wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 05:50 am BST

PDB ID	:	7PIL / pdb_00007pil
EMDB ID	:	EMD-13441
Title	:	Cryo-EM structure of the Rhodobacter sphaeroides RC-LH1-PufXY monomer complex at 2.5 A
Authors	:	Qian, P.; Hunter, C.N.
Deposited on	:	2021-08-20
Resolution	:	2.50 Å(reported)

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

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

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

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

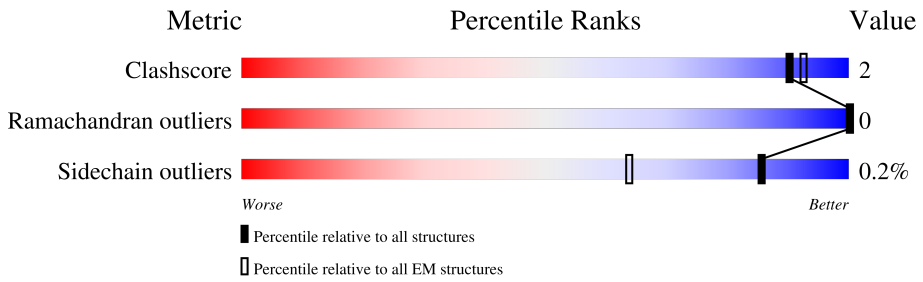
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

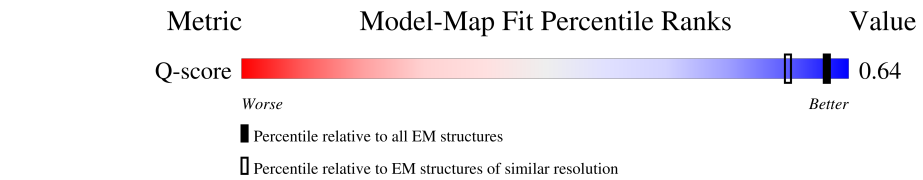
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	AA	55	82% • 16%
1	AB	55	96% •
1	AC	55	96% •
1	AD	55	93% 7%

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Mol	Chain	Length	Quality of chain
1	AE	55	96%
1	AF	55	98%
1	AG	55	100%
1	AH	55	96%
1	AI	55	98%
1	AJ	55	96%
1	AK	55	98%
1	AL	55	95% 5%
1	AM	55	5% 98%
1	AN	55	15% 91% 7%
2	BA	43	93% 7%
2	BB	43	95% 5%
2	BC	43	93% 5%
2	BD	43	95% 5%
2	BE	43	98%
2	BF	43	95% 5%
2	BG	43	100%
2	BH	43	98%
2	BI	43	5% 95% 5%
2	BJ	43	5% 100%
2	BK	43	12% 98%
2	BL	43	5% 100%
2	BM	43	16% 95% 5%
2	BN	43	26% 88% 12%
3	H	246	99%

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Mol	Chain	Length	Quality of chain
4	L	281	98%
5	M	307	98%
6	UU	49	100%
7	X	55	98%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 22480 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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	46	392	271	60	58	3	0	0
1	AB	55	461	313	74	71	3	0	0
1	AC	55	460	313	74	70	3	0	0
1	AD	55	461	313	74	71	3	0	0
1	AE	55	461	313	74	71	3	0	0
1	AF	55	461	313	74	71	3	0	0
1	AG	55	461	313	74	71	3	0	0
1	AH	55	461	313	74	71	3	0	0
1	AI	55	461	313	74	71	3	0	0
1	AJ	55	461	313	74	71	3	0	0
1	AK	55	461	313	74	71	3	0	0
1	AL	55	461	313	74	71	3	0	0
1	AM	55	461	313	74	71	3	0	0
1	AN	51	432	296	69	65	2	0	0

- Molecule 2 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BA	43	352	236	55	60	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BB	43	352	236	55	60	1	0	0
2	BC	42	344	230	54	59	1	0	0
2	BD	43	352	236	55	60	1	0	0
2	BE	43	352	236	55	60	1	0	0
2	BF	43	352	236	55	60	1	0	0
2	BG	43	352	236	55	60	1	0	0
2	BH	43	352	236	55	60	1	0	0
2	BI	43	352	236	55	60	1	0	0
2	BJ	43	352	236	55	60	1	0	0
2	BK	43	352	236	55	60	1	0	0
2	BL	43	352	236	55	60	1	0	0
2	BM	43	352	236	55	60	1	0	0
2	BN	38	317	213	50	53	1	0	0

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	246	1867	1196	316	345	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	281	2232	1507	355	362	8	0	0

- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	307	2445	1630	400	404	11	0	0

- Molecule 6 is a protein called RC-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UU	49	363	247	56	57	3	0	0

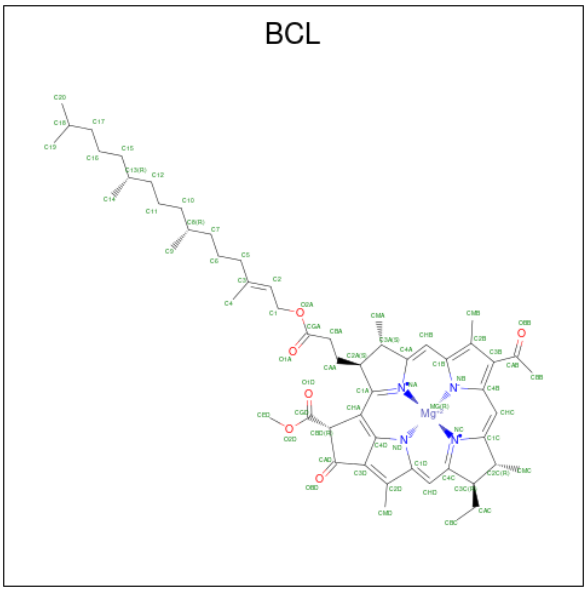
- Molecule 7 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	X	55	422	281	71	67	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	53	LEU	ARG	conflict	UNP P13402

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	AA	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	AB	1	66	55	1	4	6	0
8	AC	1	66	55	1	4	6	0
8	AD	1	66	55	1	4	6	0
8	AE	1	66	55	1	4	6	0
8	AE	1	66	55	1	4	6	0
8	AF	1	66	55	1	4	6	0
8	AG	1	66	55	1	4	6	0
8	AH	1	66	55	1	4	6	0
8	AI	1	66	55	1	4	6	0
8	AJ	1	66	55	1	4	6	0
8	AK	1	66	55	1	4	6	0
8	AK	1	66	55	1	4	6	0
8	AL	1	66	55	1	4	6	0
8	AM	1	66	55	1	4	6	0
8	AM	1	66	55	1	4	6	0
8	AN	1	66	55	1	4	6	0
8	BA	1	66	55	1	4	6	0
8	BB	1	66	55	1	4	6	0
8	BC	1	66	55	1	4	6	0
8	BD	1	66	55	1	4	6	0
8	BF	1	66	55	1	4	6	0

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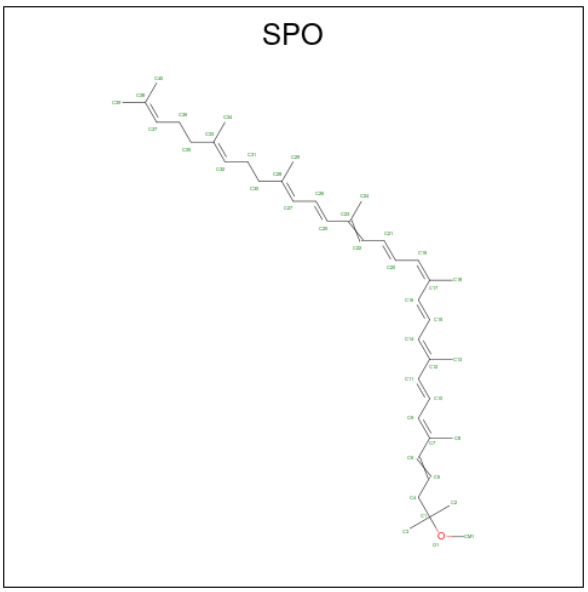
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	BG	1	66	55	1	4	6	0
8	BH	1	66	55	1	4	6	0
8	BI	1	66	55	1	4	6	0
8	BJ	1	66	55	1	4	6	0
8	BL	1	66	55	1	4	6	0
8	BN	1	66	55	1	4	6	0
8	L	1	66	55	1	4	6	0
8	L	1	66	55	1	4	6	0
8	M	1	66	55	1	4	6	0
8	M	1	66	55	1	4	6	0

- Molecule 9 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	AA	1	42	41	1	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	AB	1	42	41	1	0
9	AC	1	42	41	1	0
9	AC	1	42	41	1	0
9	AD	1	42	41	1	0
9	AD	1	42	41	1	0
9	AE	1	42	41	1	0
9	AF	1	42	41	1	0
9	AF	1	42	41	1	0
9	AG	1	42	41	1	0
9	AG	1	42	41	1	0
9	AH	1	42	41	1	0
9	AH	1	42	41	1	0
9	AI	1	42	41	1	0
9	AI	1	42	41	1	0
9	AJ	1	42	41	1	0
9	AJ	1	42	41	1	0
9	AK	1	42	41	1	0
9	AK	1	42	41	1	0
9	AL	1	42	41	1	0
9	AM	1	42	41	1	0
9	AM	1	42	41	1	0

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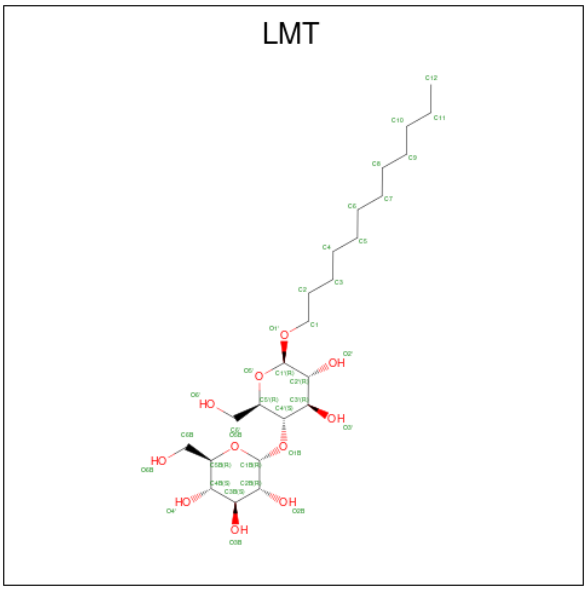
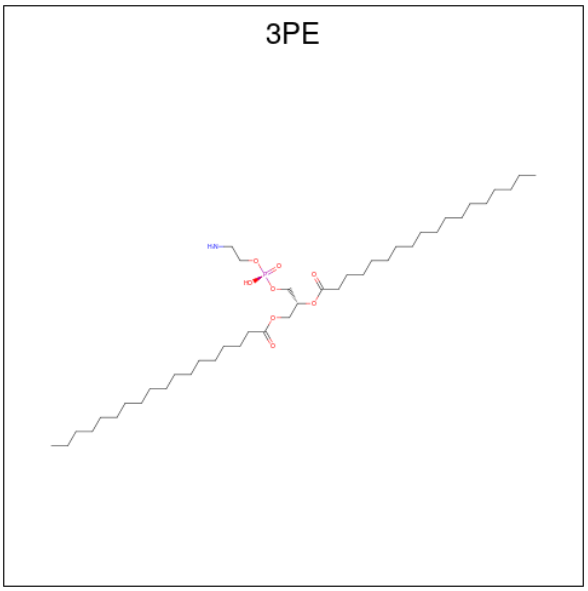
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	BA	1	42	41	1	0
9	BE	1	42	41	1	0
9	BL	1	42	41	1	0
9	M	1	42	41	1	0

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



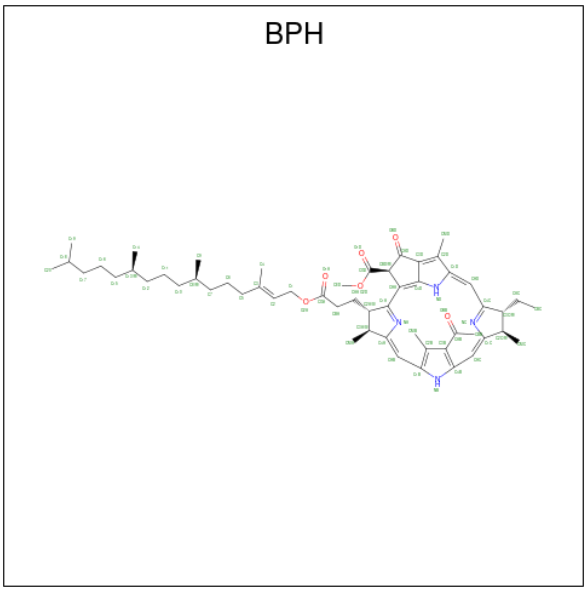
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	AA	1	35	24	11	0
10	AB	1	35	24	11	0
10	M	1	35	24	11	0
10	X	1	35	24	11	0

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



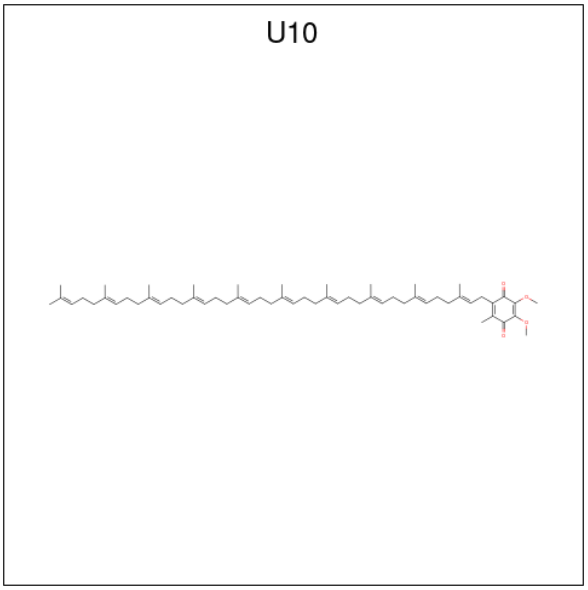
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	AB	1	51	41	1	8	1	0
			Total	C	N	O	P	
11	AC	1	51	41	1	8	1	0
			Total	C	N	O	P	
11	H	1	51	41	1	8	1	0
			Total	C	N	O	P	
11	H	1	51	41	1	8	1	0

- Molecule 12 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



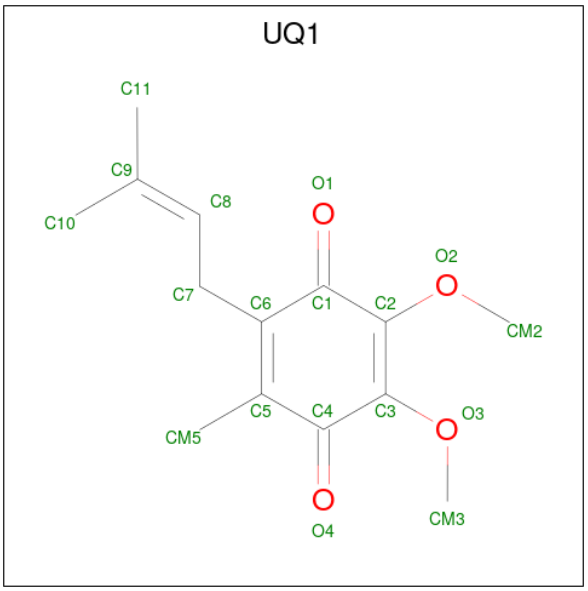
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	L	1	65	55	4	6	0
12	M	1	65	55	4	6	0

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



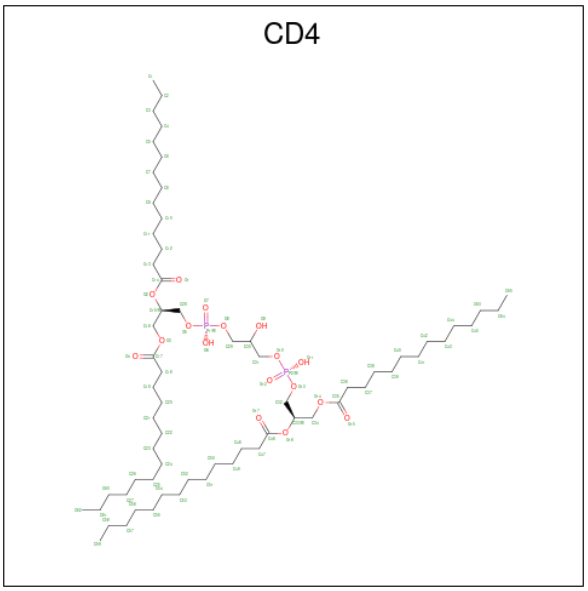
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	L	1	63	59	4	0
13	M	1	63	59	4	0

- Molecule 14 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	L	1	18	14	4	0

- Molecule 15 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecanoyloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: $C_{65}H_{126}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	M	1	84	65	17	2	0

- Molecule 16 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
16	M	1	1	1	0

- Molecule 17 is water.

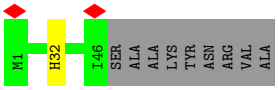
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
17	AB	1	1	1	0
			Total	O	
17	H	2	2	2	0
			Total	O	
17	X	1	1	1	0

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.

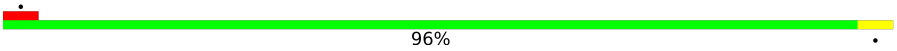
• Molecule 1: Light-harvesting protein B-875 alpha chain

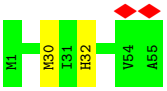
Chain AA:



• Molecule 1: Light-harvesting protein B-875 alpha chain

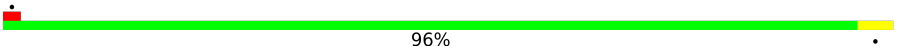
Chain AB:

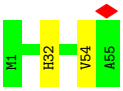




• Molecule 1: Light-harvesting protein B-875 alpha chain

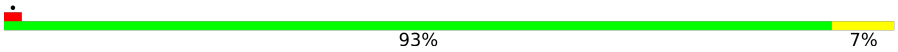
Chain AC:

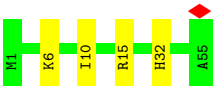




• Molecule 1: Light-harvesting protein B-875 alpha chain

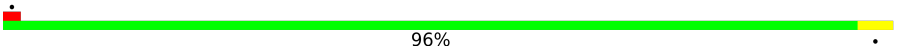
Chain AD:

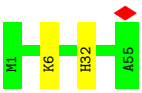




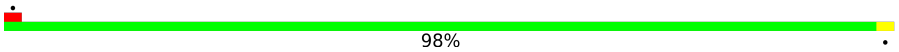
• Molecule 1: Light-harvesting protein B-875 alpha chain

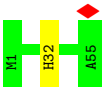
Chain AE:



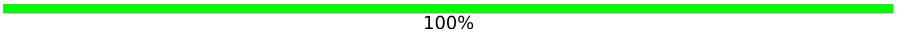


• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AF: 

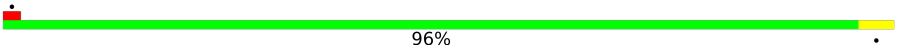


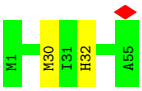
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AG: 

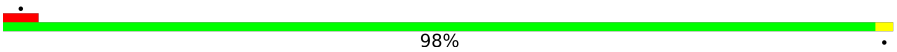
There are no outlier residues recorded for this chain.

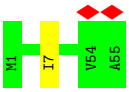
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AH: 

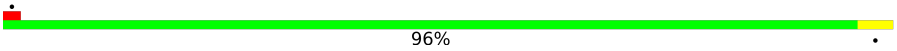


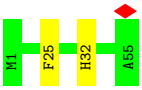
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AI: 

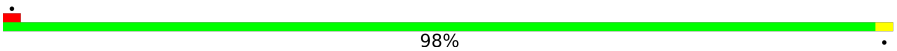


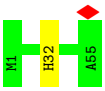
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AJ: 

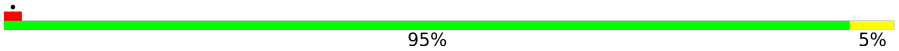


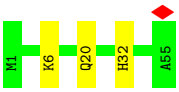
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AK: 



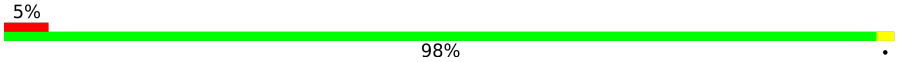
• Molecule 1: Light-harvesting protein B-875 alpha chain

Chain AL: 



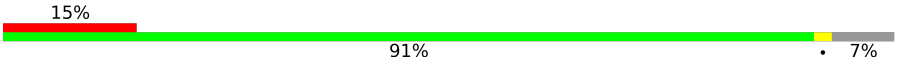
• Molecule 1: Light-harvesting protein B-875 alpha chain

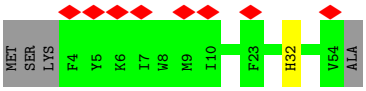
Chain AM:



• Molecule 1: Light-harvesting protein B-875 alpha chain

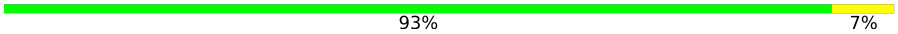
Chain AN:

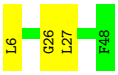




• Molecule 2: Light-harvesting protein B-875 beta chain

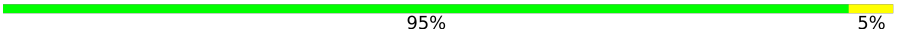
Chain BA:





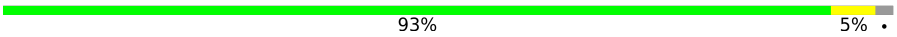
• Molecule 2: Light-harvesting protein B-875 beta chain

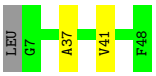
Chain BB:



• Molecule 2: Light-harvesting protein B-875 beta chain

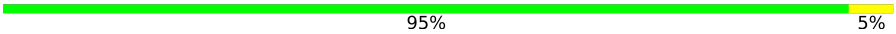
Chain BC:





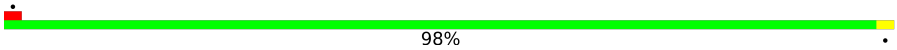
• Molecule 2: Light-harvesting protein B-875 beta chain

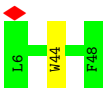
Chain BD:



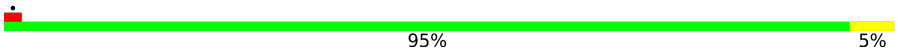
• Molecule 2: Light-harvesting protein B-875 beta chain

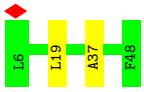
Chain BE:



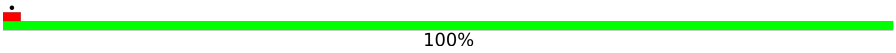


• Molecule 2: Light-harvesting protein B-875 beta chain

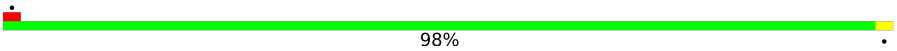
Chain BF: 

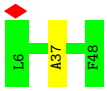


• Molecule 2: Light-harvesting protein B-875 beta chain

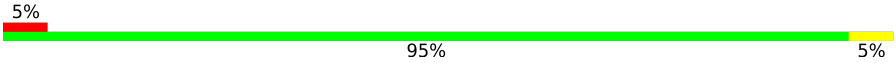
Chain BG: 

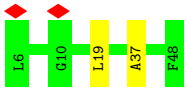
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BH: 

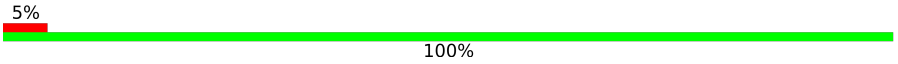


• Molecule 2: Light-harvesting protein B-875 beta chain

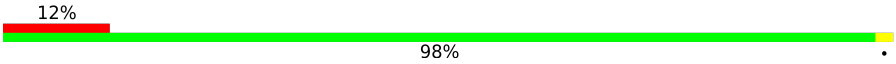
Chain BI: 

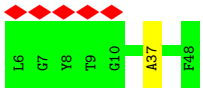


• Molecule 2: Light-harvesting protein B-875 beta chain

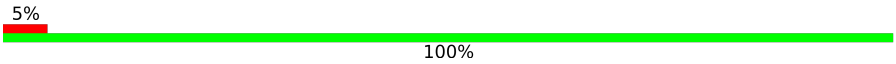
Chain BJ: 

• Molecule 2: Light-harvesting protein B-875 beta chain

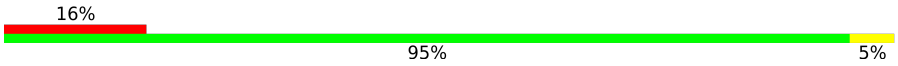
Chain BK: 

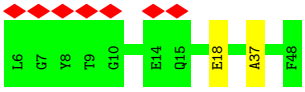


• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BL: 

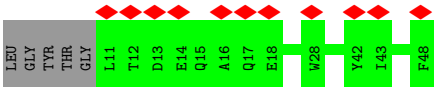
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BM: 

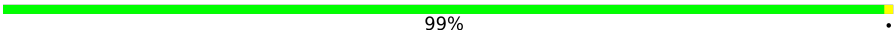


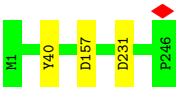
• Molecule 2: Light-harvesting protein B-875 beta chain

Chain BN:

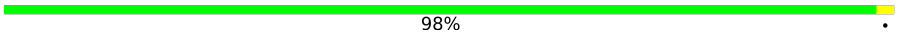


• Molecule 3: Reaction center protein H chain

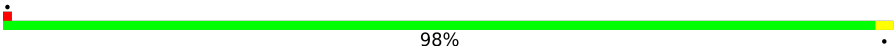
Chain H: 



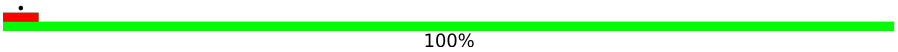
• Molecule 4: Reaction center protein L chain

Chain L: 

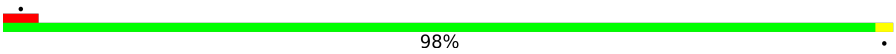
• Molecule 5: Reaction center protein M chain

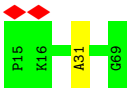
Chain M: 

• Molecule 6: RC-Y

Chain UU: 

• Molecule 7: Intrinsic membrane protein PufX

Chain X: 



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	250613	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44.94	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0187	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	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: 3PE, LMT, UQ1, U10, BPH, FE, BCL, SPO, CD4

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	AA	0.19	0/405	0.46	0/549
1	AB	0.19	0/475	0.49	0/642
1	AC	0.19	0/474	0.51	0/642
1	AD	0.17	0/475	0.45	0/642
1	AE	0.19	0/475	0.49	0/642
1	AF	0.19	0/475	0.49	0/642
1	AG	0.18	0/475	0.49	0/642
1	AH	0.19	0/475	0.50	0/642
1	AI	0.19	0/475	0.49	0/642
1	AJ	0.19	0/475	0.49	0/642
1	AK	0.18	0/475	0.50	0/642
1	AL	0.18	0/475	0.51	0/642
1	AM	0.20	0/475	0.50	0/642
1	AN	0.18	0/446	0.44	0/606
2	BA	0.15	0/365	0.40	0/499
2	BB	0.16	0/365	0.45	0/499
2	BC	0.15	0/357	0.41	0/488
2	BD	0.14	0/365	0.42	0/499
2	BE	0.14	0/365	0.43	0/499
2	BF	0.16	0/365	0.45	0/499
2	BG	0.14	0/365	0.44	0/499
2	BH	0.14	0/365	0.46	0/499
2	BI	0.15	0/365	0.44	0/499
2	BJ	0.14	0/365	0.44	0/499
2	BK	0.15	0/365	0.48	0/499
2	BL	0.16	0/365	0.45	0/499
2	BM	0.16	0/365	0.46	0/499
2	BN	0.17	0/329	0.43	0/450
3	H	0.17	0/1917	0.48	0/2609
4	L	0.18	0/2320	0.48	0/3175
5	M	0.17	0/2538	0.49	0/3464
6	UU	0.16	0/374	0.45	0/505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	X	0.19	0/434	0.51	0/586
All	All	0.17	0/19199	0.47	0/26124

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AD	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AD	15	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	392	0	412	1	0
1	AB	461	0	482	2	0
1	AC	460	0	482	3	0
1	AD	461	0	482	3	0
1	AE	461	0	482	2	0
1	AF	461	0	482	1	0
1	AG	461	0	482	0	0
1	AH	461	0	482	3	0
1	AI	461	0	482	1	0
1	AJ	461	0	482	2	0
1	AK	461	0	482	1	0
1	AL	461	0	482	4	0
1	AM	461	0	482	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	432	0	447	1	0
2	BA	352	0	336	3	0
2	BB	352	0	336	2	0
2	BC	344	0	325	2	0
2	BD	352	0	336	2	0
2	BE	352	0	336	1	0
2	BF	352	0	336	2	0
2	BG	352	0	336	0	0
2	BH	352	0	336	1	0
2	BI	352	0	336	2	0
2	BJ	352	0	336	0	0
2	BK	352	0	336	1	0
2	BL	352	0	336	0	0
2	BM	352	0	336	2	0
2	BN	317	0	303	0	0
3	H	1867	0	1864	2	0
4	L	2232	0	2187	4	0
5	M	2445	0	2359	4	0
6	UU	363	0	358	0	0
7	X	422	0	436	1	0
8	AA	66	0	74	1	0
8	AB	66	0	74	3	0
8	AC	66	0	74	1	0
8	AD	66	0	74	0	0
8	AE	132	0	148	2	0
8	AF	66	0	74	1	0
8	AG	66	0	74	0	0
8	AH	66	0	74	0	0
8	AI	66	0	74	1	0
8	AJ	66	0	74	3	0
8	AK	132	0	148	1	0
8	AL	66	0	74	0	0
8	AM	132	0	148	2	0
8	AN	66	0	74	0	0
8	BA	66	0	74	1	0
8	BB	66	0	74	1	0
8	BC	66	0	74	2	0
8	BD	66	0	74	1	0
8	BF	66	0	74	1	0
8	BG	66	0	74	0	0
8	BH	66	0	74	1	0
8	BI	66	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BJ	66	0	74	1	0
8	BL	66	0	74	1	0
8	BN	66	0	74	0	0
8	L	132	0	148	0	0
8	M	132	0	148	0	0
9	AA	42	0	60	2	0
9	AB	42	0	60	3	0
9	AC	84	0	120	2	0
9	AD	84	0	120	2	0
9	AE	42	0	60	3	0
9	AF	84	0	120	5	0
9	AG	84	0	120	0	0
9	AH	84	0	120	3	0
9	AI	84	0	120	4	0
9	AJ	84	0	120	3	0
9	AK	84	0	120	2	0
9	AL	42	0	60	2	0
9	AM	84	0	120	4	0
9	BA	42	0	60	3	0
9	BE	42	0	60	2	0
9	BL	42	0	60	0	0
9	M	42	0	60	2	0
10	AA	35	0	45	0	0
10	AB	35	0	45	0	0
10	M	35	0	46	0	0
10	X	35	0	46	0	0
11	AB	51	0	82	0	0
11	AC	51	0	82	0	0
11	H	102	0	164	1	0
12	L	65	0	76	0	0
12	M	65	0	76	1	0
13	L	63	0	90	1	0
13	M	63	0	90	1	0
14	L	18	0	18	0	0
15	M	84	0	124	1	0
16	M	1	0	0	0	0
17	AB	1	0	0	0	0
17	H	2	0	0	0	0
17	X	1	0	0	0	0
All	All	22480	0	23419	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 77 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:102:SPO:H132	8:AJ:101:BCL:H42	1.70	0.73
2:BD:48:PHE:HB3	9:BE:1000:SPO:H343	1.72	0.72
1:AH:30:MET:HE3	9:M:407:SPO:H401	1.76	0.67
1:AC:54:VAL:O	1:AC:54:VAL:HG23	1.97	0.64
2:BE:44:TRP:CD1	9:BE:1000:SPO:H342	2.32	0.64

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	44/55 (80%)	43 (98%)	1 (2%)	0	100	100
1	AB	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AC	53/55 (96%)	53 (100%)	0	0	100	100
1	AD	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AE	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AF	53/55 (96%)	53 (100%)	0	0	100	100
1	AG	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AH	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AI	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
1	AJ	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AK	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
1	AL	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AM	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
1	AN	49/55 (89%)	48 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BA	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
2	BB	41/43 (95%)	41 (100%)	0	0	100	100
2	BC	40/43 (93%)	40 (100%)	0	0	100	100
2	BD	41/43 (95%)	41 (100%)	0	0	100	100
2	BE	41/43 (95%)	41 (100%)	0	0	100	100
2	BF	41/43 (95%)	41 (100%)	0	0	100	100
2	BG	41/43 (95%)	41 (100%)	0	0	100	100
2	BH	41/43 (95%)	41 (100%)	0	0	100	100
2	BI	41/43 (95%)	41 (100%)	0	0	100	100
2	BJ	41/43 (95%)	41 (100%)	0	0	100	100
2	BK	41/43 (95%)	41 (100%)	0	0	100	100
2	BL	41/43 (95%)	41 (100%)	0	0	100	100
2	BM	41/43 (95%)	41 (100%)	0	0	100	100
2	BN	36/43 (84%)	35 (97%)	1 (3%)	0	100	100
3	H	244/246 (99%)	240 (98%)	4 (2%)	0	100	100
4	L	279/281 (99%)	273 (98%)	6 (2%)	0	100	100
5	M	305/307 (99%)	297 (97%)	8 (3%)	0	100	100
6	UU	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
7	X	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
All	All	2225/2310 (96%)	2188 (98%)	37 (2%)	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	AA	43/49 (88%)	43 (100%)	0	100	100
1	AB	49/49 (100%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	49/49 (100%)	49 (100%)	0	100	100
1	AD	49/49 (100%)	49 (100%)	0	100	100
1	AE	49/49 (100%)	49 (100%)	0	100	100
1	AF	49/49 (100%)	49 (100%)	0	100	100
1	AG	49/49 (100%)	49 (100%)	0	100	100
1	AH	49/49 (100%)	49 (100%)	0	100	100
1	AI	49/49 (100%)	49 (100%)	0	100	100
1	AJ	49/49 (100%)	49 (100%)	0	100	100
1	AK	49/49 (100%)	49 (100%)	0	100	100
1	AL	49/49 (100%)	49 (100%)	0	100	100
1	AM	49/49 (100%)	49 (100%)	0	100	100
1	AN	46/49 (94%)	46 (100%)	0	100	100
2	BA	35/35 (100%)	35 (100%)	0	100	100
2	BB	35/35 (100%)	35 (100%)	0	100	100
2	BC	34/35 (97%)	34 (100%)	0	100	100
2	BD	35/35 (100%)	35 (100%)	0	100	100
2	BE	35/35 (100%)	35 (100%)	0	100	100
2	BF	35/35 (100%)	35 (100%)	0	100	100
2	BG	35/35 (100%)	35 (100%)	0	100	100
2	BH	35/35 (100%)	35 (100%)	0	100	100
2	BI	35/35 (100%)	35 (100%)	0	100	100
2	BJ	35/35 (100%)	35 (100%)	0	100	100
2	BK	35/35 (100%)	35 (100%)	0	100	100
2	BL	35/35 (100%)	35 (100%)	0	100	100
2	BM	35/35 (100%)	35 (100%)	0	100	100
2	BN	32/35 (91%)	32 (100%)	0	100	100
3	H	198/198 (100%)	197 (100%)	1 (0%)	81	92
4	L	220/220 (100%)	218 (99%)	2 (1%)	70	87
5	M	240/240 (100%)	239 (100%)	1 (0%)	84	93
6	UU	33/33 (100%)	33 (100%)	0	100	100
7	X	42/42 (100%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1896/1909 (99%)	1892 (100%)	4 (0%)	85 95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	231	ASP
4	L	210	ASP
4	L	247	CYS
5	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	300	ASN
5	M	307	ASN
2	BJ	17	GLN
5	M	138	GLN
5	M	259	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 73 ligands modelled in this entry, 1 is monoatomic - leaving 72 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	$\#\|Z\| > 2$
9	SPO	AA	1002	-	40,41,41	0.17	0	47,50,50	0.71	2 (4%)
9	SPO	AK	104	-	40,41,41	0.19	0	47,50,50	0.40	0
9	SPO	AK	102	-	40,41,41	0.23	0	47,50,50	0.42	0
9	SPO	AD	101	-	40,41,41	0.16	0	47,50,50	0.44	0
8	BCL	AF	102	1	69,74,74	1.21	5 (7%)	83,115,115	1.46	12 (14%)
8	BCL	AB	101	1	69,74,74	1.23	6 (8%)	83,115,115	1.53	13 (15%)
9	SPO	AC	103	-	40,41,41	0.23	0	47,50,50	0.25	0
8	BCL	AN	101	1	69,74,74	1.20	6 (8%)	83,115,115	1.40	11 (13%)
8	BCL	BL	102	2	69,74,74	1.16	5 (7%)	83,115,115	1.40	13 (15%)
11	3PE	H	301	-	50,50,50	0.53	0	53,55,55	0.51	1 (1%)
9	SPO	AH	103	-	40,41,41	0.28	0	47,50,50	0.54	0
8	BCL	AM	1003	2	69,74,74	1.17	5 (7%)	83,115,115	1.41	11 (13%)
11	3PE	AC	104	-	50,50,50	0.53	0	53,55,55	0.58	1 (1%)
12	BPH	L	301	-	59,70,70	1.03	3 (5%)	61,101,101	1.93	9 (14%)
9	SPO	AF	101	-	40,41,41	0.39	0	47,50,50	0.58	1 (2%)
11	3PE	AB	102	-	50,50,50	0.53	0	53,55,55	0.54	1 (1%)
9	SPO	BL	101	-	40,41,41	0.35	0	47,50,50	0.35	0
8	BCL	BG	101	2	69,74,74	1.18	5 (7%)	83,115,115	1.41	13 (15%)
10	LMT	AA	1003	-	36,36,36	1.08	4 (11%)	47,47,47	0.94	2 (4%)
8	BCL	AE	101	1	69,74,74	1.17	5 (7%)	83,115,115	1.45	11 (13%)
11	3PE	H	302	-	50,50,50	0.51	0	53,55,55	0.66	2 (3%)
8	BCL	AA	1001	1	69,74,74	1.24	5 (7%)	83,115,115	1.39	11 (13%)
9	SPO	AD	103	-	40,41,41	0.20	0	47,50,50	0.40	0
8	BCL	BH	101	2	69,74,74	1.18	6 (8%)	83,115,115	1.41	12 (14%)
9	SPO	BE	1000	-	40,41,41	0.38	0	47,50,50	0.49	0
10	LMT	AB	104	-	36,36,36	1.12	4 (11%)	47,47,47	0.83	0
8	BCL	AM	1001	1	69,74,74	1.19	5 (7%)	83,115,115	1.50	13 (15%)
8	BCL	AH	102	1	69,74,74	1.21	6 (8%)	83,115,115	1.45	12 (14%)
9	SPO	AM	1002	-	40,41,41	0.24	0	47,50,50	0.41	0
10	LMT	M	401	-	36,36,36	1.06	5 (13%)	47,47,47	0.97	2 (4%)
8	BCL	AC	102	1	69,74,74	1.18	4 (5%)	83,115,115	1.42	11 (13%)
8	BCL	AK	101	1	69,74,74	1.22	5 (7%)	83,115,115	1.49	13 (15%)
9	SPO	AE	102	-	40,41,41	0.32	0	47,50,50	0.51	0
15	CD4	M	405	-	83,83,83	0.50	0	89,95,95	0.97	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SPO	AJ	102	-	40,41,41	0.22	0	47,50,50	0.51	0
9	SPO	AB	103	-	40,41,41	0.39	0	47,50,50	0.71	2 (4%)
8	BCL	AK	103	2	69,74,74	1.18	5 (7%)	83,115,115	1.39	12 (14%)
8	BCL	M	403	5	69,74,74	1.21	6 (8%)	83,115,115	1.42	11 (13%)
9	SPO	AH	101	-	40,41,41	0.19	0	47,50,50	0.46	1 (2%)
9	SPO	M	407	-	40,41,41	0.20	0	47,50,50	0.51	0
8	BCL	BI	101	2	69,74,74	1.17	5 (7%)	83,115,115	1.41	13 (15%)
8	BCL	BJ	101	2	69,74,74	1.18	6 (8%)	83,115,115	1.40	11 (13%)
8	BCL	BC	101	2	69,74,74	1.16	5 (7%)	83,115,115	1.40	11 (13%)
8	BCL	M	406	5	69,74,74	1.15	5 (7%)	83,115,115	1.51	13 (15%)
8	BCL	BB	1001	2	69,74,74	1.16	5 (7%)	83,115,115	1.41	12 (14%)
9	SPO	AF	103	-	40,41,41	0.31	0	47,50,50	0.34	0
8	BCL	AI	101	1	69,74,74	1.22	4 (5%)	83,115,115	1.46	12 (14%)
9	SPO	AG	103	-	40,41,41	0.30	0	47,50,50	0.51	0
9	SPO	AM	1004	-	40,41,41	0.38	0	47,50,50	0.39	0
8	BCL	BA	102	2	69,74,74	1.17	5 (7%)	83,115,115	1.45	13 (15%)
8	BCL	BN	101	2	69,74,74	1.20	5 (7%)	83,115,115	1.48	13 (15%)
8	BCL	BF	101	2	69,74,74	1.17	5 (7%)	83,115,115	1.37	11 (13%)
8	BCL	AE	103	2	69,74,74	1.18	5 (7%)	83,115,115	1.46	12 (14%)
9	SPO	AC	101	-	40,41,41	0.19	0	47,50,50	0.45	0
8	BCL	AG	102	1	69,74,74	1.18	5 (7%)	83,115,115	1.43	11 (13%)
9	SPO	AG	101	-	40,41,41	0.29	0	47,50,50	0.41	0
9	SPO	AI	103	-	40,41,41	0.33	0	47,50,50	0.86	2 (4%)
9	SPO	AJ	103	-	40,41,41	0.35	0	47,50,50	0.68	2 (4%)
10	LMT	X	101	-	36,36,36	1.11	5 (13%)	47,47,47	0.89	2 (4%)
12	BPH	M	402	-	59,70,70	1.07	4 (6%)	61,101,101	1.97	9 (14%)
13	U10	L	302	-	63,63,63	2.68	17 (26%)	76,79,79	1.56	18 (23%)
9	SPO	AL	1002	-	40,41,41	0.37	0	47,50,50	0.68	2 (4%)
13	U10	M	404	-	63,63,63	2.65	17 (26%)	76,79,79	1.67	16 (21%)
14	UQ1	L	303	-	18,18,18	0.78	0	22,25,25	1.85	6 (27%)
9	SPO	BA	101	-	40,41,41	0.18	0	47,50,50	0.66	1 (2%)
8	BCL	L	305	4	69,74,74	1.15	6 (8%)	83,115,115	1.43	12 (14%)
8	BCL	L	304	4	69,74,74	1.18	6 (8%)	83,115,115	1.36	11 (13%)
8	BCL	BD	101	2	69,74,74	1.18	5 (7%)	83,115,115	1.44	13 (15%)
8	BCL	AD	102	1	69,74,74	1.19	5 (7%)	83,115,115	1.57	13 (15%)
8	BCL	AL	1001	1	69,74,74	1.20	5 (7%)	83,115,115	1.51	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SPO	AI	102	-	40,41,41	0.37	0	47,50,50	0.79	2 (4%)
8	BCL	AJ	101	1	69,74,74	1.20	5 (7%)	83,115,115	1.57	12 (14%)

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
9	SPO	AA	1002	-	-	8/47/47/47	-
9	SPO	AK	104	-	-	8/47/47/47	-
9	SPO	AK	102	-	-	4/47/47/47	-
9	SPO	AD	101	-	-	5/47/47/47	-
8	BCL	AF	102	1	-	3/41/137/137	-
8	BCL	AB	101	1	-	7/41/137/137	-
9	SPO	AC	103	-	-	3/47/47/47	-
8	BCL	AN	101	1	-	5/41/137/137	-
8	BCL	BL	102	2	-	11/41/137/137	-
11	3PE	H	301	-	-	16/54/54/54	-
9	SPO	AH	103	-	-	3/47/47/47	-
8	BCL	AM	1003	2	-	6/41/137/137	-
11	3PE	AC	104	-	-	12/54/54/54	-
12	BPH	L	301	-	-	5/37/105/105	0/5/6/6
9	SPO	AF	101	-	-	4/47/47/47	-
11	3PE	AB	102	-	-	10/54/54/54	-
9	SPO	BL	101	-	-	5/47/47/47	-
8	BCL	BG	101	2	-	7/41/137/137	-
10	LMT	AA	1003	-	-	3/21/61/61	0/2/2/2
8	BCL	AE	101	1	-	3/41/137/137	-
11	3PE	H	302	-	-	14/54/54/54	-
8	BCL	AA	1001	1	-	6/41/137/137	-
9	SPO	AD	103	-	-	4/47/47/47	-
8	BCL	BH	101	2	-	7/41/137/137	-
9	SPO	BE	1000	-	-	7/47/47/47	-
10	LMT	AB	104	-	-	4/21/61/61	0/2/2/2
8	BCL	AM	1001	1	-	4/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	AH	102	1	-	1/41/137/137	-
9	SPO	AM	1002	-	-	2/47/47/47	-
10	LMT	M	401	-	-	4/21/61/61	0/2/2/2
8	BCL	AC	102	1	-	10/41/137/137	-
8	BCL	AK	101	1	-	5/41/137/137	-
9	SPO	AE	102	-	-	3/47/47/47	-
15	CD4	M	405	-	-	12/94/94/94	-
9	SPO	AJ	102	-	-	6/47/47/47	-
9	SPO	AB	103	-	-	9/47/47/47	-
8	BCL	AK	103	2	-	5/41/137/137	-
8	BCL	M	403	5	-	1/41/137/137	-
9	SPO	AH	101	-	-	2/47/47/47	-
9	SPO	M	407	-	-	2/47/47/47	-
8	BCL	BI	101	2	-	3/41/137/137	-
8	BCL	BJ	101	2	-	6/41/137/137	-
8	BCL	BC	101	2	-	7/41/137/137	-
8	BCL	M	406	5	-	7/41/137/137	-
8	BCL	BB	1001	2	-	7/41/137/137	-
9	SPO	AF	103	-	-	2/47/47/47	-
8	BCL	AI	101	1	-	11/41/137/137	-
9	SPO	AG	103	-	-	2/47/47/47	-
9	SPO	AM	1004	-	-	3/47/47/47	-
8	BCL	BA	102	2	-	4/41/137/137	-
8	BCL	BN	101	2	-	6/41/137/137	-
8	BCL	BF	101	2	-	8/41/137/137	-
8	BCL	AE	103	2	-	5/41/137/137	-
9	SPO	AC	101	-	-	2/47/47/47	-
8	BCL	AG	102	1	-	1/41/137/137	-
9	SPO	AG	101	-	-	2/47/47/47	-
9	SPO	AI	103	-	-	4/47/47/47	-
9	SPO	AJ	103	-	-	4/47/47/47	-
10	LMT	X	101	-	-	1/21/61/61	0/2/2/2
12	BPH	M	402	-	-	6/37/105/105	0/5/6/6
13	U10	L	302	-	-	13/63/87/87	0/1/1/1
9	SPO	AL	1002	-	-	2/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	U10	M	404	-	-	8/63/87/87	0/1/1/1
14	UQ1	L	303	-	-	4/9/33/33	0/1/1/1
9	SPO	BA	101	-	-	3/47/47/47	-
8	BCL	L	305	4	-	4/41/137/137	-
8	BCL	L	304	4	-	1/41/137/137	-
8	BCL	BD	101	2	-	2/41/137/137	-
8	BCL	AD	102	1	-	4/41/137/137	-
8	BCL	AL	1001	1	-	5/41/137/137	-
9	SPO	AI	102	-	-	4/47/47/47	-
8	BCL	AJ	101	1	-	7/41/137/137	-

The worst 5 of 225 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	302	U10	C43-C44	6.14	1.47	1.33
13	M	404	U10	C43-C44	6.11	1.47	1.33
13	L	302	U10	C48-C49	6.11	1.47	1.33
13	L	302	U10	C18-C19	6.10	1.47	1.33
13	M	404	U10	C18-C19	6.08	1.47	1.33

The worst 5 of 475 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	402	BPH	C4D-CHA-CBD	-11.03	103.53	108.52
12	L	301	BPH	C4D-CHA-CBD	-10.97	103.56	108.52
8	M	406	BCL	CHD-C1D-ND	-6.09	118.86	124.45
8	L	305	BCL	CHD-C1D-ND	-5.39	119.50	124.45
8	AI	101	BCL	CHD-C1D-ND	-5.25	119.62	124.45

There are no chirality outliers.

5 of 384 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AK	101	BCL	C2-C3-C5-C6
8	AK	101	BCL	C4-C3-C5-C6
8	AN	101	BCL	C4-C3-C5-C6
8	BA	102	BCL	C3A-C2A-CAA-CBA
8	BB	1001	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

44 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AA	1002	SPO	2	0
9	AK	104	SPO	2	0
8	AF	102	BCL	1	0
8	AB	101	BCL	3	0
9	AC	103	SPO	2	0
8	BL	102	BCL	1	0
9	AH	103	SPO	1	0
8	AM	1003	BCL	1	0
9	AF	101	SPO	3	0
8	AE	101	BCL	1	0
11	H	302	3PE	1	0
8	AA	1001	BCL	1	0
9	AD	103	SPO	2	0
8	BH	101	BCL	1	0
9	BE	1000	SPO	2	0
8	AM	1001	BCL	1	0
9	AM	1002	SPO	2	0
8	AC	102	BCL	1	0
9	AE	102	SPO	3	0
15	M	405	CD4	1	0
9	AJ	102	SPO	2	0
9	AB	103	SPO	3	0
8	AK	103	BCL	1	0
9	AH	101	SPO	2	0
9	M	407	SPO	2	0
8	BJ	101	BCL	1	0
8	BC	101	BCL	2	0
8	BB	1001	BCL	1	0
9	AF	103	SPO	2	0
8	AI	101	BCL	1	0
9	AM	1004	SPO	2	0
8	BA	102	BCL	1	0
8	BF	101	BCL	1	0
8	AE	103	BCL	1	0
9	AI	103	SPO	1	0
9	AJ	103	SPO	1	0
12	M	402	BPH	1	0
13	L	302	U10	1	0
9	AL	1002	SPO	2	0
13	M	404	U10	1	0
9	BA	101	SPO	3	0
8	BD	101	BCL	1	0

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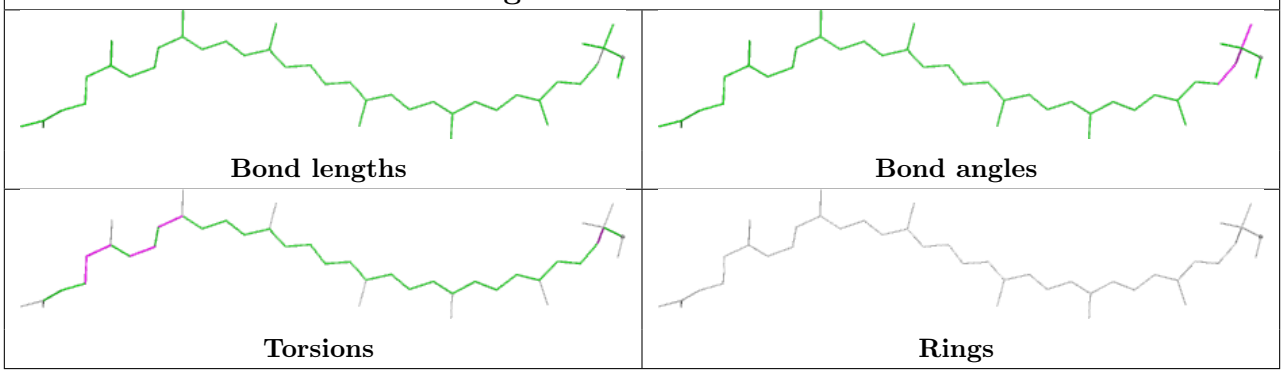
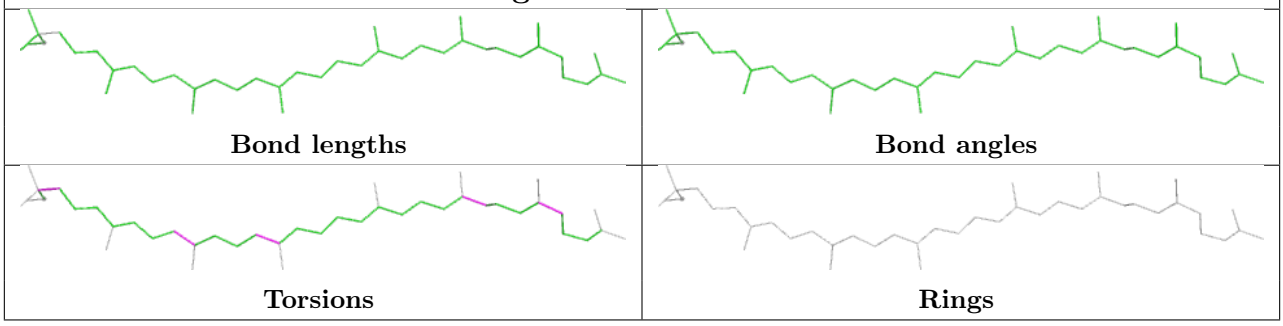
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AI	102	SPO	3	0
8	AJ	101	BCL	3	0

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

Ligand SPO AA 1002



Ligand SPO AK 104



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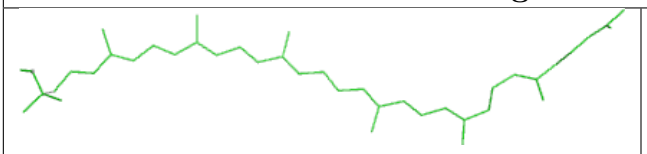
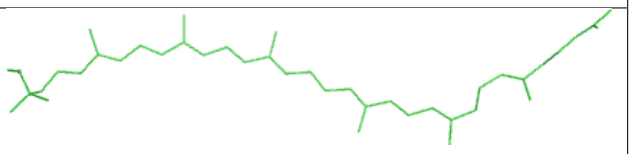
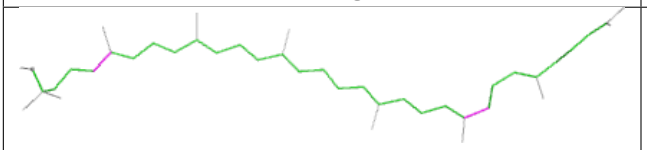
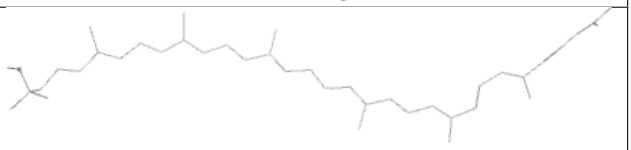
 Bond lengths	 Bond angles
 Torsions	 Rings

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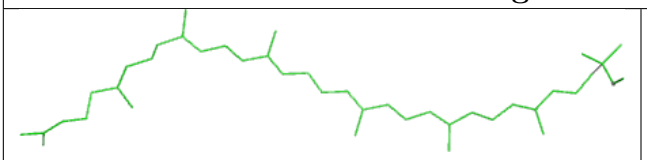
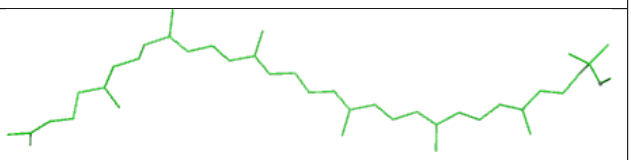
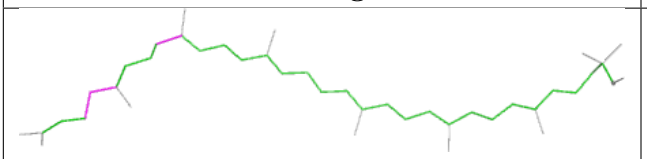
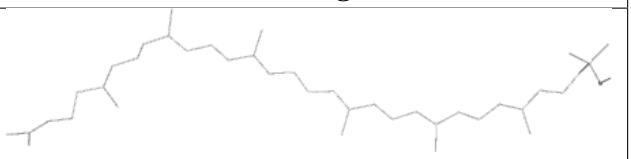
 Bond lengths	 Bond angles
 Torsions	 Rings

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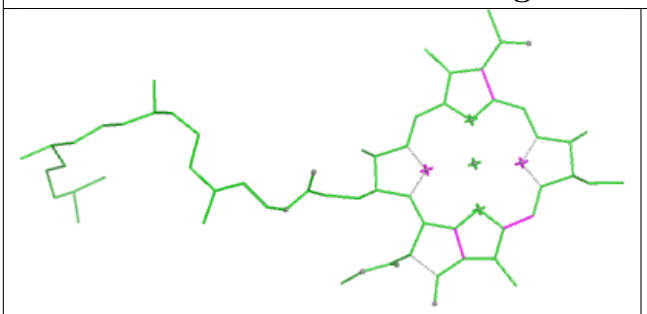
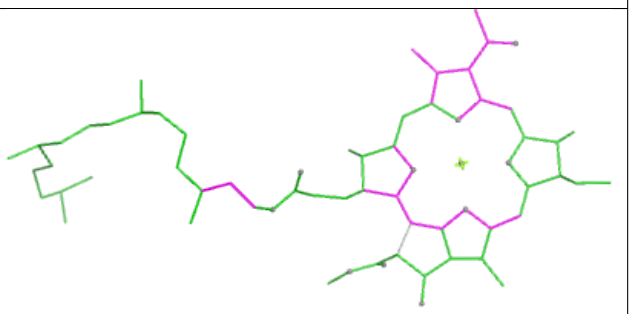
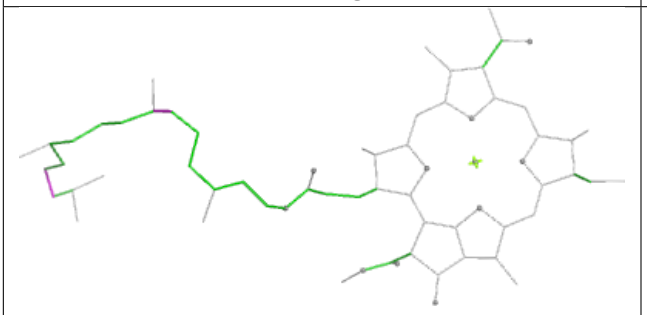
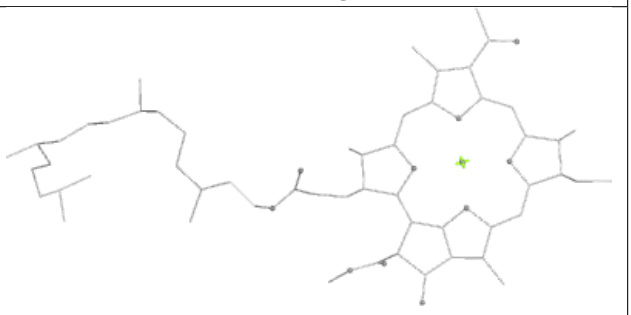
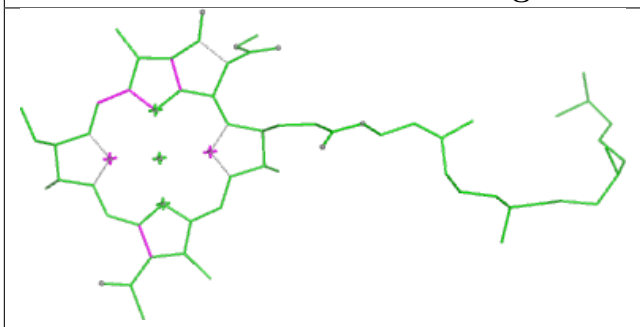
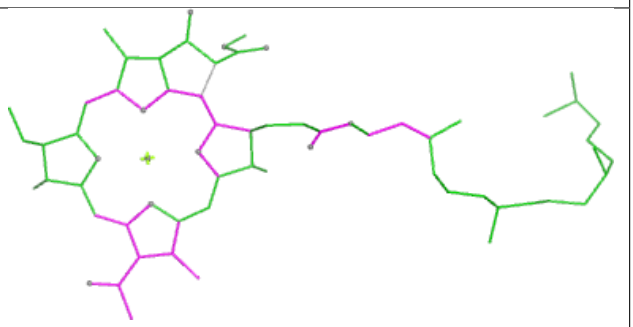
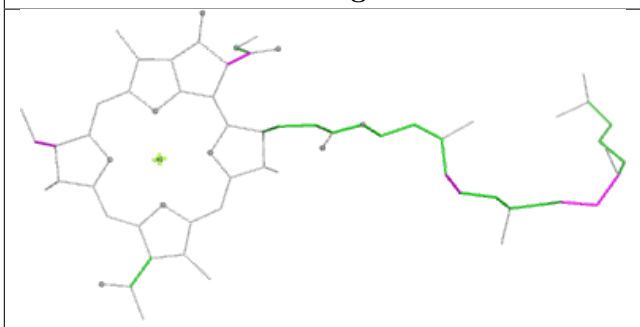
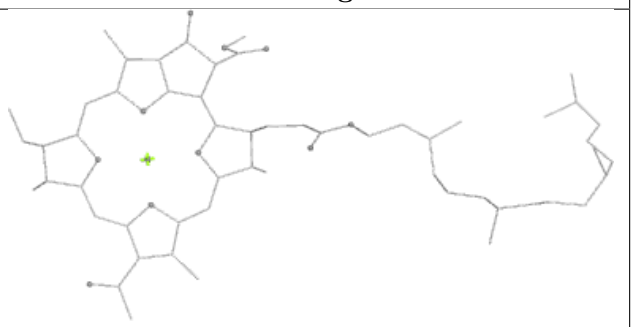
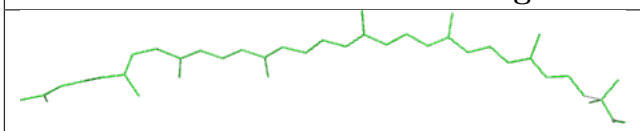
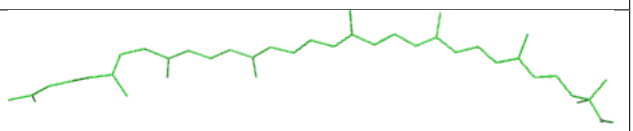
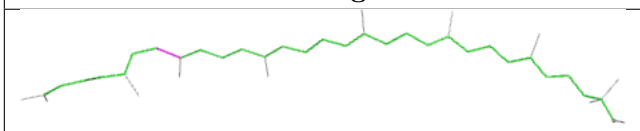
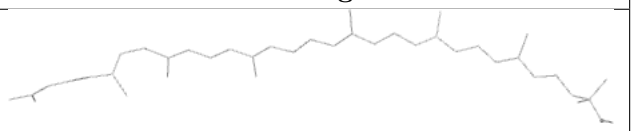
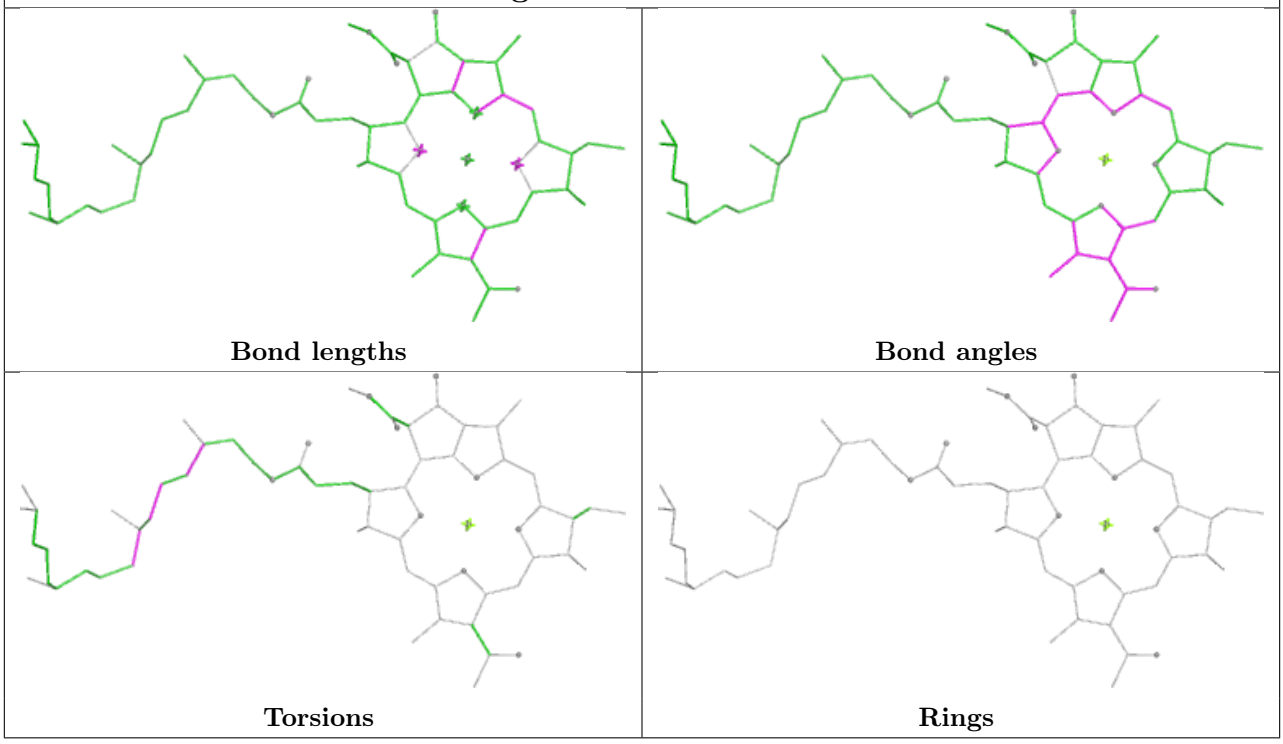
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AB 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AC 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AN 101



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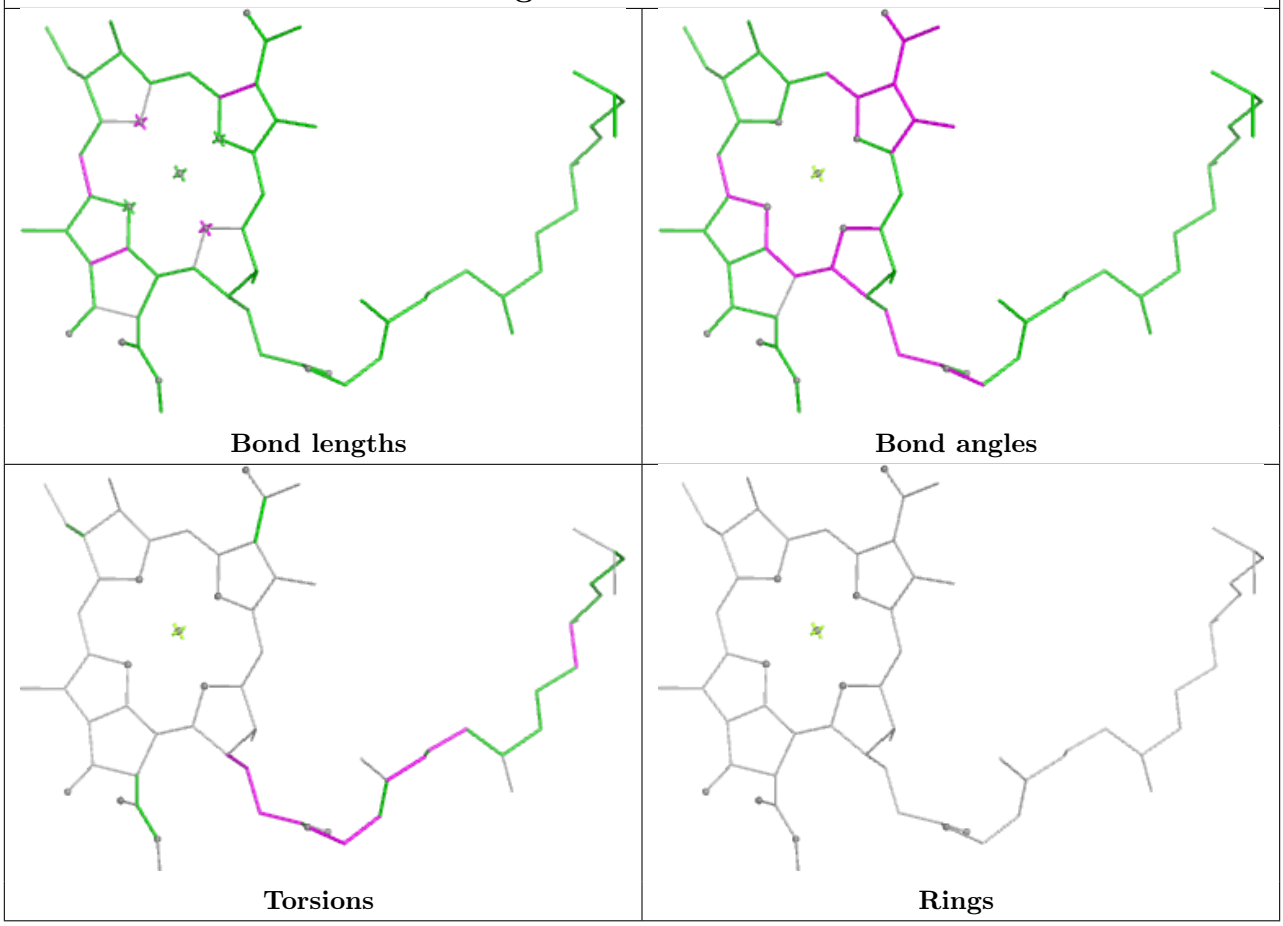
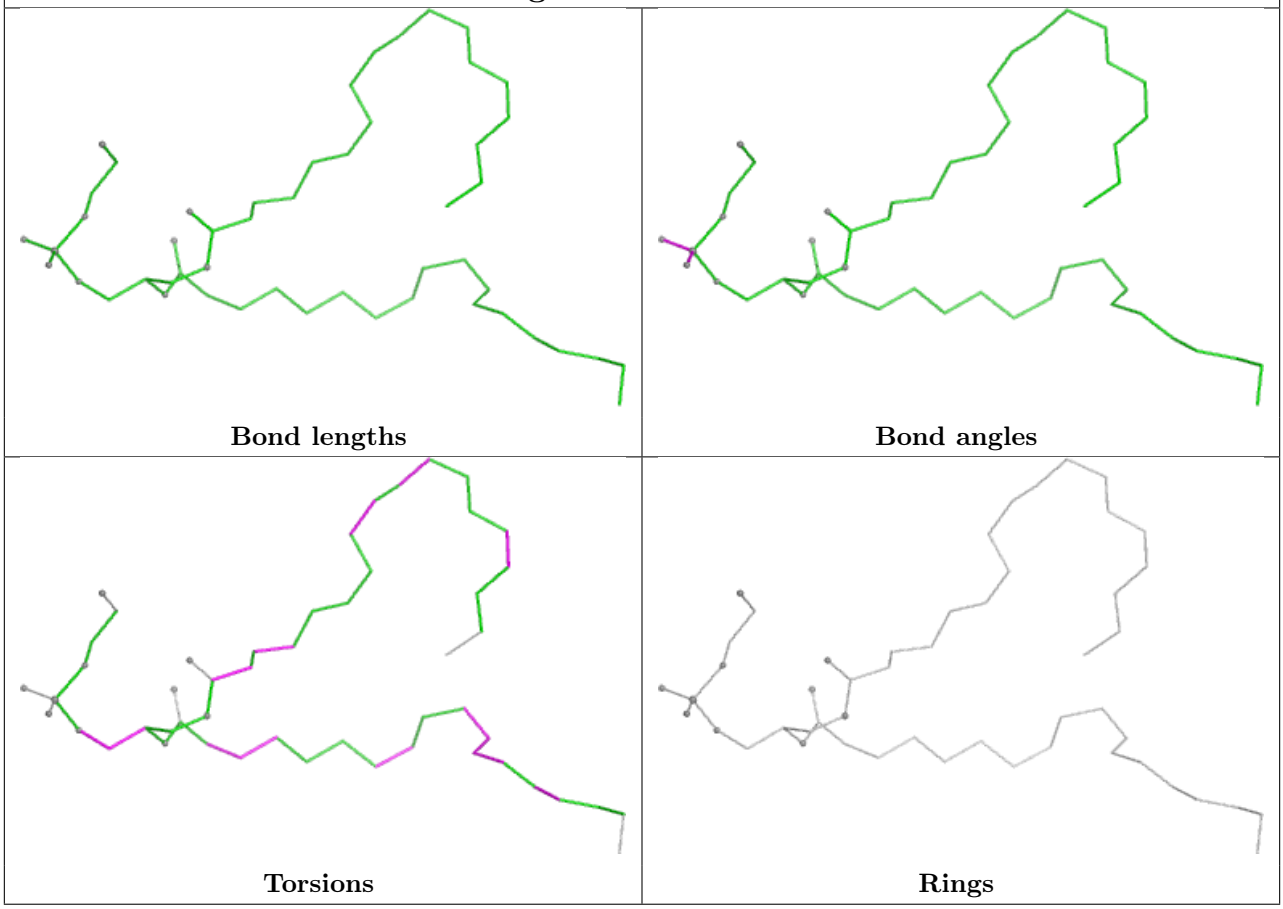


Ligand 3PE H 301



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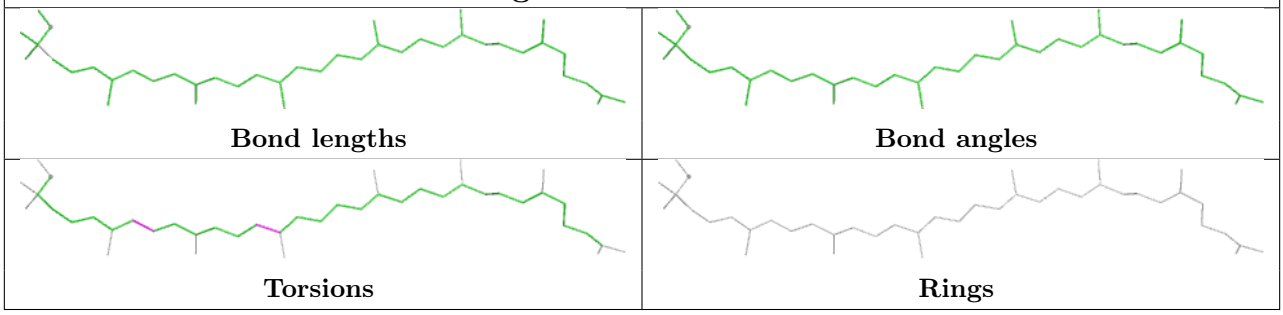

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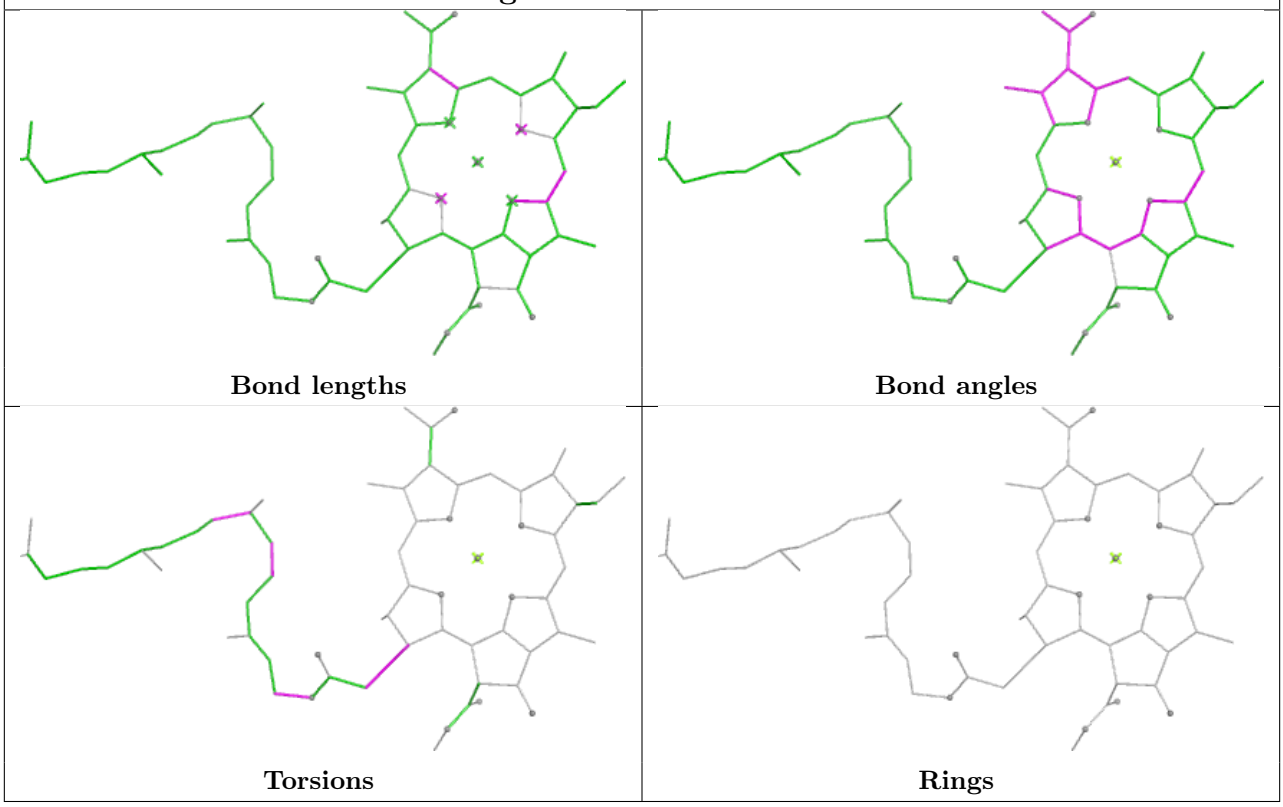

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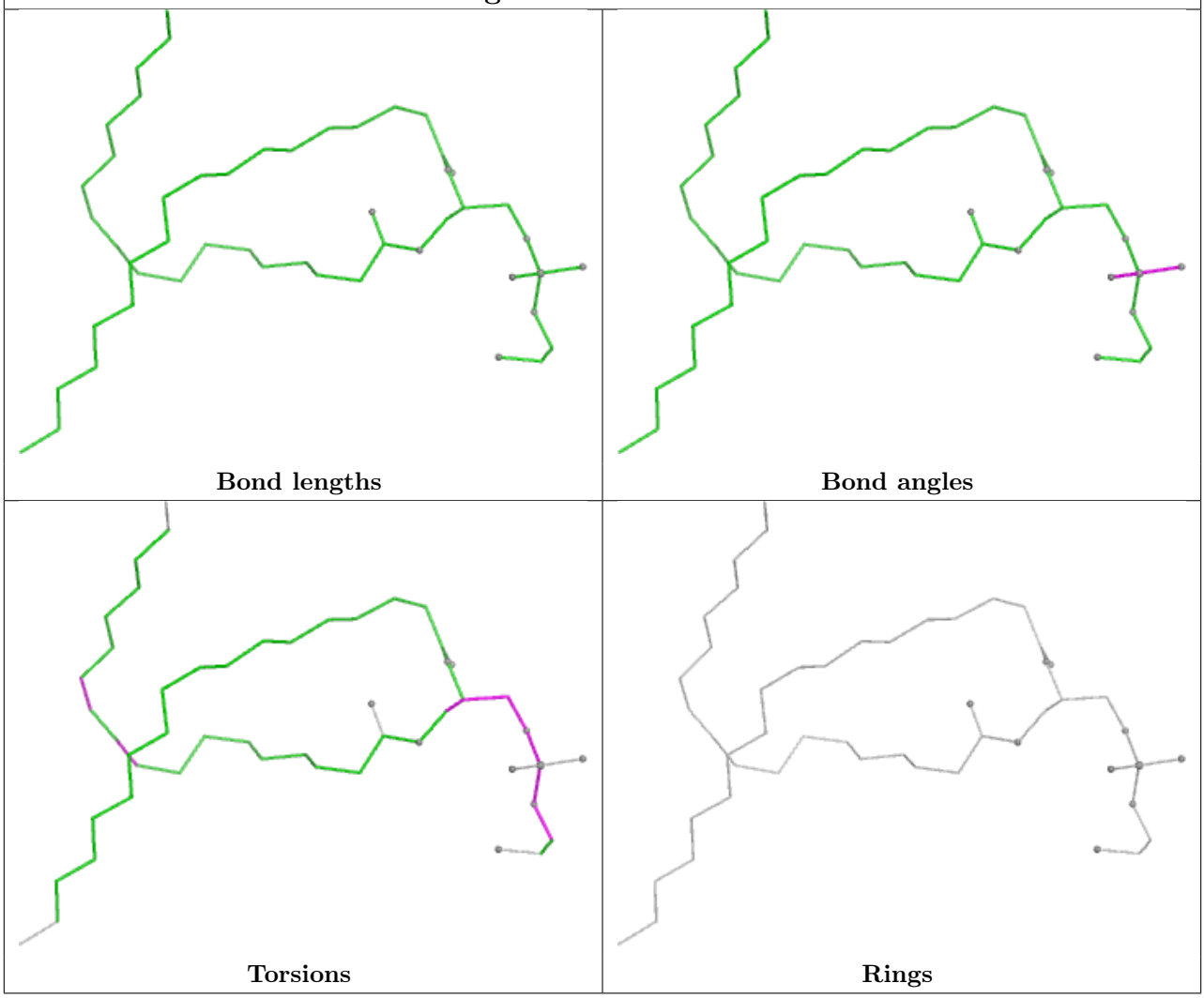

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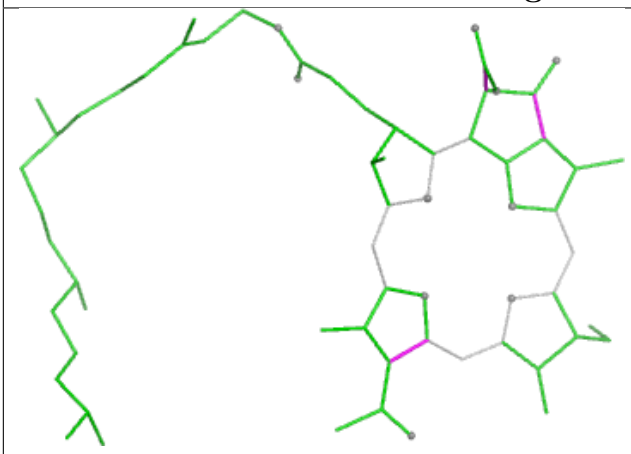
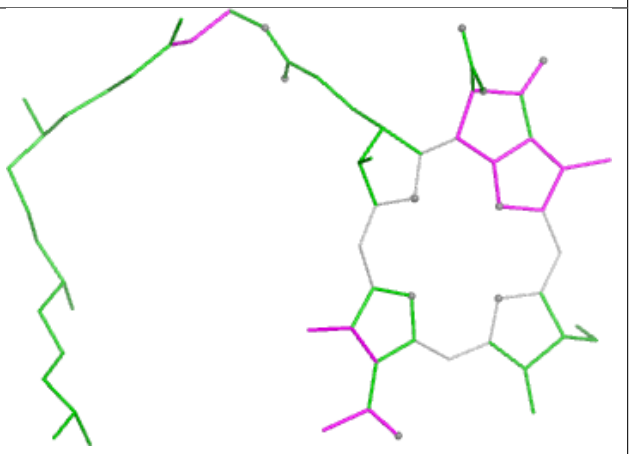
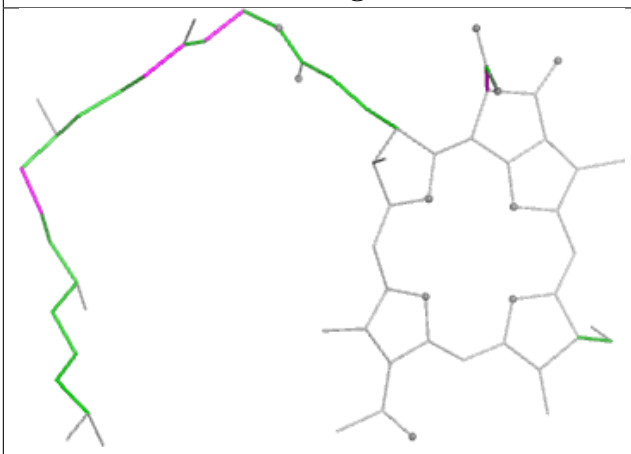


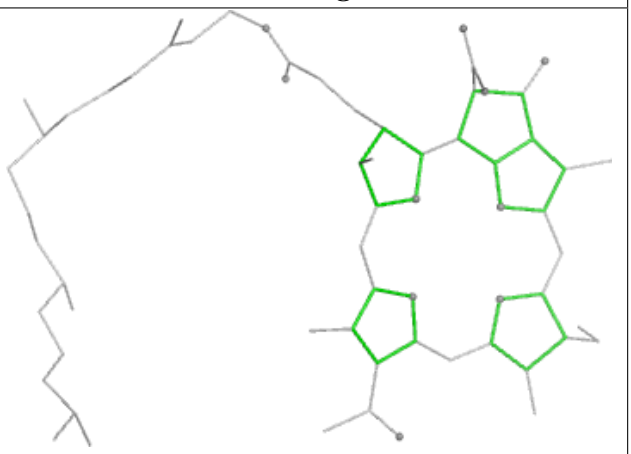
Bond lengths



Bond angles

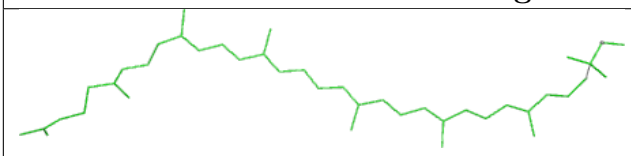


Torsions

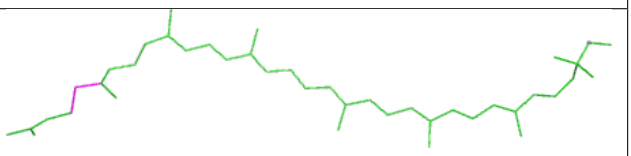


Rings

Ligand SPO AF 101



Bond lengths



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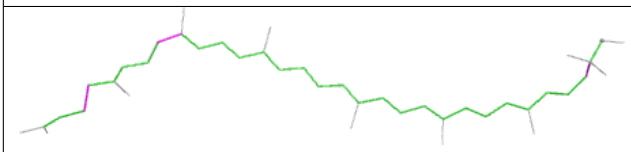
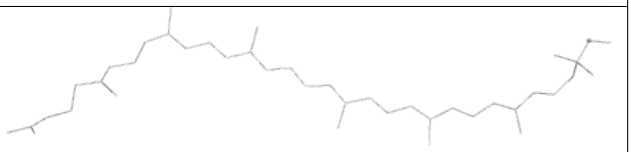
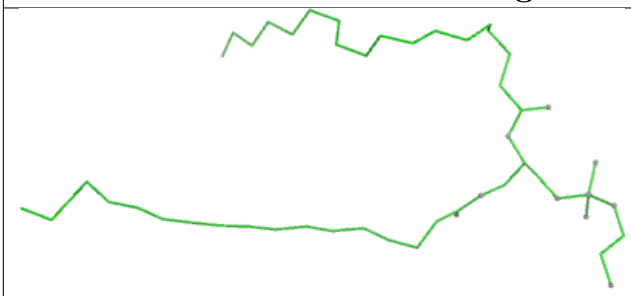
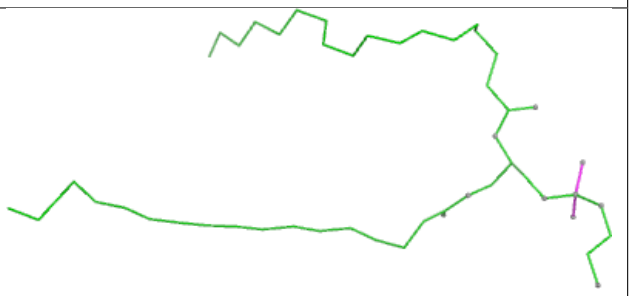
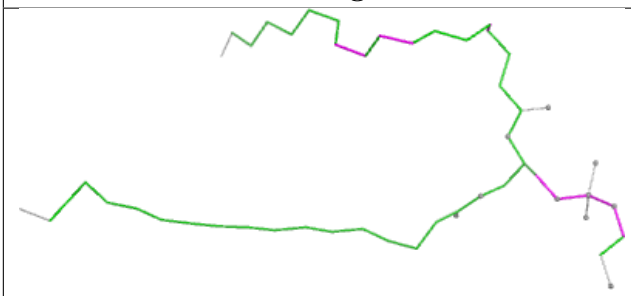
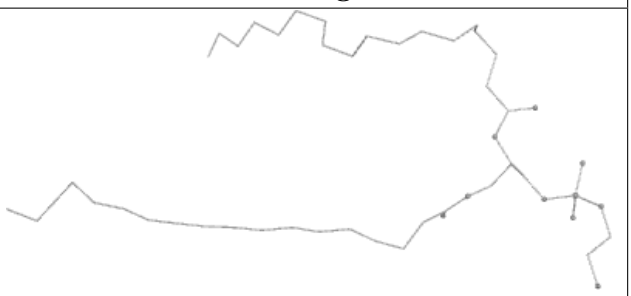
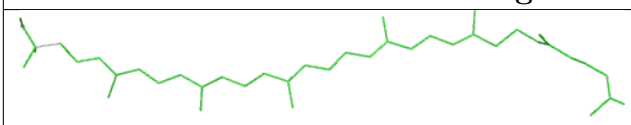
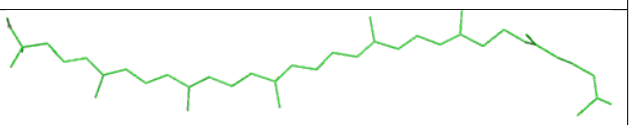
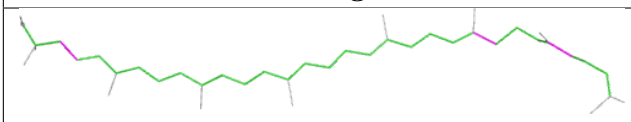
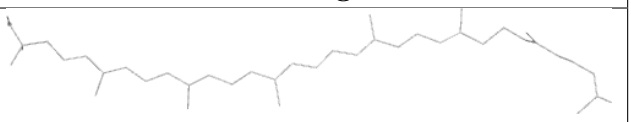


Torsions

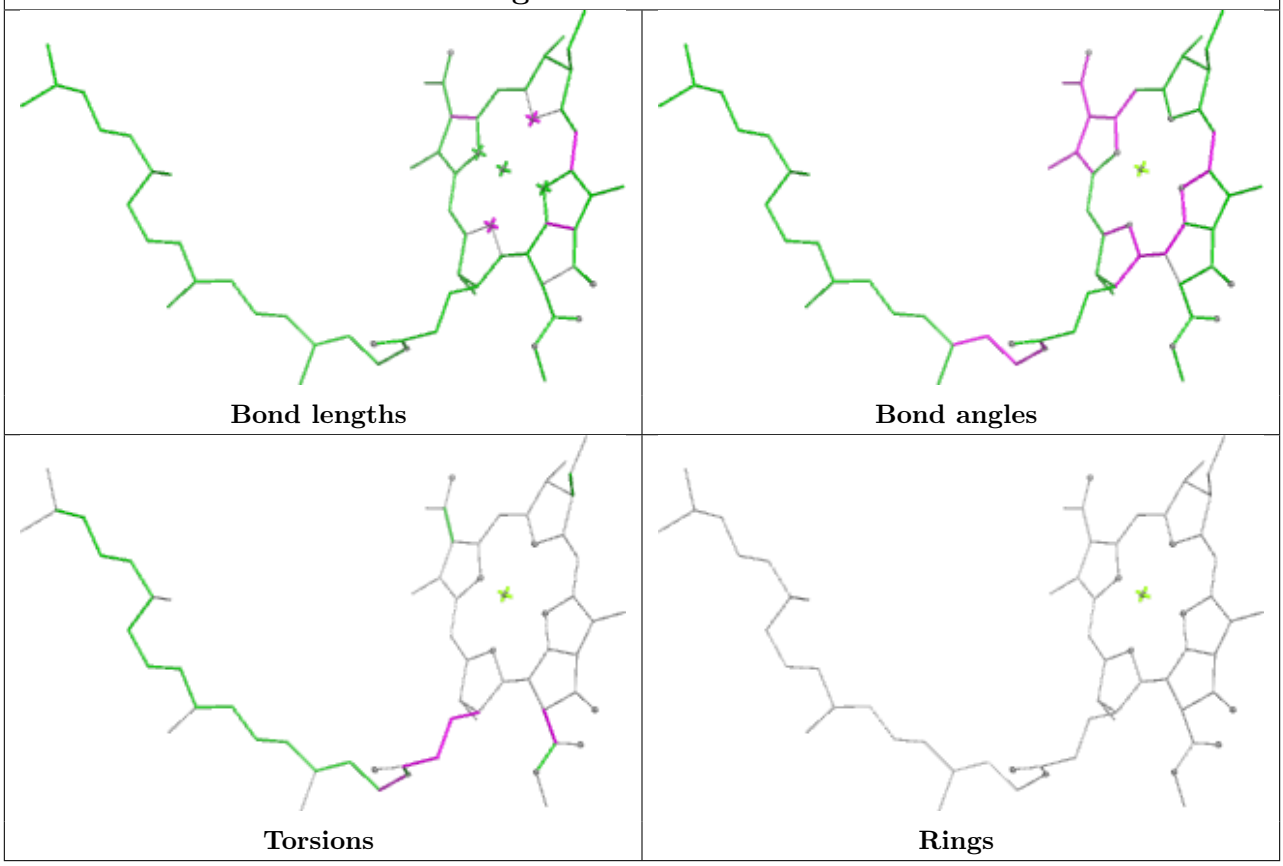


Rings

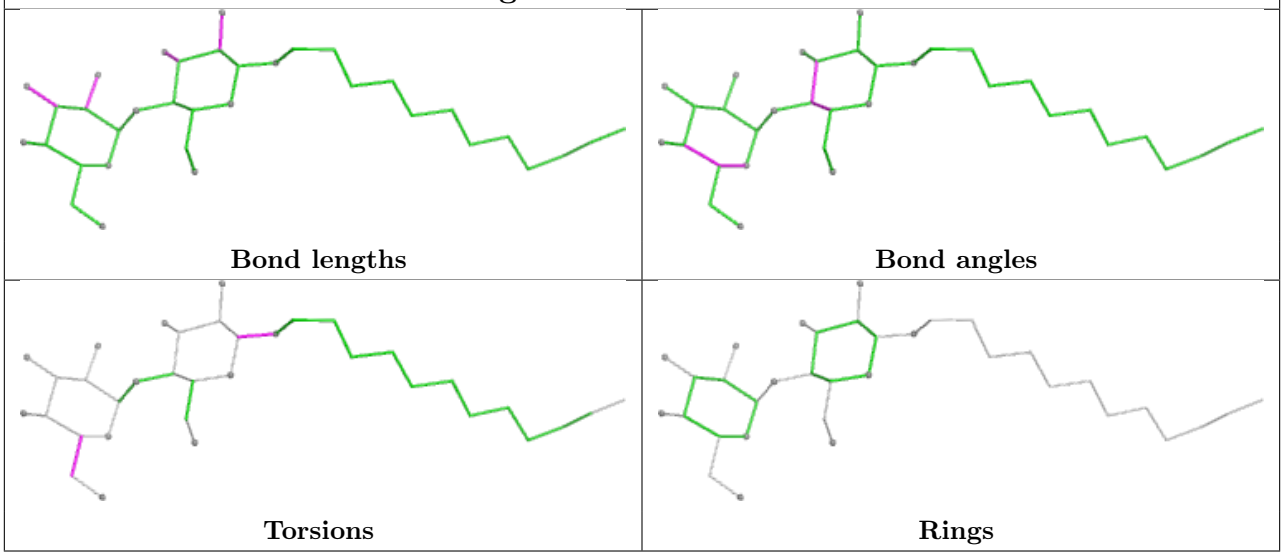
Ligand 3PE AB 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO BL 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL BG 101



Ligand LMT AA 1003



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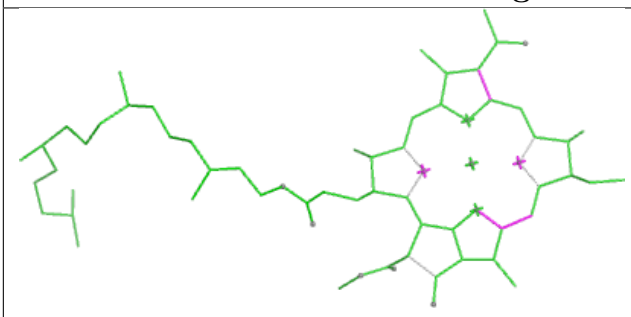
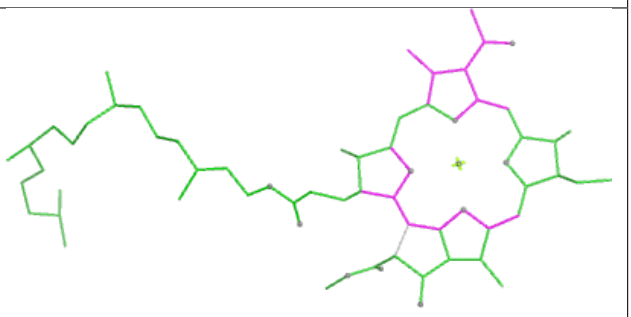
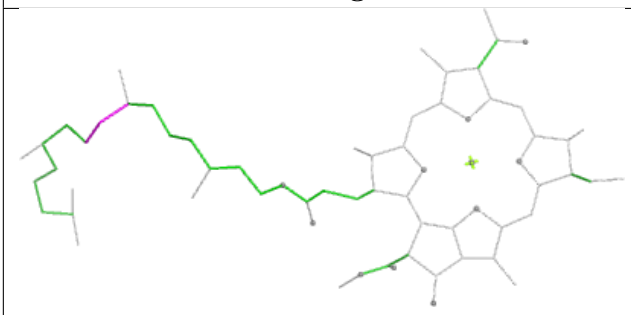
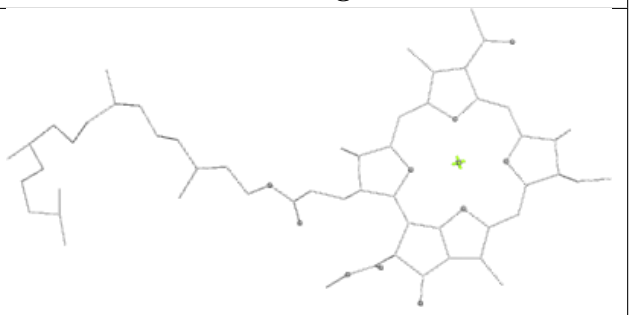
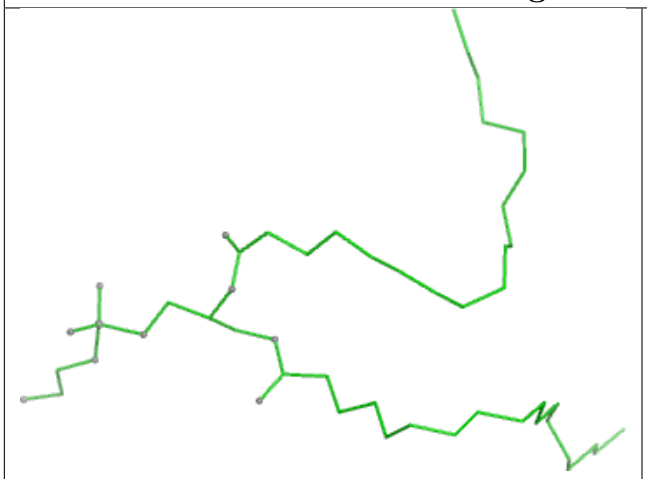
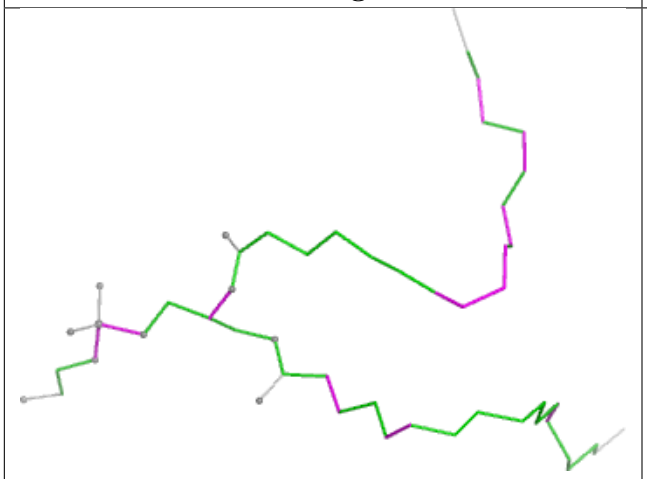
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE H 302



Bond lengths

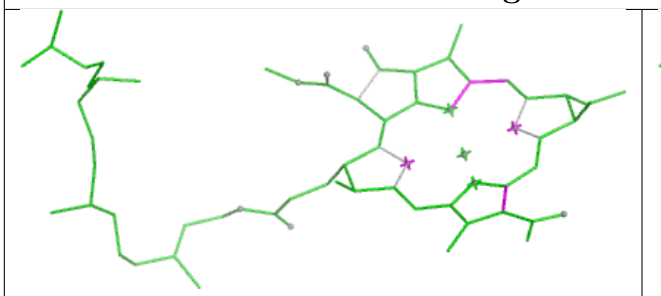
Bond angles



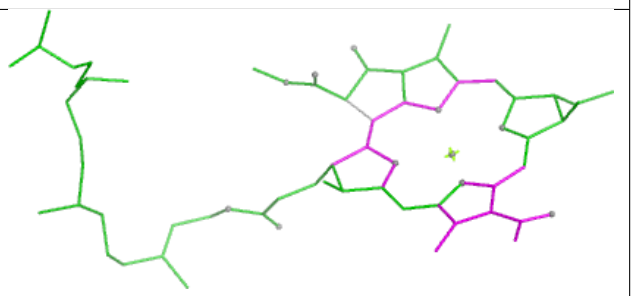
Torsions

Rings

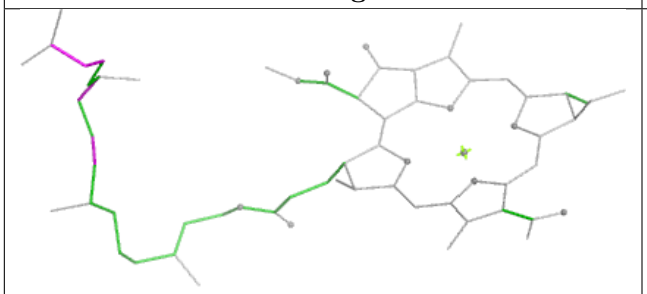
Ligand BCL AA 1001



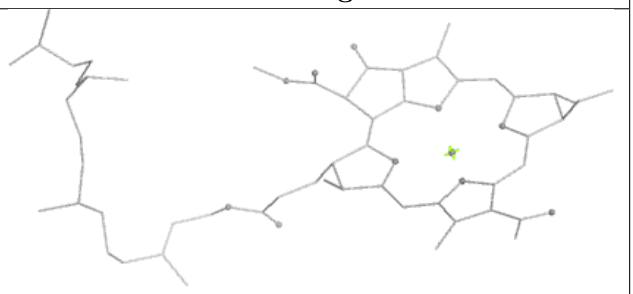
Bond lengths



Bond angles

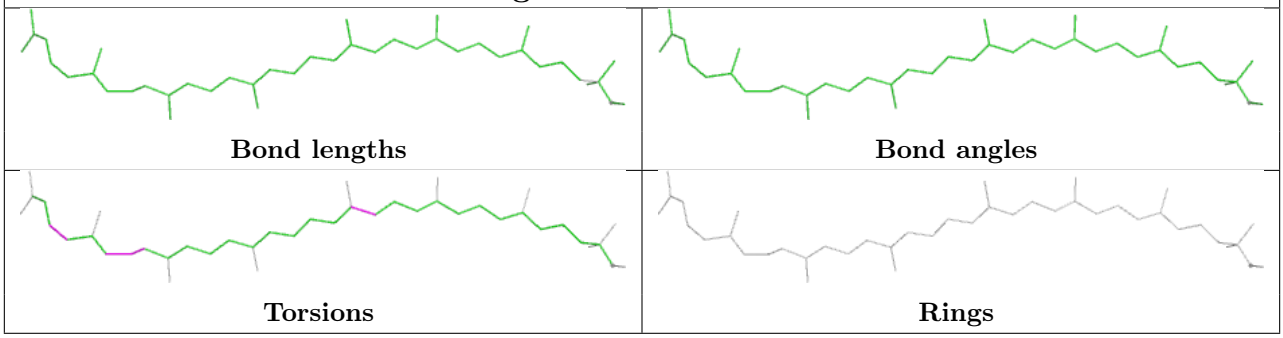


Torsions

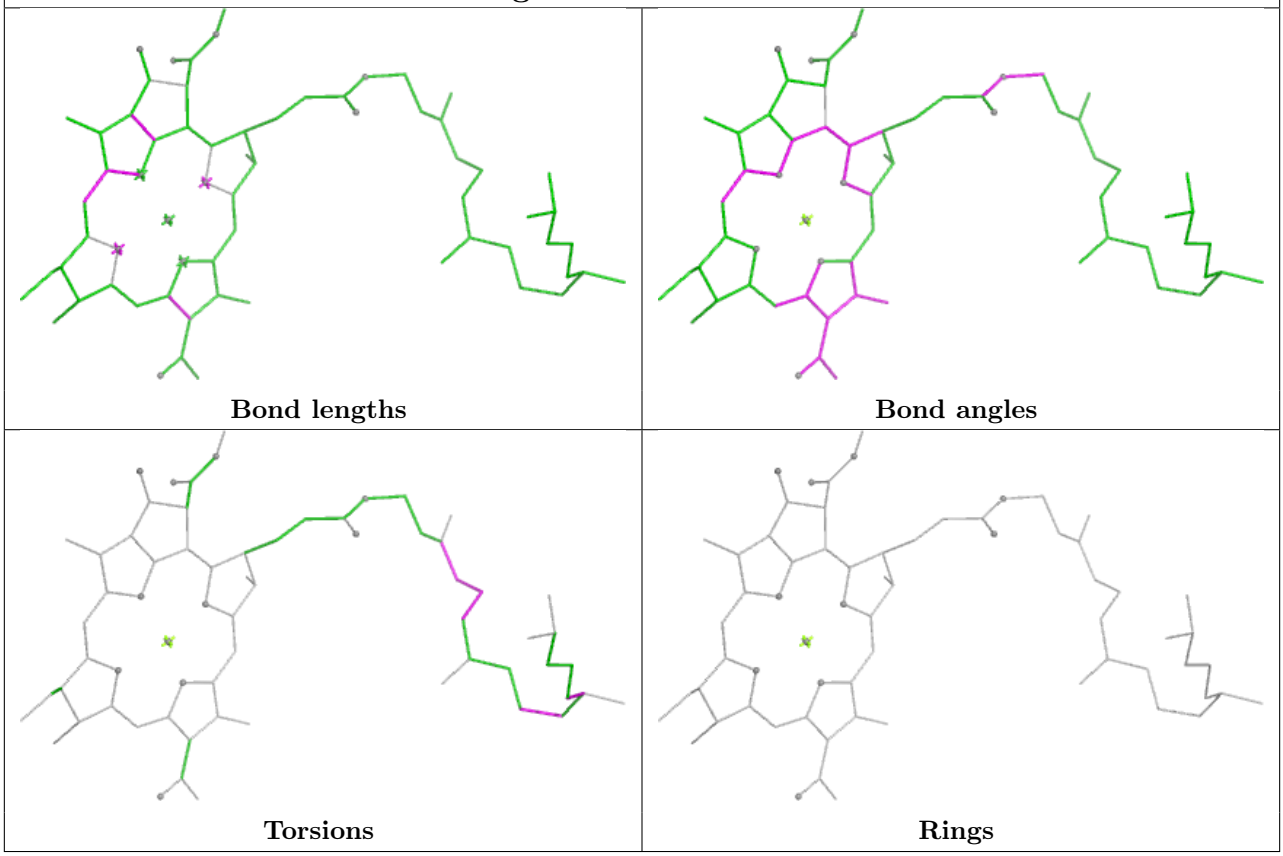


Rings

Ligand SPO AD 103



Ligand BCL BH 101



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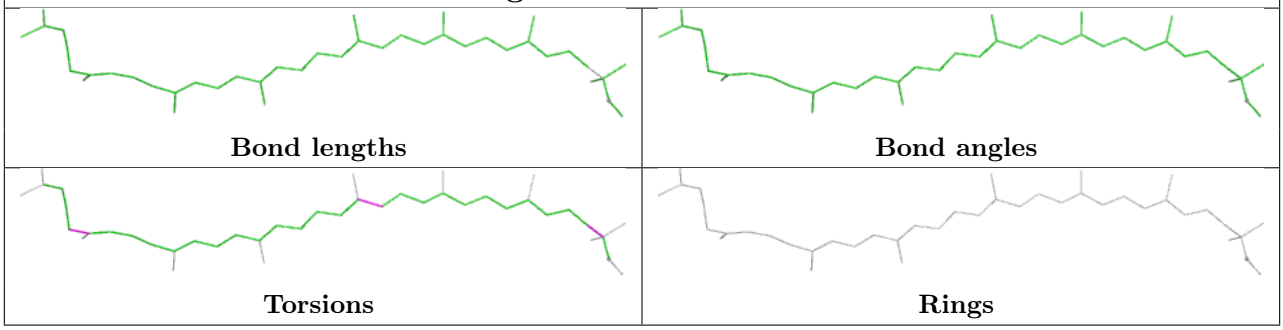
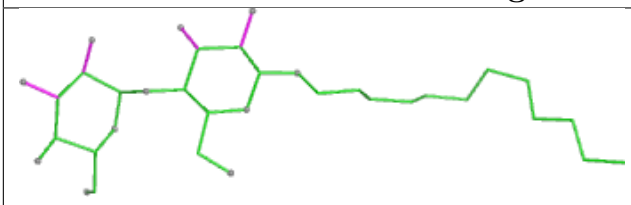
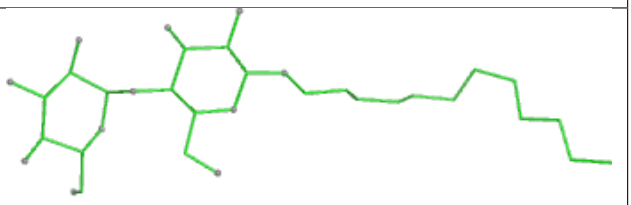
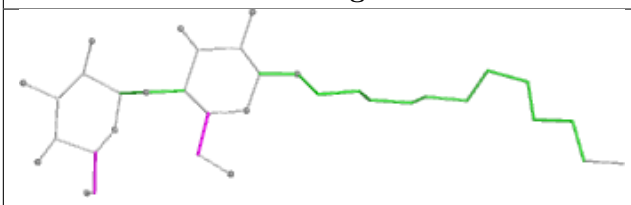
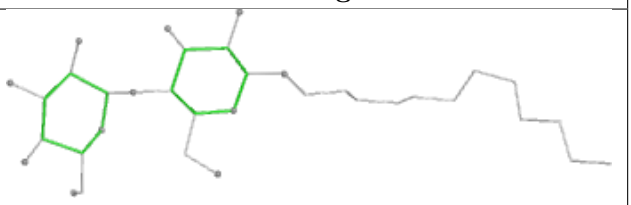
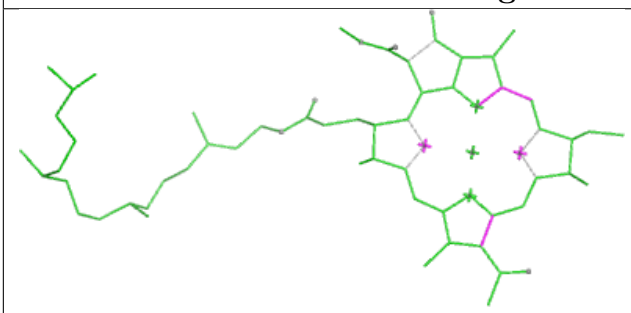
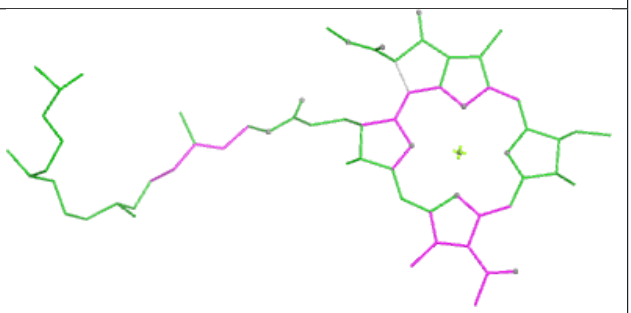
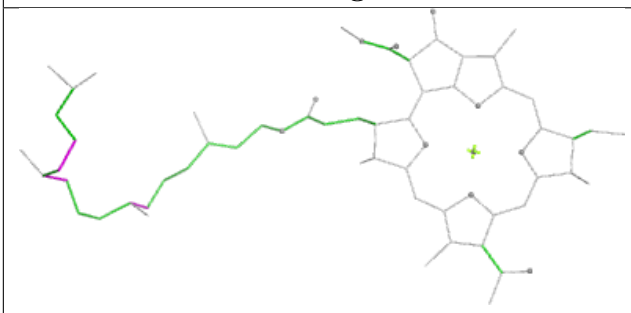
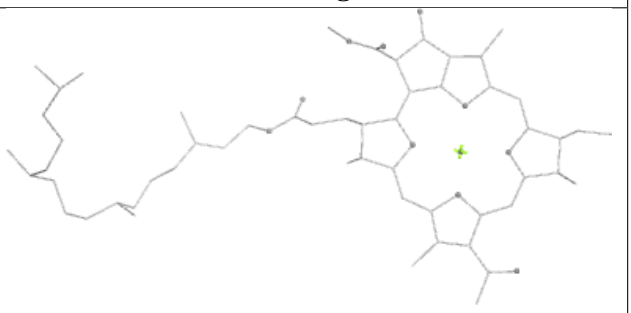
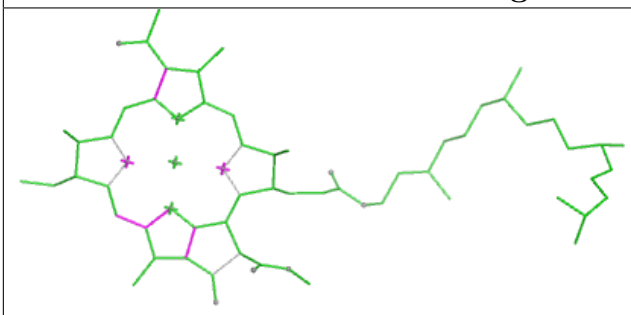


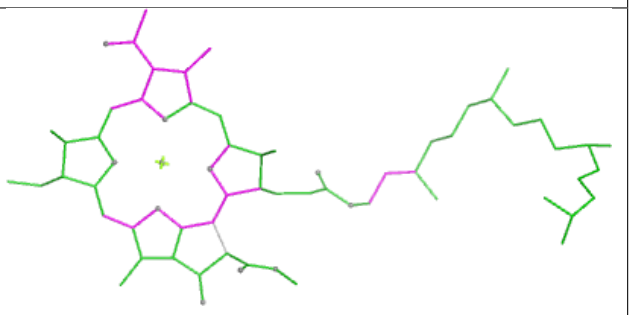
Ligand LMT AB 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AM 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

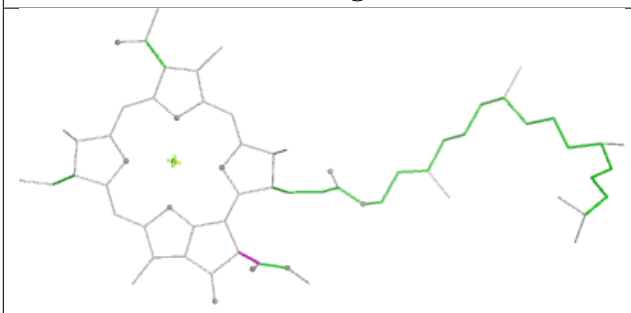
Ligand BCL AH 102



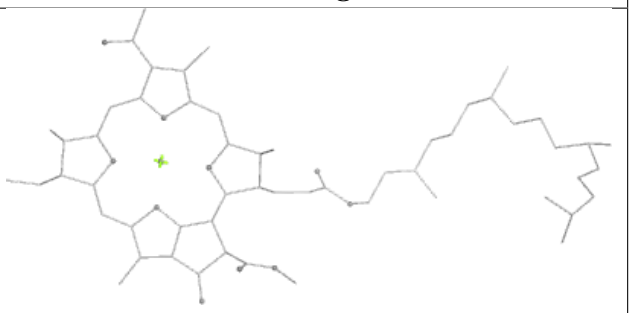
Bond lengths



Bond angles

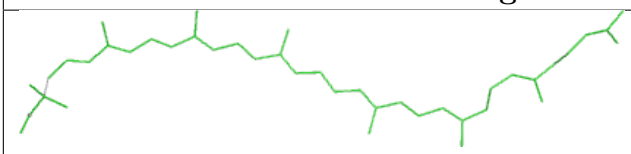


Torsions

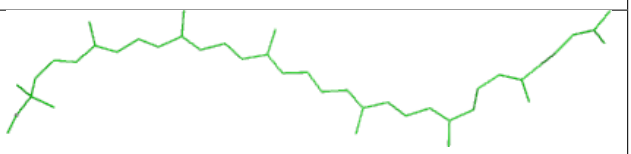


Rings

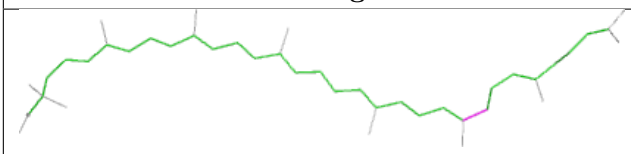
Ligand SPO AM 1002



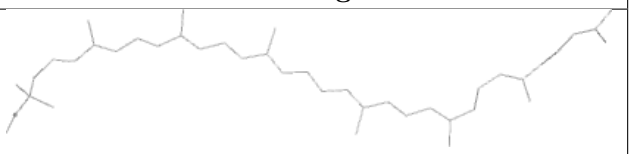
Bond lengths



Bond angles



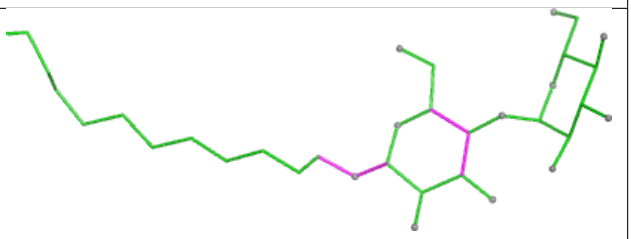
Torsions



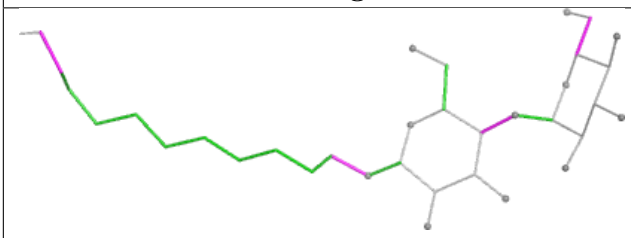
Rings

Ligand LMT M 401

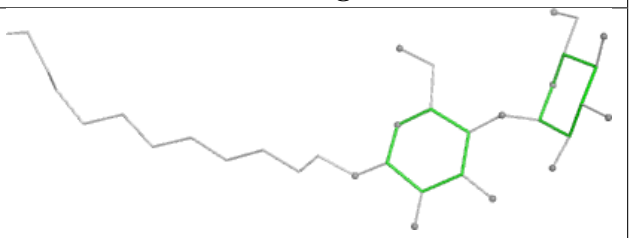
Bond lengths



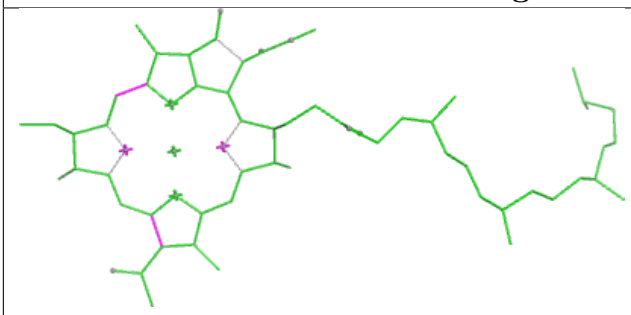
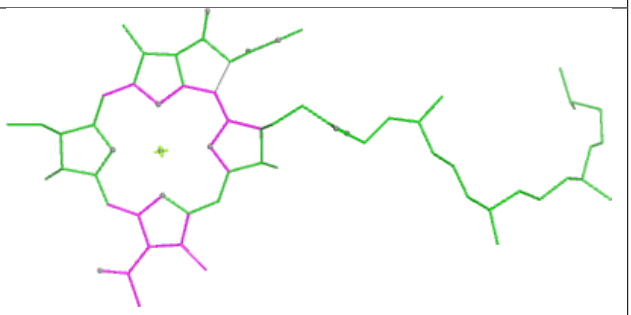
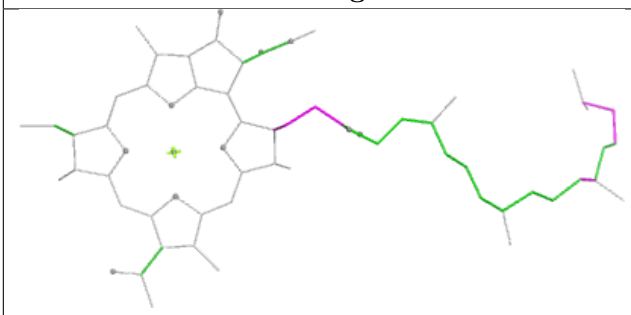
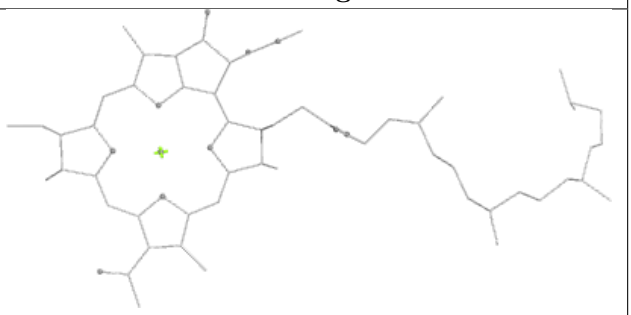
Bond angles

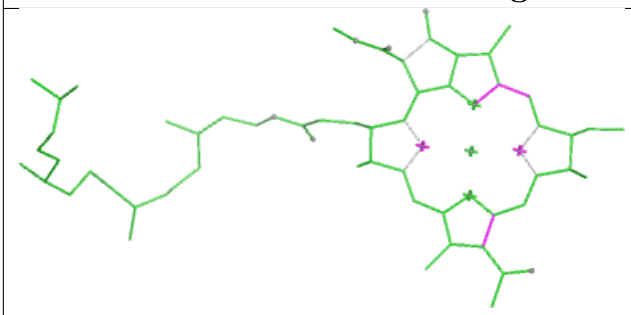
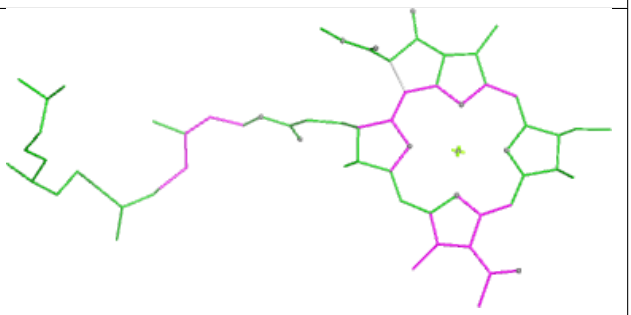
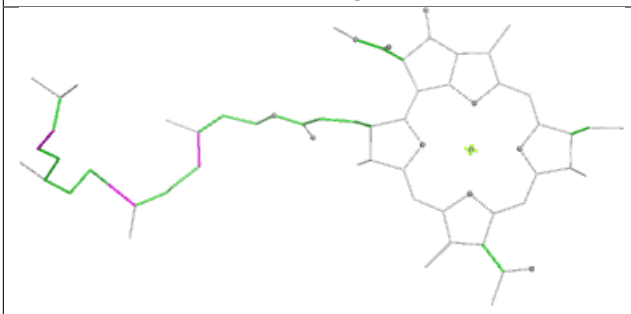
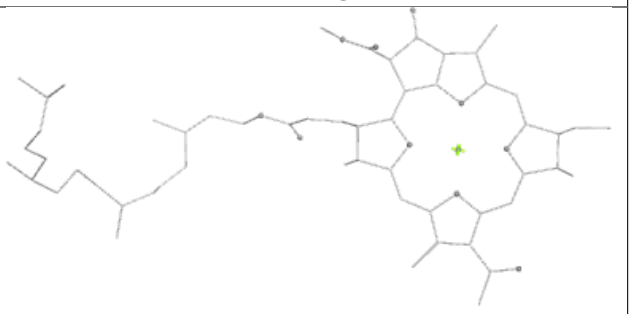


Torsions

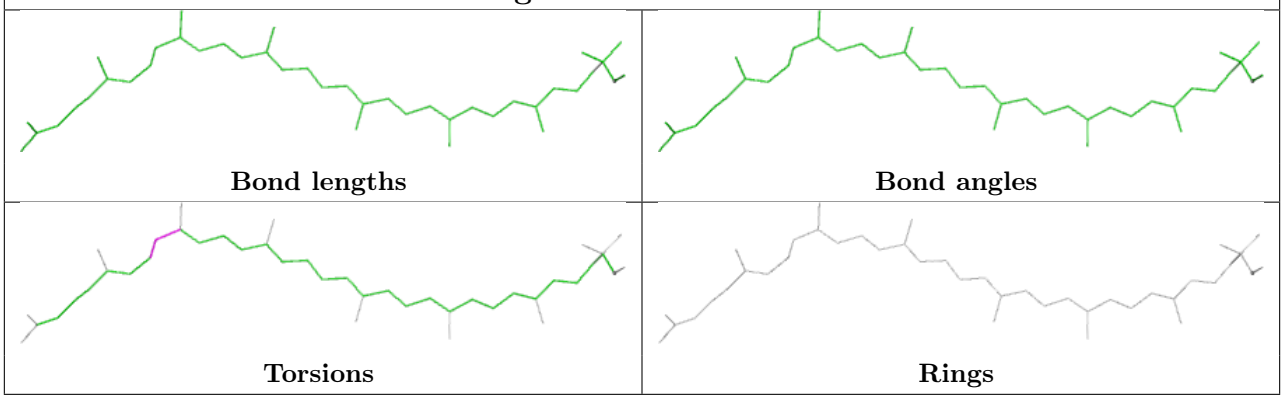


Rings

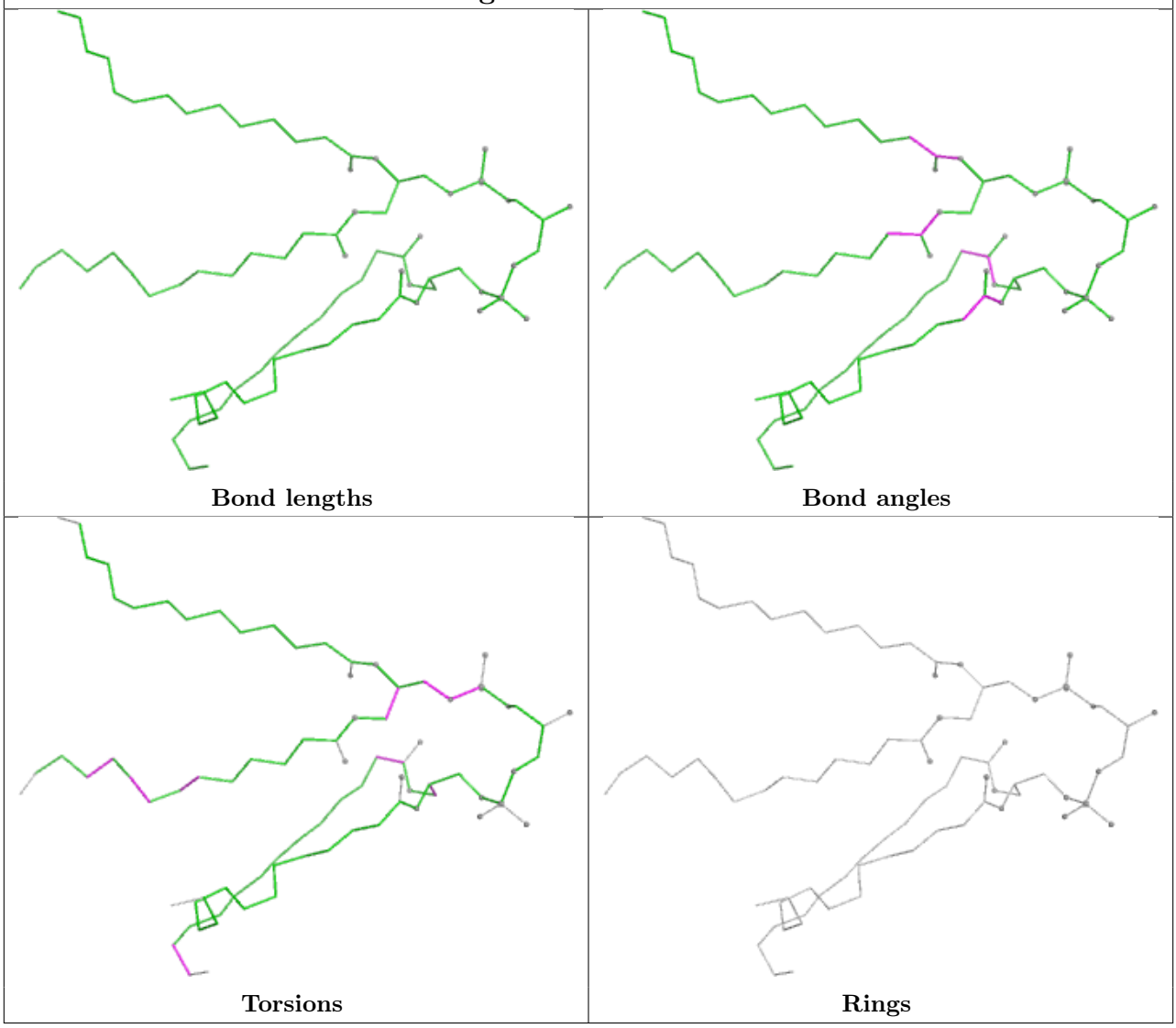
Ligand BCL AC 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

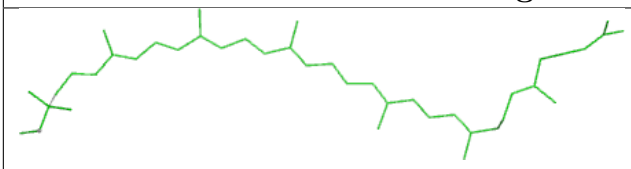
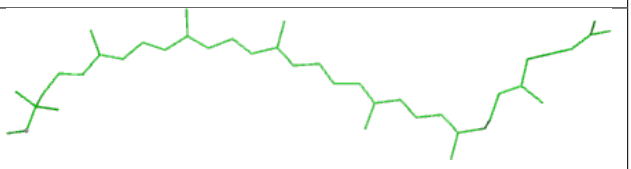
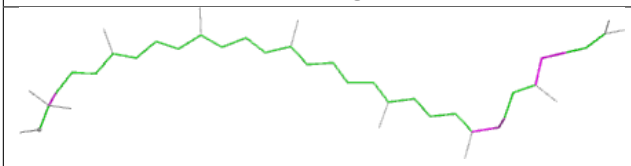
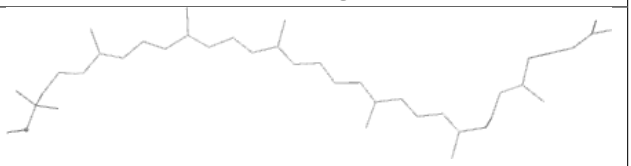
Ligand BCL AK 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

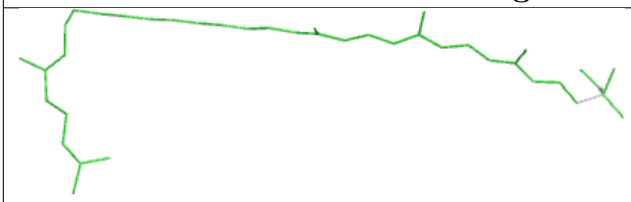
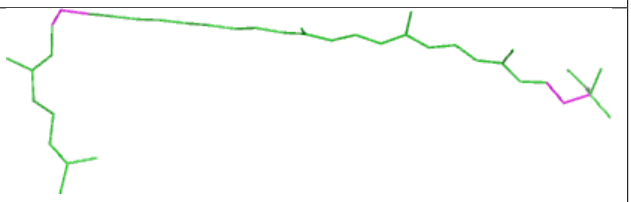
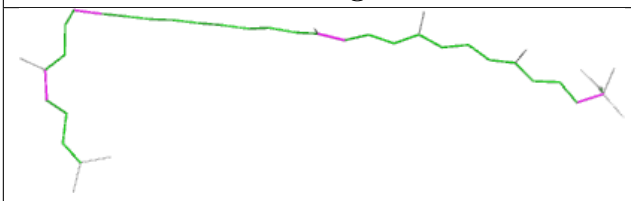
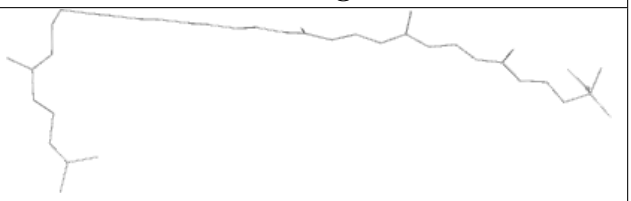
Ligand SPO AE 102



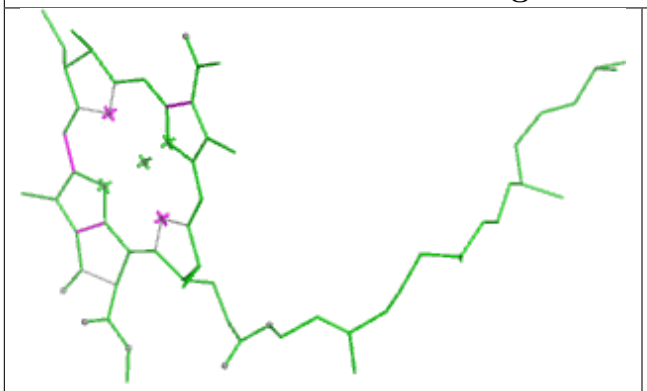
Ligand CD4 M 405



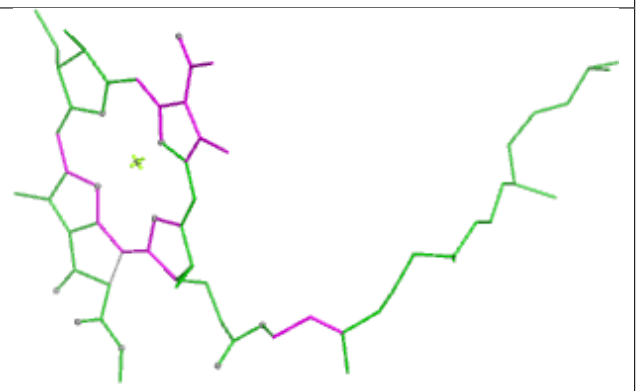
Ligand SPO AJ 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AB 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

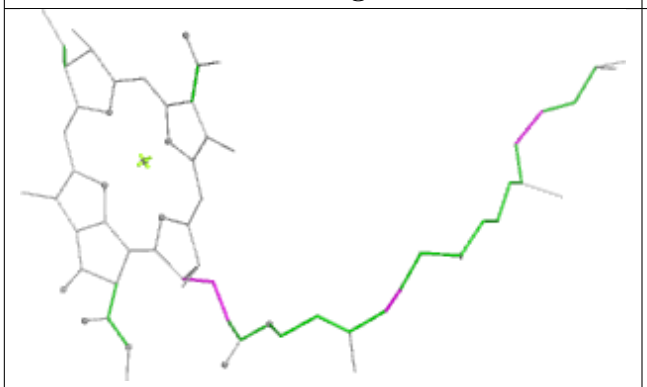
Ligand BCL AK 103



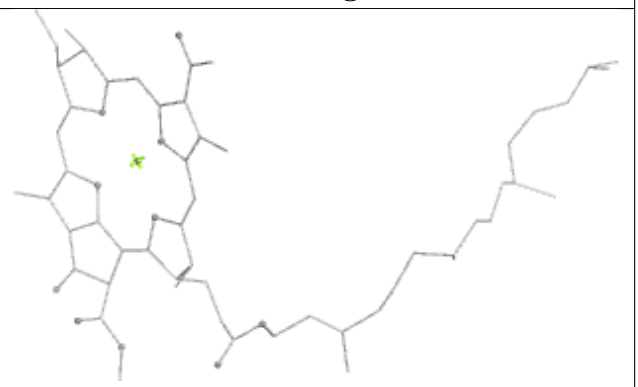
Bond lengths



Bond angles

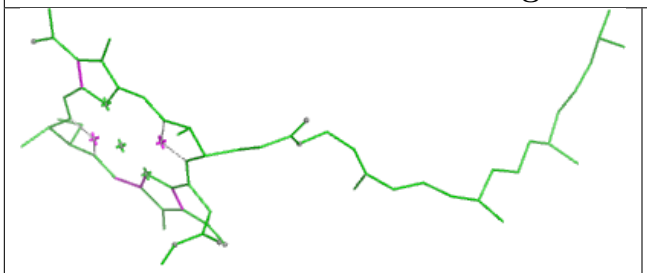


Torsions

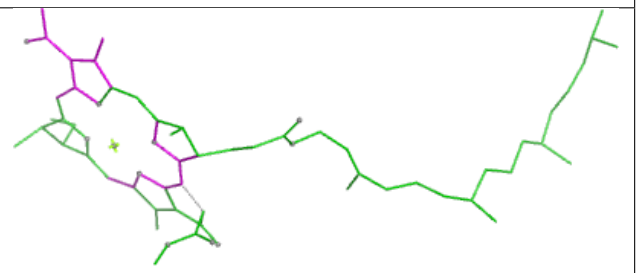


Rings

Ligand BCL M 403



Bond lengths



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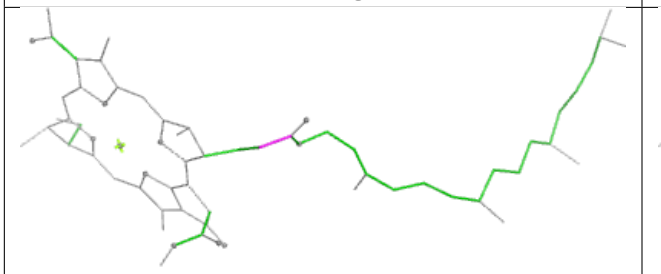
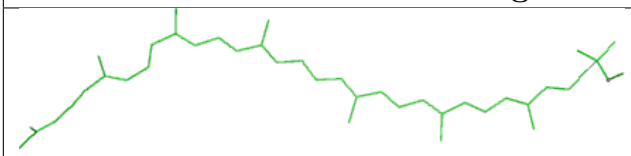
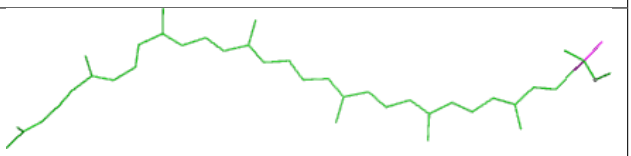
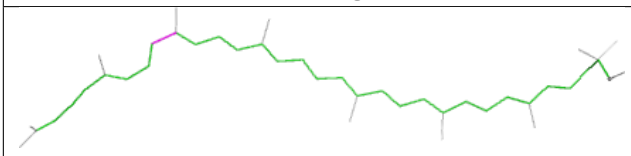
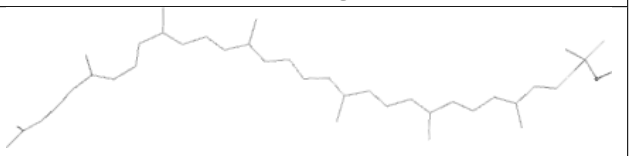
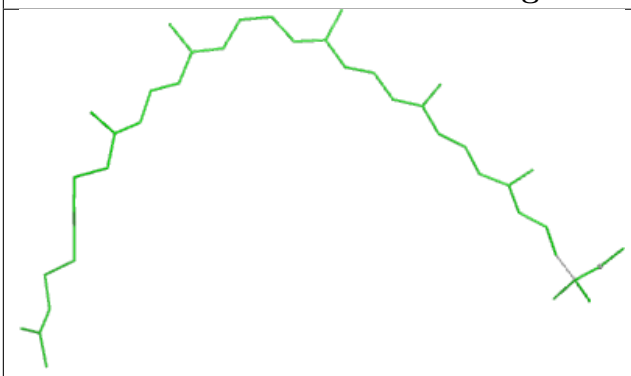
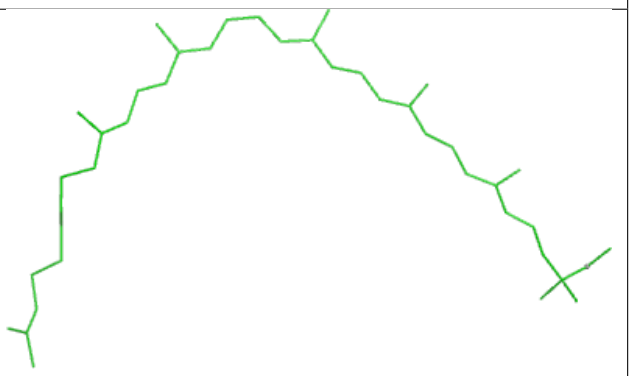
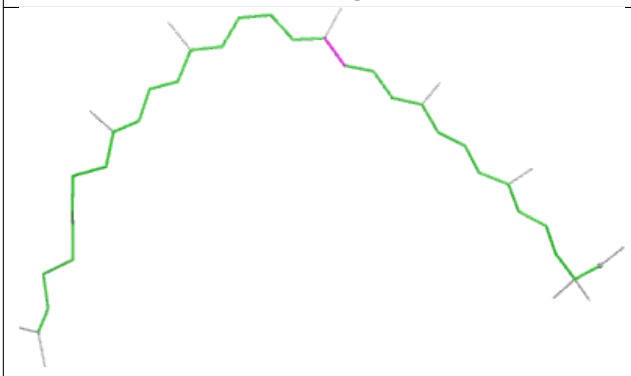
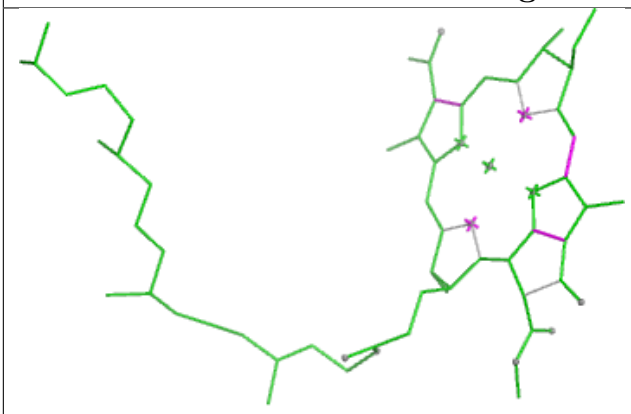
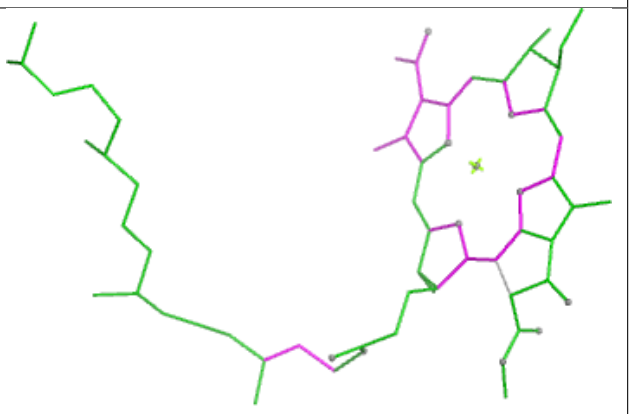
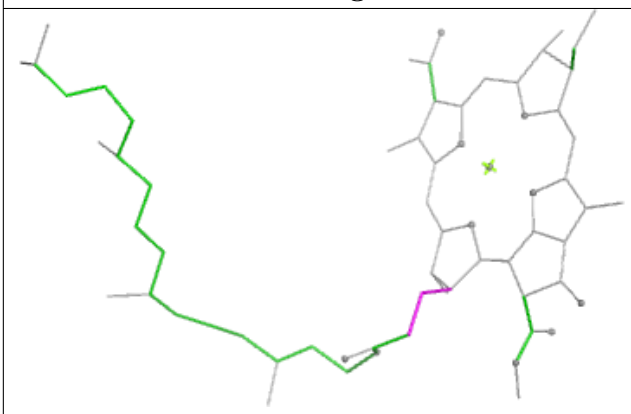
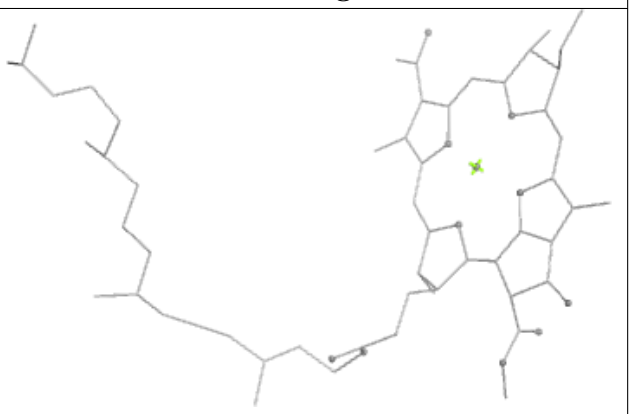


Torsions

Rings

Ligand SPO AH 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO M 407	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand BCL BI 101	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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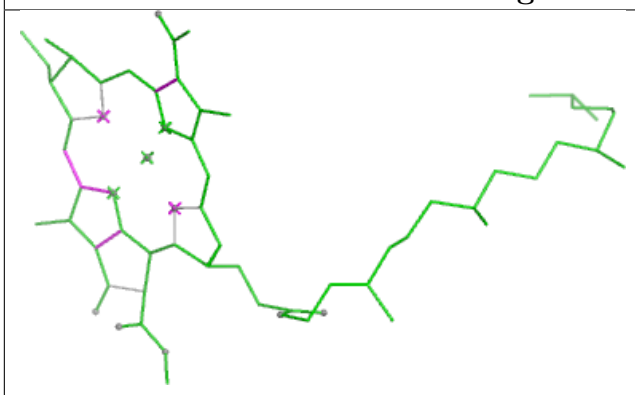
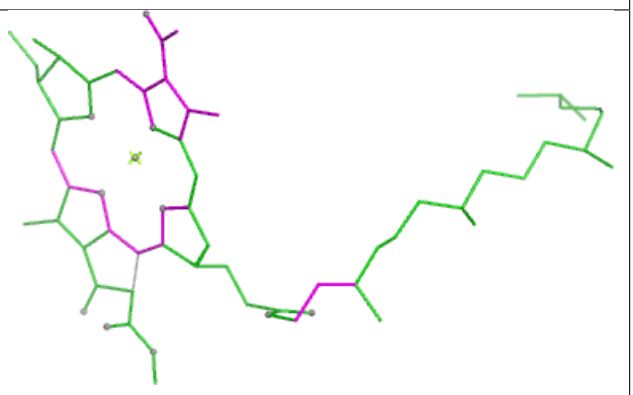
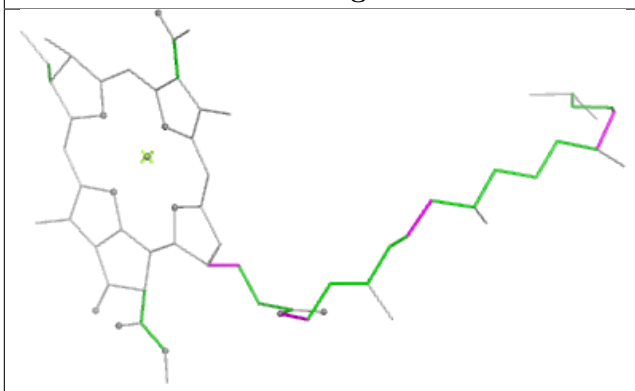
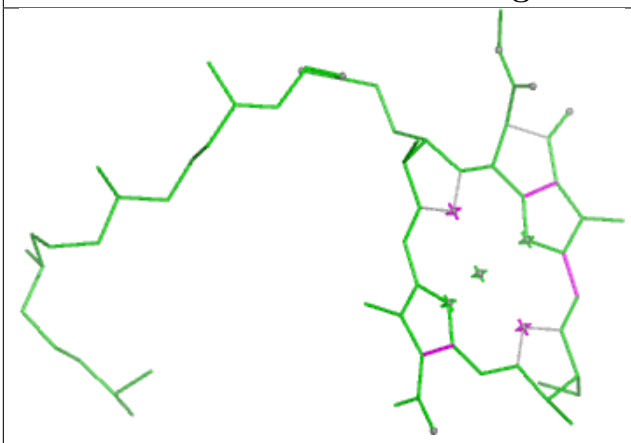
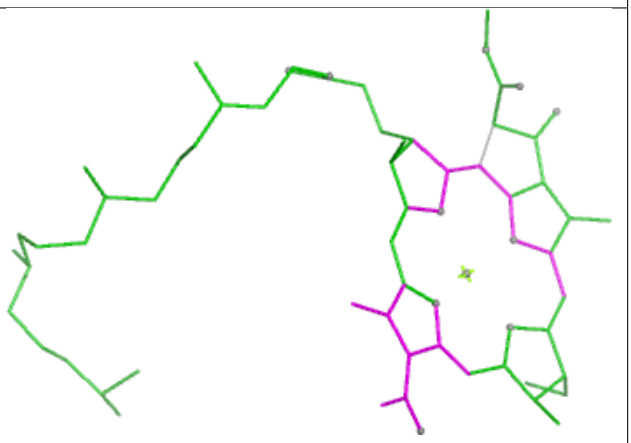
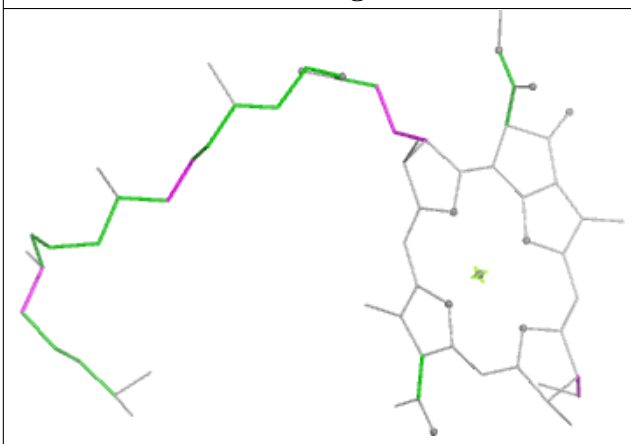
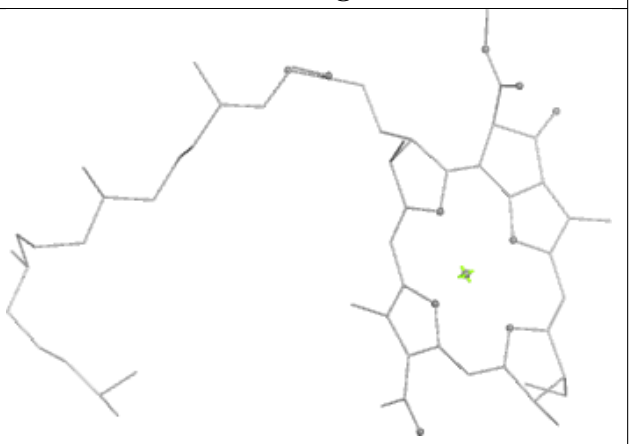
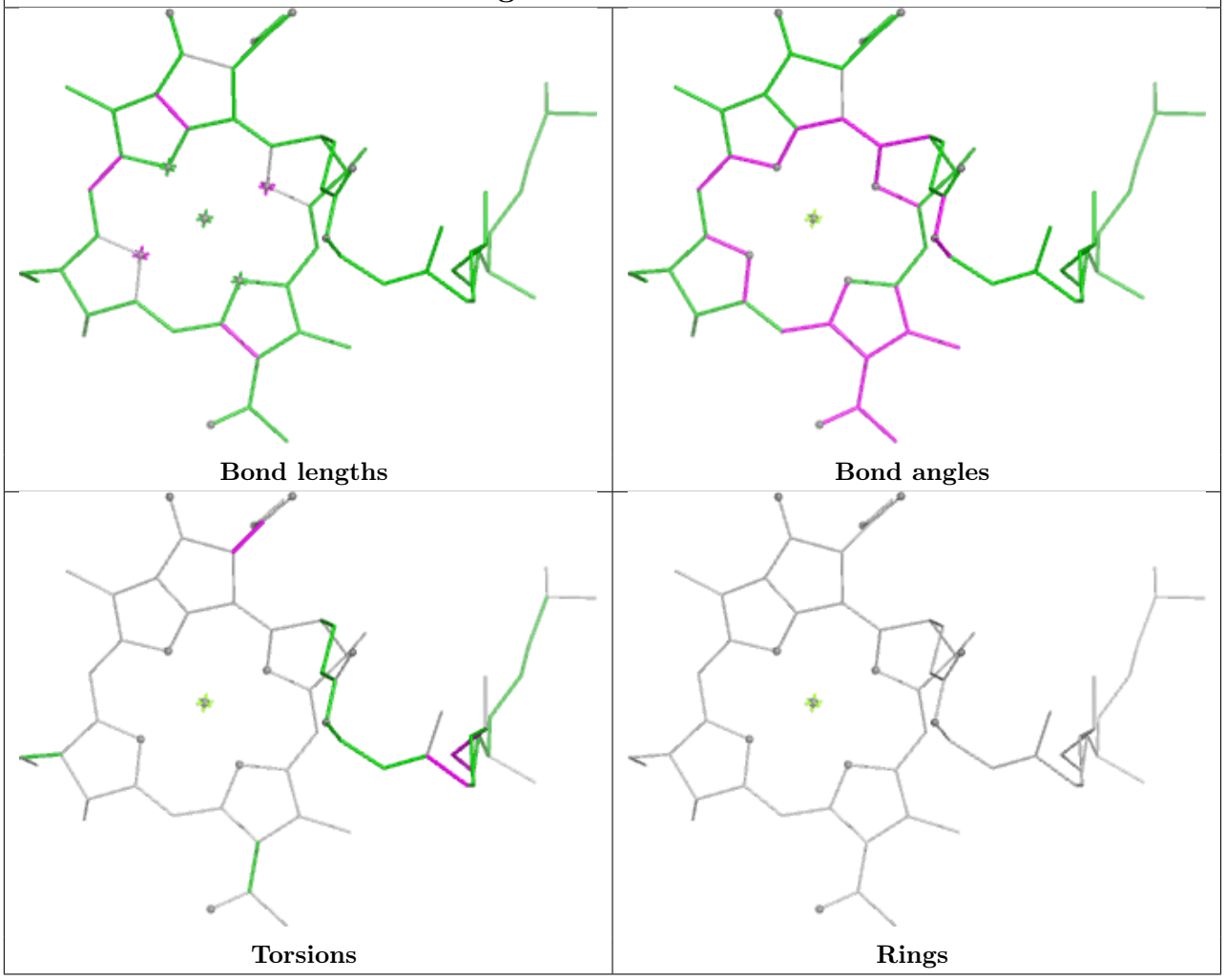
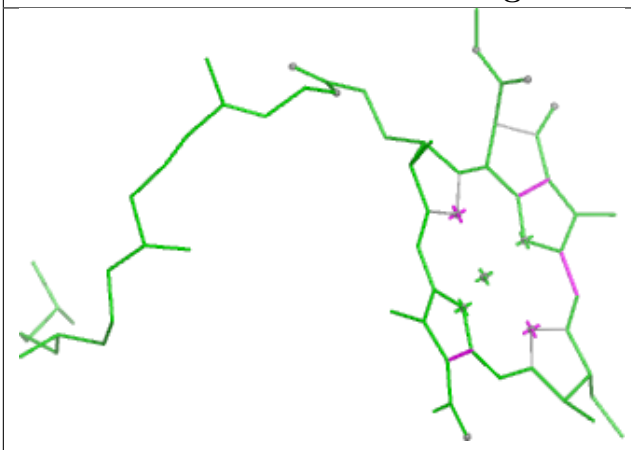
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand BCL BC 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

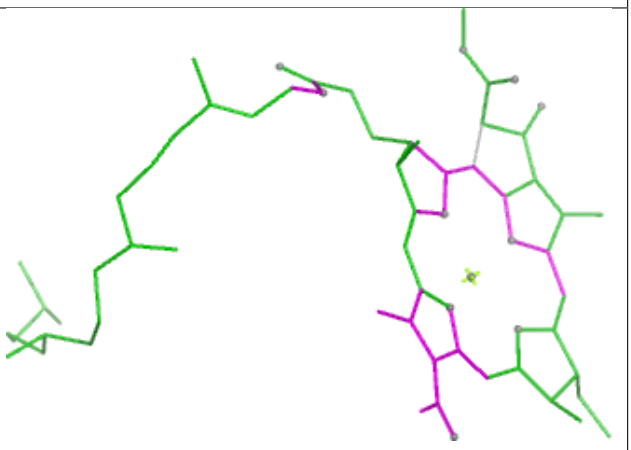
Ligand BCL M 406



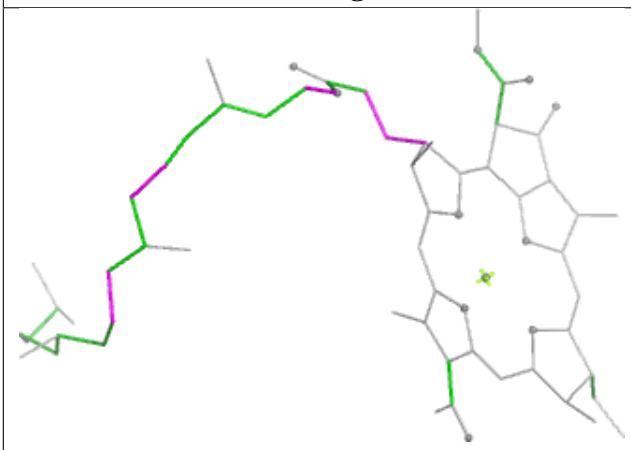
Ligand BCL BB 1001



Bond lengths



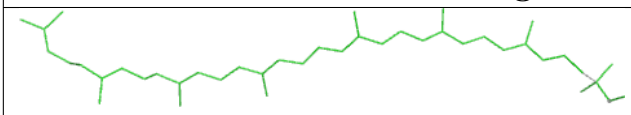
Bond angles



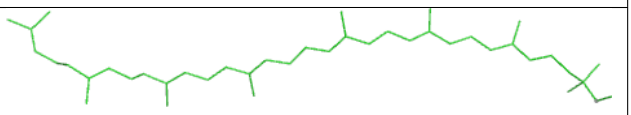
Torsions

Rings

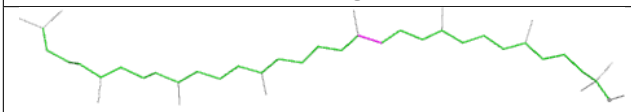
Ligand SPO AF 103



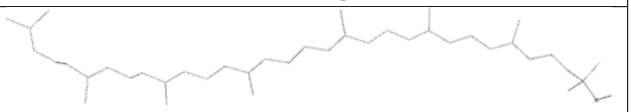
Bond lengths



Bond angles

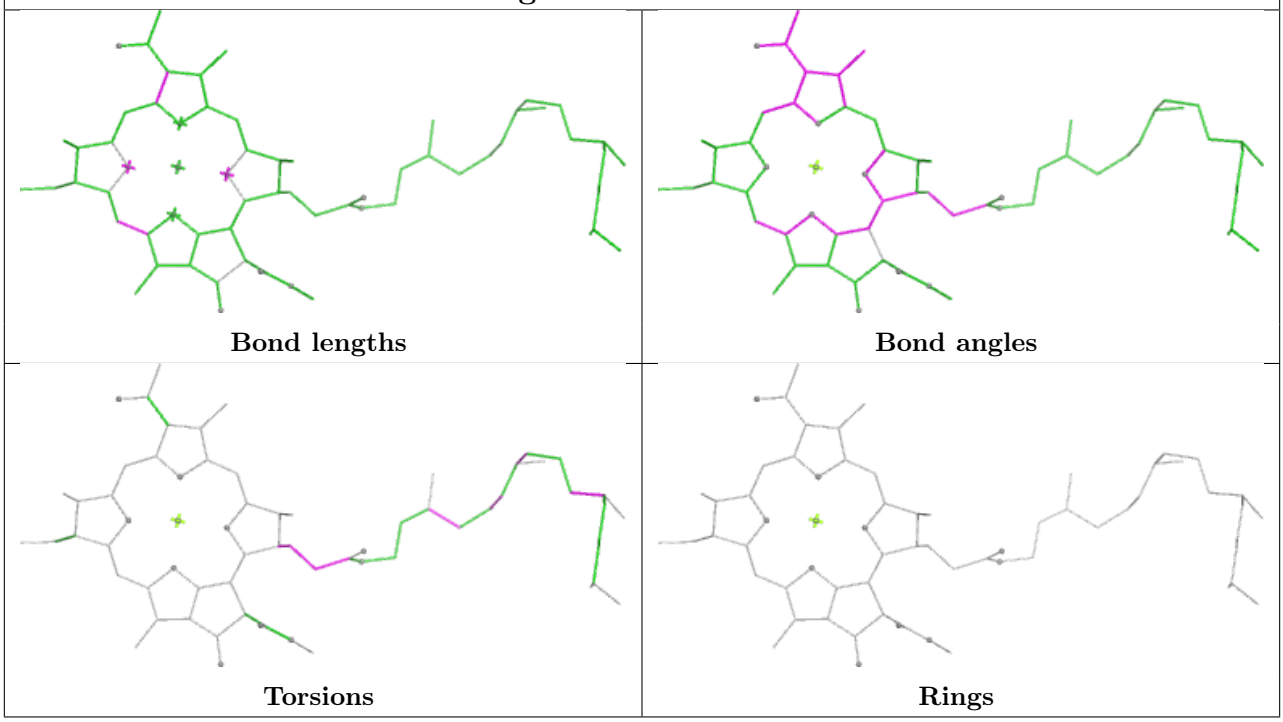


Torsions

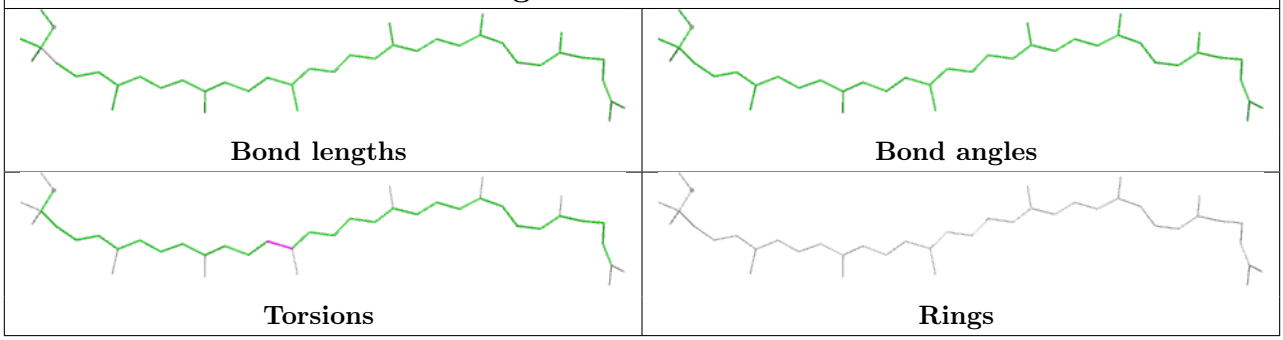


Rings

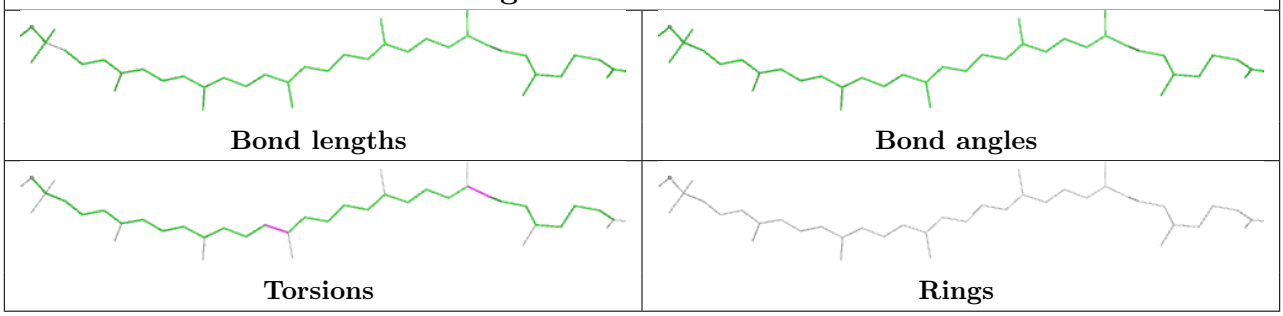
Ligand BCL AI 101



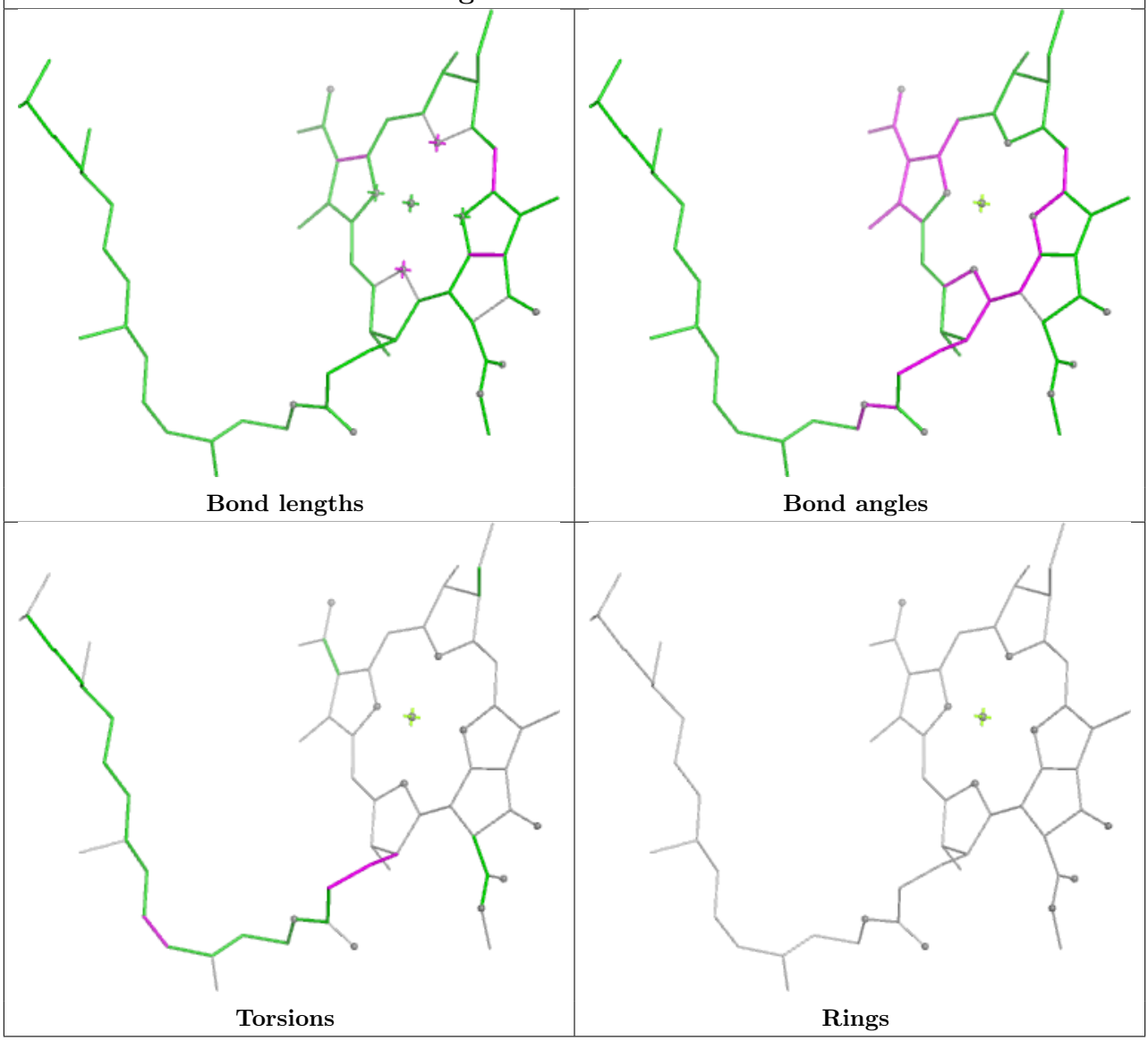
Ligand SPO AG 103



Ligand SPO AM 1004



Ligand BCL BA 102



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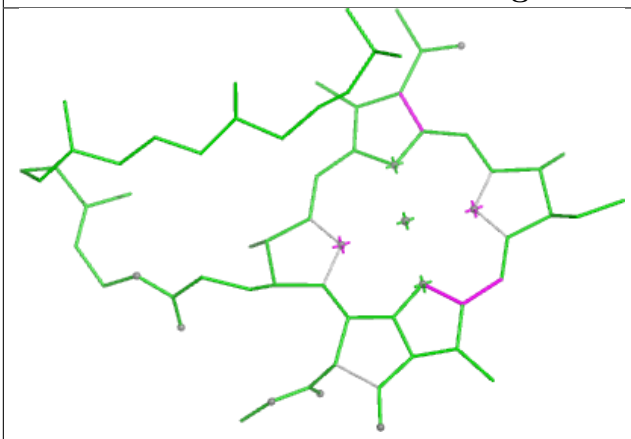
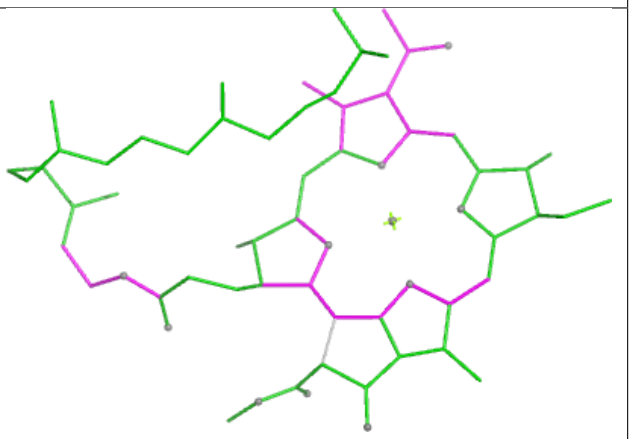
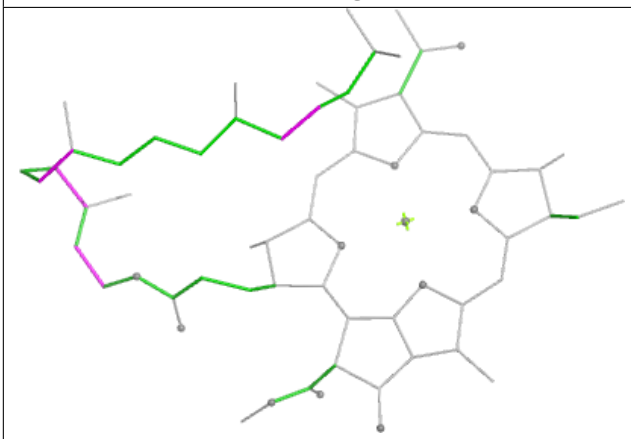
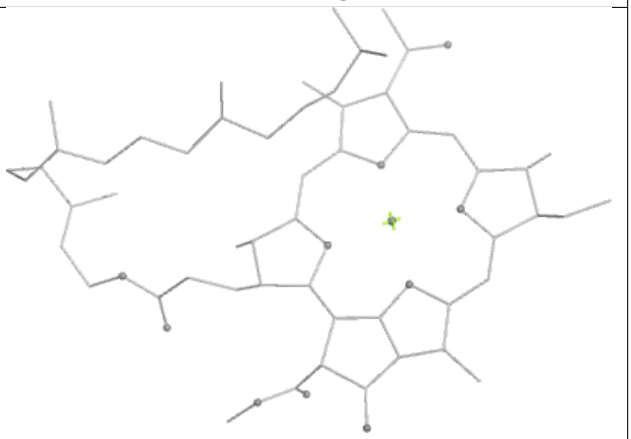
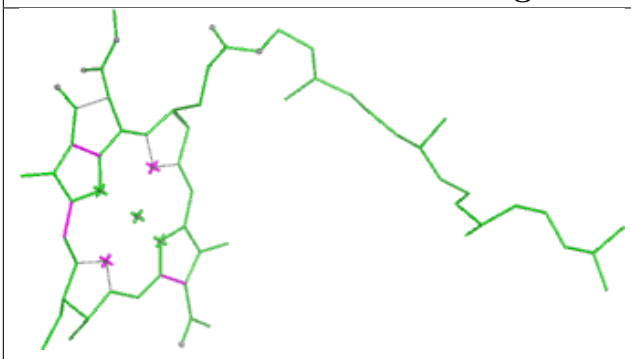
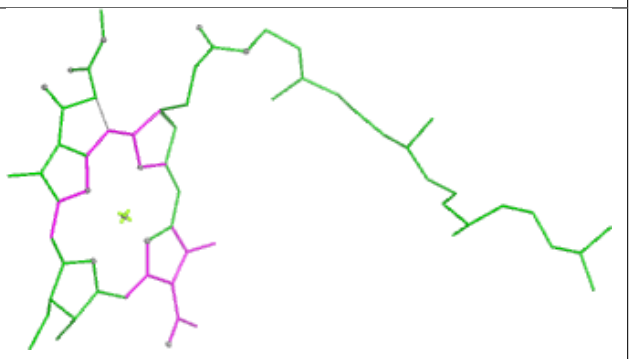
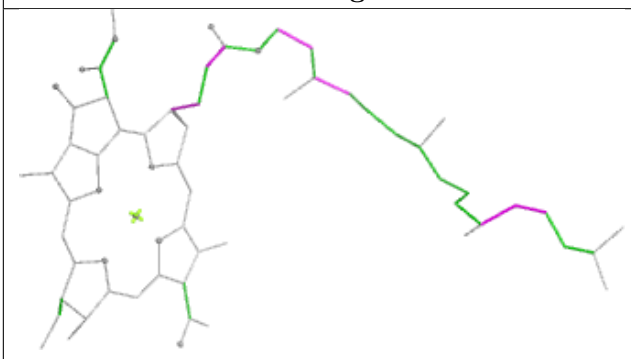
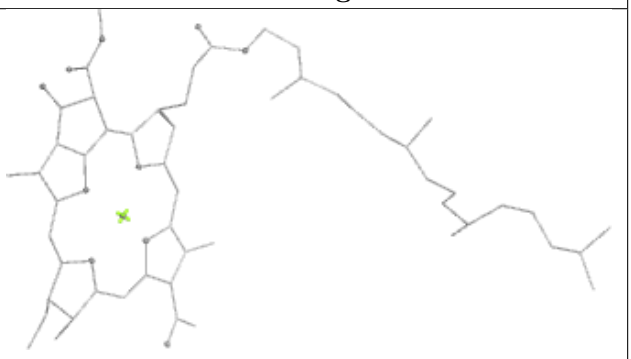
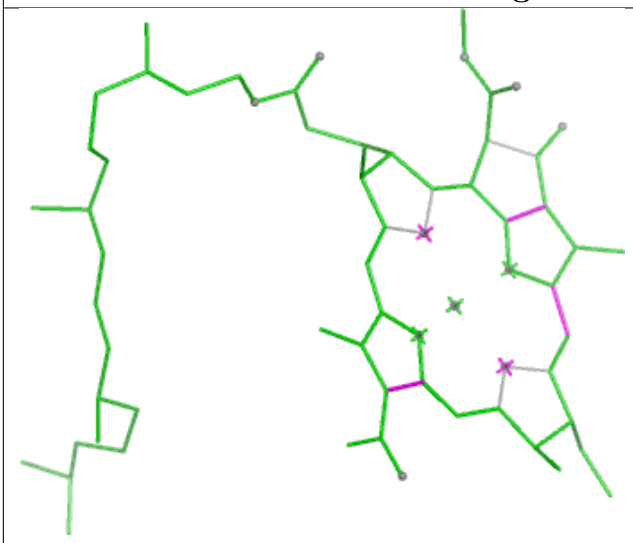
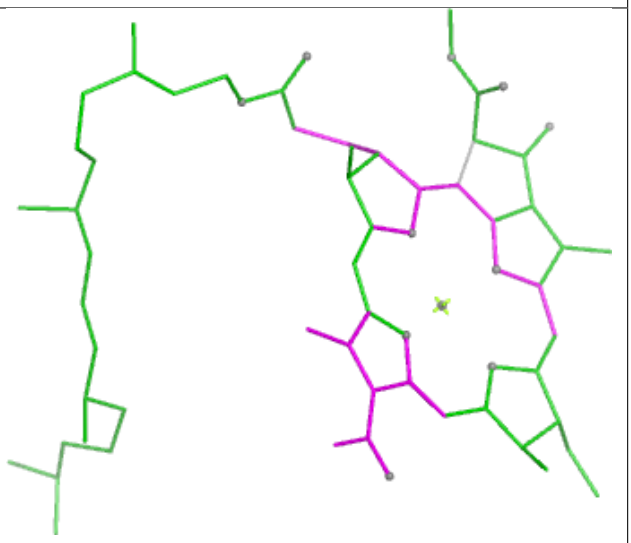
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL BF 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

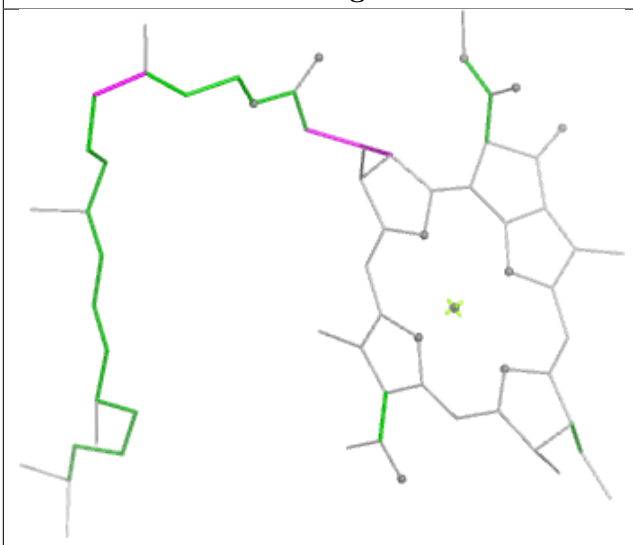
Ligand BCL AE 103



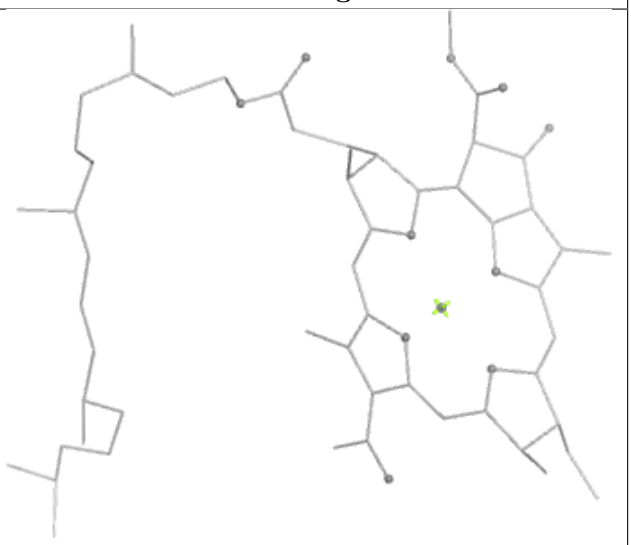
Bond lengths



Bond angles



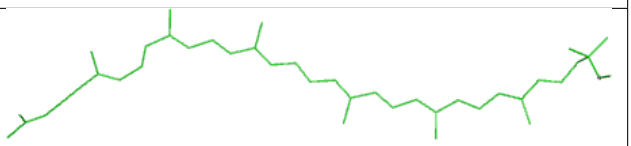
Torsions



Rings

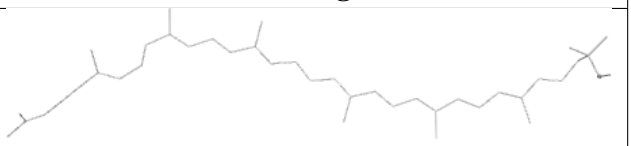
Ligand SPO AC 101

Bond lengths



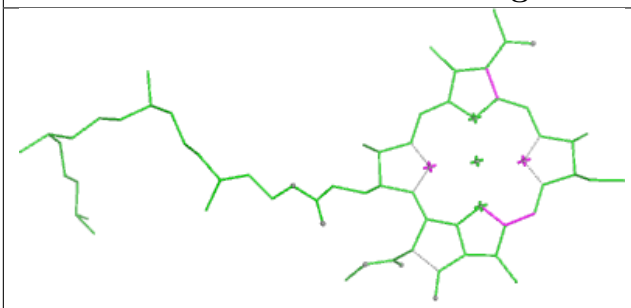
Bond angles

Torsions

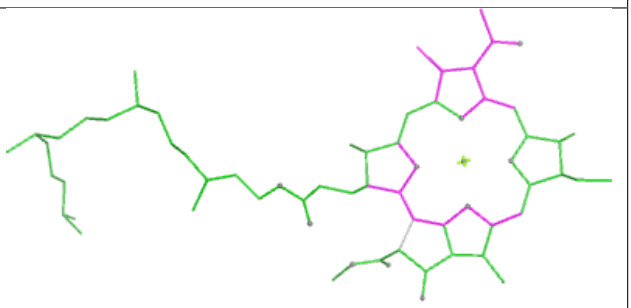


Rings

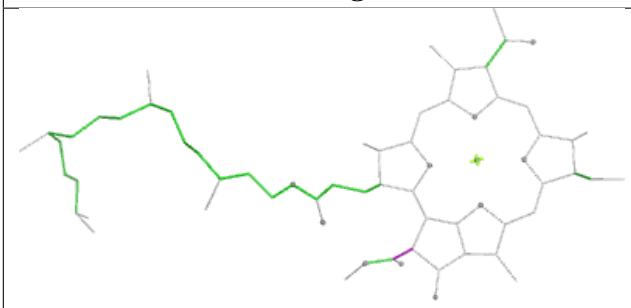
Ligand BCL AG 102



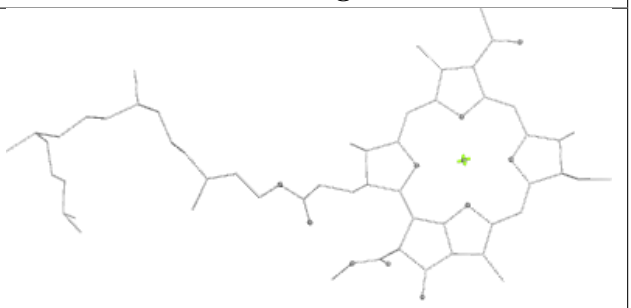
Bond lengths



Bond angles

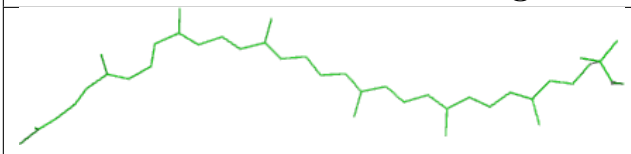


Torsions

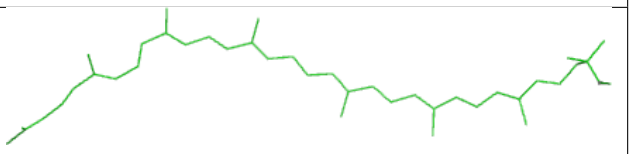


Rings

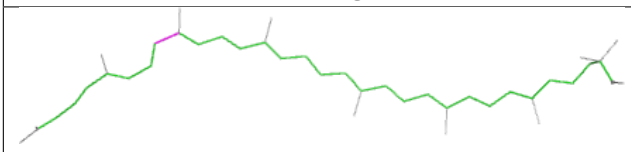
Ligand SPO AG 101



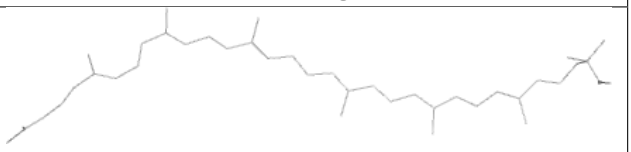
Bond lengths



Bond angles



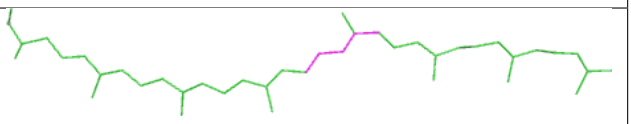
Torsions



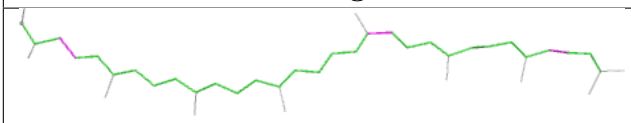
Rings

Ligand SPO AI 103

Bond lengths



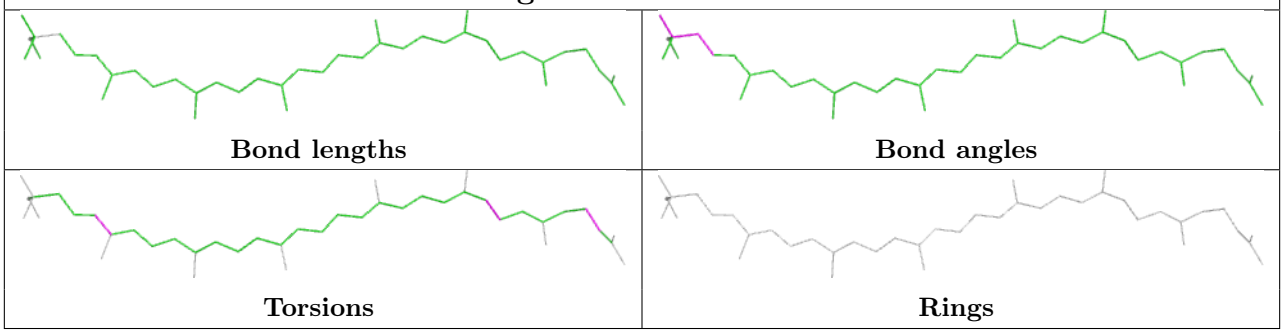
Bond angles



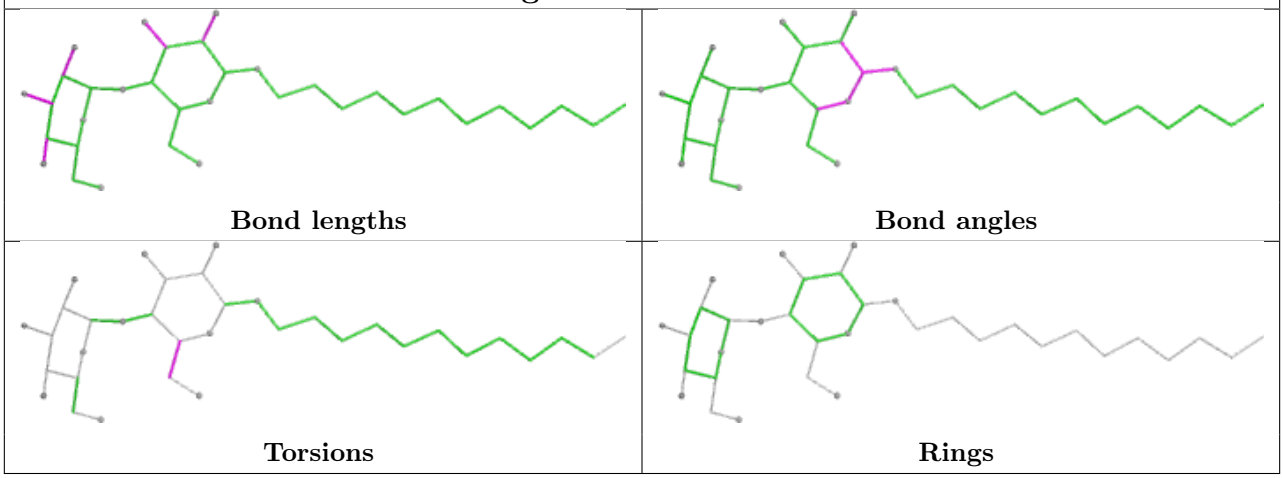
Torsions

Rings

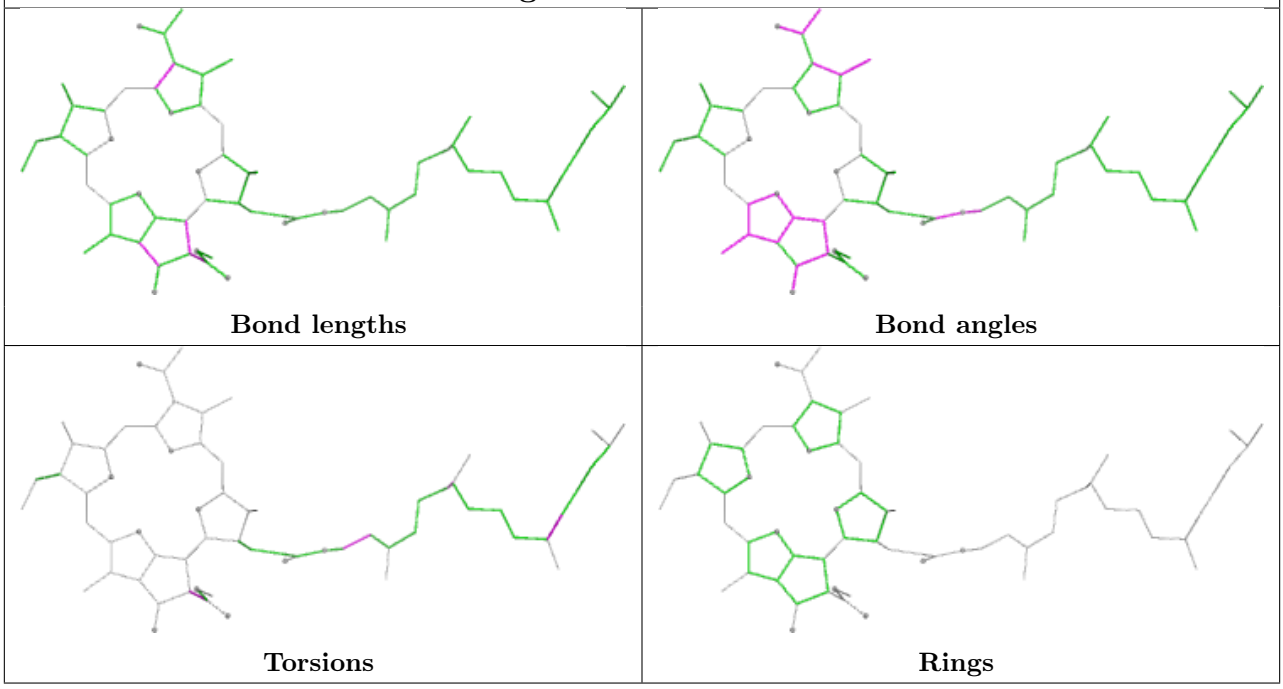
Ligand SPO AJ 103

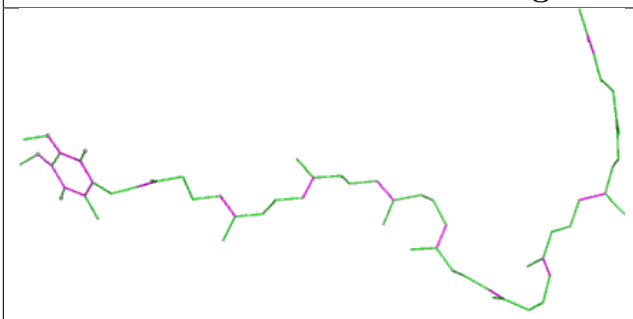
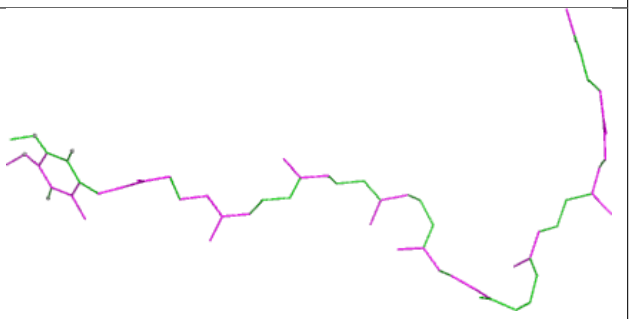
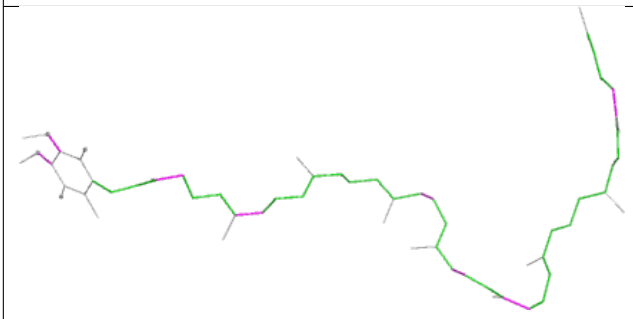
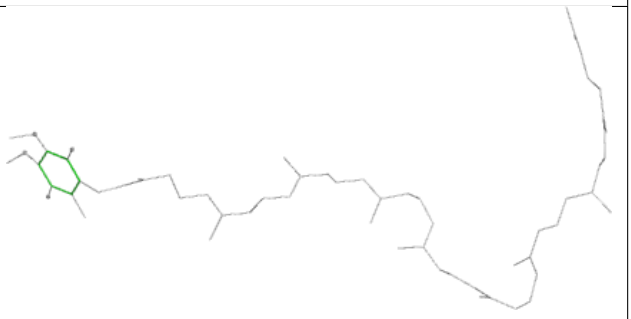


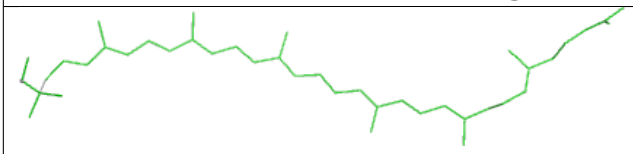
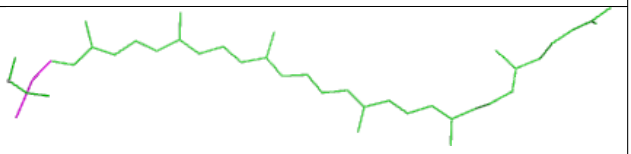
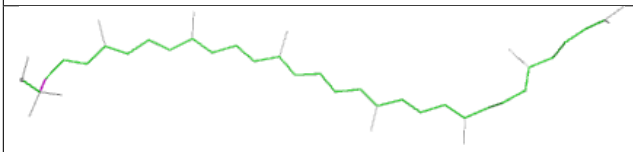
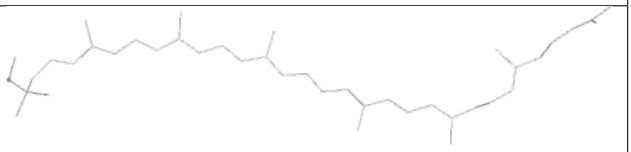
Ligand LMT X 101



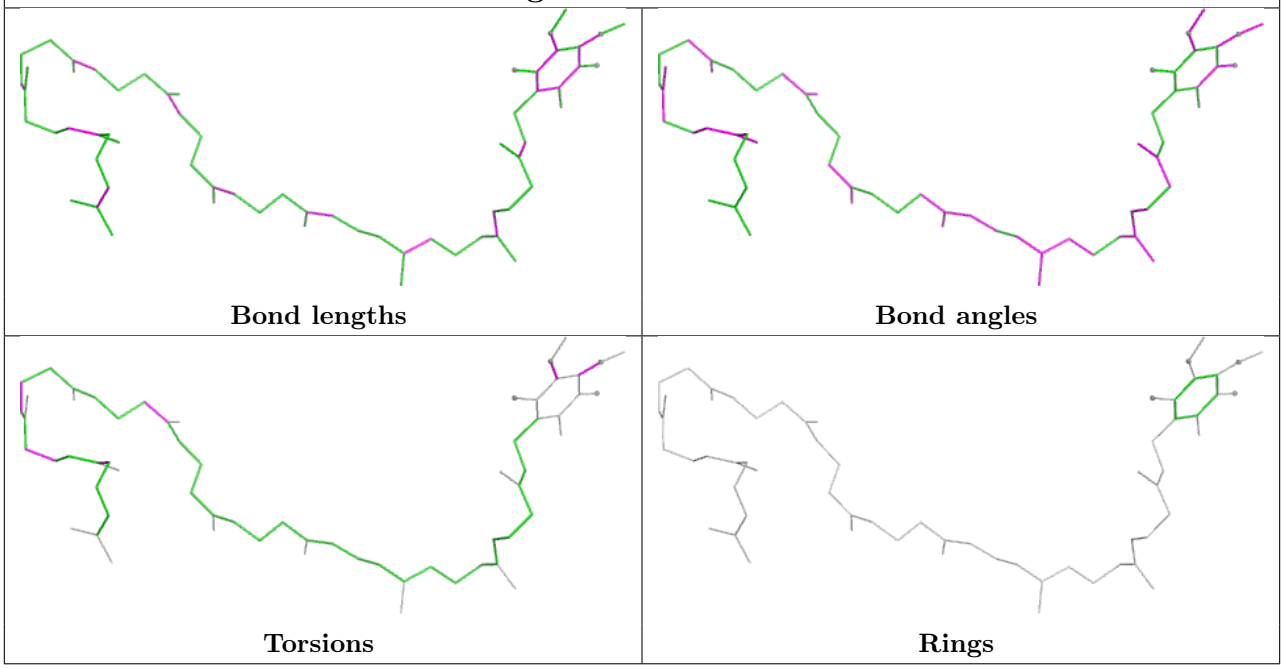
Ligand BPH M 402



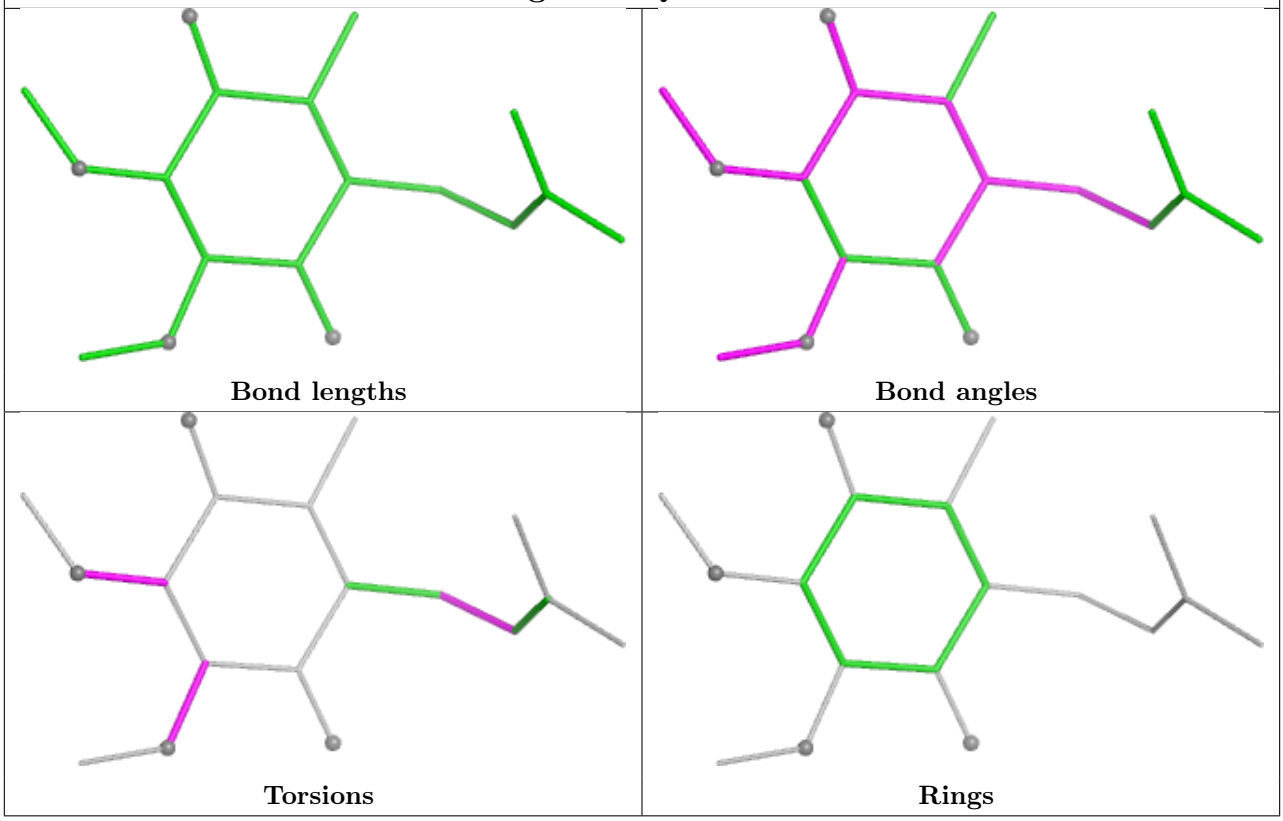
Ligand U10 L 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPO AL 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

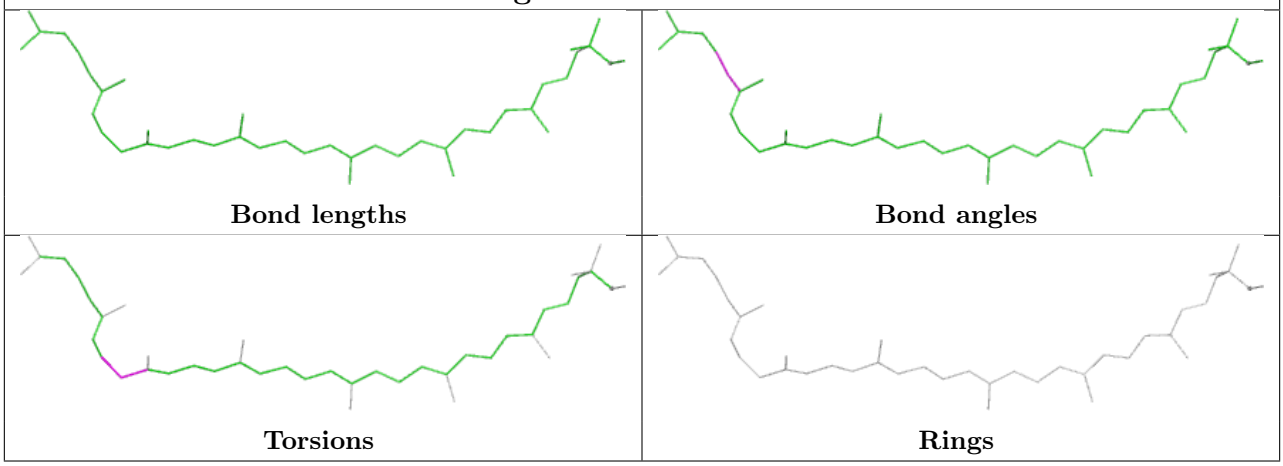
Ligand U10 M 404



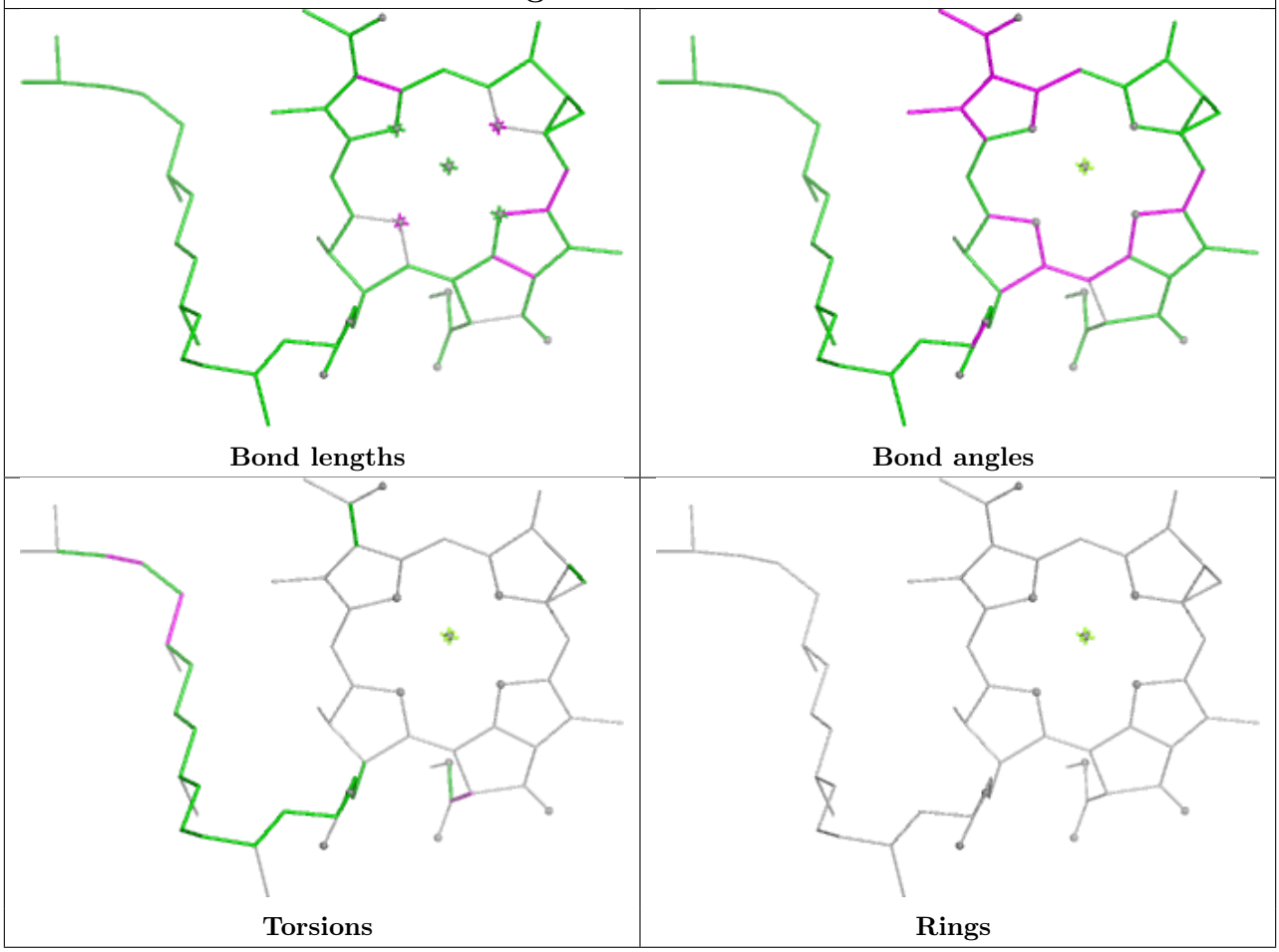
Ligand UQ1 L 303



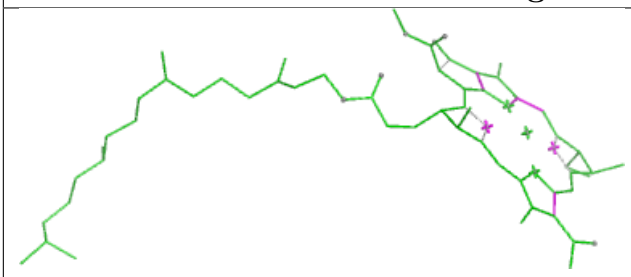
Ligand SPO BA 101



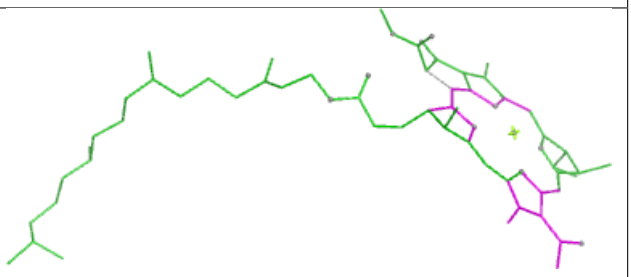
Ligand BCL L 305



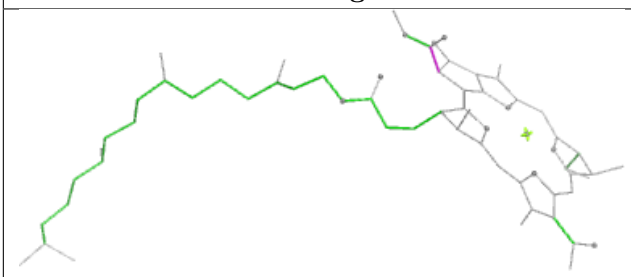
Ligand BCL L 304



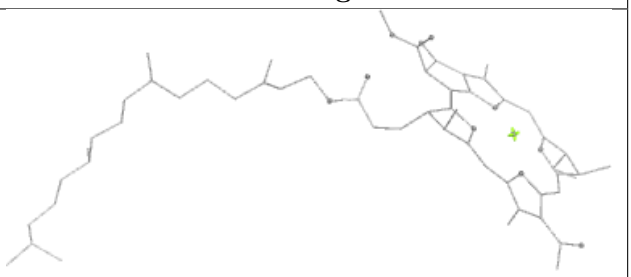
Bond lengths



Bond angles

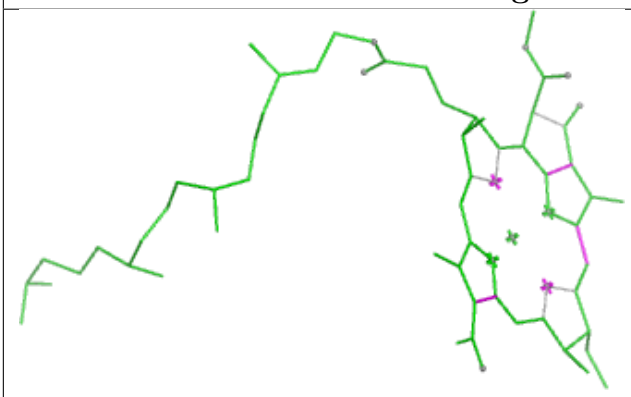


Torsions

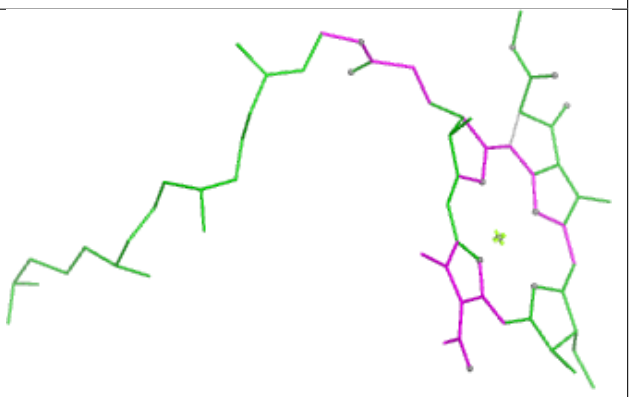


Rings

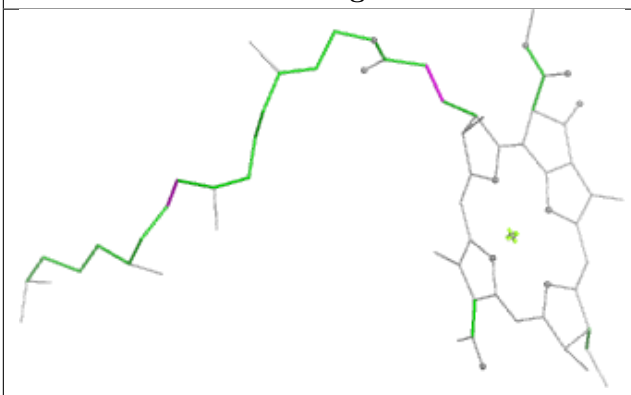
Ligand BCL BD 101



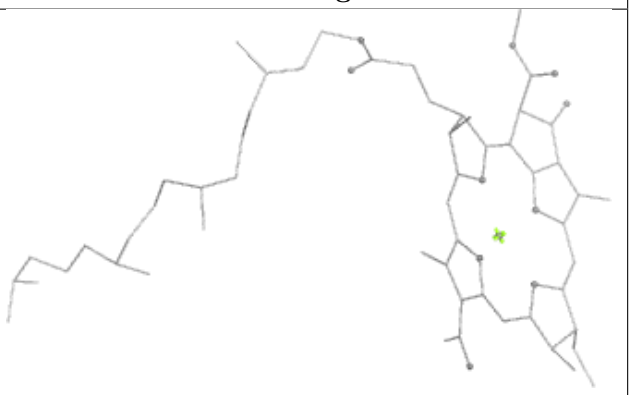
Bond lengths



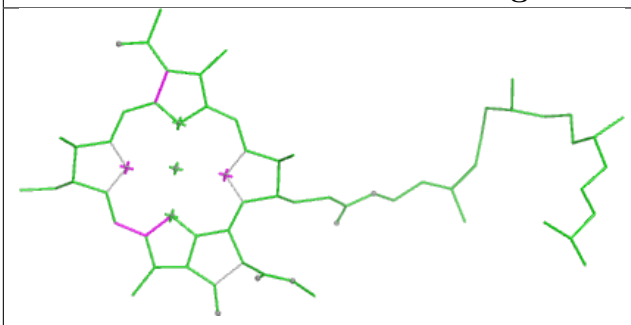
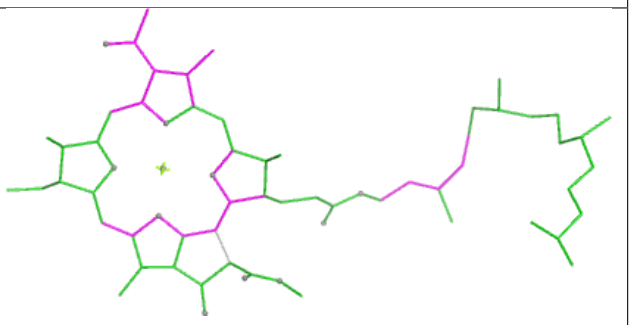
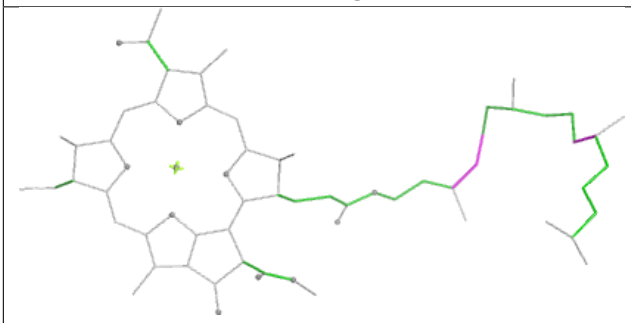
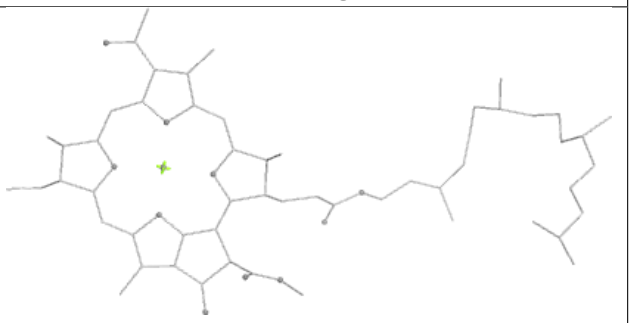
Bond angles

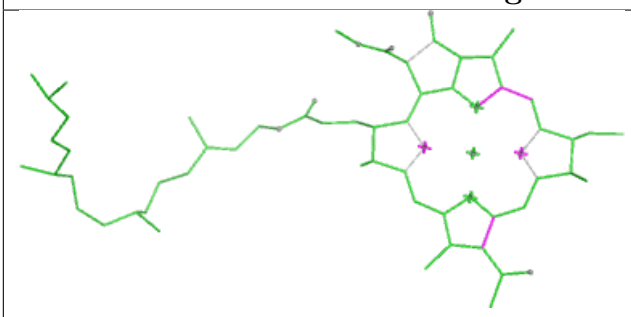
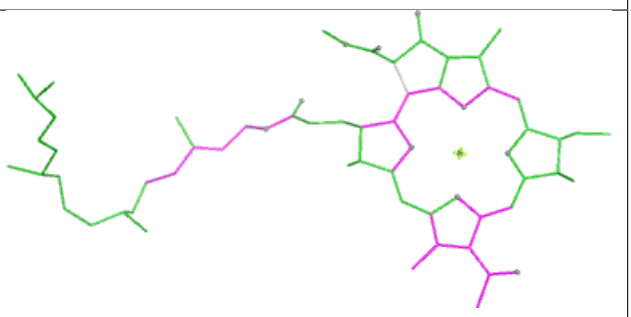
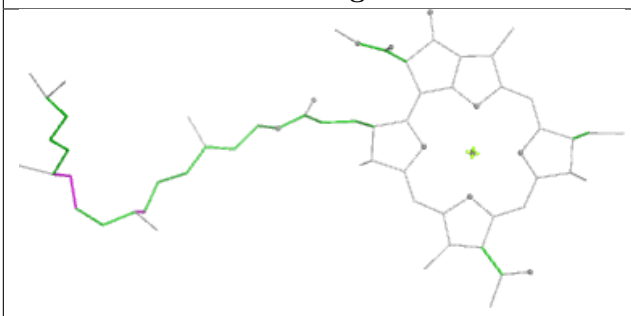
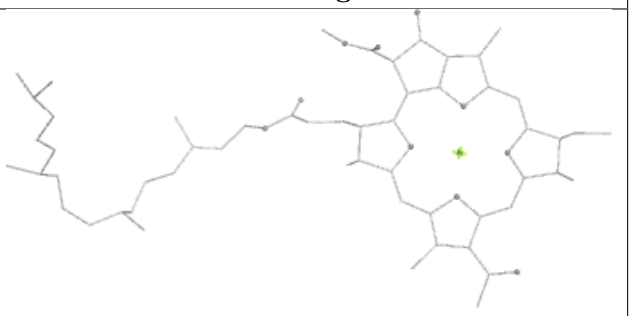


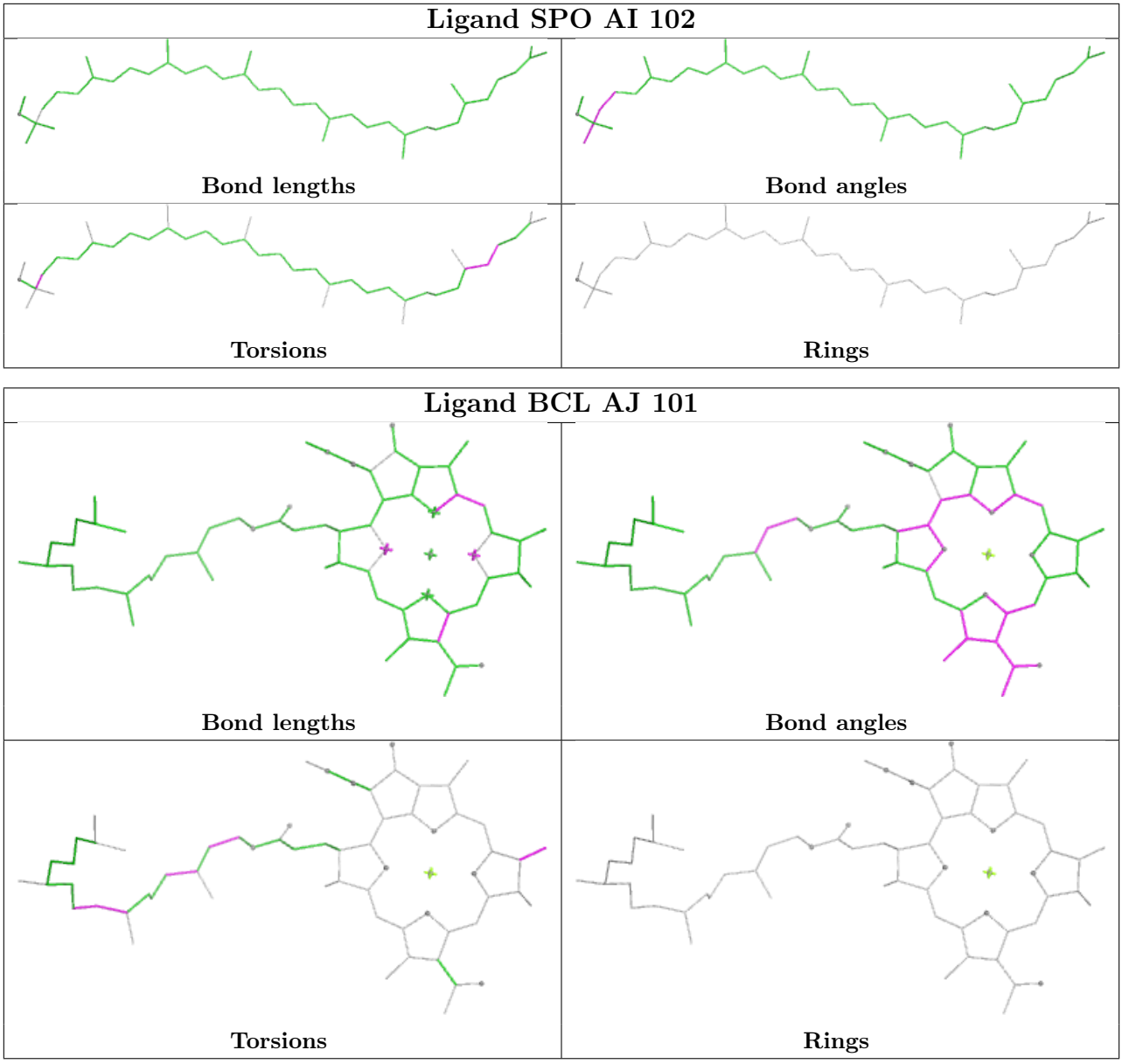
Torsions



Rings

Ligand BCL AD 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL AL 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

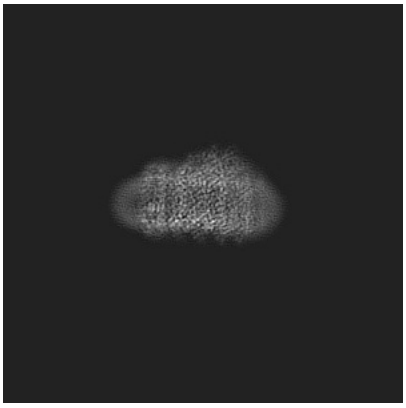
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13441. These allow visual inspection of the internal detail of the map and identification of artifacts.

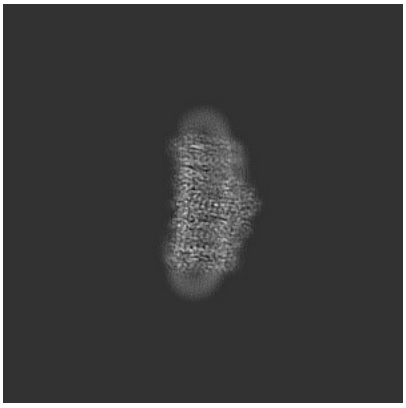
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

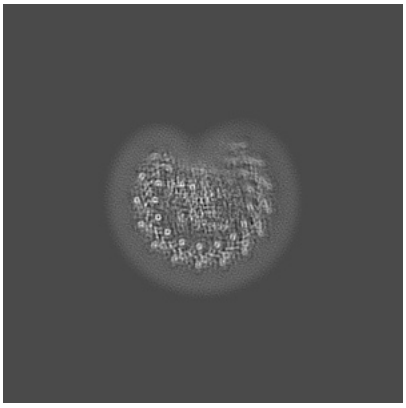
6.1.1 Primary map



X



Y

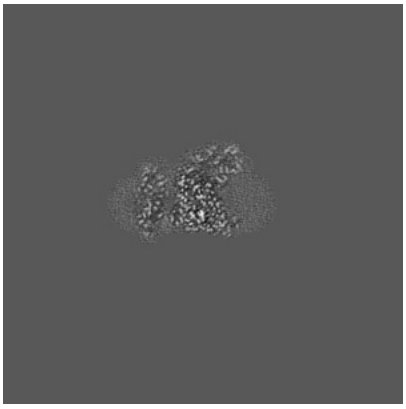


Z

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

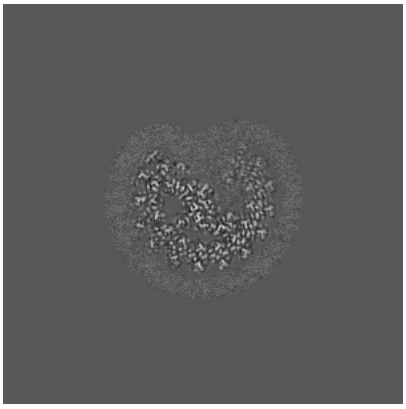
6.2 Central slices (i)

6.2.1 Primary map



X Index: 256

Y Index: 256

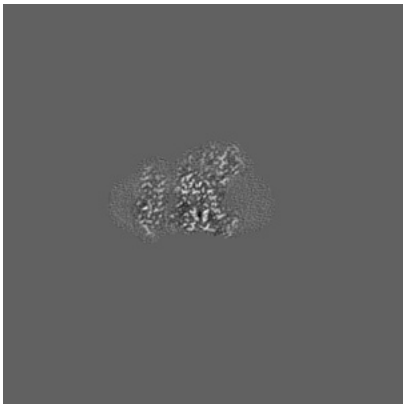


Z Index: 256

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

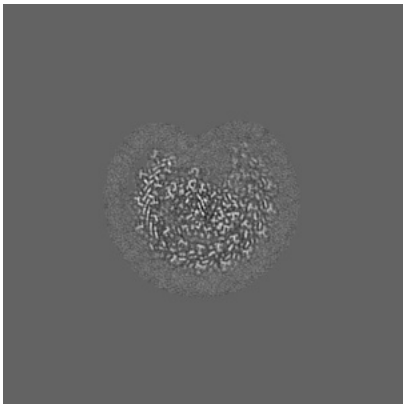
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 254

Y Index: 279

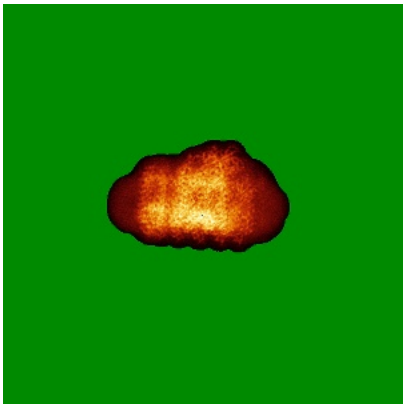


Z Index: 240

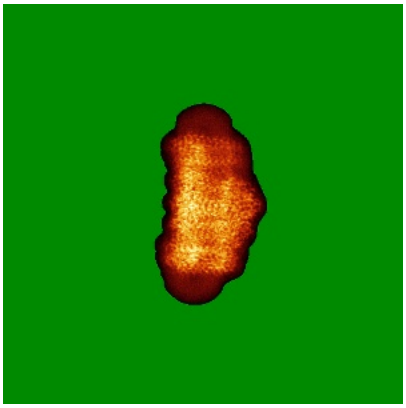
The images above show the largest variance slices of the map in three orthogonal directions.

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

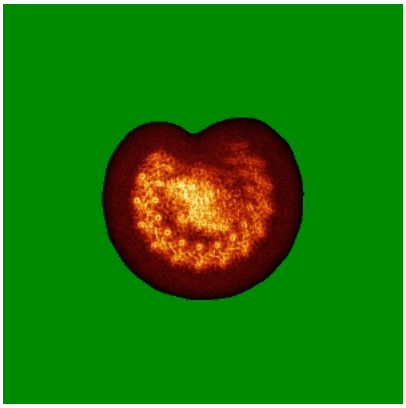
6.4.1 Primary map



X



Y

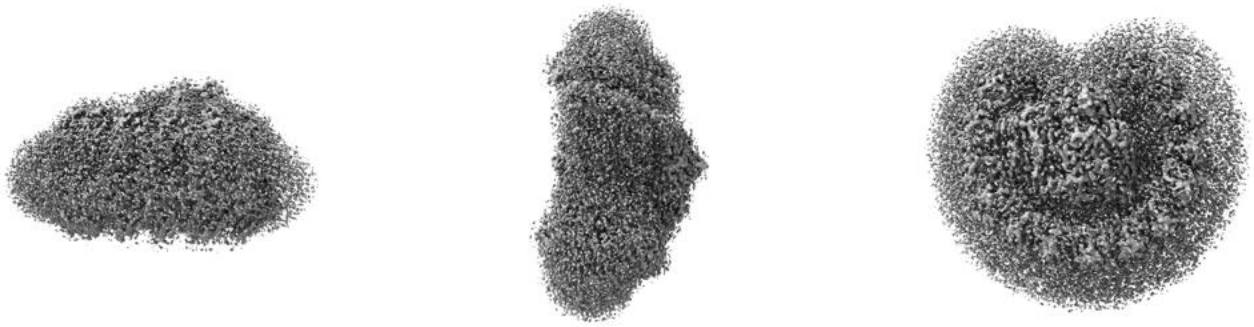


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

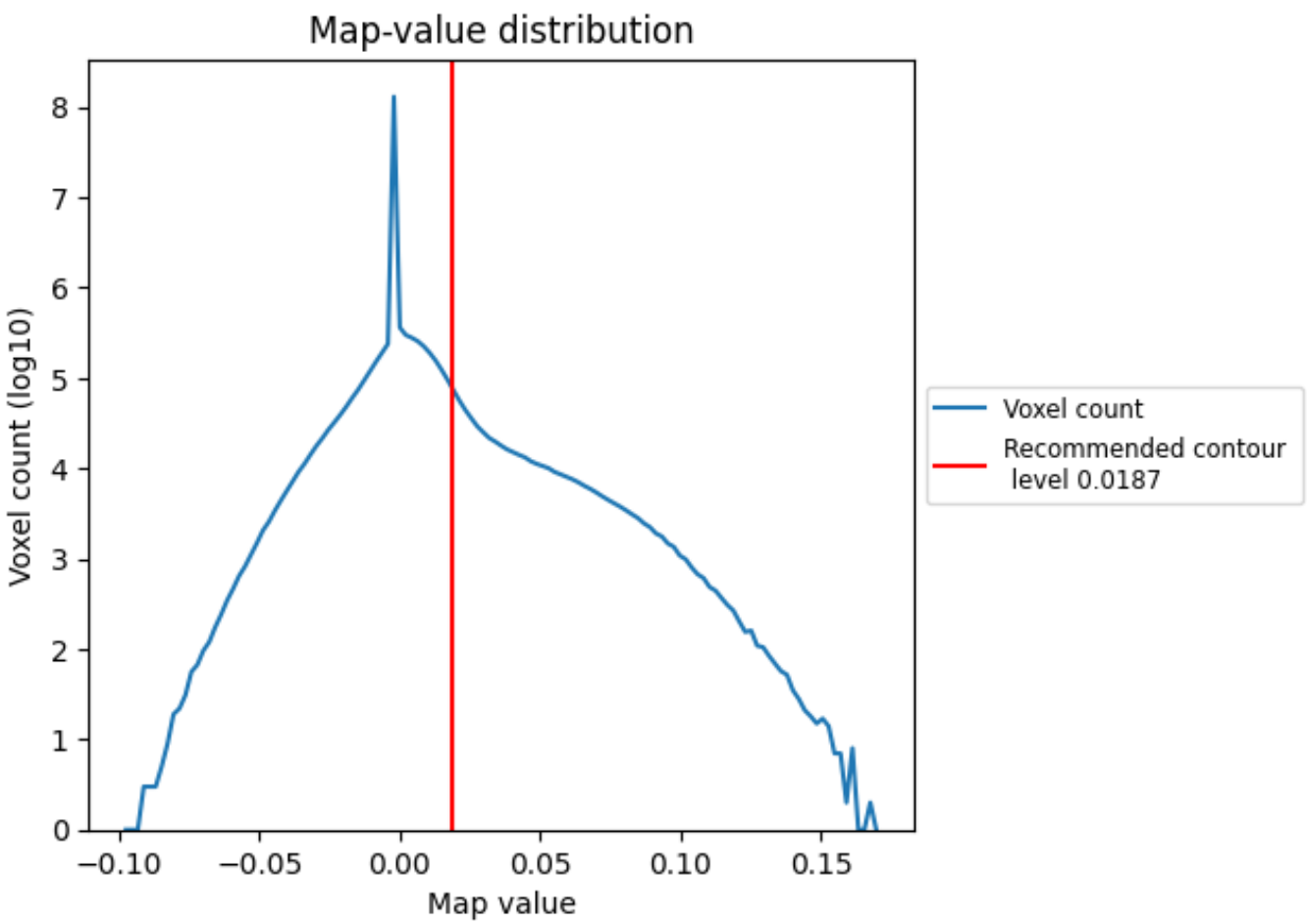
6.6 Mask visualisation (i)

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

7 Map analysis (i)

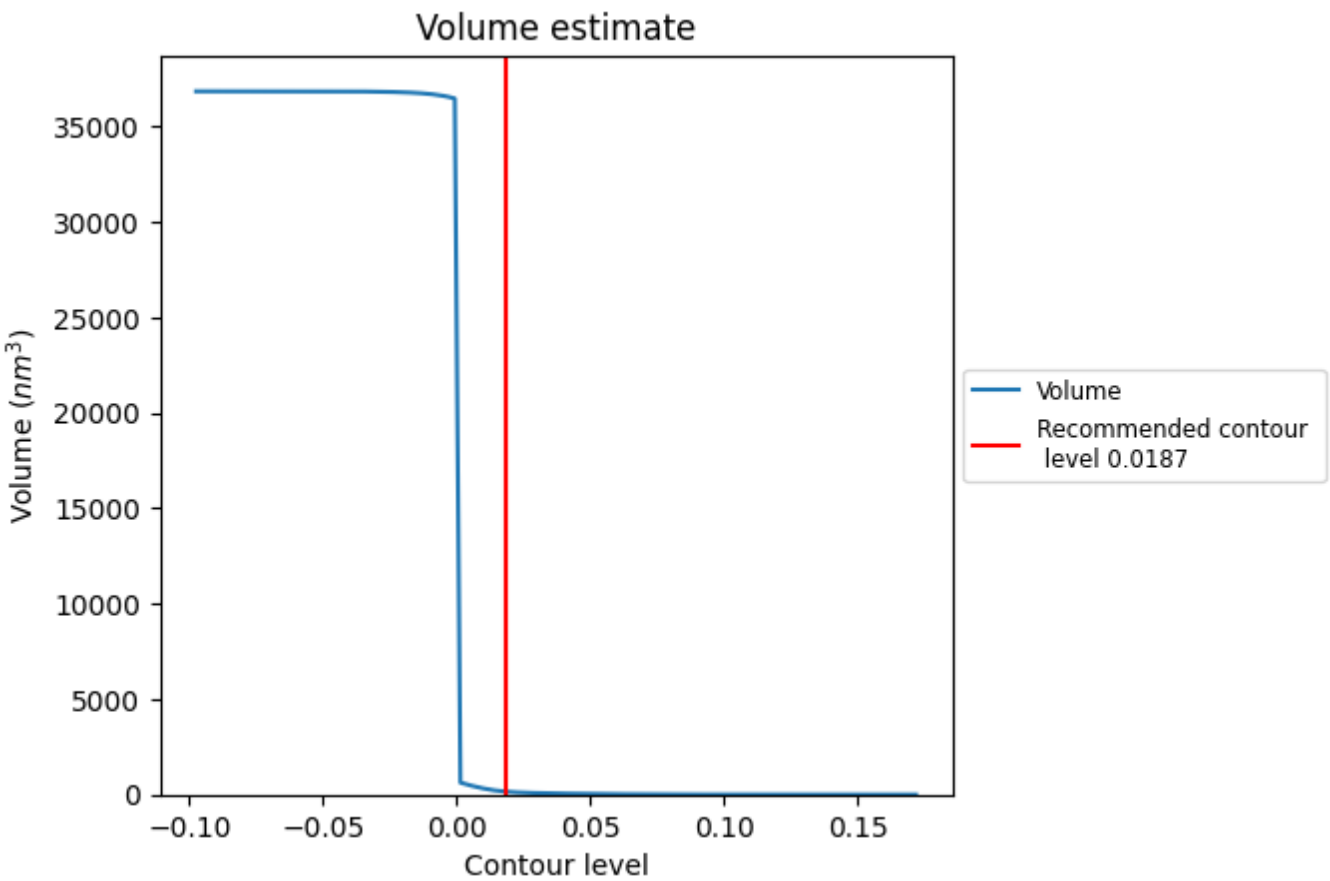
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

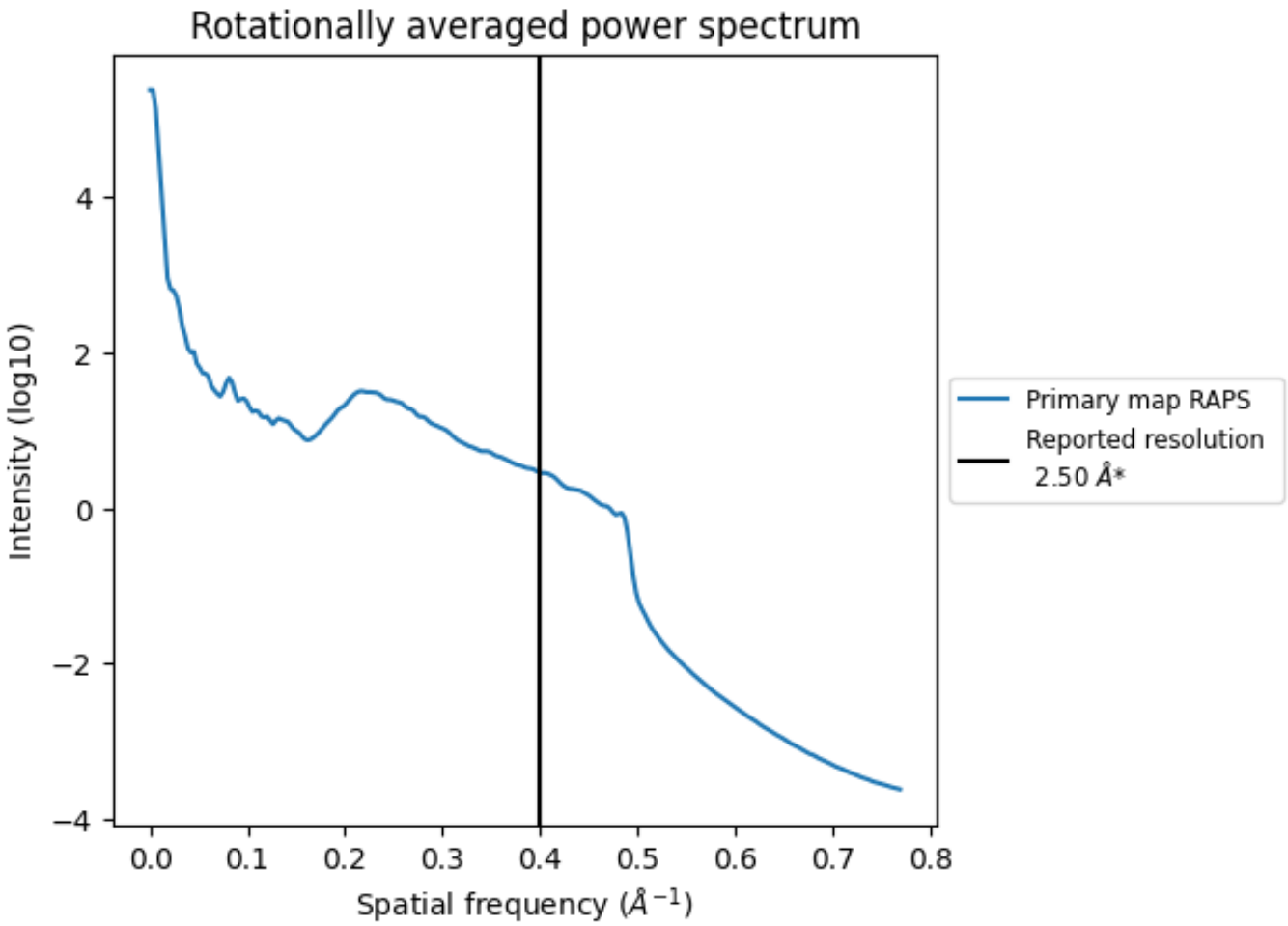
7.2 Volume estimate (i)



The volume at the recommended contour level is 151 nm^3; this corresponds to an approximate mass of 136 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)

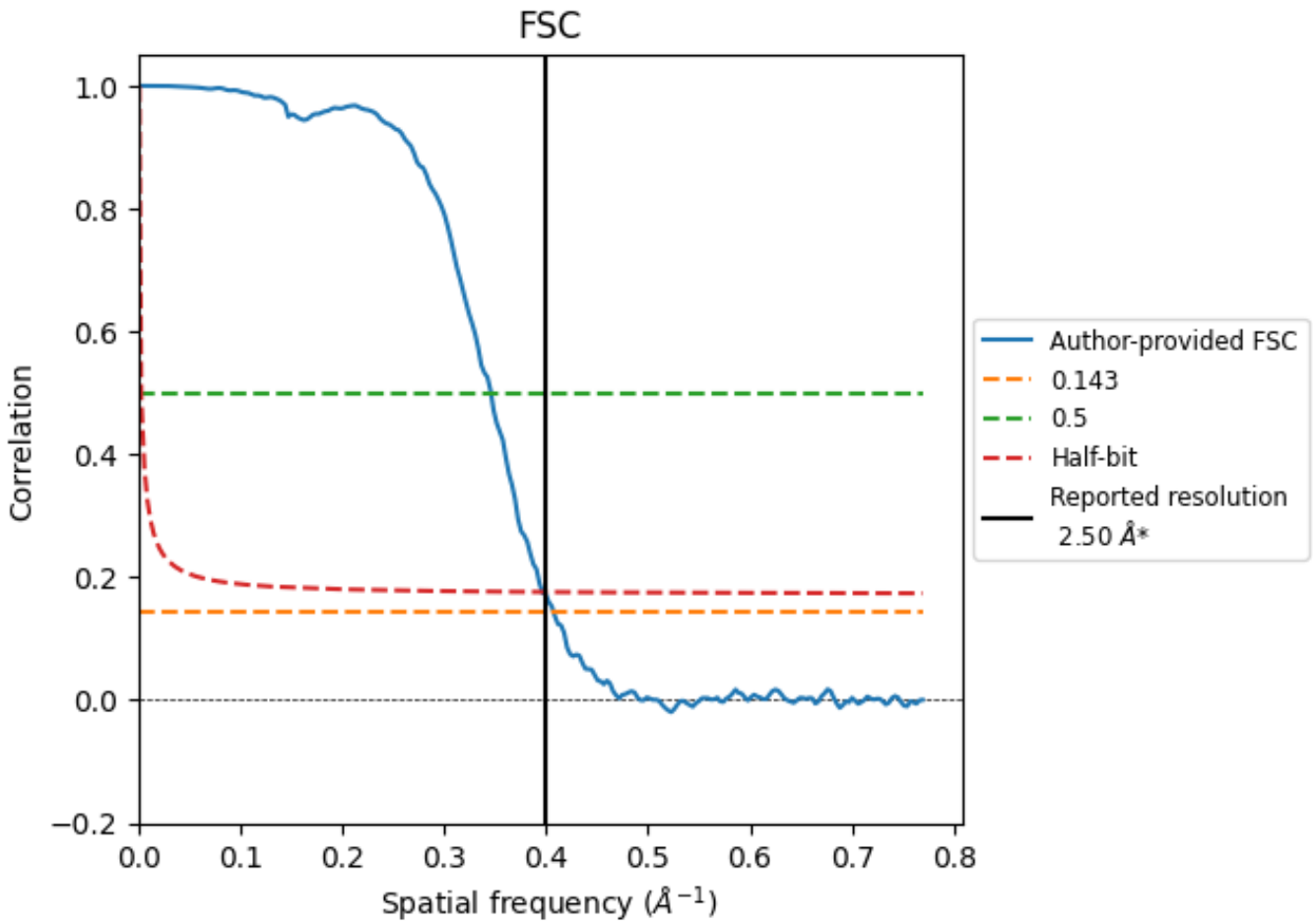


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

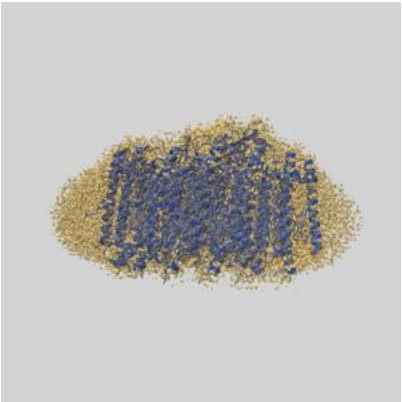
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.45	2.89	2.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

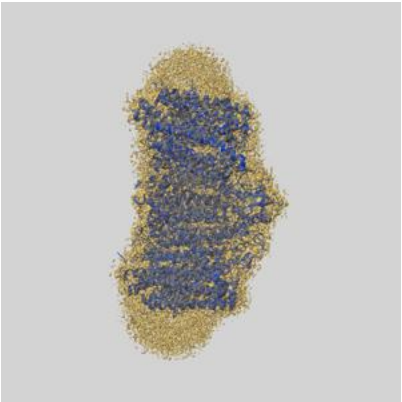
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13441 and PDB model 7PIL. Per-residue inclusion information can be found in section 3 on page 16.

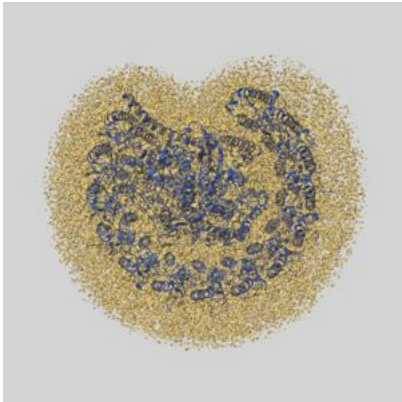
9.1 Map-model overlay (i)



X



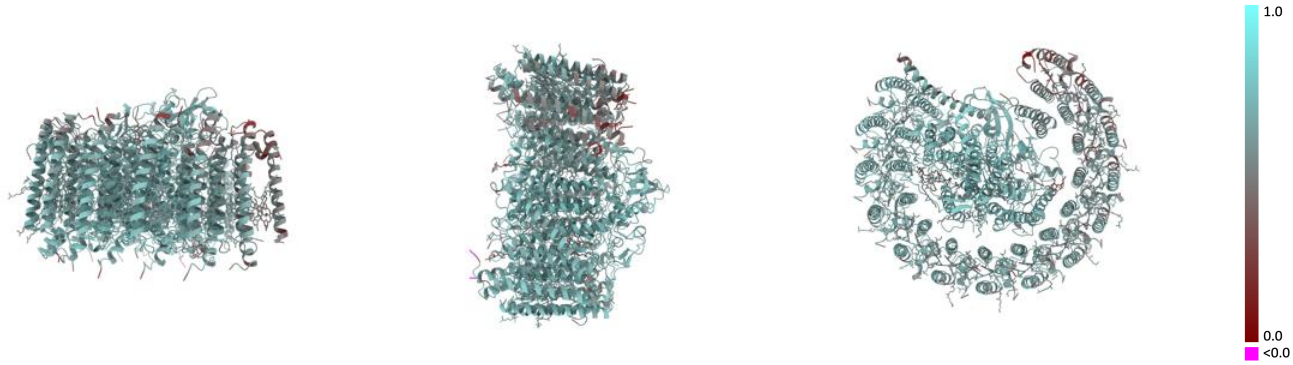
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187 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.

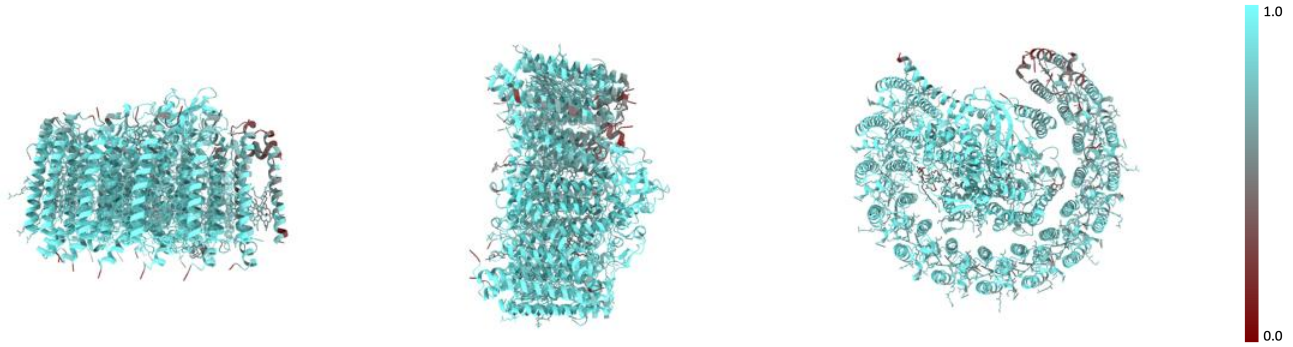
9.2 Q-score mapped to coordinate model (i)



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.

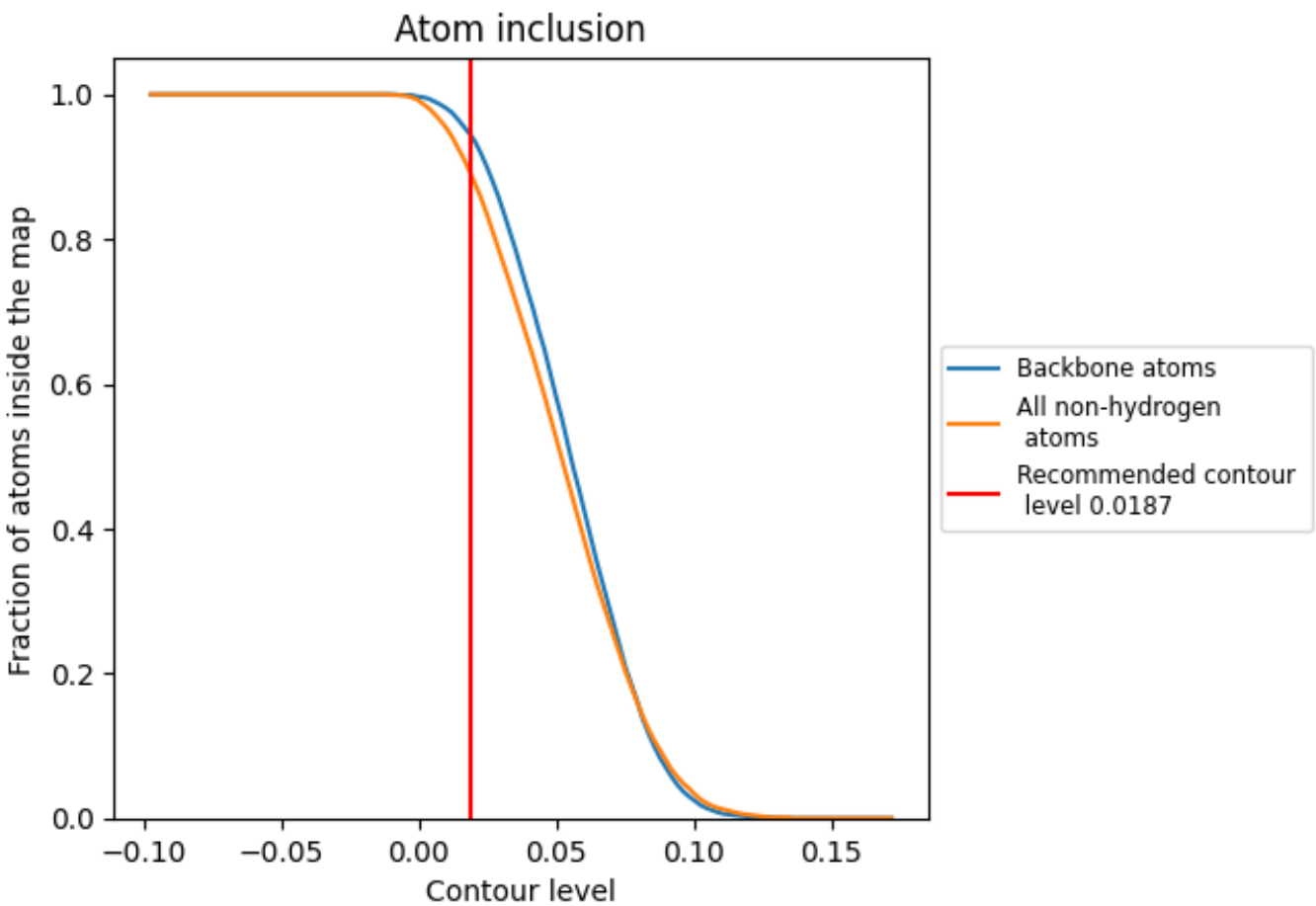
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0187).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.6400
AA	0.9020	0.6480
AB	0.8900	0.6350
AC	0.8960	0.6520
AD	0.9310	0.6620
AE	0.9350	0.6610
AF	0.9230	0.6490
AG	0.9110	0.6440
AH	0.9040	0.6410
AI	0.8710	0.6270
AJ	0.8930	0.6250
AK	0.8680	0.6100
AL	0.8480	0.5940
AM	0.7610	0.5700
AN	0.6710	0.4990
BA	0.8970	0.6450
BB	0.9260	0.6680
BC	0.9200	0.6660
BD	0.9140	0.6490
BE	0.9330	0.6400
BF	0.8770	0.6160
BG	0.8920	0.6240
BH	0.8790	0.6230
BI	0.8620	0.5950
BJ	0.8450	0.5890
BK	0.8340	0.5740
BL	0.7810	0.5550
BM	0.7040	0.4850
BN	0.5460	0.4280
H	0.9390	0.6620
L	0.9760	0.7140
M	0.9530	0.6990
UU	0.8440	0.5950
X	0.8470	0.6020