wwPDB EM Validation Summary Report (i)

Aug 7, 2026 – 03:14 AM JST

PDB ID	:	9LTS / pdb_00009lts
EMDB ID	:	EMD-63379
Title	:	Cryo-EM structure of the Dinoroseobacter shibae RC-LH1 supercomplex
Authors	:	Liu, Z.K.; Wang, P.; Liu, L.N.
Deposited on	:	2025-02-06
Resolution	:	2.49 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 (1)) were used in the production of this report:

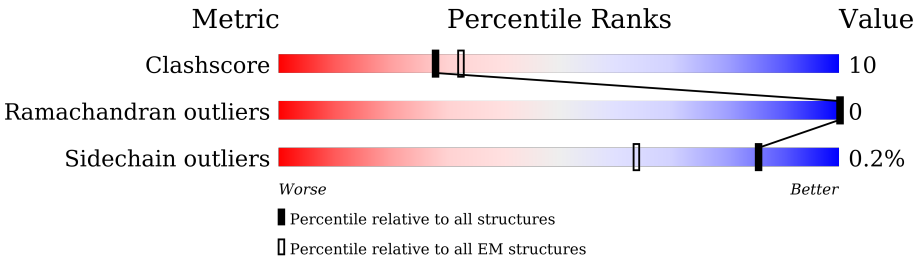
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

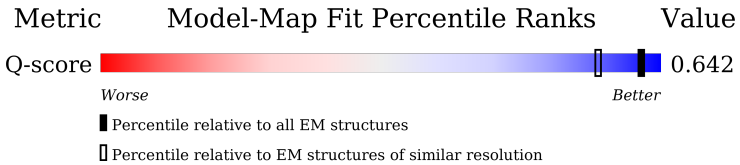
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.49 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	6237 (2.00 - 2.99)

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

Mol	Chain	Length	Quality of chain
1	A	76	76% 21%
2	1	51	94% 6%
2	3	51	86% 14%
2	5	51	86% 14%

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Mol	Chain	Length	Quality of chain
2	7	51	86% 14%
2	9	51	90% 10%
2	a	51	92% 8%
2	c	51	90% 10%
2	e	51	84% 16%
2	g	51	94% 6%
2	i	51	80% 20%
2	k	51	82% 18%
2	m	51	94% 6%
2	o	51	80% 18%
2	q	51	84% 16%
2	s	51	82% 18%
2	u	51	84% 16%
2	w	51	92% 8%
3	0	44	91% 9%
3	2	44	80% 20%
3	4	44	86% 14%
3	6	44	84% 16%
3	8	44	82% 18%
3	b	44	80% 20%
3	d	44	89% 11%
3	f	44	84% 16%
3	h	44	70% 27%
3	j	44	86% 14%
3	l	44	91% 9%

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Mol	Chain	Length	Quality of chain
3	n	44	82% 18%
3	p	44	86% 14%
3	r	44	7% 82% 18%
3	t	44	77% 23%
3	v	44	77% 23%
3	x	44	91% 9%
4	C	357	82% 18%
5	H	255	94% 6%
6	L	273	91% 8%
7	M	325	91% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SPN	1	102	-	X	-	-
10	SPN	1	103	-	X	-	-
10	SPN	1	104	-	X	-	-
10	SPN	1	105	-	X	-	-
10	SPN	3	102	-	X	-	-
10	SPN	5	102	-	X	-	-
10	SPN	5	103	-	X	-	-
10	SPN	7	102	-	X	-	-
10	SPN	7	103	-	X	-	-
10	SPN	9	103	-	X	-	-
10	SPN	a	102	-	X	-	-
10	SPN	a	103	-	X	-	-
10	SPN	c	102	-	X	-	-
10	SPN	c	103	-	X	-	-
10	SPN	e	102	-	X	-	-
10	SPN	h	102	-	X	-	-
10	SPN	h	103	-	X	-	-
10	SPN	i	102	-	X	-	-
10	SPN	j	102	-	X	-	-
10	SPN	k	102	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SPN	l	102	-	X	-	-
10	SPN	m	102	-	X	-	-
10	SPN	n	102	-	X	-	-
10	SPN	p	102	-	X	-	-
10	SPN	p	103	-	X	-	-
10	SPN	q	102	-	X	-	-
10	SPN	r	102	-	X	-	-
10	SPN	s	102	-	X	-	-
10	SPN	t	102	-	X	-	-
10	SPN	u	102	-	X	-	-
10	SPN	w	102	-	X	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 28463 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 Protein LRC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	76	552	353	95	96	8	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP A8LIU2
A	?	-	THR	deletion	UNP A8LIU2
A	?	-	GLY	deletion	UNP A8LIU2
A	?	-	ARG	deletion	UNP A8LIU2
A	?	-	PRO	deletion	UNP A8LIU2

- Molecule 2 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	51	425	291	68	64	2	0	0
2	5	51	425	291	68	64	2	0	0
2	3	51	425	291	68	64	2	0	0
2	w	51	425	291	68	64	2	0	0
2	u	51	425	291	68	64	2	0	0
2	s	51	425	291	68	64	2	0	0
2	q	51	425	291	68	64	2	0	0
2	o	51	425	291	68	64	2	0	0
2	m	51	425	291	68	64	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	k	51	425	291	68	64	2	0	0
2	g	51	425	291	68	64	2	0	0
2	e	51	425	291	68	64	2	0	0
2	c	51	425	291	68	64	2	0	0
2	a	51	425	291	68	64	2	0	0
2	i	51	425	291	68	64	2	0	0
2	7	51	425	291	68	64	2	0	0
2	9	51	425	291	68	64	2	0	0

- Molecule 3 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	44	358	239	56	62	1	0	0
3	6	44	358	239	56	62	1	0	0
3	4	44	358	239	56	62	1	0	0
3	x	44	358	239	56	62	1	0	0
3	v	44	358	239	56	62	1	0	0
3	t	44	358	239	56	62	1	0	0
3	r	44	358	239	56	62	1	0	0
3	p	44	358	239	56	62	1	0	0
3	n	44	358	239	56	62	1	0	0
3	l	44	358	239	56	62	1	0	0
3	h	44	358	239	56	62	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	f	44	358	239	56	62	1	0	0
3	d	44	358	239	56	62	1	0	0
3	b	44	358	239	56	62	1	0	0
3	j	44	358	239	56	62	1	0	0
3	8	44	358	239	56	62	1	0	0
3	0	44	358	239	56	62	1	0	0

- Molecule 4 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	357	2785	1761	461	548	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	40	MET	TRP	conflict	UNP A8LQ18

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	255	2015	1279	345	383	8	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	44	GLU	ASP	conflict	UNP A8LQ33
H	181	LEU	ILE	conflict	UNP A8LQ33
H	197	GLN	GLU	conflict	UNP A8LQ33

- Molecule 6 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	273	2172	1466	345	352	9	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	176	LEU	ILE	conflict	UNP A8LQ16

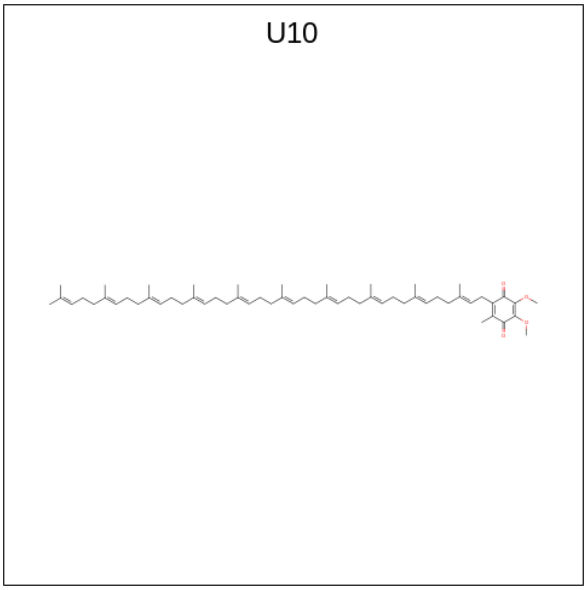
- Molecule 7 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	325	2634	1753	421	452	8	0	0

There is a discrepancy between the modelled and reference sequences:

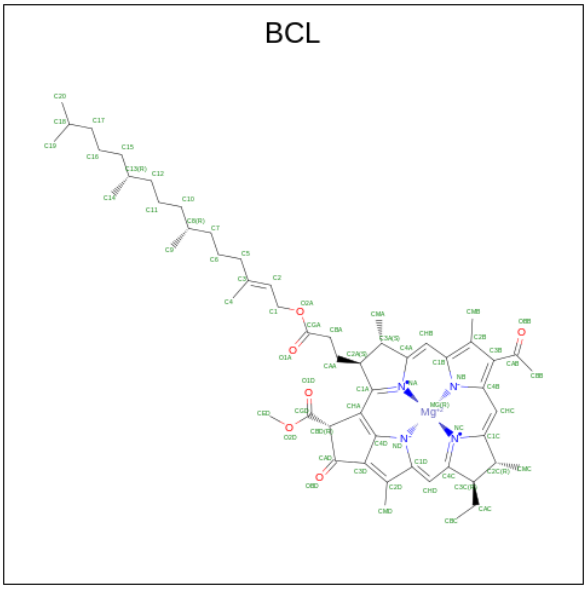
Chain	Residue	Modelled	Actual	Comment	Reference
M	134	THR	SER	conflict	UNP A8LQ17

- Molecule 8 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	
8	A	1	43	39	4	0
8	L	1	38	34	4	0
8	L	1	38	34	4	0
8	M	1	63	59	4	0

- Molecule 9 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	
9	1	1	66	55	1	4	6	0
9	2	1	66	55	1	4	6	0
9	5	1	66	55	1	4	6	0
9	6	1	66	55	1	4	6	0
9	3	1	66	55	1	4	6	0
9	4	1	66	55	1	4	6	0
9	w	1	66	55	1	4	6	0
9	x	1	66	55	1	4	6	0
9	u	1	66	55	1	4	6	0
9	v	1	66	55	1	4	6	0
9	s	1	66	55	1	4	6	0
9	t	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	q	1	66	55	1	4	6	0
9	r	1	66	55	1	4	6	0
9	o	1	66	55	1	4	6	0
9	p	1	66	55	1	4	6	0
9	m	1	66	55	1	4	6	0
9	n	1	66	55	1	4	6	0
9	k	1	66	55	1	4	6	0
9	l	1	66	55	1	4	6	0
9	g	1	66	55	1	4	6	0
9	h	1	66	55	1	4	6	0
9	e	1	66	55	1	4	6	0
9	f	1	66	55	1	4	6	0
9	c	1	66	55	1	4	6	0
9	d	1	66	55	1	4	6	0
9	a	1	66	55	1	4	6	0
9	b	1	66	55	1	4	6	0
9	i	1	66	55	1	4	6	0
9	j	1	66	55	1	4	6	0
9	7	1	66	55	1	4	6	0
9	8	1	66	55	1	4	6	0
9	L	1	66	55	1	4	6	0

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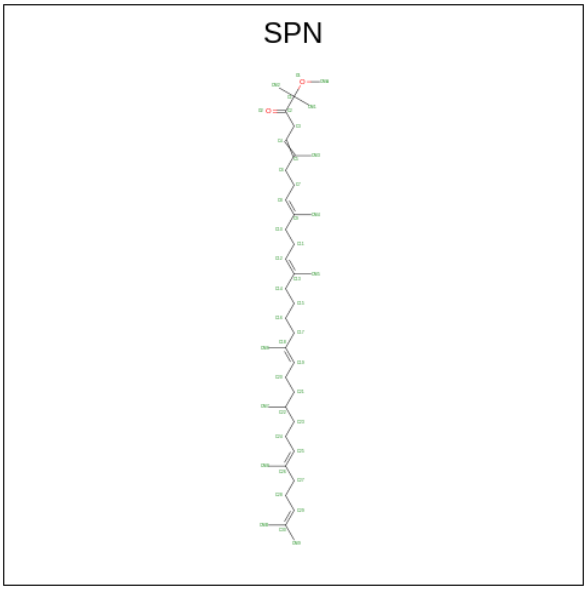
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	L	1	66	55	1	4	6	0
9	M	1	66	55	1	4	6	0
9	M	1	66	55	1	4	6	0
9	9	1	66	55	1	4	6	0
9	0	1	66	55	1	4	6	0

- Molecule 10 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	1	1	43	41	2	0
10	1	1	43	41	2	0
10	1	1	43	41	2	0
10	1	1	43	41	2	0
10	5	1	43	41	2	0
10	5	1	43	41	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	3	1	43	41	2	0
10	w	1	43	41	2	0
10	u	1	43	41	2	0
10	v	1	43	41	2	0
10	s	1	43	41	2	0
10	t	1	43	41	2	0
10	q	1	43	41	2	0
10	r	1	43	41	2	0
10	p	1	43	41	2	0
10	p	1	43	41	2	0
10	m	1	43	41	2	0
10	n	1	43	41	2	0
10	k	1	43	41	2	0
10	l	1	43	41	2	0
10	h	1	43	41	2	0
10	h	1	43	41	2	0
10	e	1	43	41	2	0
10	f	1	43	41	2	0
10	c	1	43	41	2	0
10	c	1	43	41	2	0
10	a	1	43	41	2	0

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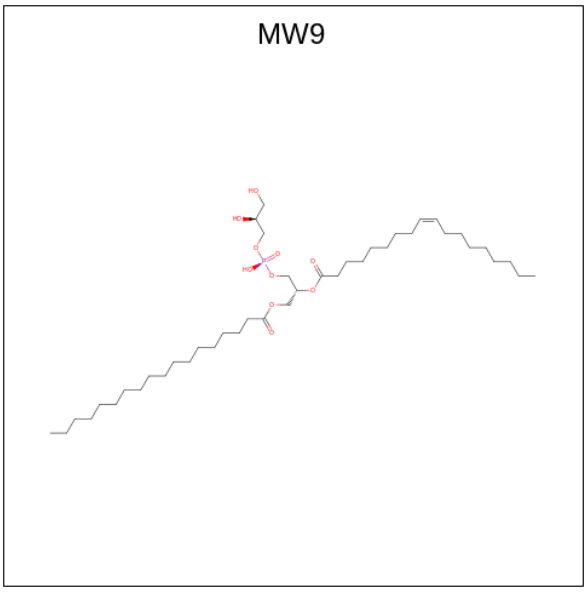
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	a	1	43	41	2	0
10	i	1	43	41	2	0
10	j	1	43	41	2	0
10	7	1	43	41	2	0
10	7	1	43	41	2	0
10	M	1	43	41	2	0
10	9	1	43	41	2	0
10	0	1	43	41	2	0

- Molecule 11 is (21R,24R,27S)-24,27,28-trihydroxy-18,24-dioxo-19,23,25-trioxa-24lambda 5 -phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (CCD ID: MW9) (formula: $C_{42}H_{81}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	g	1	53	42	10	1	0
11	g	1	50	39	10	1	0

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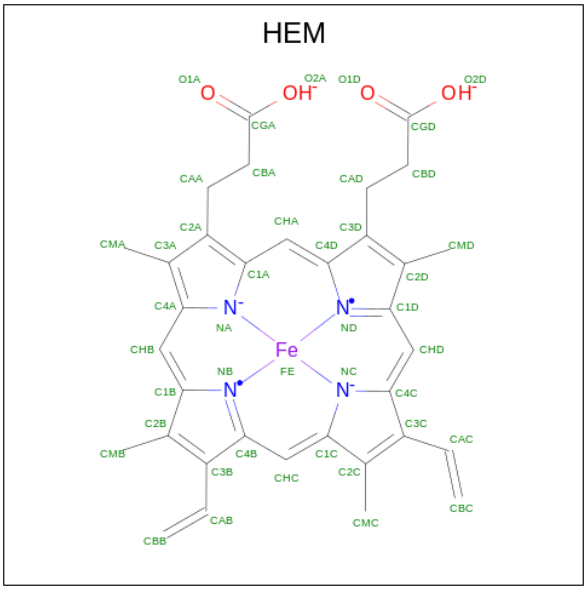
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
11	H	1	53	42	10	1	0
11	H	1	53	42	10	1	0
11	H	1	53	42	10	1	0
11	H	1	53	42	10	1	0
11	M	1	53	42	10	1	0
11	M	1	53	42	10	1	0
11	9	1	53	42	10	1	0

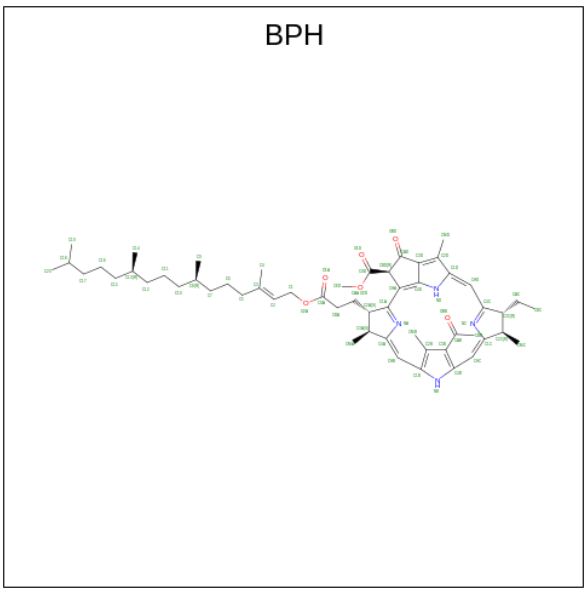
- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (la-

beled as "Ligand of Interest" by depositor).



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

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

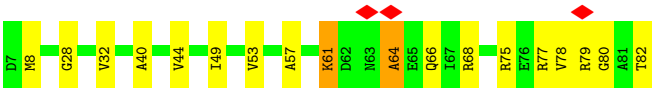
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
14	M	1	1	1	0

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.

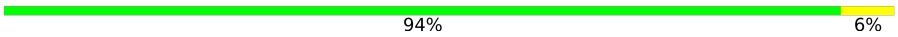
- Molecule 1: Protein LRC

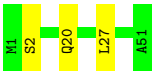
Chain A:



- Molecule 2: Antenna pigment protein alpha chain

Chain 1:



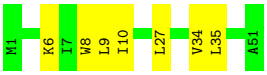


- Molecule 2: Antenna pigment protein alpha chain

Chain 5:

- Molecule 2: Antenna pigment protein alpha chain

Chain 3:

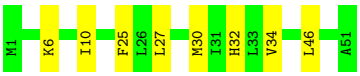


- Molecule 2: Antenna pigment protein alpha chain

Chain w:

- Molecule 2: Antenna pigment protein alpha chain

Chain u: 84% 16%

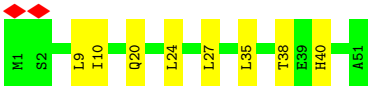


- Molecule 2: Antenna pigment protein alpha chain

Chain s: 82% 18%

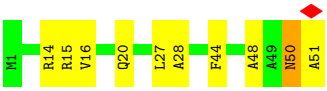
- Molecule 2: Antenna pigment protein alpha chain

Chain q: 84% 16%



- Molecule 2: Antenna pigment protein alpha chain

Chain o: 80% 18%

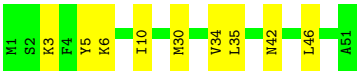


- Molecule 2: Antenna pigment protein alpha chain

Chain m: 94% 6%

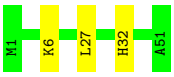
- Molecule 2: Antenna pigment protein alpha chain

Chain k: 82% 18%



- Molecule 2: Antenna pigment protein alpha chain

Chain g: 94% 6%



- Molecule 2: Antenna pigment protein alpha chain

Chain e: 84% 16%

- Molecule 2: Antenna pigment protein alpha chain

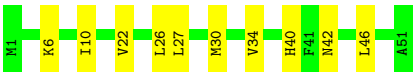
Chain c: 90% 10%

- Molecule 2: Antenna pigment protein alpha chain

Chain a: 92% 8%

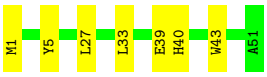
- Molecule 2: Antenna pigment protein alpha chain

Chain i: 80% 20%



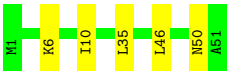
- Molecule 2: Antenna pigment protein alpha chain

Chain 7: 86% 14%



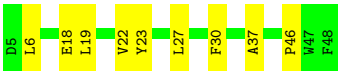
- Molecule 2: Antenna pigment protein alpha chain

Chain 9: 90% 10%



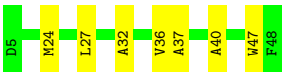
- Molecule 3: Antenna pigment protein beta chain

Chain 2: 80% 20%



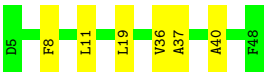
- Molecule 3: Antenna pigment protein beta chain

Chain 6: 84% 16%



• Molecule 3: Antenna pigment protein beta chain

Chain 4: 86% 14%

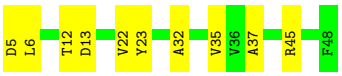


• Molecule 3: Antenna pigment protein beta chain

Chain x: 91% 9%

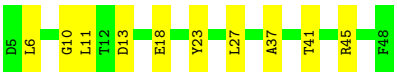
• Molecule 3: Antenna pigment protein beta chain

Chain v: 77% 23%



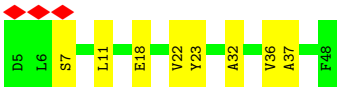
• Molecule 3: Antenna pigment protein beta chain

Chain t: 77% 23%



• Molecule 3: Antenna pigment protein beta chain

Chain r: 7% 82% 18%

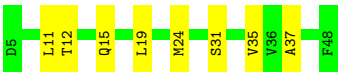


• Molecule 3: Antenna pigment protein beta chain

Chain p: 86% 14%

• Molecule 3: Antenna pigment protein beta chain

Chain n: 82% 18%



- Molecule 3: Antenna pigment protein beta chain

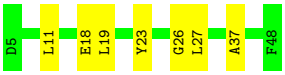
Chain l: 91% 9%

- Molecule 3: Antenna pigment protein beta chain

Chain h: 70% 27%

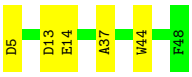
- Molecule 3: Antenna pigment protein beta chain

Chain f: 84% 16%



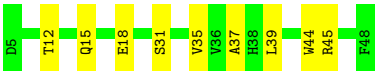
- Molecule 3: Antenna pigment protein beta chain

Chain d: 89% 11%



- Molecule 3: Antenna pigment protein beta chain

Chain b: 80% 20%



- Molecule 3: Antenna pigment protein beta chain

Chain j: 86% 14%

- Molecule 3: Antenna pigment protein beta chain

Chain 8: 82% 18%

D5 D13 Q17 E18 Y23 A34 V35 V36 A37 W44 F48

• Molecule 3: Antenna pigment protein beta chain

Chain 0: 91% 9%

D5 E18 V22 A37 P46 W47 F48

• Molecule 4: Photosynthetic reaction center cytochrome c subunit

Chain C: 82% 18%

K4 W5 F6 D7 E8 W9 N10 S11 K12 N13 P14 T15 D16 I17 P20 G28 M40 T46 P53 T56 G57 M58 S59 V60 P61 E62 D71 I74 E89 Y98 E99 N100 V101 D102 P103 V104 L116 L117 A118 A119 M120 W123 T124 L129 L130 I142

N143 M144 I145 Q146 M147 T150 C169 C172 P179 D187 S194 G195 W196 L206 Y218 L222 E233 V236 E237 N256 L262 N265 C269 T282 A288 G307 L311 V319 Y320 C331 H332 Q337 P338 L352 V355

D370

• Molecule 5: Reaction center protein H chain

Chain H: 94% 6%

E2 M35 L41 P54 L57 E60 R69 L123 V153 W168 Y178 L181 V199 K207 V208 R209 S210 D234 L256

• Molecule 6: Reaction center protein L chain

Chain L: 91% 8%

A2 D21 D24 V32 V37 L44 L132 V133 V134 F135 R136 P137 M140 L166 H167 F168 H169 L176 L186 N212 S245 A246 V247 C248 I249 I250 I251 S252 G253 P254 P274

• Molecule 7: Reaction center protein M chain

Chain M: 91% 9%

P2 N6 E30 Y53 W56 G65 F69 V80 Q90 L94 P109 L110 D111 I117 S120 W131 T134 Y135 Q136 E139 M140 M143 G162 Y178 F181 P182 H183 V208 F217 T228 W271 V275 Y312 R326

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT, POINT, POINT, POINT, POINT	Depositor
Number of particles used	123390, 123390, 123390, 123390, 123390, 123390, 123390, 123390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.072	Depositor
Minimum map value	-0.968	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	291.0, 291.0, 291.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	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: FE, SPN, U10, BPH, MW9, BCL, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.90	0/559	1.33	9/757 (1.2%)
2	1	0.51	0/439	0.64	1/595 (0.2%)
2	3	0.75	0/439	0.76	2/595 (0.3%)
2	5	1.02	0/439	0.96	2/595 (0.3%)
2	7	0.55	0/439	0.70	1/595 (0.2%)
2	9	0.49	0/439	0.50	0/595
2	a	0.34	0/439	0.48	0/595
2	c	0.39	0/439	0.39	0/595
2	e	0.22	0/439	0.38	0/595
2	g	0.22	0/439	0.35	0/595
2	i	0.59	0/439	0.68	1/595 (0.2%)
2	k	0.22	0/439	0.31	0/595
2	m	0.57	0/439	0.73	1/595 (0.2%)
2	o	0.68	0/439	0.63	1/595 (0.2%)
2	q	0.42	0/439	0.49	0/595
2	s	0.43	0/439	0.55	0/595
2	u	0.24	0/439	0.32	0/595
2	w	0.13	0/439	0.28	0/595
3	0	0.43	0/371	0.55	1/508 (0.2%)
3	2	0.40	0/371	0.57	1/508 (0.2%)
3	4	0.79	0/371	0.81	1/508 (0.2%)
3	6	0.91	0/371	0.95	2/508 (0.4%)
3	8	0.79	0/371	0.77	2/508 (0.4%)
3	b	0.45	0/371	0.67	1/508 (0.2%)
3	d	0.58	0/371	0.56	0/508
3	f	0.16	0/371	0.31	0/508
3	h	0.38	0/371	0.55	1/508 (0.2%)
3	j	0.72	0/371	0.69	1/508 (0.2%)
3	l	0.18	0/371	0.34	0/508
3	n	0.36	0/371	0.39	0/508
3	p	0.29	0/371	0.48	0/508
3	r	0.59	0/371	0.76	1/508 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	t	0.67	0/371	0.65	0/508
3	v	0.53	0/371	0.63	0/508
3	x	0.25	0/371	0.36	0/508
4	C	0.69	2/2864 (0.1%)	0.93	16/3929 (0.4%)
5	H	0.44	0/2065	0.58	3/2795 (0.1%)
6	L	0.69	3/2261 (0.1%)	0.73	5/3097 (0.2%)
7	M	0.59	2/2732 (0.1%)	0.61	2/3737 (0.1%)
All	All	0.58	7/24251 (0.0%)	0.68	55/33066 (0.2%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	136	ARG	C-O	-5.96	1.18	1.24
7	M	181	PHE	C-N	5.79	1.41	1.33
4	C	117	LEU	CA-C	-5.64	1.45	1.53
7	M	136	GLN	C-O	-5.46	1.17	1.24
6	L	252	SER	CA-C	-5.30	1.46	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	187	ASP	N-CA-C	14.22	132.08	112.75
4	C	7	ASP	N-CA-C	-11.51	98.67	113.17
1	A	66	GLN	N-CA-C	-10.86	99.61	113.72
1	A	64	ALA	N-CA-C	-10.59	91.23	108.07
3	6	47	TRP	N-CA-C	-10.28	95.16	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	552	0	570	6	0
2	1	425	0	433	3	0
2	3	425	0	433	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5	425	0	433	3	0
2	7	425	0	433	6	0
2	9	425	0	433	6	0
2	a	425	0	433	10	0
2	c	425	0	433	4	0
2	e	425	0	433	8	0
2	g	425	0	433	3	0
2	i	425	0	433	12	0
2	k	425	0	433	10	0
2	m	425	0	433	1	0
2	o	425	0	433	13	0
2	q	425	0	433	13	0
2	s	425	0	433	16	0
2	u	425	0	433	12	0
2	w	425	0	433	6	0
3	0	358	0	338	4	0
3	2	358	0	338	10	0
3	4	358	0	338	8	0
3	6	358	0	338	3	0
3	8	358	0	338	8	0
3	b	358	0	338	13	0
3	d	358	0	338	4	0
3	f	358	0	338	7	0
3	h	358	0	338	18	0
3	j	358	0	338	10	0
3	l	358	0	338	4	0
3	n	358	0	338	8	0
3	p	358	0	338	7	0
3	r	358	0	338	6	0
3	t	358	0	338	18	0
3	v	358	0	338	18	0
3	x	358	0	338	4	0
4	C	2785	0	2631	50	0
5	H	2015	0	1963	8	0
6	L	2172	0	2113	17	0
7	M	2634	0	2526	22	0
8	A	43	0	55	0	0
8	L	76	0	94	5	0
8	M	63	0	90	0	0
9	0	66	0	73	7	0
9	1	66	0	74	2	0
9	2	66	0	73	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	3	66	0	74	7	0
9	4	66	0	73	4	0
9	5	66	0	74	5	0
9	6	66	0	73	4	0
9	7	66	0	74	5	0
9	8	66	0	73	8	0
9	9	66	0	74	5	0
9	L	132	0	148	8	0
9	M	132	0	148	12	0
9	a	66	0	74	4	0
9	b	66	0	73	6	0
9	c	66	0	74	3	0
9	d	66	0	74	6	0
9	e	66	0	74	3	0
9	f	66	0	74	7	0
9	g	66	0	74	3	0
9	h	66	0	74	10	0
9	i	66	0	74	5	0
9	j	66	0	74	7	0
9	k	66	0	74	7	0
9	l	66	0	74	5	0
9	m	66	0	74	6	0
9	n	66	0	74	4	0
9	o	66	0	74	13	0
9	p	66	0	74	11	0
9	q	66	0	74	4	0
9	r	66	0	74	7	0
9	s	66	0	74	7	0
9	t	66	0	74	4	0
9	u	66	0	74	5	0
9	v	66	0	74	7	0
9	w	66	0	74	4	0
9	x	66	0	74	6	0
10	0	43	0	69	4	0
10	1	172	0	276	21	0
10	3	43	0	69	4	0
10	5	86	0	138	7	0
10	7	86	0	138	5	0
10	9	43	0	69	1	0
10	M	43	0	69	11	0
10	a	86	0	138	3	0
10	c	86	0	138	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	e	43	0	69	2	0
10	f	43	0	69	8	0
10	h	86	0	138	16	0
10	i	43	0	69	2	0
10	j	43	0	69	5	0
10	k	43	0	69	2	0
10	l	43	0	69	6	0
10	m	43	0	69	1	0
10	n	43	0	69	4	0
10	p	86	0	138	20	0
10	q	43	0	69	8	0
10	r	43	0	69	1	0
10	s	43	0	69	1	0
10	t	43	0	69	4	0
10	u	43	0	69	3	0
10	v	43	0	69	14	0
10	w	43	0	69	2	0
11	9	53	0	0	0	0
11	H	212	0	0	3	0
11	M	106	0	0	1	0
11	g	103	0	0	0	0
12	C	129	0	90	15	0
13	L	65	0	76	2	0
13	M	130	0	152	2	0
14	M	1	0	0	0	0
All	All	28463	0	28688	550	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 10.

The worst 5 of 550 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)
4:C:101:VAL:HG12	4:C:103:PRO:HD2	1.16	1.15
2:s:46:LEU:HD21	3:t:45:ARG:HH12	1.16	1.09
2:k:42:ASN:O	2:k:46:LEU:HD13	1.56	1.04
2:a:40:HIS:CE1	3:b:45:ARG:HH11	1.78	1.02
2:s:40:HIS:CE1	3:t:45:ARG:HD2	1.99	0.96

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
2	1	49/51 (96%)	49 (100%)	0	0	100	100
2	3	49/51 (96%)	49 (100%)	0	0	100	100
2	5	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
2	7	49/51 (96%)	49 (100%)	0	0	100	100
2	9	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
2	a	49/51 (96%)	49 (100%)	0	0	100	100
2	c	49/51 (96%)	49 (100%)	0	0	100	100
2	e	49/51 (96%)	49 (100%)	0	0	100	100
2	g	49/51 (96%)	49 (100%)	0	0	100	100
2	i	49/51 (96%)	49 (100%)	0	0	100	100
2	k	49/51 (96%)	49 (100%)	0	0	100	100
2	m	49/51 (96%)	49 (100%)	0	0	100	100
2	o	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
2	q	49/51 (96%)	49 (100%)	0	0	100	100
2	s	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	u	49/51 (96%)	49 (100%)	0	0	100	100
2	w	49/51 (96%)	49 (100%)	0	0	100	100
3	0	42/44 (96%)	42 (100%)	0	0	100	100
3	2	42/44 (96%)	42 (100%)	0	0	100	100
3	4	42/44 (96%)	42 (100%)	0	0	100	100
3	6	42/44 (96%)	42 (100%)	0	0	100	100
3	8	42/44 (96%)	42 (100%)	0	0	100	100
3	b	42/44 (96%)	42 (100%)	0	0	100	100
3	d	42/44 (96%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	f	42/44 (96%)	42 (100%)	0	0	100	100
3	h	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	j	42/44 (96%)	42 (100%)	0	0	100	100
3	l	42/44 (96%)	42 (100%)	0	0	100	100
3	n	42/44 (96%)	42 (100%)	0	0	100	100
3	p	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	r	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
3	t	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
3	v	42/44 (96%)	42 (100%)	0	0	100	100
3	x	42/44 (96%)	42 (100%)	0	0	100	100
4	C	355/357 (99%)	338 (95%)	17 (5%)	0	100	100
5	H	253/255 (99%)	248 (98%)	5 (2%)	0	100	100
6	L	271/273 (99%)	266 (98%)	5 (2%)	0	100	100
7	M	323/325 (99%)	317 (98%)	6 (2%)	0	100	100
All	All	2823/2901 (97%)	2772 (98%)	51 (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	A	55/55 (100%)	55 (100%)	0	100	100
2	1	43/43 (100%)	43 (100%)	0	100	100
2	3	43/43 (100%)	43 (100%)	0	100	100
2	5	43/43 (100%)	43 (100%)	0	100	100
2	7	43/43 (100%)	43 (100%)	0	100	100
2	9	43/43 (100%)	43 (100%)	0	100	100
2	a	43/43 (100%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	43/43 (100%)	43 (100%)	0	100	100
2	e	43/43 (100%)	42 (98%)	1 (2%)	44	72
2	g	43/43 (100%)	43 (100%)	0	100	100
2	i	43/43 (100%)	43 (100%)	0	100	100
2	k	43/43 (100%)	43 (100%)	0	100	100
2	m	43/43 (100%)	43 (100%)	0	100	100
2	o	43/43 (100%)	43 (100%)	0	100	100
2	q	43/43 (100%)	43 (100%)	0	100	100
2	s	43/43 (100%)	43 (100%)	0	100	100
2	u	43/43 (100%)	43 (100%)	0	100	100
2	w	43/43 (100%)	43 (100%)	0	100	100
3	0	37/37 (100%)	37 (100%)	0	100	100
3	2	37/37 (100%)	37 (100%)	0	100	100
3	4	37/37 (100%)	37 (100%)	0	100	100
3	6	37/37 (100%)	37 (100%)	0	100	100
3	8	37/37 (100%)	37 (100%)	0	100	100
3	b	37/37 (100%)	37 (100%)	0	100	100
3	d	37/37 (100%)	37 (100%)	0	100	100
3	f	37/37 (100%)	37 (100%)	0	100	100
3	h	37/37 (100%)	37 (100%)	0	100	100
3	j	37/37 (100%)	37 (100%)	0	100	100
3	l	37/37 (100%)	37 (100%)	0	100	100
3	n	37/37 (100%)	37 (100%)	0	100	100
3	p	37/37 (100%)	37 (100%)	0	100	100
3	r	37/37 (100%)	37 (100%)	0	100	100
3	t	37/37 (100%)	37 (100%)	0	100	100
3	v	37/37 (100%)	37 (100%)	0	100	100
3	x	37/37 (100%)	37 (100%)	0	100	100
4	C	304/304 (100%)	303 (100%)	1 (0%)	86	94
5	H	213/213 (100%)	212 (100%)	1 (0%)	81	92
6	L	217/217 (100%)	217 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	M	266/266 (100%)	263 (99%)	3 (1%)	65 84
All	All	2415/2415 (100%)	2409 (100%)	6 (0%)	85 95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	M	117	ILE
7	M	183	HIS
7	M	217	PHE
4	C	104	VAL
2	e	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	i	40	HIS
7	M	294	ASN
4	C	223	ASN
3	0	20	HIS
7	M	79	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 93 ligands modelled in this entry, 1 is monoatomic - leaving 92 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	$\#\|Z\| > 2$
8	U10	L	302	-	38,38,63	0.20	0	46,49,79	0.52	1 (2%)
10	SPN	a	102	-	40,42,42	3.86	19 (47%)	50,52,52	2.48	20 (40%)
13	BPH	M	405	-	59,70,70	1.19	4 (6%)	61,101,101	0.98	3 (4%)
10	SPN	j	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.63	18 (36%)
10	SPN	1	102	-	40,42,42	3.87	19 (47%)	50,52,52	2.45	20 (40%)
10	SPN	7	103	-	40,42,42	3.93	19 (47%)	50,52,52	2.47	19 (38%)
9	BCL	d	101	3	69,74,74	0.83	1 (1%)	83,115,115	1.19	10 (12%)
9	BCL	e	101	2	69,74,74	0.81	2 (2%)	83,115,115	1.20	12 (14%)
9	BCL	L	304	6	69,74,74	0.96	2 (2%)	83,115,115	1.35	14 (16%)
9	BCL	i	101	2	69,74,74	0.91	1 (1%)	83,115,115	1.27	11 (13%)
9	BCL	M	404	7	69,74,74	0.92	2 (2%)	83,115,115	1.23	12 (14%)
9	BCL	k	101	2	69,74,74	0.80	1 (1%)	83,115,115	1.22	11 (13%)
10	SPN	r	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.44	20 (40%)
11	MW9	H	301	-	52,52,52	0.60	1 (1%)	55,58,58	0.61	2 (3%)
12	HEM	C	402	4	50,50,50	0.84	1 (2%)	66,82,82	1.52	5 (7%)
10	SPN	s	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.44	21 (42%)
11	MW9	H	303	-	52,52,52	0.58	1 (1%)	55,58,58	0.61	2 (3%)
11	MW9	M	408	-	52,52,52	0.59	1 (1%)	55,58,58	0.52	2 (3%)
10	SPN	3	102	-	40,42,42	3.86	19 (47%)	50,52,52	2.49	20 (40%)
9	BCL	h	101	3	69,74,74	0.86	3 (4%)	83,115,115	1.17	10 (12%)
10	SPN	f	102	-	40,42,42	3.93	19 (47%)	50,52,52	2.55	17 (34%)
9	BCL	b	101	3	69,74,74	1.75	19 (27%)	83,115,115	2.79	27 (32%)
10	SPN	w	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.45	21 (42%)
9	BCL	7	101	2	69,74,74	0.83	1 (1%)	83,115,115	1.25	11 (13%)
9	BCL	n	101	3	69,74,74	0.82	1 (1%)	83,115,115	1.22	9 (10%)
12	HEM	C	401	4	50,50,50	0.86	2 (4%)	66,82,82	0.77	2 (3%)
9	BCL	f	101	3	69,74,74	0.84	1 (1%)	83,115,115	1.21	11 (13%)
10	SPN	5	102	-	40,42,42	3.86	19 (47%)	50,52,52	2.50	20 (40%)
11	MW9	M	407	-	52,52,52	0.58	1 (1%)	55,58,58	0.83	3 (5%)
13	BPH	L	303	-	59,70,70	1.14	3 (5%)	61,101,101	1.19	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
11	MW9	g	102	-	52,52,52	0.58	1 (1%)	55,58,58	0.64	2 (3%)
10	SPN	0	102	-	40,42,42	3.92	19 (47%)	50,52,52	2.45	18 (36%)
9	BCL	c	101	2	69,74,74	0.82	1 (1%)	83,115,115	1.21	11 (13%)
10	SPN	1	105	-	40,42,42	3.99	19 (47%)	50,52,52	2.43	20 (40%)
9	BCL	q	101	2	69,74,74	0.89	1 (1%)	83,115,115	1.24	9 (10%)
10	SPN	9	103	-	40,42,42	3.89	19 (47%)	50,52,52	2.46	22 (44%)
10	SPN	M	406	-	40,42,42	3.91	19 (47%)	50,52,52	2.74	18 (36%)
9	BCL	p	101	3	69,74,74	0.81	2 (2%)	83,115,115	1.23	10 (12%)
9	BCL	0	101	3	69,74,74	1.76	17 (24%)	83,115,115	2.84	26 (31%)
11	MW9	g	103	-	49,49,52	0.60	1 (2%)	52,55,58	0.66	2 (3%)
10	SPN	n	102	-	40,42,42	3.93	19 (47%)	50,52,52	2.46	20 (40%)
9	BCL	a	101	2	69,74,74	0.82	2 (2%)	83,115,115	1.20	12 (14%)
9	BCL	8	101	3	69,74,74	1.75	18 (26%)	83,115,115	2.88	27 (32%)
10	SPN	p	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.59	19 (38%)
9	BCL	j	101	3	69,74,74	0.80	1 (1%)	83,115,115	1.19	11 (13%)
9	BCL	1	101	2	69,74,74	0.86	1 (1%)	83,115,115	1.30	10 (12%)
9	BCL	6	101	3	69,74,74	1.76	19 (27%)	83,115,115	2.82	26 (31%)
9	BCL	g	101	2	69,74,74	0.82	1 (1%)	83,115,115	1.19	12 (14%)
9	BCL	M	402	7	69,74,74	1.80	17 (24%)	83,115,115	2.78	31 (37%)
10	SPN	c	103	-	40,42,42	3.95	19 (47%)	50,52,52	2.50	20 (40%)
10	SPN	7	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.45	21 (42%)
13	BPH	M	409	-	59,70,70	1.06	4 (6%)	61,101,101	1.05	5 (8%)
10	SPN	m	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.44	21 (42%)
10	SPN	c	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.45	22 (44%)
9	BCL	t	101	3	69,74,74	0.84	1 (1%)	83,115,115	1.19	9 (10%)
10	SPN	h	103	-	40,42,42	3.91	19 (47%)	50,52,52	2.56	18 (36%)
10	SPN	l	102	-	40,42,42	3.92	19 (47%)	50,52,52	2.55	18 (36%)
9	BCL	3	101	2	69,74,74	0.88	2 (2%)	83,115,115	1.23	11 (13%)
10	SPN	q	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.55	20 (40%)
10	SPN	1	104	-	40,42,42	3.92	19 (47%)	50,52,52	2.63	18 (36%)
10	SPN	i	102	-	40,42,42	3.89	19 (47%)	50,52,52	2.45	21 (42%)
10	SPN	k	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.45	21 (42%)
10	SPN	a	103	-	40,42,42	3.91	19 (47%)	50,52,52	2.64	21 (42%)
9	BCL	l	101	3	69,74,74	0.80	1 (1%)	83,115,115	1.23	11 (13%)
9	BCL	m	101	2	69,74,74	0.80	2 (2%)	83,115,115	1.23	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	U10	L	305	-	38,38,63	1.29	2 (5%)	46,49,79	2.18	12 (26%)
9	BCL	v	101	3	69,74,74	0.77	1 (1%)	83,115,115	1.27	11 (13%)
10	SPN	1	103	-	40,42,42	3.89	19 (47%)	50,52,52	2.79	21 (42%)
10	SPN	t	102	-	40,42,42	3.90	19 (47%)	50,52,52	2.46	21 (42%)
10	SPN	u	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.45	21 (42%)
10	SPN	e	102	-	40,42,42	3.91	19 (47%)	50,52,52	2.45	22 (44%)
9	BCL	o	101	2	69,74,74	0.94	2 (2%)	83,115,115	1.30	12 (14%)
12	HEM	C	403	4	50,50,50	0.79	1 (2%)	66,82,82	0.83	2 (3%)
10	SPN	h	102	-	40,42,42	3.89	19 (47%)	50,52,52	2.45	22 (44%)
9	BCL	x	101	3	69,74,74	0.82	1 (1%)	83,115,115	1.22	10 (12%)
9	BCL	u	101	2	69,74,74	0.81	2 (2%)	83,115,115	1.19	11 (13%)
9	BCL	9	102	2	69,74,74	0.82	2 (2%)	83,115,115	1.19	10 (12%)
9	BCL	L	301	6	69,74,74	0.91	2 (2%)	83,115,115	1.24	12 (14%)
9	BCL	r	101	3	69,74,74	0.82	1 (1%)	83,115,115	1.26	13 (15%)
10	SPN	5	103	-	40,42,42	3.94	19 (47%)	50,52,52	2.48	18 (36%)
8	U10	A	101	-	43,43,63	1.27	2 (4%)	52,55,79	1.87	15 (28%)
9	BCL	2	101	3	69,74,74	1.75	17 (24%)	83,115,115	2.82	26 (31%)
11	MW9	H	302	-	52,52,52	0.59	1 (1%)	55,58,58	0.72	3 (5%)
9	BCL	s	101	2	69,74,74	0.91	3 (4%)	83,115,115	1.30	12 (14%)
8	U10	M	403	-	63,63,63	1.16	2 (3%)	76,79,79	1.57	15 (19%)
9	BCL	w	101	2	69,74,74	0.81	2 (2%)	83,115,115	1.23	10 (12%)
10	SPN	p	103	-	40,42,42	3.91	19 (47%)	50,52,52	2.50	21 (42%)
10	SPN	v	102	-	40,42,42	3.93	19 (47%)	50,52,52	2.58	18 (36%)
11	MW9	9	101	-	52,52,52	0.57	1 (1%)	55,58,58	0.53	2 (3%)
9	BCL	5	101	2	69,74,74	0.87	2 (2%)	83,115,115	1.24	10 (12%)
11	MW9	H	304	-	52,52,52	0.57	1 (1%)	55,58,58	0.55	2 (3%)
9	BCL	4	101	3	69,74,74	1.75	19 (27%)	83,115,115	2.79	28 (33%)

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
8	U10	L	302	-	-	6/33/57/87	0/1/1/1
10	SPN	a	102	-	-	23/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BPH	M	405	-	-	11/37/105/105	0/5/6/6
10	SPN	j	102	-	-	23/50/51/51	-
10	SPN	1	102	-	-	24/50/51/51	-
10	SPN	7	103	-	-	21/50/51/51	-
9	BCL	d	101	3	-	20/41/137/137	-
9	BCL	e	101	2	-	20/41/137/137	-
9	BCL	L	304	6	-	28/41/137/137	-
9	BCL	i	101	2	-	12/41/137/137	-
9	BCL	M	404	7	-	13/41/137/137	-
9	BCL	k	101	2	-	17/41/137/137	-
10	SPN	r	102	-	-	19/50/51/51	-
11	MW9	H	301	-	-	38/57/57/57	-
12	HEM	C	402	4	-	4/14/54/54	-
10	SPN	s	102	-	-	18/50/51/51	-
11	MW9	H	303	-	-	34/57/57/57	-
11	MW9	M	408	-	-	26/57/57/57	-
10	SPN	3	102	-	-	25/50/51/51	-
9	BCL	h	101	3	-	20/41/137/137	-
10	SPN	f	102	-	-	20/50/51/51	-
9	BCL	b	101	3	-	22/41/137/137	-
10	SPN	w	102	-	-	18/50/51/51	-
9	BCL	7	101	2	-	20/41/137/137	-
9	BCL	n	101	3	-	20/41/137/137	-
12	HEM	C	401	4	-	6/14/54/54	-
9	BCL	f	101	3	-	16/41/137/137	-
10	SPN	5	102	-	-	24/50/51/51	-
11	MW9	M	407	-	-	20/57/57/57	-
13	BPH	L	303	-	-	13/37/105/105	0/5/6/6
11	MW9	g	102	-	-	21/57/57/57	-
10	SPN	0	102	-	-	20/50/51/51	-
9	BCL	c	101	2	-	22/41/137/137	-
10	SPN	1	105	-	-	22/50/51/51	-
9	BCL	q	101	2	-	18/41/137/137	-
10	SPN	9	103	-	-	19/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPN	M	406	-	-	17/50/51/51	-
9	BCL	p	101	3	-	17/41/137/137	-
9	BCL	0	101	3	-	19/41/137/137	-
11	MW9	g	103	-	-	21/54/54/57	-
10	SPN	n	102	-	-	21/50/51/51	-
9	BCL	a	101	2	-	20/41/137/137	-
9	BCL	8	101	3	-	12/41/137/137	-
10	SPN	p	102	-	-	25/50/51/51	-
9	BCL	j	101	3	-	21/41/137/137	-
9	BCL	1	101	2	-	18/41/137/137	-
9	BCL	6	101	3	-	15/41/137/137	-
9	BCL	g	101	2	-	27/41/137/137	-
9	BCL	M	402	7	-	16/41/137/137	-
10	SPN	c	103	-	-	20/50/51/51	-
10	SPN	7	102	-	-	22/50/51/51	-
13	BPH	M	409	-	-	17/37/105/105	0/5/6/6
10	SPN	m	102	-	-	18/50/51/51	-
10	SPN	c	102	-	-	20/50/51/51	-
9	BCL	t	101	3	-	18/41/137/137	-
10	SPN	h	103	-	-	21/50/51/51	-
10	SPN	l	102	-	-	21/50/51/51	-
9	BCL	3	101	2	-	18/41/137/137	-
10	SPN	q	102	-	-	23/50/51/51	-
10	SPN	1	104	-	-	22/50/51/51	-
10	SPN	i	102	-	-	22/50/51/51	-
10	SPN	k	102	-	-	22/50/51/51	-
10	SPN	a	103	-	-	21/50/51/51	-
9	BCL	l	101	3	-	20/41/137/137	-
9	BCL	m	101	2	-	25/41/137/137	-
8	U10	L	305	-	-	11/33/57/87	0/1/1/1
9	BCL	v	101	3	-	15/41/137/137	-
10	SPN	1	103	-	-	18/50/51/51	-
10	SPN	t	102	-	-	18/50/51/51	-
10	SPN	u	102	-	-	21/50/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SPN	e	102	-	-	19/50/51/51	-
9	BCL	o	101	2	-	15/41/137/137	-
12	HEM	C	403	4	-	4/14/54/54	-
10	SPN	h	102	-	-	20/50/51/51	-
9	BCL	x	101	3	-	19/41/137/137	-
9	BCL	u	101	2	-	16/41/137/137	-
9	BCL	9	102	2	-	18/41/137/137	-
9	BCL	L	301	6	-	11/41/137/137	-
9	BCL	r	101	3	-	24/41/137/137	-
10	SPN	5	103	-	-	21/50/51/51	-
8	U10	A	101	-	-	7/39/63/87	0/1/1/1
9	BCL	2	101	3	-	18/41/137/137	-
11	MW9	H	302	-	-	21/57/57/57	-
9	BCL	s	101	2	-	22/41/137/137	-
8	U10	M	403	-	-	19/63/87/87	0/1/1/1
9	BCL	w	101	2	-	19/41/137/137	-
10	SPN	p	103	-	-	22/50/51/51	-
10	SPN	v	102	-	-	18/50/51/51	-
11	MW9	9	101	-	-	34/57/57/57	-
9	BCL	5	101	2	-	21/41/137/137	-
11	MW9	H	304	-	-	36/57/57/57	-
9	BCL	4	101	3	-	19/41/137/137	-

The worst 5 of 869 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	103	SPN	C3-C4	-12.57	1.32	1.50
10	5	103	SPN	C3-C4	-12.56	1.32	1.50
10	c	103	SPN	C3-C4	-12.54	1.32	1.50
10	7	103	SPN	C3-C4	-12.50	1.32	1.50
10	1	104	SPN	C3-C4	-12.42	1.32	1.50

The worst 5 of 1313 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	6	101	BCL	C2B-C1B-NB	11.18	117.73	110.23
9	8	101	BCL	O2D-CGD-CBD	10.93	130.70	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	101	BCL	C2B-C1B-NB	10.92	117.56	110.23
9	0	101	BCL	O2D-CGD-CBD	10.91	130.66	111.27
9	4	101	BCL	C2B-C1B-NB	10.69	117.40	110.23

There are no chirality outliers.

5 of 1788 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	101	U10	C29-C31-C32-C33
8	L	305	U10	C1-C6-C7-C8
8	L	305	U10	C5-C6-C7-C8
8	L	305	U10	C15-C14-C16-C17
9	1	101	BCL	C2C-C3C-CAC-CBC

There are no ring outliers.

83 monomers are involved in 365 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	302	U10	1	0
10	a	102	SPN	1	0
10	j	102	SPN	5	0
10	1	102	SPN	2	0
10	7	103	SPN	4	0
9	d	101	BCL	6	0
9	e	101	BCL	3	0
9	L	304	BCL	5	0
9	i	101	BCL	5	0
9	M	404	BCL	3	0
9	k	101	BCL	7	0
10	r	102	SPN	1	0
11	H	301	MW9	2	0
12	C	402	HEM	4	0
10	s	102	SPN	1	0
11	H	303	MW9	1	0
10	3	102	SPN	4	0
9	h	101	BCL	10	0
10	f	102	SPN	8	0
9	b	101	BCL	6	0
10	w	102	SPN	2	0
9	7	101	BCL	5	0
9	n	101	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	401	HEM	6	0
9	f	101	BCL	7	0
10	5	102	SPN	4	0
11	M	407	MW9	1	0
13	L	303	BPH	2	0
10	0	102	SPN	4	0
9	c	101	BCL	3	0
10	1	105	SPN	3	0
9	q	101	BCL	4	0
10	9	103	SPN	1	0
10	M	406	SPN	11	0
9	p	101	BCL	11	0
9	0	101	BCL	7	0
10	n	102	SPN	4	0
9	a	101	BCL	4	0
9	8	101	BCL	8	0
10	p	102	SPN	13	0
9	j	101	BCL	7	0
9	1	101	BCL	2	0
9	6	101	BCL	4	0
9	g	101	BCL	3	0
9	M	402	BCL	10	0
10	c	103	SPN	1	0
10	7	102	SPN	1	0
13	M	409	BPH	2	0
10	m	102	SPN	1	0
10	c	102	SPN	2	0
9	t	101	BCL	4	0
10	h	103	SPN	9	0
10	l	102	SPN	6	0
9	3	101	BCL	7	0
10	q	102	SPN	8	0
10	1	104	SPN	4	0
10	i	102	SPN	2	0
10	k	102	SPN	2	0
10	a	103	SPN	2	0
9	l	101	BCL	5	0
9	m	101	BCL	6	0
8	L	305	U10	5	0
9	v	101	BCL	7	0
10	1	103	SPN	12	0
10	t	102	SPN	4	0

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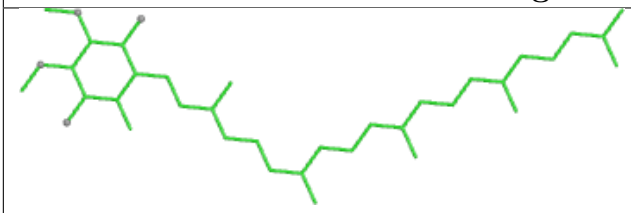
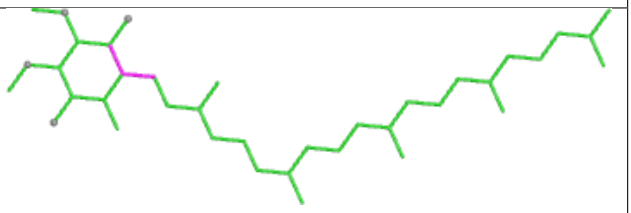
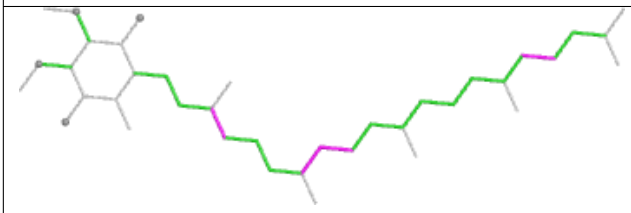
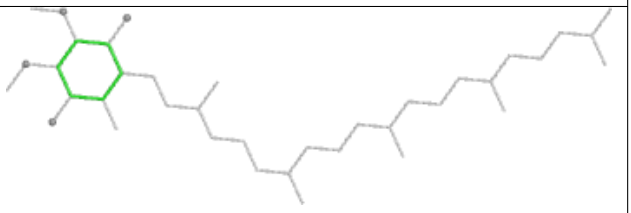
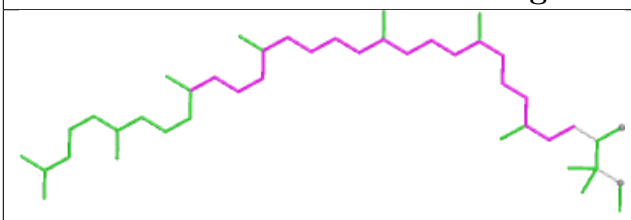
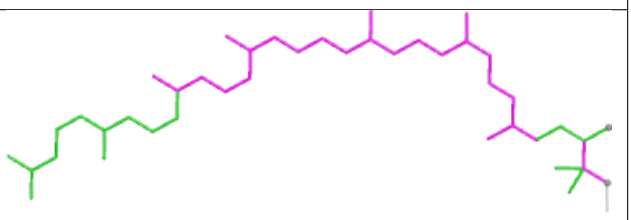
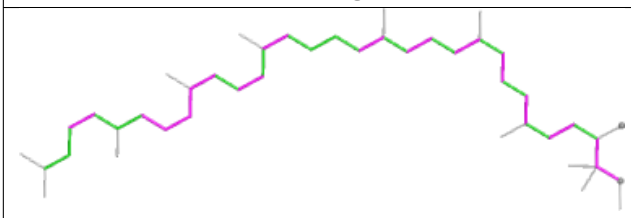
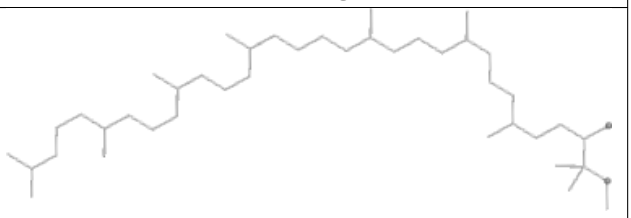
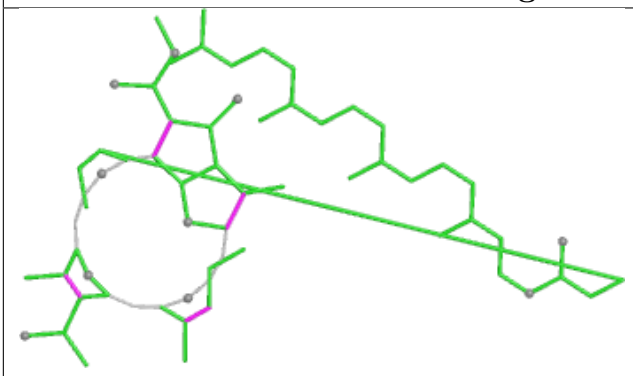
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	u	102	SPN	3	0
10	e	102	SPN	2	0
9	o	101	BCL	13	0
12	C	403	HEM	5	0
10	h	102	SPN	8	0
9	x	101	BCL	6	0
9	u	101	BCL	5	0
9	9	102	BCL	5	0
9	L	301	BCL	4	0
9	r	101	BCL	7	0
10	5	103	SPN	3	0
9	2	101	BCL	6	0
9	s	101	BCL	7	0
9	w	101	BCL	4	0
10	p	103	SPN	7	0
10	v	102	SPN	14	0
9	5	101	BCL	5	0
9	4	101	BCL	4	0

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

Ligand U10 L 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPN a 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH M 405



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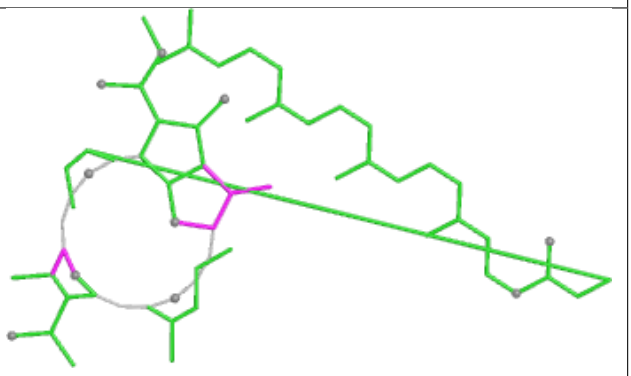

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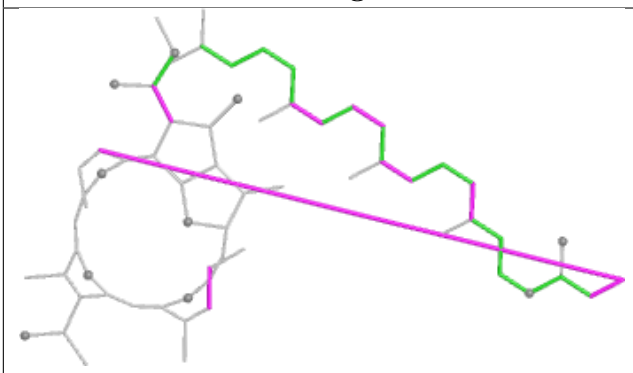

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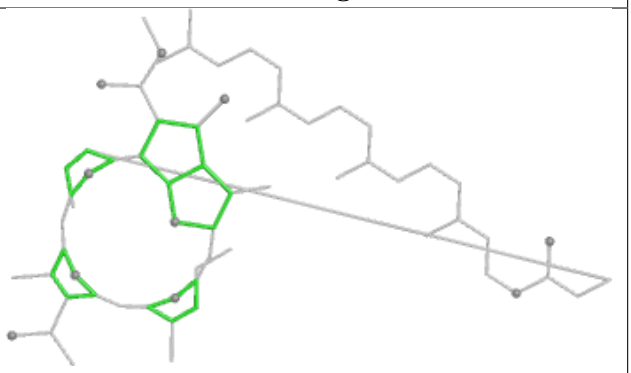

Rings

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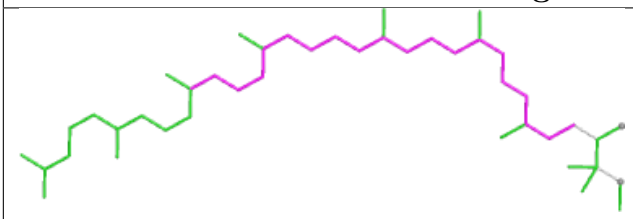

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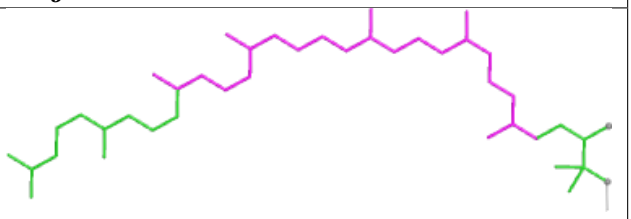

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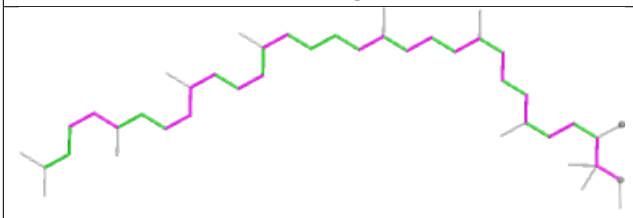

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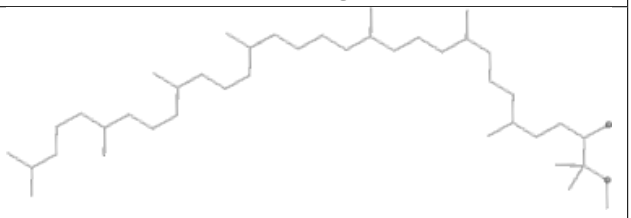

Rings

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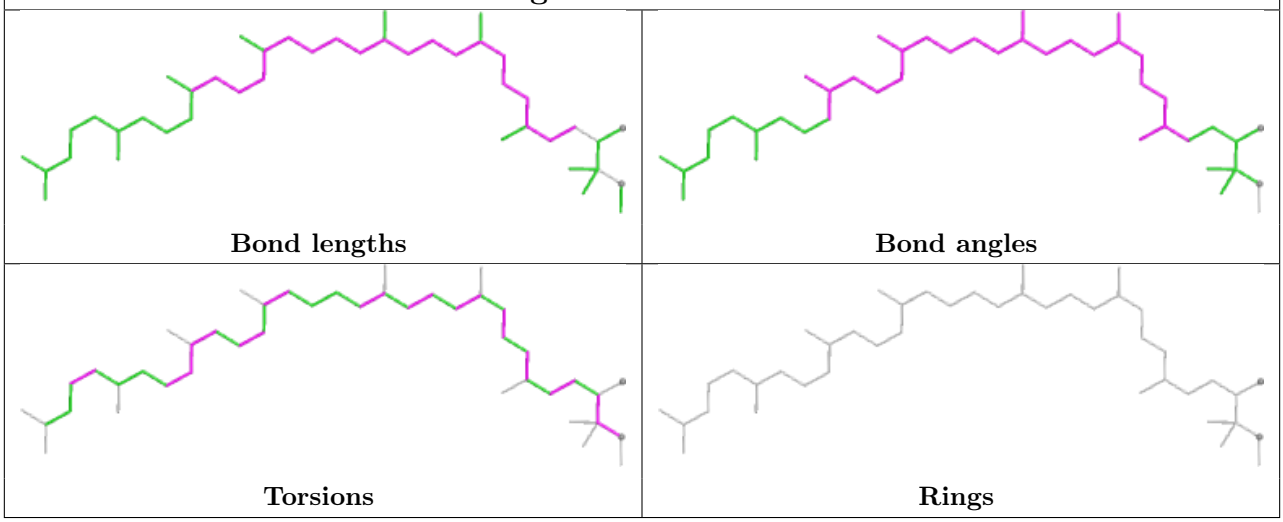

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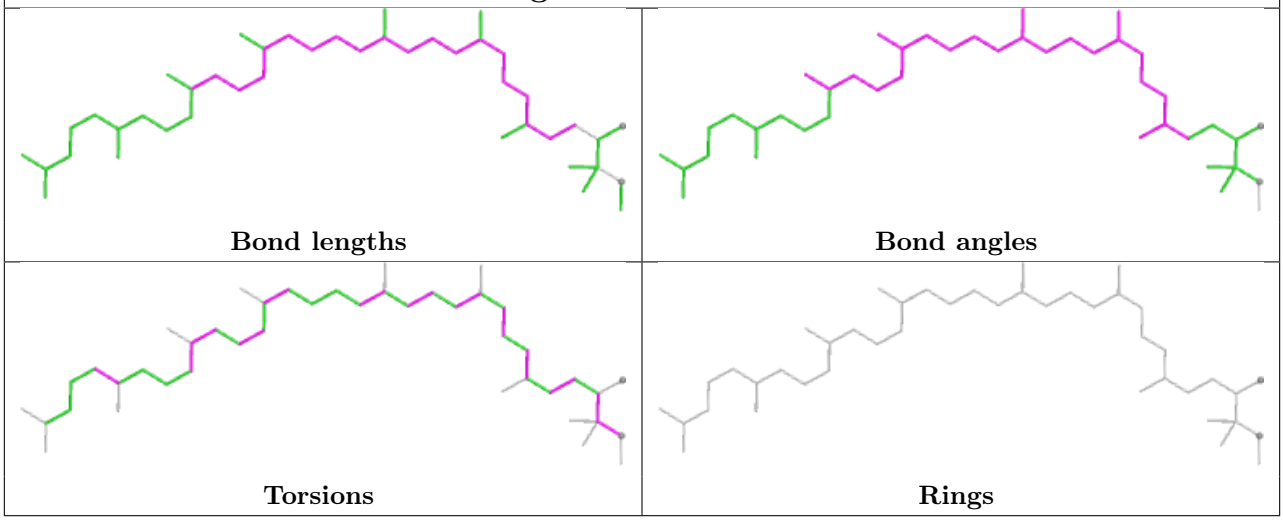

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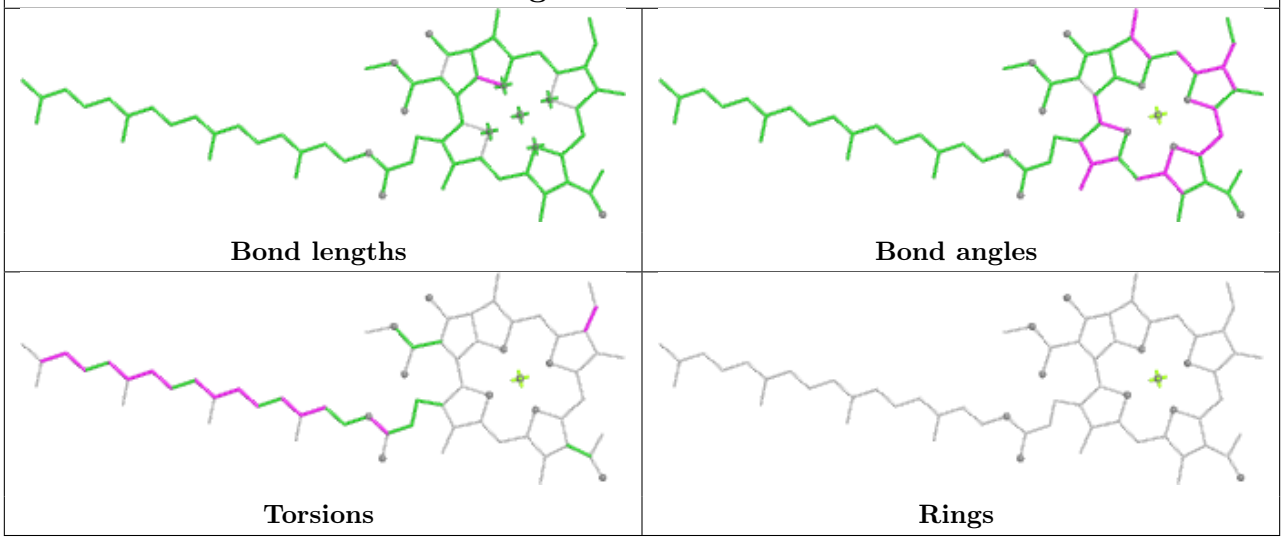

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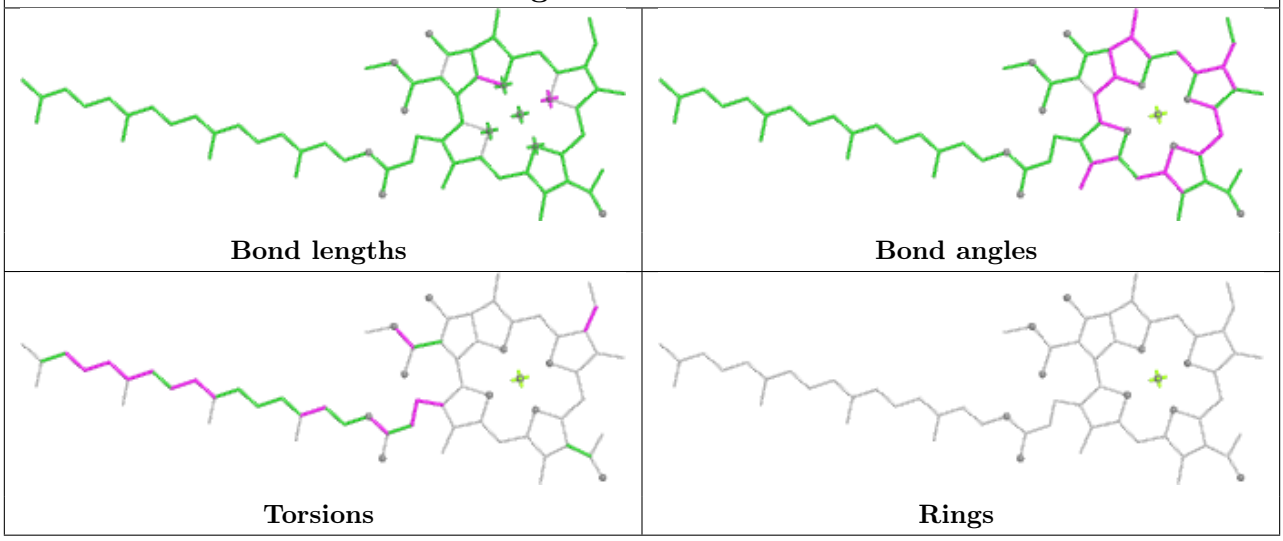

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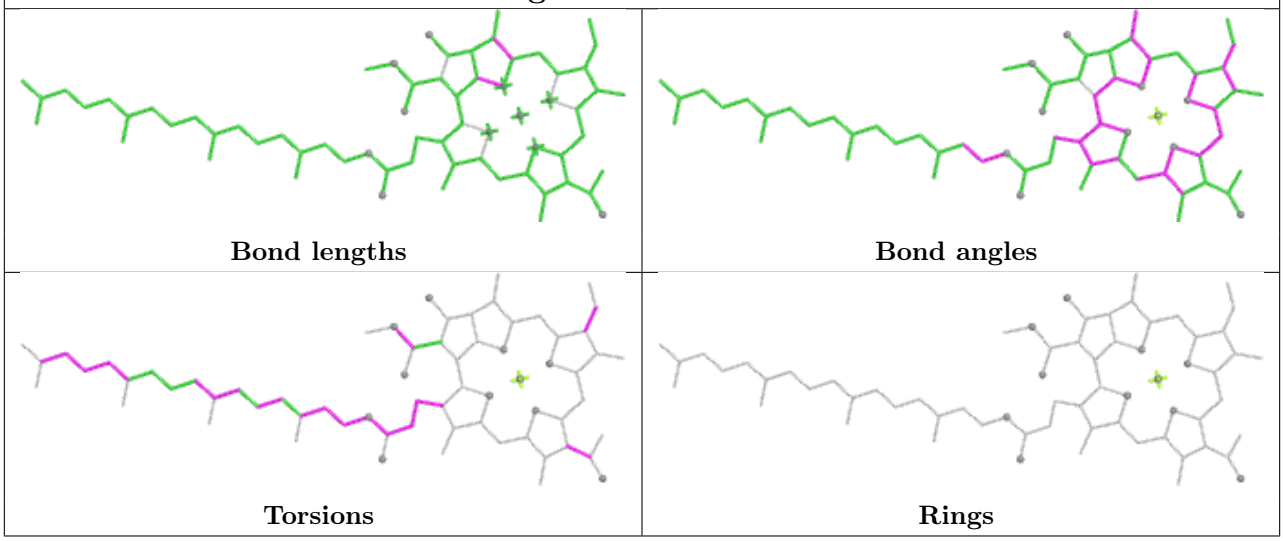

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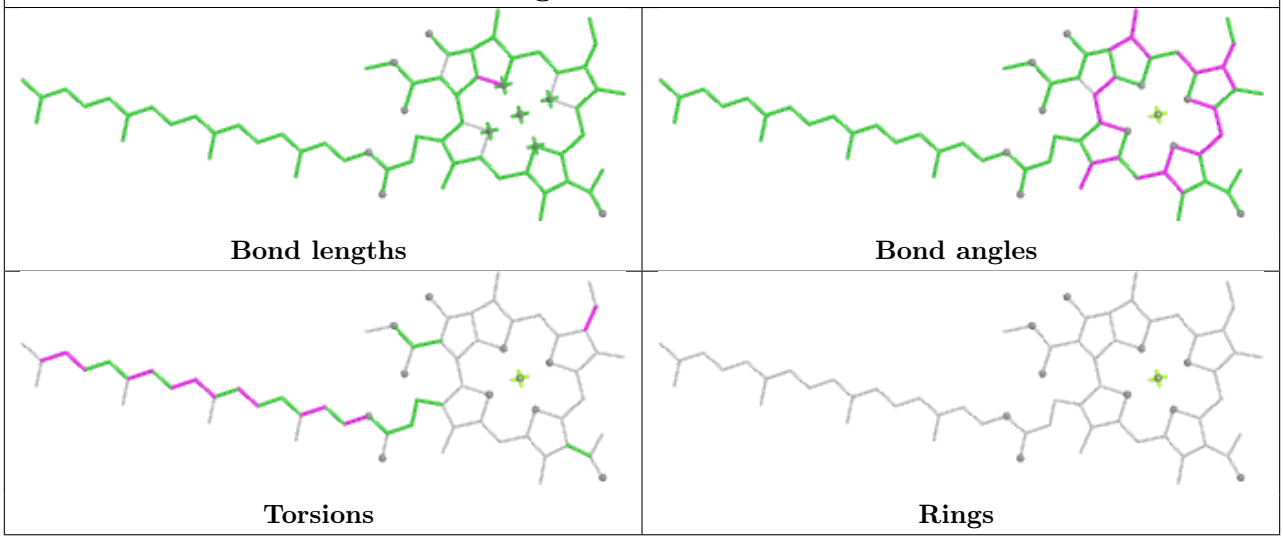

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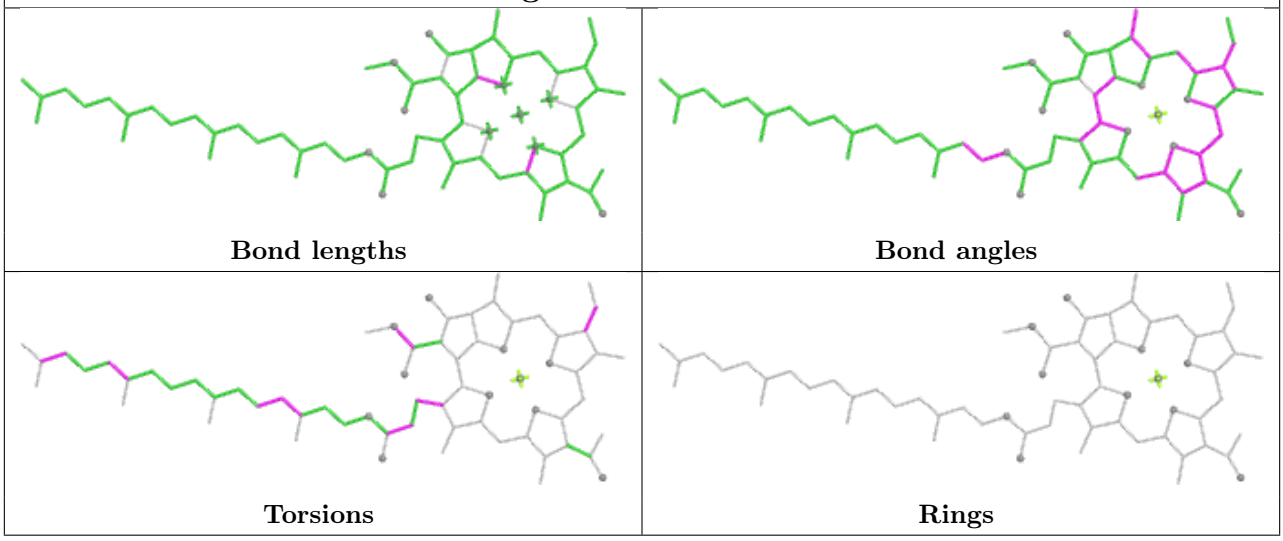

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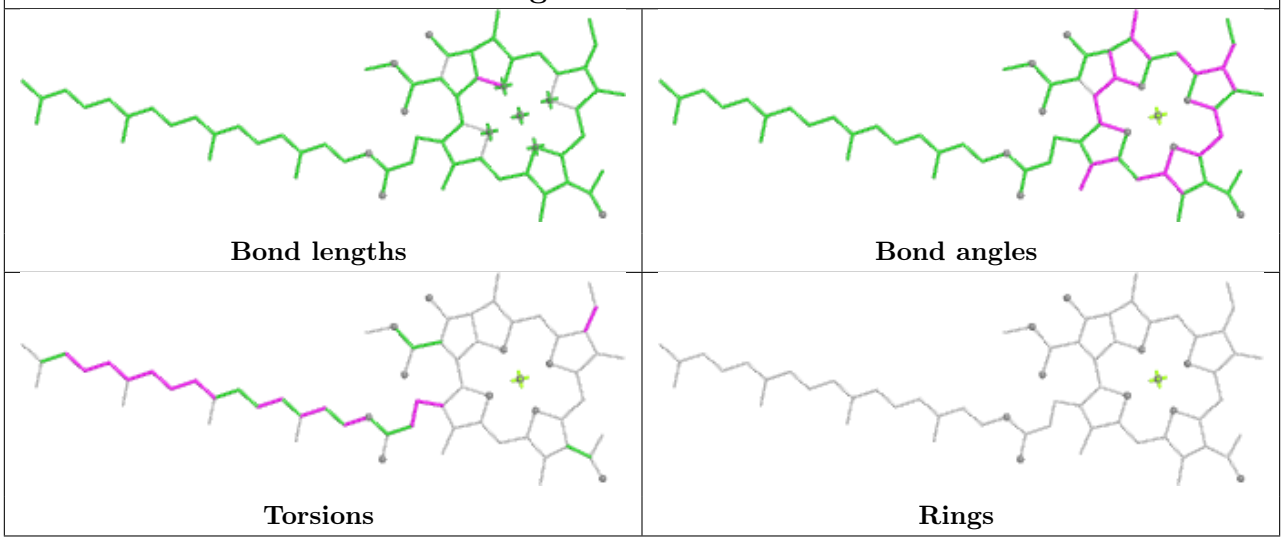

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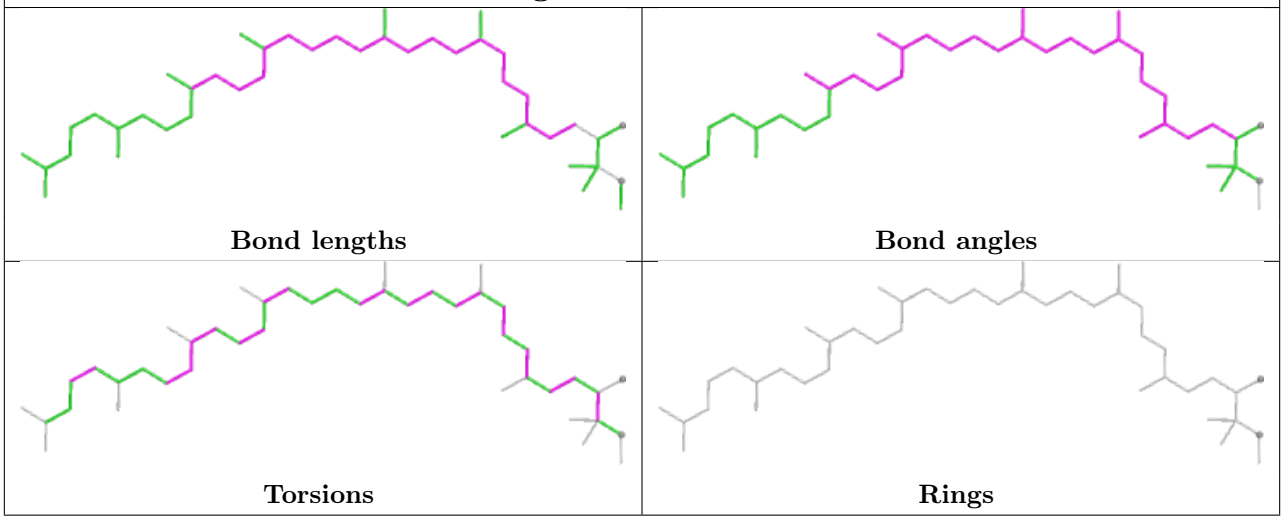
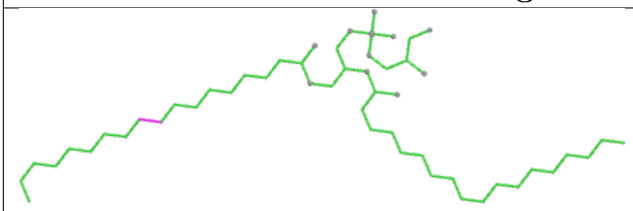
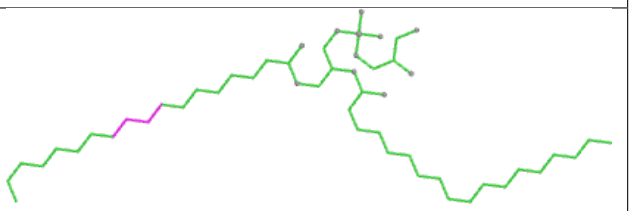


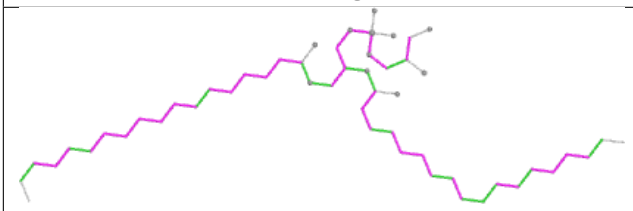
Ligand MW9 H 301



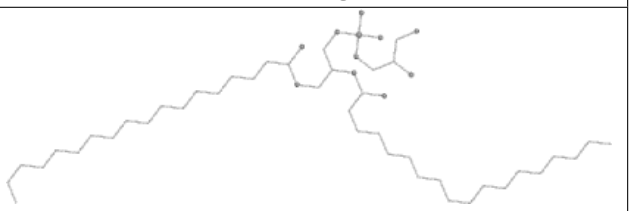
Bond lengths



Bond angles

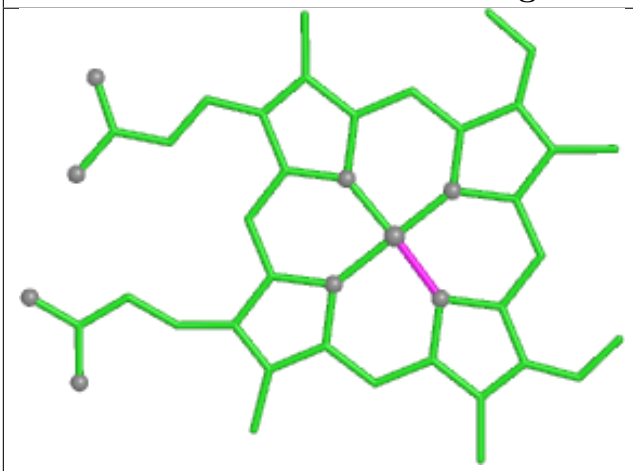


Torsions



Rings

Ligand HEM C 402



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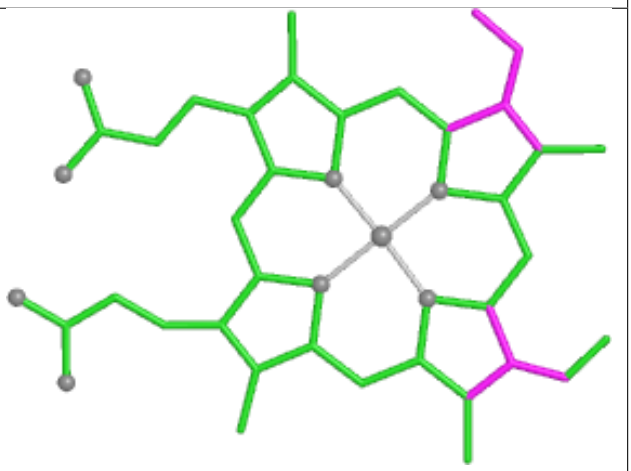
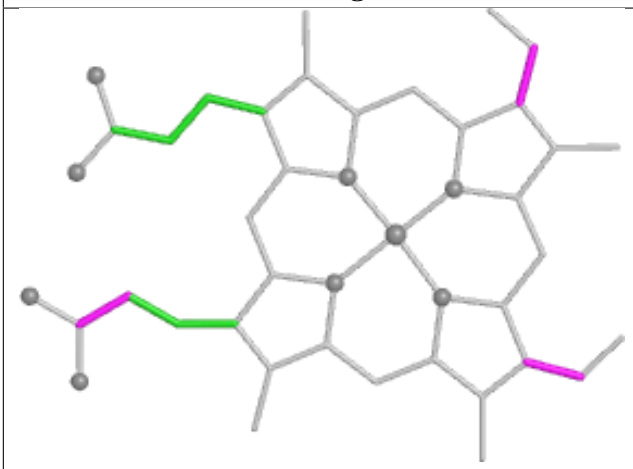


Bond angles



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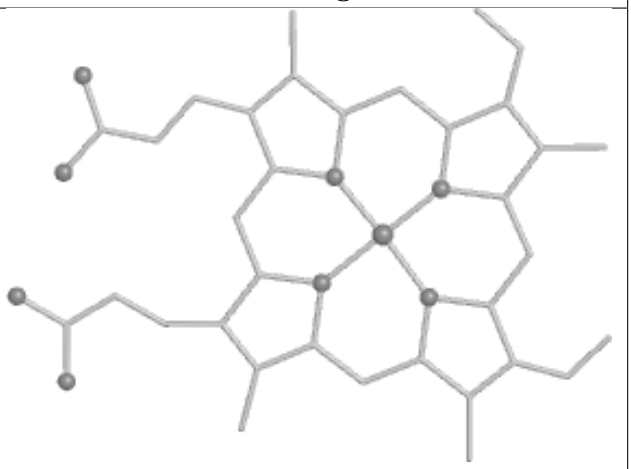
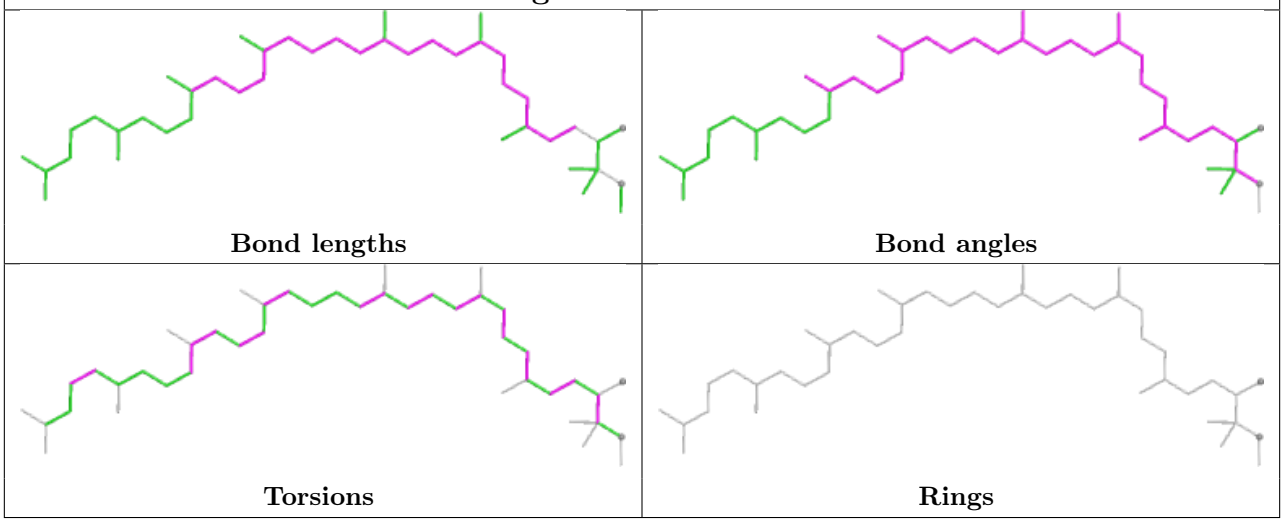
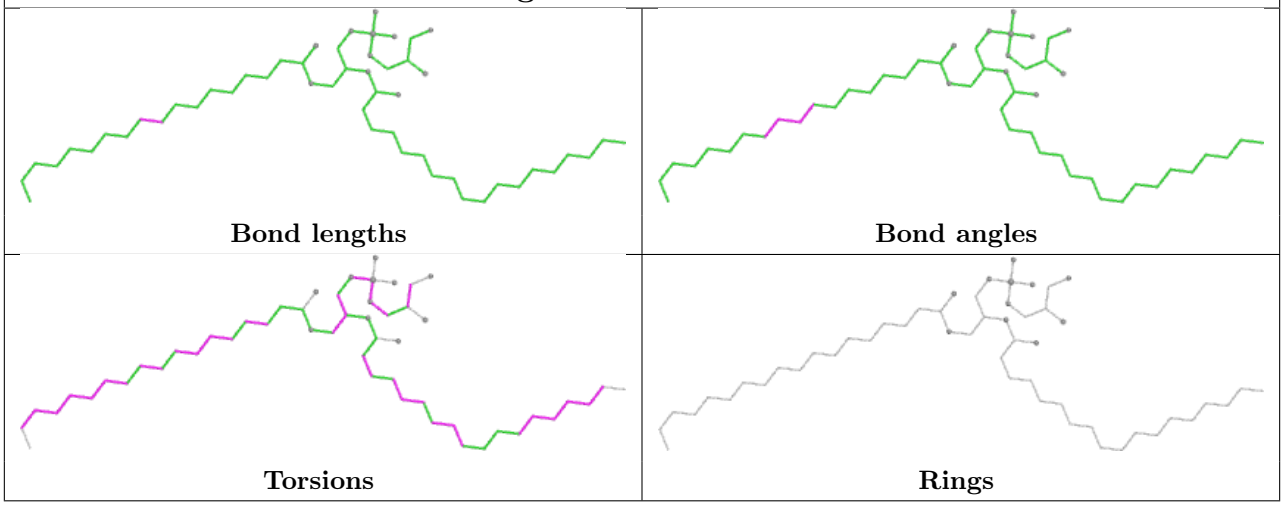


Rings

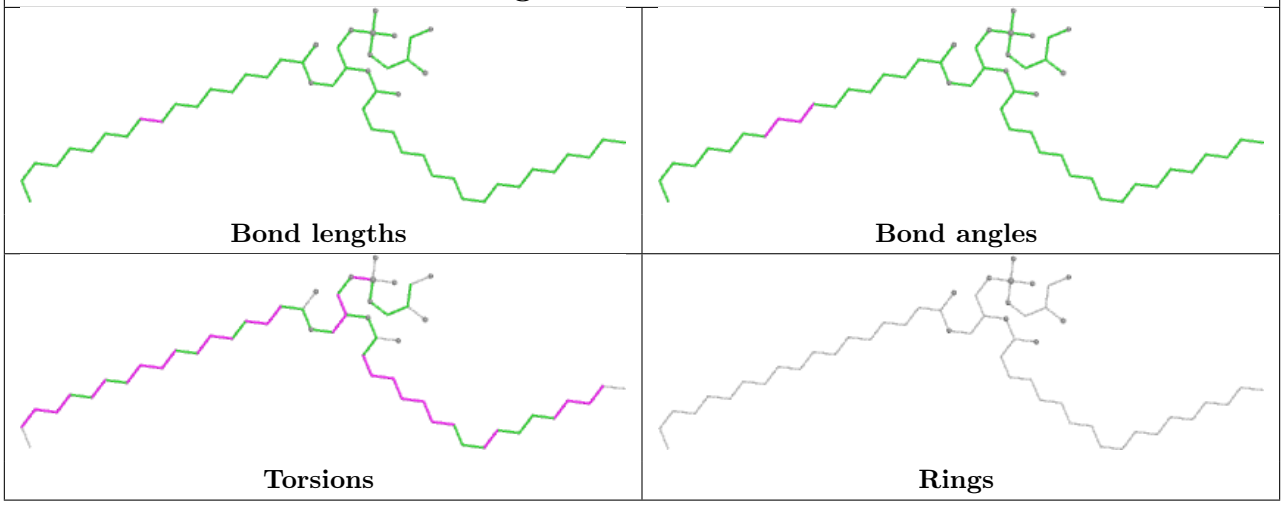
Ligand SPN s 102



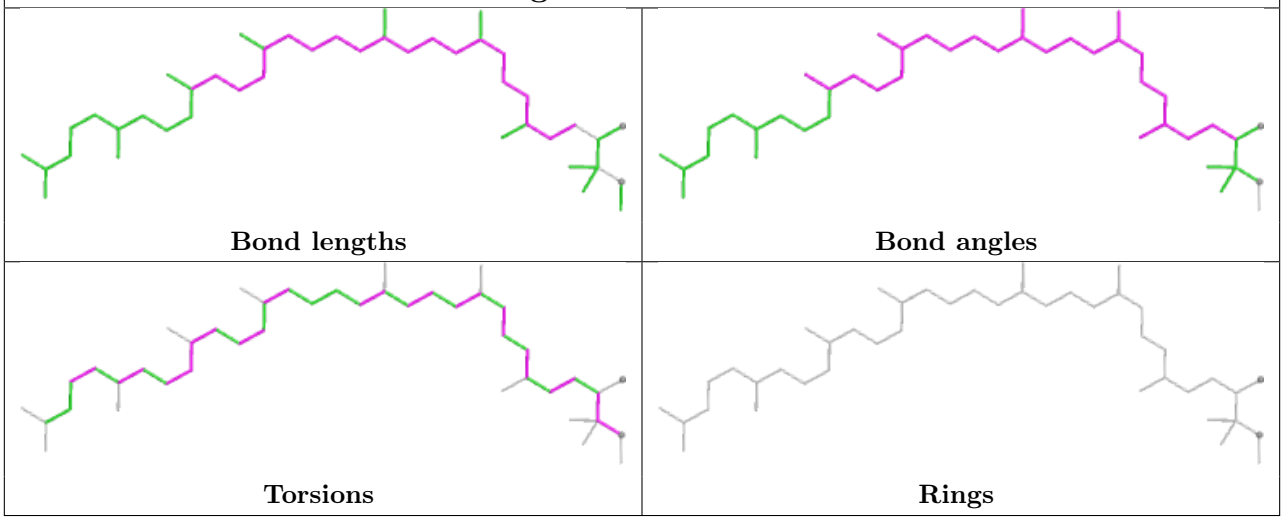
Ligand MW9 H 303



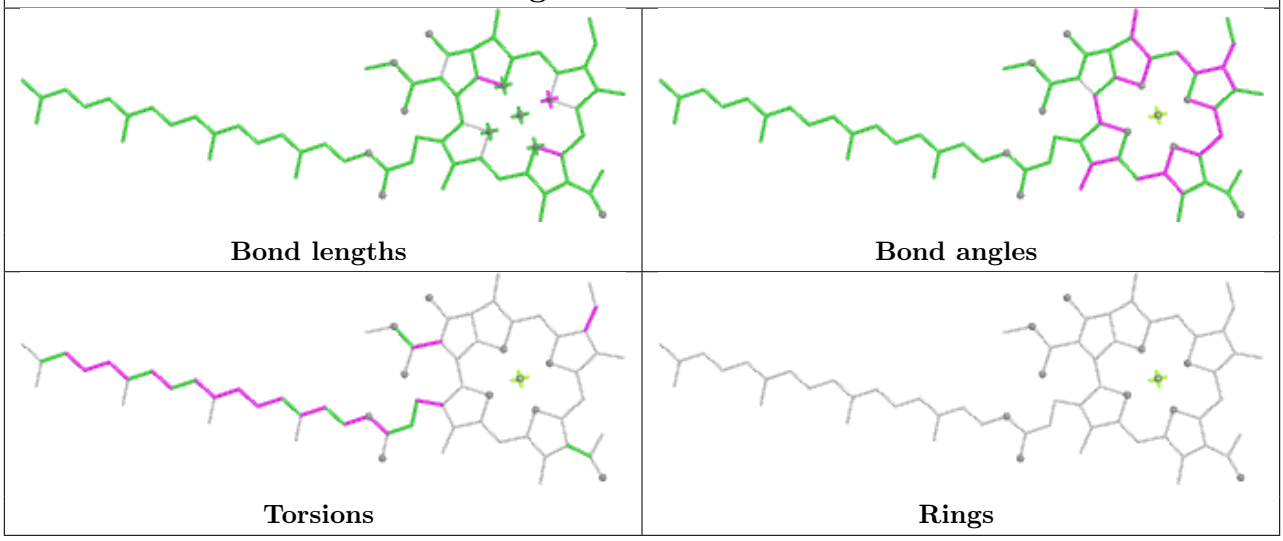
Ligand MW9 M 408



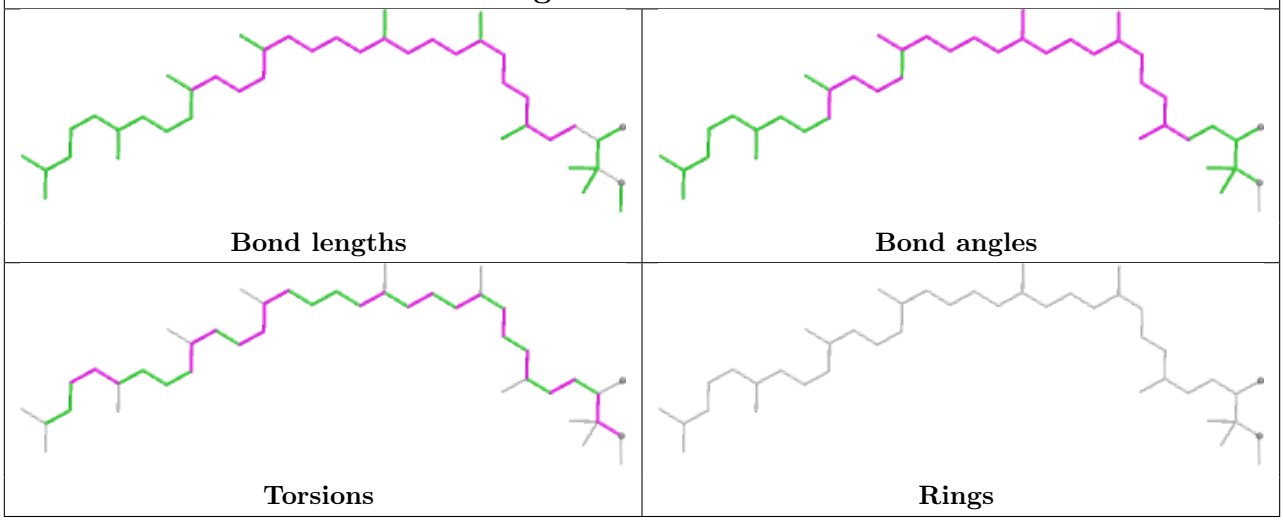
Ligand SPN 3 102



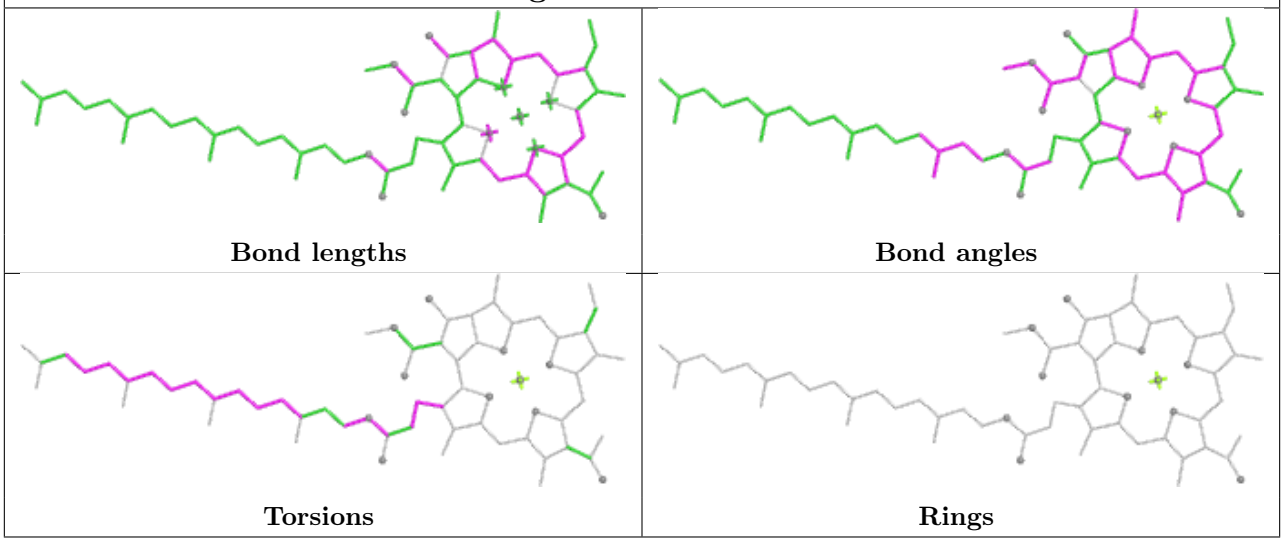
Ligand BCL h 101



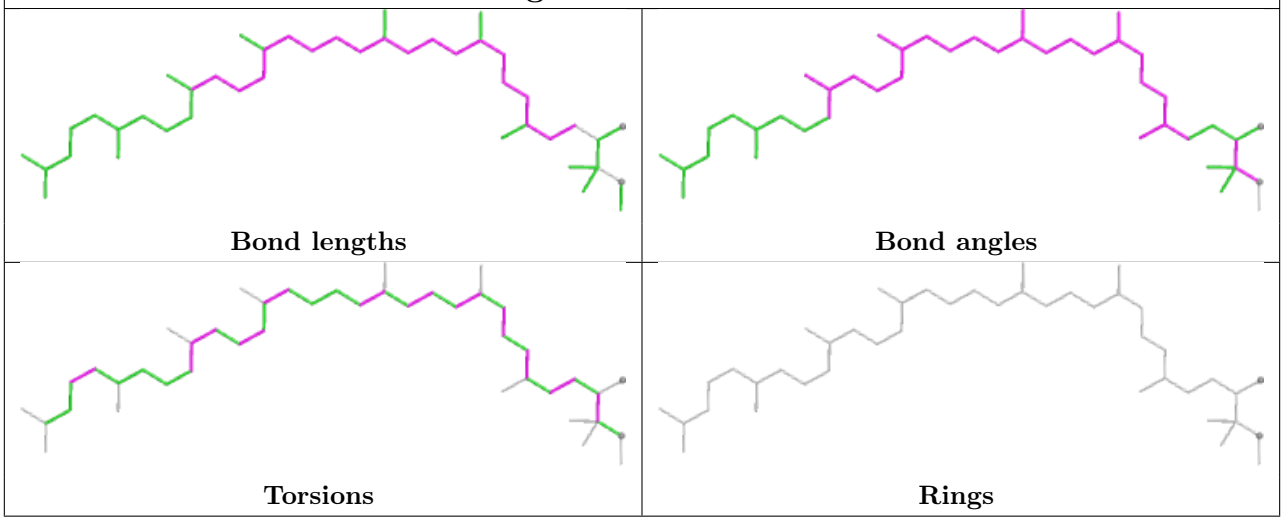
Ligand SPN f 102



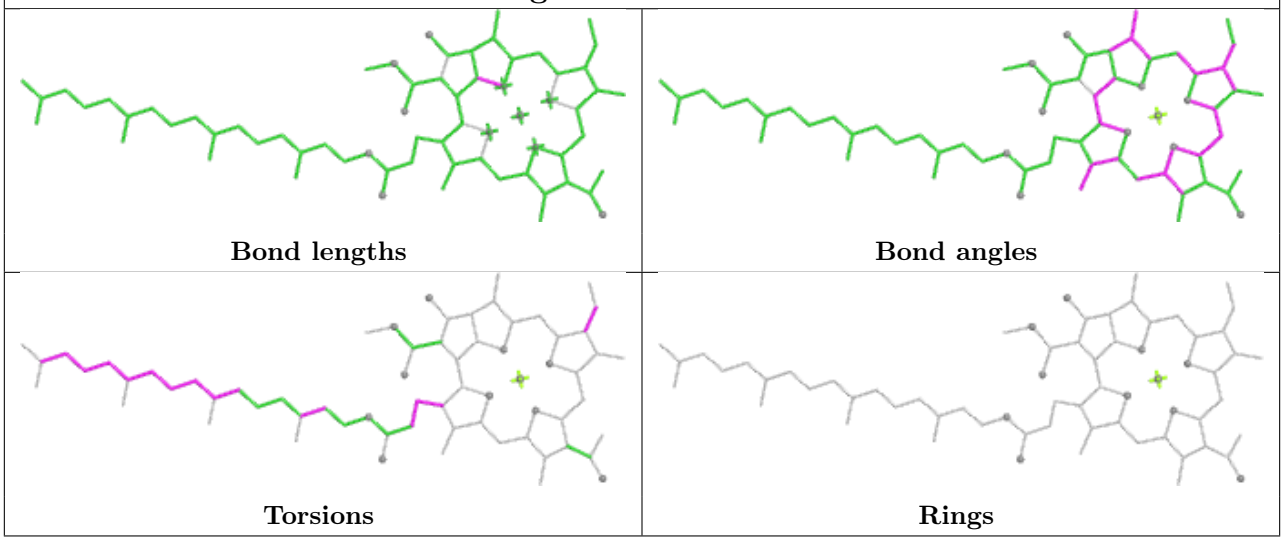
Ligand BCL b 101



Ligand SPN w 102



Ligand BCL 7 101



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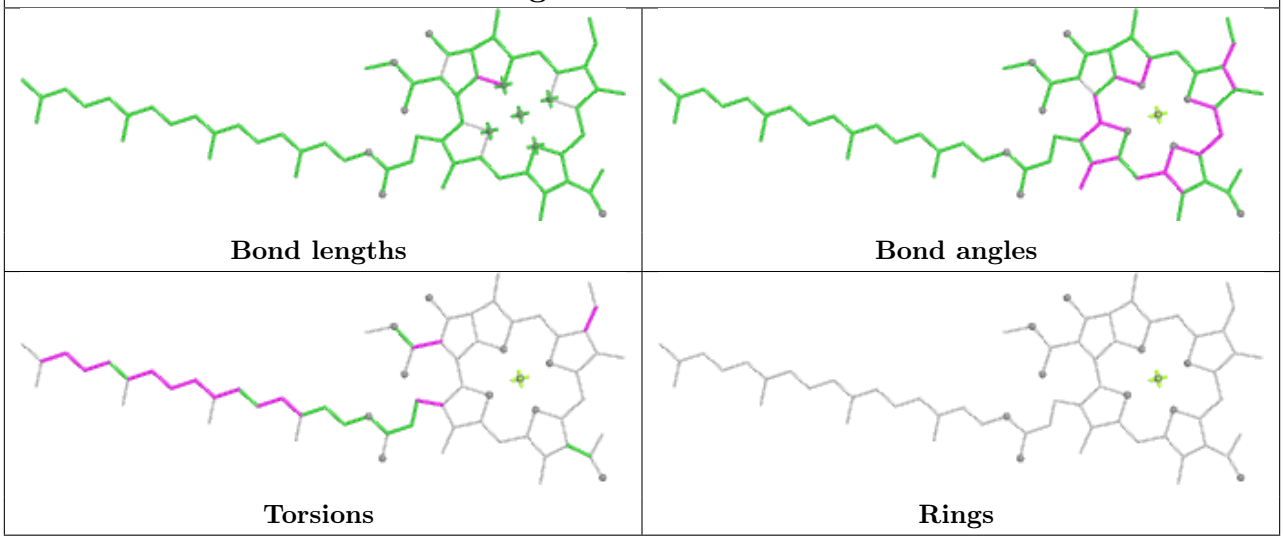
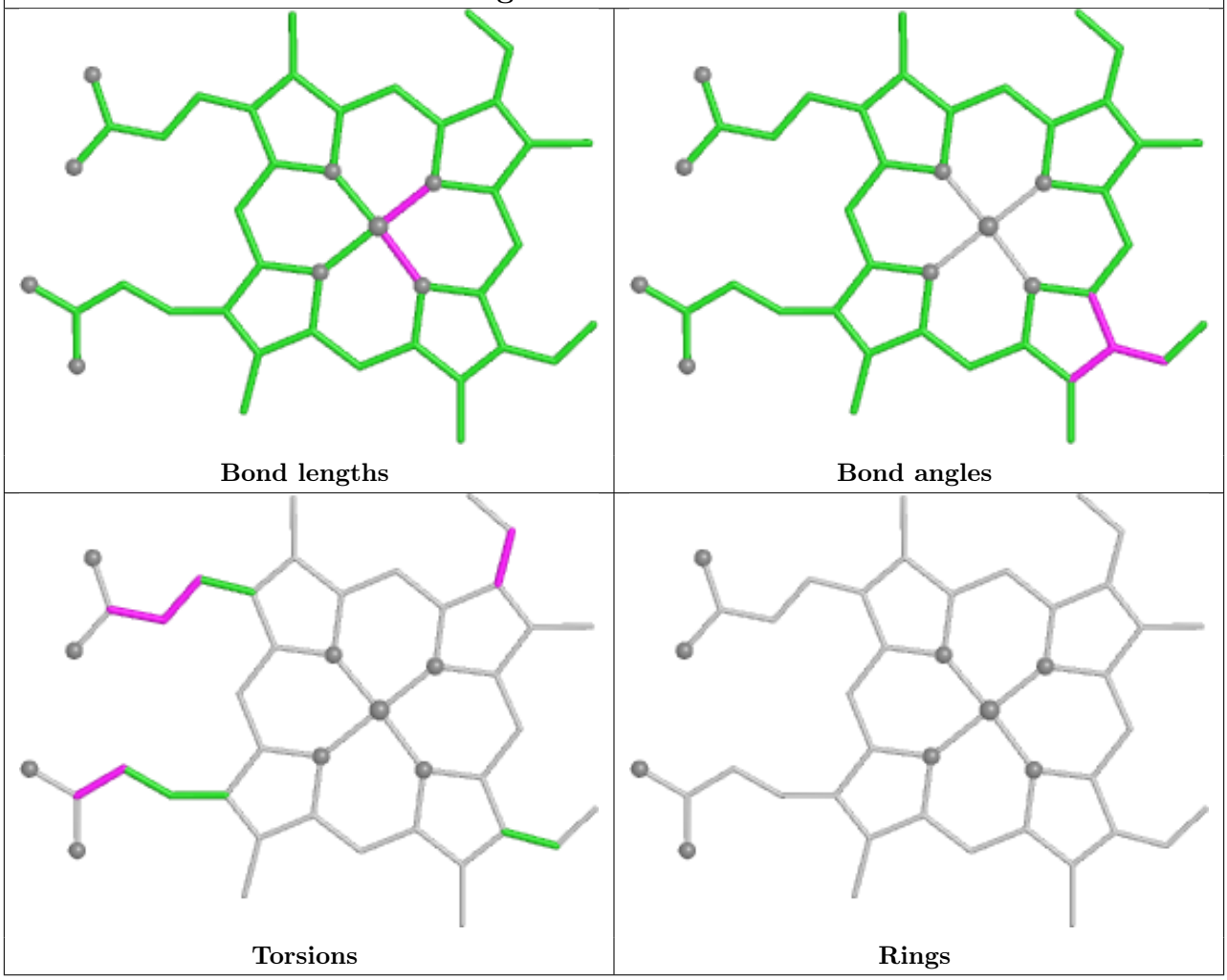
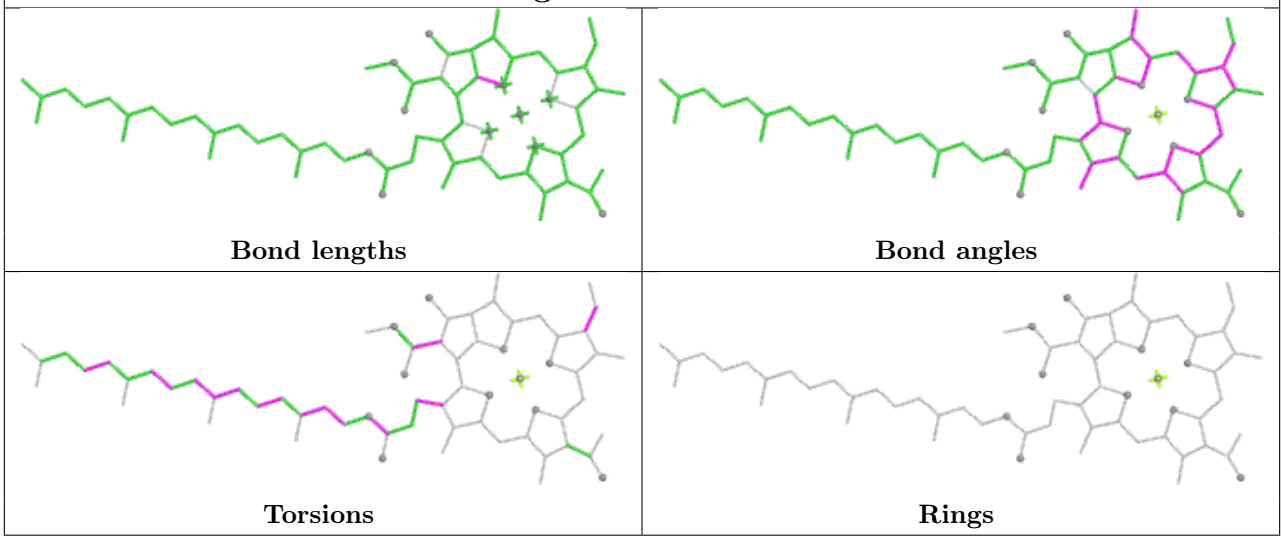


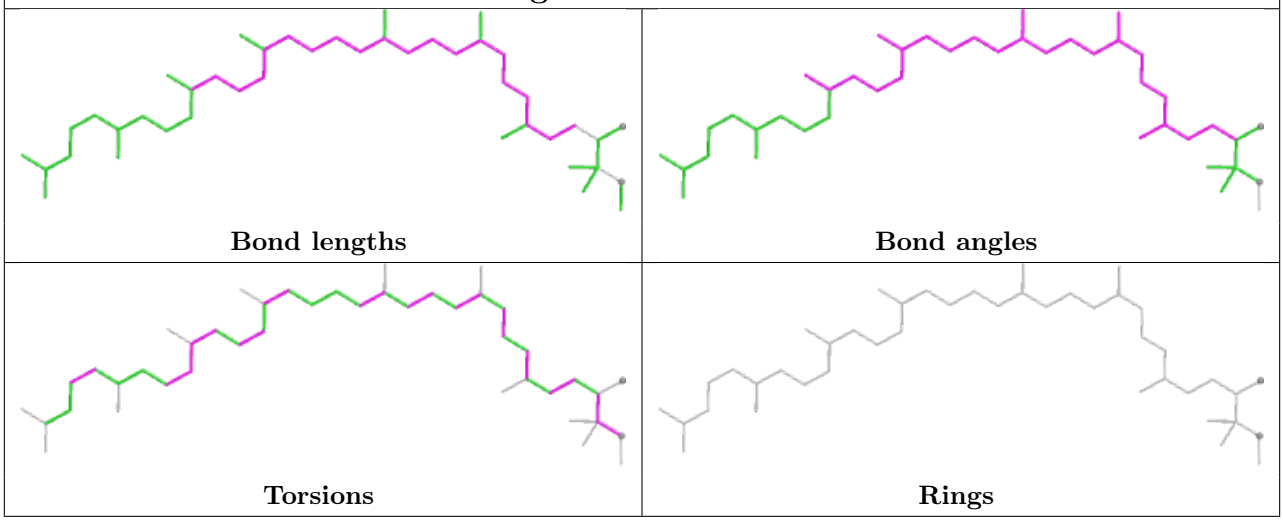
Ligand HEM C 401



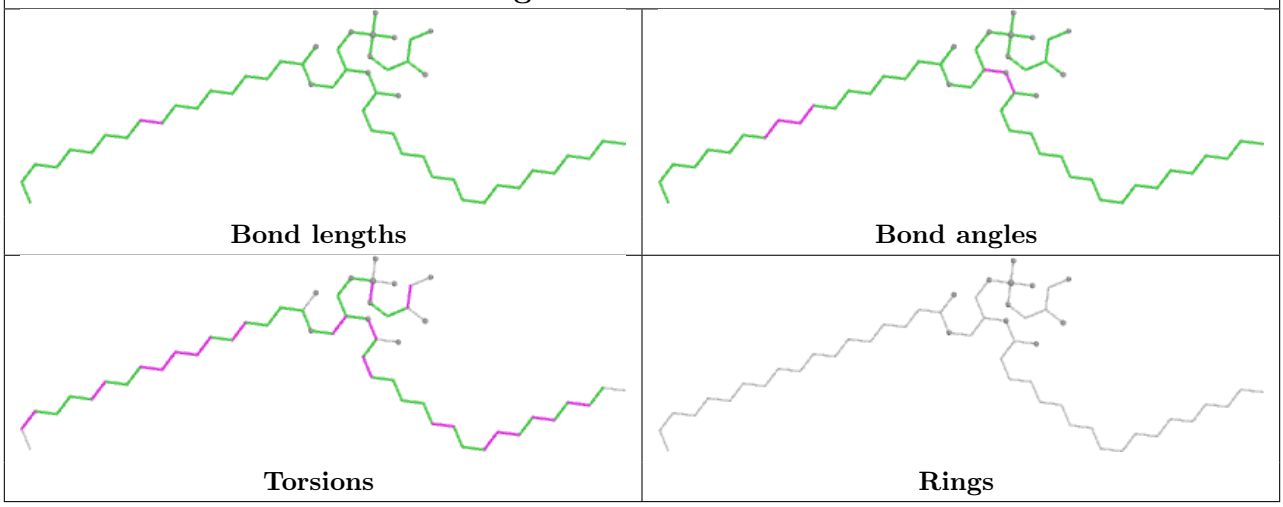
Ligand BCL f 101



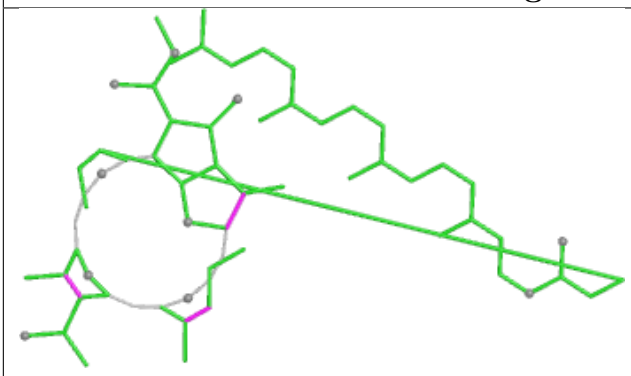
Ligand SPN 5 102



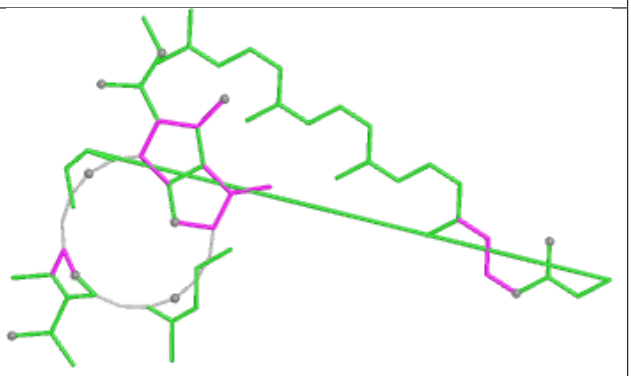
Ligand MW9 M 407



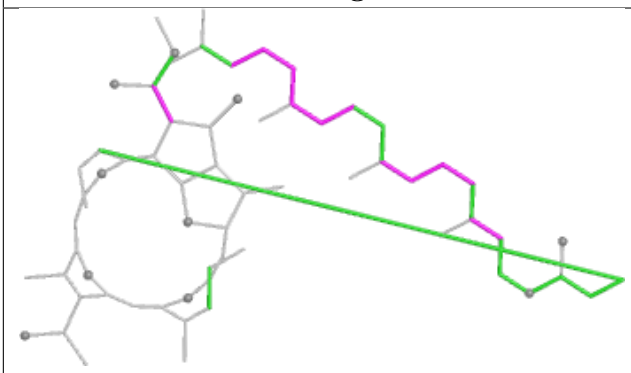
Ligand BPH L 303



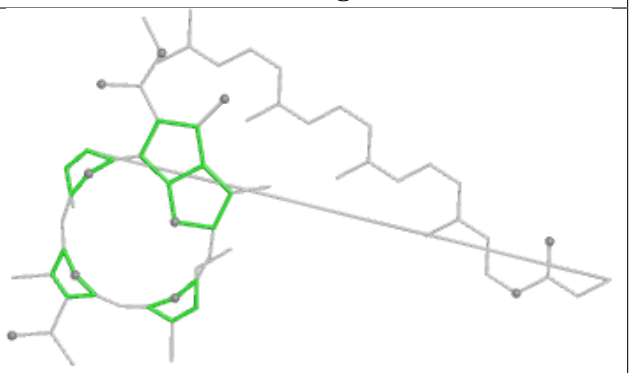
Bond lengths



Bond angles

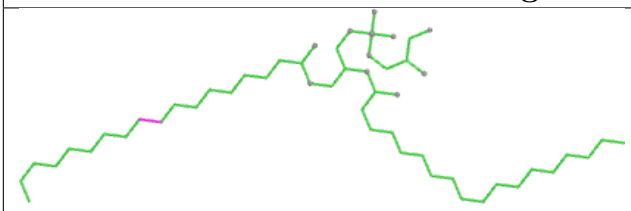


Torsions

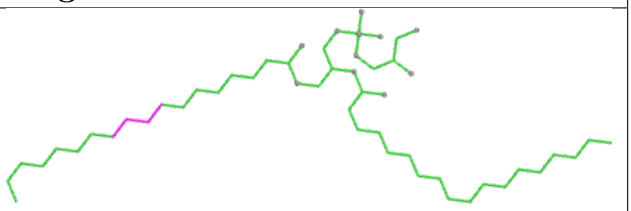


Rings

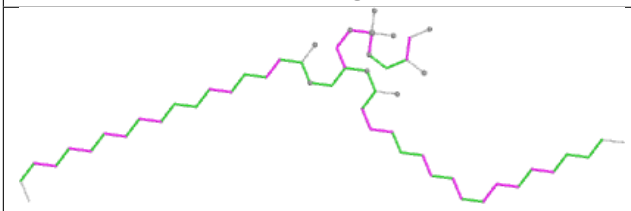
Ligand MW9 g 102



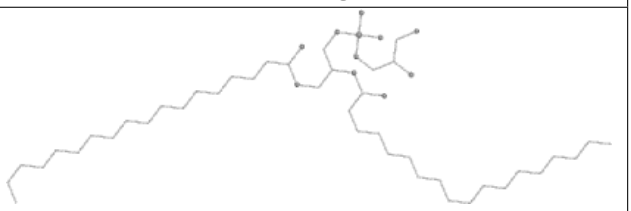
Bond lengths



Bond angles

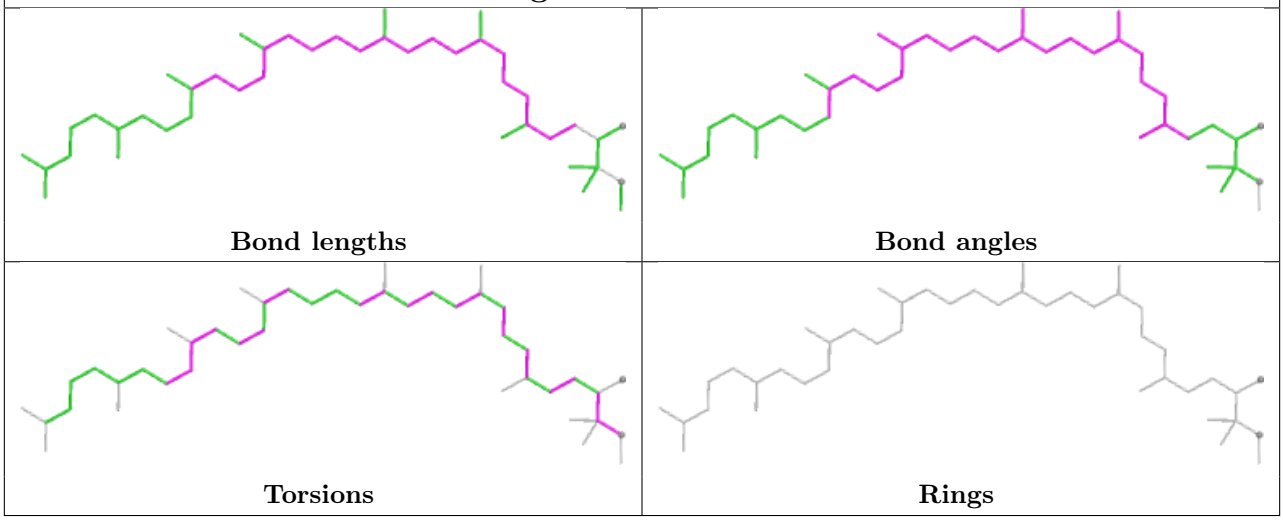


Torsions

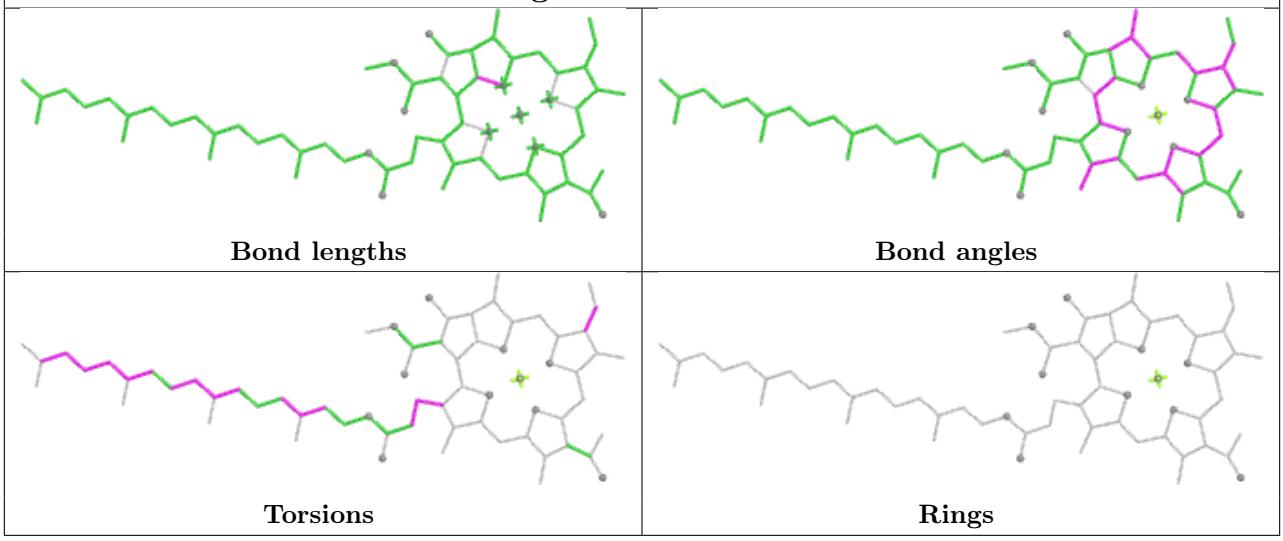


Rings

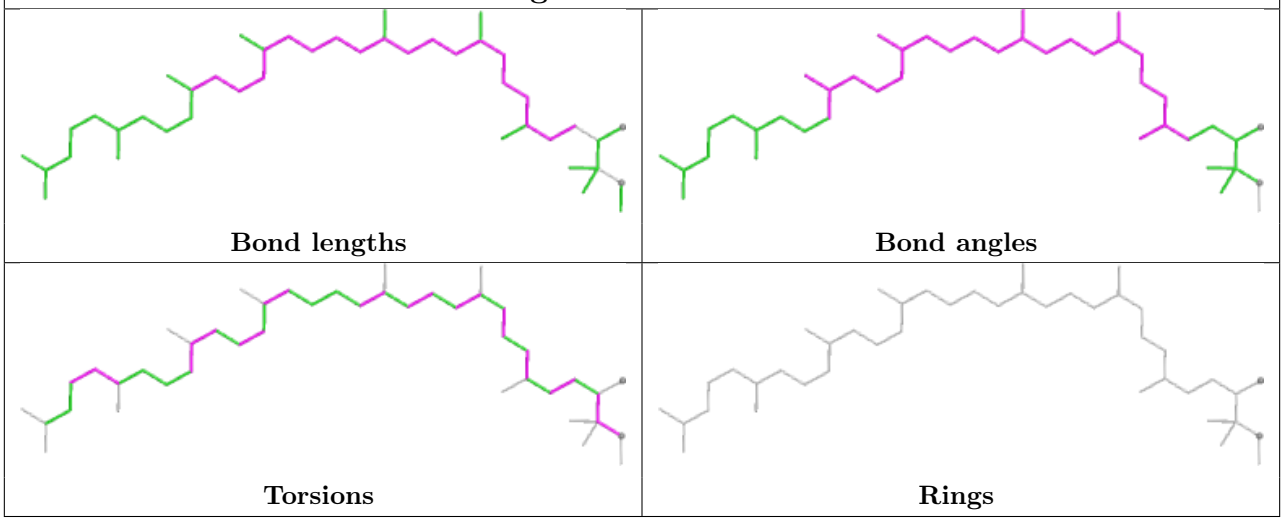
Ligand SPN 0 102



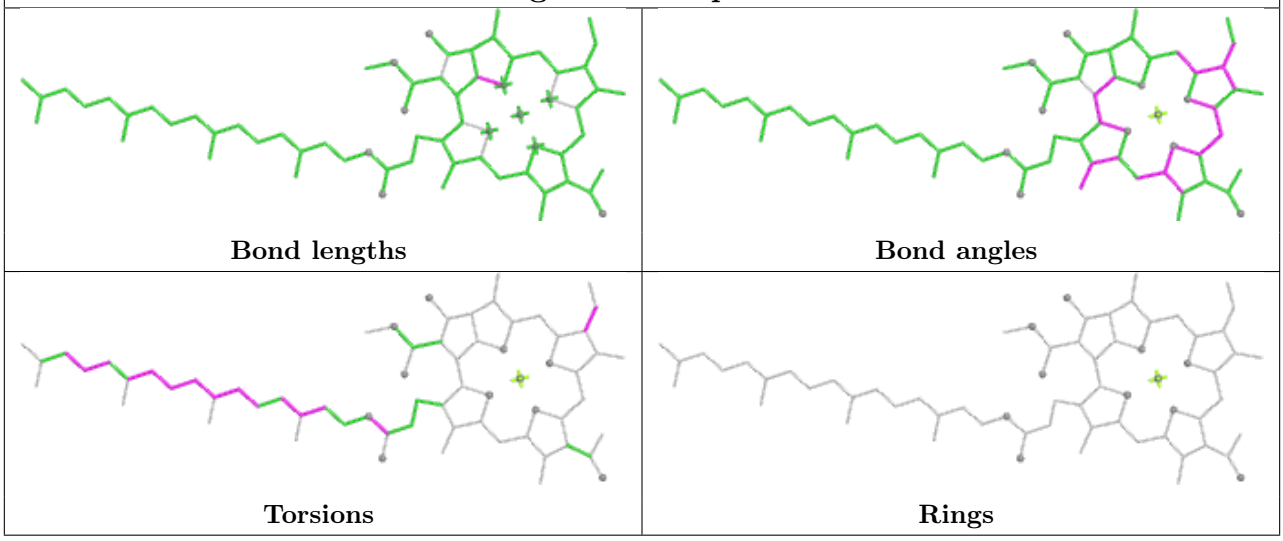
Ligand BCL c 101



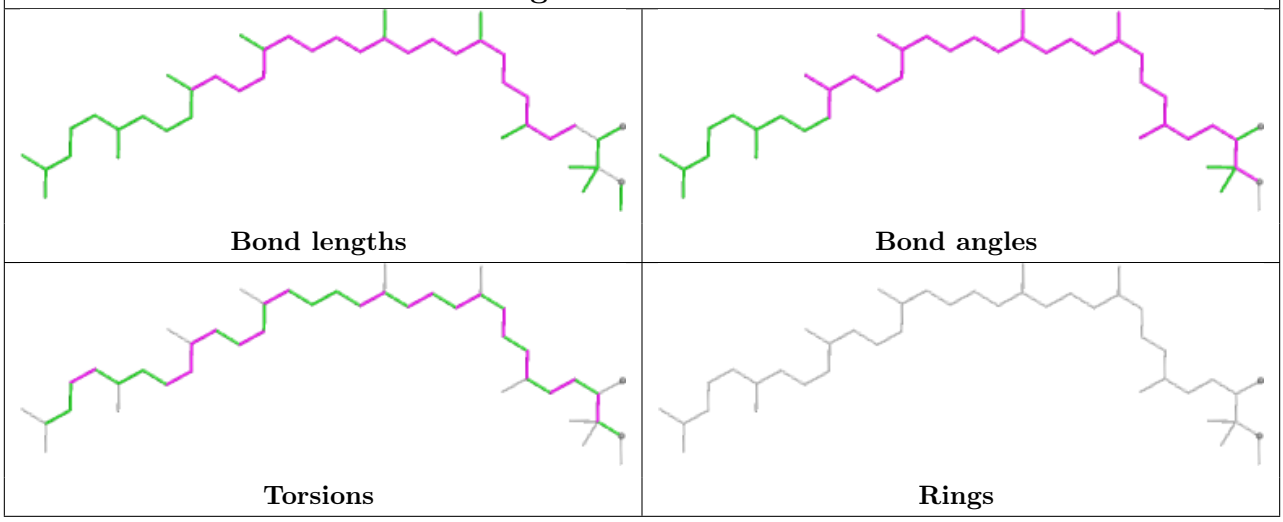
Ligand SPN 1 105



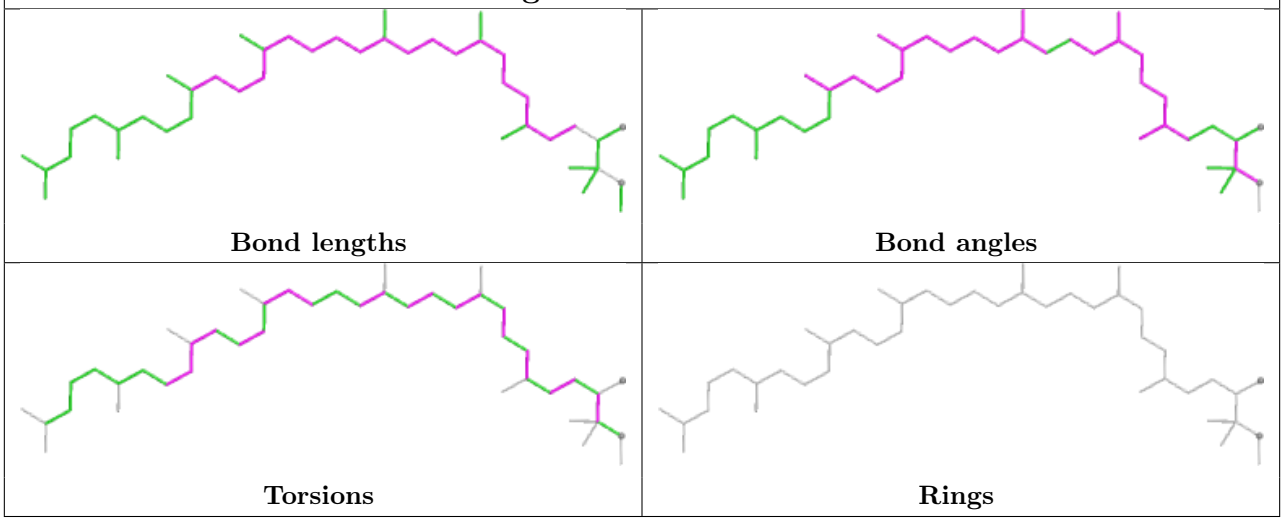
Ligand BCL q 101



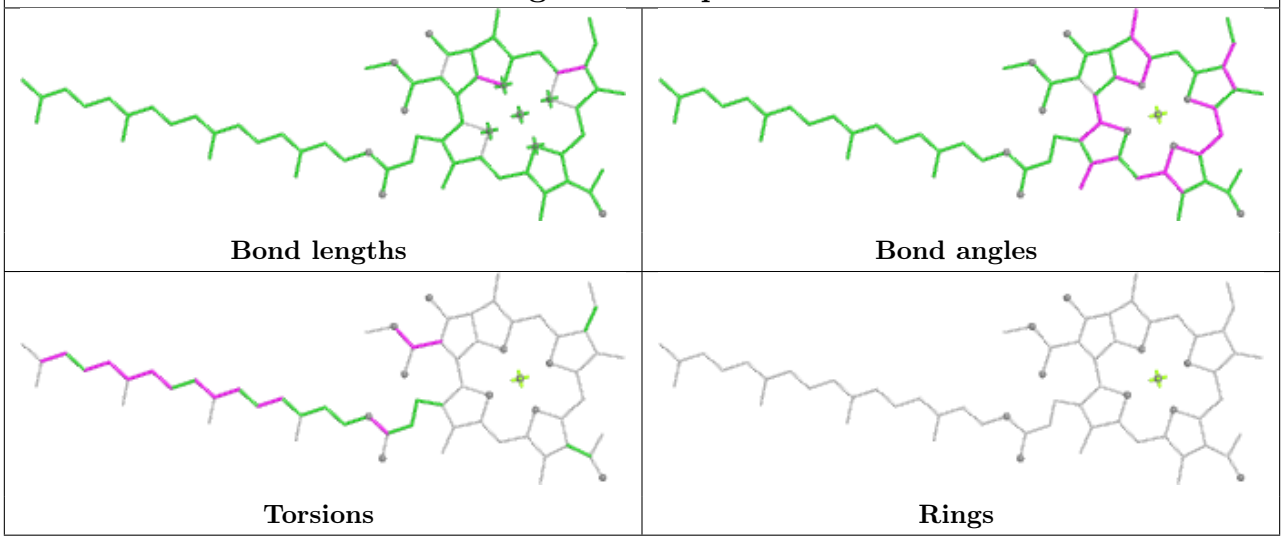
Ligand SPN 9 103



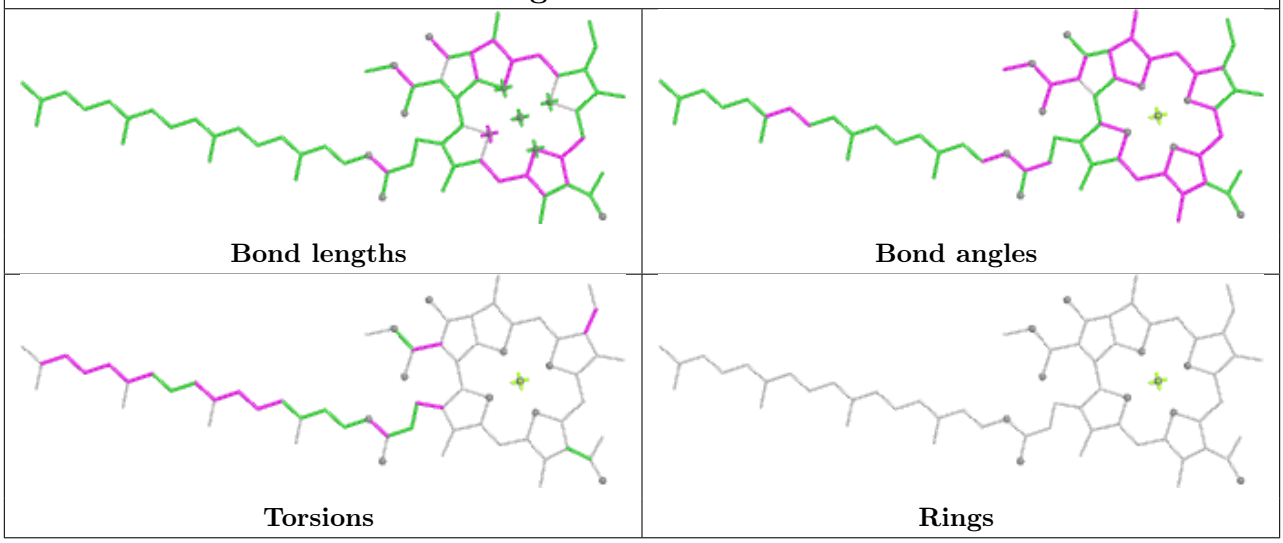
Ligand SPN M 406



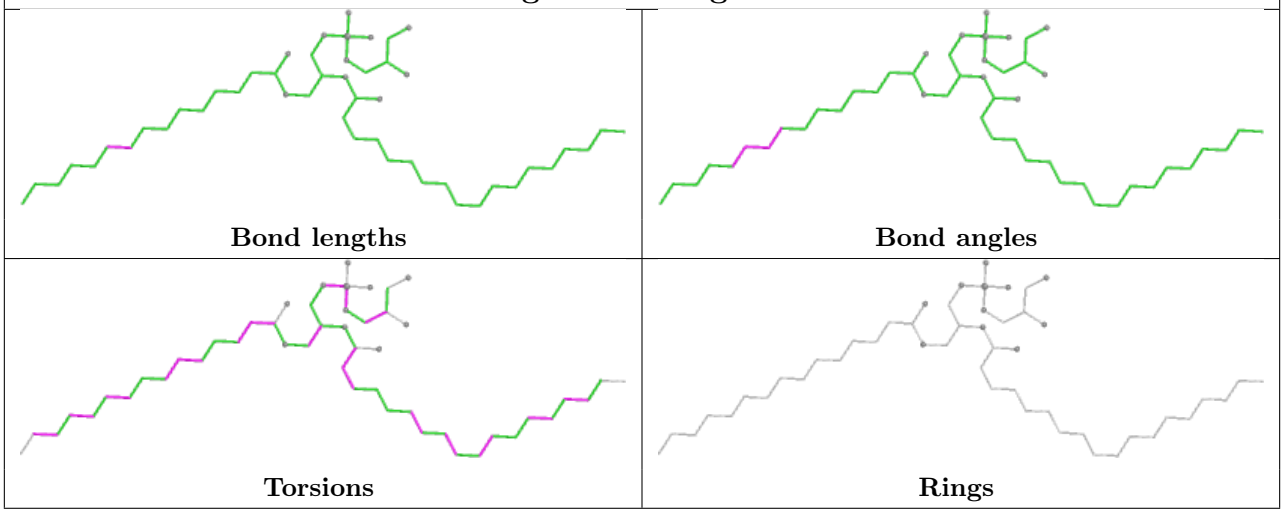
Ligand BCL p 101



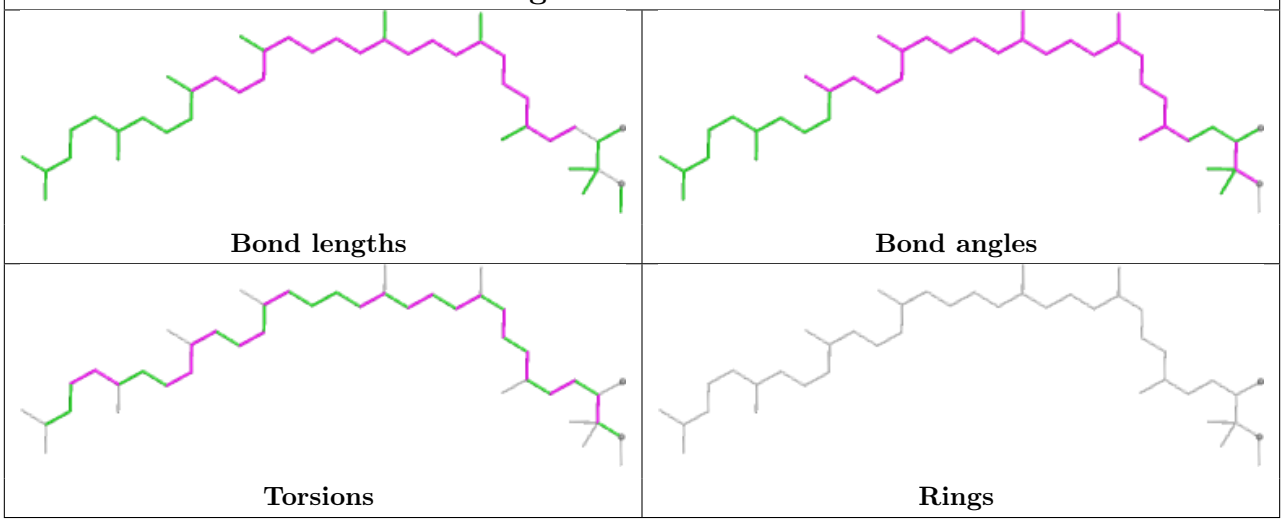
Ligand BCL 0 101



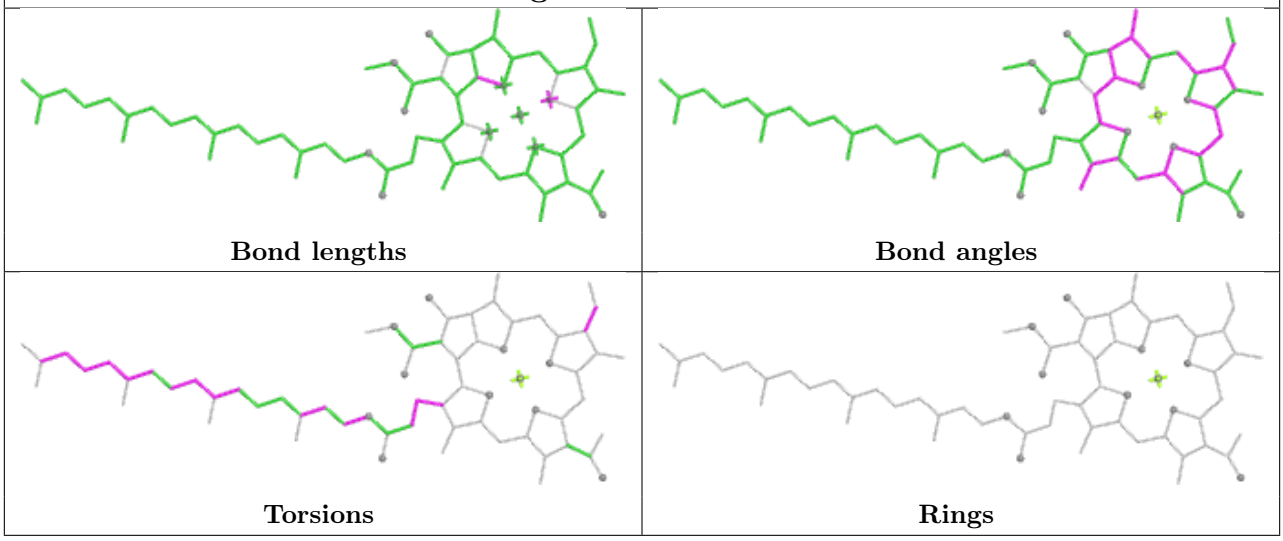
Ligand MW9 g 103



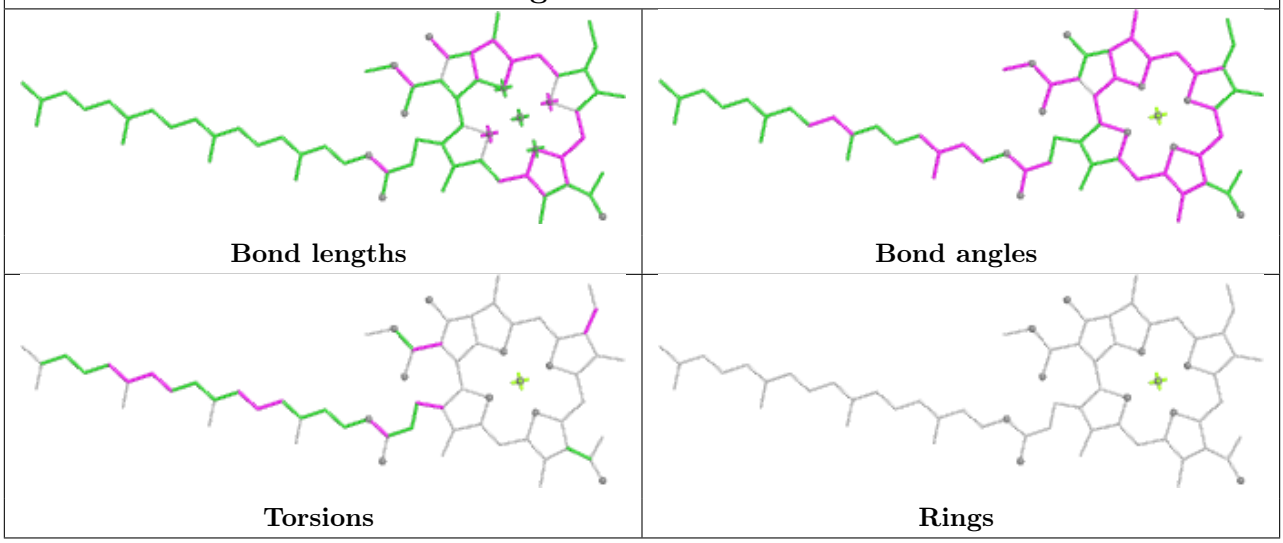
Ligand SPN n 102



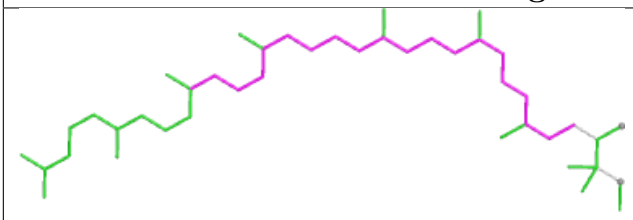
Ligand BCL a 101



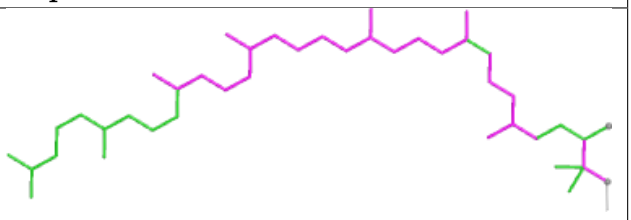
Ligand BCL 8 101



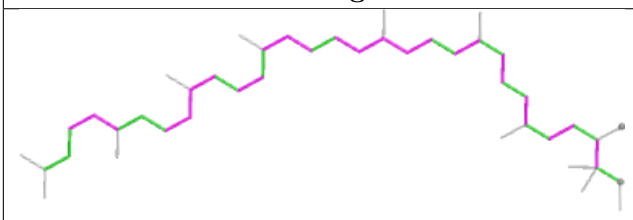
Ligand SPN p 102



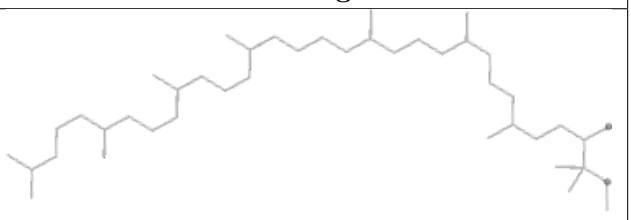
Bond lengths



Bond angles

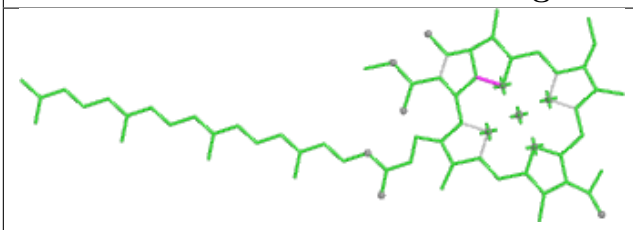


Torsions

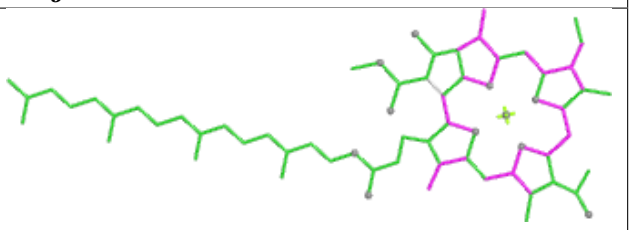


Rings

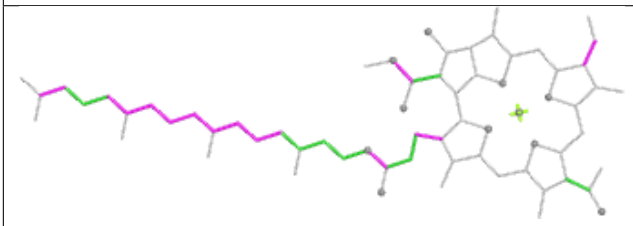
Ligand BCL j 101



Bond lengths



Bond angles



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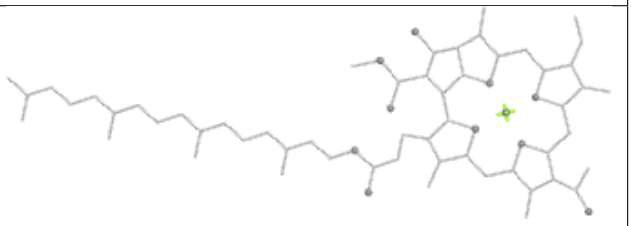
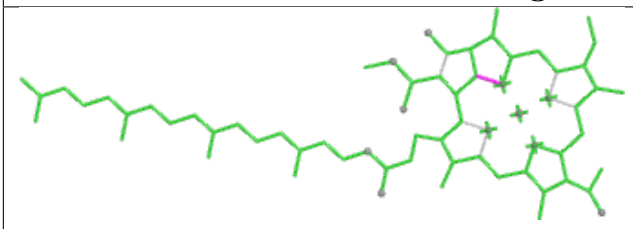
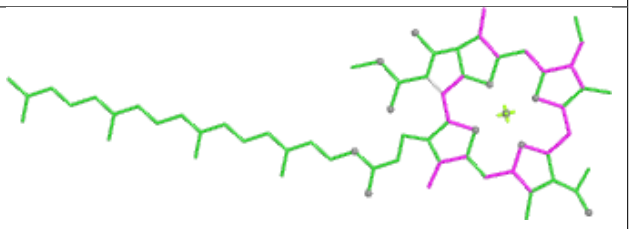


Rings

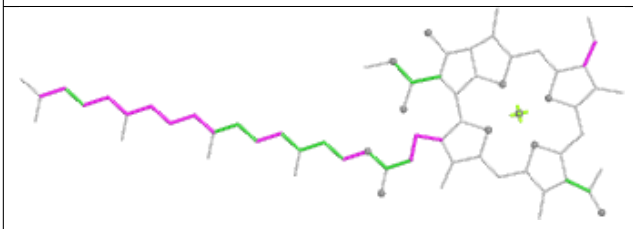
Ligand BCL 1 101



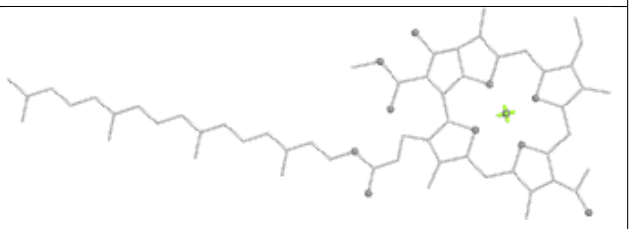
Bond lengths



Bond angles

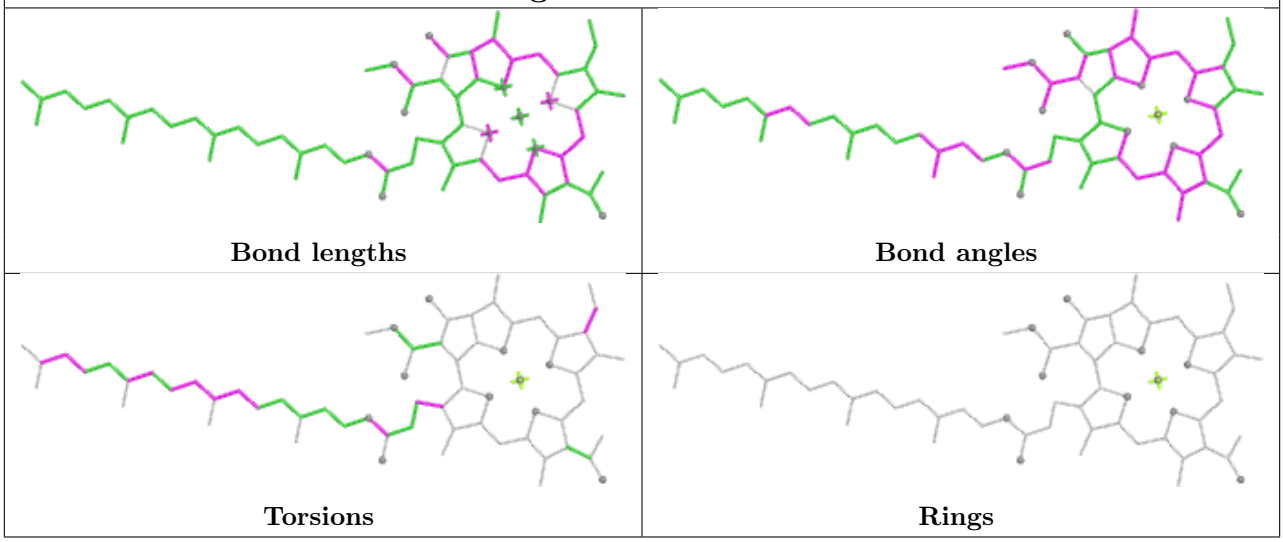


Torsions

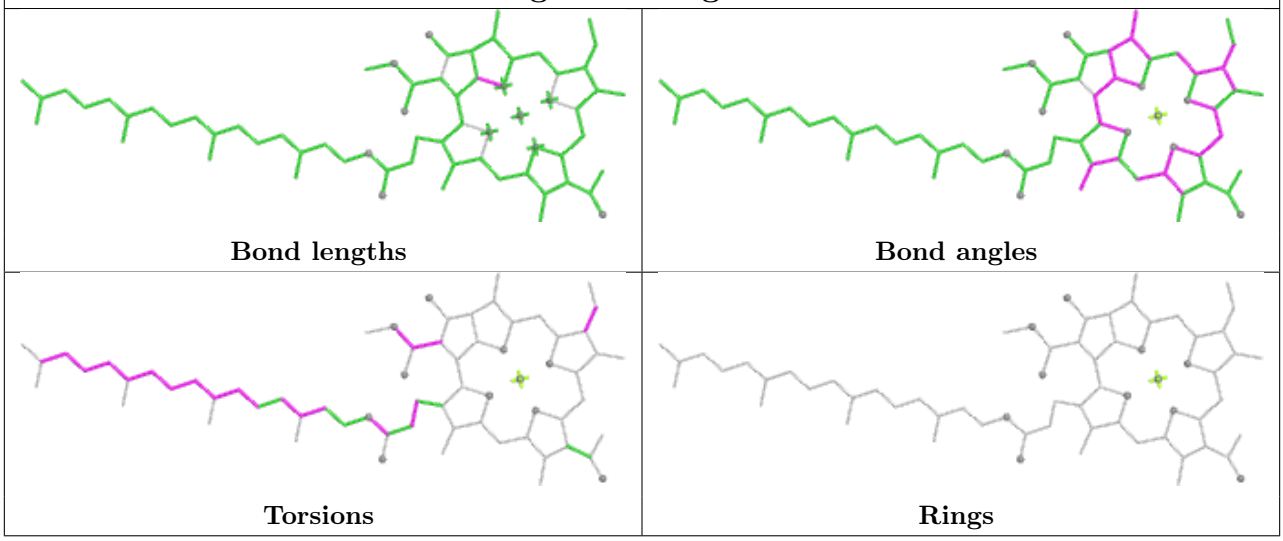


Rings

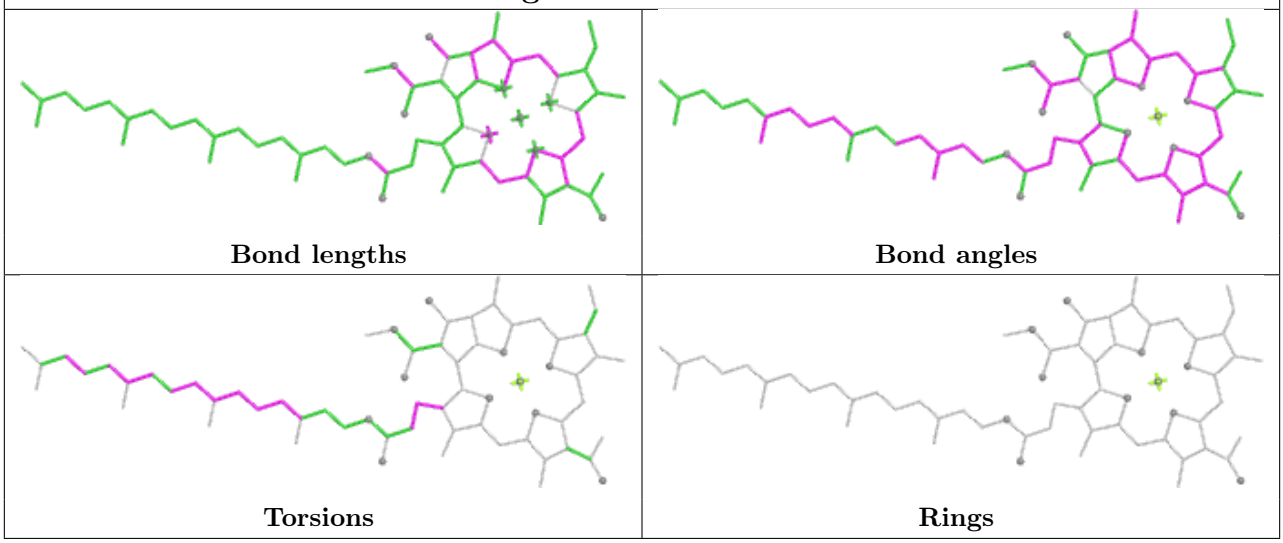
Ligand BCL 6 101

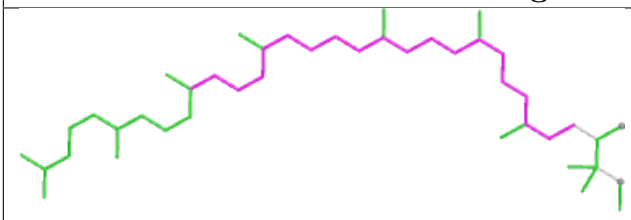
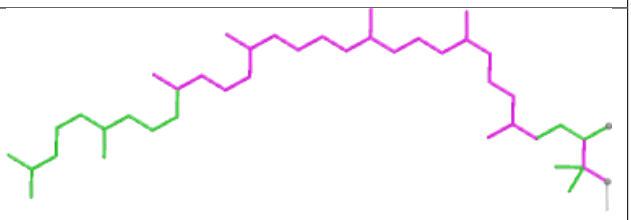
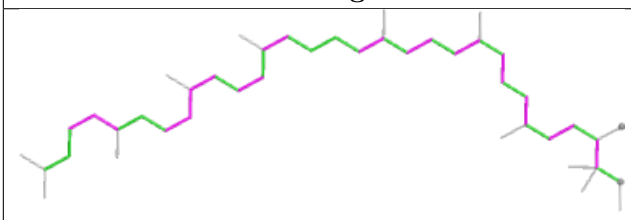
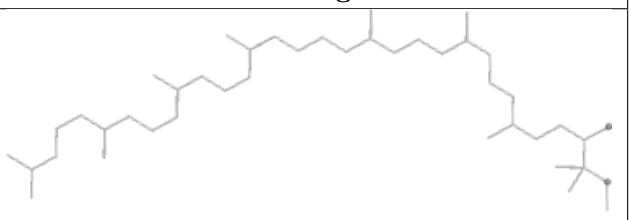


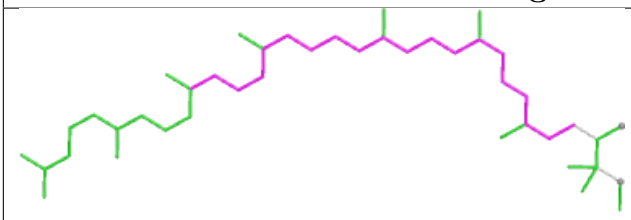
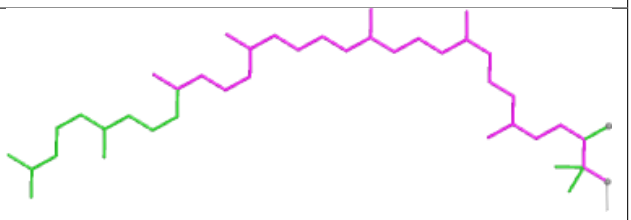
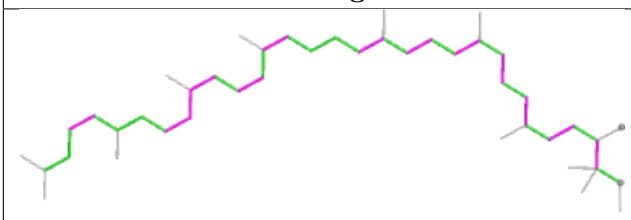
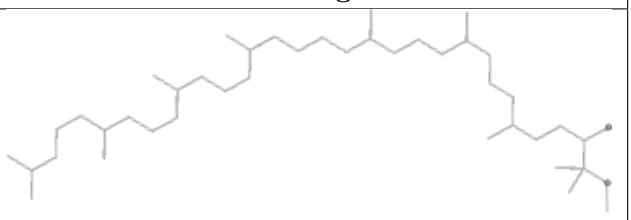
Ligand BCL g 101



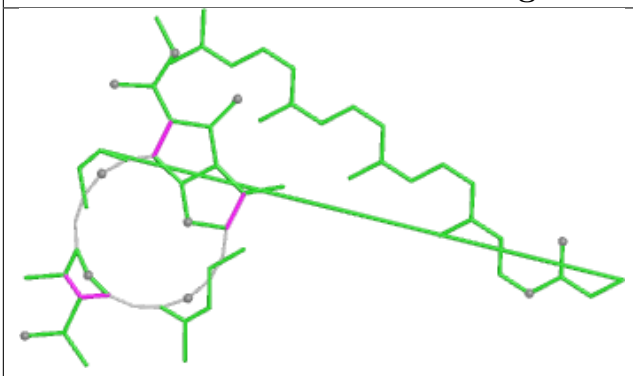
Ligand BCL M 402



Ligand SPN c 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPN 7 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH M 409



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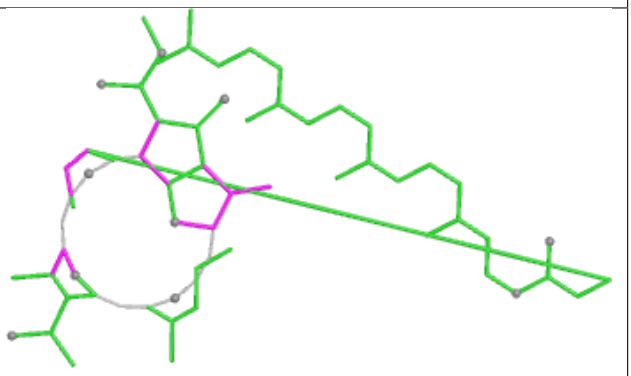

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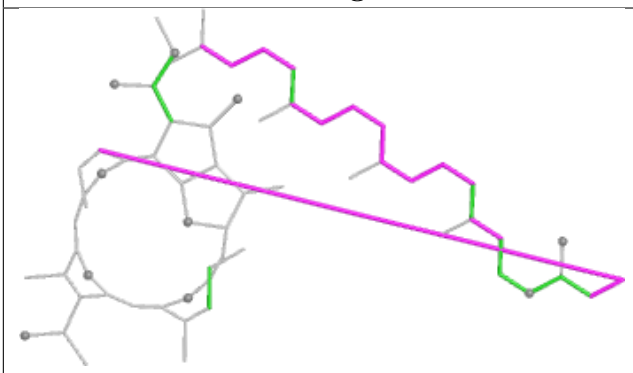
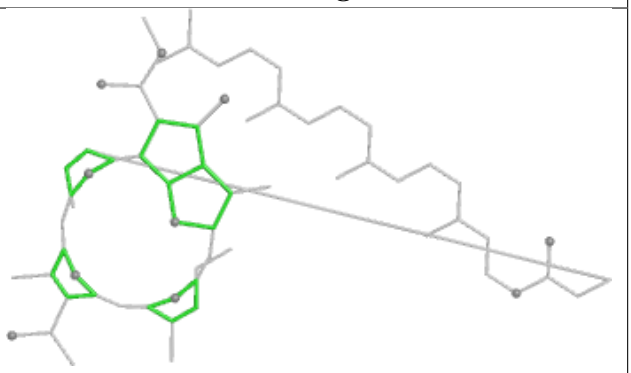
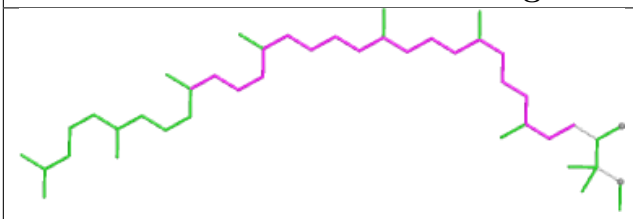


Torsions



Rings

Ligand SPN m 102



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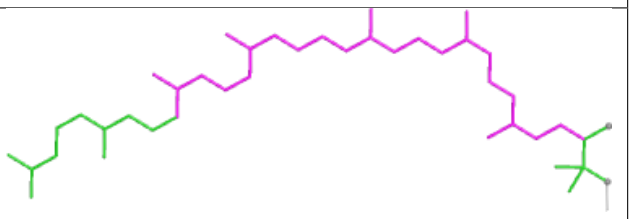

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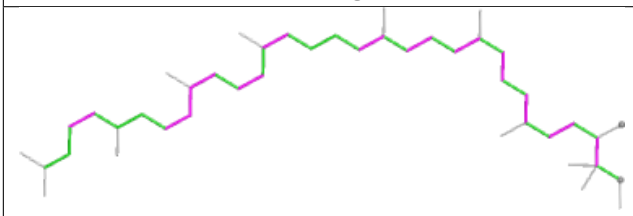

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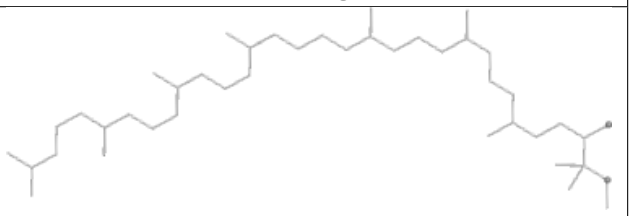
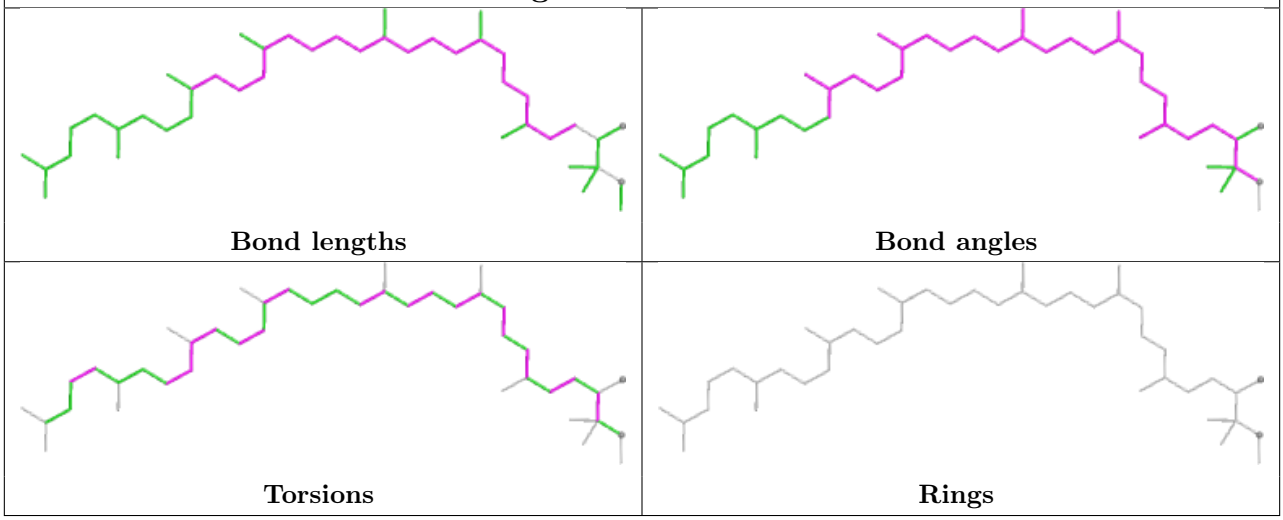
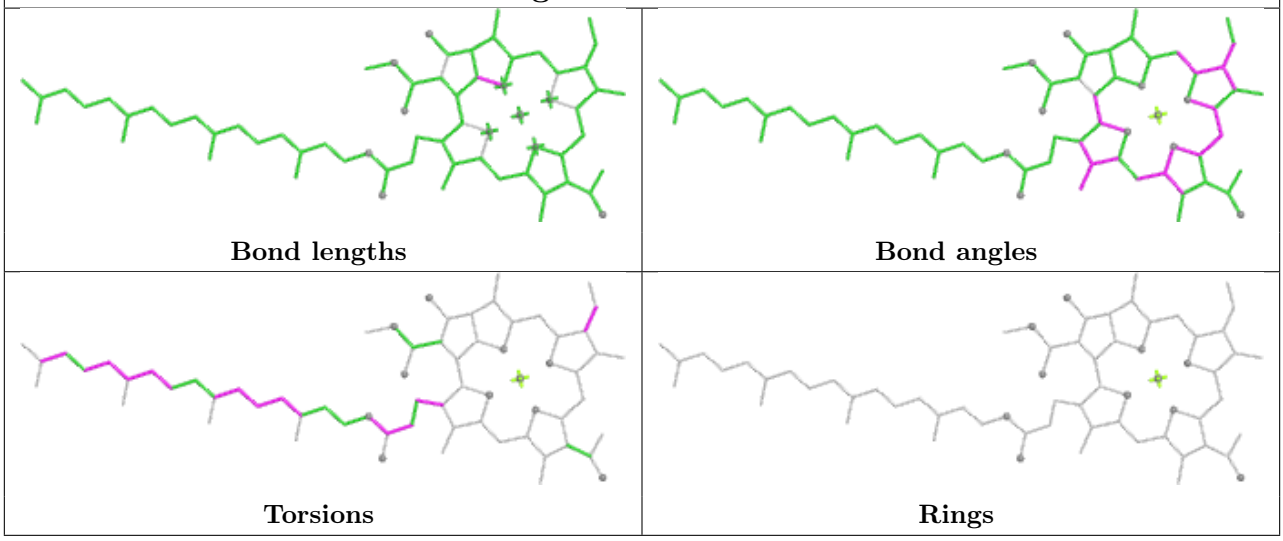


Rings

Ligand SPN c 102



Ligand BCL t 101



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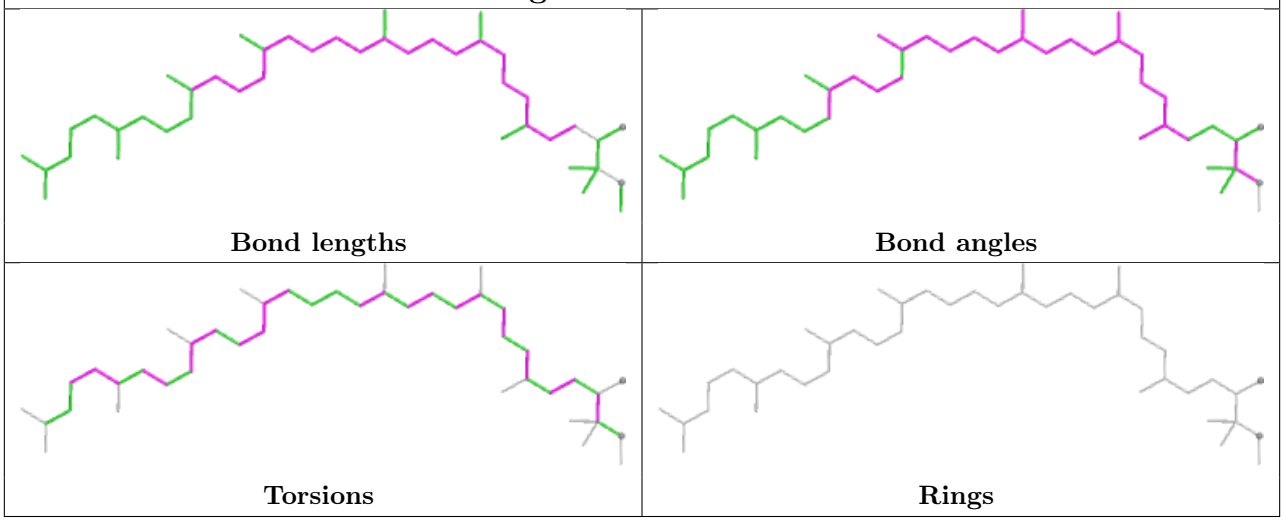
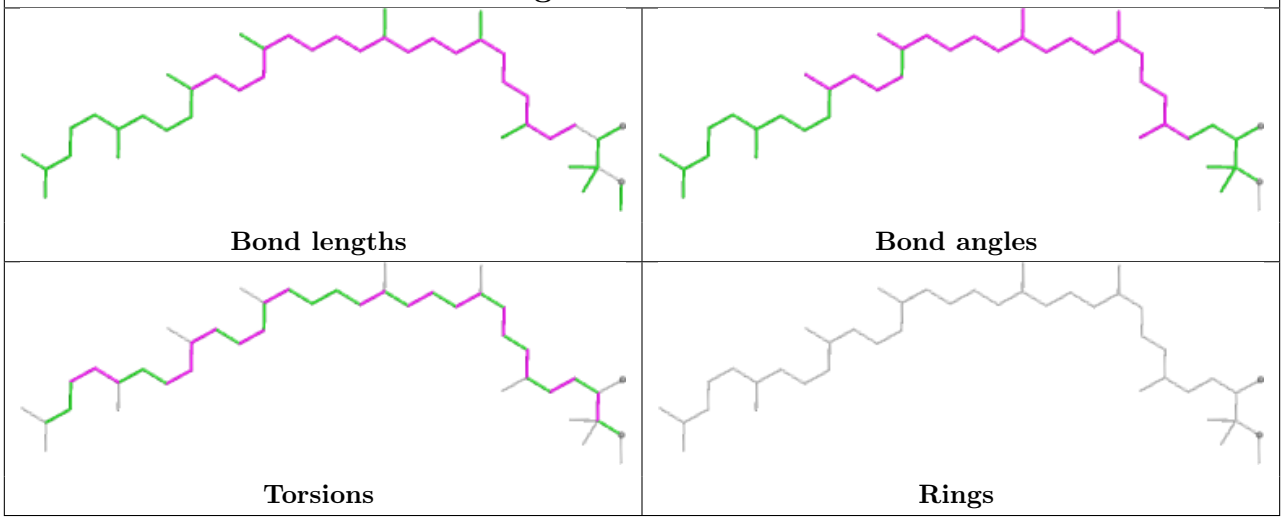


Ligand SPN l 102



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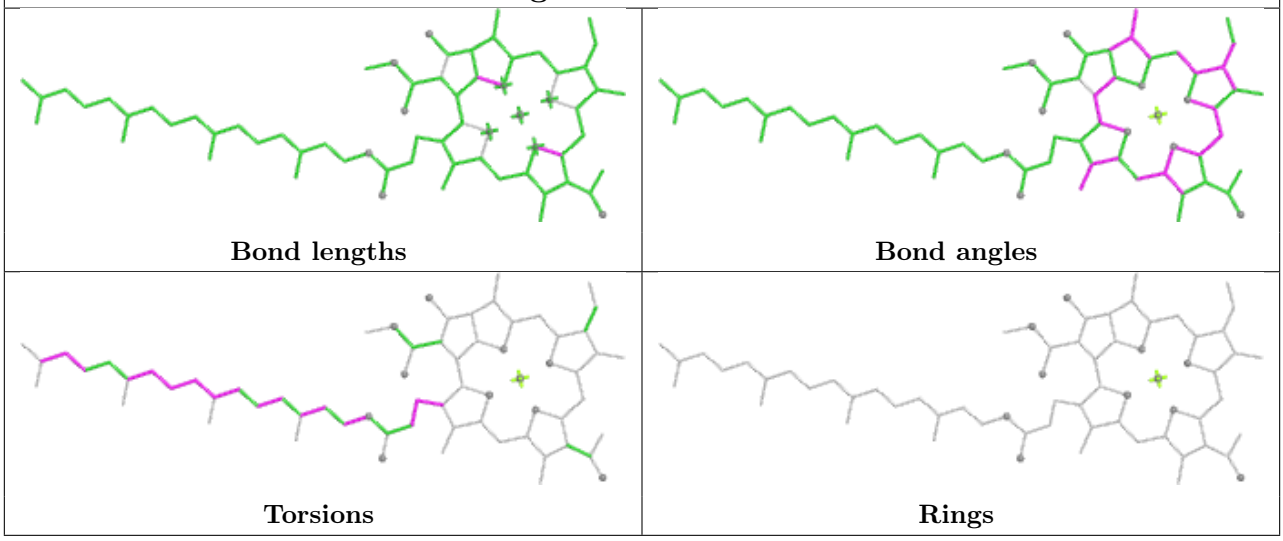

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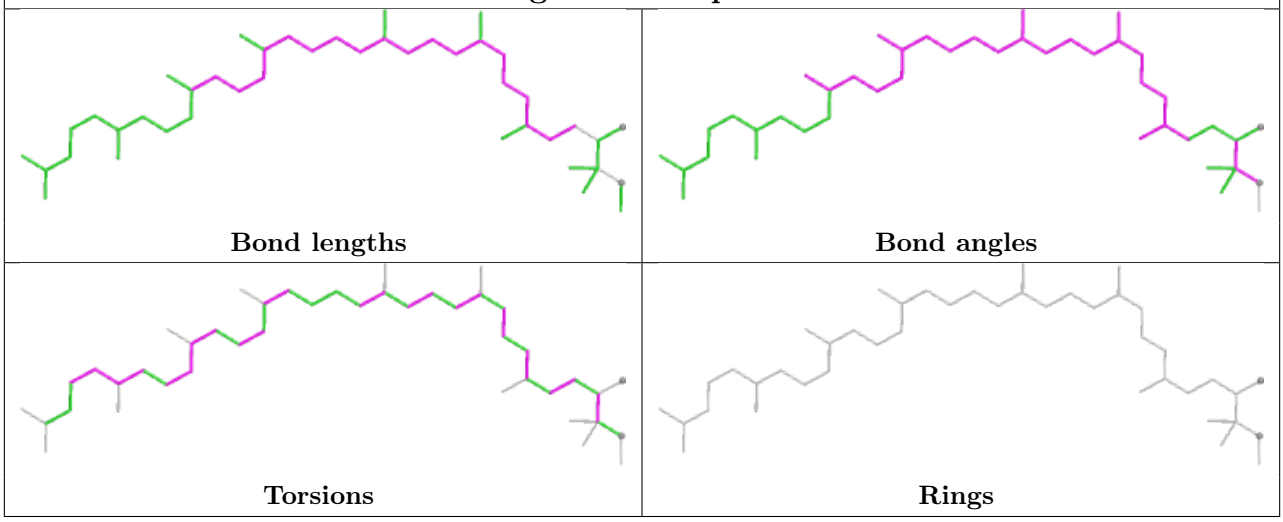

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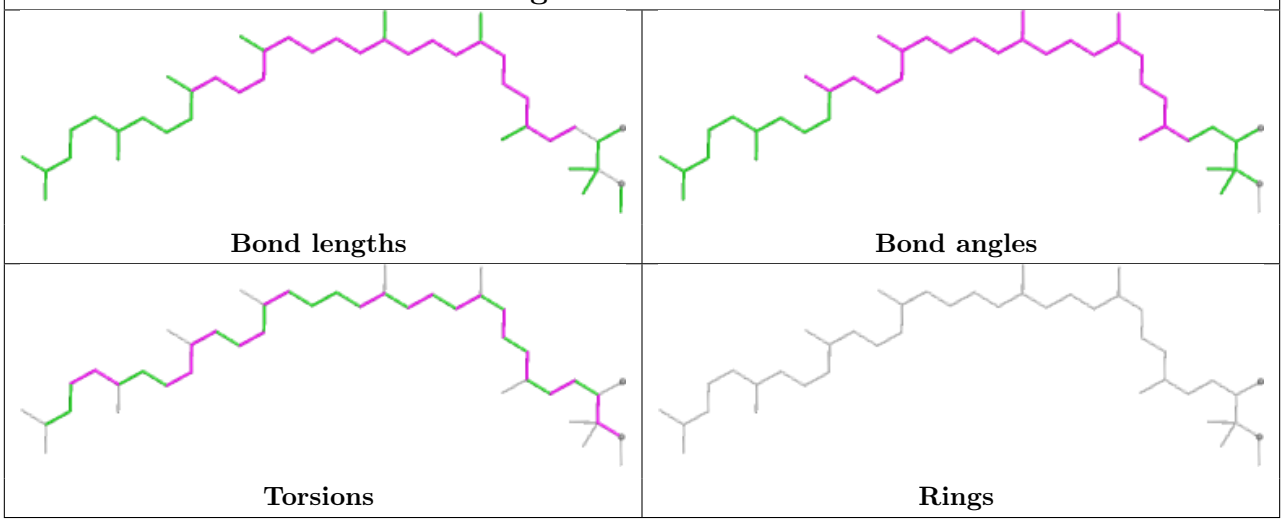

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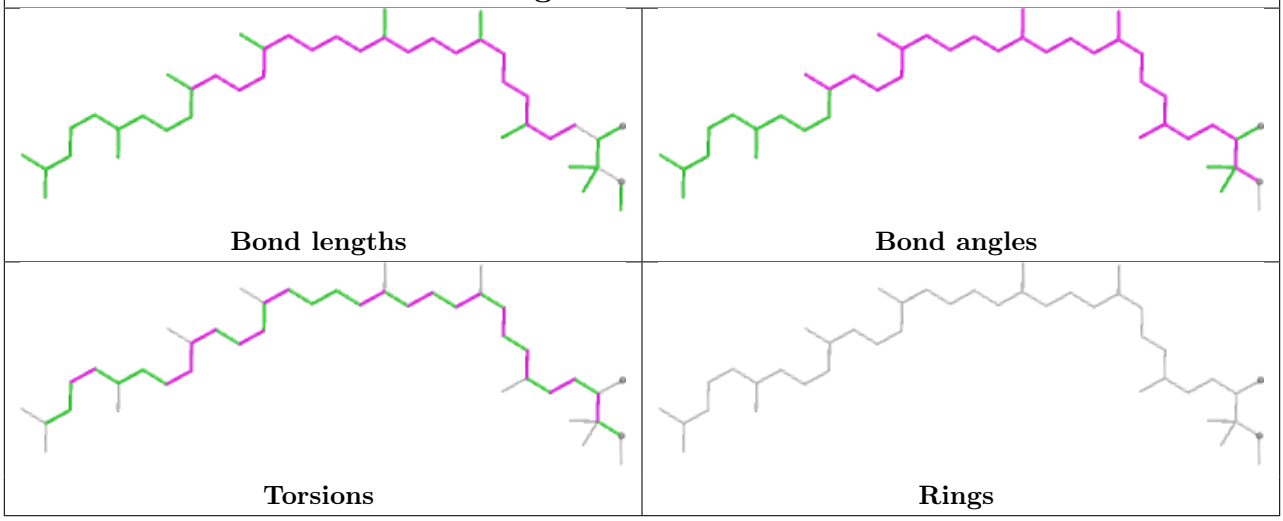

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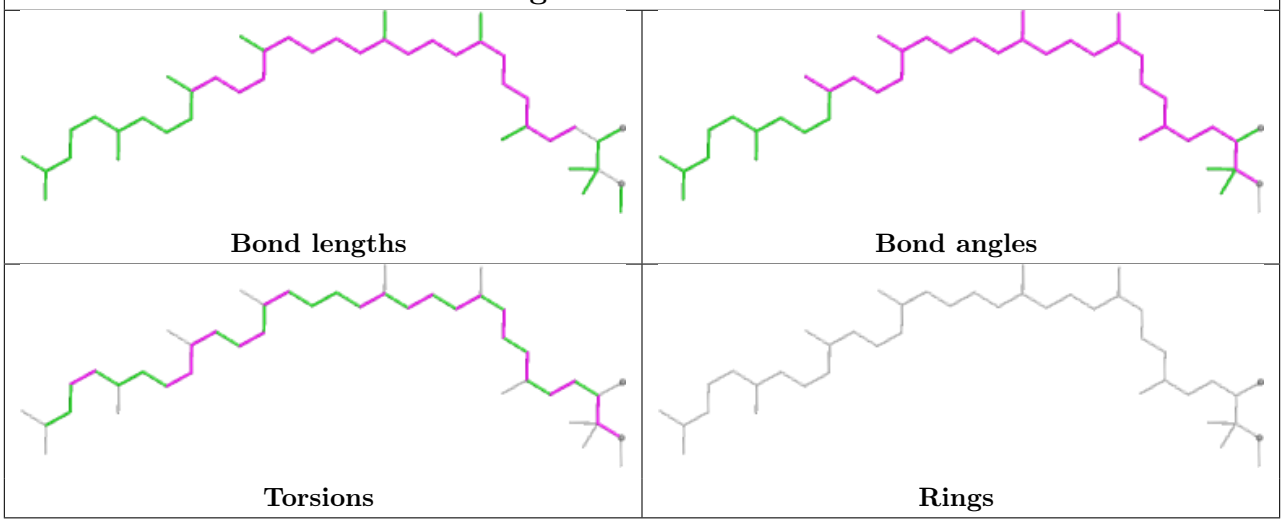

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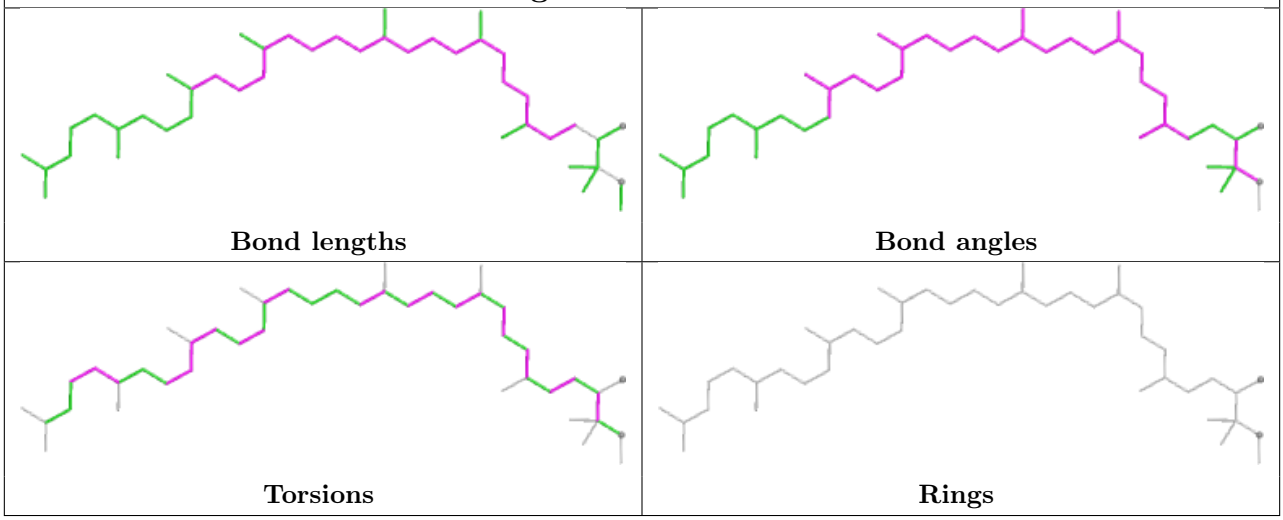

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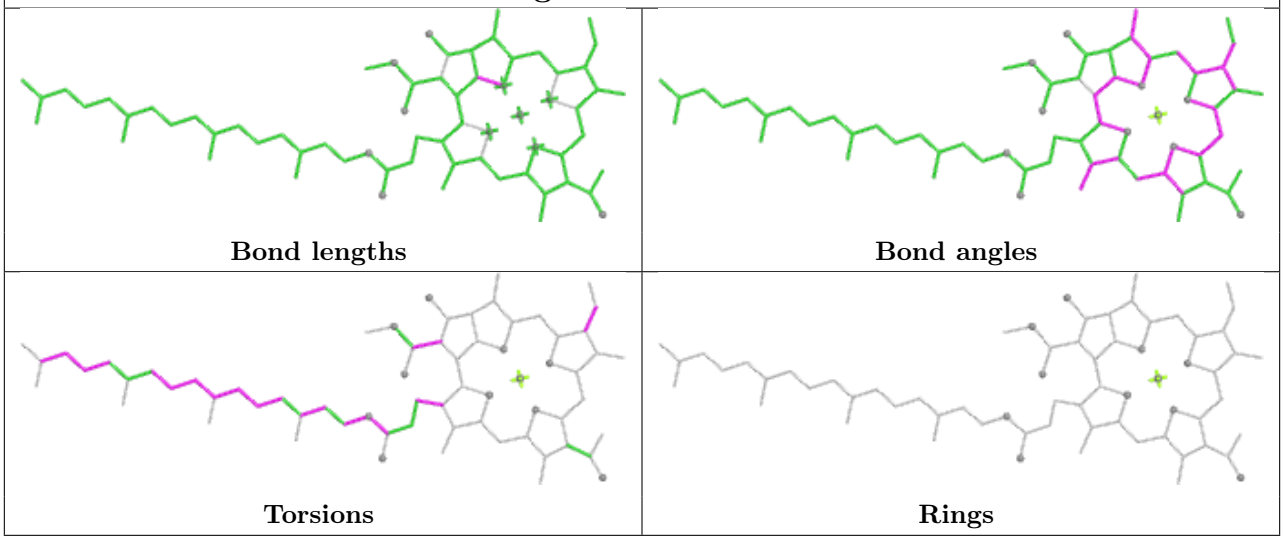

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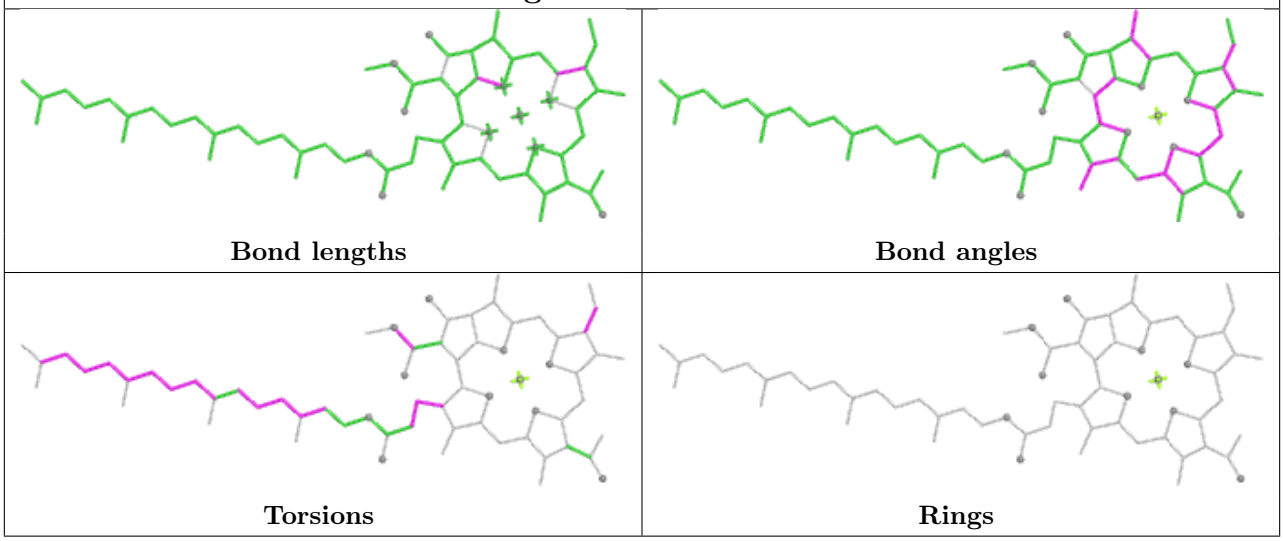
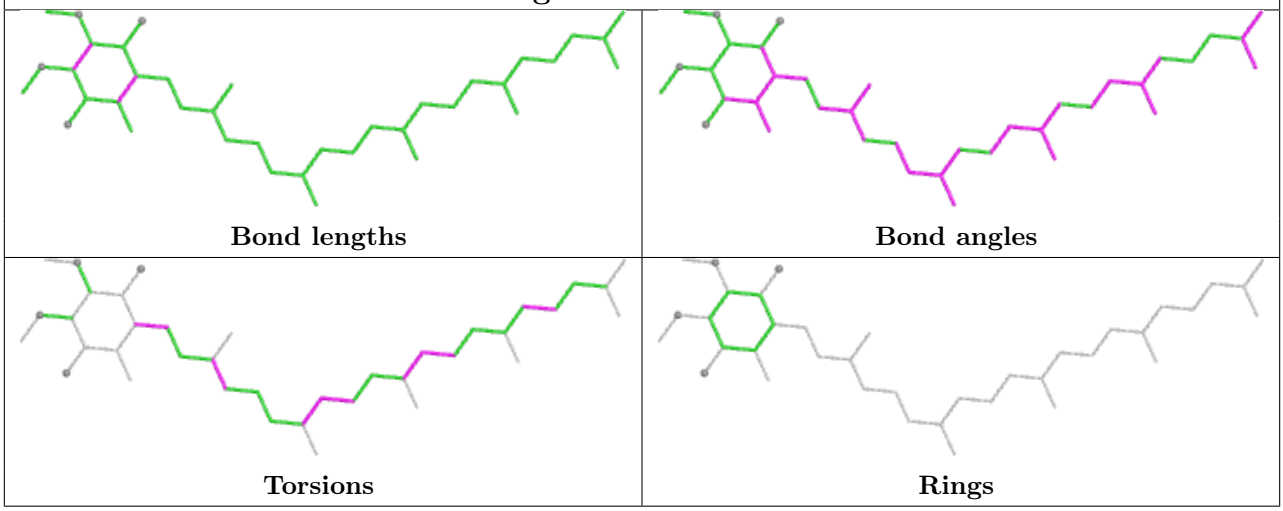


Ligand U10 L 305



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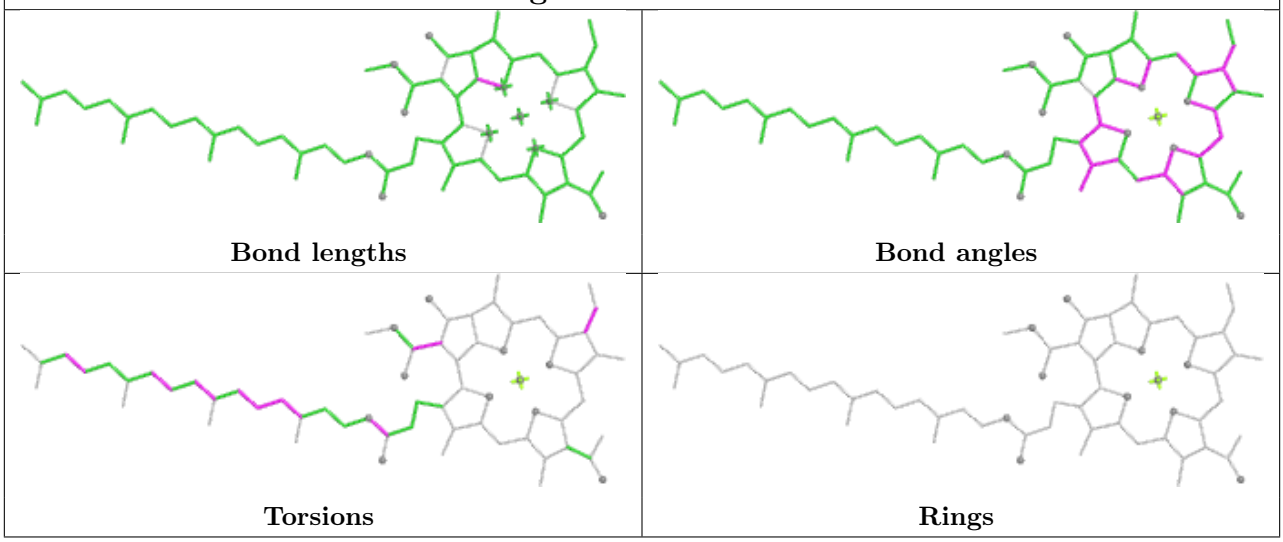

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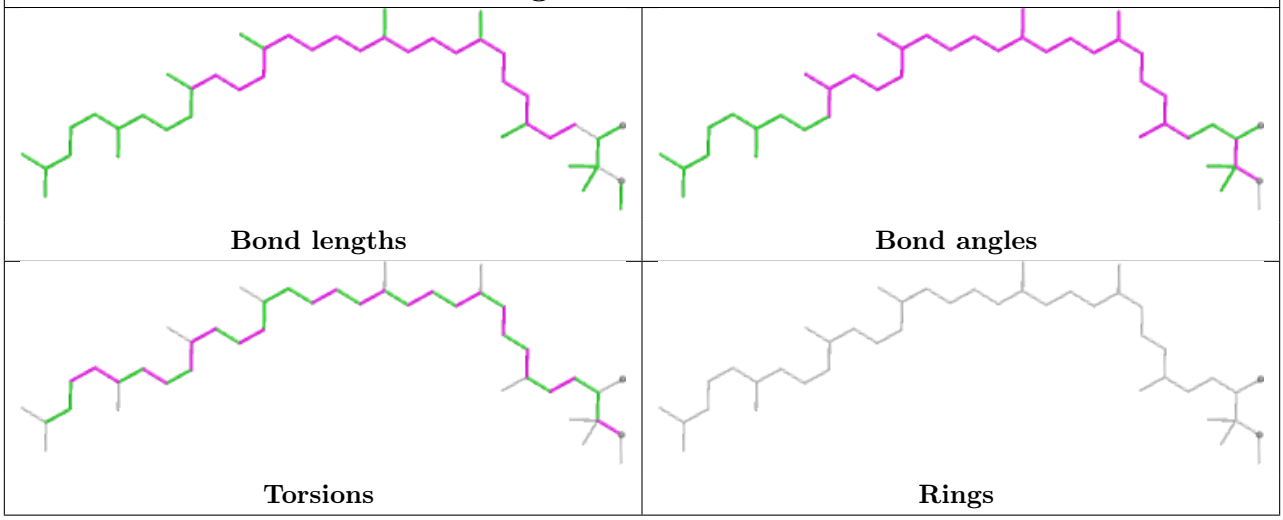

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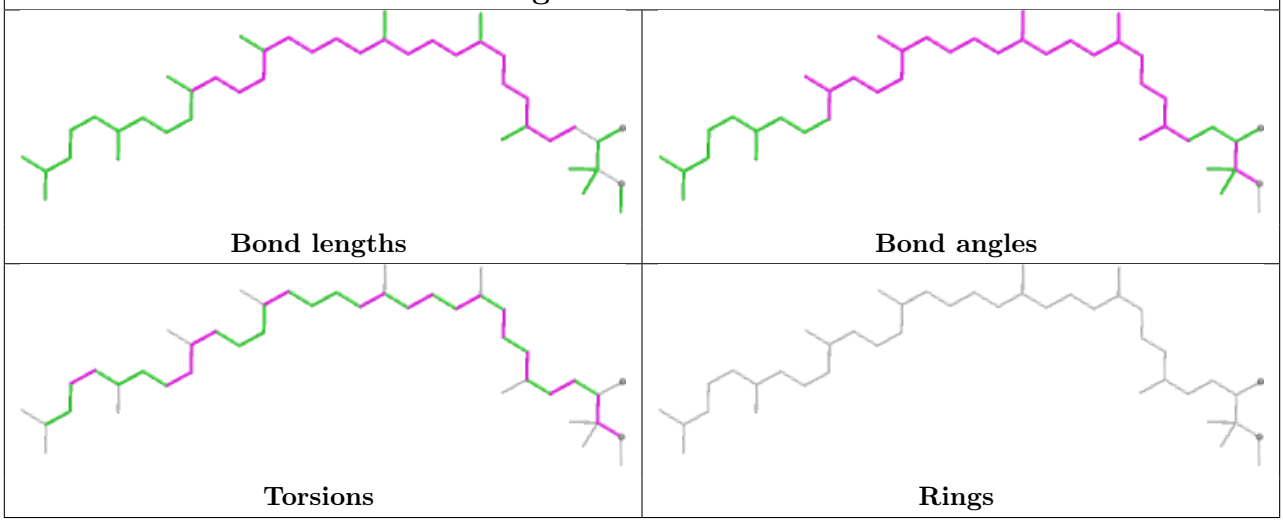

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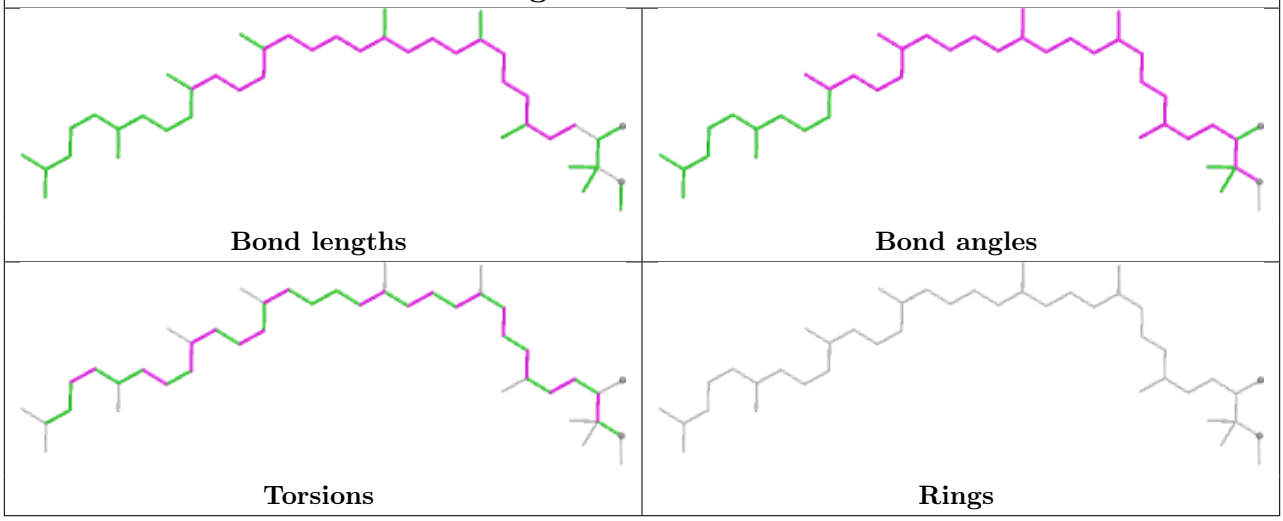

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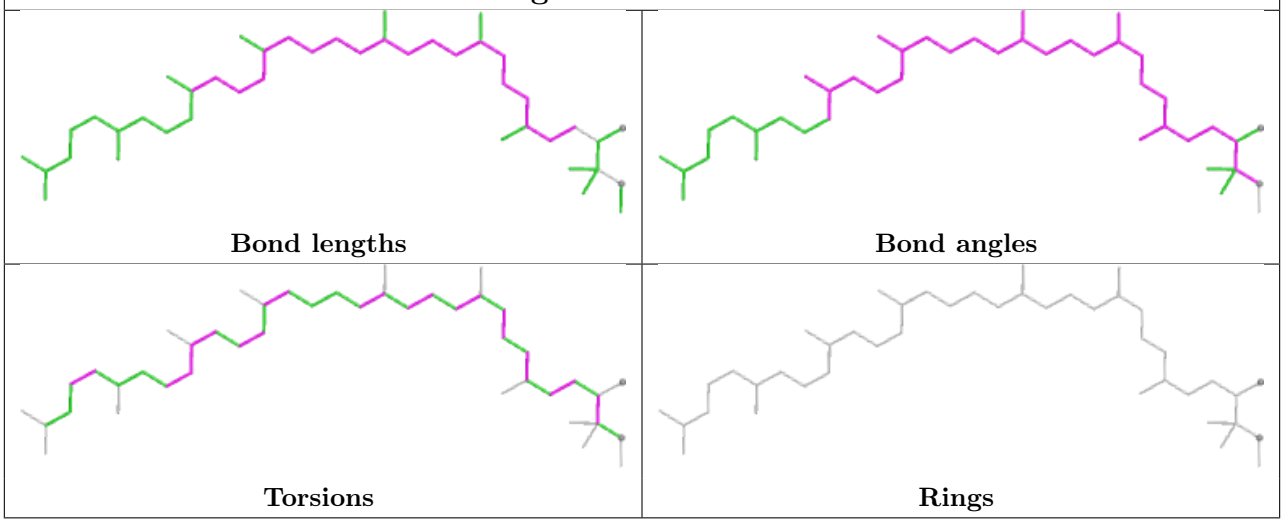

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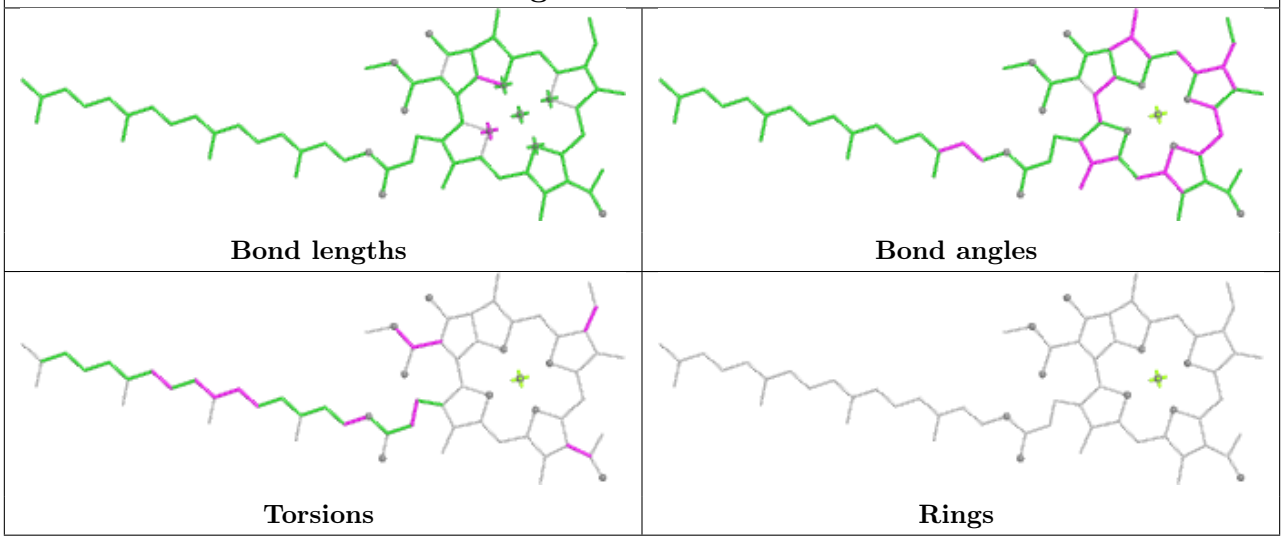
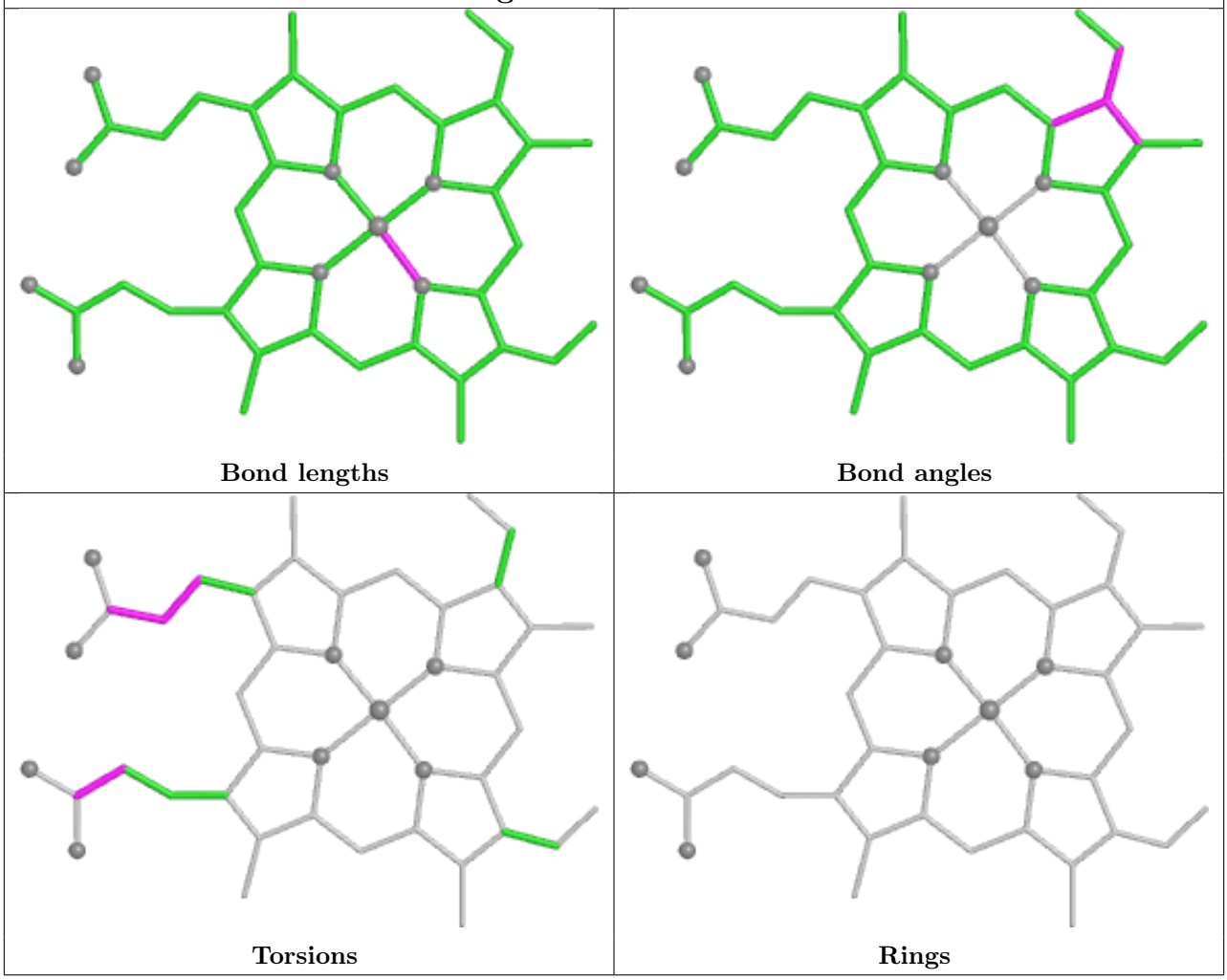


Ligand HEM C 403



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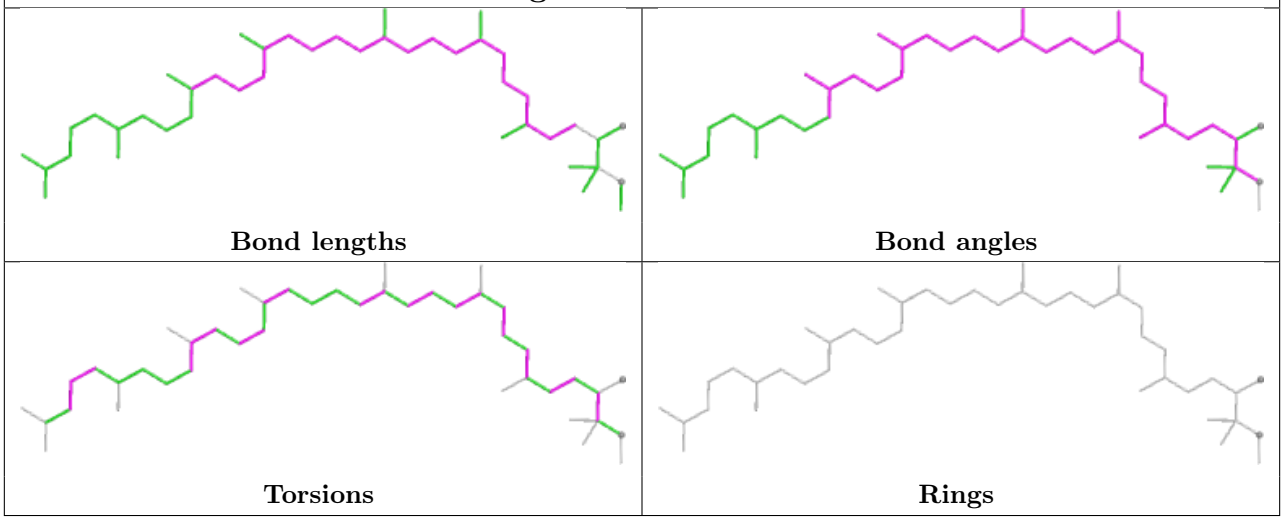

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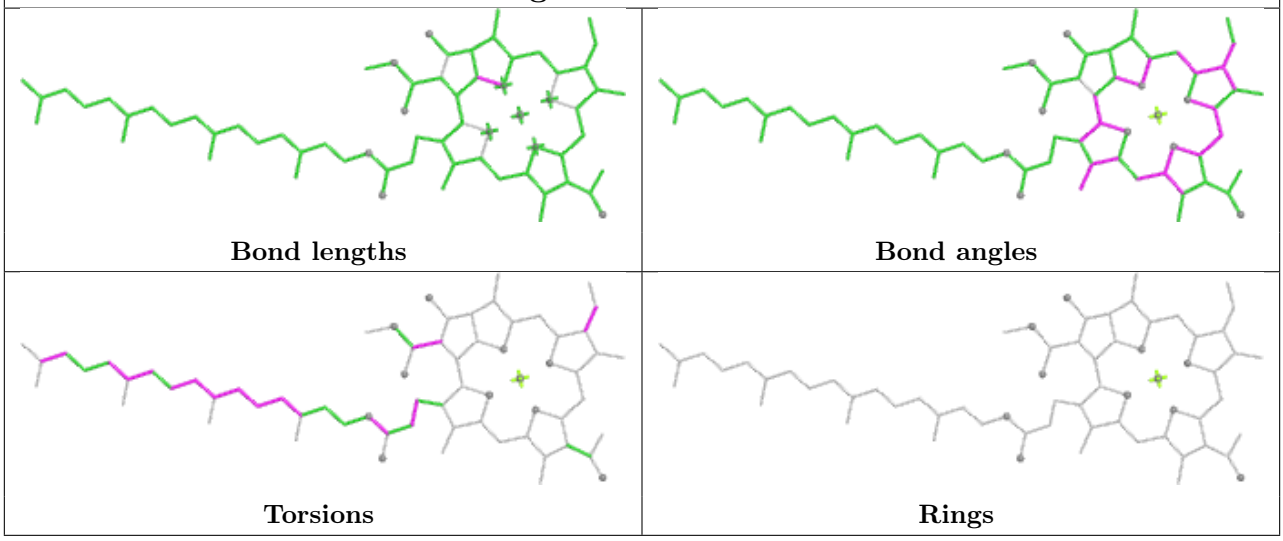

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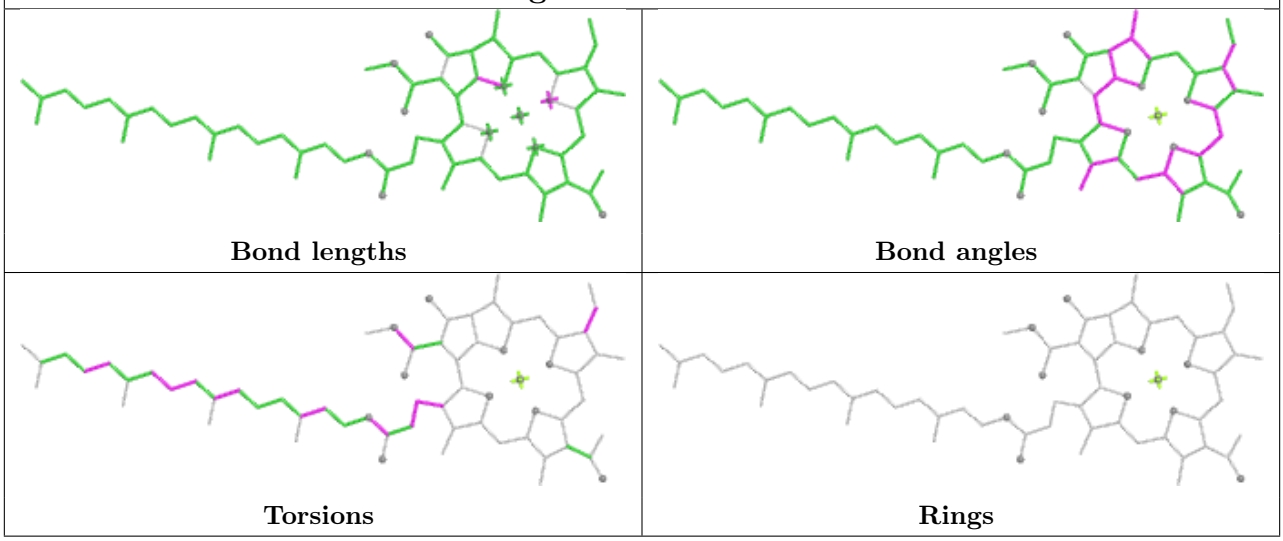
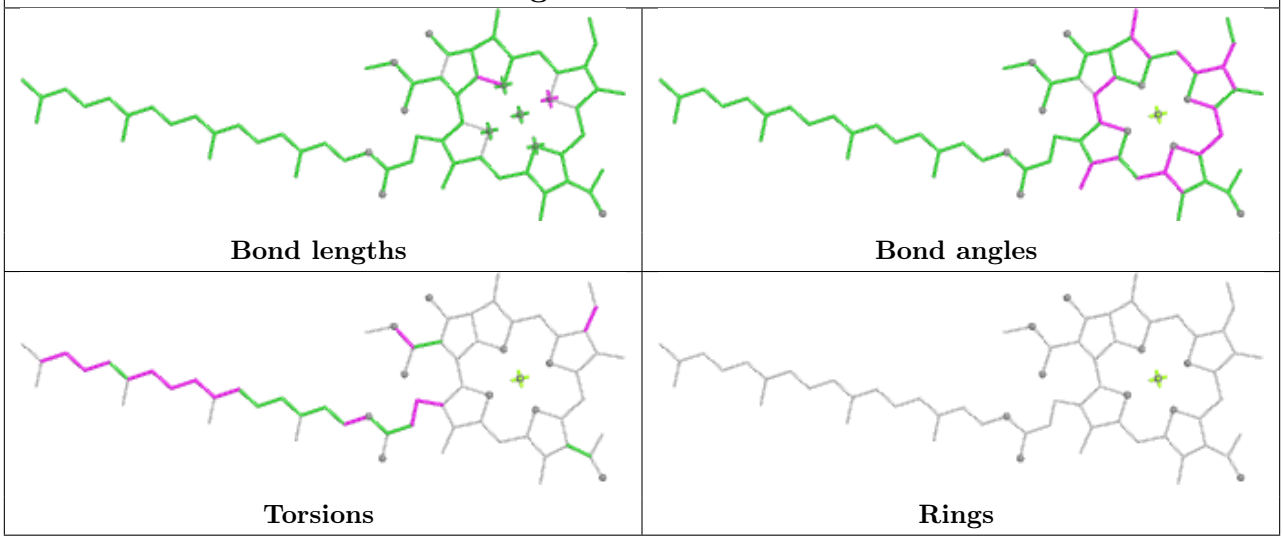
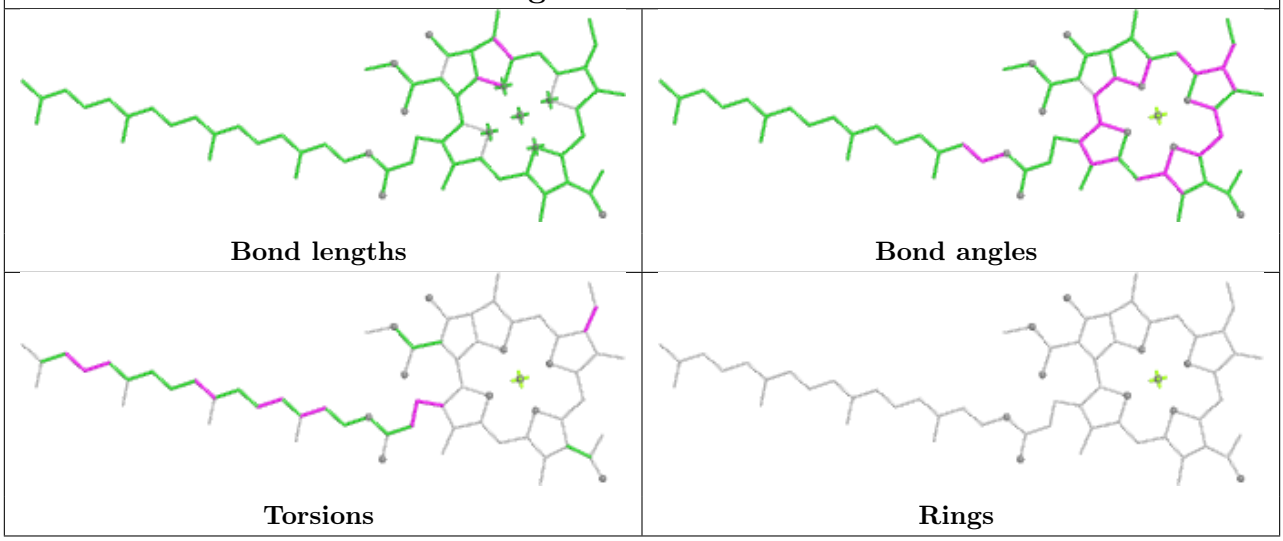


Ligand BCL 9 102



Ligand BCL L 301



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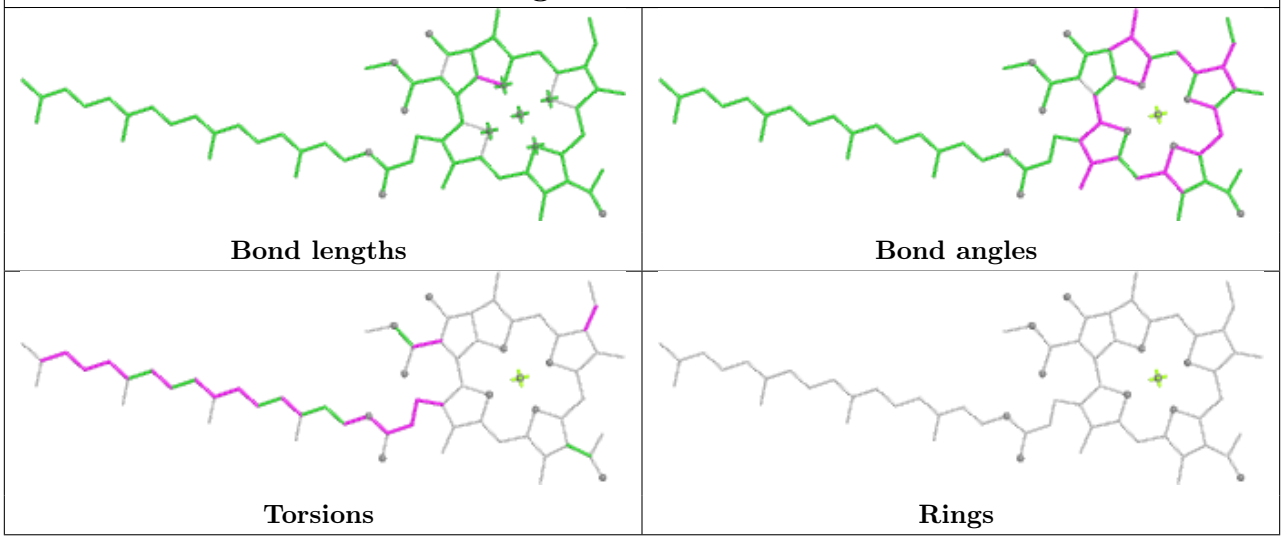
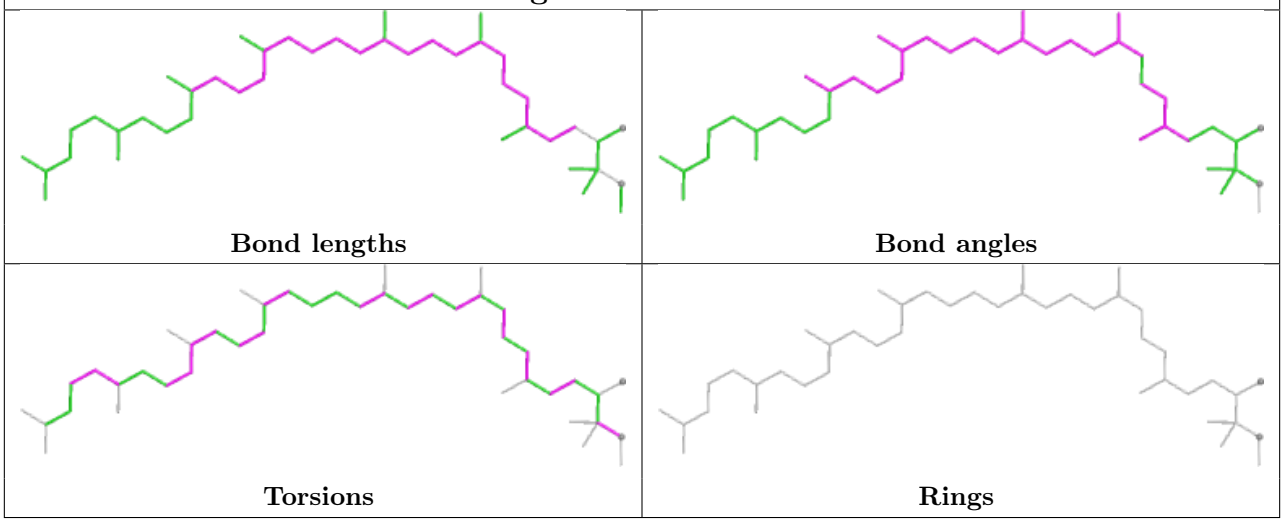
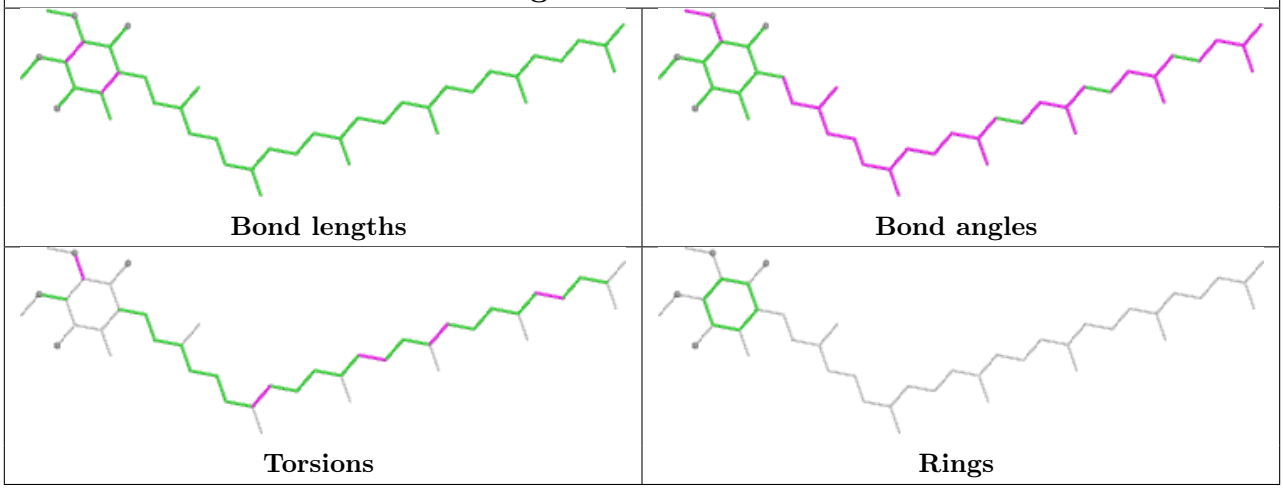


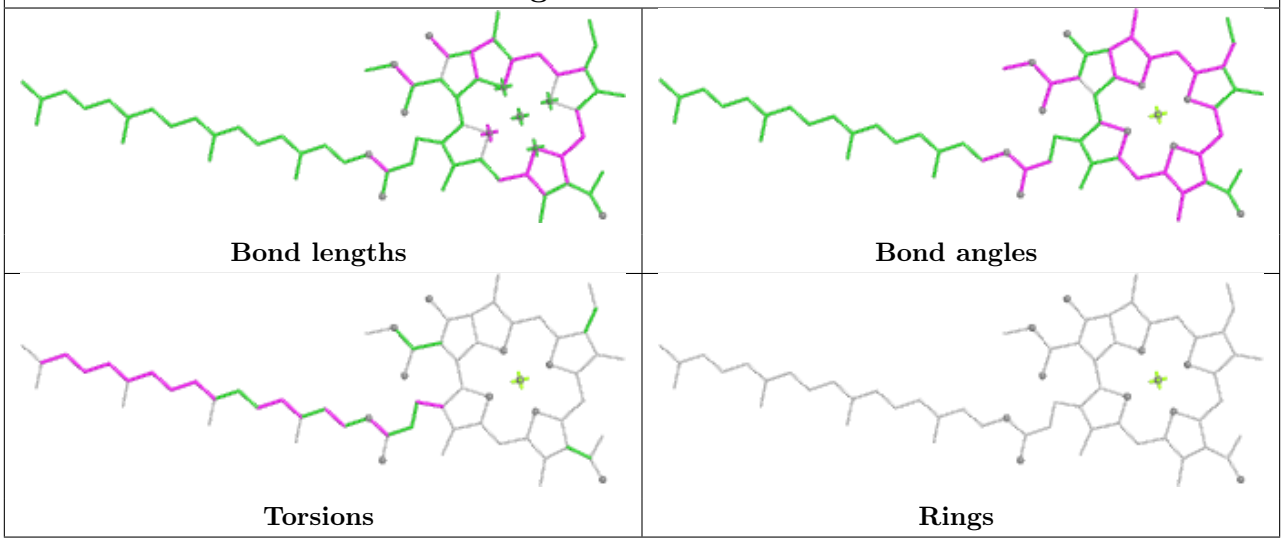
Ligand SPN 5 103



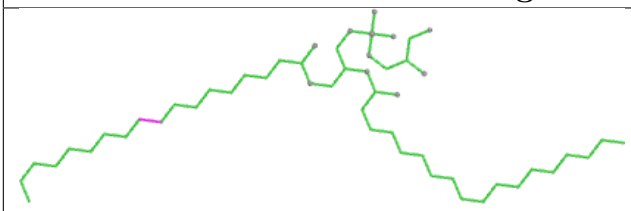
Ligand U10 A 101



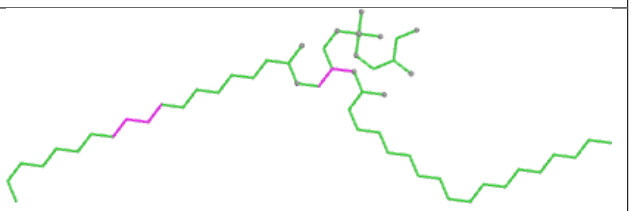
Ligand BCL 2 101



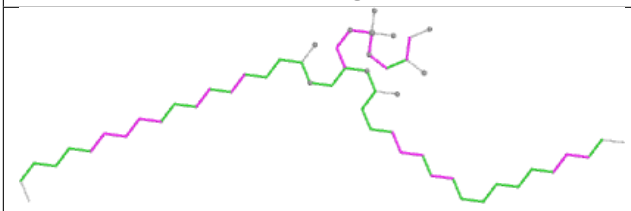
Ligand MW9 H 302



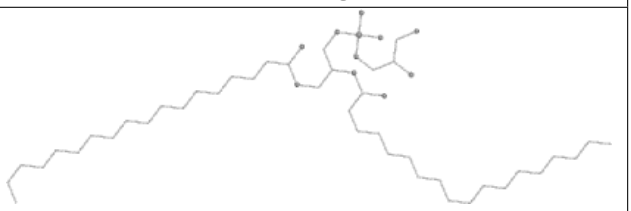
Bond lengths



Bond angles

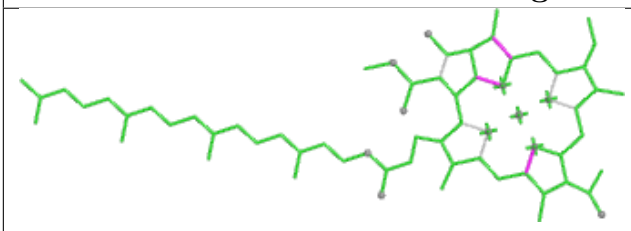


Torsions



Rings

Ligand BCL s 101



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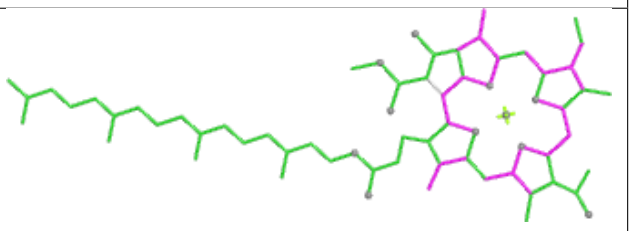
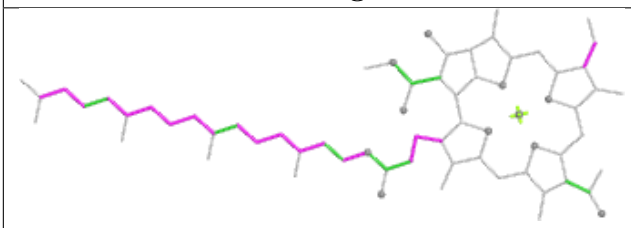


Bond angles



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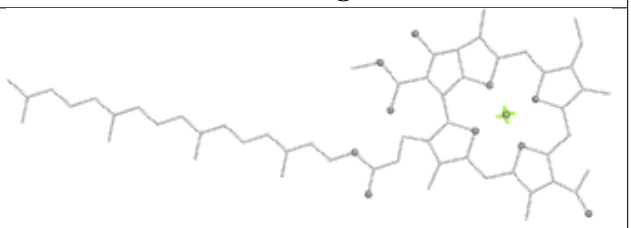
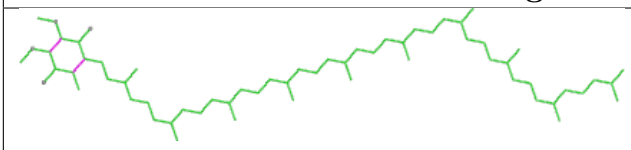
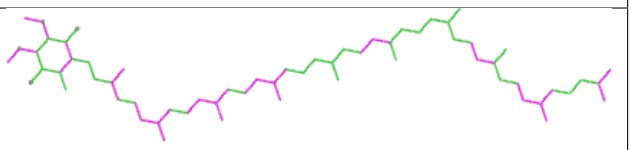


Rings

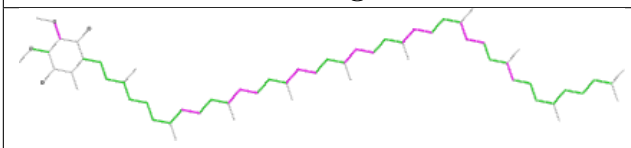
Ligand U10 M 403



Bond lengths



Bond angles



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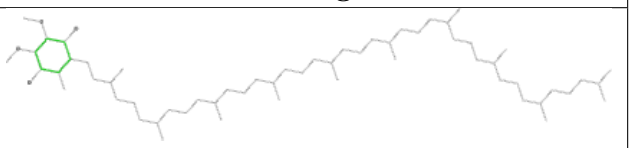
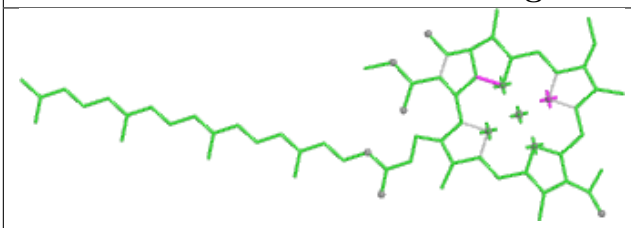
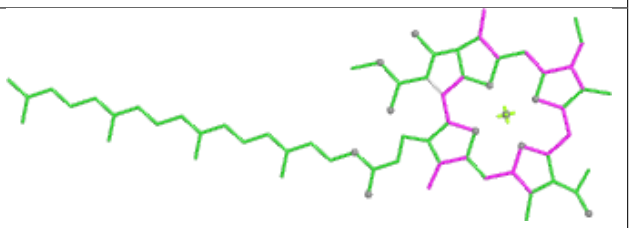
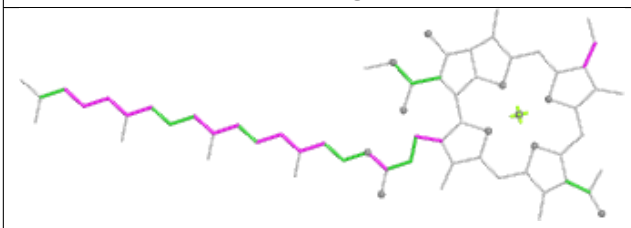
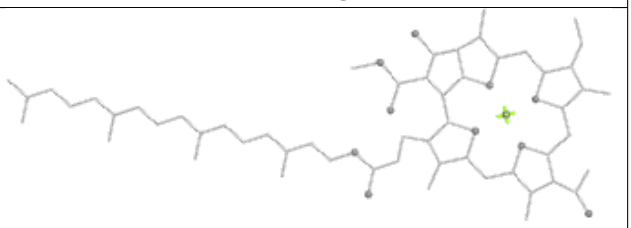
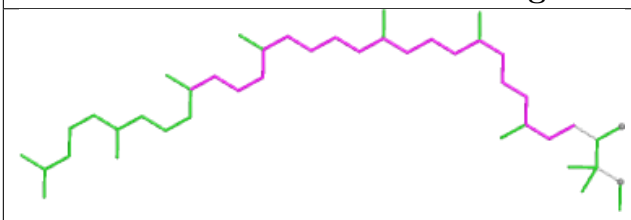
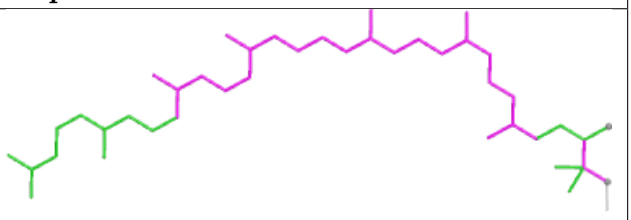
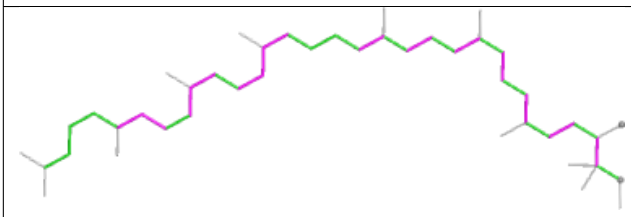
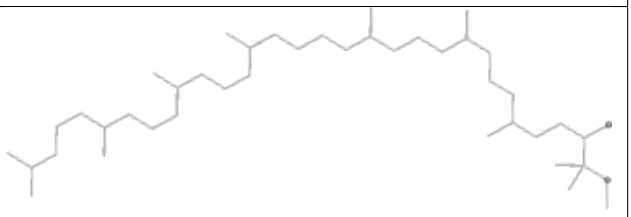
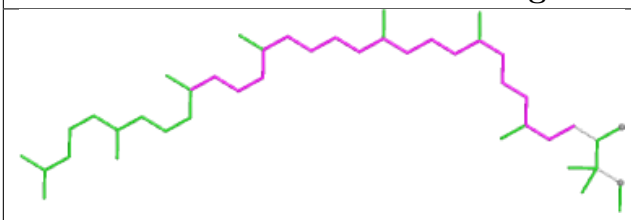
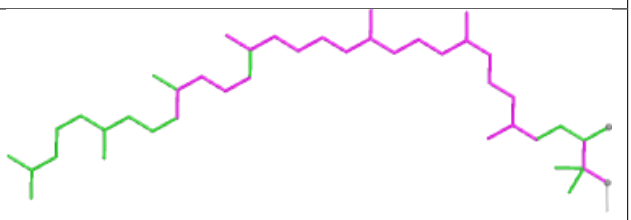
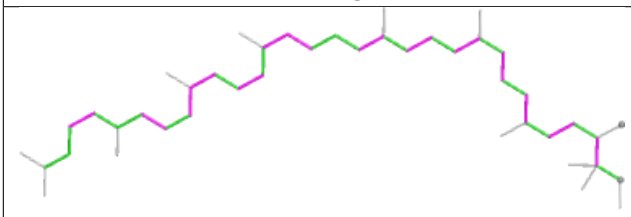
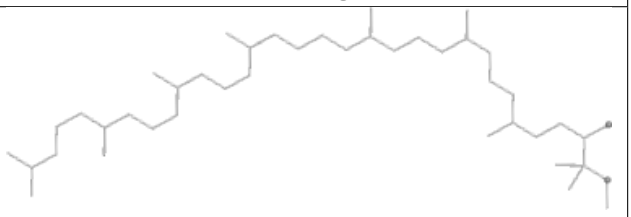


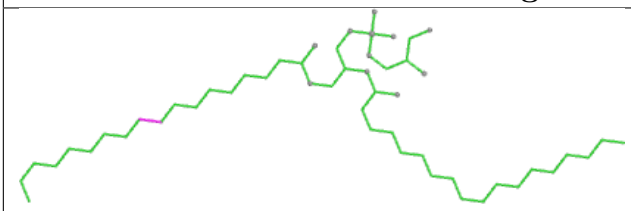
Rings

Ligand BCL w 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

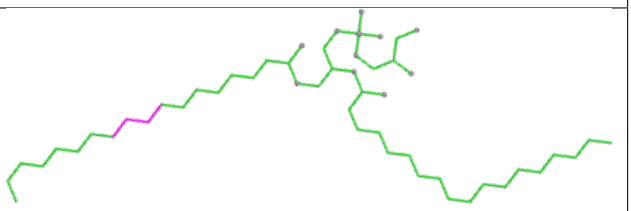
Ligand SPN p 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPN v 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

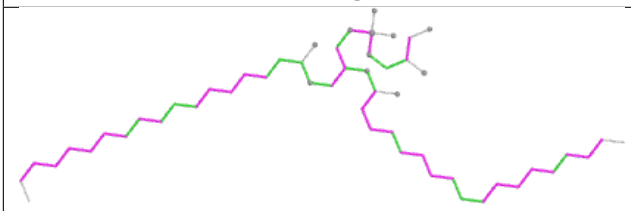
Ligand MW9 9 101



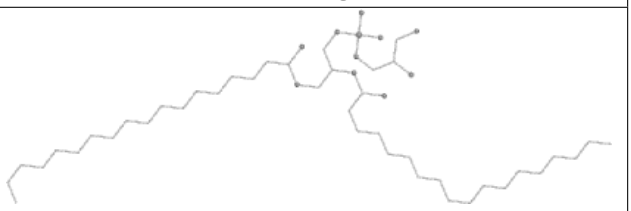
Bond lengths



Bond angles

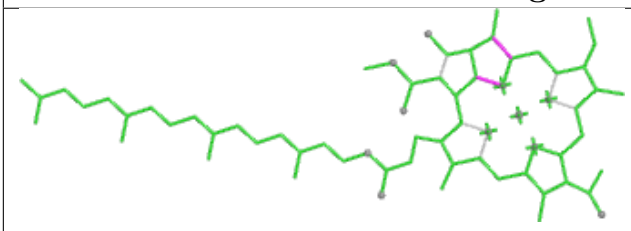


Torsions

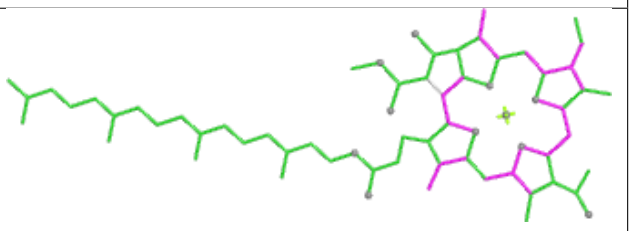


Rings

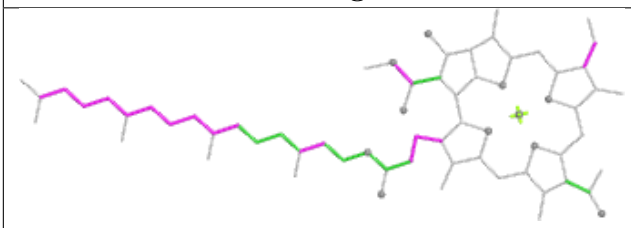
Ligand BCL 5 101



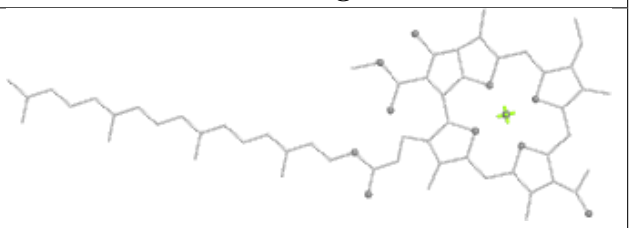
Bond lengths



Bond angles

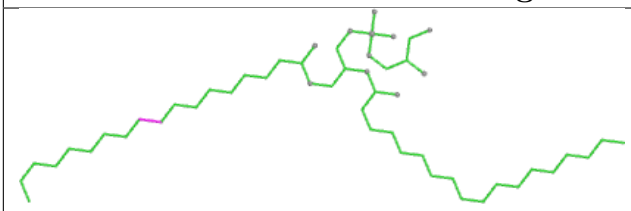


Torsions

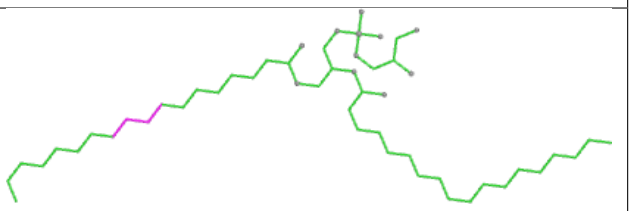


Rings

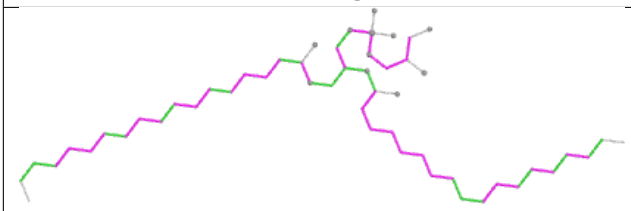
Ligand MW9 H 304



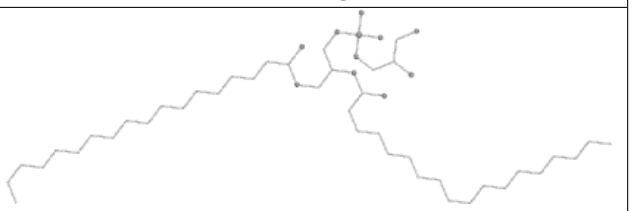
Bond lengths



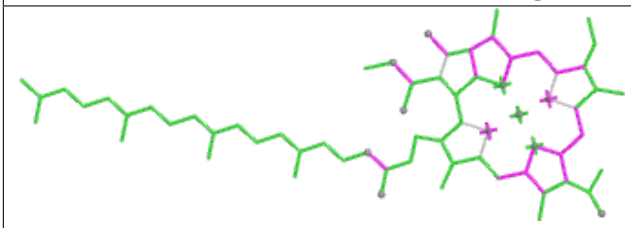
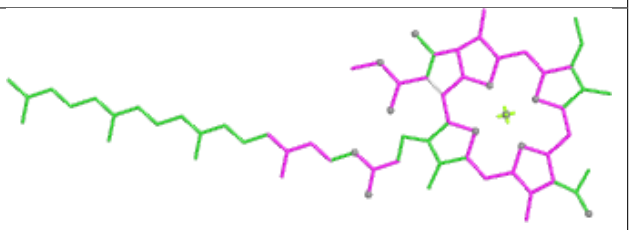
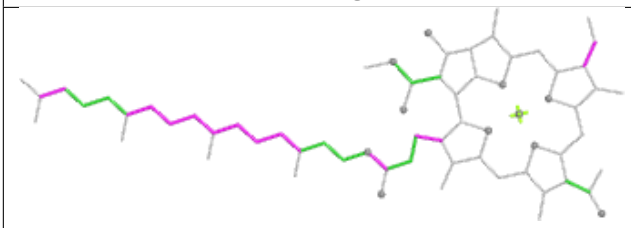
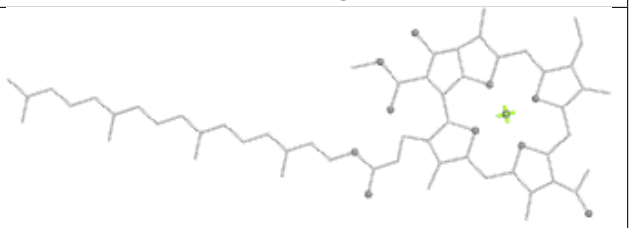
Bond angles



Torsions



Rings

Ligand BCL 4 101	
 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.

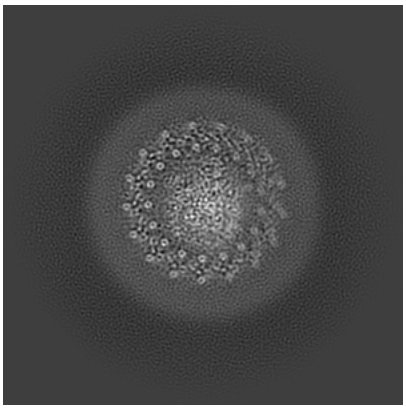
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-63379. These allow visual inspection of the internal detail of the map and identification of artifacts.

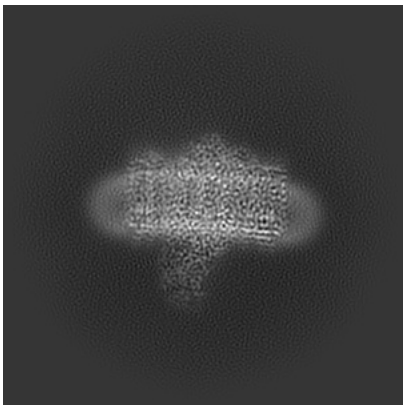
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

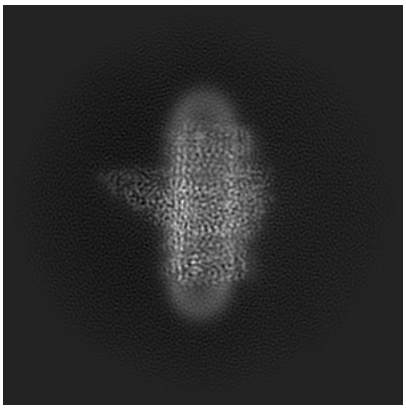
6.1.1 Primary map



X

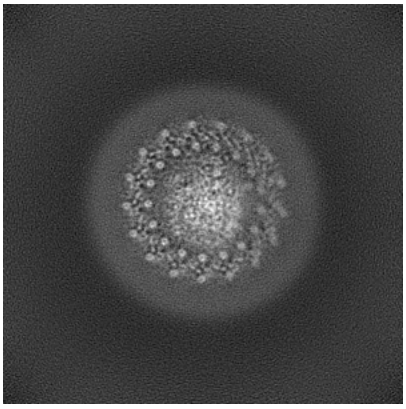


Y

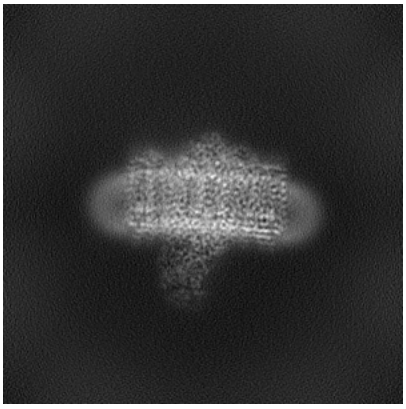


Z

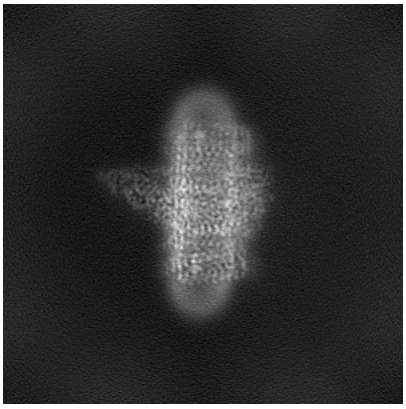
6.1.2 Raw map



X



Y

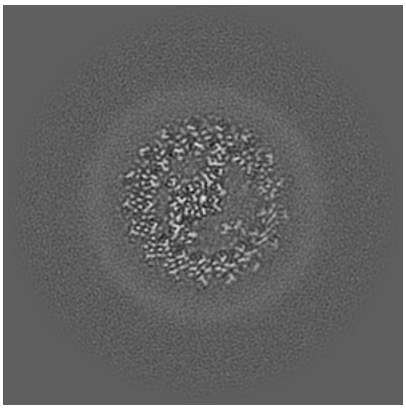


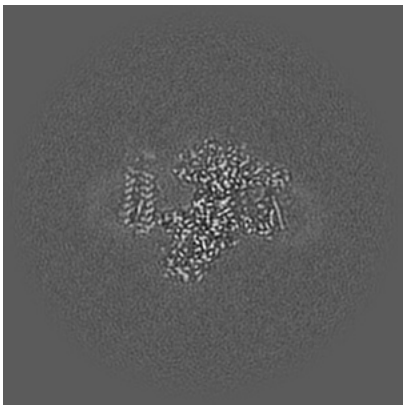
Z

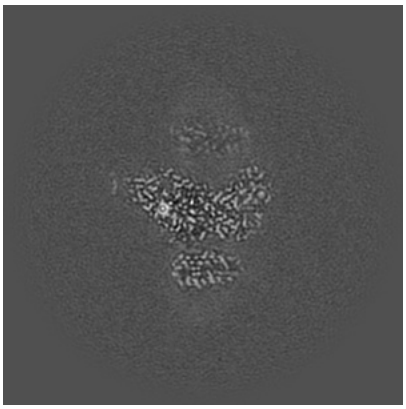
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

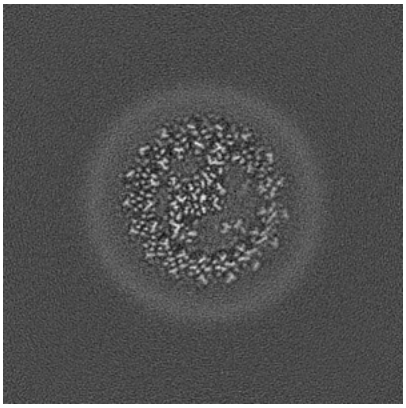
6.2.1 Primary map

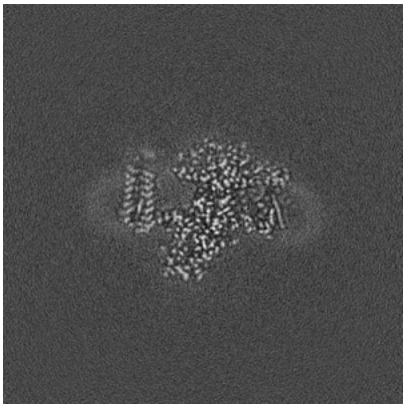

X Index: 150

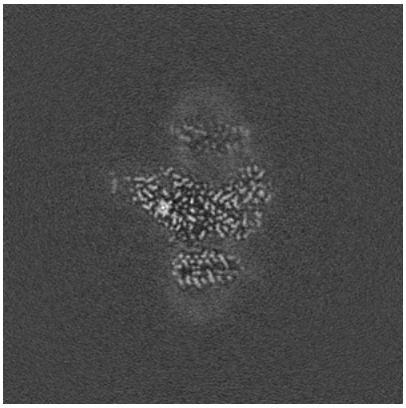

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

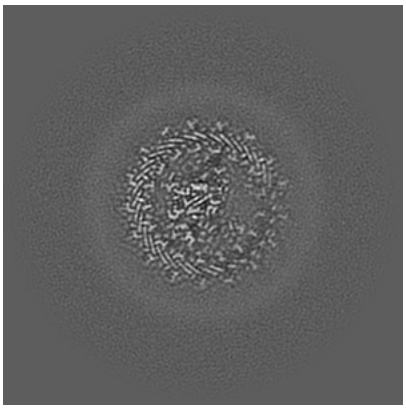

Y Index: 150

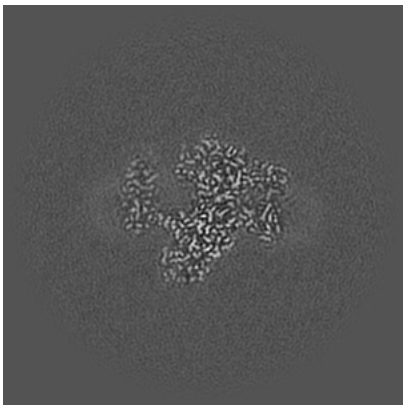

Z Index: 150

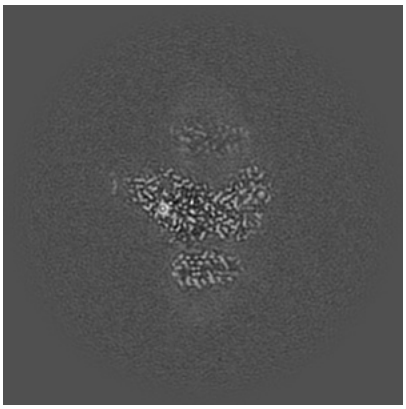
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

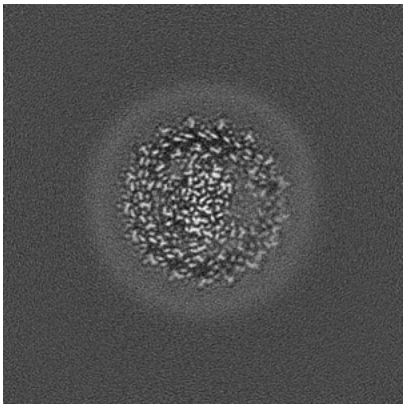
6.3.1 Primary map

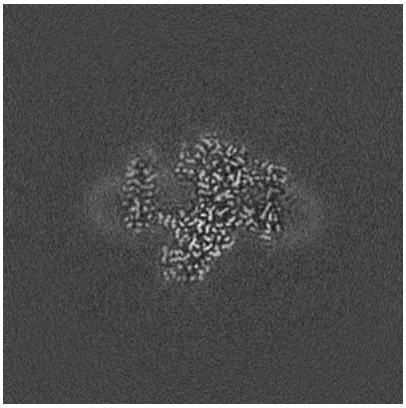

X Index: 143

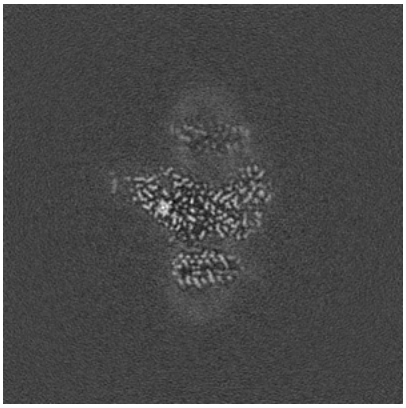

Y Index: 152


Z Index: 150

6.3.2 Raw map


X Index: 137

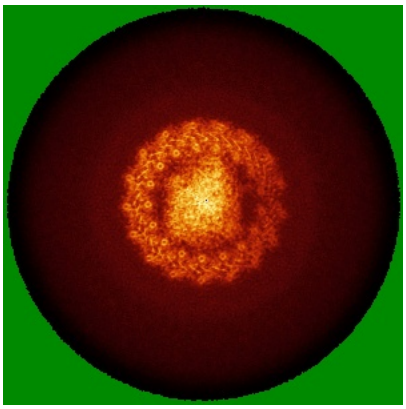

Y Index: 152

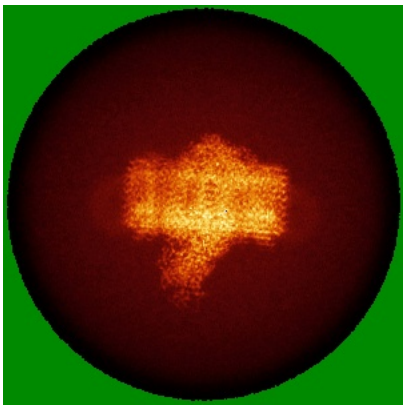

Z Index: 150

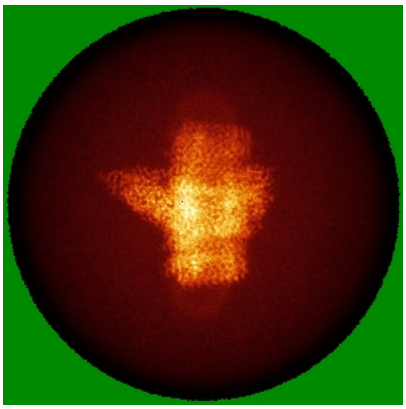
The images above show the largest variance slices of the map in three orthogonal directions.

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

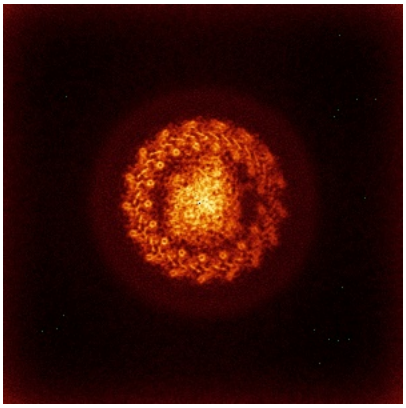
6.4.1 Primary map

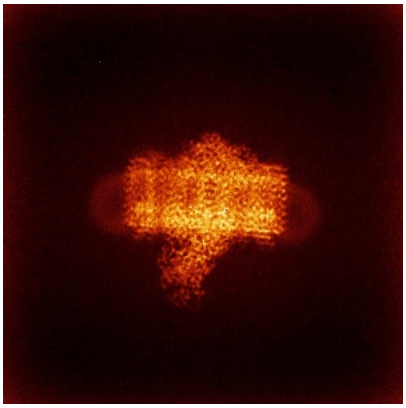

X

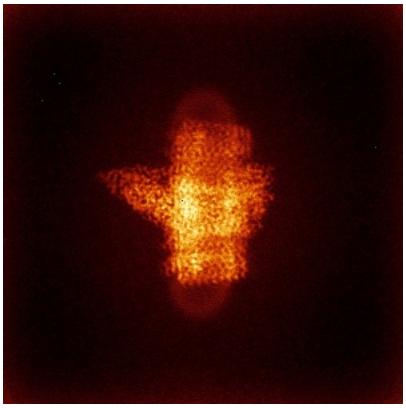

Y


Z

6.4.2 Raw map


X


Y


Z

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

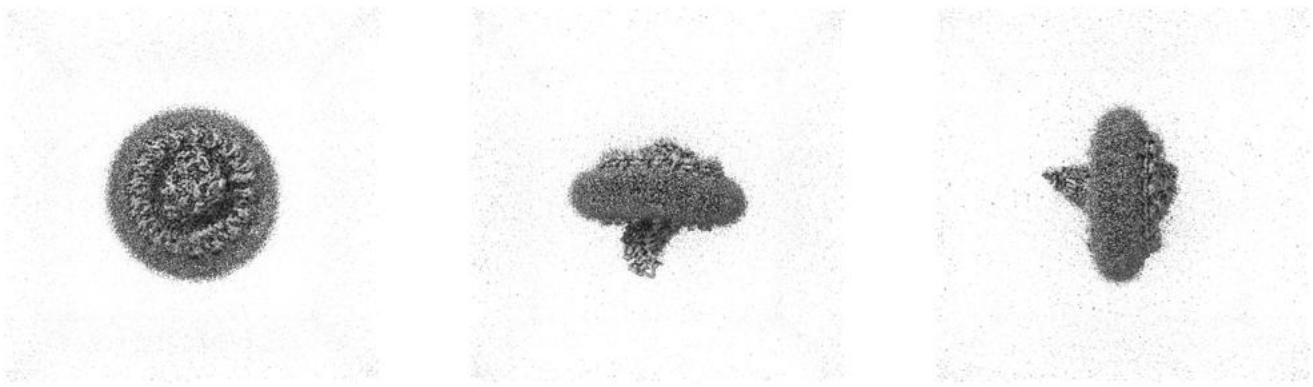
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

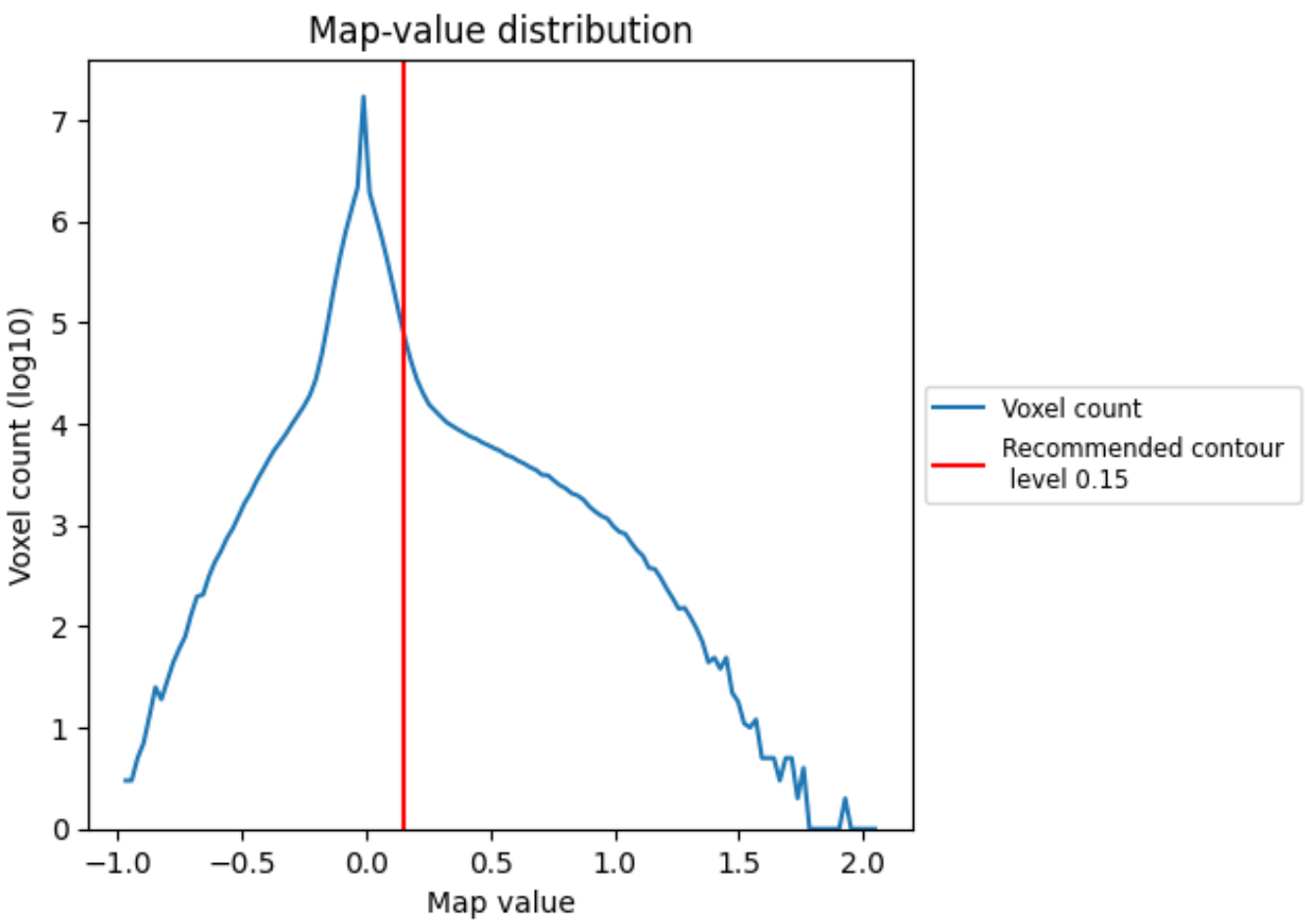
6.6 Mask visualisation (i)

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

7 Map analysis (i)

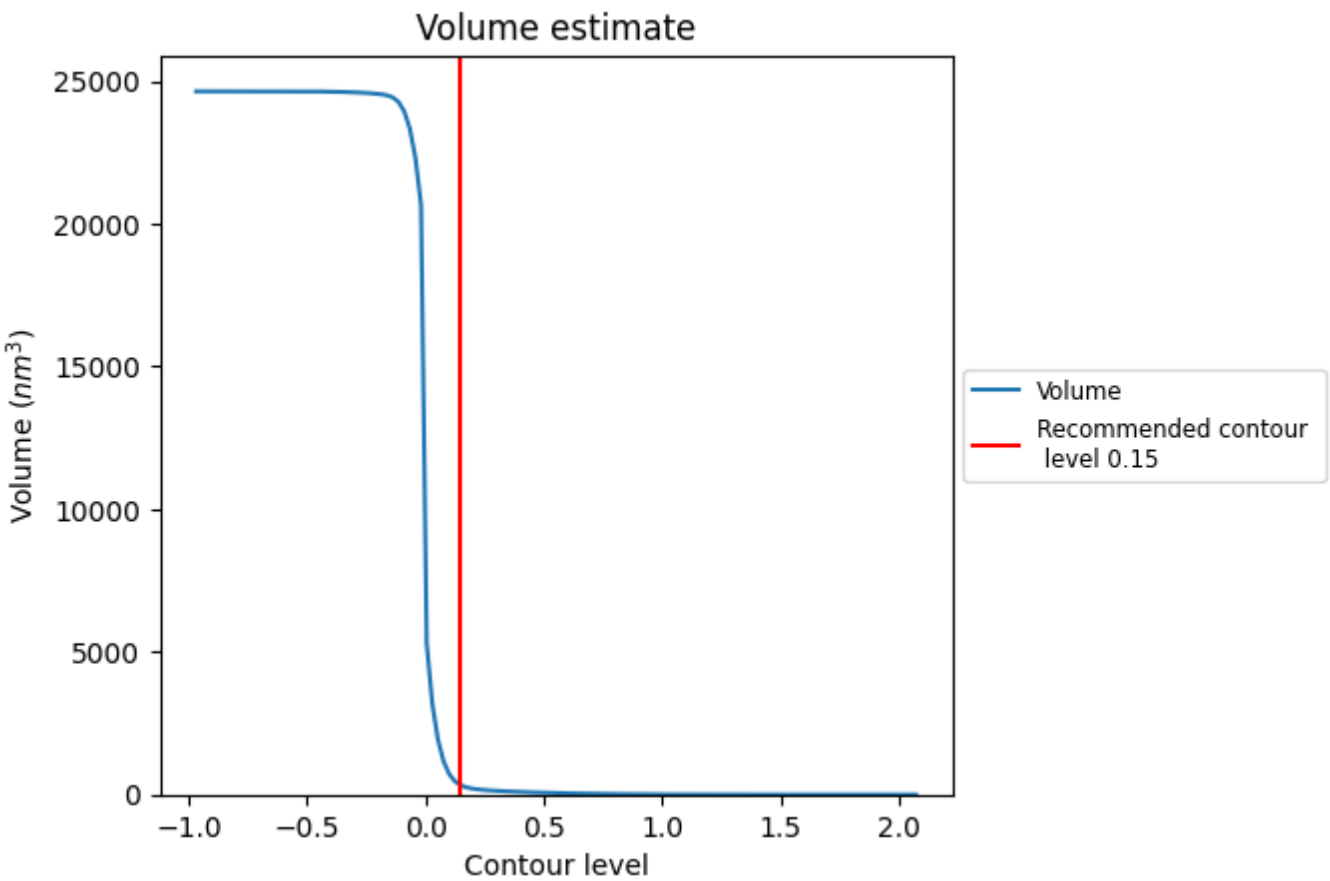
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

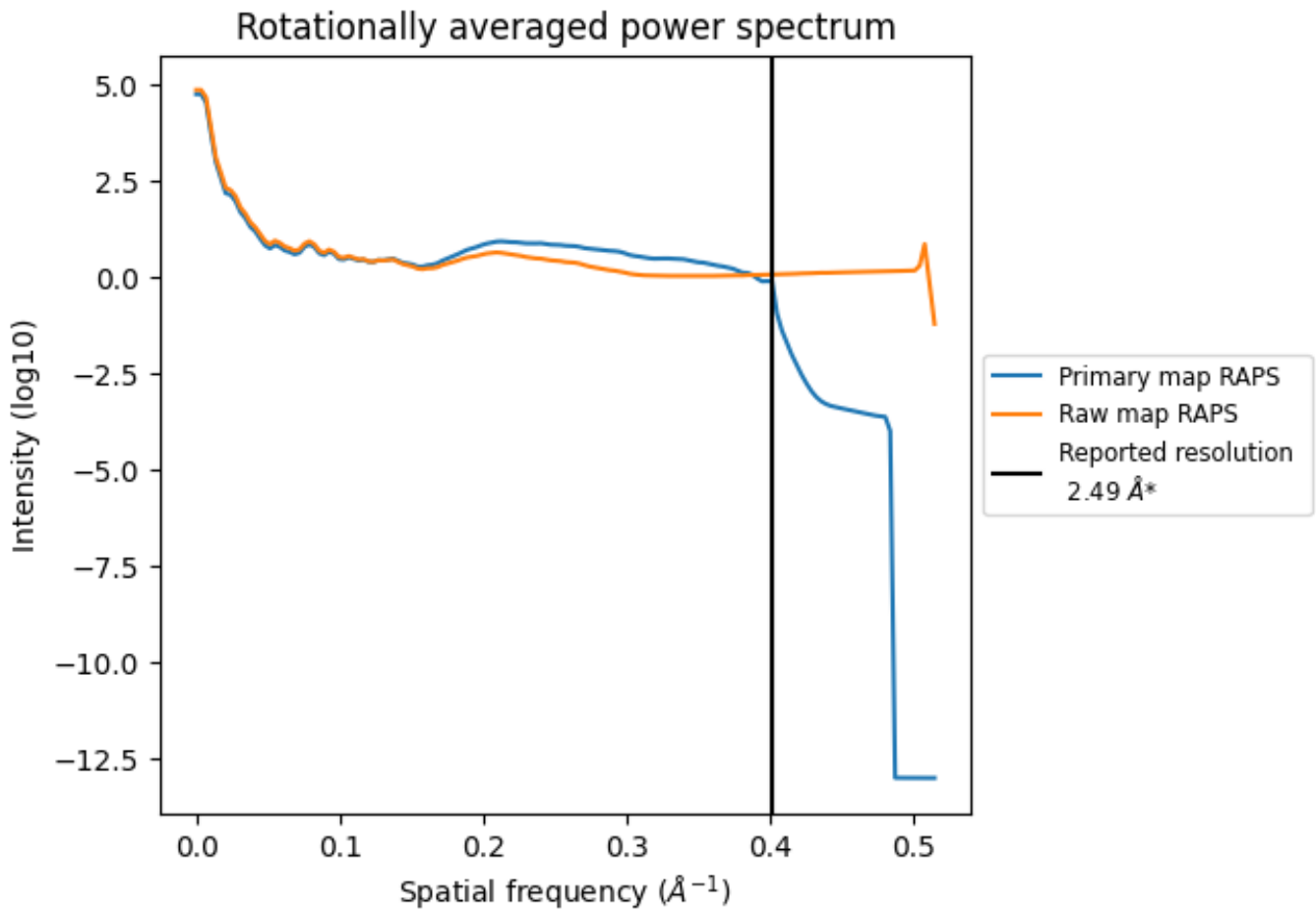
7.2 Volume estimate (i)



The volume at the recommended contour level is 326 nm^3; this corresponds to an approximate mass of 295 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)

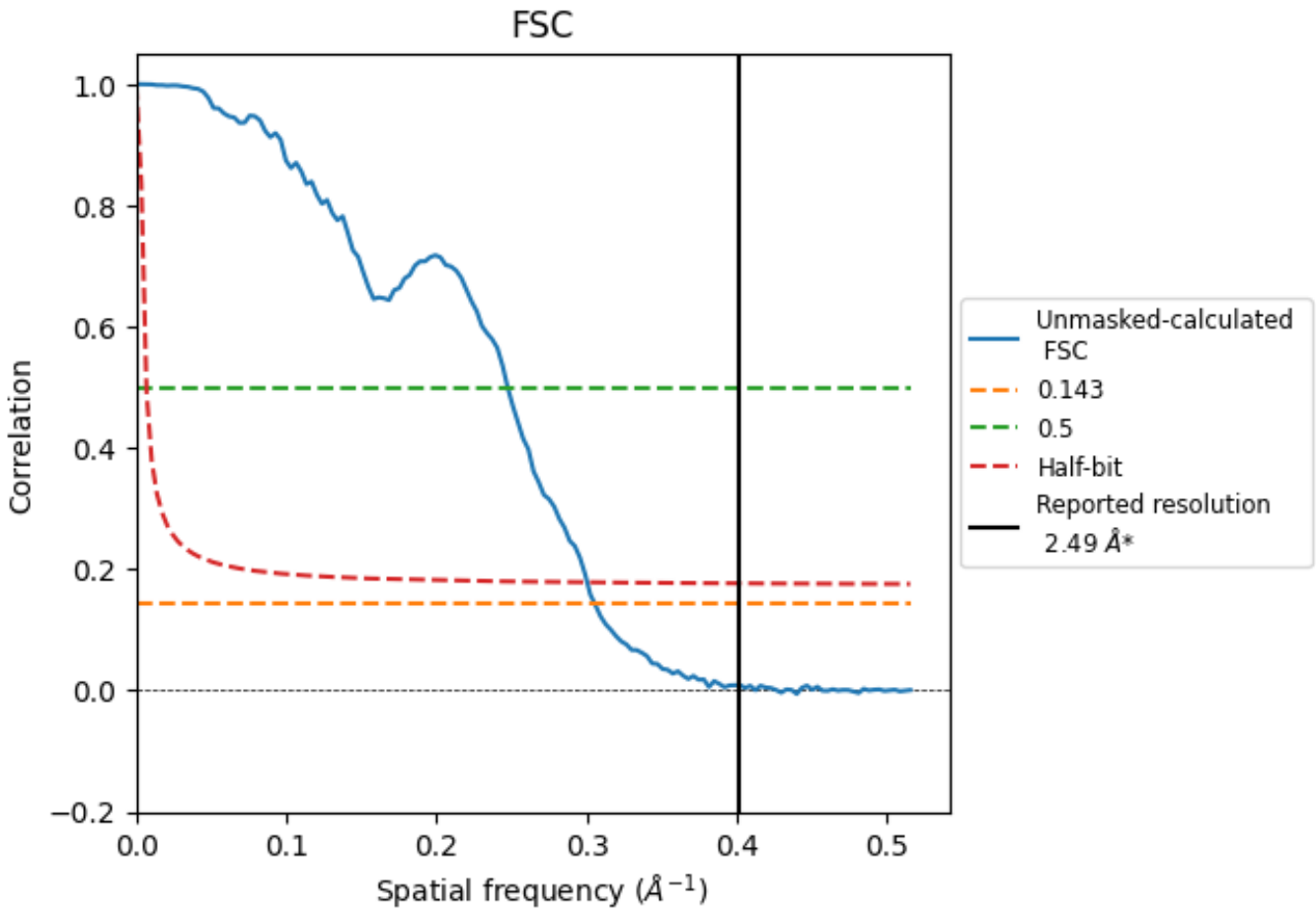


*Reported resolution corresponds to spatial frequency of 0.402 Å^{-1}

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 0.402 Å^{-1}

8.2 Resolution estimates (i)

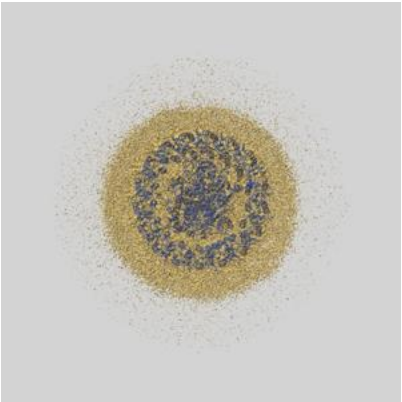
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	4.04	3.33

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

9 Map-model fit (i)

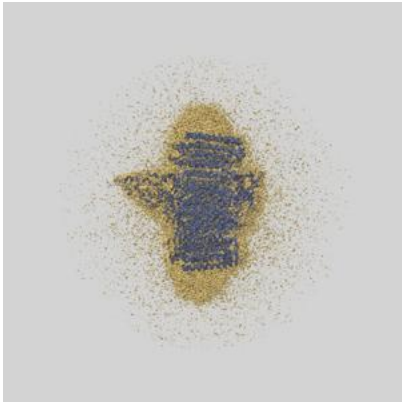
This section contains information regarding the fit between EMDB map EMD-63379 and PDB model 9LTS. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay (i)



X

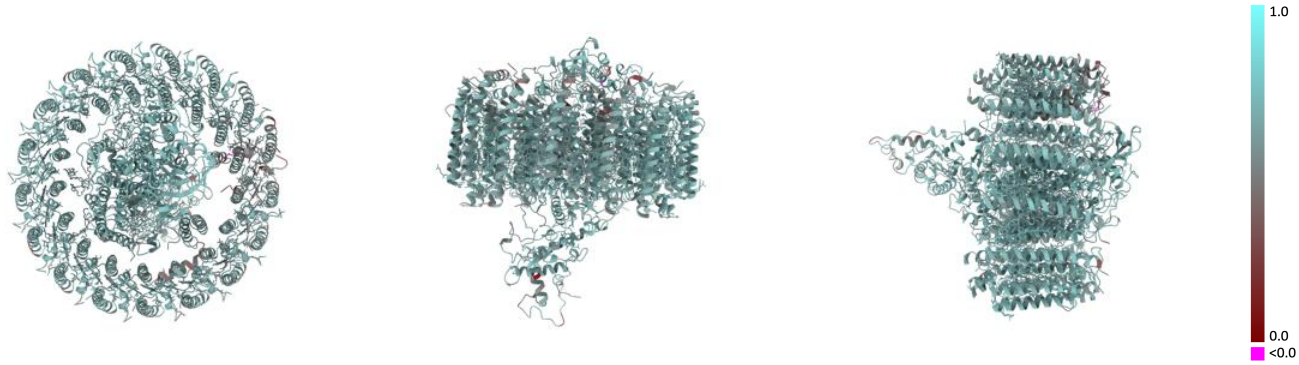
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

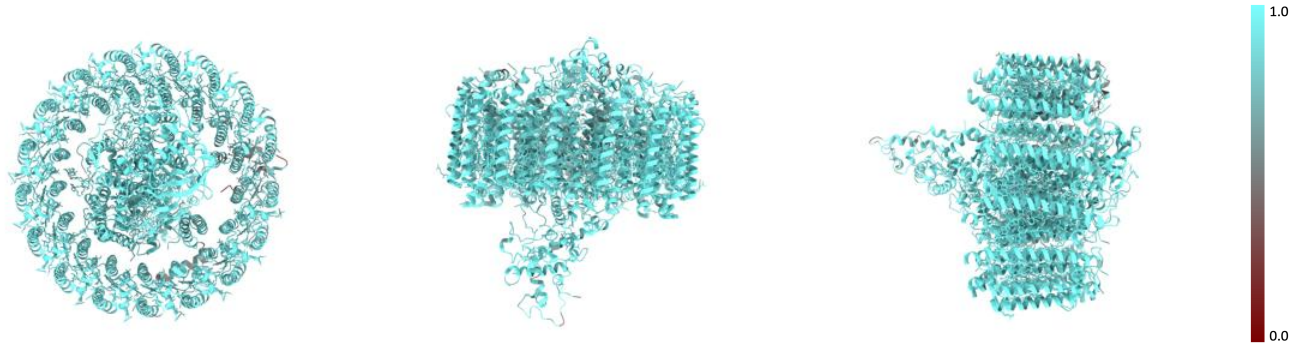
9.2 Q-score mapped to coordinate model (i)



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.

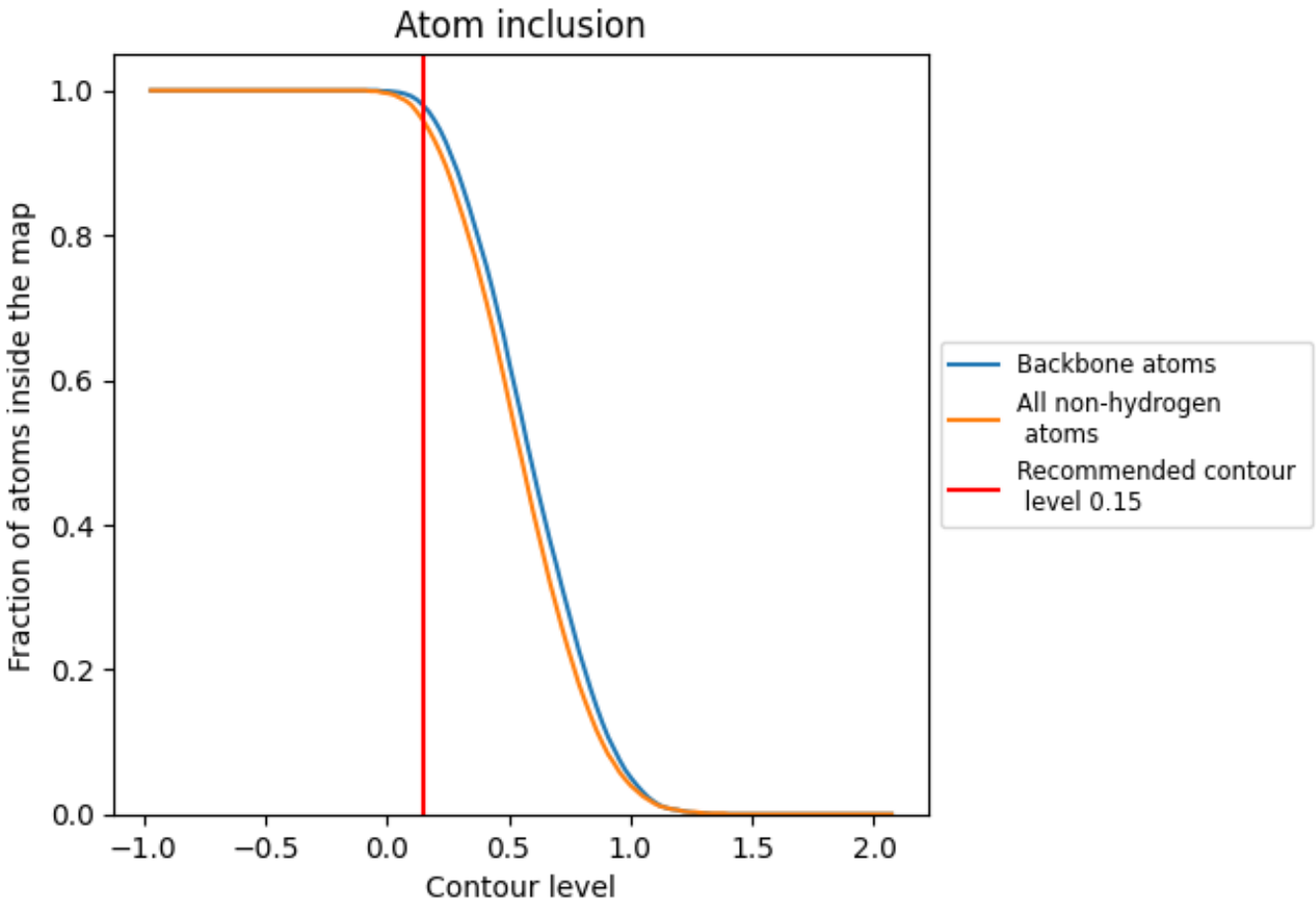
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.6420
0	0.9720	0.6510
1	0.9760	0.6460
2	0.9520	0.6300
3	0.9710	0.6510
4	0.9610	0.6450
5	0.9810	0.6680
6	0.9590	0.6450
7	0.9820	0.6590
8	0.9640	0.6360
9	0.9720	0.6470
A	0.8660	0.5790
C	0.9400	0.6240
H	0.9700	0.6540
L	0.9860	0.6810
M	0.9860	0.6750
a	0.9810	0.6620
b	0.9730	0.6480
c	0.9840	0.6620
d	0.9710	0.6450
e	0.9790	0.6690
f	0.9720	0.6420
g	0.9830	0.6550
h	0.9700	0.6430
i	0.9710	0.6580
j	0.9780	0.6470
k	0.9640	0.6440
l	0.9630	0.6390
m	0.9560	0.6310
n	0.9580	0.6230
o	0.9150	0.5820
p	0.8640	0.5570
q	0.8640	0.5600
r	0.8270	0.5610
s	0.9520	0.6160

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Chain	Atom inclusion	Q-score
t	0.9150	0.5970
u	0.9560	0.6270
v	0.9300	0.5980
w	0.9540	0.6390
x	0.9470	0.6240