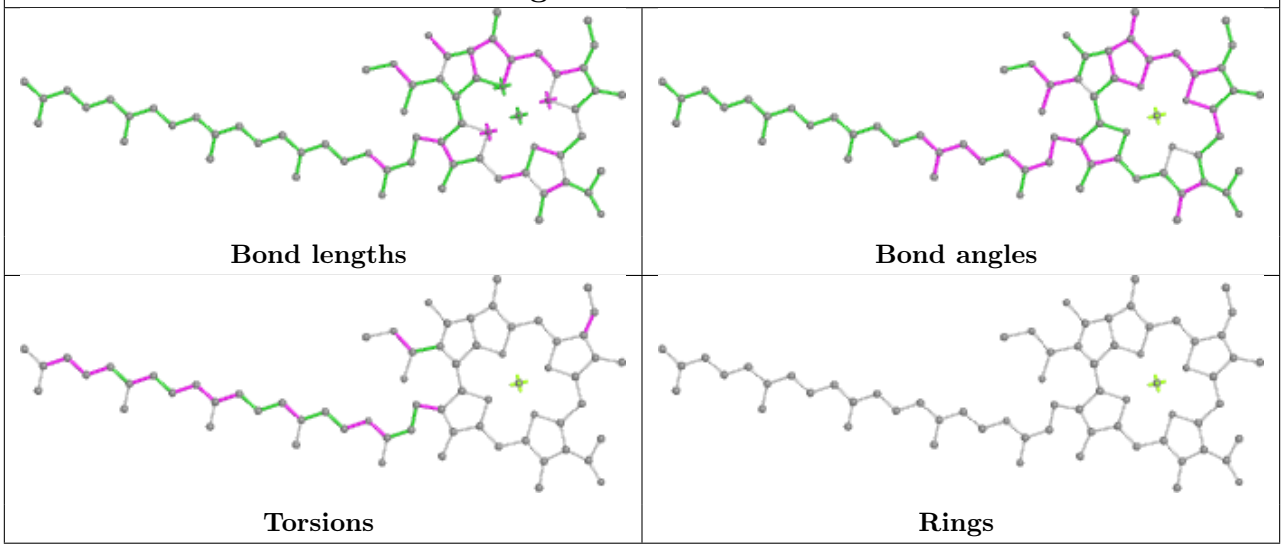
Ligand BCL Q 103



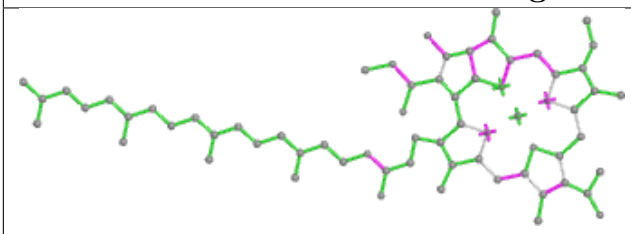
Ligand BGL Y 101



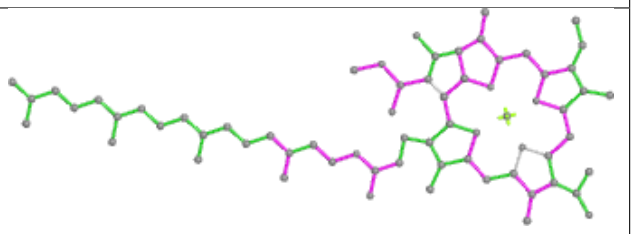
Ligand BCL 2 102



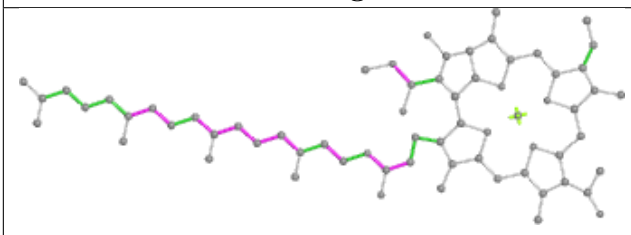
Ligand BCL 2 101



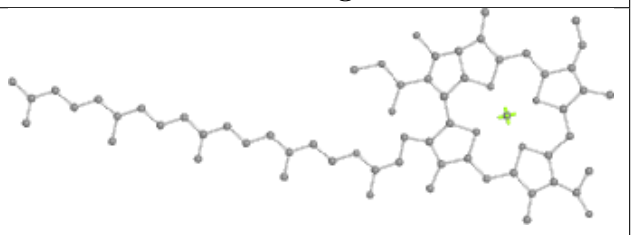
Bond lengths



Bond angles

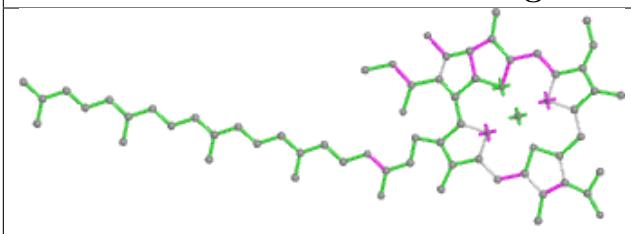


Torsions

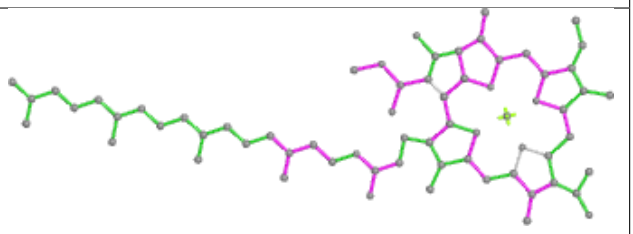


Rings

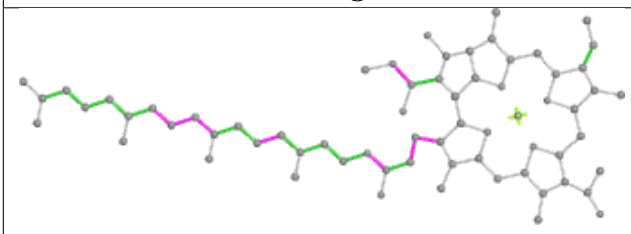
Ligand BCL O 102



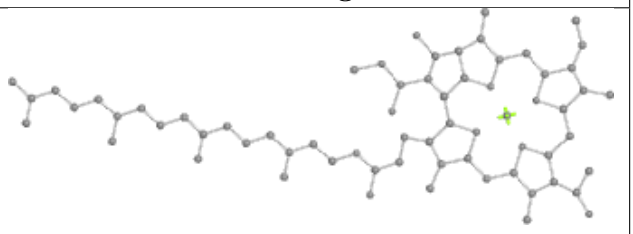
Bond lengths



Bond angles

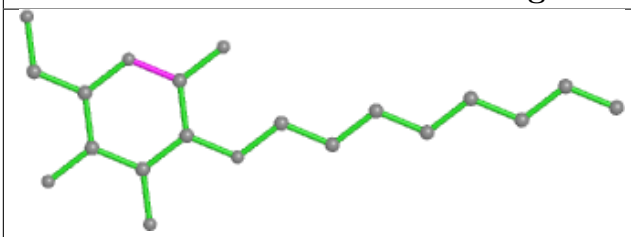


Torsions



Rings

Ligand BGL 3 103



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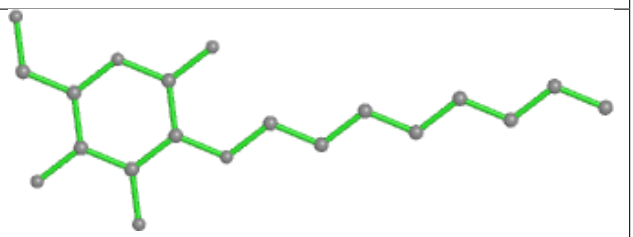
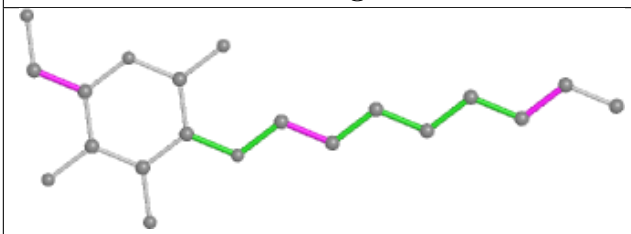


Bond angles



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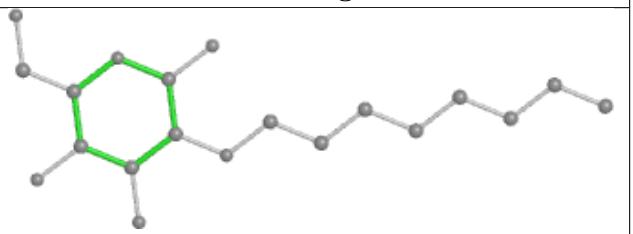
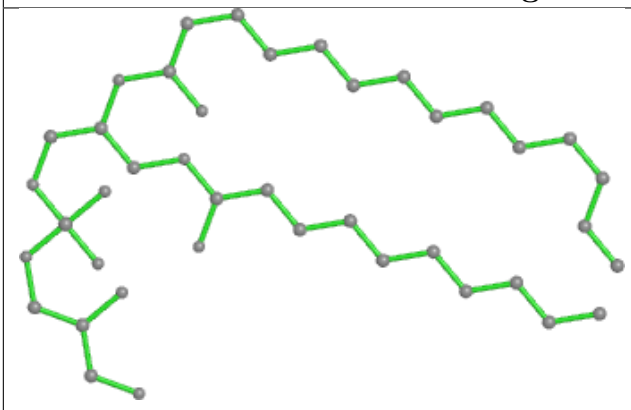


Rings

Ligand PGV C 407



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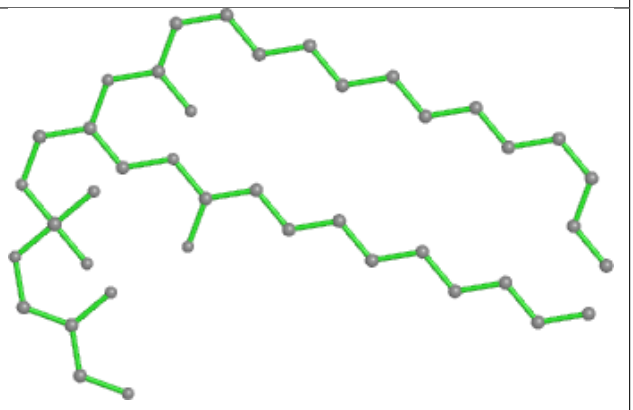
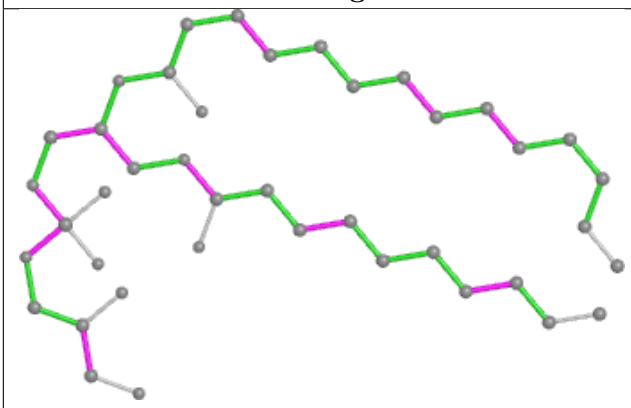
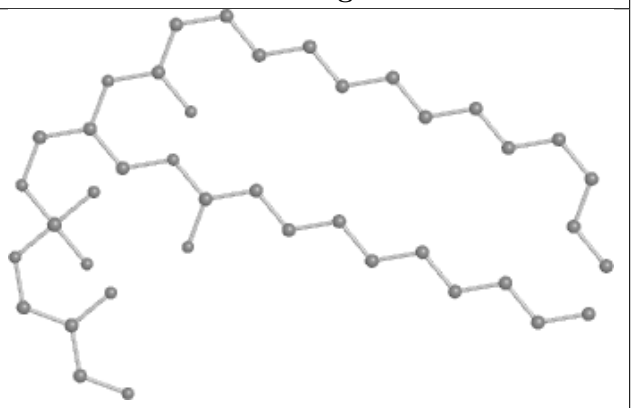


Bond angles

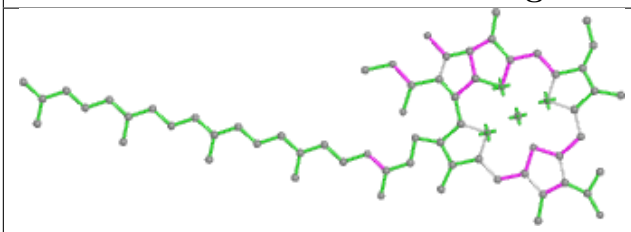


Torsions



Rings

Ligand BCL P 101



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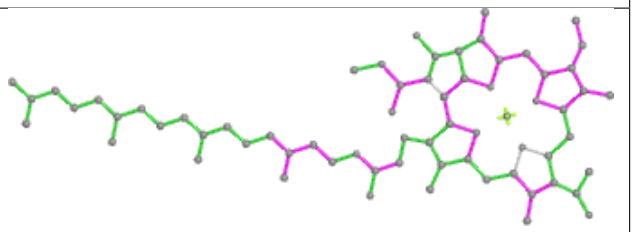
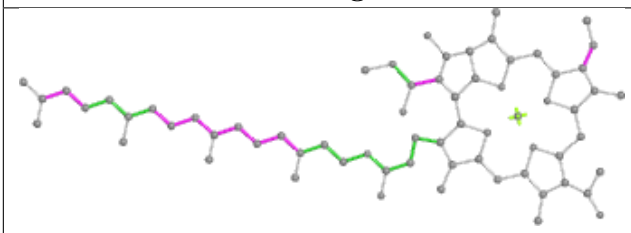


Bond angles



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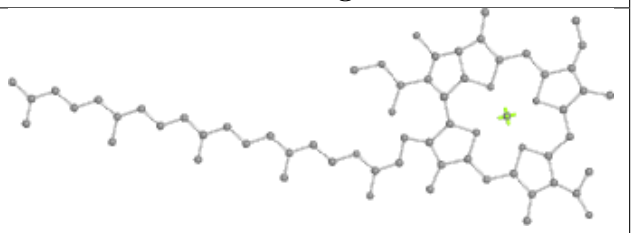
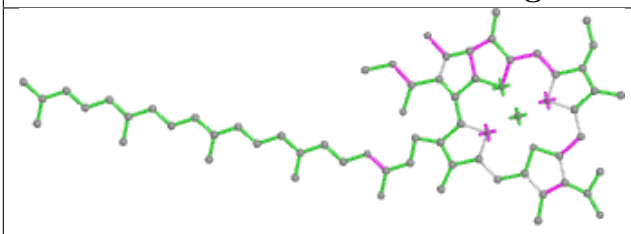


Rings

Ligand BCL U 102



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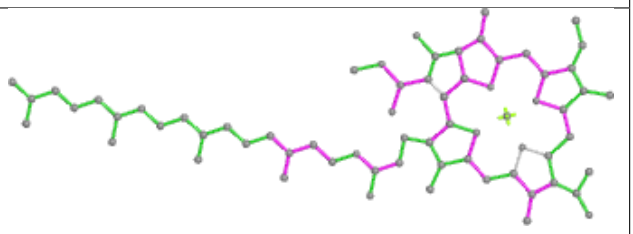
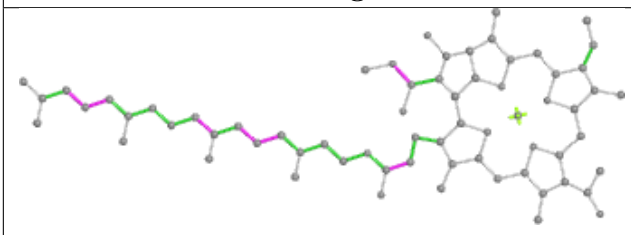


Bond angles



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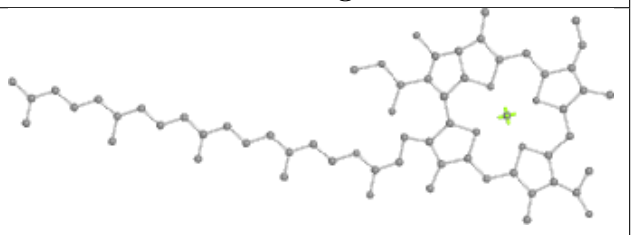
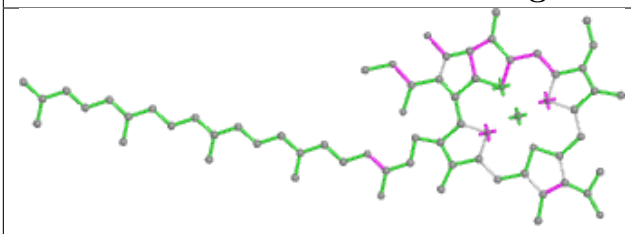


Rings

Ligand BCL 9 102



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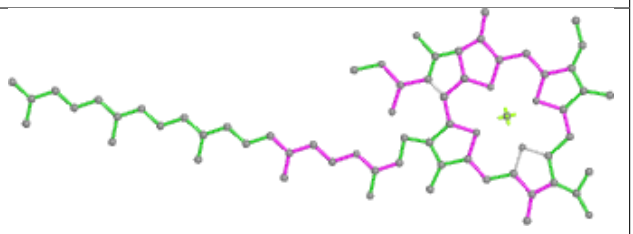
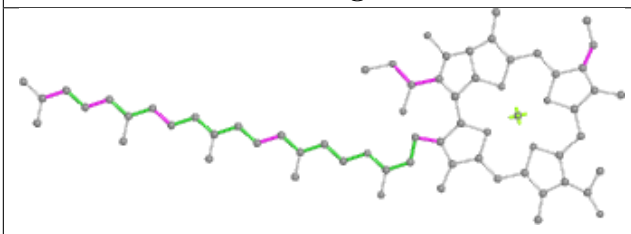


Bond angles



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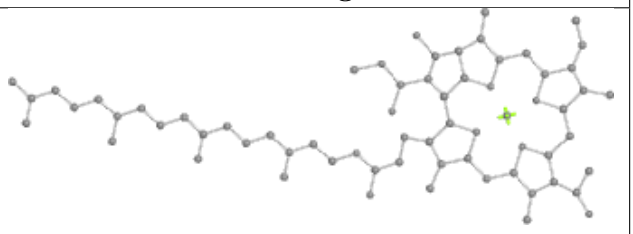
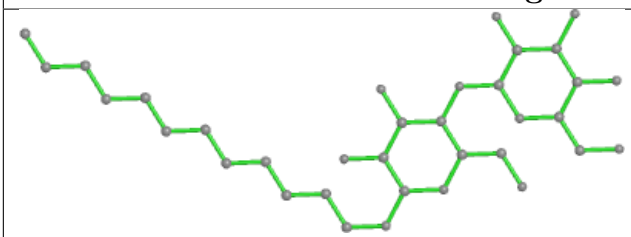


Rings

Ligand LMT 1 103



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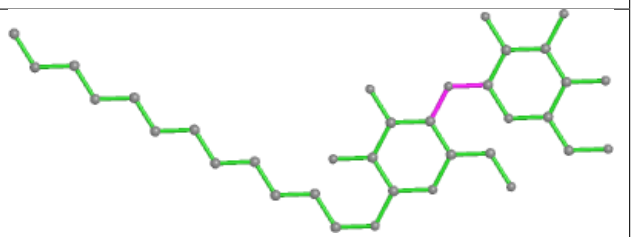
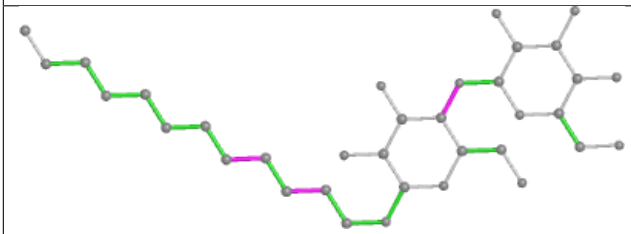


Bond angles



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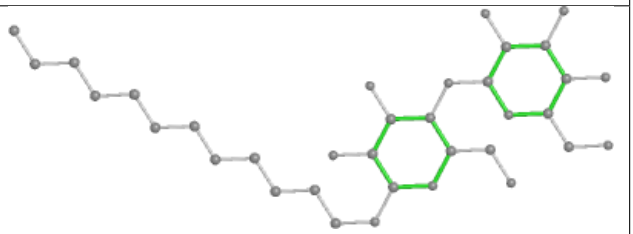
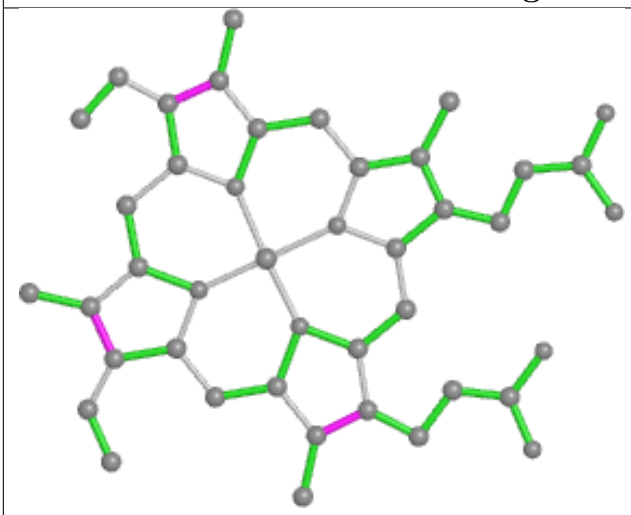


Rings

Ligand HEC C 404



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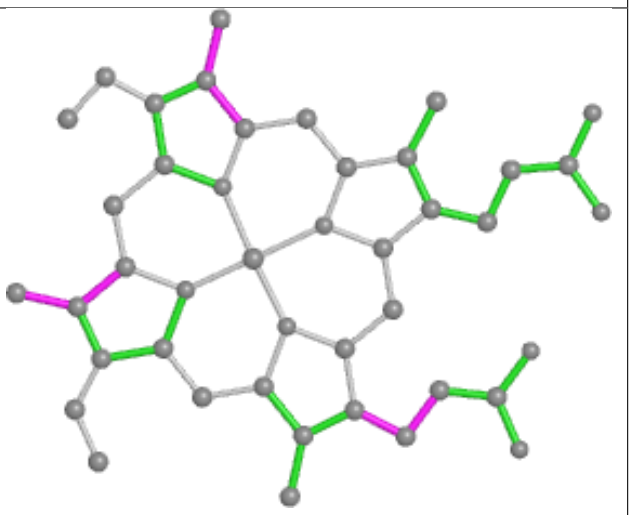
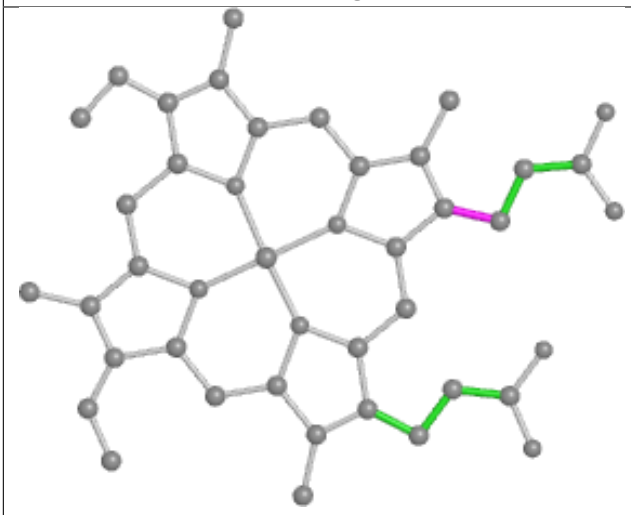


Bond angles



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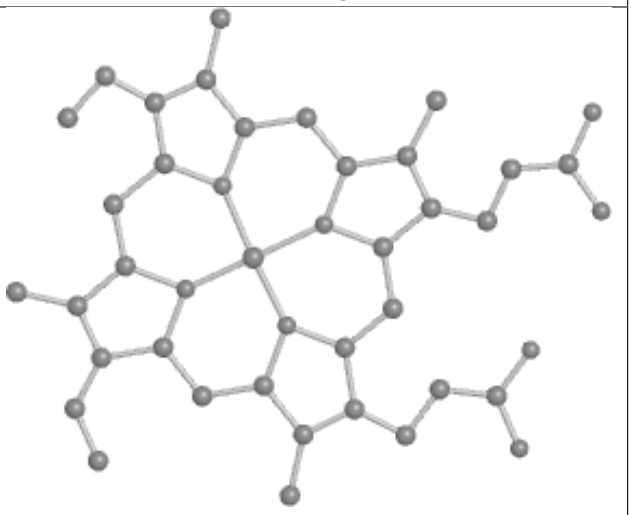
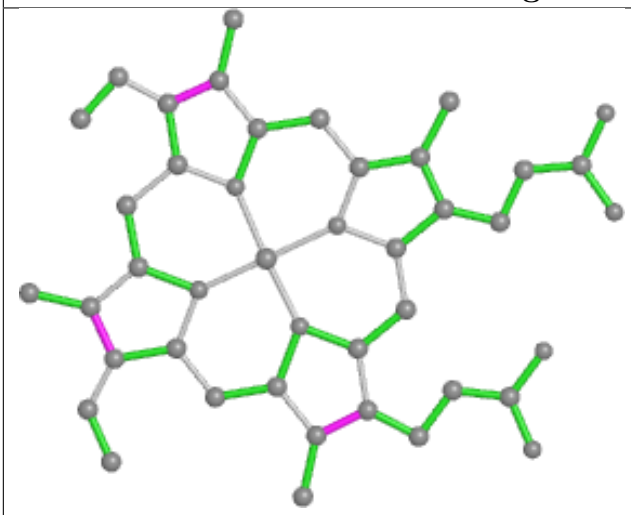


Rings

Ligand HEC C 403



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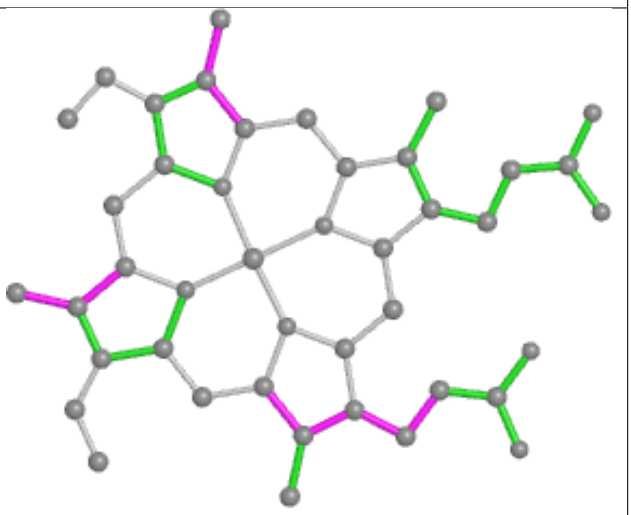
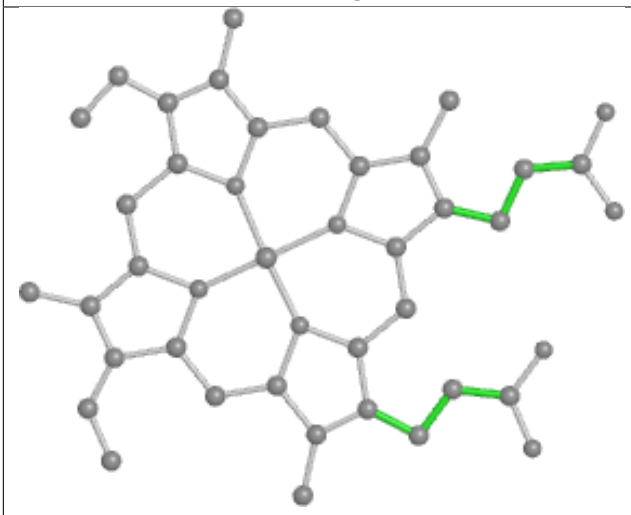


Bond angles



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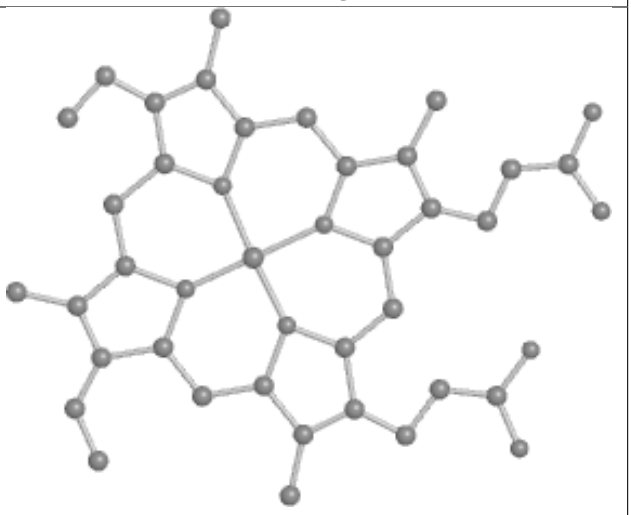
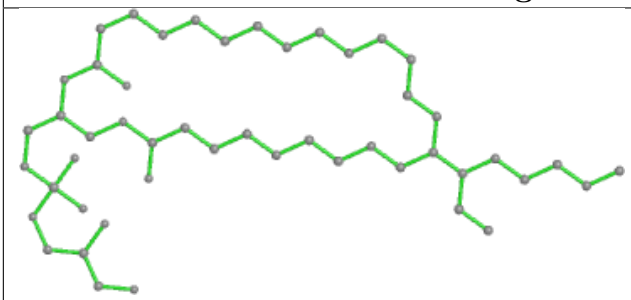


Rings

Ligand PGV L 1007



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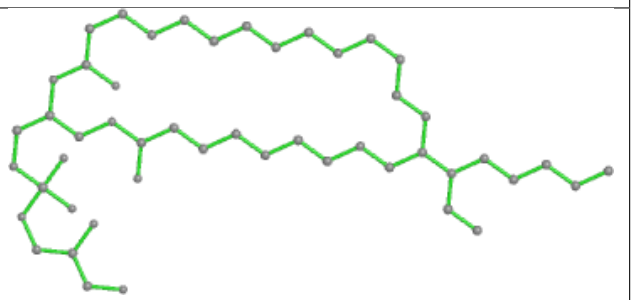
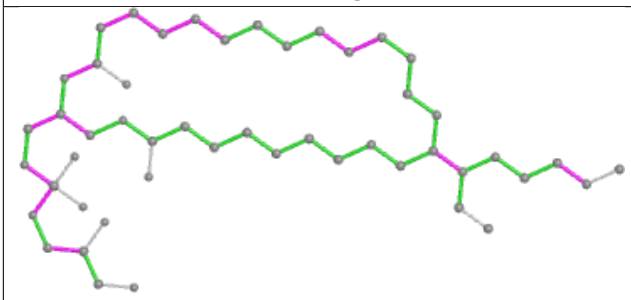


Bond angles



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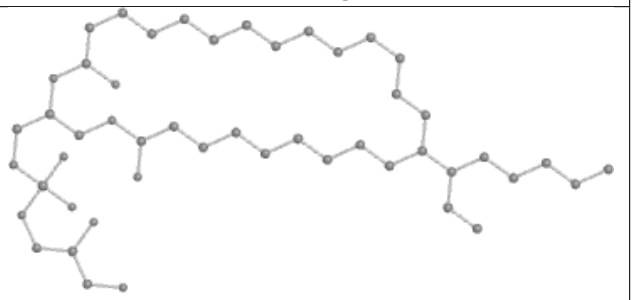
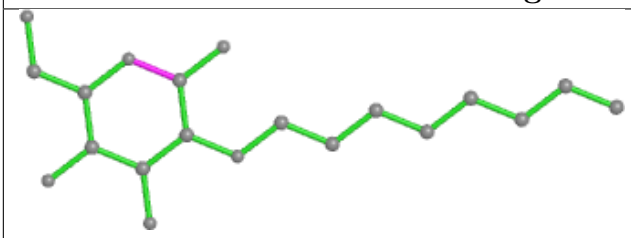


Rings

Ligand BGL C 410



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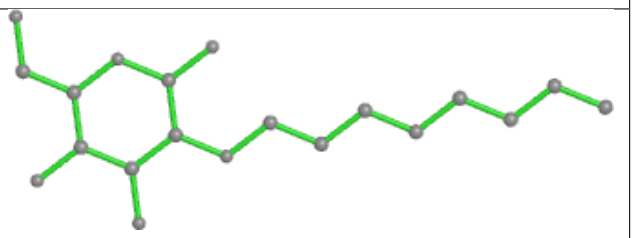
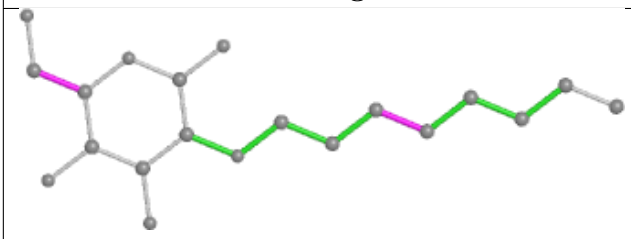


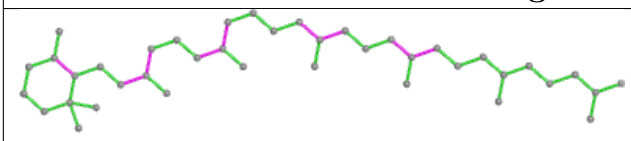
Bond angles



Torsions

Rings

Ligand U4Z T 102



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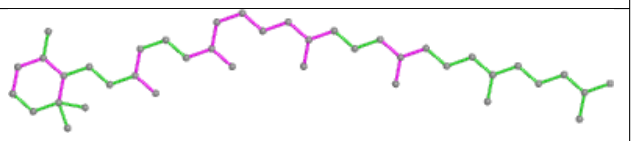
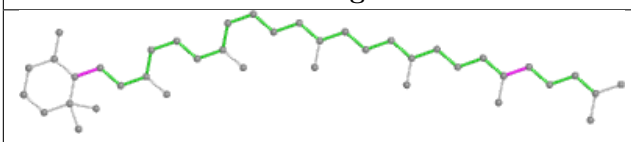
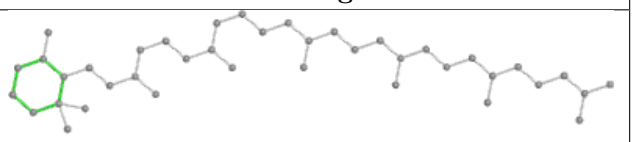


Bond angles

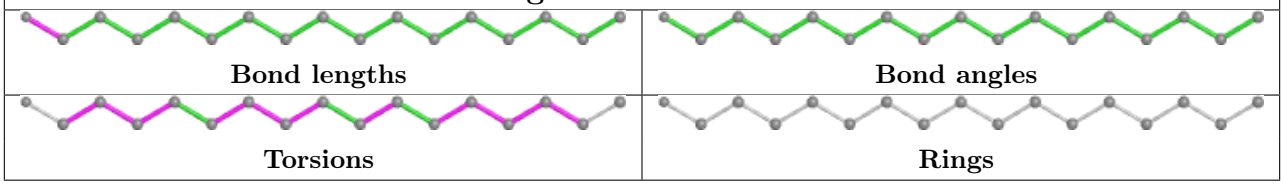


Torsions

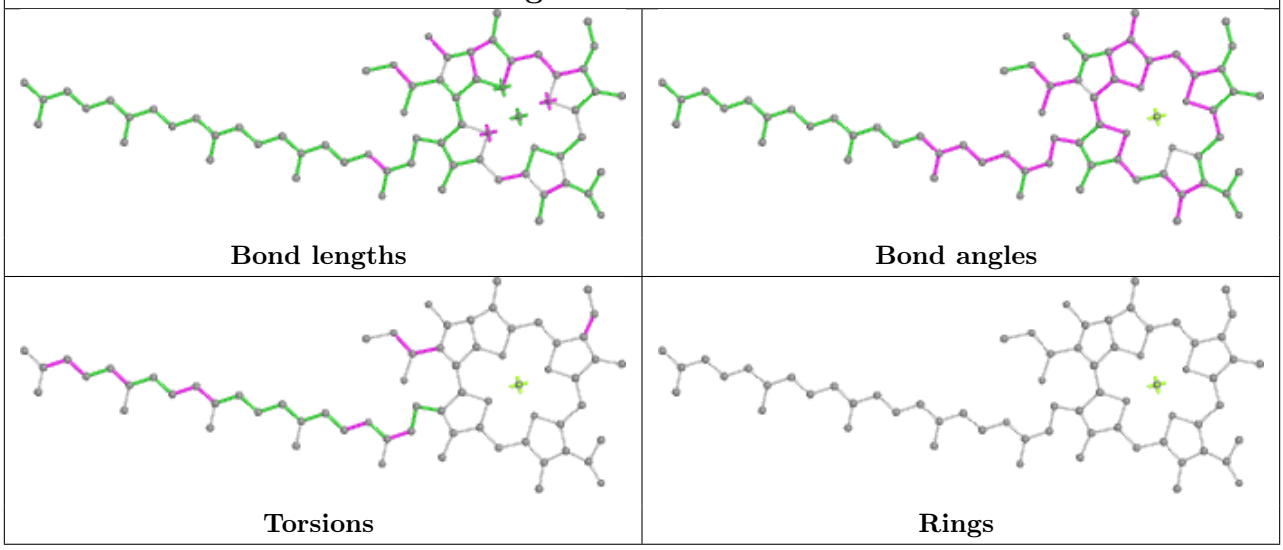


Rings

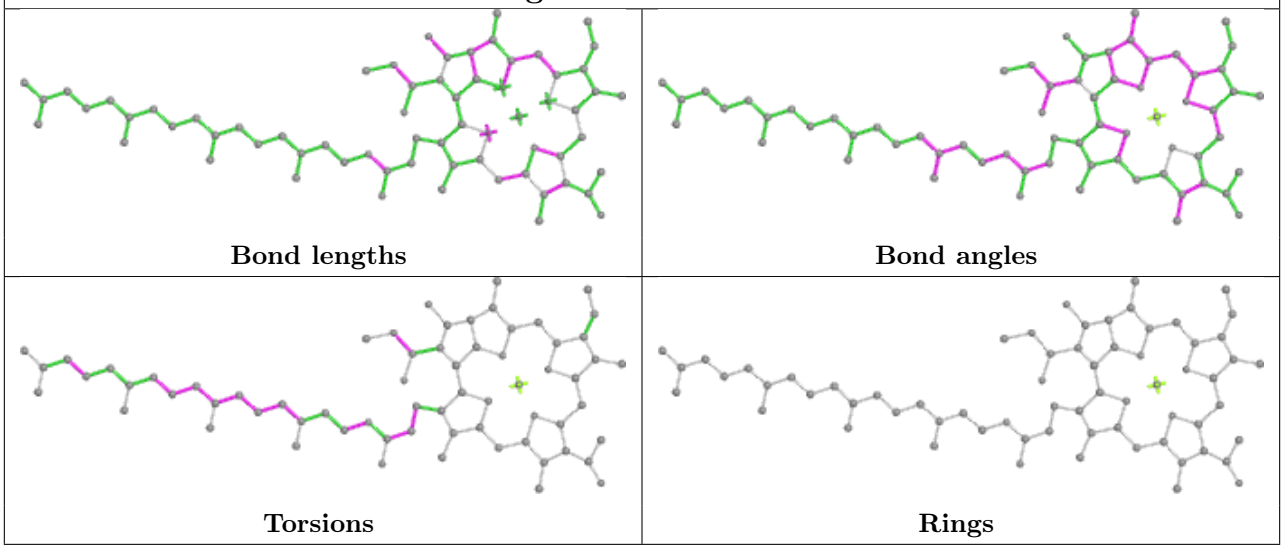
Ligand LHG h 101



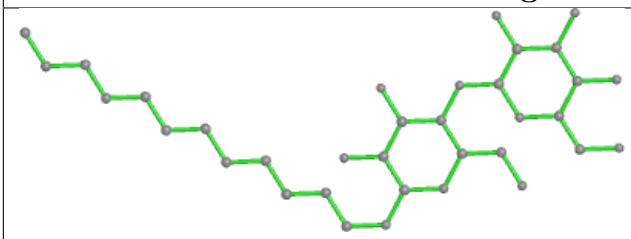
Ligand BCL D 101



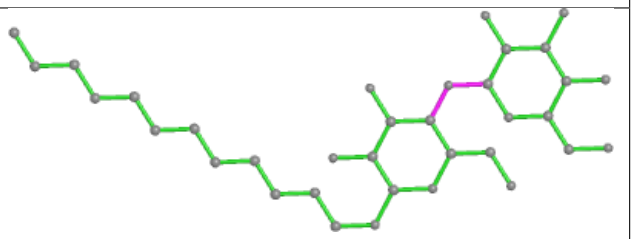
Ligand BCL O 103



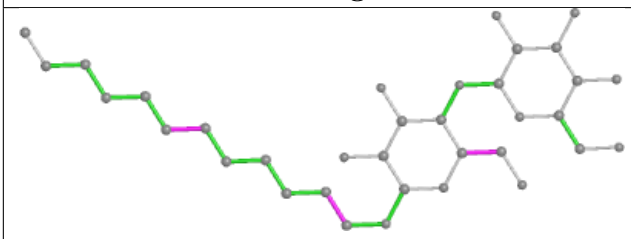
Ligand LMT D 105



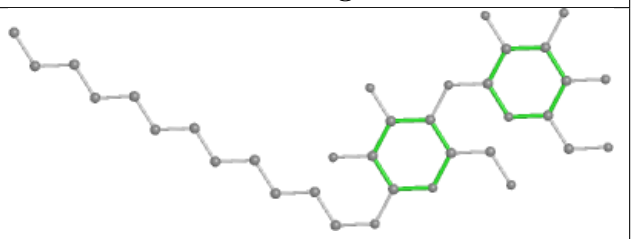
Bond lengths



Bond angles

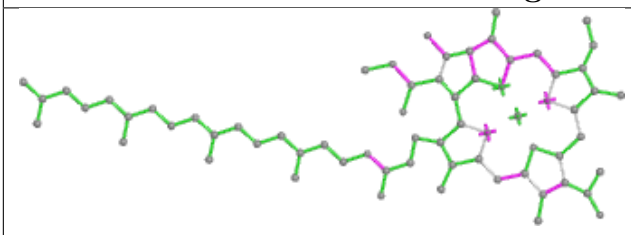


Torsions



Rings

Ligand BCL U 103



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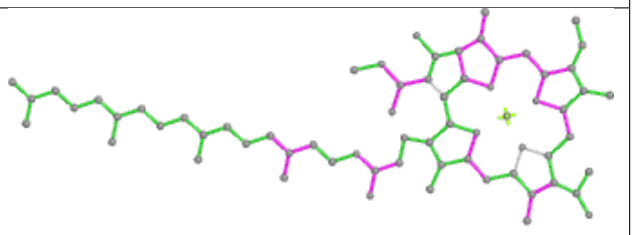
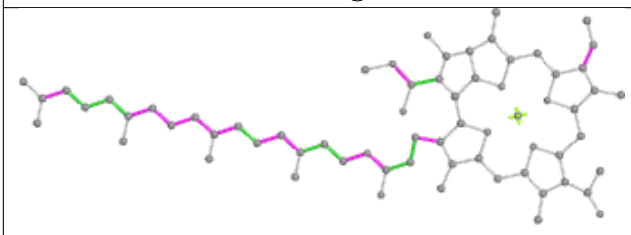


Bond angles



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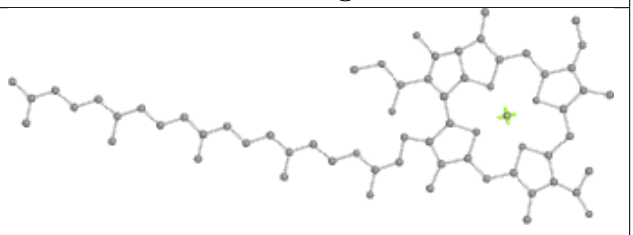
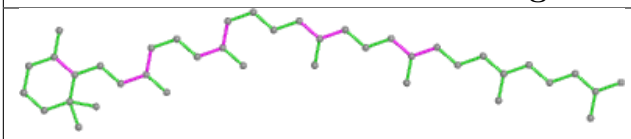
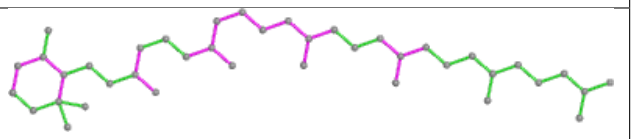


Rings

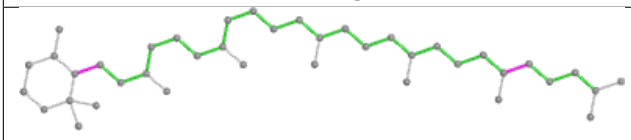
Ligand U4Z F 103



Bond lengths



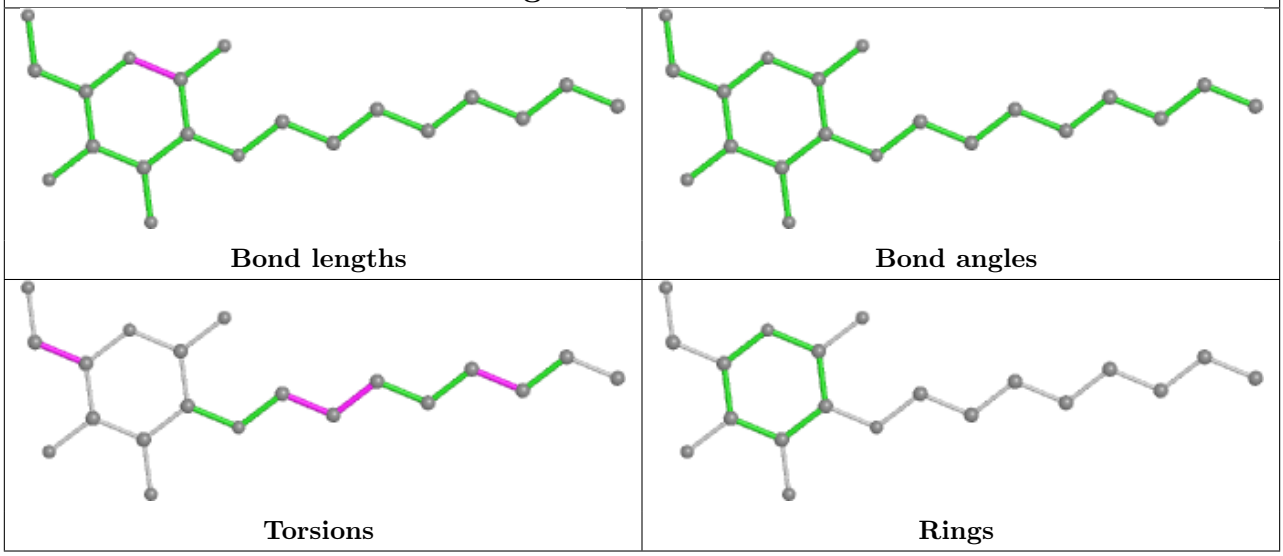
Bond angles



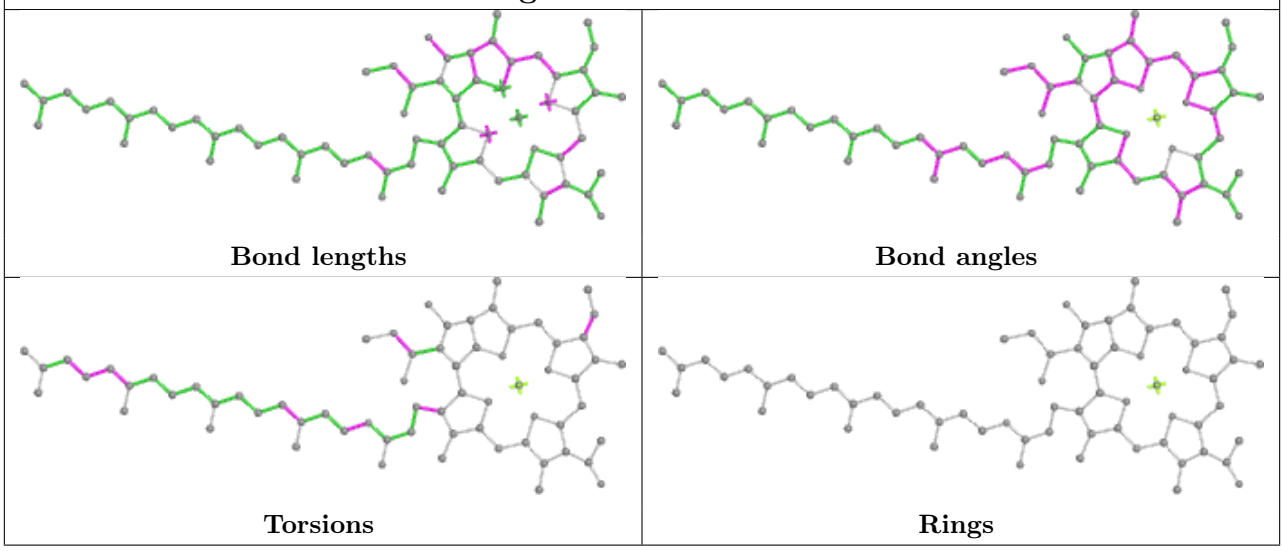
Torsions

Rings

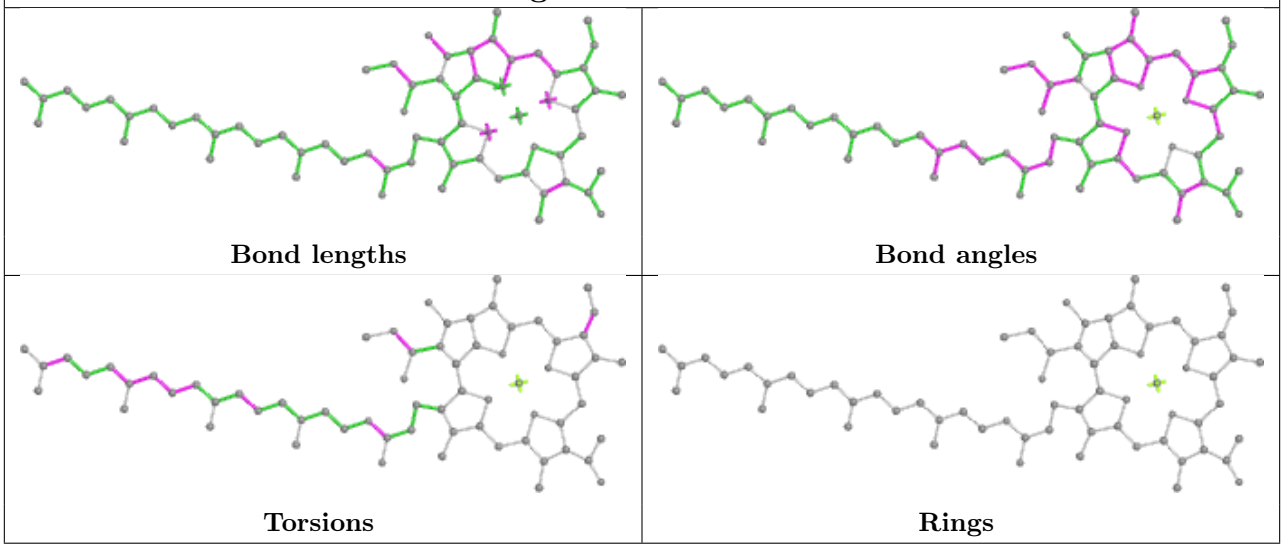
Ligand BGL H 107



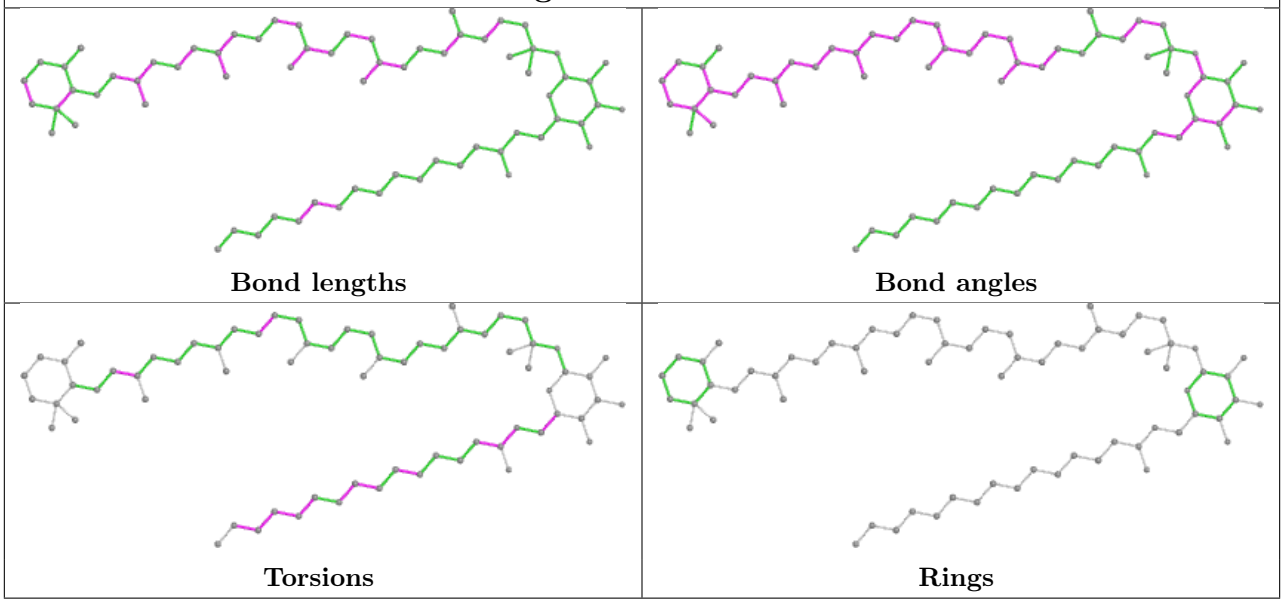
Ligand BCL L 1002



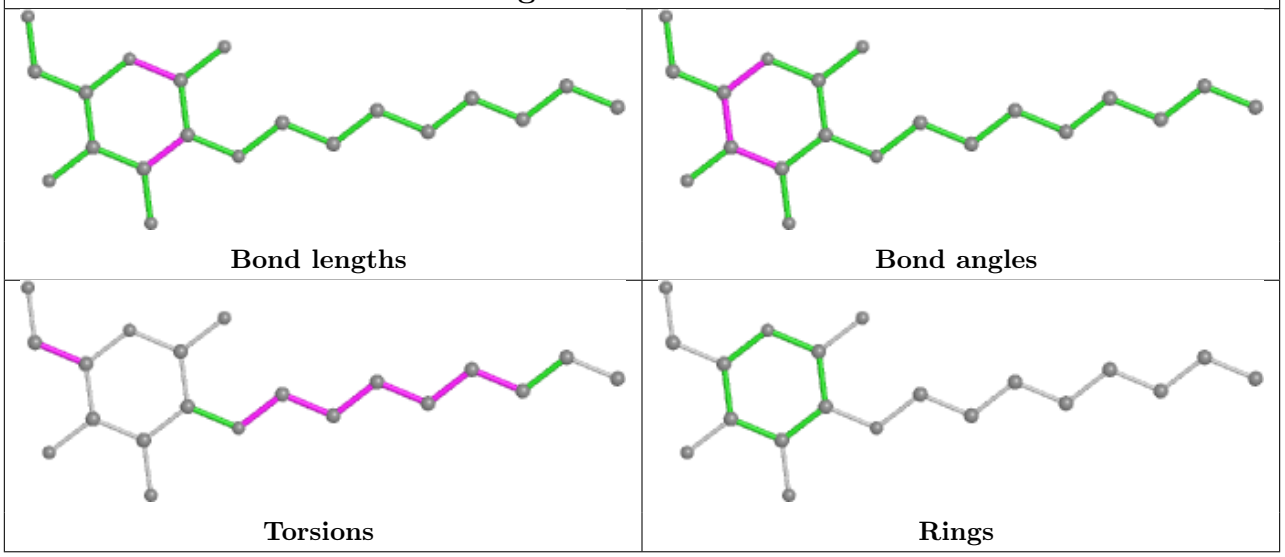
Ligand BCL 0 102



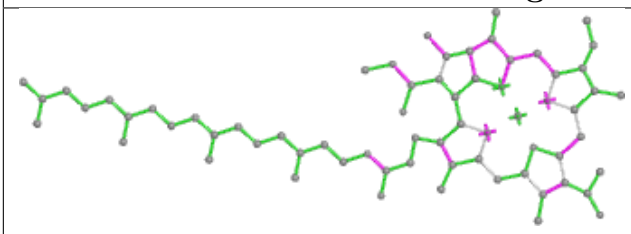
Ligand U42 4 104



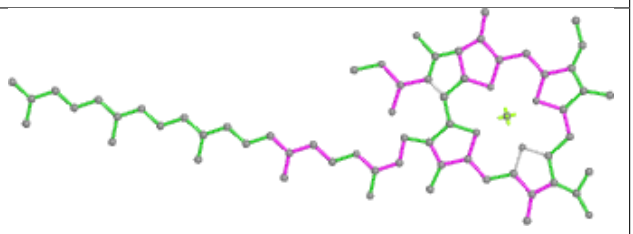
Ligand BGL L 1015



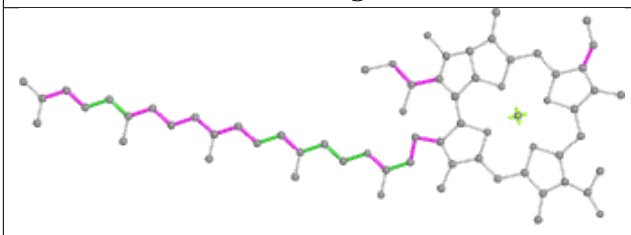
Ligand BCL E 102



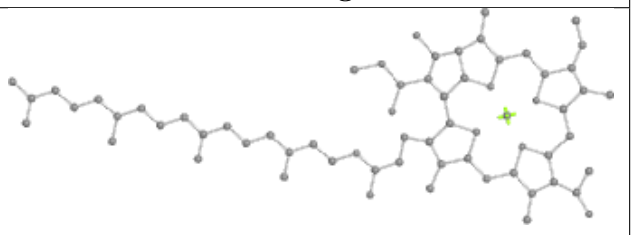
Bond lengths



Bond angles

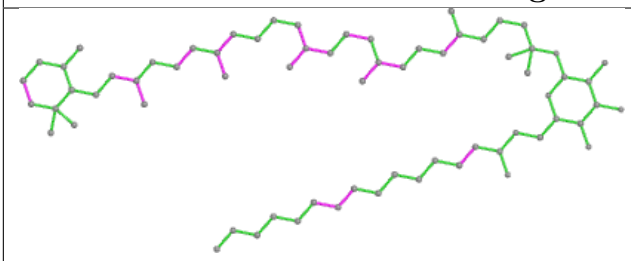


Torsions

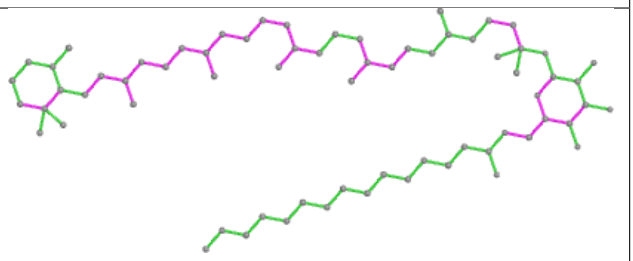


Rings

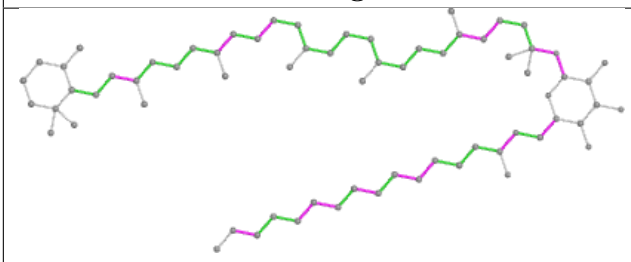
Ligand U42 U 101



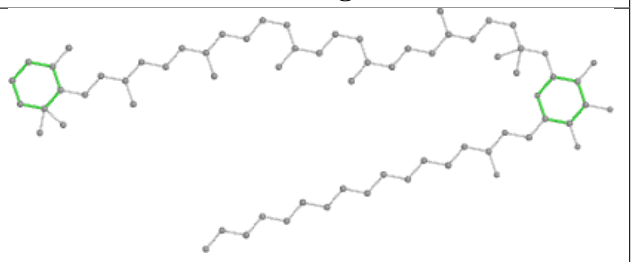
Bond lengths



Bond angles

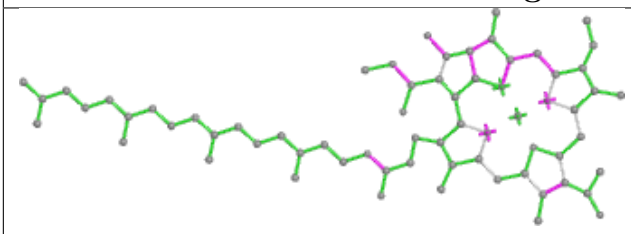


Torsions

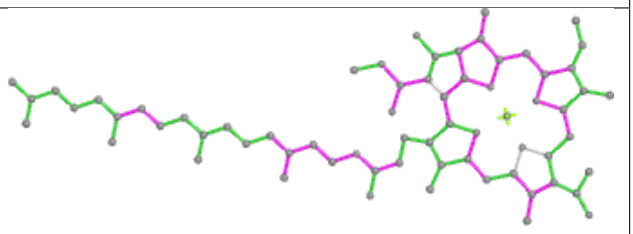


Rings

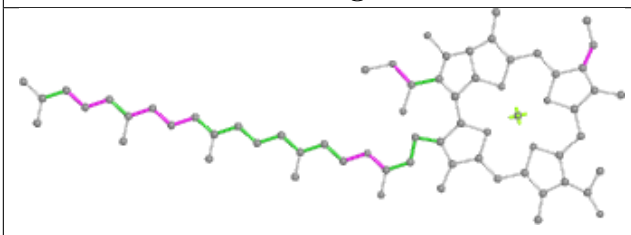
Ligand BCL K 101



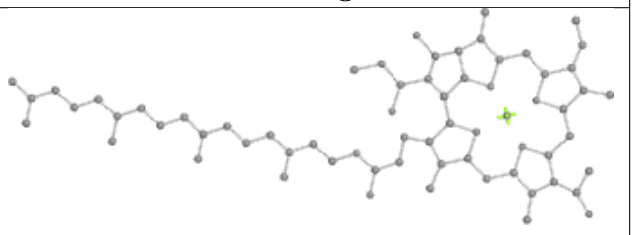
Bond lengths



Bond angles

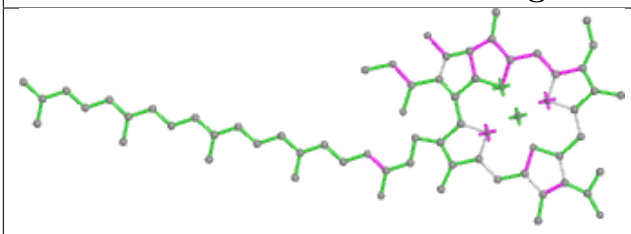


Torsions

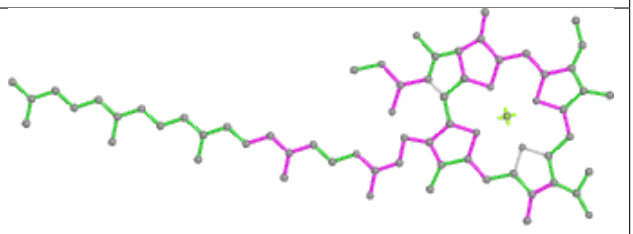


Rings

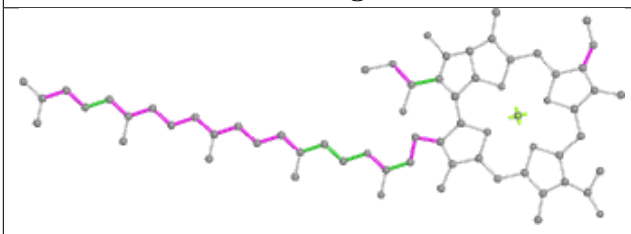
Ligand BCL S 103



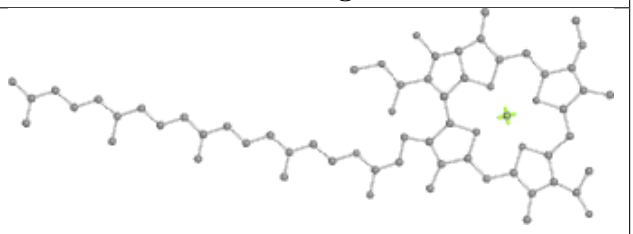
Bond lengths



Bond angles

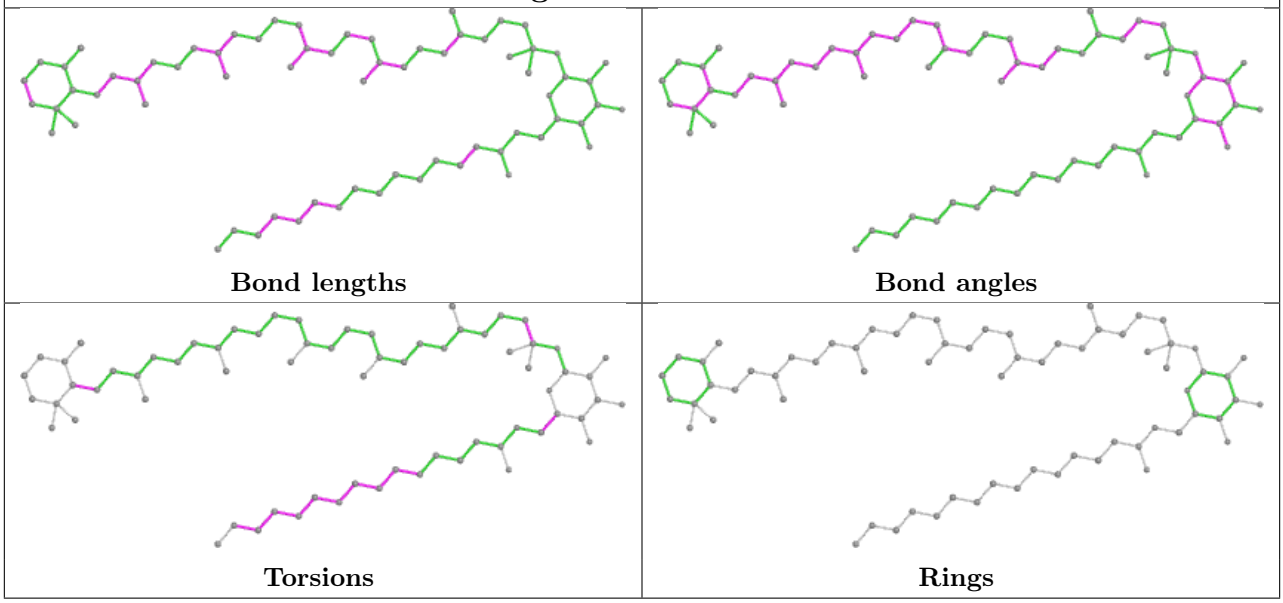


Torsions

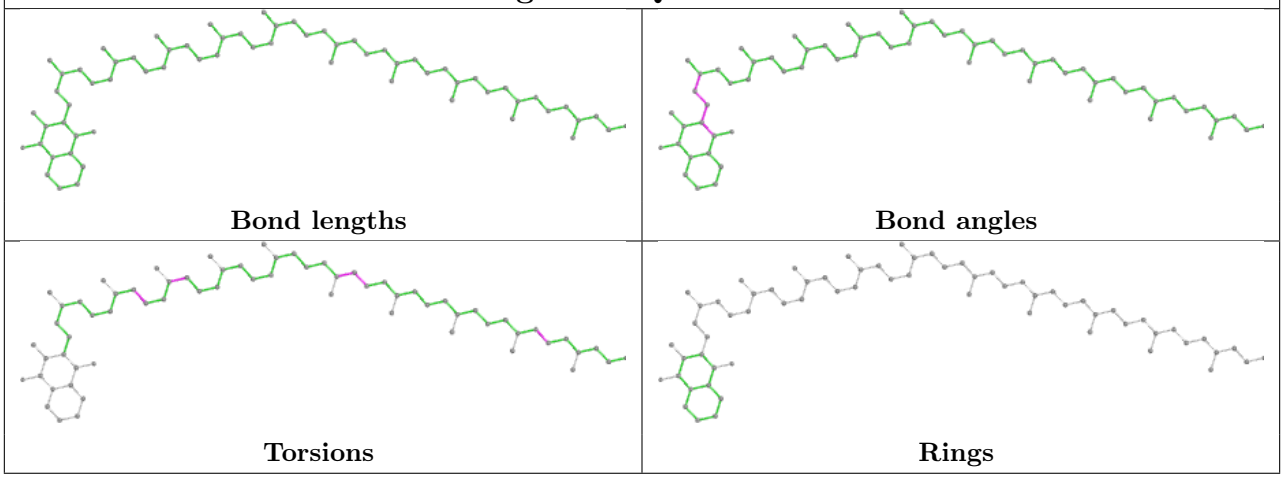


Rings

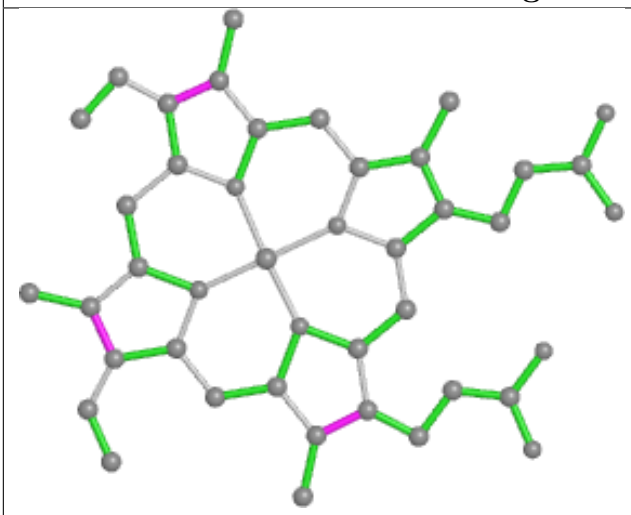
Ligand U42 B 101



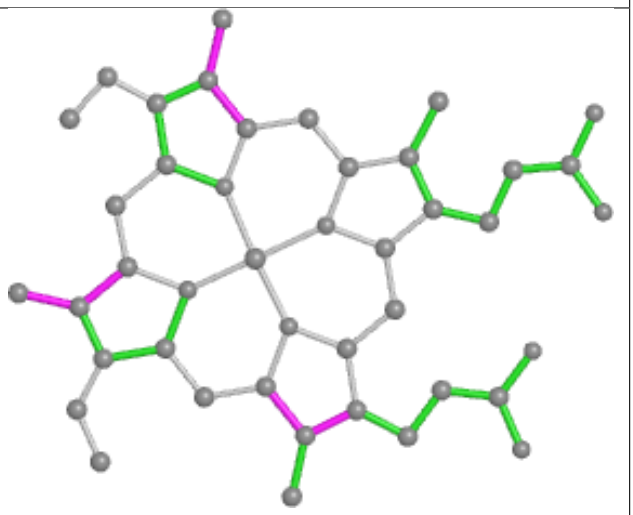
Ligand MQE M 704



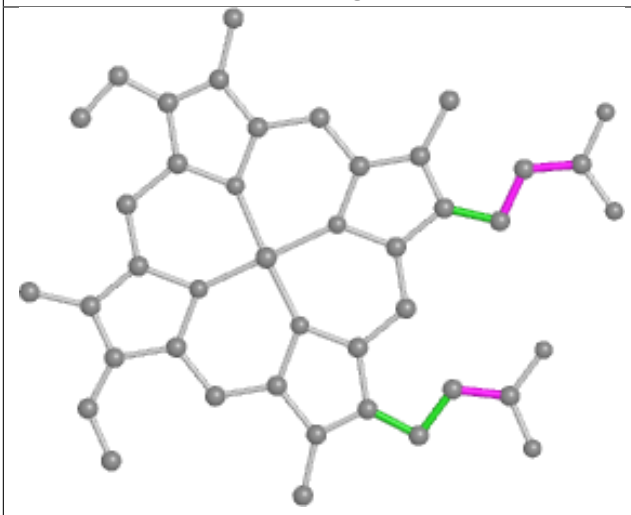
Ligand HEC C 402



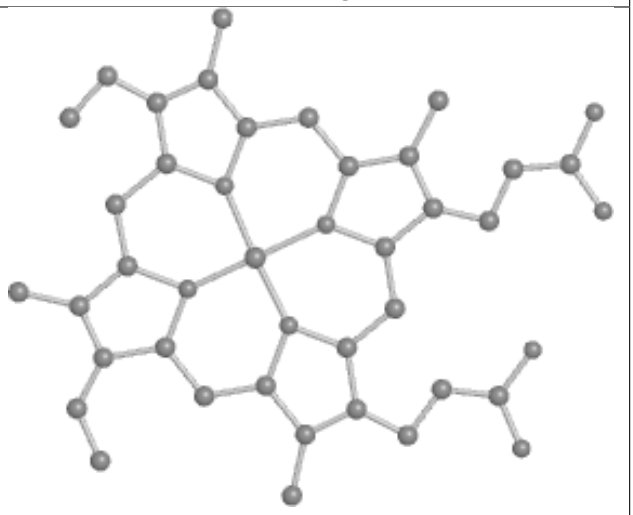
Bond lengths



Bond angles

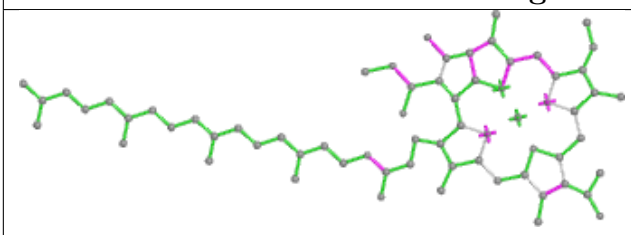


Torsions

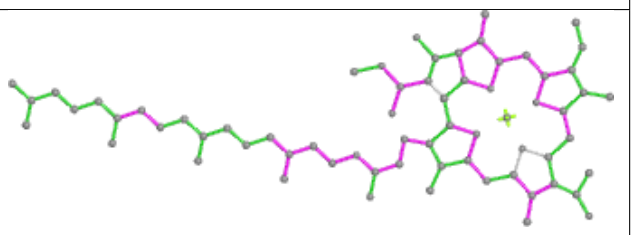


Rings

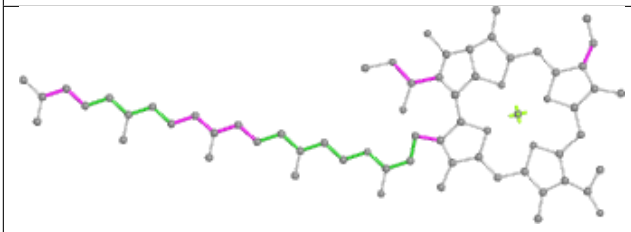
Ligand BCL 5 101



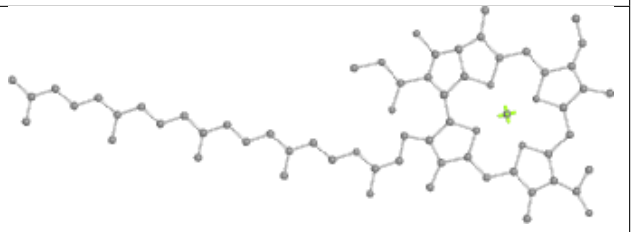
Bond lengths



Bond angles

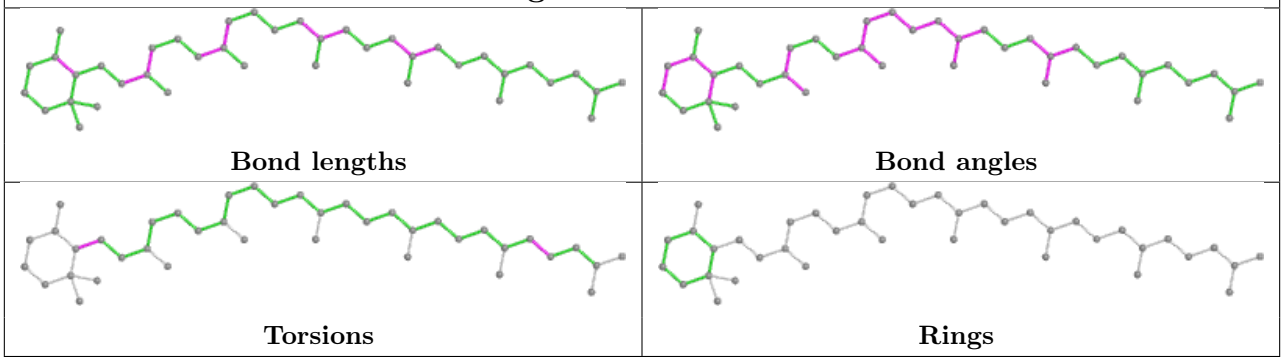


Torsions

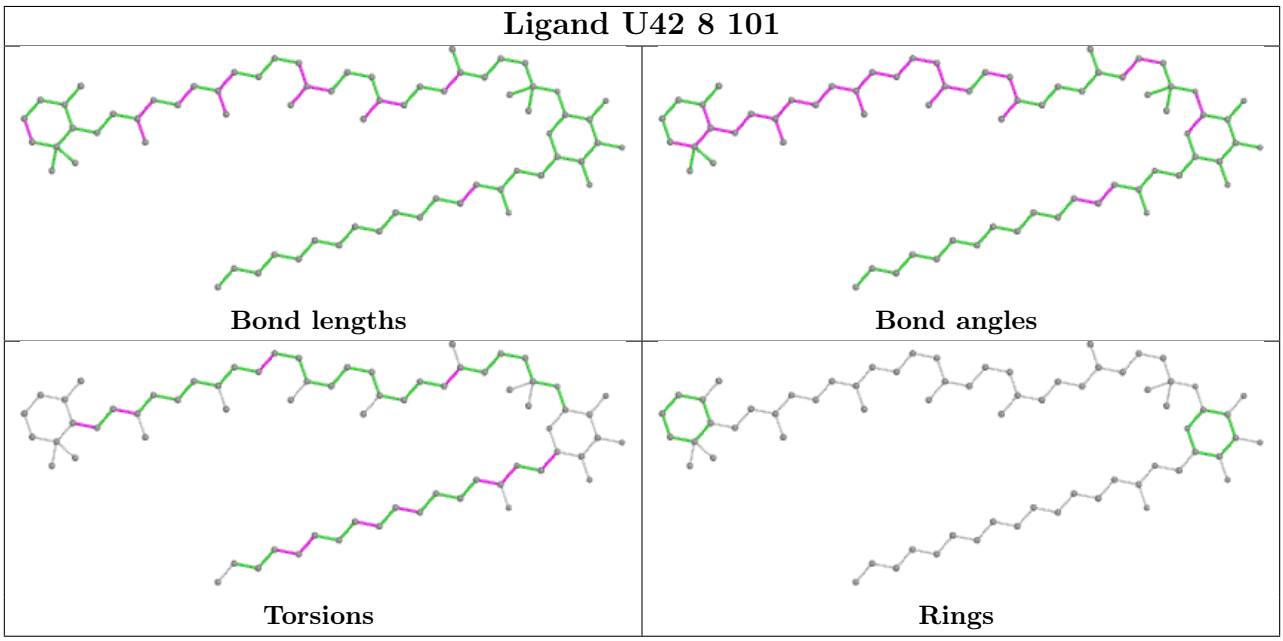


Rings

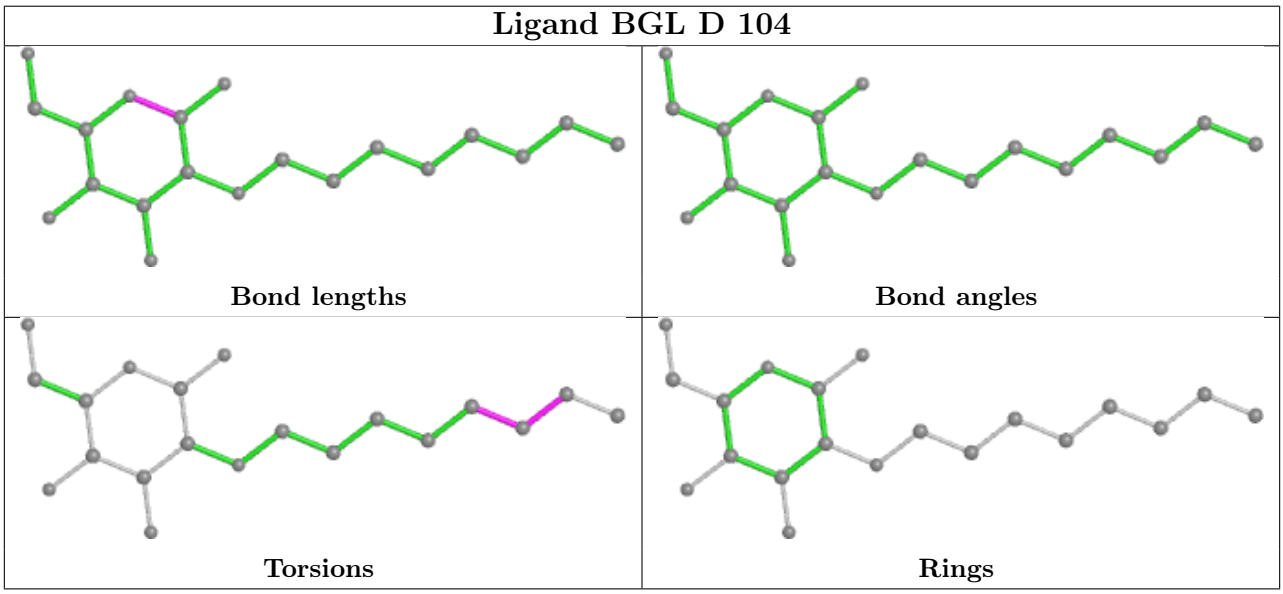
Ligand U4Z H 102



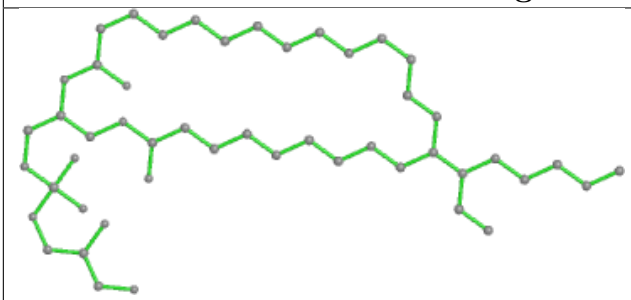
Ligand U42 8 101



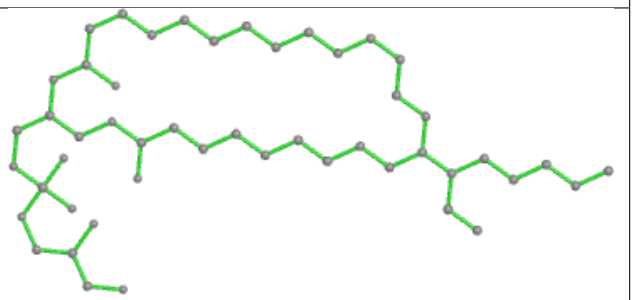
Ligand BGL D 104



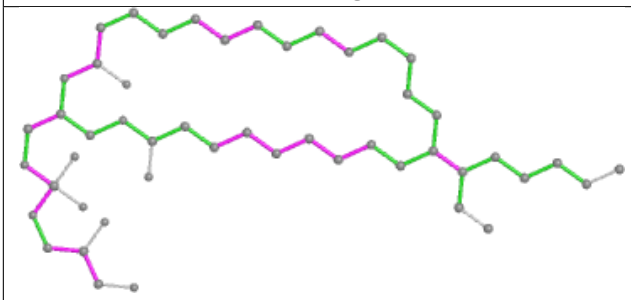
Ligand PGV L 1008



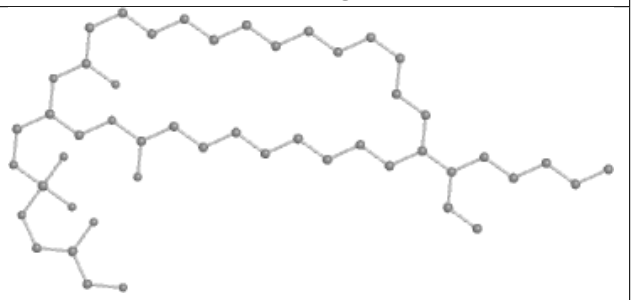
Bond lengths



Bond angles

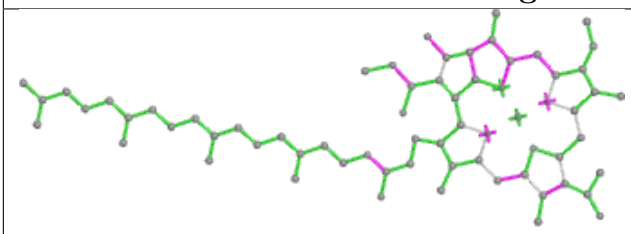


Torsions

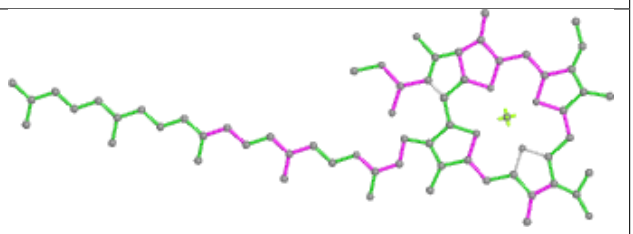


Rings

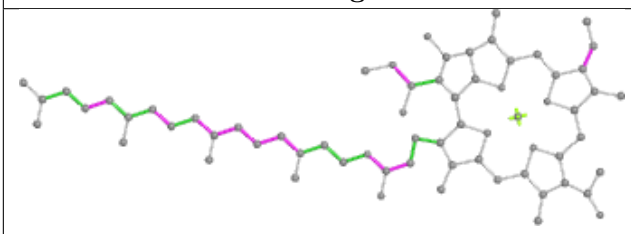
Ligand BCL W 102



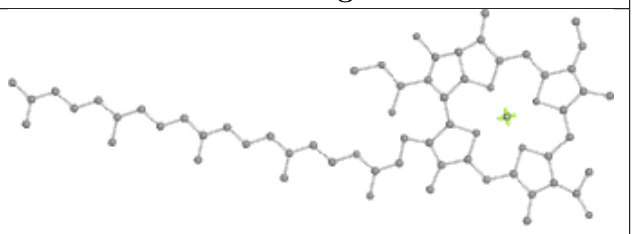
Bond lengths



Bond angles

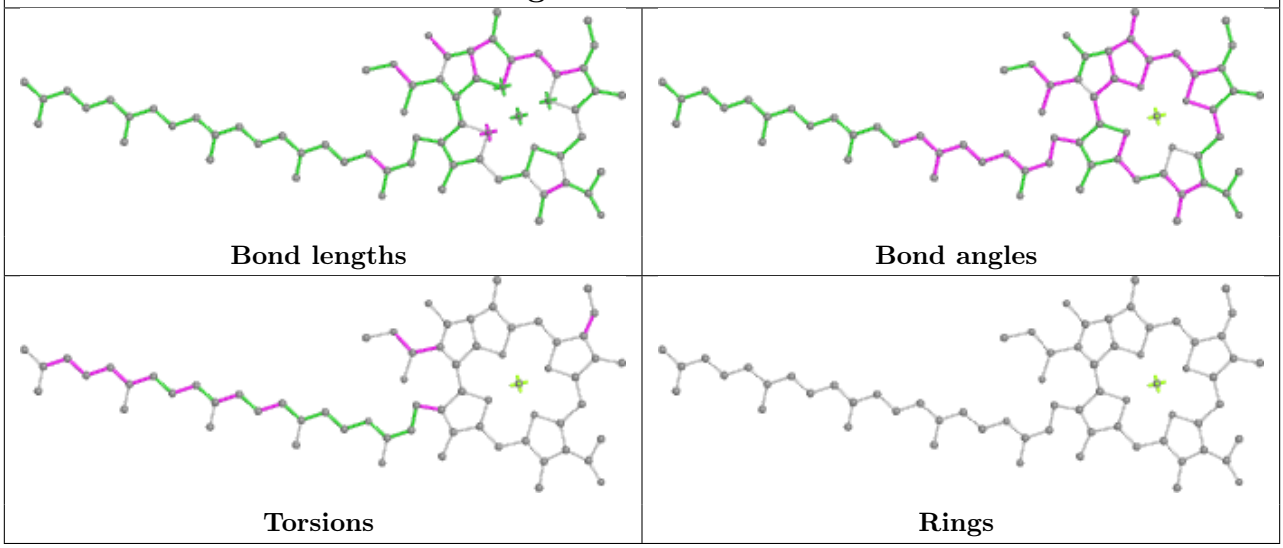


Torsions

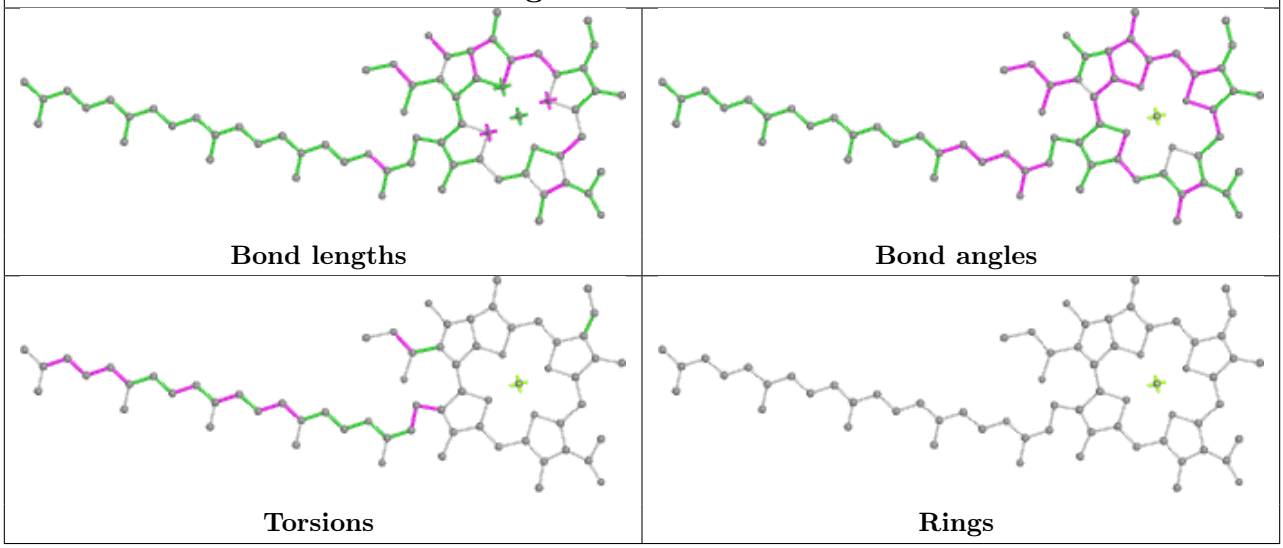


Rings

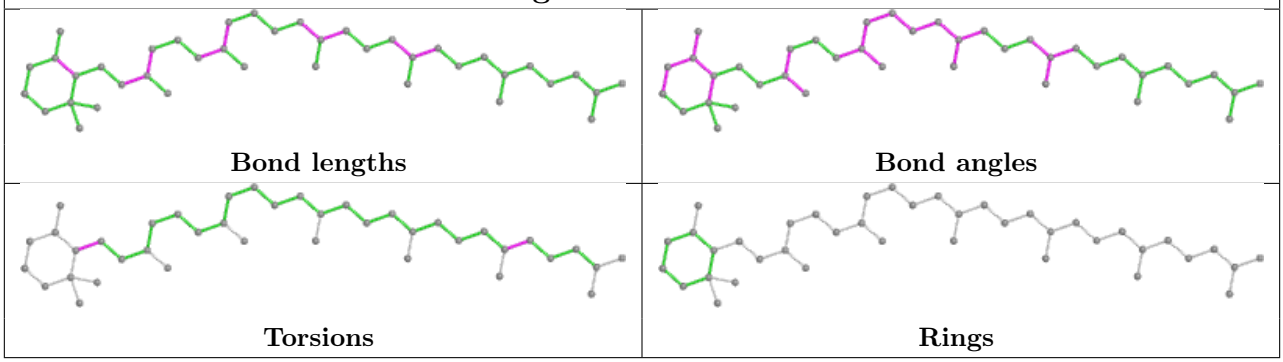
Ligand BCL F 101



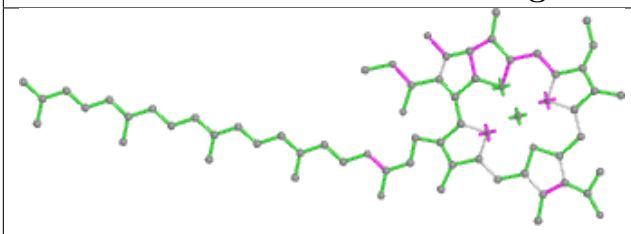
Ligand BCL V 101



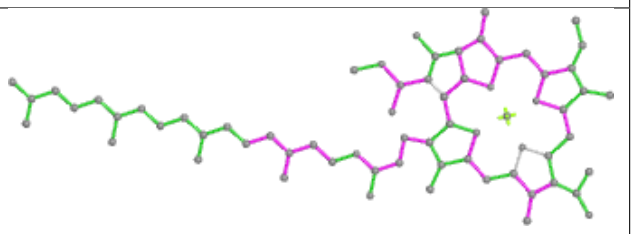
Ligand U4Z J 102



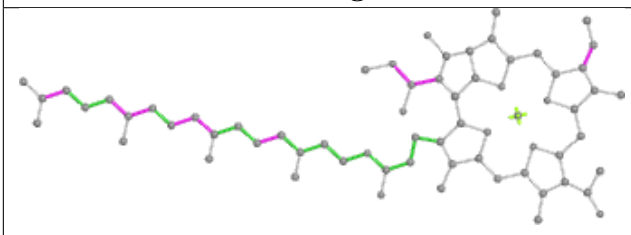
Ligand BCL J 101



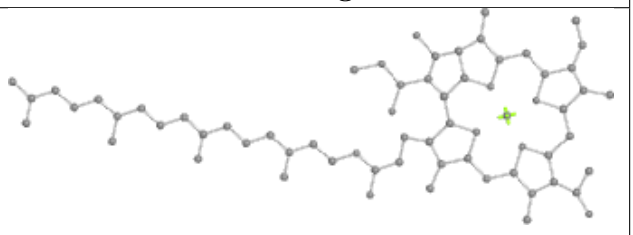
Bond lengths



Bond angles

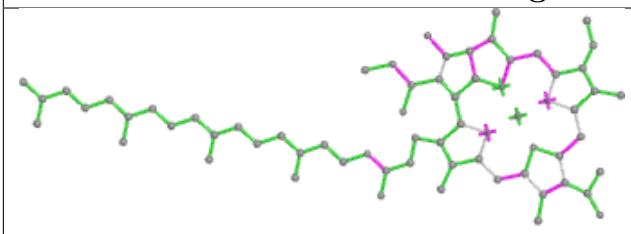


Torsions

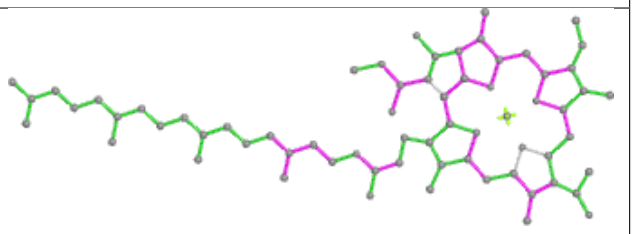


Rings

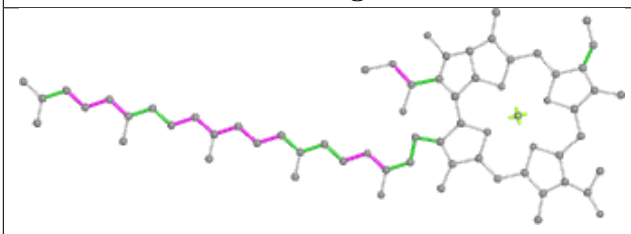
Ligand BCL 8 102



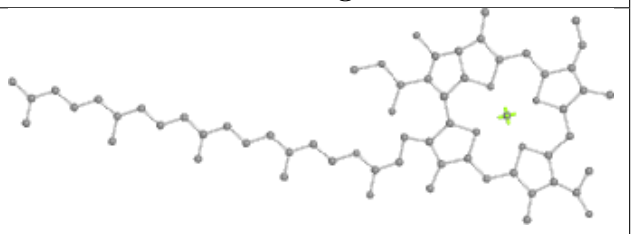
Bond lengths



Bond angles

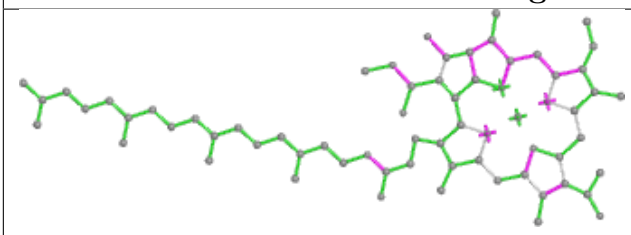


Torsions

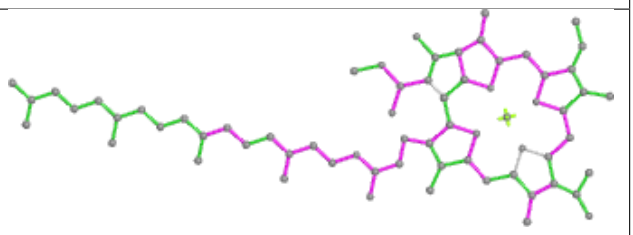


Rings

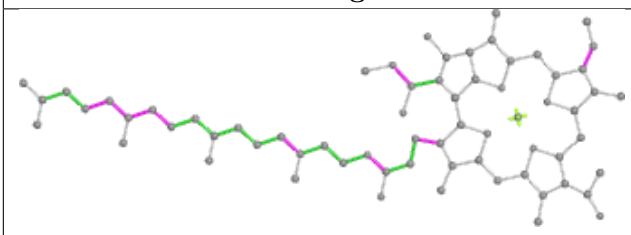
Ligand BCL 4 103



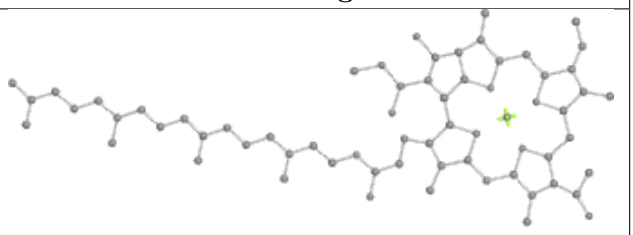
Bond lengths



Bond angles

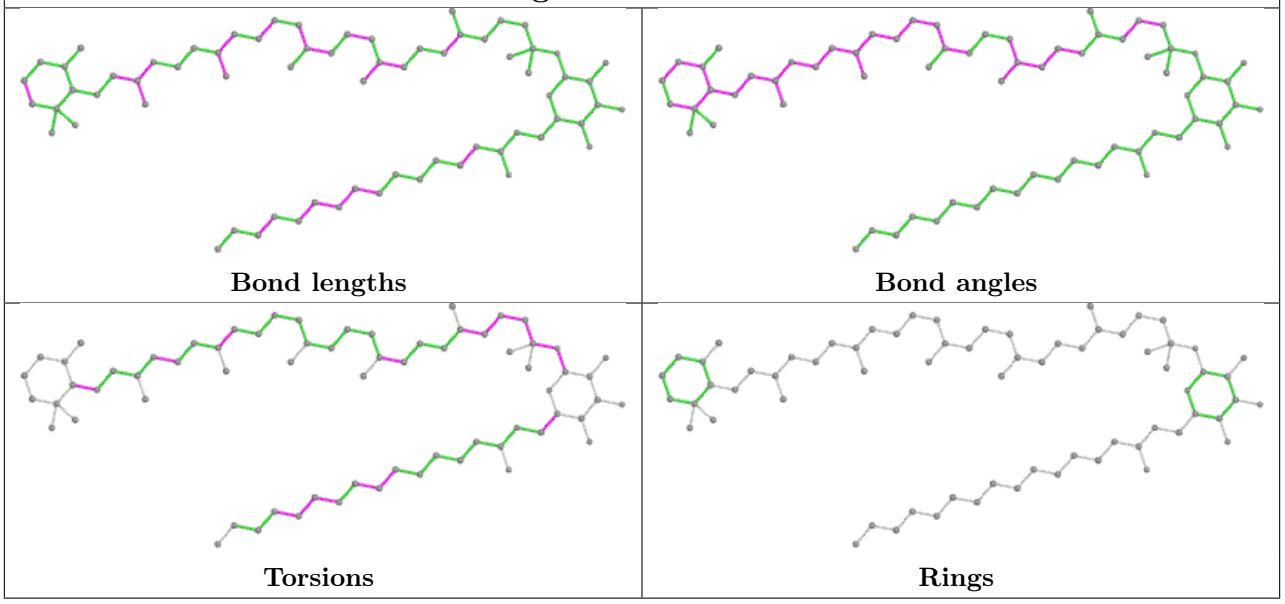


Torsions

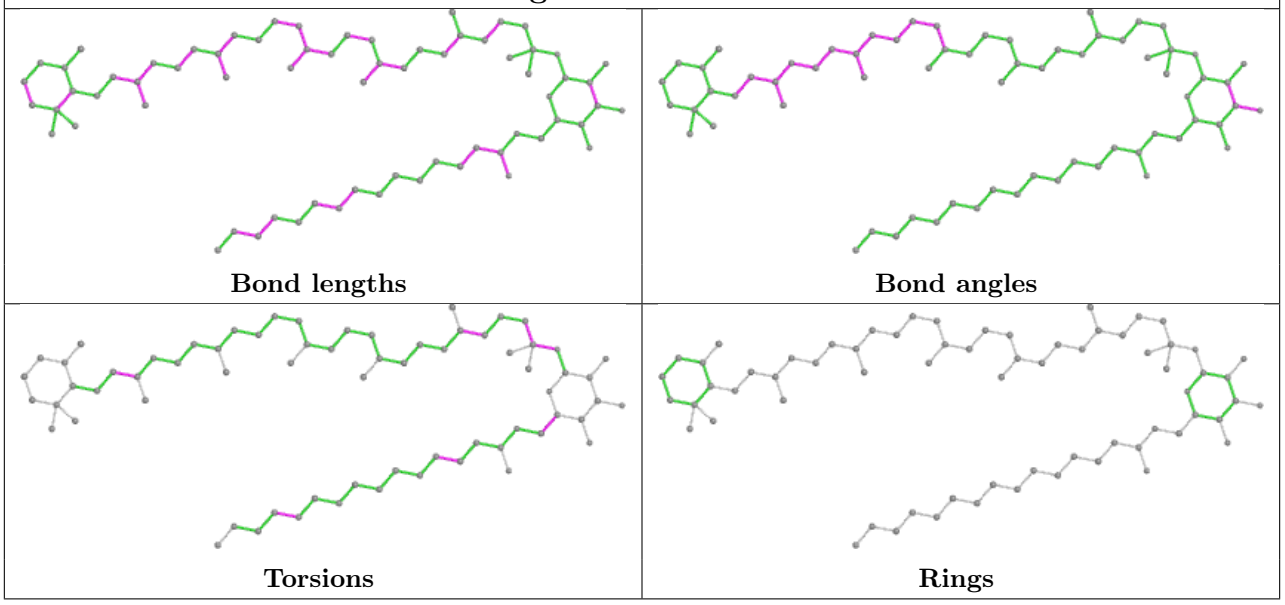


Rings

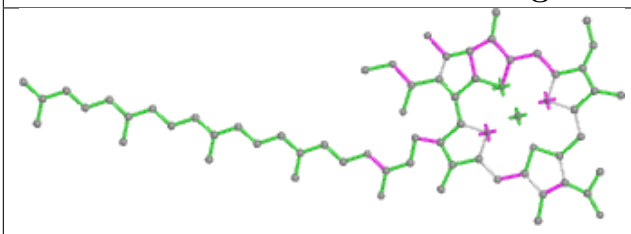
Ligand U42 E 101



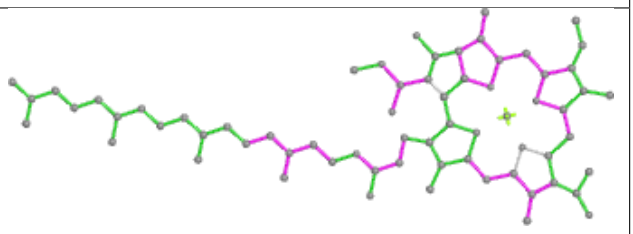
Ligand U42 G 101



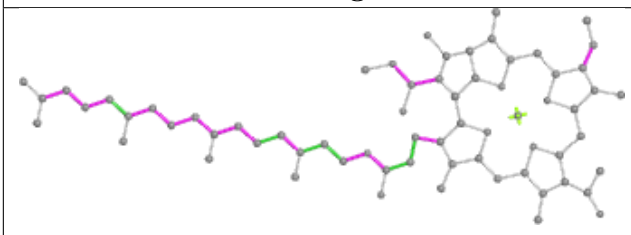
Ligand BCL I 103



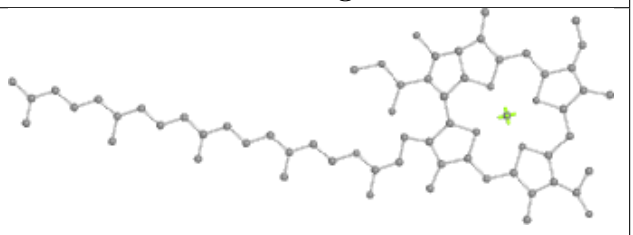
Bond lengths



Bond angles

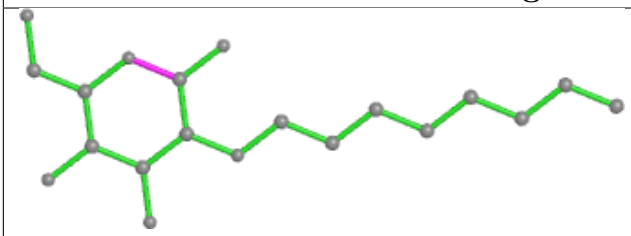


Torsions

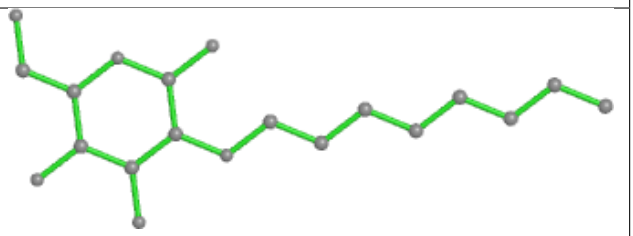


Rings

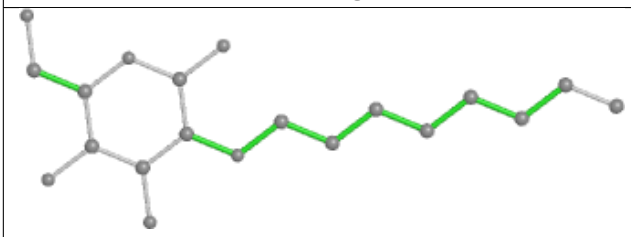
Ligand BGL H 103



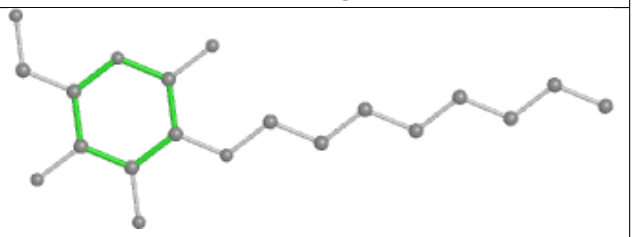
Bond lengths



Bond angles

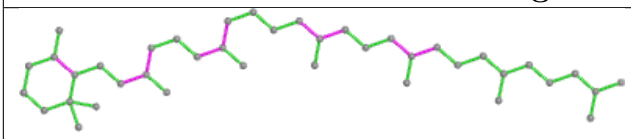


Torsions

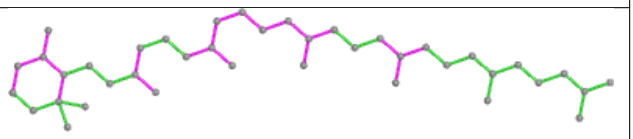


Rings

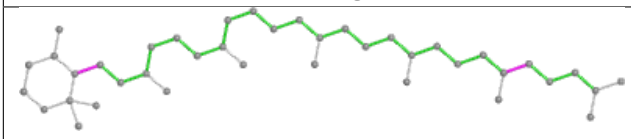
Ligand U4Z 3 102



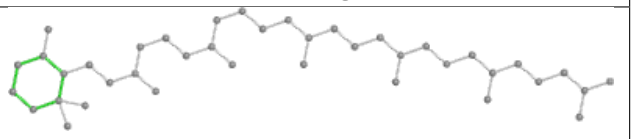
Bond lengths



Bond angles

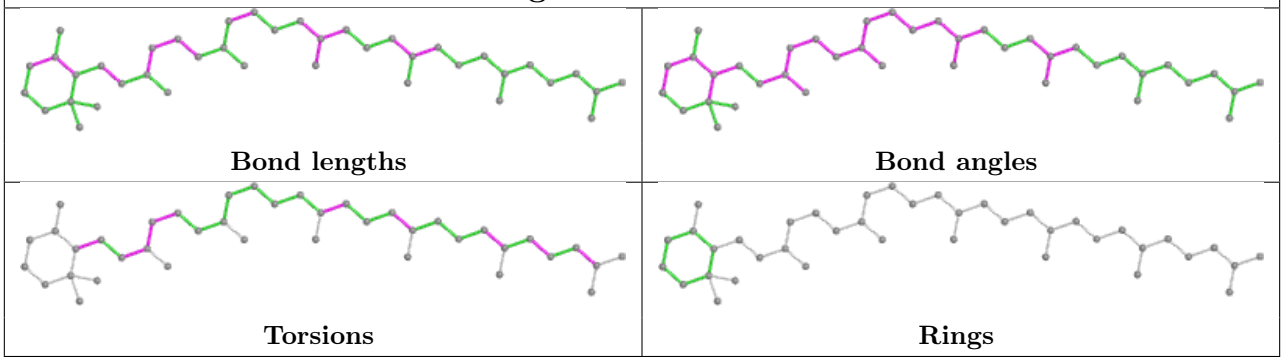


Torsions

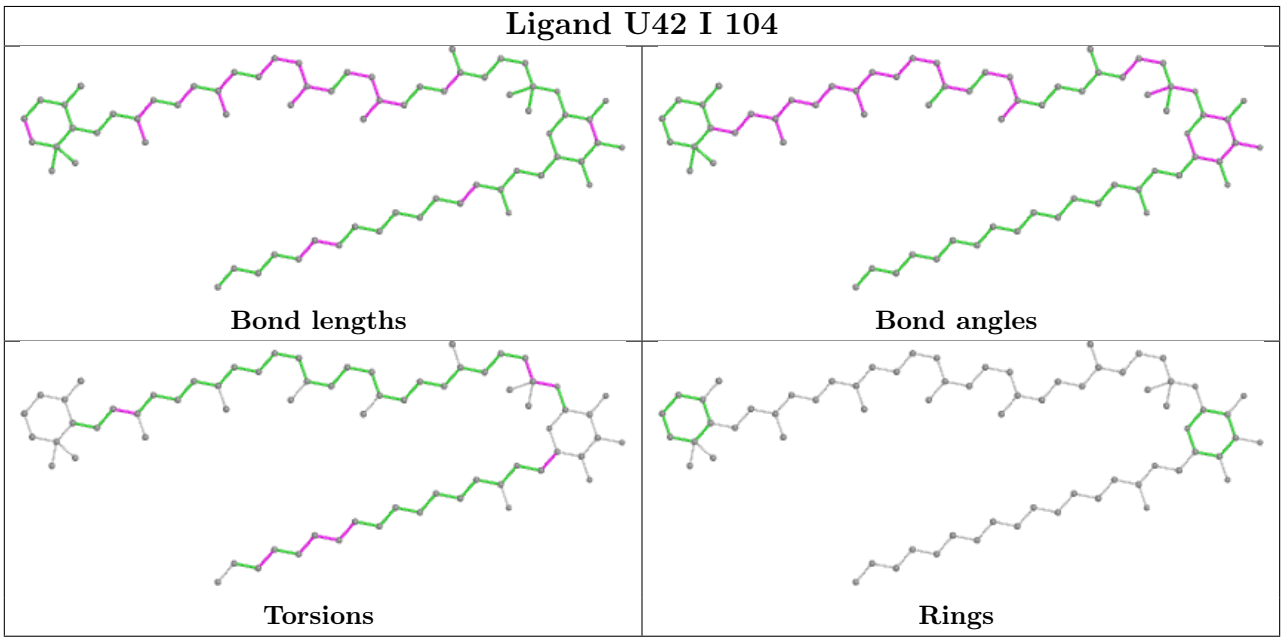


Rings

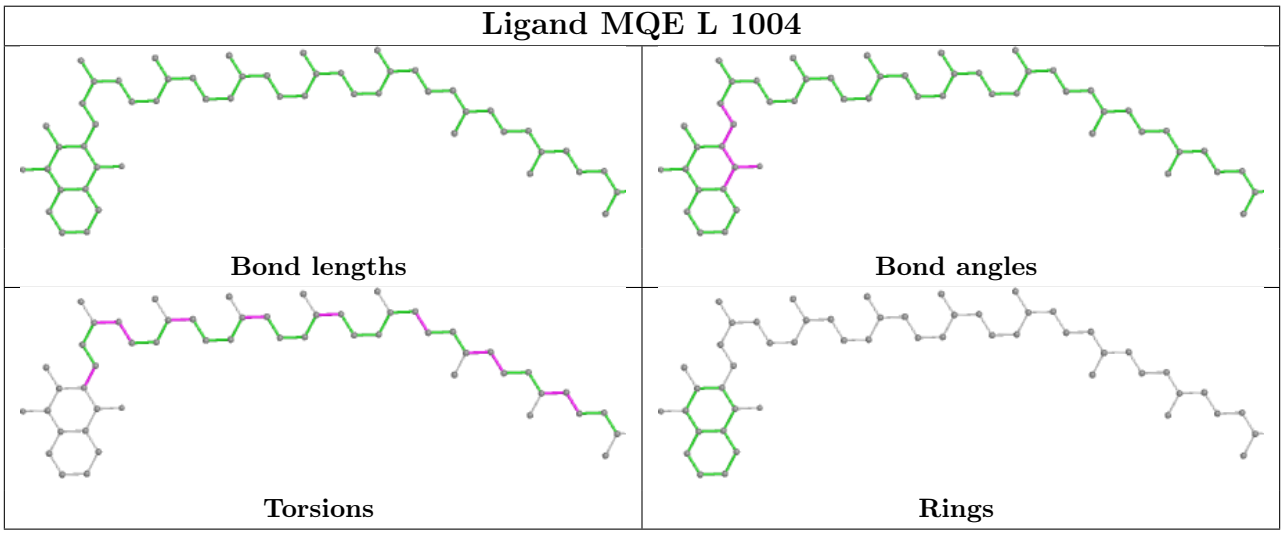
Ligand U4Z C 401



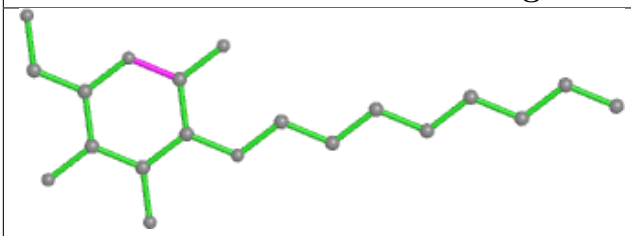
Ligand U42 I 104



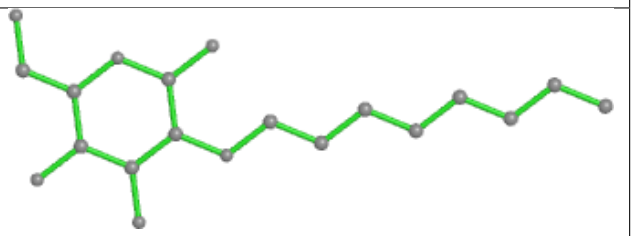
Ligand MQE L 1004



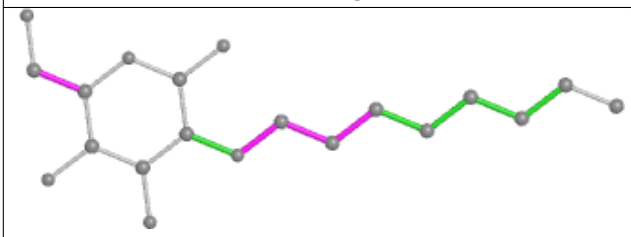
Ligand BGL N 103



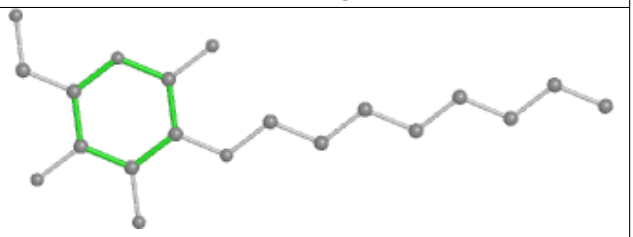
Bond lengths



Bond angles

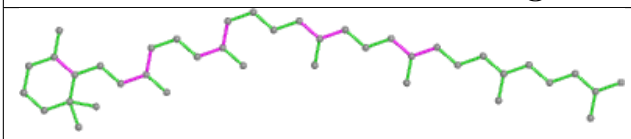


Torsions

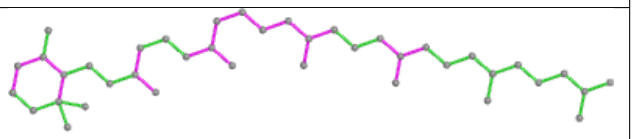


Rings

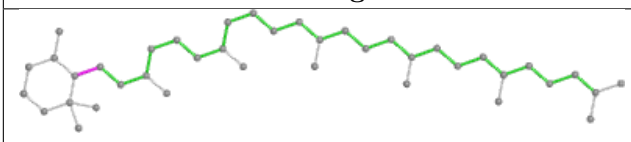
Ligand U4Z N 102



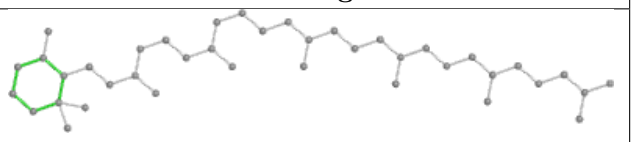
Bond lengths



Bond angles

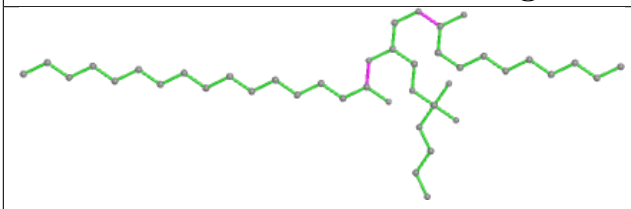


Torsions

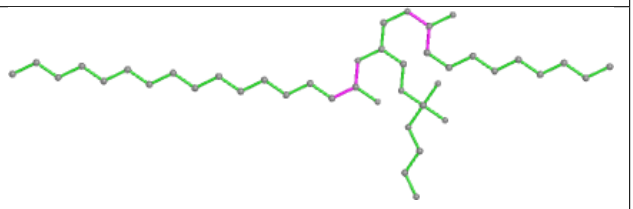


Rings

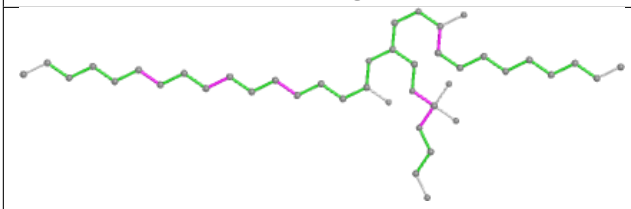
Ligand PEF L 1017



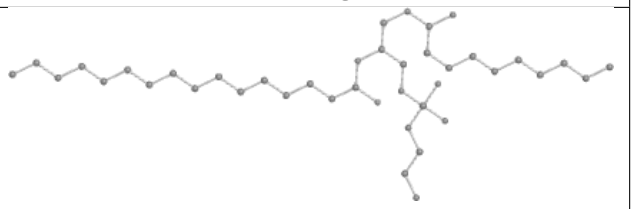
Bond lengths



Bond angles

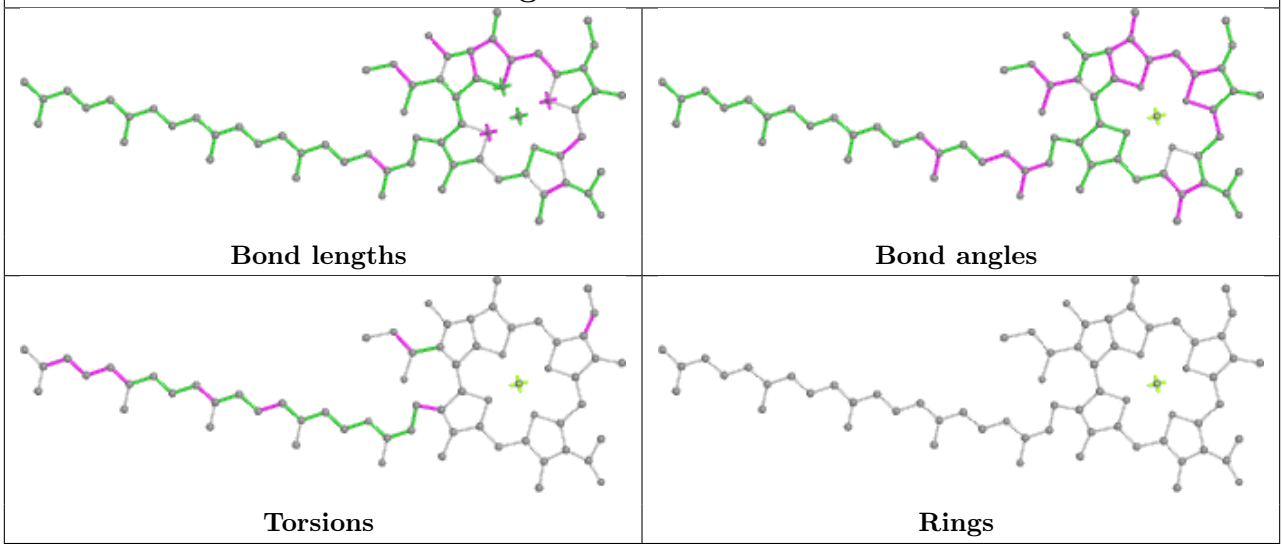


Torsions



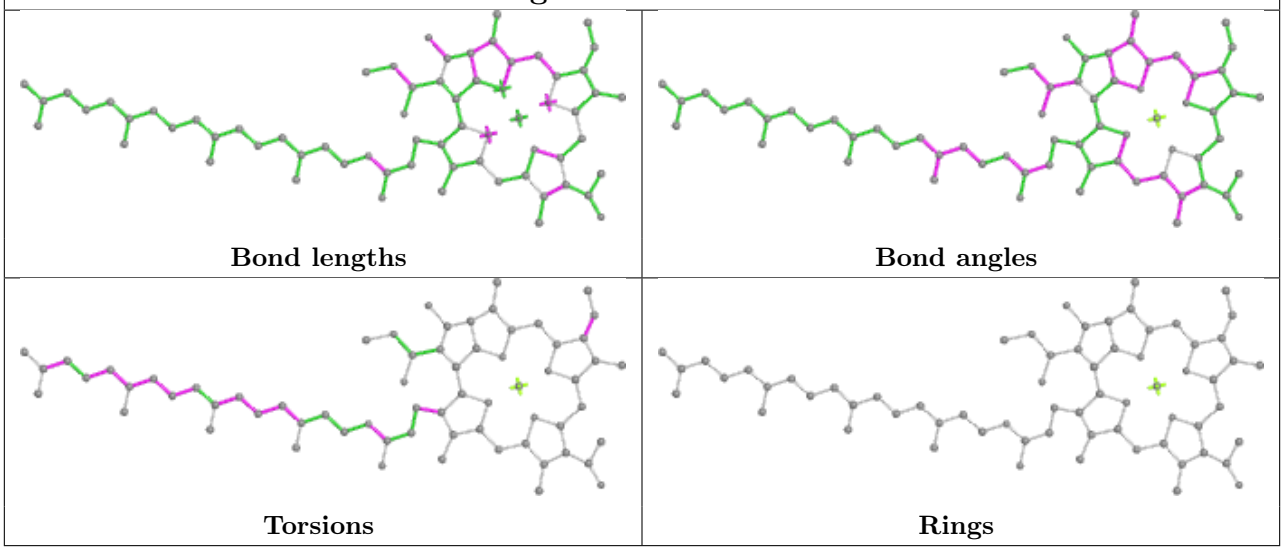
Rings

Ligand BCL L 1001

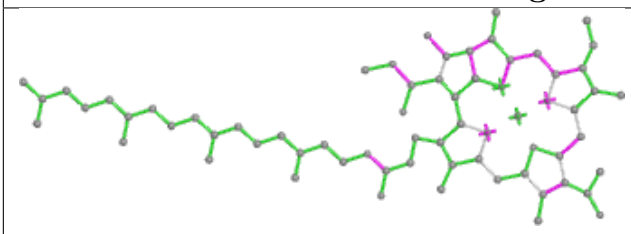


Ligand U4Z 9 101

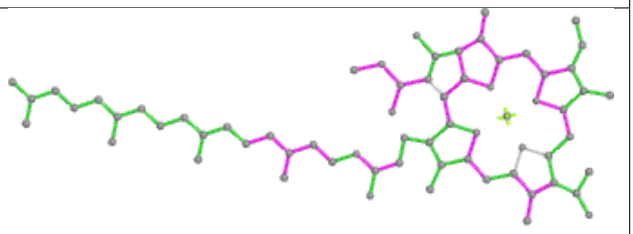
Ligand BCL 6 102



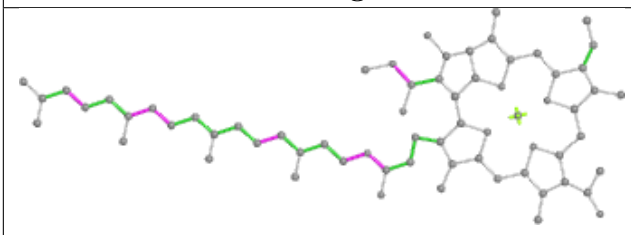
Ligand BCL 6 101



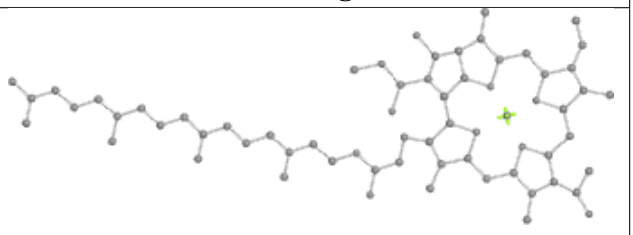
Bond lengths



Bond angles

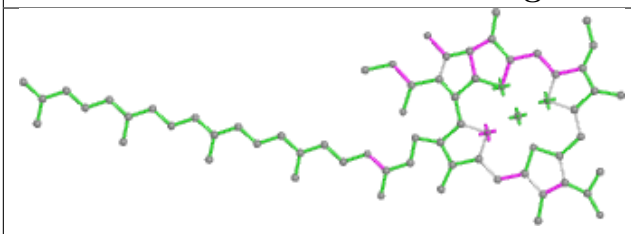


Torsions

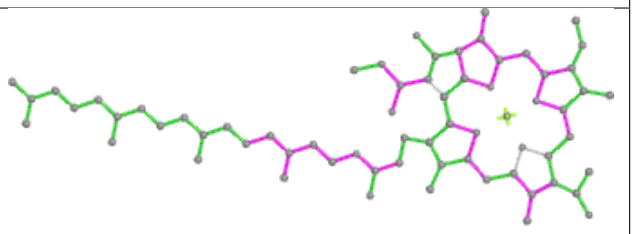


Rings

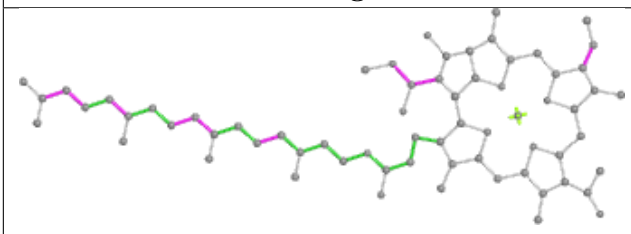
Ligand BCL H 101



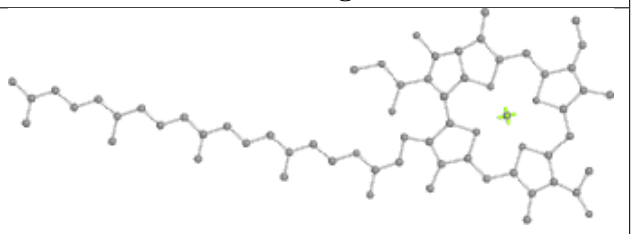
Bond lengths



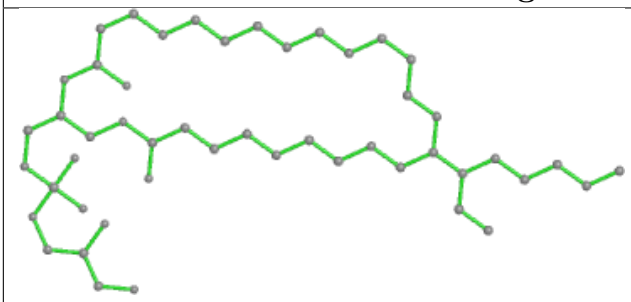
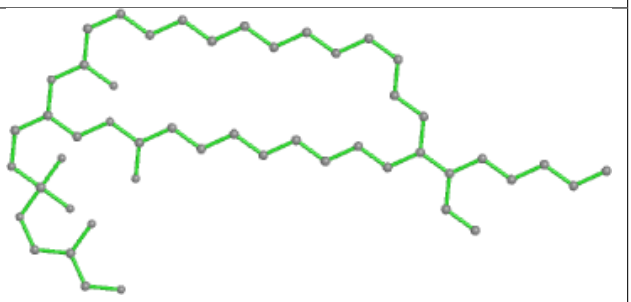
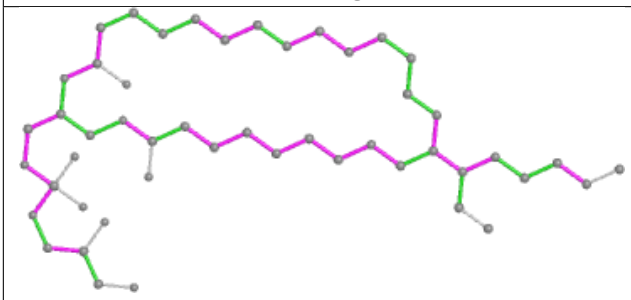
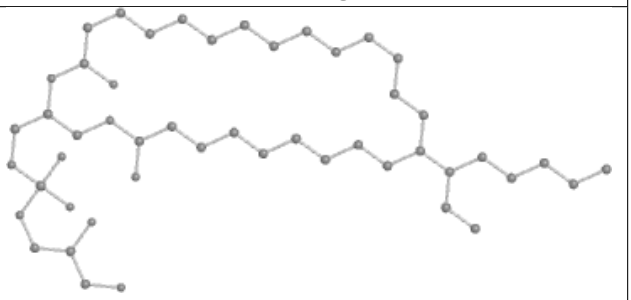
Bond angles

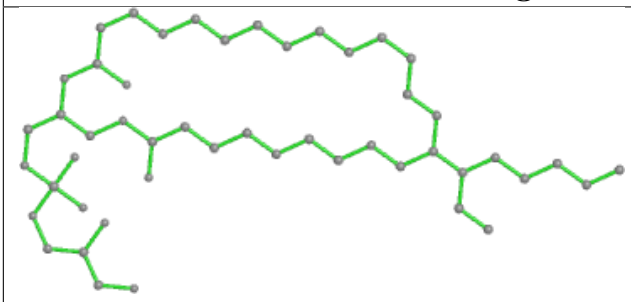
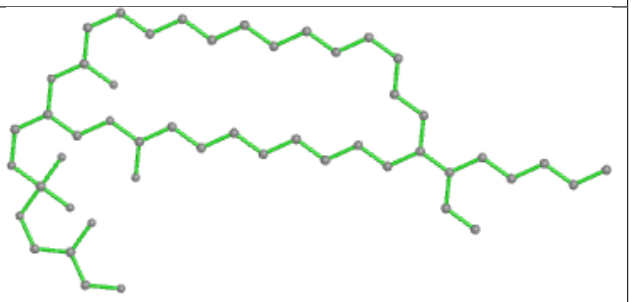
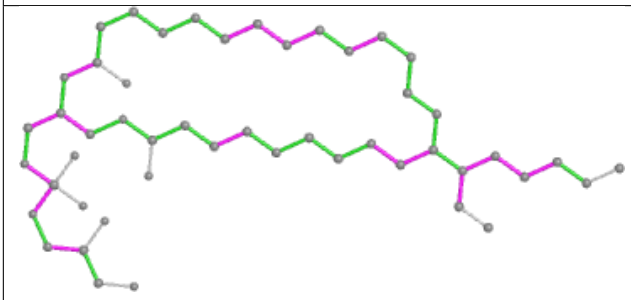
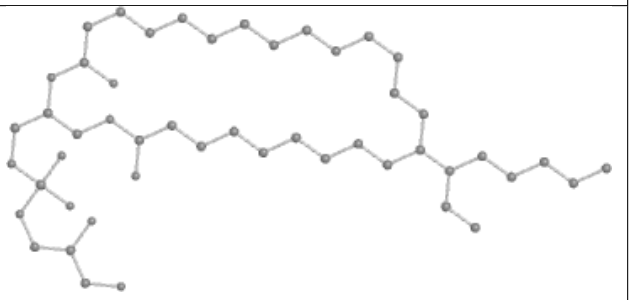


Torsions

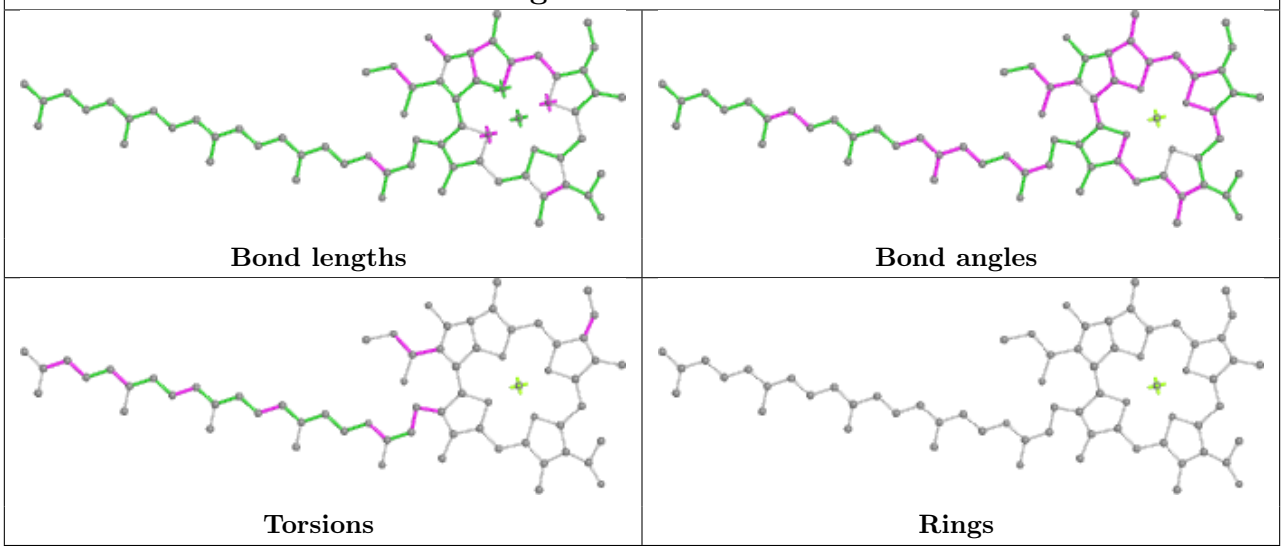


Rings

Ligand PGV M 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV L 1006	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 3 101



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.

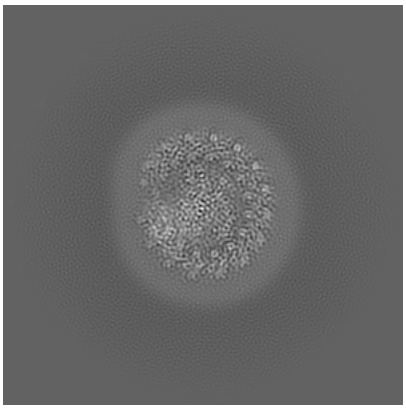
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35721. These allow visual inspection of the internal detail of the map and identification of artifacts.

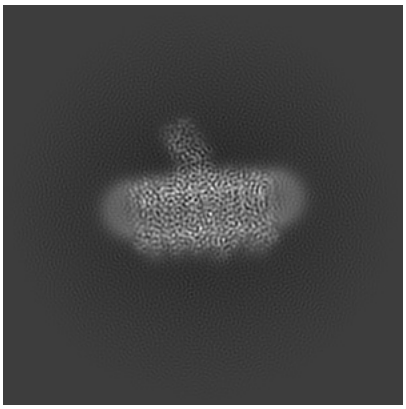
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

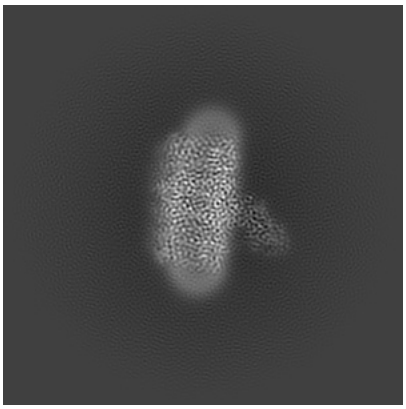
6.1.1 Primary map



X

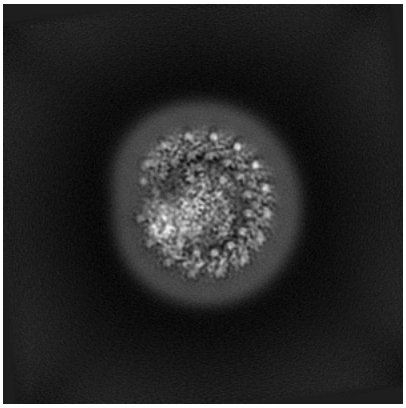


Y

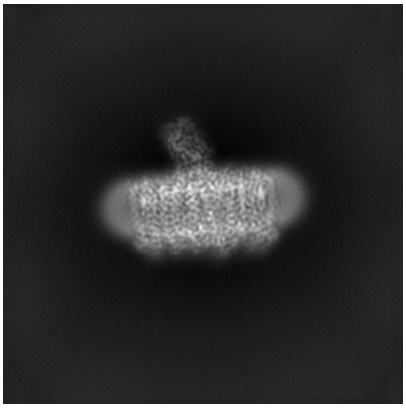


Z

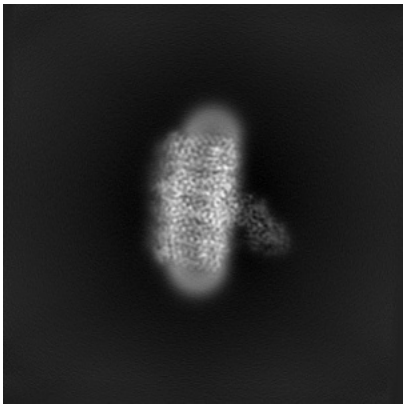
6.1.2 Raw map



X



Y

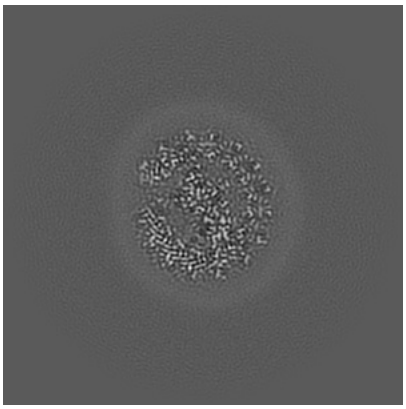


Z

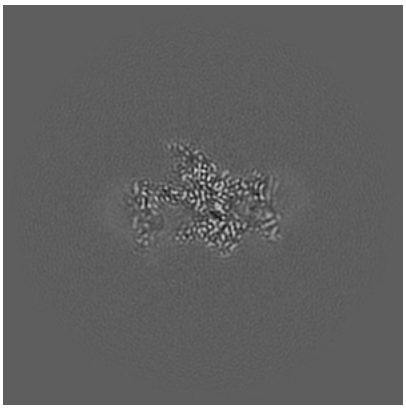
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

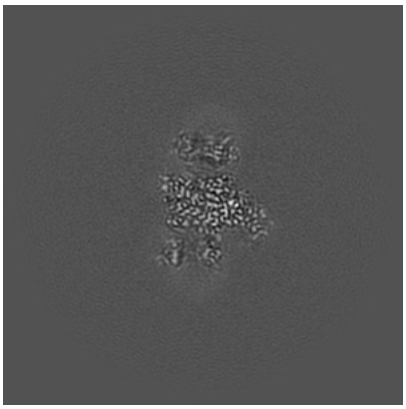
6.2.1 Primary map



X Index: 180

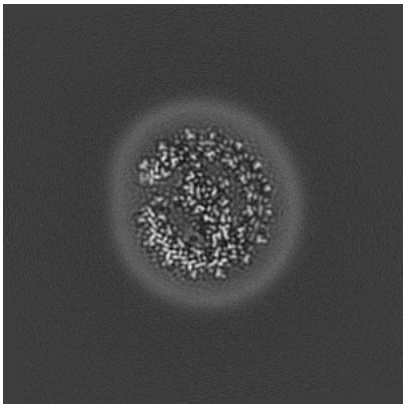


Y Index: 180

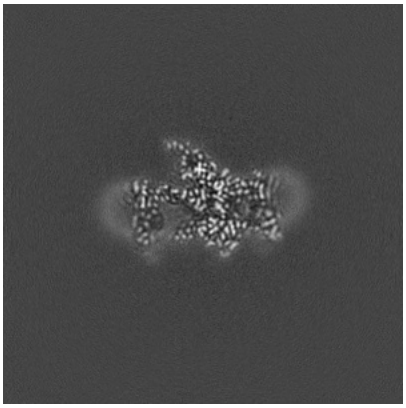


Z Index: 180

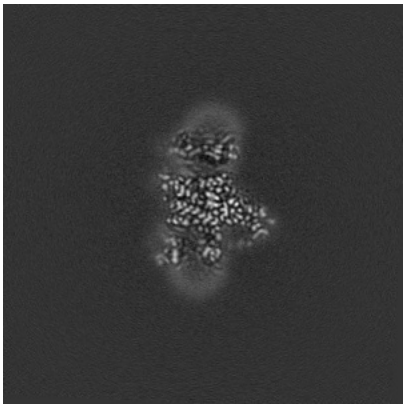
6.2.2 Raw map



X Index: 180



Y Index: 180

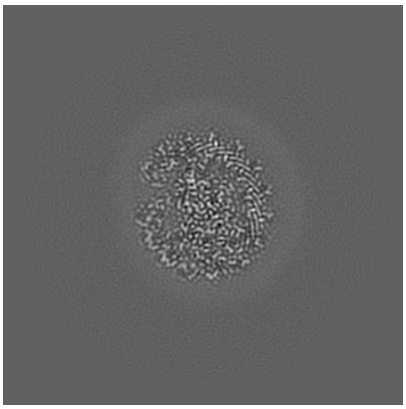


Z Index: 180

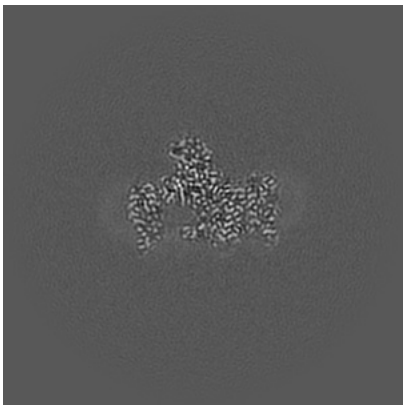
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

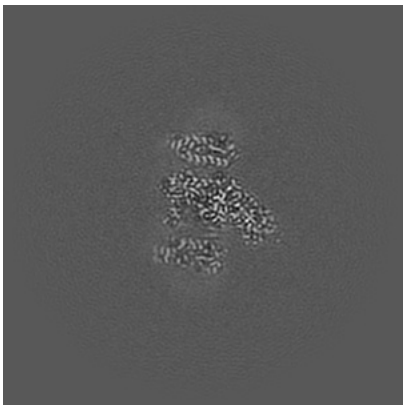
6.3.1 Primary map



X Index: 192

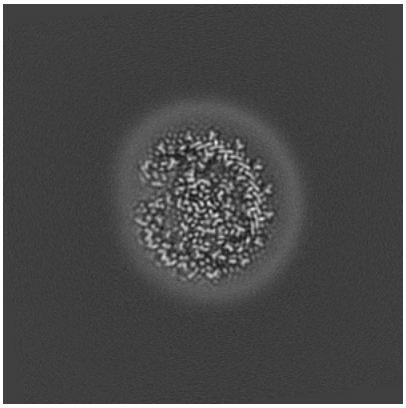


Y Index: 171

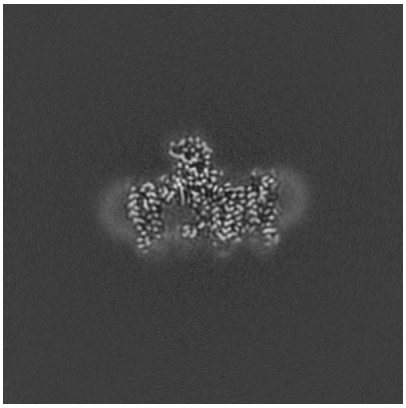


Z Index: 173

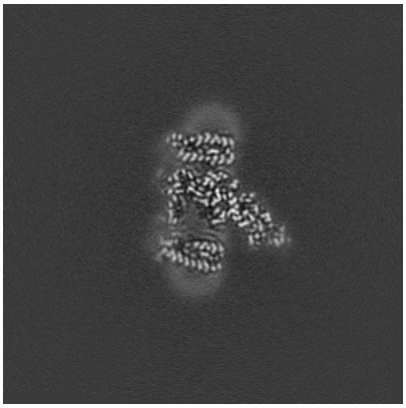
6.3.2 Raw map



X Index: 192



Y Index: 171

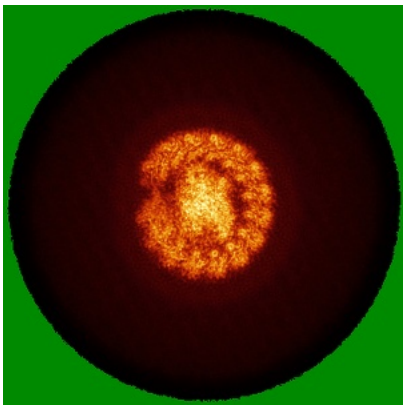


Z Index: 169

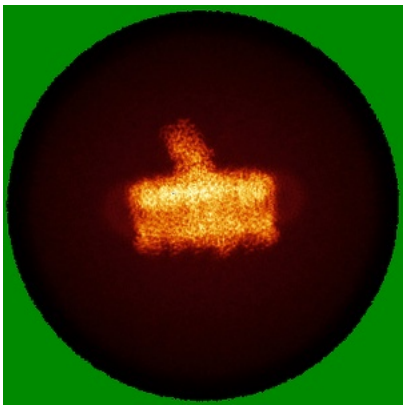
The images above show the largest variance slices of the map in three orthogonal directions.

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

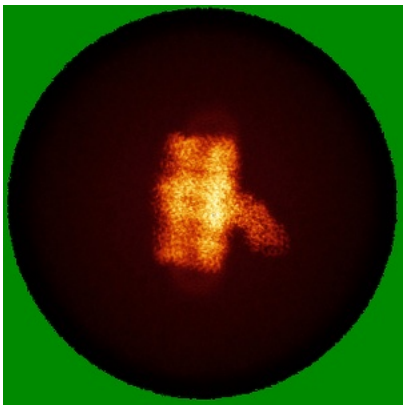
6.4.1 Primary map



X

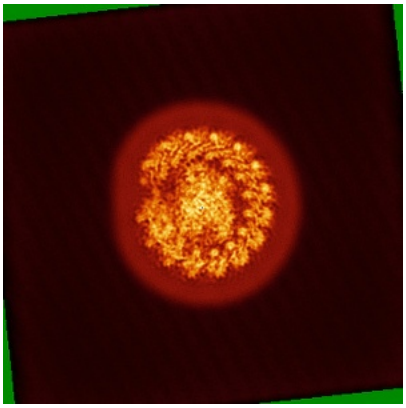


Y

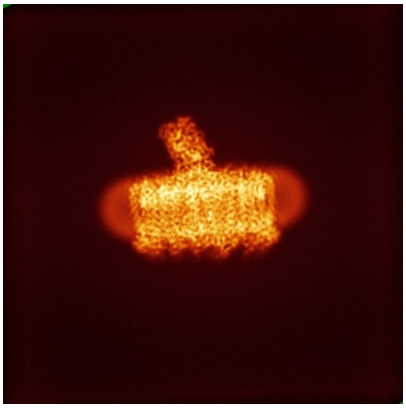


Z

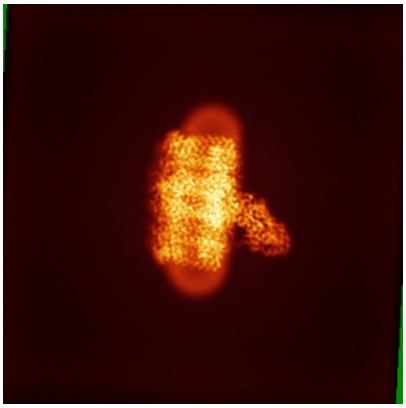
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.226. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

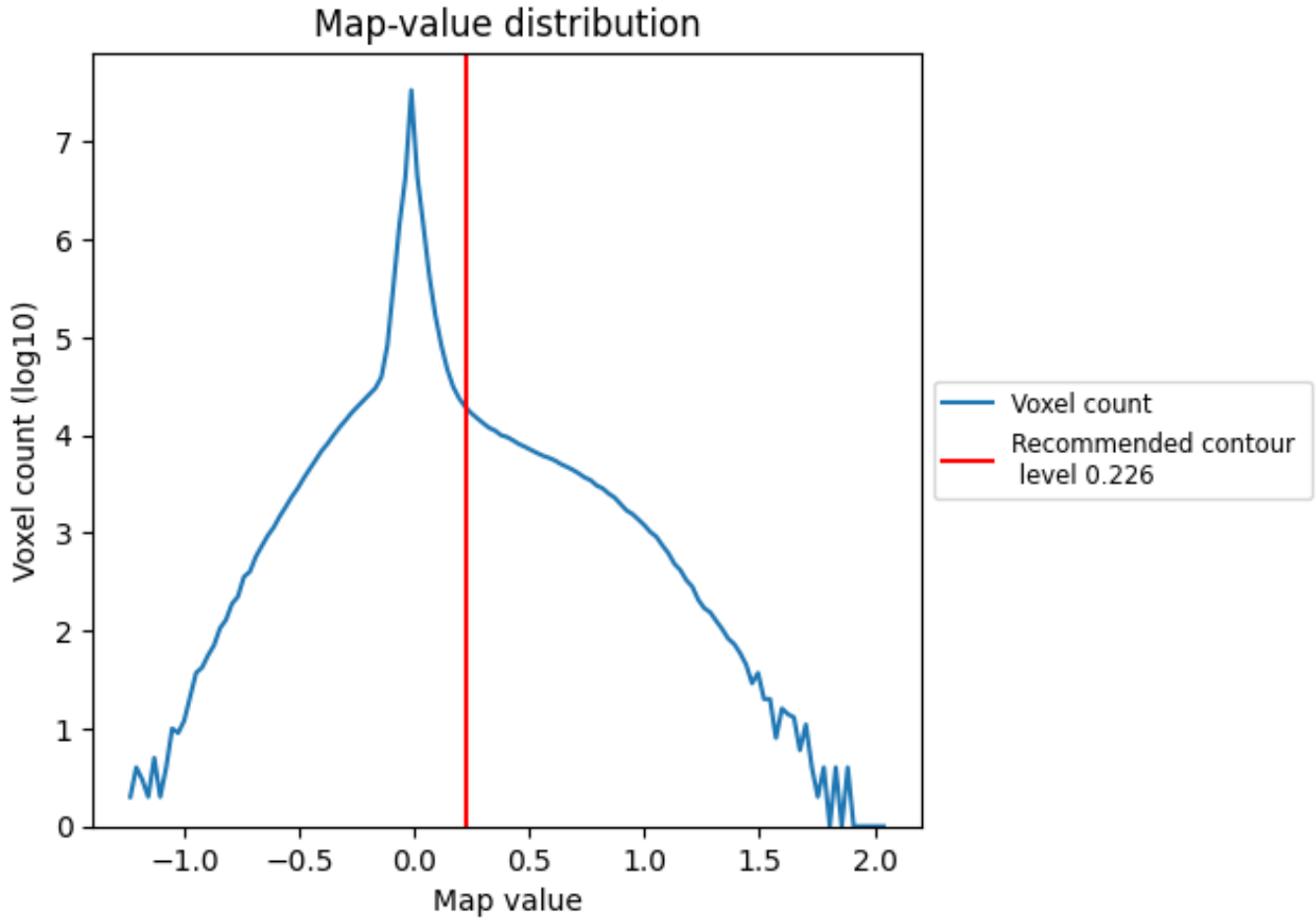
6.6 Mask visualisation (i)

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

7 Map analysis

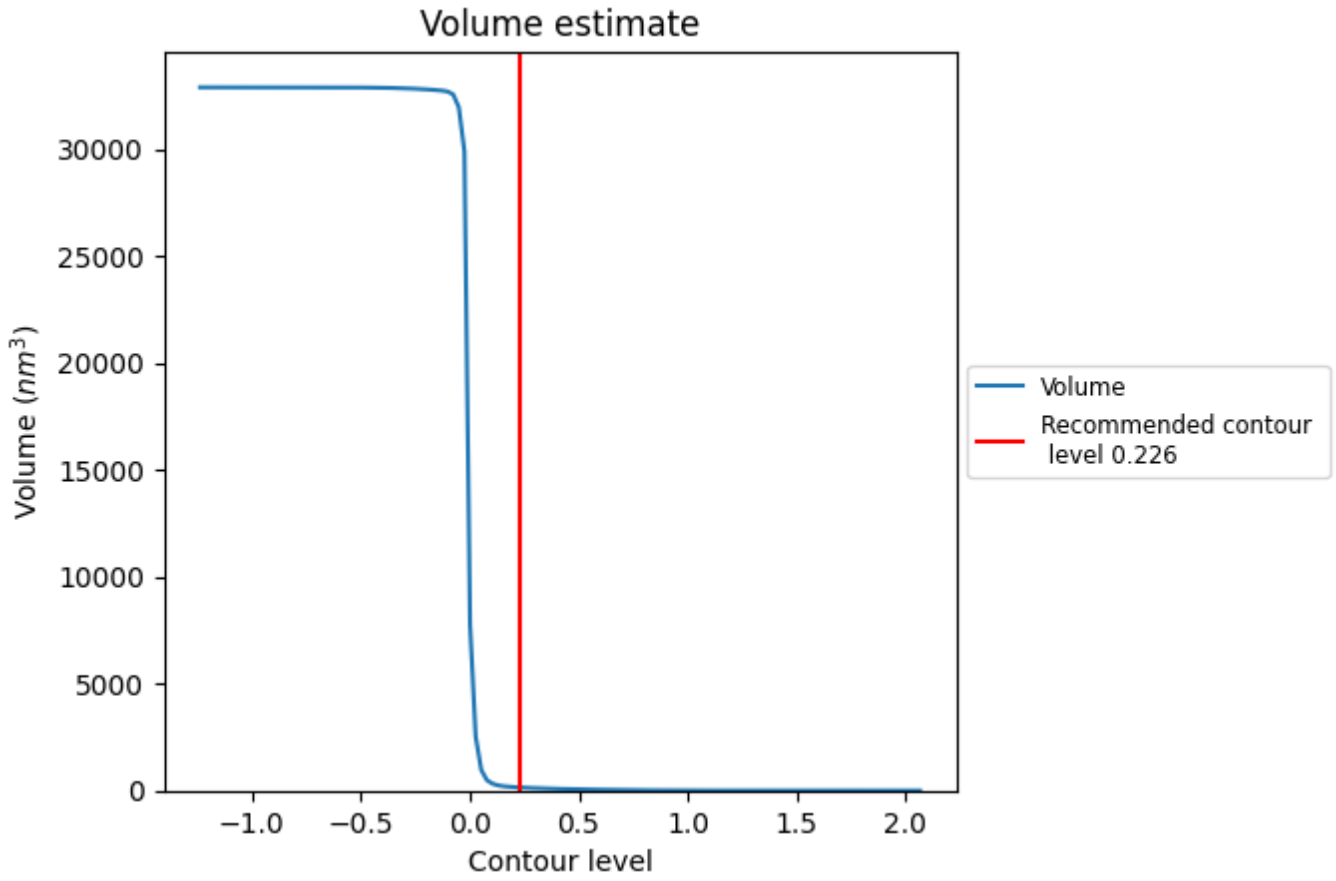
This section contains the results of statistical analysis of the map.

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.

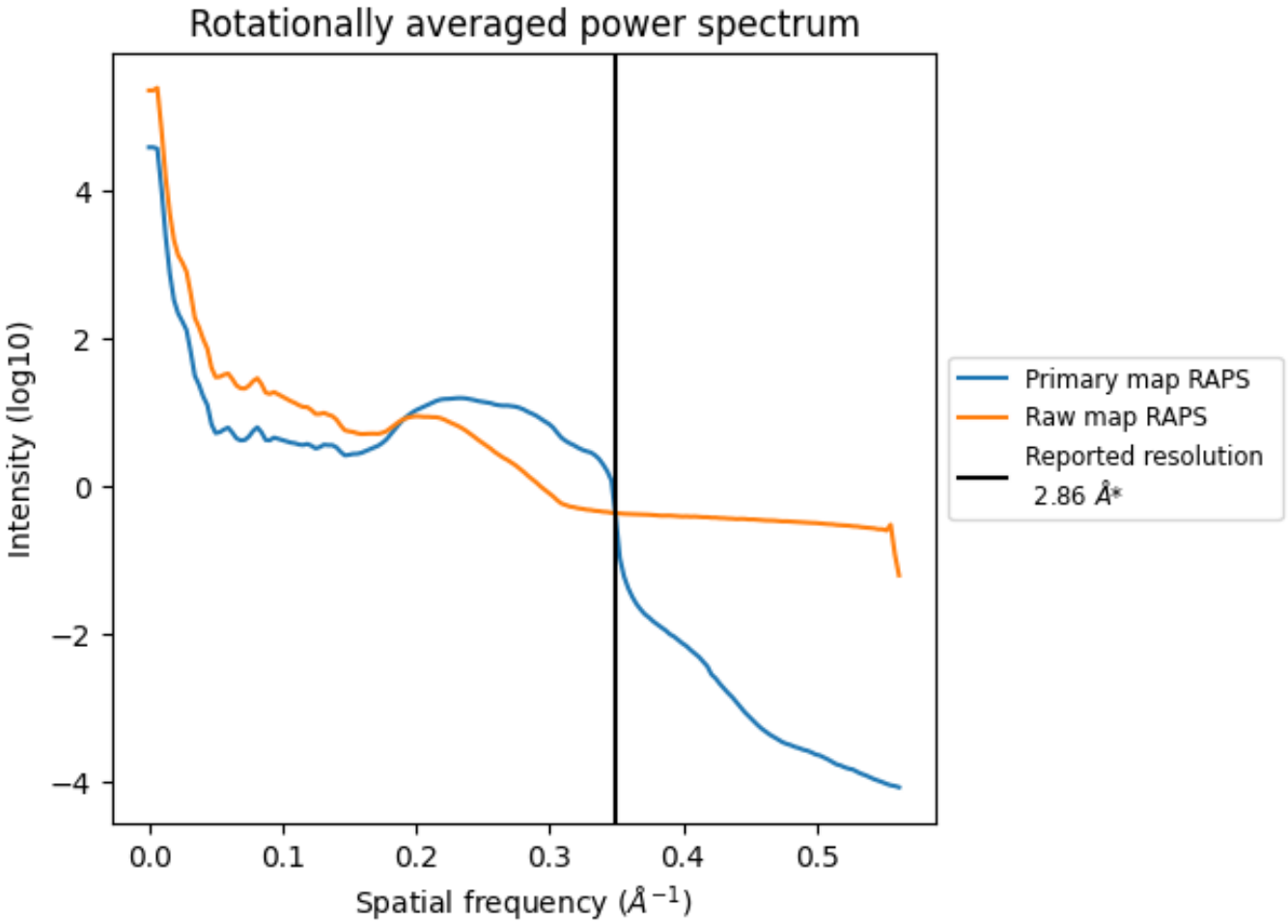
7.2 Volume estimate (i)



The volume at the recommended contour level is 146 nm^3; this corresponds to an approximate mass of 132 kDa.

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

7.3 Rotationally averaged power spectrum (i)

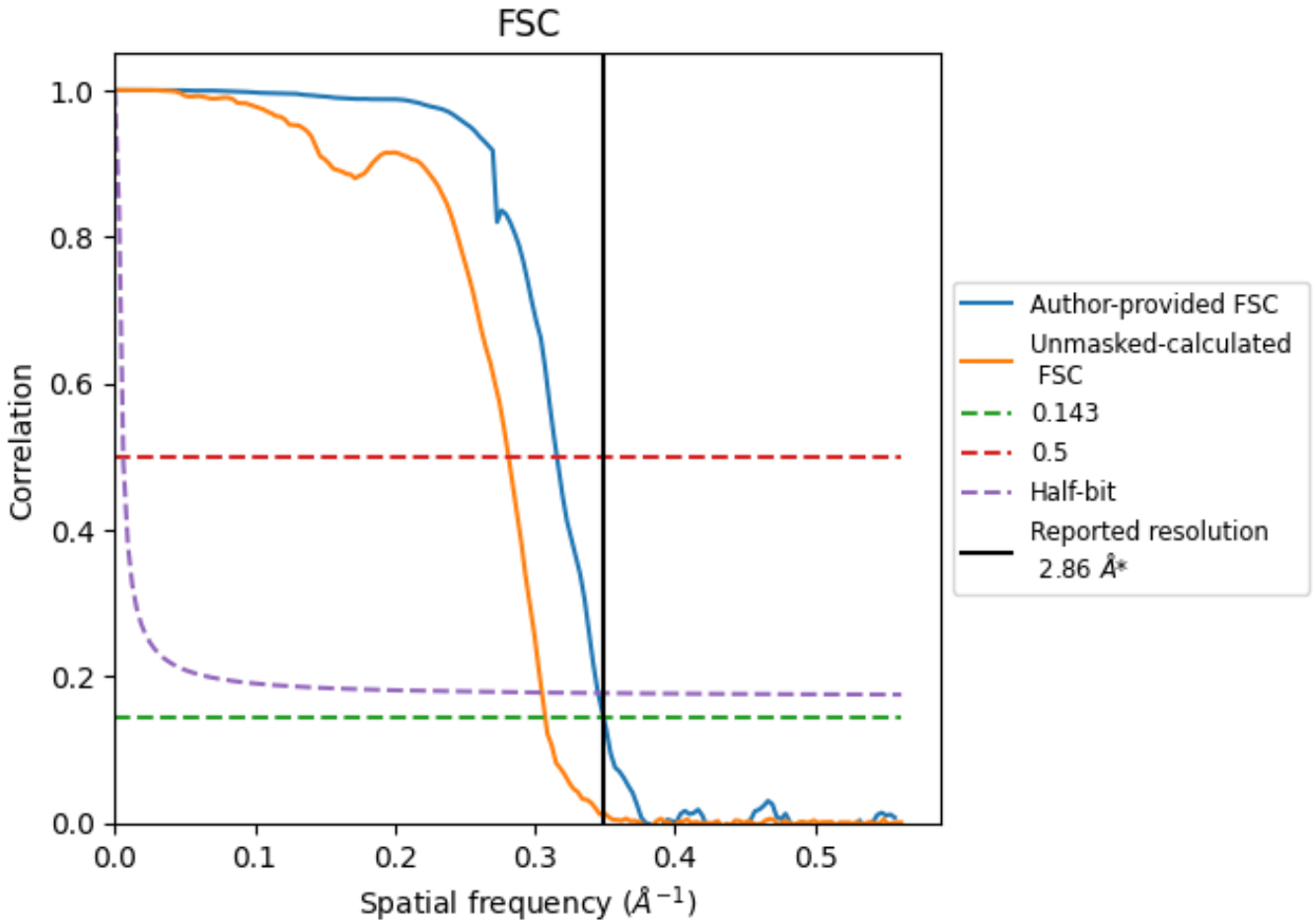


*Reported resolution corresponds to spatial frequency of 0.350 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.350 Å^{-1}

8.2 Resolution estimates (i)

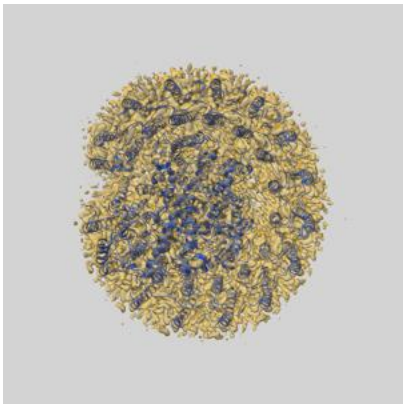
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.17	2.90
Unmasked-calculated*	3.25	3.56	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.86 by more than 10 %

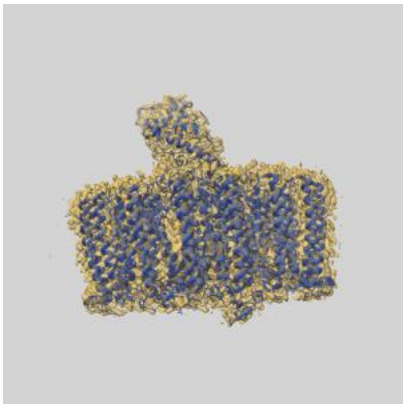
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35721 and PDB model 8IUG. Per-residue inclusion information can be found in section 3 on page 20.

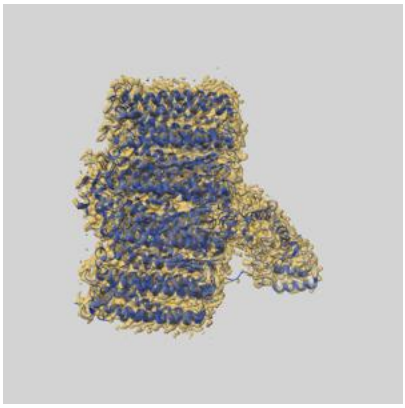
9.1 Map-model overlay



X



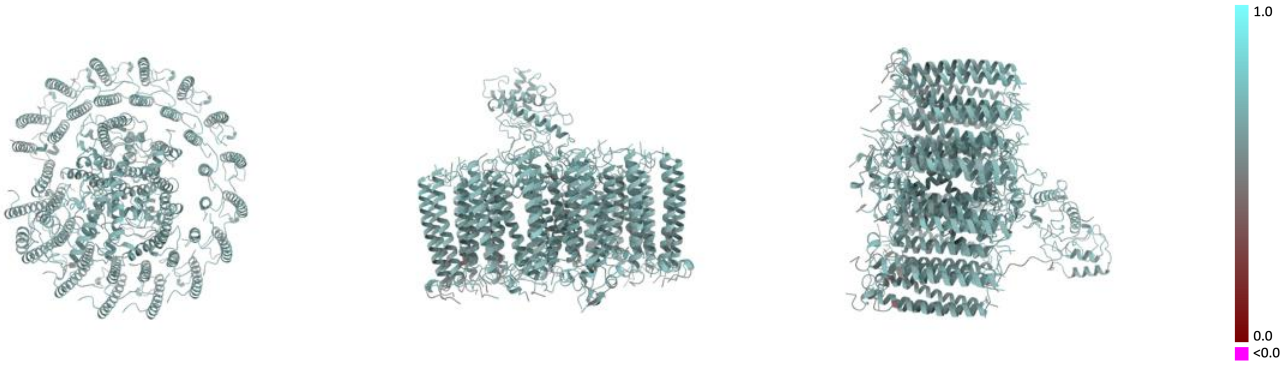
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.226 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

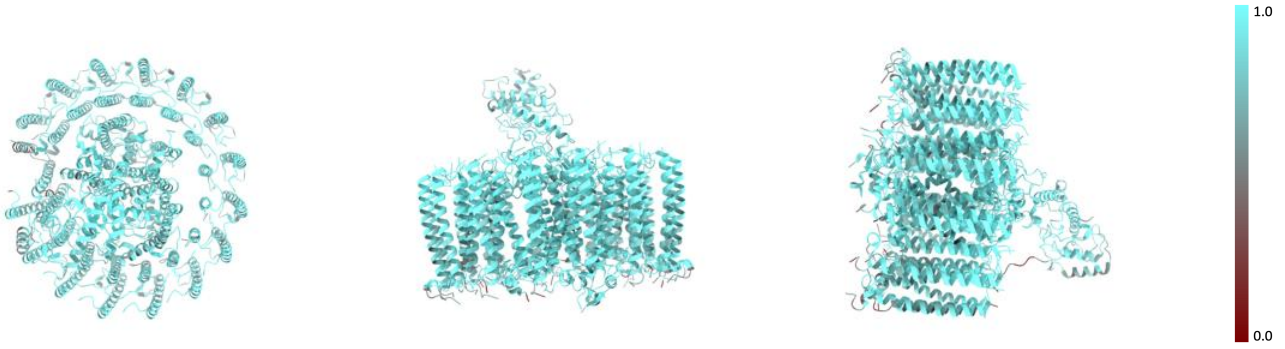
9.2 Q-score mapped to coordinate model (i)



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.

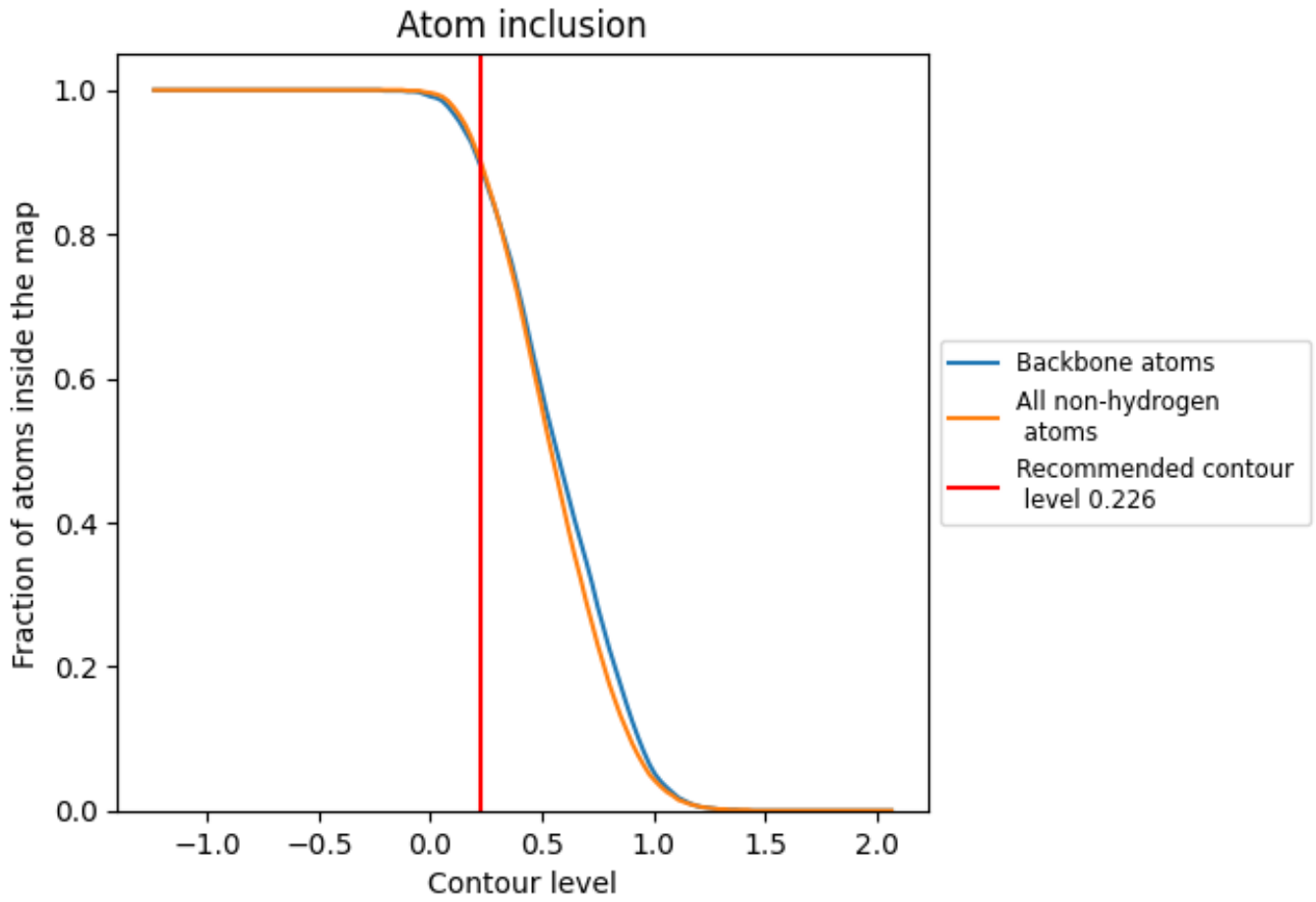
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.226).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 90% 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 (0.226) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.6220
0	0.8560	0.6100
1	0.8530	0.6070
2	0.8570	0.5980
3	0.9190	0.6220
4	0.8790	0.6190
5	0.9180	0.6260
6	0.8850	0.6120
7	0.9000	0.6250
8	0.8710	0.6090
9	0.9080	0.6230
A	0.9210	0.6260
B	0.8800	0.6100
C	0.8780	0.6150
D	0.8980	0.6170
E	0.8820	0.6100
F	0.9200	0.6220
G	0.8820	0.6160
H	0.8780	0.6180
I	0.8850	0.6220
J	0.9480	0.6430
K	0.8950	0.6130
L	0.9390	0.6390
M	0.9480	0.6420
N	0.9260	0.6310
O	0.8960	0.6170
P	0.9010	0.6290
Q	0.8830	0.6150
R	0.9390	0.6340
S	0.9020	0.6220
T	0.9090	0.6150
U	0.8710	0.6140
V	0.8730	0.6110
W	0.8520	0.6020
X	0.6620	0.5670

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Chain	Atom inclusion	Q-score
Y	0.9070	0.6180
Z	0.9410	0.6260
h	0.9340	0.6330