wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 01:18 AM JST

PDB ID	:	8ZK2 / pdb_00008zk2
EMDB ID	:	EMD-60165
Title	:	Cryo-EM structure of photosynthetic LH1-RC core complex of Roseospirillum parvum
Authors	:	Wang, G.-L.; Wang, X.-P.; Yu, L.-J.
Deposited on	:	2024-05-15
Resolution	:	2.65 Å(reported)

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

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

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

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

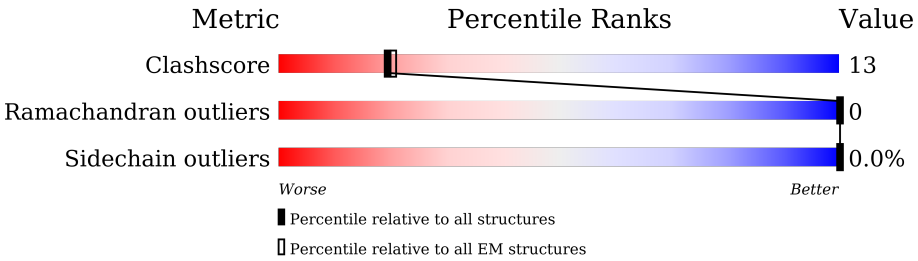
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

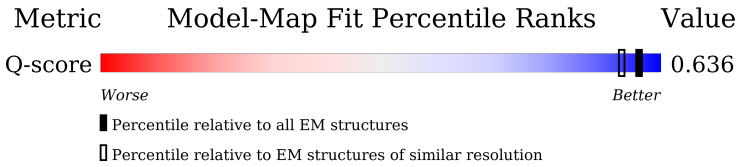
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	9050 (2.15 - 3.15)

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	C	362	10% 75% 20% 6%
2	L	275	6% 69% 30% •
3	M	323	7% 64% 24% 11%
4	H	254	11% 80% 17% •

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Mol	Chain	Length	Quality of chain
5	B	68	19% 62% 10% 28%
5	D	68	12% 63% 9% 28%
5	F	68	10% 51% 21% 28%
5	I	68	13% 63% 9% 28%
5	K	68	7% 59% 13% 28%
5	O	68	10% 62% 10% 28%
5	Q	68	12% 66% 6% 28%
5	S	68	7% 66% 6% 28%
5	U	68	9% 60% 12% 28%
5	W	68	6% 62% 10% 28%
5	Y	68	21% 59% 13% 28%
5	a	68	60% 12% 28%
5	c	68	18% 59% 13% 28%
5	e	68	9% 62% 10% 28%
5	g	68	10% 59% 13% 28%
5	i	68	59% 13% 28%
6	A	67	12% 57% 22% 21%
6	E	67	64% 15% 21%
6	G	67	73% 6% 21%
6	J	67	64% 15% 21%
6	N	67	58% 21% 21%
6	P	67	6% 55% 24% 21%
6	R	67	64% 15% 21%
6	T	67	55% 24% 21%
6	V	67	60% 19% 21%

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Mol	Chain	Length	Quality of chain
6	X	67	58% 21% 21%
6	Z	67	12% 48% 21% 31%
6	b	67	55% 24% 21%
6	d	67	7% 55% 24% 21%
6	f	67	60% 19% 21%
6	h	67	52% 27% 21%
6	j	67	54% 25% 21%

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
7	HEC	C	501	X	-	-	-
7	HEC	C	504	X	-	-	-
9	PGV	L	410	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 26948 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	342	2618	1646	446	501	25	0	0

- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	273	2163	1458	344	350	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	287	2269	1514	369	376	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	245	1906	1214	327	357	8	0	0

- Molecule 5 is a protein called Beta subunit of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	49	377	248	62	65	2	0	0
5	D	49	377	248	62	65	2	0	0
5	F	49	377	248	62	65	2	0	0
5	I	49	377	248	62	65	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	49	377	248	62	65	2	0	0
5	O	49	377	248	62	65	2	0	0
5	Q	49	377	248	62	65	2	0	0
5	S	49	377	248	62	65	2	0	0
5	U	49	377	248	62	65	2	0	0
5	W	49	377	248	62	65	2	0	0
5	Y	49	377	248	62	65	2	0	0
5	a	49	377	248	62	65	2	0	0
5	c	49	377	248	62	65	2	0	0
5	e	49	377	248	62	65	2	0	0
5	g	49	377	248	62	65	2	0	0
5	i	49	377	248	62	65	2	0	0

- Molecule 6 is a protein called Alpha subunit of light-harvesting 1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	A	53	424	283	71	67	3	0	0
6	E	53	424	283	71	67	3	0	0
6	G	53	424	283	71	67	3	0	0
6	J	53	424	283	71	67	3	0	0
6	N	53	424	283	71	67	3	0	0
6	P	53	424	283	71	67	3	0	0
6	R	53	424	283	71	67	3	0	0

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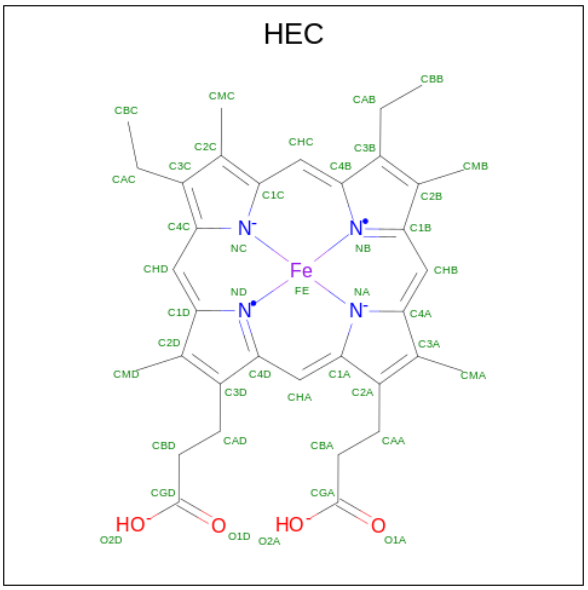
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	53	424	283	71	67	3	0	0
			Total	C	N	O	S		
6	V	53	424	283	71	67	3	0	0
			Total	C	N	O	S		
6	X	53	424	283	71	67	3	0	0
			Total	C	N	O	S		
6	Z	46	369	248	63	56	2	0	0
			Total	C	N	O	S		
6	b	53	424	283	71	67	3	0	0
			Total	C	N	O	S		
6	d	53	424	283	71	67	3	0	0
			Total	C	N	O	S		
6	f	53	424	283	71	67	3	0	0
			Total	C	N	O	S		
6	h	53	424	283	71	67	3	0	0
			Total	C	N	O	S		
6	j	53	424	283	71	67	3	0	0

- Molecule 7 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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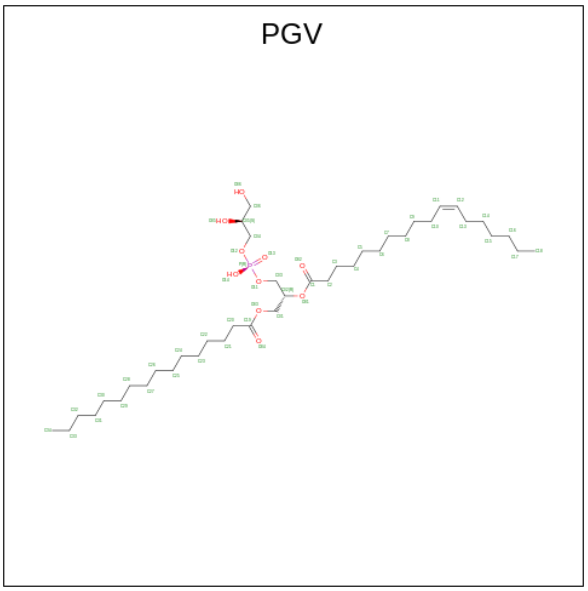
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
7	C	1	43	34	1	4	4	0
7	C	1	43	34	1	4	4	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	C	3	3	3	0
8	H	1	1	1	0

- Molecule 9 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	C	1	38	27	10	1	0
9	L	1	Total	C	O		0
			22	17	5		
9	M	1	Total	C	O	P	0
			46	37	8	1	
9	M	1	Total	C	O	P	0
			42	33	8	1	

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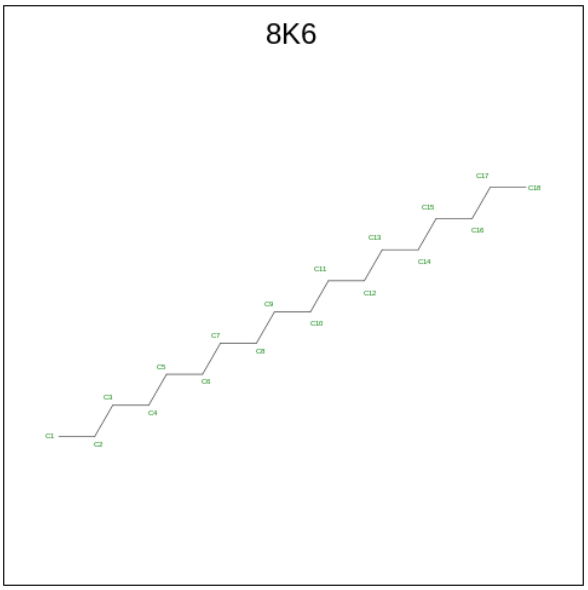
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	H	1	51	40	10	1	0
			Total	C	O	P	
9	H	1	51	40	10	1	0
			Total	C	O	P	
9	R	1	51	40	10	1	0
			Total	C	O	P	
9	Z	1	42	31	10	1	0

- Molecule 10 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
10	C	1	16	16	0
			Total	C	
10	L	1	15	15	0
			Total	C	
10	L	1	18	18	0
			Total	C	
10	L	1	18	18	0
			Total	C	
10	L	1	18	18	0
			Total	C	
10	L	1	18	18	0
			Total	C	
10	M	1	18	18	0

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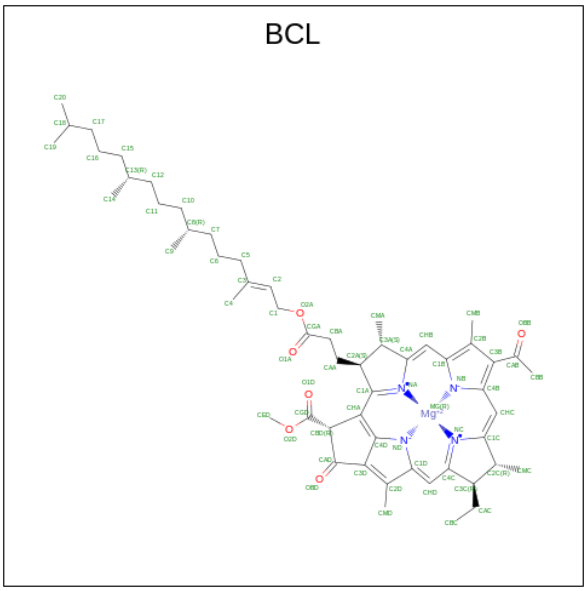
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
10	H	1	17	17	0
			Total	C	
10	H	1	18	18	0
			Total	C	
10	H	1	18	18	0
			Total	C	
10	H	1	15	15	0
			Total	C	
10	J	1	13	13	0
			Total	C	
10	J	1	18	18	0
			Total	C	
10	N	1	18	18	0
			Total	C	
10	P	1	18	18	0
			Total	C	
10	V	1	18	18	0
			Total	C	
10	V	1	18	18	0
			Total	C	
10	X	1	18	18	0
			Total	C	
10	d	1	18	18	0
			Total	C	
10	f	1	18	18	0
			Total	C	
10	j	1	18	18	0
			Total	C	
10	j	1	18	18	0

- Molecule 11 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	
11	L	1	66	55	1	4	6	0
11	L	1	66	55	1	4	6	0
11	M	1	66	55	1	4	6	0
11	M	1	66	55	1	4	6	0
11	B	1	66	55	1	4	6	0
11	A	1	66	55	1	4	6	0
11	A	1	66	55	1	4	6	0
11	D	1	66	55	1	4	6	0
11	E	1	66	55	1	4	6	0
11	E	1	66	55	1	4	6	0
11	F	1	66	55	1	4	6	0
11	G	1	66	55	1	4	6	0
11	G	1	66	55	1	4	6	0
11	I	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
11	J	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	J	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	K	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	N	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	O	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	P	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	Q	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	R	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	R	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	S	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	T	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	T	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	U	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	V	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	W	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	X	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	X	1	66	55	1	4	6	0
			Total	C	Mg	N	O	
11	Y	1	66	55	1	4	6	0

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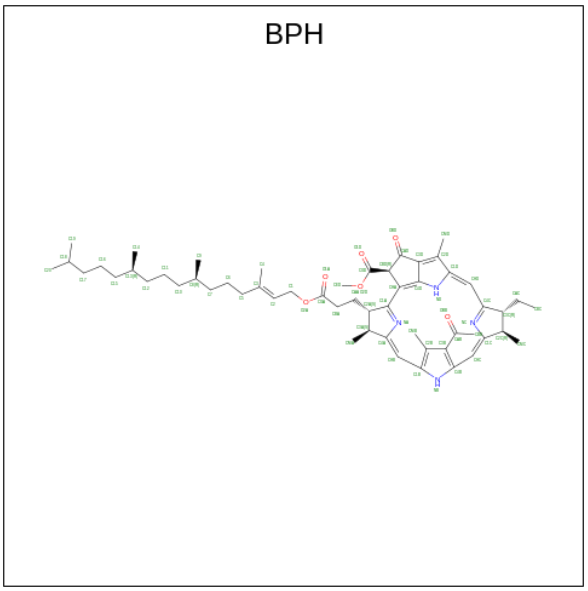
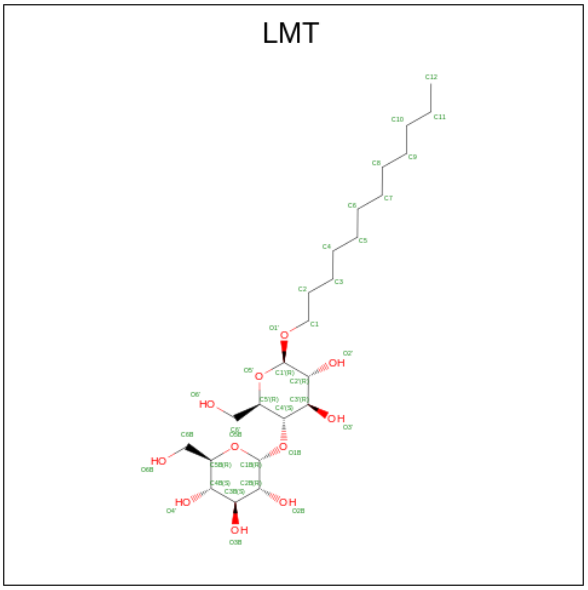
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
11	Z	1	66	55	1	4	6	0
11	a	1	66	55	1	4	6	0
11	b	1	66	55	1	4	6	0
11	b	1	66	55	1	4	6	0
11	c	1	66	55	1	4	6	0
11	d	1	66	55	1	4	6	0
11	d	1	66	55	1	4	6	0
11	e	1	66	55	1	4	6	0
11	f	1	66	55	1	4	6	0
11	f	1	66	55	1	4	6	0
11	g	1	66	55	1	4	6	0
11	h	1	66	55	1	4	6	0
11	h	1	66	55	1	4	6	0
11	i	1	66	55	1	4	6	0
11	j	1	66	55	1	4	6	0
11	j	1	66	55	1	4	6	0

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



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

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



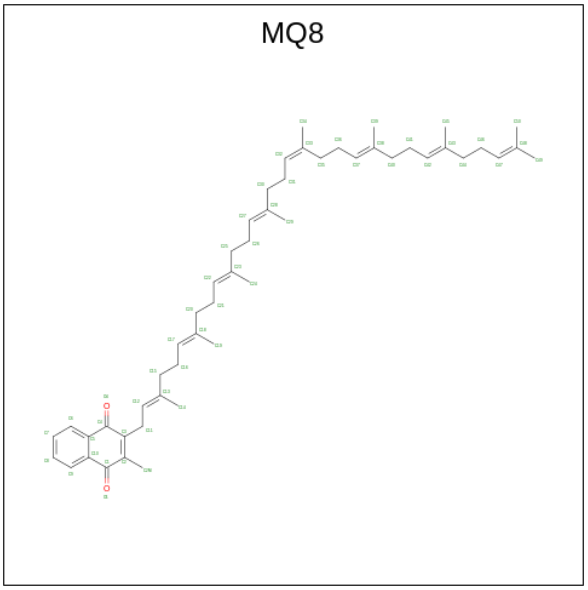
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
13	L	1	32	21	11		0

- 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

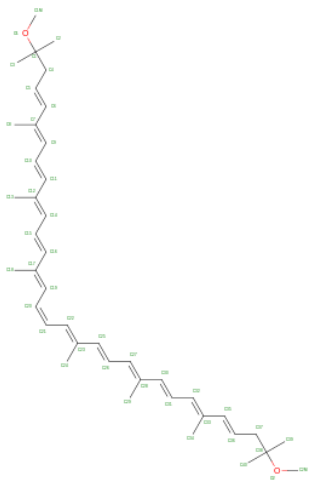
- Molecule 15 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	M	1	53	51	2	0

- Molecule 16 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$) (labeled as "Ligand of Interest" by depositor).

CRT



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	M	1	44	42	2	0
16	B	1	44	42	2	0
16	A	1	44	42	2	0
16	E	1	44	42	2	0
16	I	1	44	42	2	0
16	K	1	44	42	2	0
16	N	1	44	42	2	0
16	P	1	44	42	2	0
16	R	1	44	42	2	0
16	U	1	44	42	2	0
16	W	1	44	42	2	0
16	Y	1	44	42	2	0
16	Z	1	44	42	2	0
16	a	1	44	42	2	0

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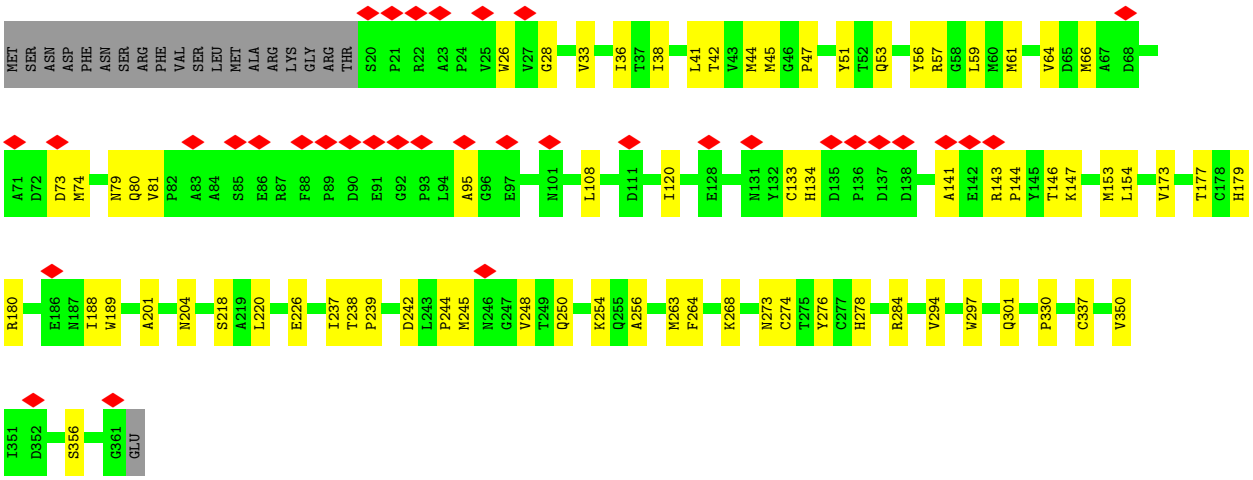
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	e	1	44	42	2	0
			Total	C	O	
16	i	1	44	42	2	0
			Total	C	O	
16	j	1	44	42	2	0

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.

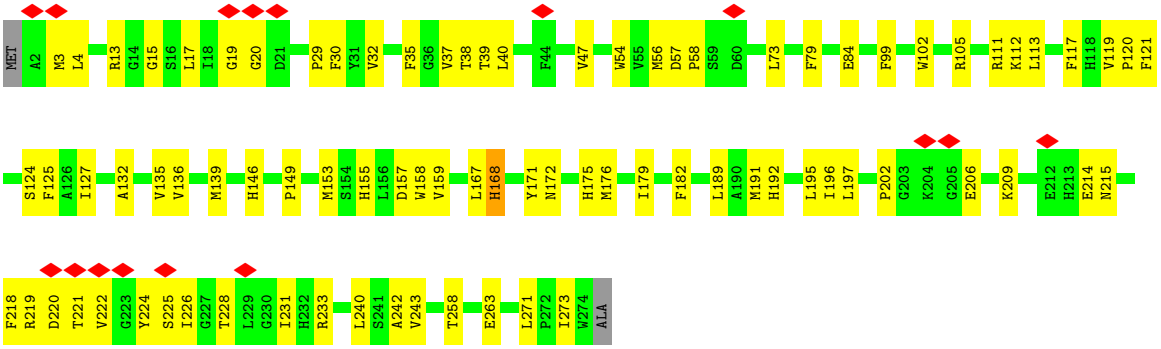
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



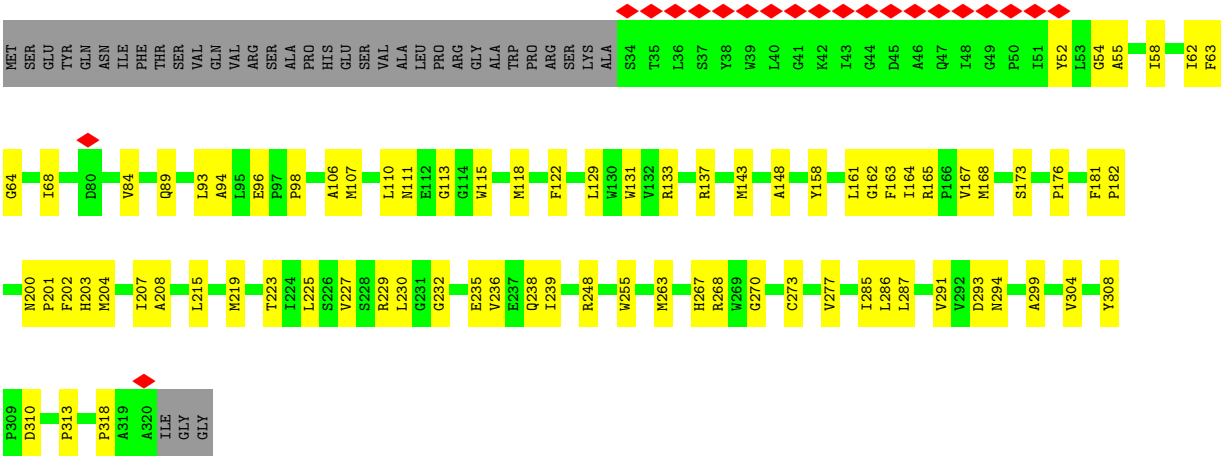
• Molecule 2: Reaction center protein L chain

Chain L:



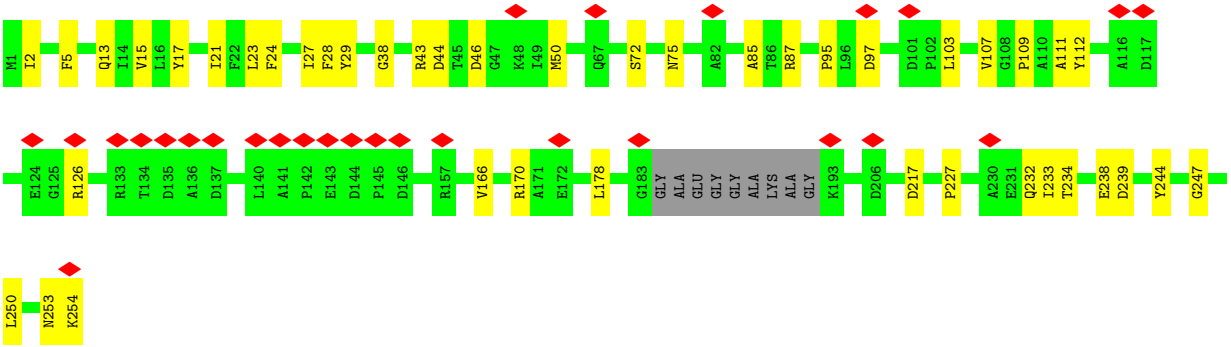
• Molecule 3: Reaction center protein M chain

Chain M:



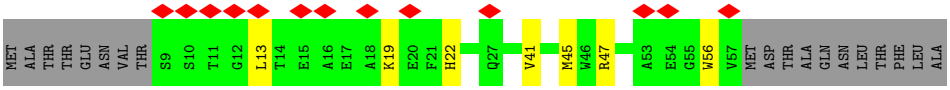
• Molecule 4: Photosynthetic reaction center H subunit

Chain H:



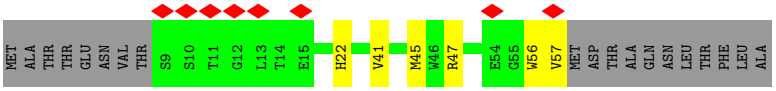
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain B:



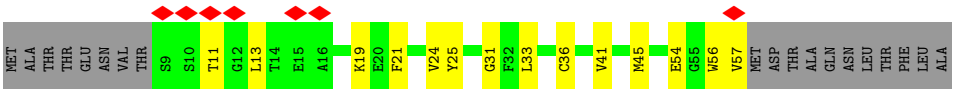
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain D:



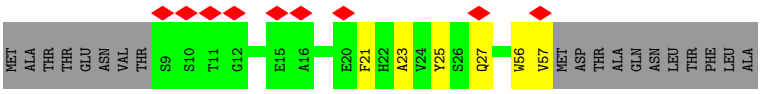
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain F:



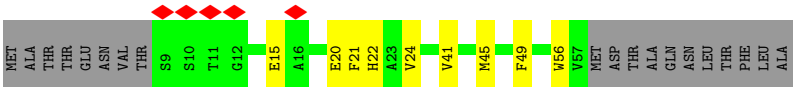
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain I:



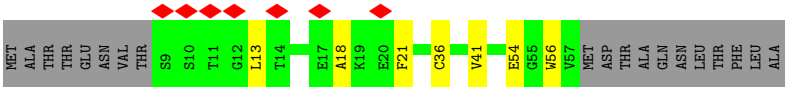
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain K:



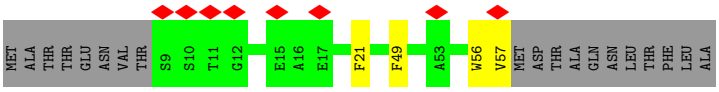
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain O:



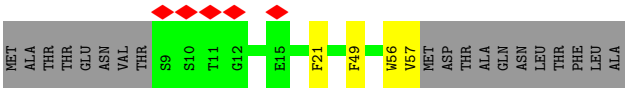
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain Q:



• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain S:

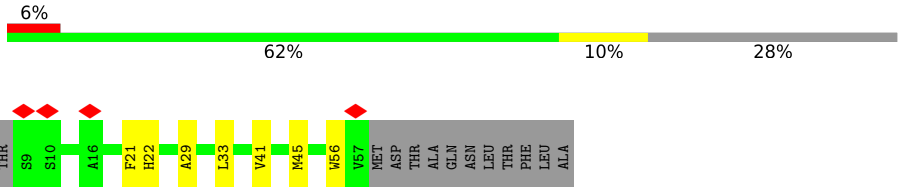


• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain U:

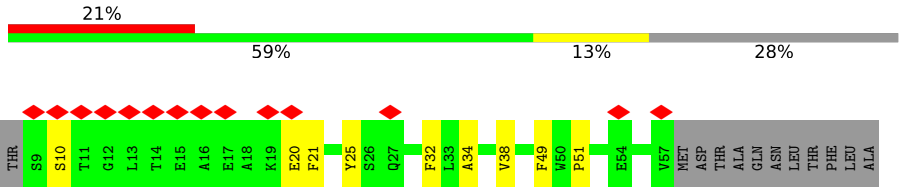
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain W:



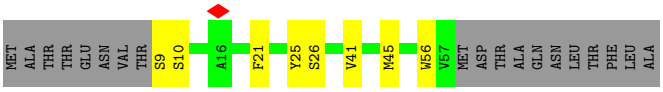
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain Y:



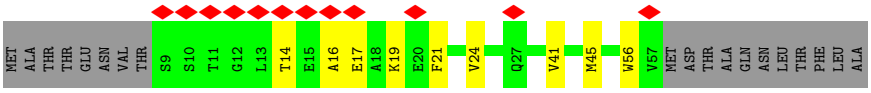
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain a:



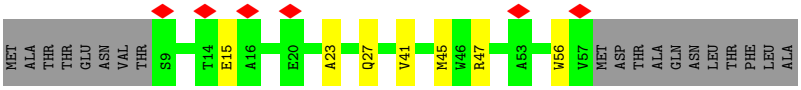
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain c:



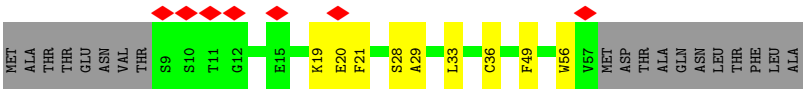
• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain e:



• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain g:

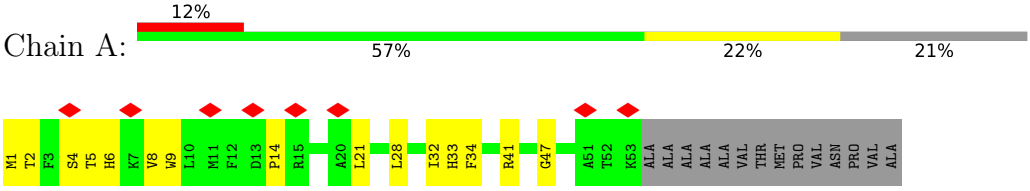


• Molecule 5: Beta subunit of light-harvesting 1 complex

Chain i:

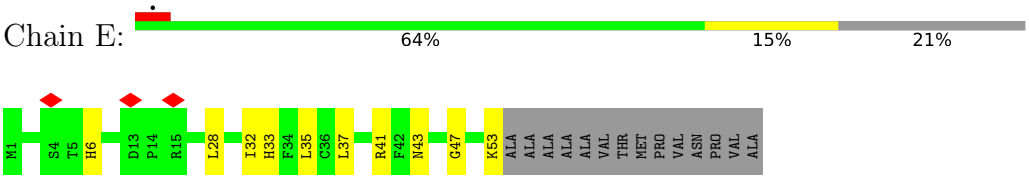
- Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain A:



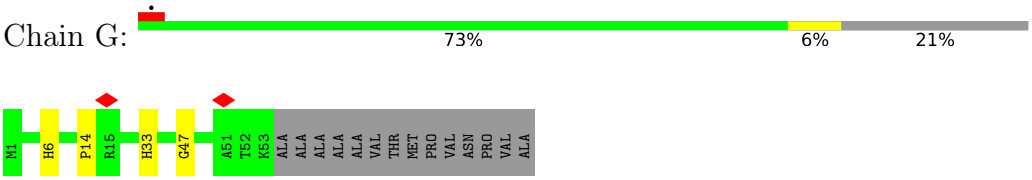
- Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain E:



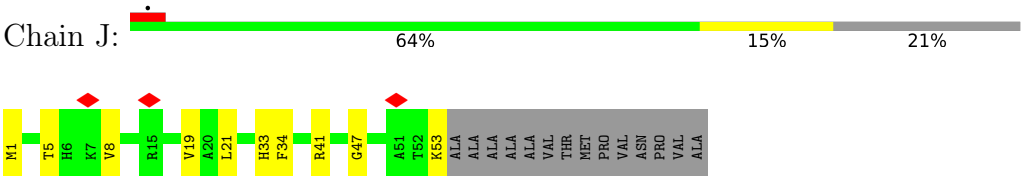
- Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain G:



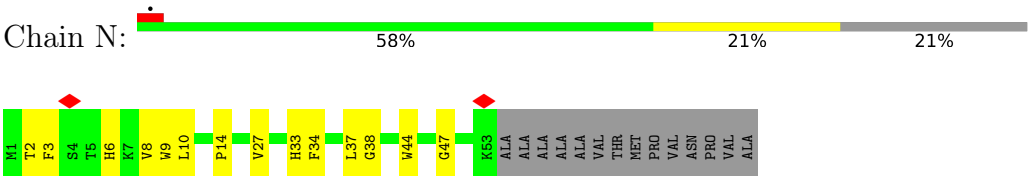
- Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain J:



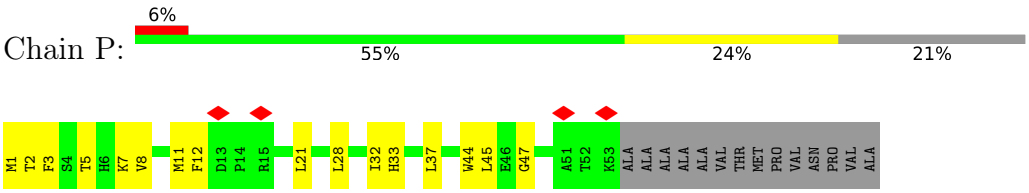
- Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain N:



- Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain P:

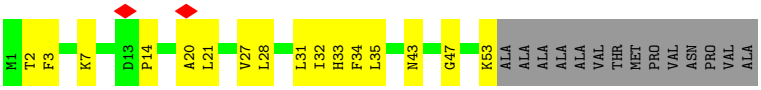


- Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain R:

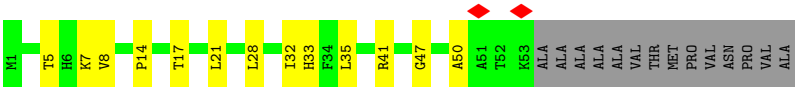
• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain T:



• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain V:

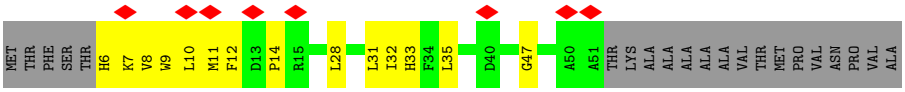


• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain X:

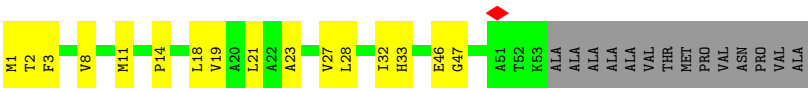
• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain Z:



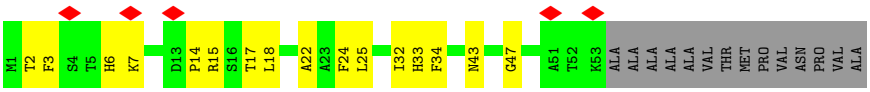
• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain b:



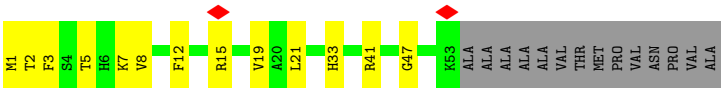
• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain d:



• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain f:



• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain h:

• Molecule 6: Alpha subunit of light-harvesting 1 complex

Chain j:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.289	Depositor
Minimum map value	-1.682	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.562	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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, MQ8, BCL, LMT, 8K6, MG, BPH, CRT, PGV, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	C	0.19	0/2693	0.42	0/3681
2	L	0.26	0/2250	0.45	0/3075
3	M	0.26	0/2357	0.43	0/3230
4	H	0.18	0/1952	0.37	0/2658
5	B	0.15	0/392	0.42	0/537
5	D	0.15	0/392	0.36	0/537
5	F	0.16	0/392	0.42	0/537
5	I	0.18	0/392	0.47	0/537
5	K	0.15	0/392	0.36	0/537
5	O	0.15	0/392	0.40	0/537
5	Q	0.17	0/392	0.38	0/537
5	S	0.25	0/392	0.39	0/537
5	U	0.16	0/392	0.34	0/537
5	W	0.19	0/392	0.43	0/537
5	Y	0.14	0/392	0.37	0/537
5	a	0.16	0/392	0.34	0/537
5	c	0.15	0/392	0.34	0/537
5	e	0.18	0/392	0.42	0/537
5	g	0.15	0/392	0.37	0/537
5	i	0.17	0/392	0.36	0/537
6	A	0.36	0/437	0.59	0/595
6	E	0.37	0/437	0.53	0/595
6	G	0.25	0/437	0.44	0/595
6	J	0.20	0/437	0.41	0/595
6	N	0.20	0/437	0.41	0/595
6	P	0.22	0/437	0.46	0/595
6	R	0.19	0/437	0.40	0/595
6	T	0.16	0/437	0.37	0/595
6	V	0.19	0/437	0.38	0/595
6	X	0.20	0/437	0.41	0/595
6	Z	0.27	0/381	0.59	1/520 (0.2%)
6	b	0.17	0/437	0.38	0/595

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	d	0.18	0/437	0.42	0/595
6	f	0.20	0/437	0.42	0/595
6	h	0.19	0/437	0.38	0/595
6	j	0.26	0/437	0.44	0/595
All	All	0.21	0/22460	0.42	1/30681 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Z	10	LEU	N-CA-C	-5.62	106.09	113.17

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	C	2618	0	2465	65	0
2	L	2163	0	2111	118	0
3	M	2269	0	2210	67	0
4	H	1906	0	1894	32	0
5	B	377	0	349	6	0
5	D	377	0	349	5	0
5	F	377	0	349	12	0
5	I	377	0	349	8	0
5	K	377	0	349	12	0
5	O	377	0	349	7	0
5	Q	377	0	349	5	0
5	S	377	0	349	4	0
5	U	377	0	349	7	0
5	W	377	0	349	6	0
5	Y	377	0	349	11	0
5	a	377	0	349	7	0
5	c	377	0	349	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	e	377	0	349	5	0
5	g	377	0	349	9	0
5	i	377	0	349	9	0
6	A	424	0	434	15	0
6	E	424	0	434	9	0
6	G	424	0	434	5	0
6	J	424	0	434	12	0
6	N	424	0	434	15	0
6	P	424	0	434	12	0
6	R	424	0	434	10	0
6	T	424	0	434	16	0
6	V	424	0	434	15	0
6	X	424	0	434	13	0
6	Z	369	0	374	14	0
6	b	424	0	434	17	0
6	d	424	0	434	20	0
6	f	424	0	434	14	0
6	h	424	0	434	17	0
6	j	424	0	434	19	0
7	C	172	0	120	16	0
8	C	3	0	0	0	0
8	H	1	0	0	0	0
9	C	38	0	47	0	0
9	H	102	0	152	12	0
9	L	22	0	25	40	0
9	M	88	0	127	11	0
9	R	51	0	76	2	0
9	Z	42	0	55	3	0
10	C	16	0	31	2	0
10	H	68	0	138	4	0
10	J	31	0	63	2	0
10	L	87	0	181	12	0
10	M	18	0	38	0	0
10	N	18	0	38	4	0
10	P	18	0	38	2	0
10	V	36	0	76	2	0
10	X	18	0	38	1	0
10	d	18	0	38	1	0
10	f	18	0	38	3	0
10	j	36	0	76	2	0
11	A	132	0	148	7	0
11	B	66	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	66	0	74	4	0
11	E	132	0	148	4	0
11	F	66	0	74	3	0
11	G	132	0	148	6	0
11	I	66	0	74	5	0
11	J	132	0	148	5	0
11	K	66	0	74	5	0
11	L	132	0	148	10	0
11	M	132	0	148	2	0
11	N	132	0	148	4	0
11	O	66	0	74	6	0
11	P	132	0	148	6	0
11	Q	66	0	74	4	0
11	R	132	0	148	5	0
11	S	66	0	74	2	0
11	T	132	0	148	7	0
11	U	66	0	74	5	0
11	V	132	0	148	3	0
11	W	66	0	74	3	0
11	X	132	0	148	8	0
11	Y	66	0	74	4	0
11	Z	66	0	74	3	0
11	a	66	0	74	4	0
11	b	132	0	148	7	0
11	c	66	0	74	7	0
11	d	132	0	148	7	0
11	e	66	0	74	1	0
11	f	132	0	148	11	0
11	g	66	0	74	5	0
11	h	132	0	148	8	0
11	i	66	0	74	7	0
11	j	132	0	148	6	0
12	L	65	0	76	4	0
12	M	65	0	76	3	0
13	L	32	0	37	0	0
14	M	1	0	0	0	0
15	M	53	0	72	7	0
16	A	44	0	60	6	0
16	B	44	0	60	4	0
16	E	44	0	60	10	0
16	I	44	0	60	10	0
16	K	44	0	60	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	M	44	0	60	3	0
16	N	44	0	60	6	0
16	P	44	0	60	7	0
16	R	44	0	60	8	0
16	U	44	0	60	8	0
16	W	44	0	60	5	0
16	Y	44	0	60	7	0
16	Z	44	0	60	15	0
16	a	44	0	60	5	0
16	e	44	0	60	5	0
16	i	44	0	60	8	0
16	j	44	0	60	8	0
All	All	26948	0	27598	686	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 13.

The worst 5 of 686 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)
2:L:195:LEU:HD23	9:L:410:PGV:H221	1.30	1.11
2:L:228:THR:HG22	9:L:410:PGV:H241	1.33	1.08
4:H:250:LEU:O	4:H:254:LYS:HD2	1.51	1.06
2:L:195:LEU:HD13	2:L:218:PHE:CE2	1.97	1.00
2:L:192:HIS:HA	9:L:410:PGV:H202	1.43	0.97

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	C	340/362 (94%)	325 (96%)	15 (4%)	0	100	100
2	L	271/275 (98%)	265 (98%)	6 (2%)	0	100	100
3	M	285/323 (88%)	277 (97%)	8 (3%)	0	100	100
4	H	241/254 (95%)	237 (98%)	4 (2%)	0	100	100
5	B	47/68 (69%)	47 (100%)	0	0	100	100
5	D	47/68 (69%)	47 (100%)	0	0	100	100
5	F	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	I	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	K	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	O	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	Q	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	S	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	U	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	W	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	Y	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	a	47/68 (69%)	47 (100%)	0	0	100	100
5	c	47/68 (69%)	47 (100%)	0	0	100	100
5	e	47/68 (69%)	45 (96%)	2 (4%)	0	100	100
5	g	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
5	i	47/68 (69%)	46 (98%)	1 (2%)	0	100	100
6	A	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
6	E	51/67 (76%)	51 (100%)	0	0	100	100
6	G	51/67 (76%)	51 (100%)	0	0	100	100
6	J	51/67 (76%)	51 (100%)	0	0	100	100
6	N	51/67 (76%)	51 (100%)	0	0	100	100
6	P	51/67 (76%)	51 (100%)	0	0	100	100
6	R	51/67 (76%)	51 (100%)	0	0	100	100
6	T	51/67 (76%)	51 (100%)	0	0	100	100
6	V	51/67 (76%)	51 (100%)	0	0	100	100
6	X	51/67 (76%)	51 (100%)	0	0	100	100
6	Z	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
6	b	51/67 (76%)	51 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	d	51/67 (76%)	51 (100%)	0	0	100	100
6	f	51/67 (76%)	51 (100%)	0	0	100	100
6	h	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
6	j	51/67 (76%)	51 (100%)	0	0	100	100
All	All	2698/3374 (80%)	2645 (98%)	53 (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	C	278/296 (94%)	278 (100%)	0	100	100
2	L	218/219 (100%)	217 (100%)	1 (0%)	81	91
3	M	225/254 (89%)	225 (100%)	0	100	100
4	H	200/202 (99%)	200 (100%)	0	100	100
5	B	35/51 (69%)	35 (100%)	0	100	100
5	D	35/51 (69%)	35 (100%)	0	100	100
5	F	35/51 (69%)	35 (100%)	0	100	100
5	I	35/51 (69%)	35 (100%)	0	100	100
5	K	35/51 (69%)	35 (100%)	0	100	100
5	O	35/51 (69%)	35 (100%)	0	100	100
5	Q	35/51 (69%)	35 (100%)	0	100	100
5	S	35/51 (69%)	35 (100%)	0	100	100
5	U	35/51 (69%)	35 (100%)	0	100	100
5	W	35/51 (69%)	35 (100%)	0	100	100
5	Y	35/51 (69%)	35 (100%)	0	100	100
5	a	35/51 (69%)	35 (100%)	0	100	100
5	c	35/51 (69%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	35/51 (69%)	35 (100%)	0	100	100
5	g	35/51 (69%)	35 (100%)	0	100	100
5	i	35/51 (69%)	35 (100%)	0	100	100
6	A	45/53 (85%)	45 (100%)	0	100	100
6	E	45/53 (85%)	45 (100%)	0	100	100
6	G	45/53 (85%)	45 (100%)	0	100	100
6	J	45/53 (85%)	45 (100%)	0	100	100
6	N	45/53 (85%)	45 (100%)	0	100	100
6	P	45/53 (85%)	45 (100%)	0	100	100
6	R	45/53 (85%)	45 (100%)	0	100	100
6	T	45/53 (85%)	45 (100%)	0	100	100
6	V	45/53 (85%)	45 (100%)	0	100	100
6	X	45/53 (85%)	45 (100%)	0	100	100
6	Z	38/53 (72%)	38 (100%)	0	100	100
6	b	45/53 (85%)	45 (100%)	0	100	100
6	d	45/53 (85%)	45 (100%)	0	100	100
6	f	45/53 (85%)	45 (100%)	0	100	100
6	h	45/53 (85%)	45 (100%)	0	100	100
6	j	45/53 (85%)	45 (100%)	0	100	100
All	All	2194/2635 (83%)	2193 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	168	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
6	J	6	HIS
6	R	48	ASN
6	j	48	ASN
6	Z	48	ASN
6	f	6	HIS

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 111 ligands modelled in this entry, 5 are monoatomic - leaving 106 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	$\#\|Z\| > 2$
11	BCL	V	101	6	69,74,74	1.83	16 (23%)	83,115,115	2.61	24 (28%)
15	MQ8	M	405	-	54,54,54	0.40	0	66,69,69	0.38	0
11	BCL	S	101	5	69,74,74	1.86	19 (27%)	83,115,115	2.24	28 (33%)
11	BCL	E	102	6	69,74,74	1.80	19 (27%)	83,115,115	2.61	24 (28%)
10	8K6	j	104	-	17,17,17	0.09	0	16,16,16	0.11	0
11	BCL	G	102	6	69,74,74	1.76	17 (24%)	83,115,115	2.60	26 (31%)
11	BCL	N	102	6	69,74,74	1.77	18 (26%)	83,115,115	2.81	29 (34%)
16	CRT	I	102	-	41,43,43	1.91	12 (29%)	50,54,54	1.92	16 (32%)
11	BCL	N	101	6	69,74,74	1.84	18 (26%)	83,115,115	2.71	27 (32%)
10	8K6	H	304	-	17,17,17	0.09	0	16,16,16	0.07	0
9	PGV	C	508	-	37,37,50	1.06	2 (5%)	40,43,56	1.19	3 (7%)
11	BCL	P	101	6	69,74,74	1.84	17 (24%)	83,115,115	2.74	25 (30%)
11	BCL	i	101	5	69,74,74	1.85	16 (23%)	83,115,115	2.35	24 (28%)
11	BCL	A	102	6	69,74,74	1.80	19 (27%)	83,115,115	2.65	28 (33%)
10	8K6	j	105	-	17,17,17	0.08	0	16,16,16	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
11	BCL	R	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.60	25 (30%)
10	8K6	L	409	-	17,17,17	0.08	0	16,16,16	0.16	0
10	8K6	f	103	-	17,17,17	0.08	0	16,16,16	0.10	0
10	8K6	X	103	-	17,17,17	0.08	0	16,16,16	0.08	0
12	BPH	M	404	-	59,70,70	1.06	3 (5%)	61,101,101	1.99	9 (14%)
11	BCL	R	101	6	69,74,74	1.90	16 (23%)	83,115,115	2.47	24 (28%)
16	CRT	M	406	-	41,43,43	1.93	12 (29%)	50,54,54	1.49	11 (22%)
7	HEC	C	503	1	50,50,50	1.90	5 (10%)	68,82,82	1.45	8 (11%)
11	BCL	U	101	5	69,74,74	1.91	18 (26%)	83,115,115	2.44	25 (30%)
11	BCL	j	103	6	69,74,74	1.81	18 (26%)	83,115,115	2.65	24 (28%)
11	BCL	M	402	3	69,74,74	1.84	16 (23%)	83,115,115	2.68	22 (26%)
16	CRT	Y	102	-	41,43,43	1.98	12 (29%)	50,54,54	1.74	16 (32%)
10	8K6	H	303	-	16,16,17	0.08	0	15,15,16	0.12	0
16	CRT	U	102	-	41,43,43	1.94	12 (29%)	50,54,54	1.71	14 (28%)
11	BCL	Z	101	6	69,74,74	1.84	18 (26%)	83,115,115	2.55	26 (31%)
16	CRT	B	102	-	41,43,43	1.92	12 (29%)	50,54,54	1.68	12 (24%)
11	BCL	E	101	6	69,74,74	1.86	21 (30%)	83,115,115	2.71	27 (32%)
10	8K6	N	104	-	17,17,17	0.08	0	16,16,16	0.12	0
7	HEC	C	504	1	50,50,50	1.77	5 (10%)	68,82,82	1.46	9 (13%)
16	CRT	E	103	-	41,43,43	1.90	12 (29%)	50,54,54	1.87	16 (32%)
11	BCL	b	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.64	25 (30%)
11	BCL	b	101	6	69,74,74	1.86	17 (24%)	83,115,115	2.52	27 (32%)
10	8K6	L	407	-	17,17,17	0.09	0	16,16,16	0.08	0
7	HEC	C	502	1	50,50,50	2.32	5 (10%)	68,82,82	1.34	7 (10%)
11	BCL	J	101	6	69,74,74	1.87	18 (26%)	83,115,115	2.58	26 (31%)
11	BCL	g	101	5	69,74,74	1.83	16 (23%)	83,115,115	2.46	23 (27%)
11	BCL	I	101	5	69,74,74	1.86	18 (26%)	83,115,115	2.40	24 (28%)
10	8K6	L	404	-	14,14,17	0.08	0	13,13,16	0.14	0
16	CRT	R	103	-	41,43,43	1.92	12 (29%)	50,54,54	1.67	13 (26%)
9	PGV	M	408	-	41,41,50	1.04	2 (4%)	44,46,56	1.20	5 (11%)
10	8K6	C	509	-	15,15,17	0.09	0	14,14,16	0.11	0
11	BCL	d	102	6	69,74,74	1.79	17 (24%)	83,115,115	2.57	25 (30%)
10	8K6	H	305	-	17,17,17	0.09	0	16,16,16	0.10	0
16	CRT	e	102	-	41,43,43	1.93	12 (29%)	50,54,54	1.67	13 (26%)
10	8K6	L	405	-	17,17,17	0.09	0	16,16,16	0.11	0
13	LMT	L	408	-	33,33,36	0.39	0	44,44,47	0.78	1 (2%)
10	8K6	H	306	-	14,14,17	0.08	0	13,13,16	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	PGV	H	301	-	50,50,50	0.91	2 (4%)	53,56,56	1.09	4 (7%)
10	8K6	V	104	-	17,17,17	0.09	0	16,16,16	0.07	0
11	BCL	L	402	2	69,74,74	1.86	17 (24%)	83,115,115	2.57	27 (32%)
11	BCL	A	101	6	69,74,74	1.89	18 (26%)	83,115,115	2.65	26 (31%)
11	BCL	a	101	5	69,74,74	1.87	15 (21%)	83,115,115	2.35	25 (30%)
11	BCL	j	102	6	69,74,74	1.89	18 (26%)	83,115,115	2.67	26 (31%)
11	BCL	f	102	6	69,74,74	1.76	17 (24%)	83,115,115	2.54	24 (28%)
11	BCL	f	101	6	69,74,74	1.87	17 (24%)	83,115,115	2.62	24 (28%)
10	8K6	P	104	-	17,17,17	0.09	0	16,16,16	0.10	0
11	BCL	e	101	5	69,74,74	1.87	15 (21%)	83,115,115	2.43	25 (30%)
11	BCL	K	101	5	69,74,74	1.86	17 (24%)	83,115,115	2.41	25 (30%)
11	BCL	X	101	6	69,74,74	1.85	20 (28%)	83,115,115	2.71	27 (32%)
11	BCL	F	101	5	69,74,74	1.89	16 (23%)	83,115,115	2.34	29 (34%)
10	8K6	d	103	-	17,17,17	0.08	0	16,16,16	0.07	0
16	CRT	K	102	-	41,43,43	1.96	12 (29%)	50,54,54	1.73	14 (28%)
16	CRT	Z	102	-	41,43,43	2.02	12 (29%)	50,54,54	2.02	18 (36%)
9	PGV	M	407	-	45,45,50	0.98	2 (4%)	49,50,56	1.03	4 (8%)
11	BCL	d	101	6	69,74,74	1.86	18 (26%)	83,115,115	2.61	27 (32%)
9	PGV	R	104	-	50,50,50	0.92	2 (4%)	53,56,56	0.95	2 (3%)
11	BCL	J	102	6	69,74,74	1.78	16 (23%)	83,115,115	2.62	29 (34%)
11	BCL	G	101	6	69,74,74	1.85	17 (24%)	83,115,115	2.65	26 (31%)
16	CRT	P	103	-	41,43,43	1.91	12 (29%)	50,54,54	1.64	13 (26%)
10	8K6	L	406	-	17,17,17	0.09	0	16,16,16	0.10	0
11	BCL	h	102	6	69,74,74	1.78	18 (26%)	83,115,115	2.64	24 (28%)
11	BCL	L	401	2	69,74,74	1.85	17 (24%)	83,115,115	2.62	24 (28%)
11	BCL	h	101	6	69,74,74	1.83	16 (23%)	83,115,115	2.58	22 (26%)
11	BCL	B	101	5	69,74,74	1.85	16 (23%)	83,115,115	2.34	26 (31%)
9	PGV	H	302	-	50,50,50	0.91	2 (4%)	53,56,56	1.05	3 (5%)
11	BCL	c	101	5	69,74,74	1.84	18 (26%)	83,115,115	2.41	25 (30%)
11	BCL	V	102	6	69,74,74	1.77	19 (27%)	83,115,115	2.58	26 (31%)
11	BCL	T	102	6	69,74,74	1.79	17 (24%)	83,115,115	2.63	27 (32%)
16	CRT	j	101	-	41,43,43	1.94	12 (29%)	50,54,54	1.69	13 (26%)
11	BCL	T	101	6	69,74,74	1.86	16 (23%)	83,115,115	2.57	25 (30%)
7	HEC	C	501	1	50,50,50	1.82	5 (10%)	68,82,82	1.35	7 (10%)
16	CRT	a	102	-	41,43,43	1.91	12 (29%)	50,54,54	1.65	14 (28%)
10	8K6	M	409	-	17,17,17	0.07	0	16,16,16	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	CRT	i	102	-	41,43,43	1.90	12 (29%)	50,54,54	1.65	14 (28%)
11	BCL	O	101	5	69,74,74	1.88	17 (24%)	83,115,115	2.37	26 (31%)
11	BCL	P	102	6	69,74,74	1.76	17 (24%)	83,115,115	2.72	27 (32%)
11	BCL	Q	101	5	69,74,74	1.86	17 (24%)	83,115,115	2.36	27 (32%)
10	8K6	J	103	-	12,12,17	0.08	0	11,11,16	0.10	0
9	PGV	Z	103	-	41,41,50	1.00	2 (4%)	44,47,56	1.07	4 (9%)
11	BCL	W	101	5	69,74,74	1.85	17 (24%)	83,115,115	2.38	24 (28%)
16	CRT	N	103	-	41,43,43	1.92	12 (29%)	50,54,54	1.65	13 (26%)
11	BCL	M	403	3	69,74,74	1.95	18 (26%)	83,115,115	2.91	26 (31%)
10	8K6	V	103	-	17,17,17	0.08	0	16,16,16	0.07	0
12	BPH	L	403	-	59,70,70	1.08	3 (5%)	61,101,101	1.94	8 (13%)
16	CRT	W	102	-	41,43,43	1.91	12 (29%)	50,54,54	1.63	13 (26%)
11	BCL	X	102	6	69,74,74	1.80	18 (26%)	83,115,115	2.59	24 (28%)
9	PGV	L	410	-	21,21,50	1.28	2 (9%)	23,23,56	1.69	5 (21%)
10	8K6	J	104	-	17,17,17	0.07	0	16,16,16	0.11	0
11	BCL	Y	101	5	69,74,74	1.86	19 (27%)	83,115,115	2.38	30 (36%)
16	CRT	A	103	-	41,43,43	1.90	12 (29%)	50,54,54	1.69	13 (26%)
11	BCL	D	101	5	69,74,74	1.89	18 (26%)	83,115,115	2.42	26 (31%)

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
11	BCL	V	101	6	-	23/41/137/137	-
15	MQ8	M	405	-	-	12/47/67/67	0/2/2/2
11	BCL	S	101	5	-	13/41/137/137	-
11	BCL	E	102	6	-	17/41/137/137	-
10	8K6	j	104	-	-	2/15/15/15	-
11	BCL	G	102	6	-	19/41/137/137	-
11	BCL	N	102	6	-	15/41/137/137	-
16	CRT	I	102	-	-	5/51/51/51	-
11	BCL	N	101	6	-	20/41/137/137	-
10	8K6	H	304	-	-	0/15/15/15	-
9	PGV	C	508	-	-	7/42/42/55	-
11	BCL	P	101	6	-	21/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	i	101	5	-	16/41/137/137	-
11	BCL	A	102	6	-	15/41/137/137	-
10	8K6	j	105	-	-	2/15/15/15	-
11	BCL	R	102	6	-	15/41/137/137	-
10	8K6	L	409	-	-	0/15/15/15	-
10	8K6	f	103	-	-	1/15/15/15	-
10	8K6	X	103	-	-	1/15/15/15	-
12	BPH	M	404	-	-	8/37/105/105	0/5/6/6
11	BCL	R	101	6	-	19/41/137/137	-
16	CRT	M	406	-	-	0/51/51/51	-
7	HEC	C	503	1	-	3/14/54/54	-
11	BCL	U	101	5	-	17/41/137/137	-
11	BCL	j	103	6	-	16/41/137/137	-
11	BCL	M	402	3	-	14/41/137/137	-
16	CRT	Y	102	-	-	3/51/51/51	-
10	8K6	H	303	-	-	2/14/14/15	-
16	CRT	U	102	-	-	7/51/51/51	-
11	BCL	Z	101	6	-	24/41/137/137	-
16	CRT	B	102	-	-	5/51/51/51	-
11	BCL	E	101	6	-	25/41/137/137	-
10	8K6	N	104	-	-	0/15/15/15	-
7	HEC	C	504	1	1/1/3/7	6/14/54/54	-
16	CRT	E	103	-	-	3/51/51/51	-
11	BCL	b	102	6	-	24/41/137/137	-
11	BCL	b	101	6	-	24/41/137/137	-
10	8K6	L	407	-	-	1/15/15/15	-
7	HEC	C	502	1	-	2/14/54/54	-
11	BCL	J	101	6	-	21/41/137/137	-
11	BCL	g	101	5	-	15/41/137/137	-
11	BCL	I	101	5	-	15/41/137/137	-
10	8K6	L	404	-	-	0/12/12/15	-
16	CRT	R	103	-	-	4/51/51/51	-
9	PGV	M	408	-	-	11/43/43/55	-
10	8K6	C	509	-	-	2/13/13/15	-
11	BCL	d	102	6	-	22/41/137/137	-
10	8K6	H	305	-	-	0/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CRT	e	102	-	-	6/51/51/51	-
10	8K6	L	405	-	-	1/15/15/15	-
13	LMT	L	408	-	-	7/18/58/61	0/2/2/2
10	8K6	H	306	-	-	0/12/12/15	-
9	PGV	H	301	-	-	21/55/55/55	-
10	8K6	V	104	-	-	0/15/15/15	-
11	BCL	L	402	2	-	8/41/137/137	-
11	BCL	A	101	6	-	24/41/137/137	-
11	BCL	a	101	5	-	14/41/137/137	-
11	BCL	j	102	6	-	15/41/137/137	-
11	BCL	f	102	6	-	20/41/137/137	-
11	BCL	f	101	6	-	23/41/137/137	-
10	8K6	P	104	-	-	1/15/15/15	-
11	BCL	e	101	5	-	20/41/137/137	-
11	BCL	K	101	5	-	16/41/137/137	-
11	BCL	X	101	6	-	22/41/137/137	-
11	BCL	F	101	5	-	18/41/137/137	-
10	8K6	d	103	-	-	3/15/15/15	-
16	CRT	K	102	-	-	3/51/51/51	-
16	CRT	Z	102	-	-	11/51/51/51	-
9	PGV	M	407	-	-	13/47/47/55	-
11	BCL	d	101	6	-	14/41/137/137	-
9	PGV	R	104	-	-	15/55/55/55	-
11	BCL	J	102	6	-	17/41/137/137	-
11	BCL	G	101	6	-	17/41/137/137	-
16	CRT	P	103	-	-	4/51/51/51	-
10	8K6	L	406	-	-	2/15/15/15	-
11	BCL	h	102	6	-	22/41/137/137	-
11	BCL	L	401	2	-	10/41/137/137	-
11	BCL	h	101	6	-	12/41/137/137	-
11	BCL	B	101	5	-	15/41/137/137	-
9	PGV	H	302	-	-	12/55/55/55	-
11	BCL	c	101	5	-	13/41/137/137	-
11	BCL	V	102	6	-	19/41/137/137	-
11	BCL	T	102	6	-	17/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CRT	j	101	-	-	5/51/51/51	-
11	BCL	T	101	6	-	22/41/137/137	-
7	HEC	C	501	1	1/1/3/7	2/14/54/54	-
16	CRT	a	102	-	-	5/51/51/51	-
10	8K6	M	409	-	-	0/15/15/15	-
16	CRT	i	102	-	-	4/51/51/51	-
11	BCL	O	101	5	-	12/41/137/137	-
11	BCL	P	102	6	-	18/41/137/137	-
11	BCL	Q	101	5	-	16/41/137/137	-
10	8K6	J	103	-	-	0/10/10/15	-
9	PGV	Z	103	-	-	11/46/46/55	-
11	BCL	W	101	5	-	17/41/137/137	-
16	CRT	N	103	-	-	4/51/51/51	-
11	BCL	M	403	3	-	17/41/137/137	-
10	8K6	V	103	-	-	1/15/15/15	-
12	BPH	L	403	-	-	4/37/105/105	0/5/6/6
16	CRT	W	102	-	-	7/51/51/51	-
11	BCL	X	102	6	-	20/41/137/137	-
9	PGV	L	410	-	-	9/23/23/55	-
10	8K6	J	104	-	-	1/15/15/15	-
11	BCL	Y	101	5	-	17/41/137/137	-
16	CRT	A	103	-	-	4/51/51/51	-
11	BCL	D	101	5	-	18/41/137/137	-

The worst 5 of 1133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	502	HEC	FE-ND	8.36	2.20	1.94
7	C	502	HEC	C3D-C2D	8.05	1.53	1.36
7	C	504	HEC	C3D-C2D	7.92	1.53	1.36
7	C	501	HEC	C3D-C2D	7.78	1.53	1.36
7	C	503	HEC	C3D-C2D	7.74	1.53	1.36

The worst 5 of 1622 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	N	102	BCL	C2B-C1B-NB	13.35	119.18	110.23
11	j	103	BCL	C2B-C1B-NB	12.50	118.61	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	102	BCL	C2B-C1B-NB	12.41	118.55	110.23
11	P	102	BCL	C2B-C1B-NB	12.25	118.44	110.23
11	G	102	BCL	C2B-C1B-NB	12.11	118.35	110.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	501	HEC	NA
7	C	504	HEC	NA

5 of 1146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	410	PGV	C01-C02-C03-O11
9	L	410	PGV	O01-C02-C03-O11
9	M	407	PGV	C03-O11-P-O12
9	M	407	PGV	C03-O11-P-O14
9	H	301	PGV	C03-O11-P-O14

There are no ring outliers.

98 monomers are involved in 393 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	V	101	BCL	3	0
15	M	405	MQ8	7	0
11	S	101	BCL	2	0
11	E	102	BCL	3	0
10	j	104	8K6	1	0
11	G	102	BCL	2	0
16	I	102	CRT	10	0
11	N	101	BCL	4	0
10	H	304	8K6	2	0
11	P	101	BCL	3	0
11	i	101	BCL	7	0
11	A	102	BCL	4	0
10	j	105	8K6	1	0
11	R	102	BCL	2	0
10	L	409	8K6	5	0
10	f	103	8K6	3	0
10	X	103	8K6	1	0
12	M	404	BPH	3	0
11	R	101	BCL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	M	406	CRT	3	0
7	C	503	HEC	6	0
11	U	101	BCL	5	0
11	j	103	BCL	2	0
11	M	402	BCL	2	0
16	Y	102	CRT	7	0
10	H	303	8K6	2	0
16	U	102	CRT	8	0
11	Z	101	BCL	3	0
16	B	102	CRT	4	0
11	E	101	BCL	1	0
10	N	104	8K6	4	0
7	C	504	HEC	1	0
16	E	103	CRT	10	0
11	b	102	BCL	3	0
11	b	101	BCL	4	0
10	L	407	8K6	2	0
7	C	502	HEC	8	0
11	J	101	BCL	3	0
11	g	101	BCL	5	0
11	I	101	BCL	5	0
10	L	404	8K6	2	0
16	R	103	CRT	8	0
9	M	408	PGV	7	0
10	C	509	8K6	2	0
11	d	102	BCL	3	0
16	e	102	CRT	5	0
10	L	405	8K6	2	0
9	H	301	PGV	7	0
10	V	104	8K6	1	0
11	L	402	BCL	4	0
11	A	101	BCL	3	0
11	a	101	BCL	4	0
11	j	102	BCL	4	0
11	f	102	BCL	5	0
11	f	101	BCL	6	0
10	P	104	8K6	2	0
11	e	101	BCL	1	0
11	K	101	BCL	5	0
11	X	101	BCL	4	0
11	F	101	BCL	3	0
10	d	103	8K6	1	0

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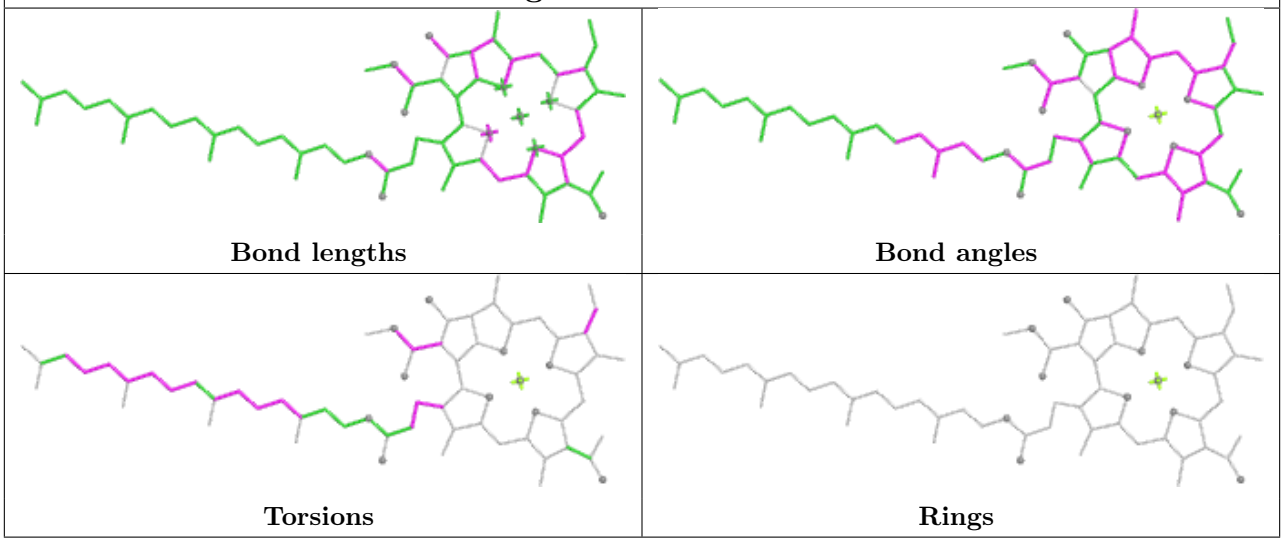
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	102	CRT	8	0
16	Z	102	CRT	15	0
9	M	407	PGV	4	0
11	d	101	BCL	4	0
9	R	104	PGV	2	0
11	J	102	BCL	2	0
11	G	101	BCL	4	0
16	P	103	CRT	7	0
10	L	406	8K6	1	0
11	h	102	BCL	3	0
11	L	401	BCL	8	0
11	h	101	BCL	5	0
11	B	101	BCL	2	0
9	H	302	PGV	5	0
11	c	101	BCL	7	0
11	T	102	BCL	2	0
16	j	101	CRT	8	0
11	T	101	BCL	5	0
7	C	501	HEC	1	0
16	a	102	CRT	5	0
16	i	102	CRT	8	0
11	O	101	BCL	6	0
11	P	102	BCL	3	0
11	Q	101	BCL	4	0
10	J	103	8K6	1	0
9	Z	103	PGV	3	0
11	W	101	BCL	3	0
16	N	103	CRT	6	0
10	V	103	8K6	1	0
12	L	403	BPH	4	0
16	W	102	CRT	5	0
11	X	102	BCL	4	0
9	L	410	PGV	40	0
10	J	104	8K6	2	0
11	Y	101	BCL	4	0
16	A	103	CRT	6	0
11	D	101	BCL	4	0

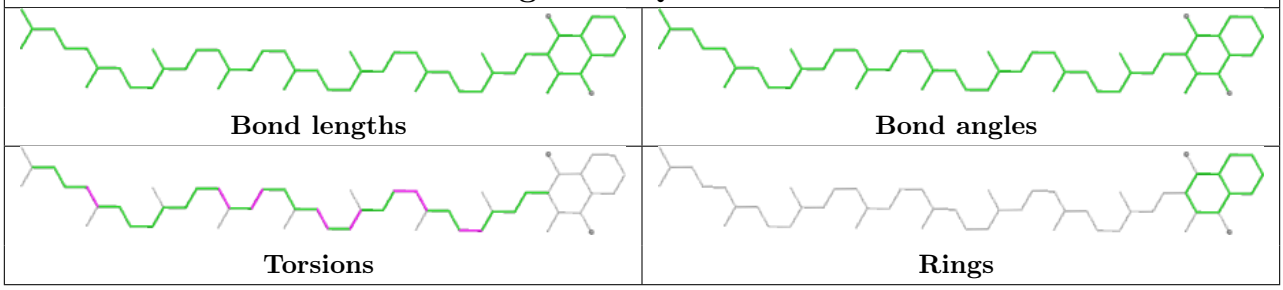
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

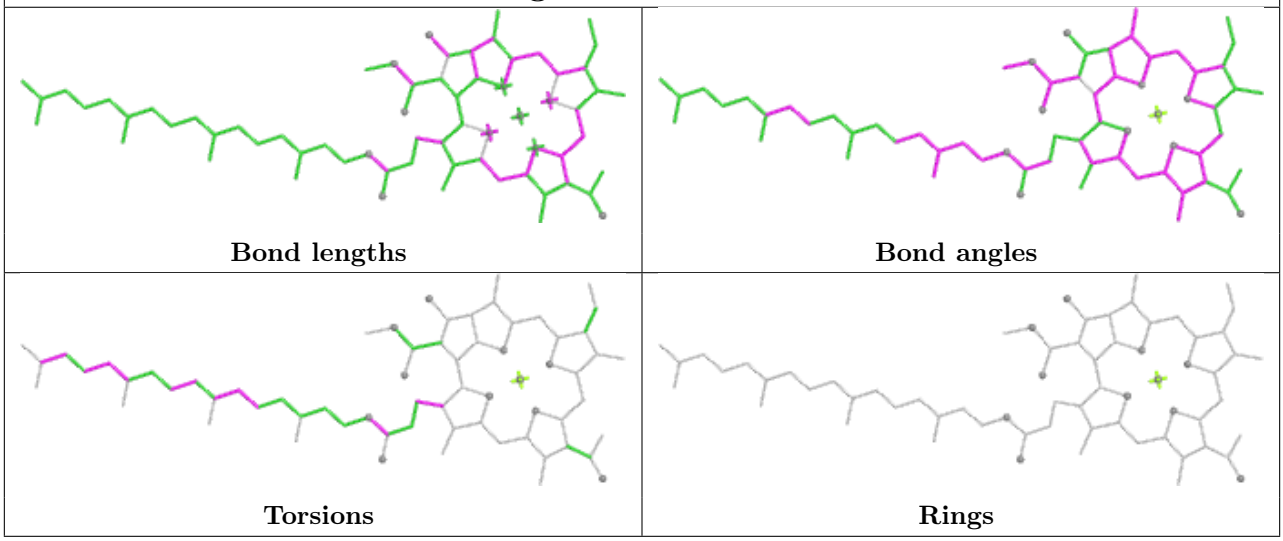
Ligand BCL V 101



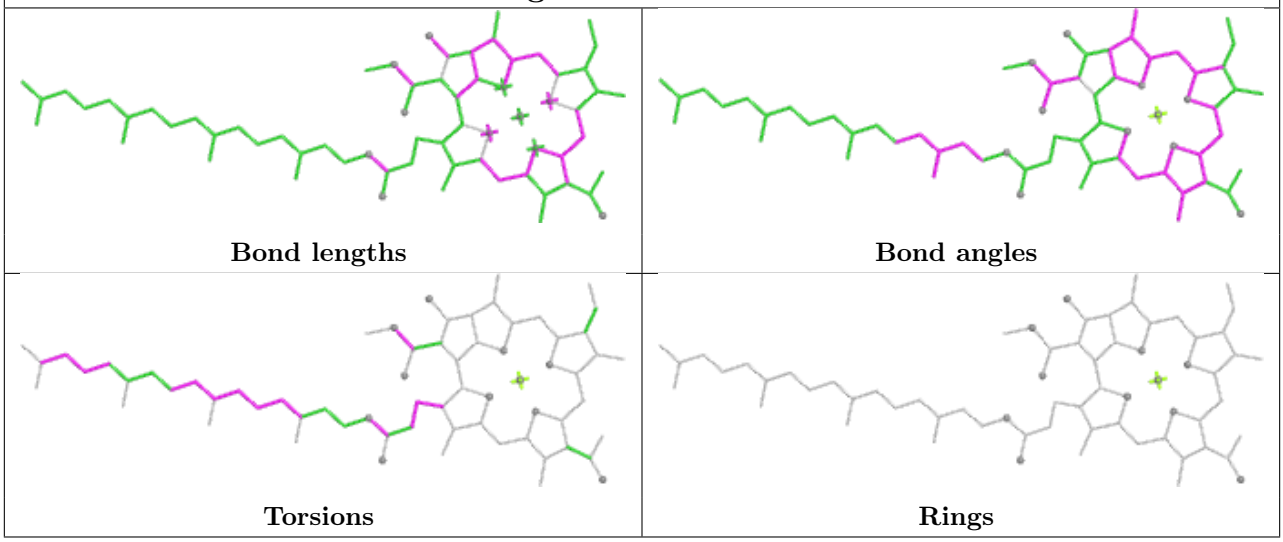
Ligand MQ8 M 405



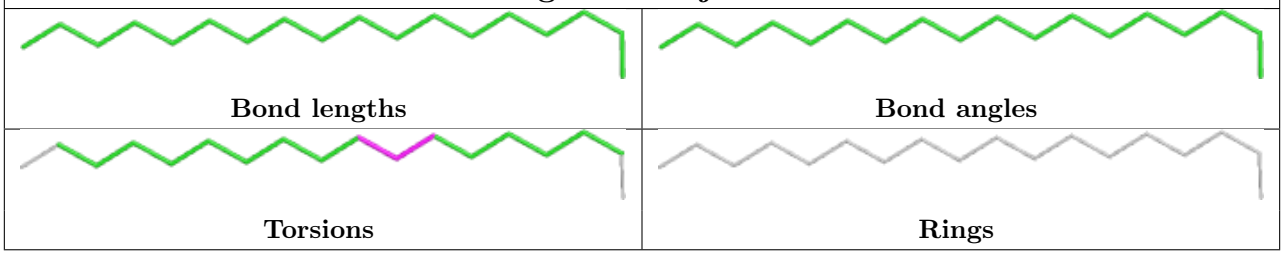
Ligand BCL S 101



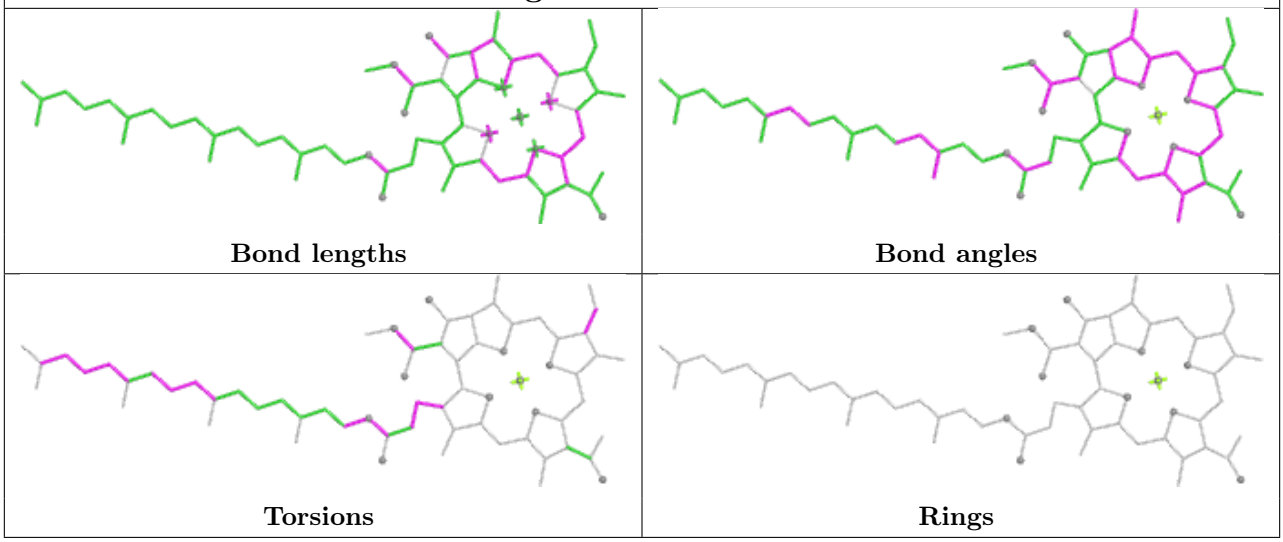
Ligand BCL E 102



Ligand 8K6 j 104



Ligand BCL G 102



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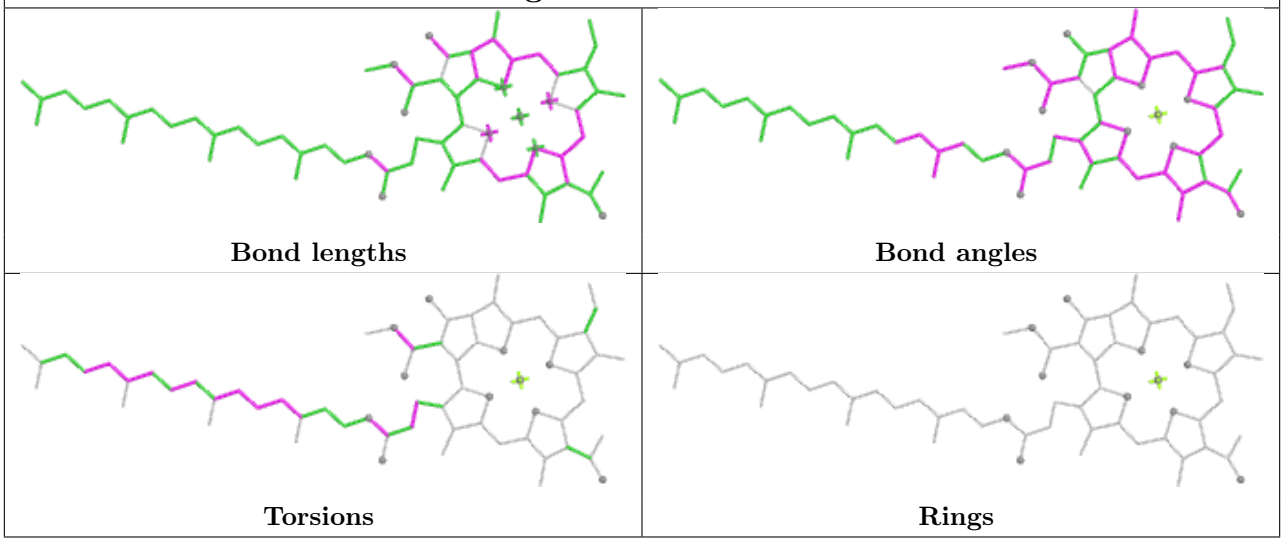
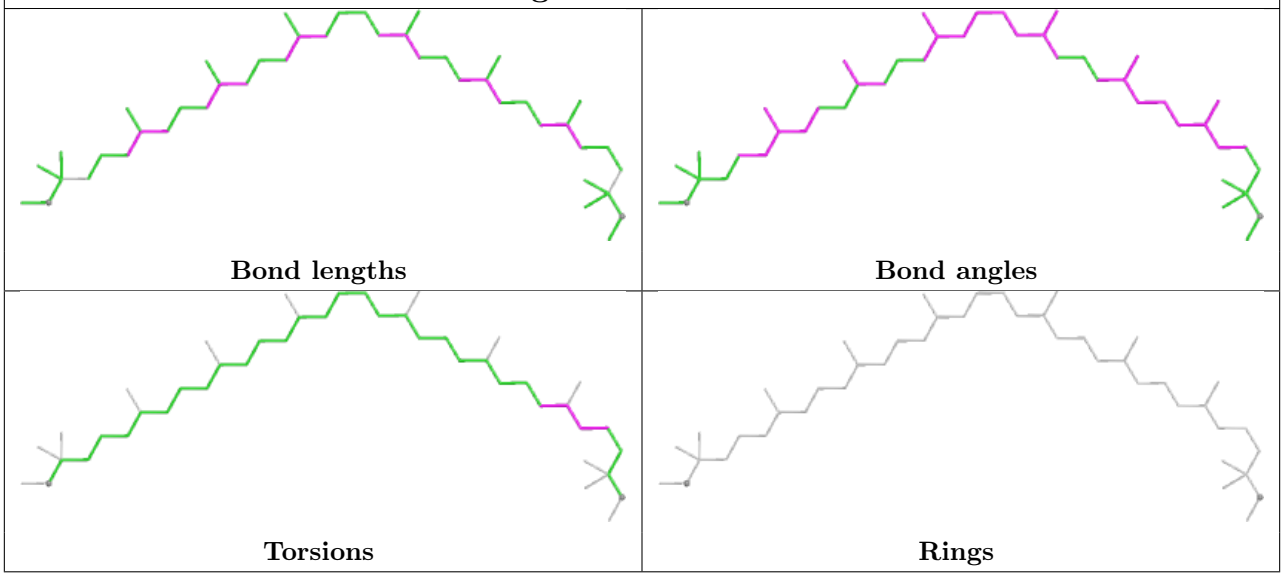


Ligand CRT I 102



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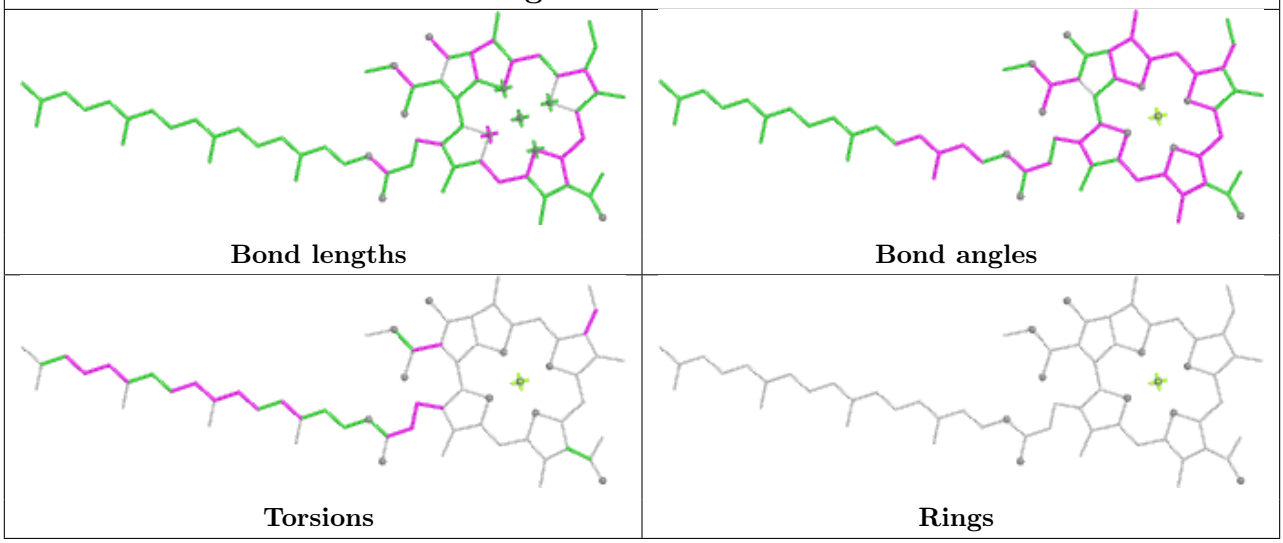
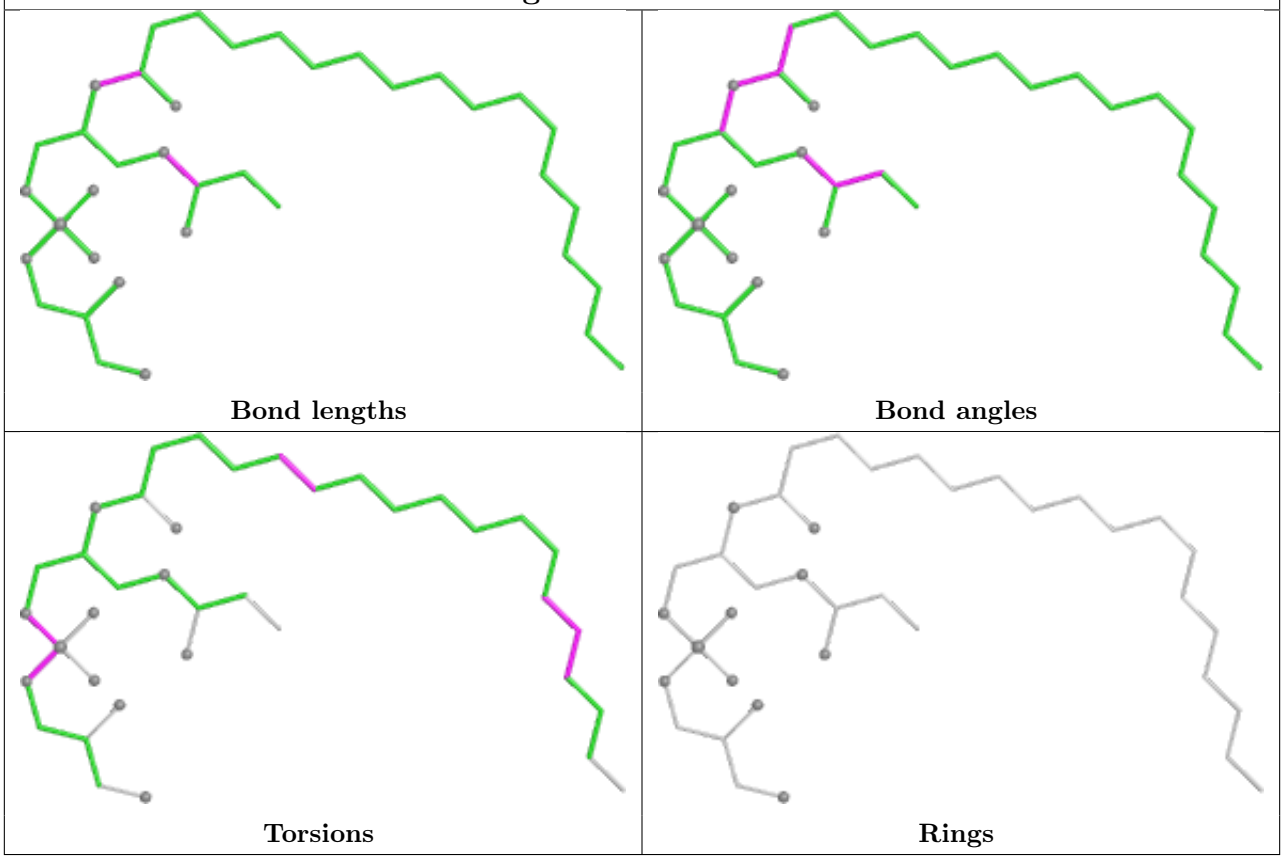
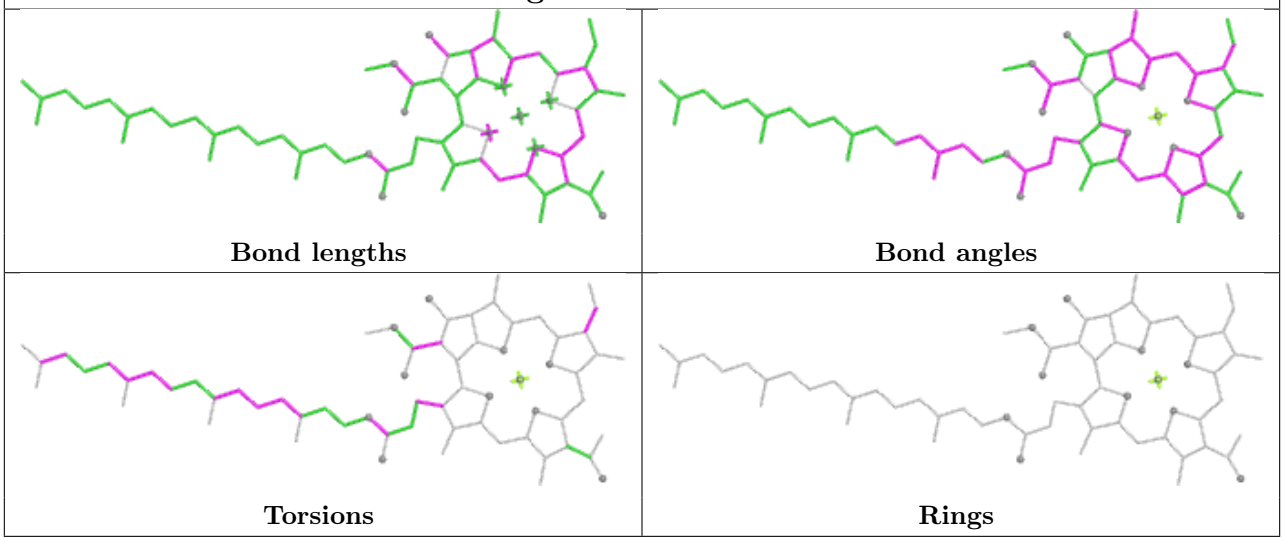


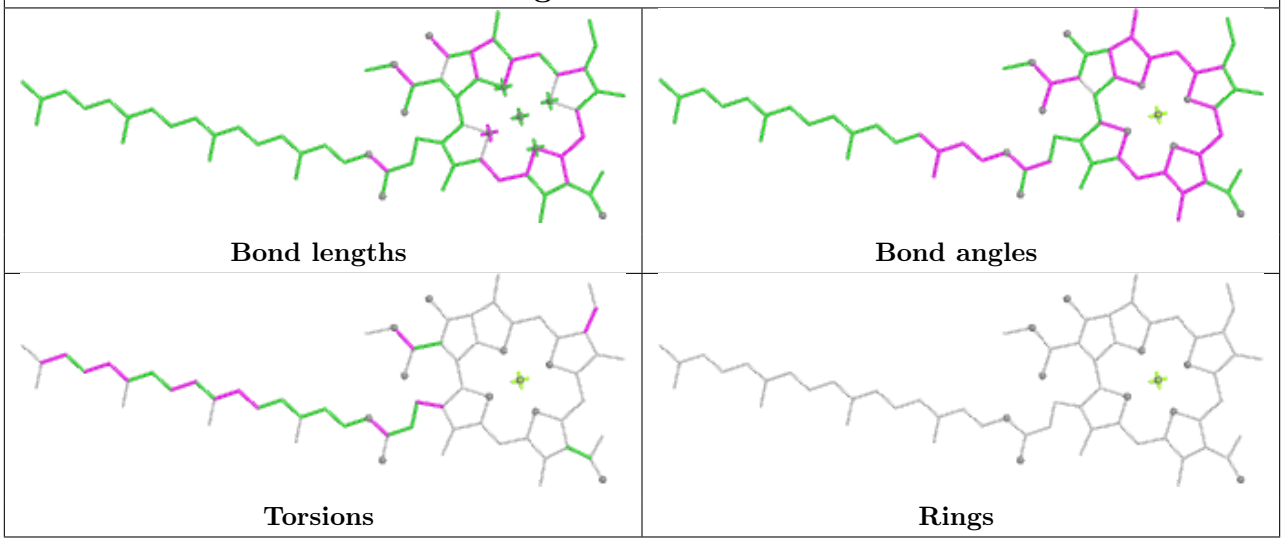
Ligand PGV C 508



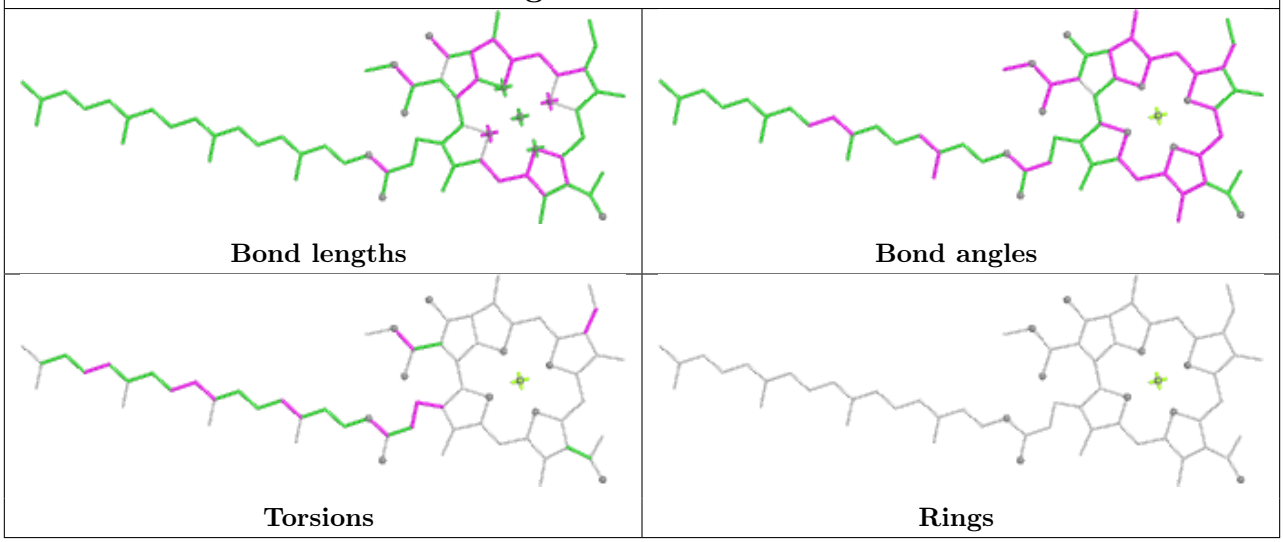
Ligand BCL P 101



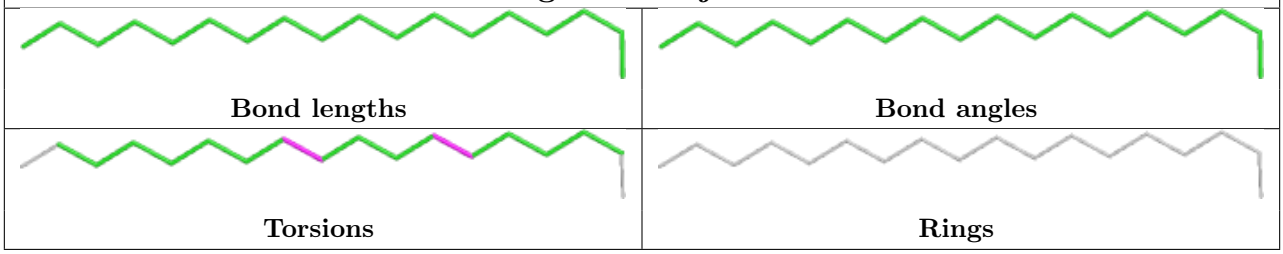
Ligand BCL i 101

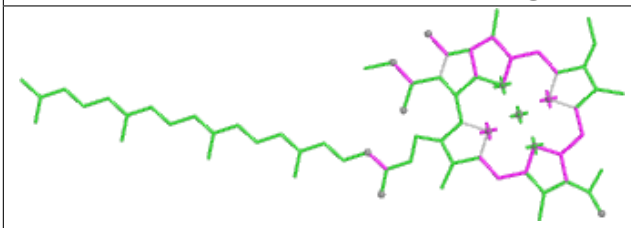
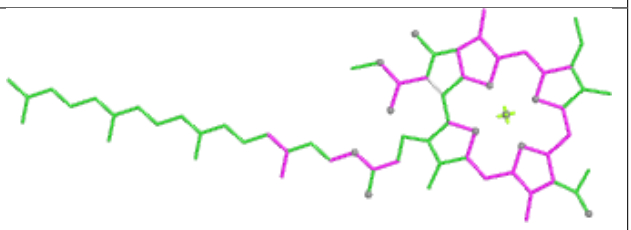
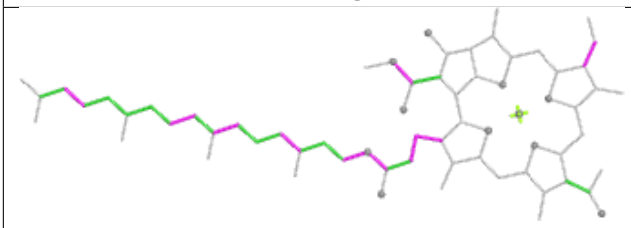
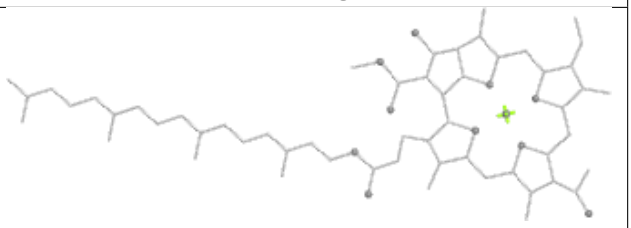


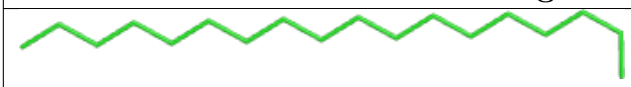
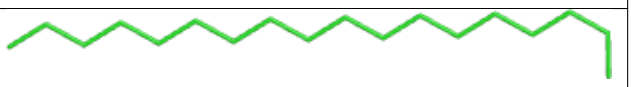
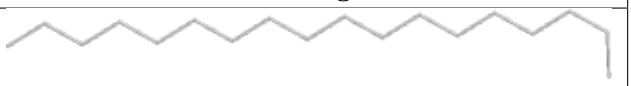
Ligand BCL A 102

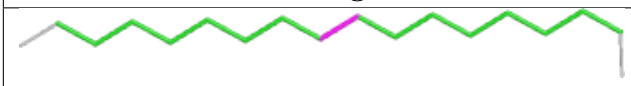
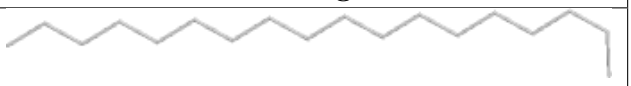


Ligand 8K6 j 105

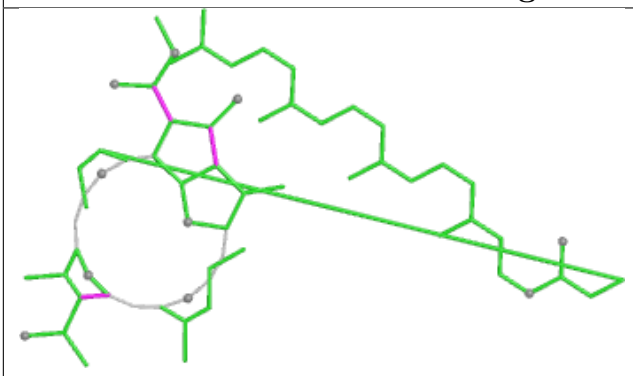


Ligand BCL R 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

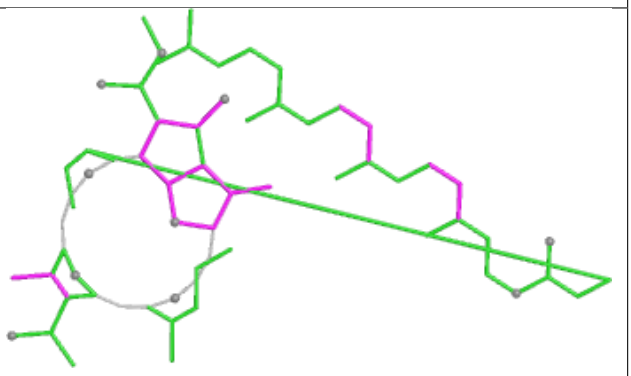
Ligand 8K6 f 103	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand 8K6 X 103	
Bond lengths	Bond angles
 Torsions	 Rings

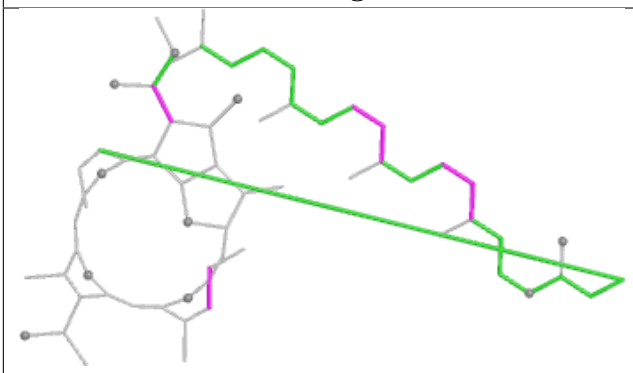
Ligand BPH M 404



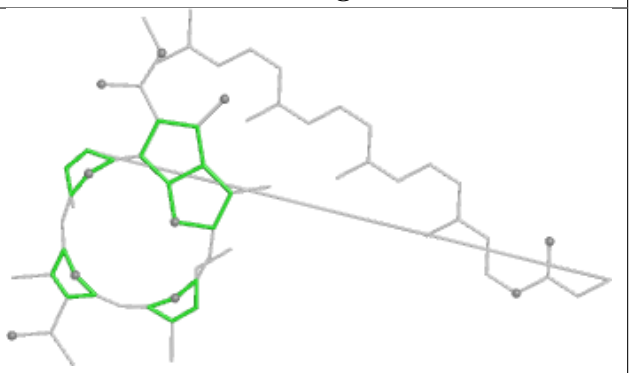
Bond lengths



Bond angles

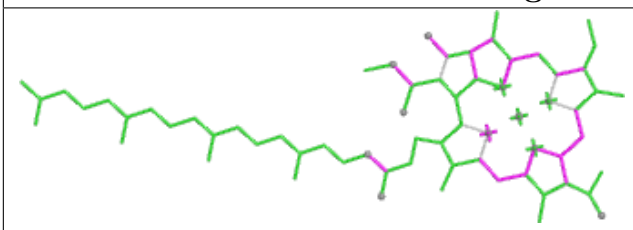


Torsions

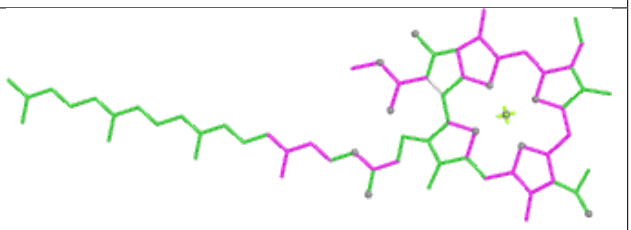


Rings

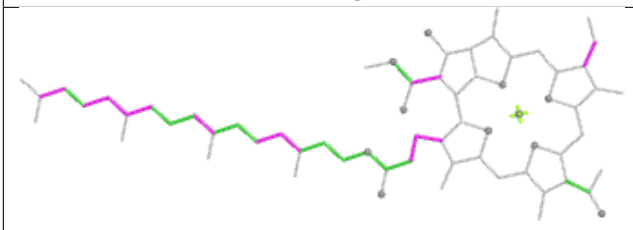
Ligand BCL R 101



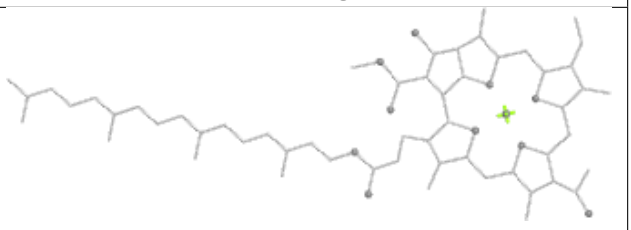
Bond lengths



Bond angles

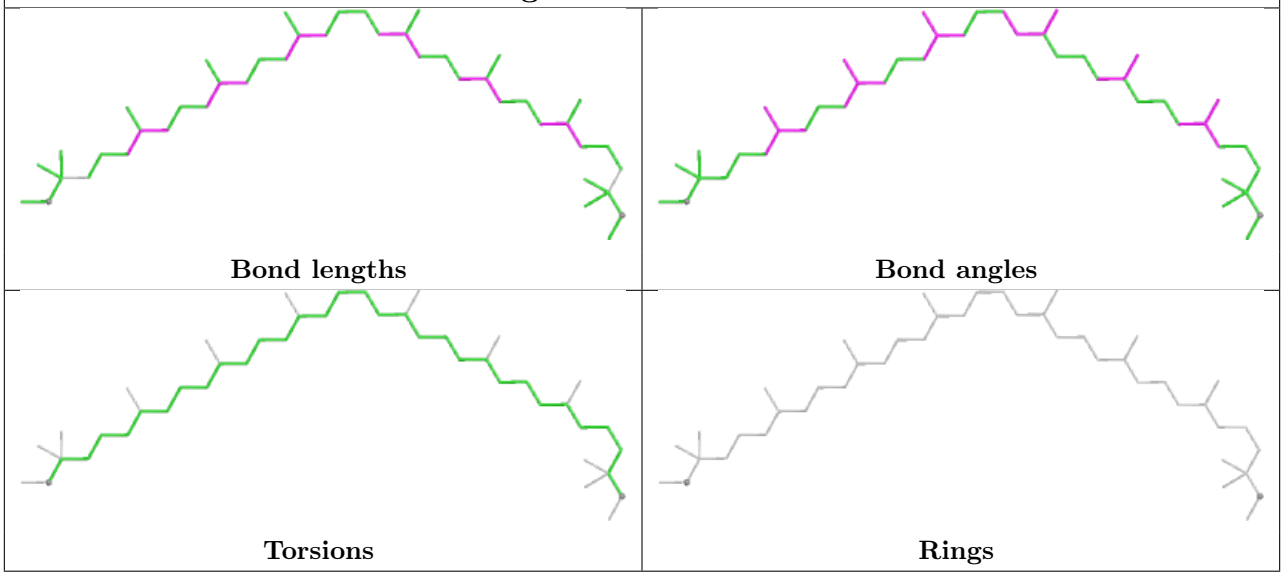


Torsions

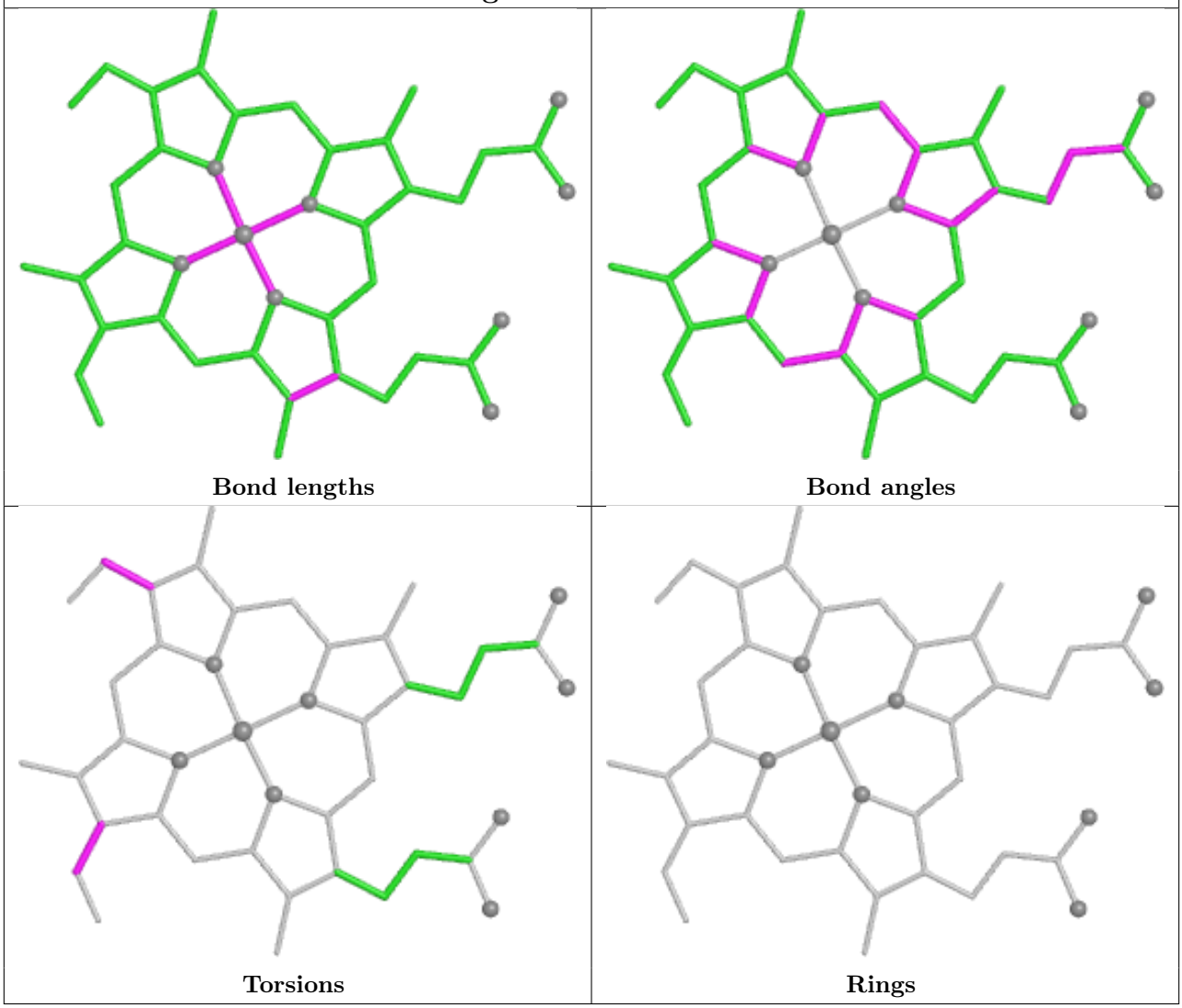


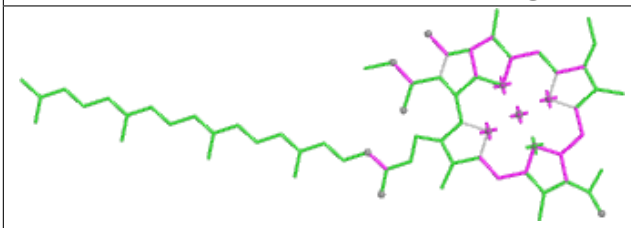
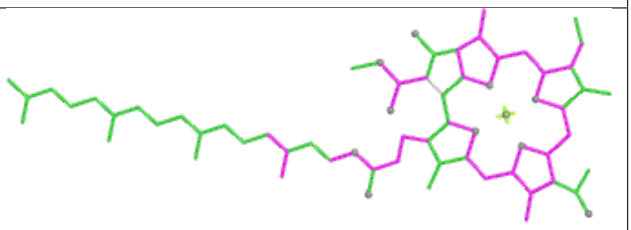
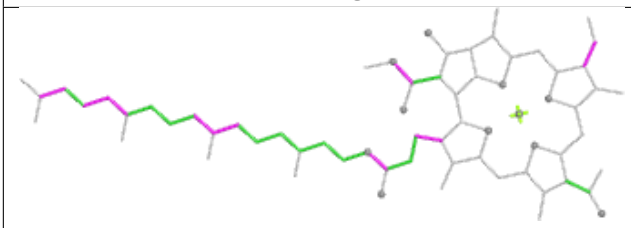
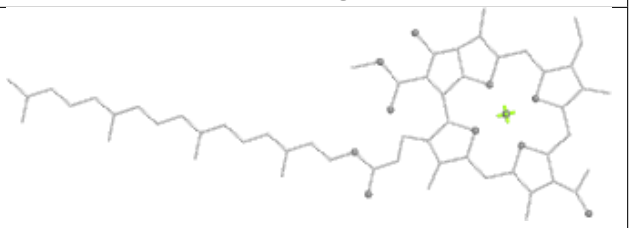
Rings

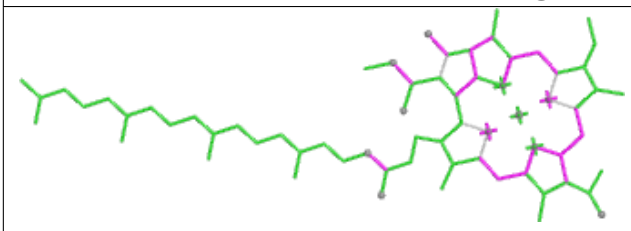
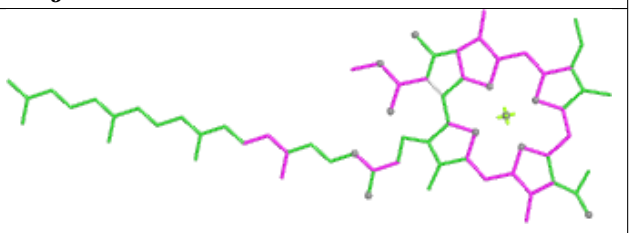
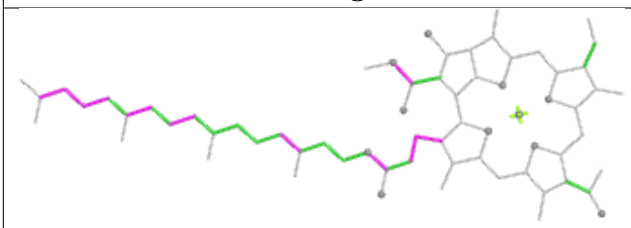
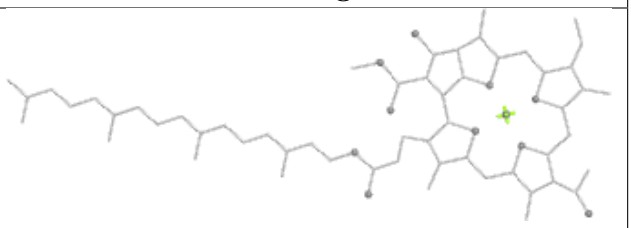
Ligand CRT M 406

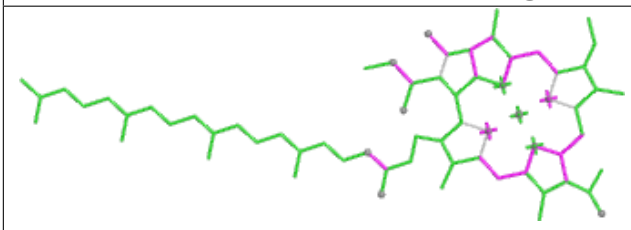
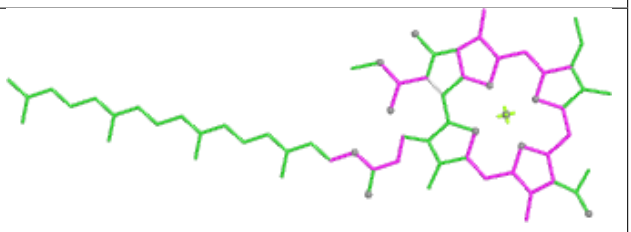
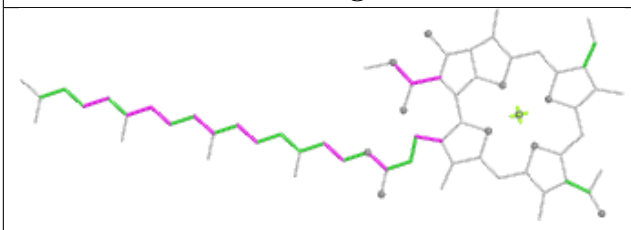
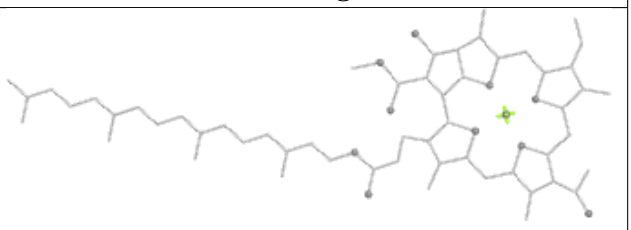


Ligand HEC C 503

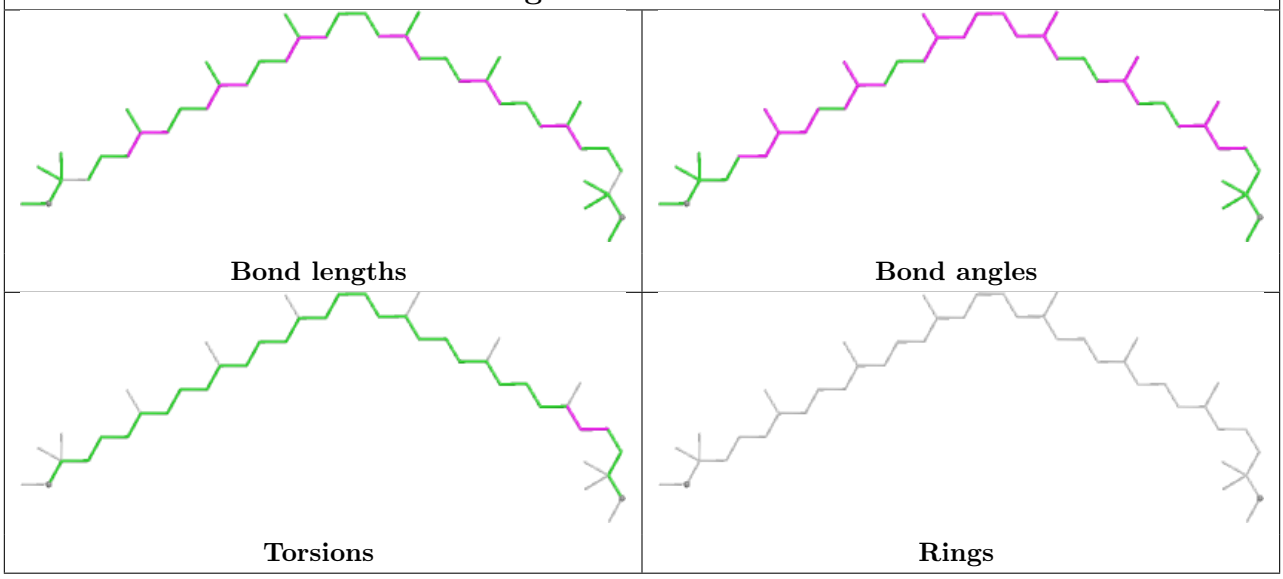


Ligand BCL U 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

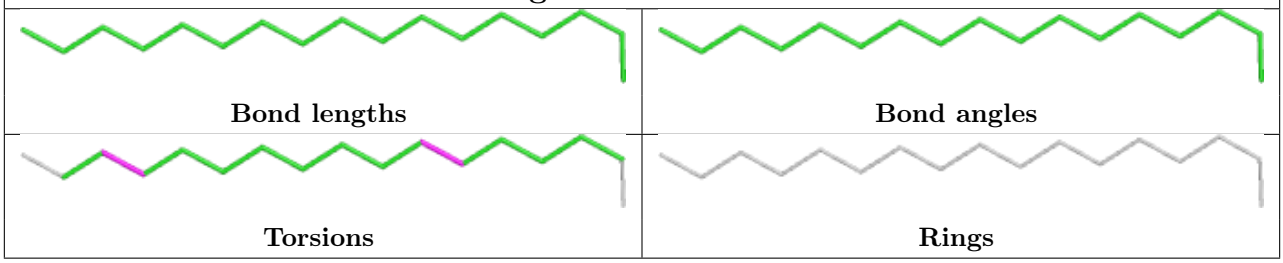
Ligand BCL j 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL M 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

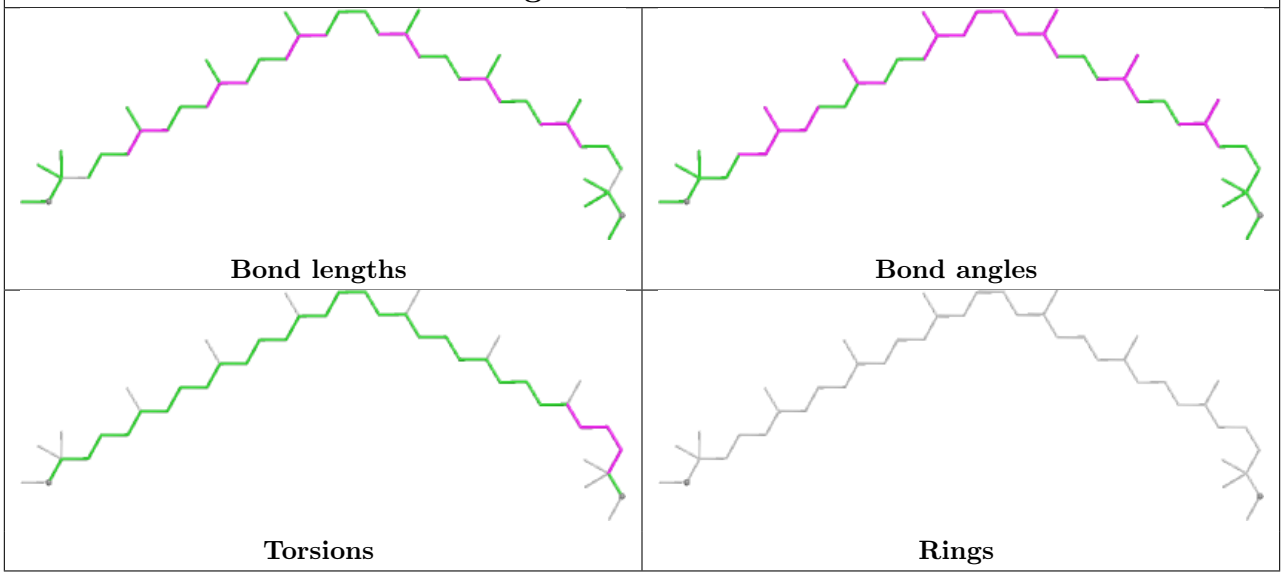
Ligand CRT Y 102



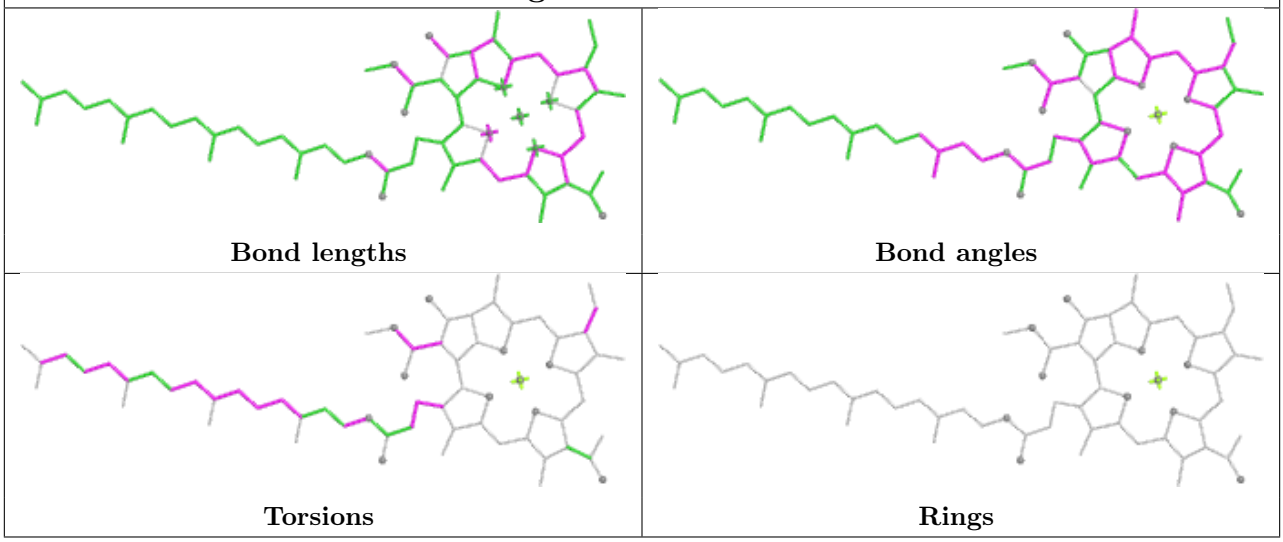
Ligand 8K6 H 303



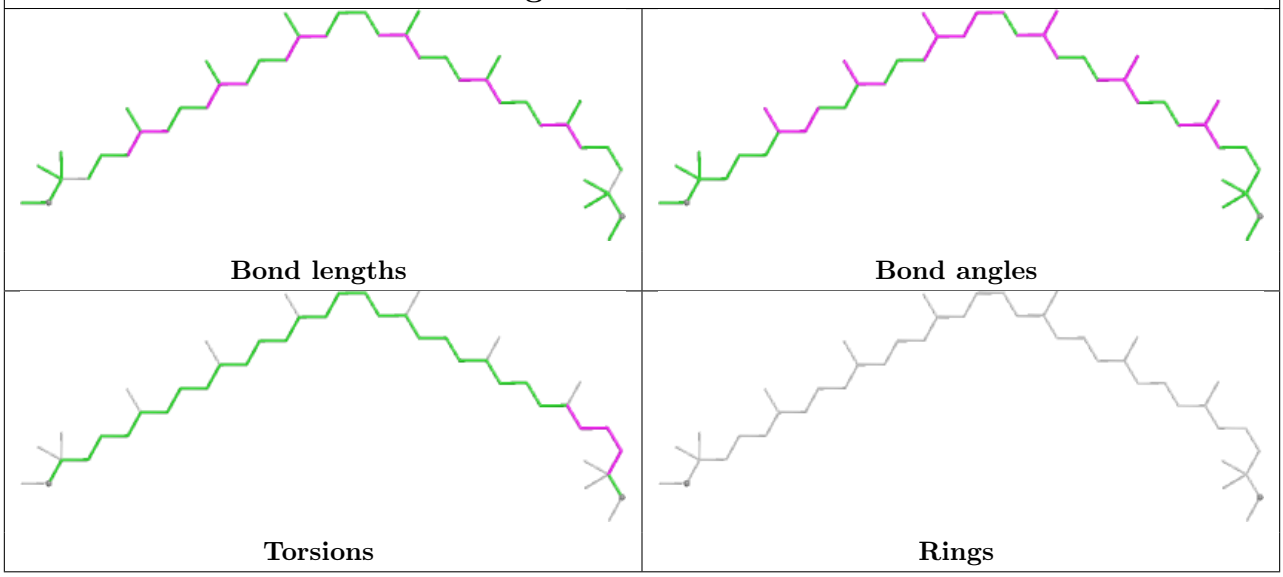
Ligand CRT U 102



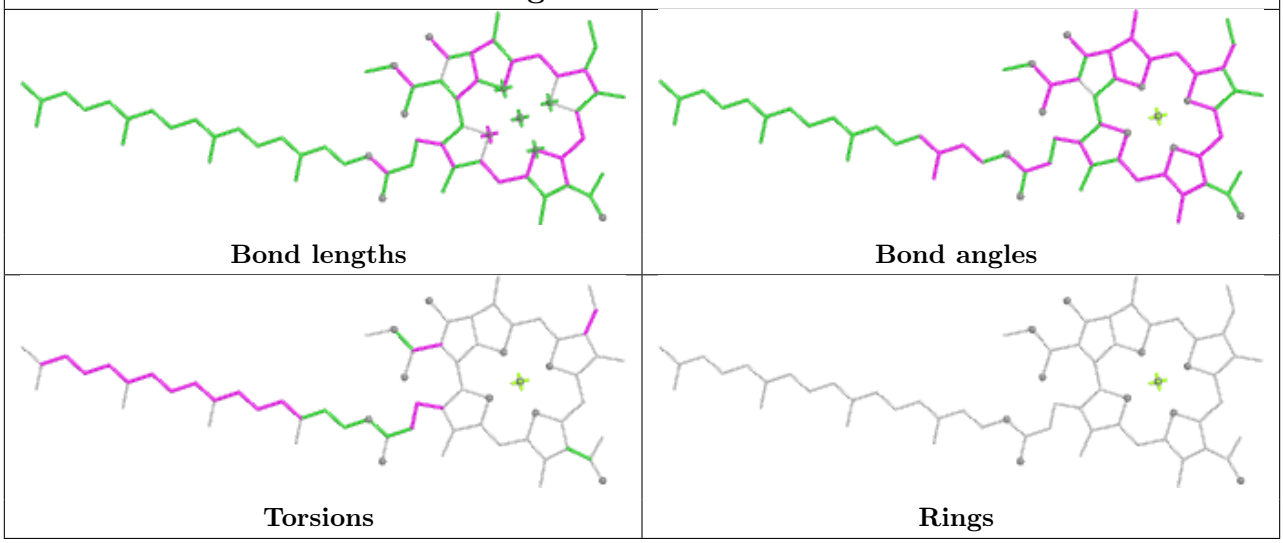
Ligand BCL Z 101



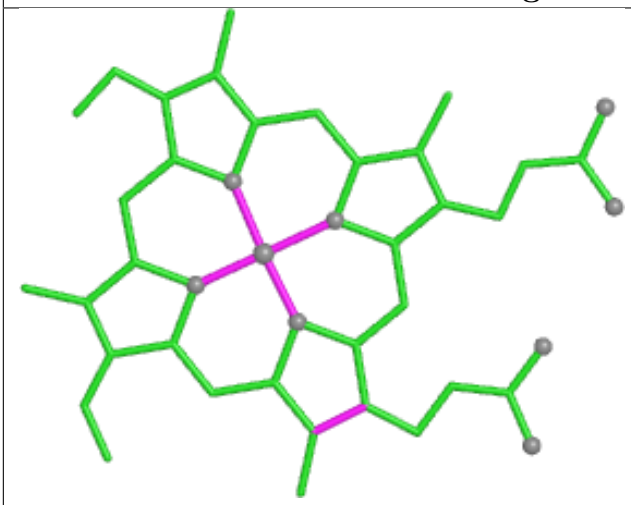
Ligand CRT B 102



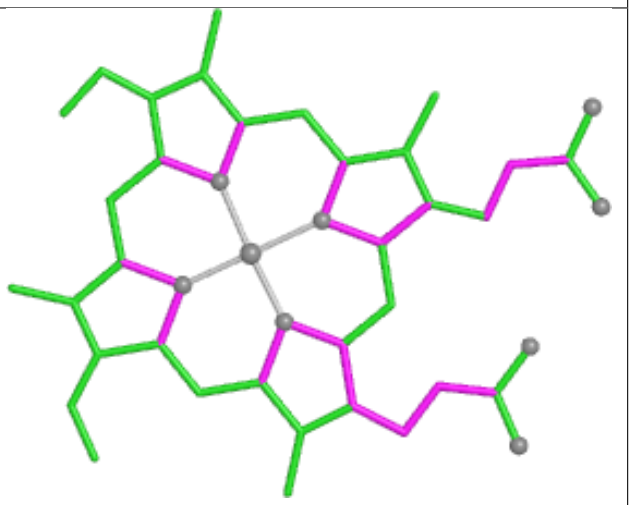
Ligand BCL E 101



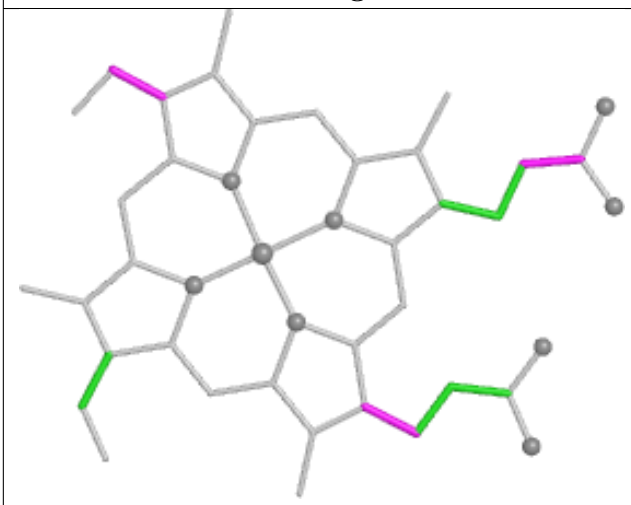
Ligand HEC C 504



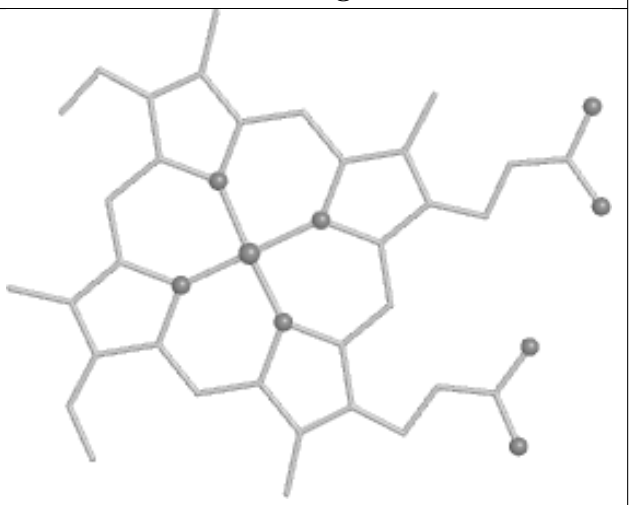
Bond lengths



Bond angles

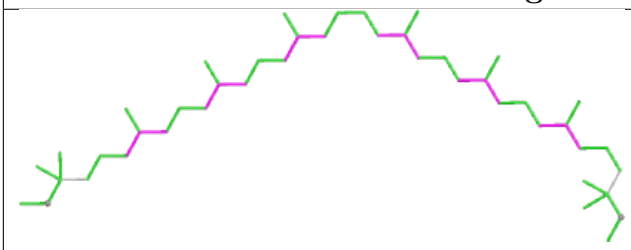


Torsions

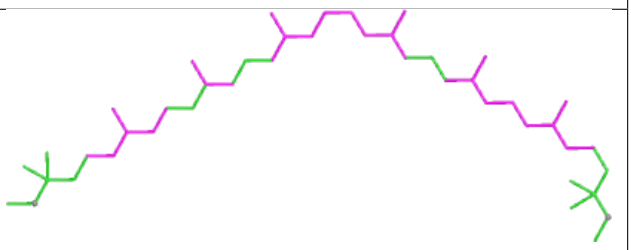


Rings

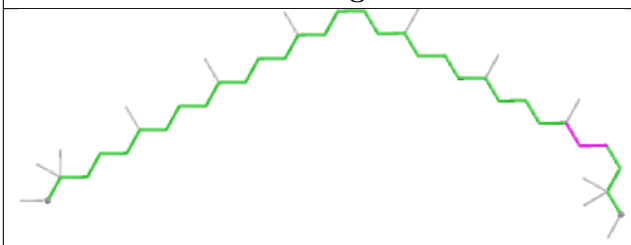
Ligand CRT E 103



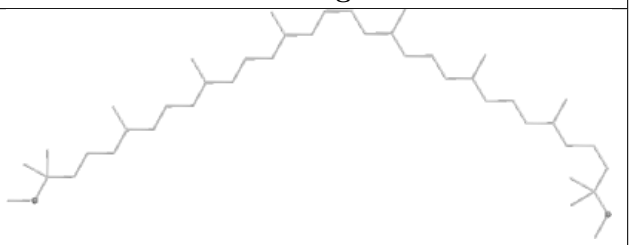
Bond lengths



Bond angles

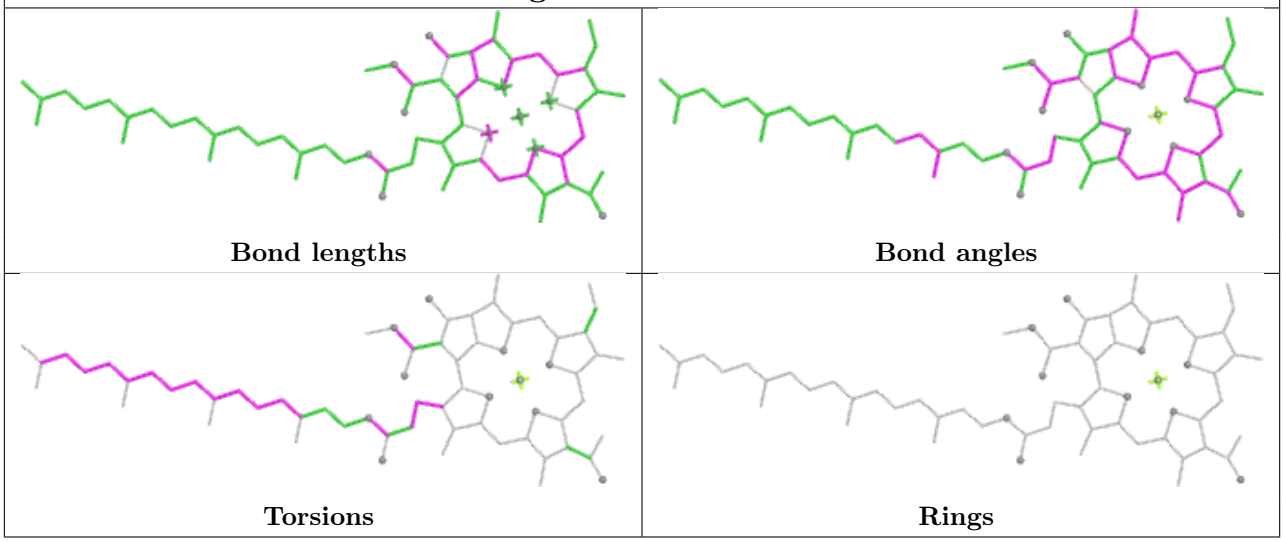


Torsions

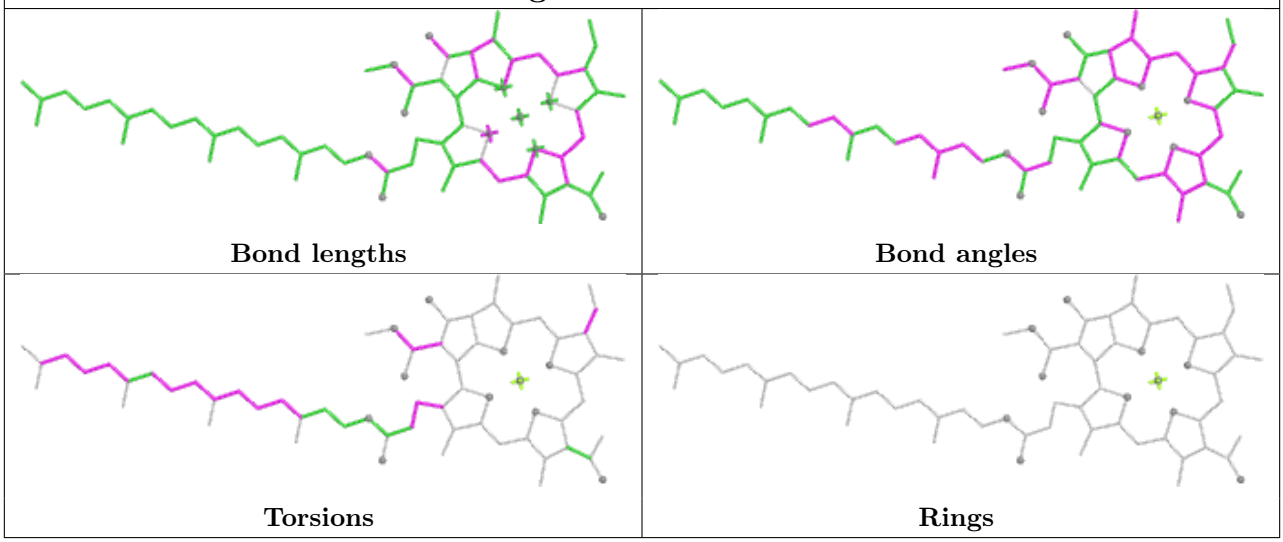


Rings

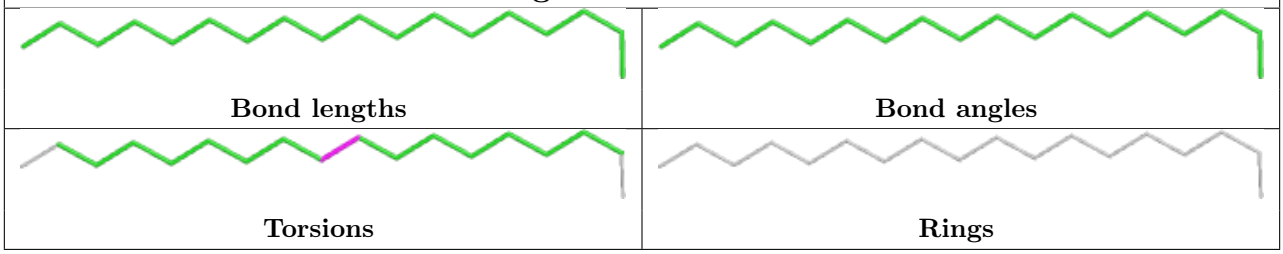
Ligand BCL b 102



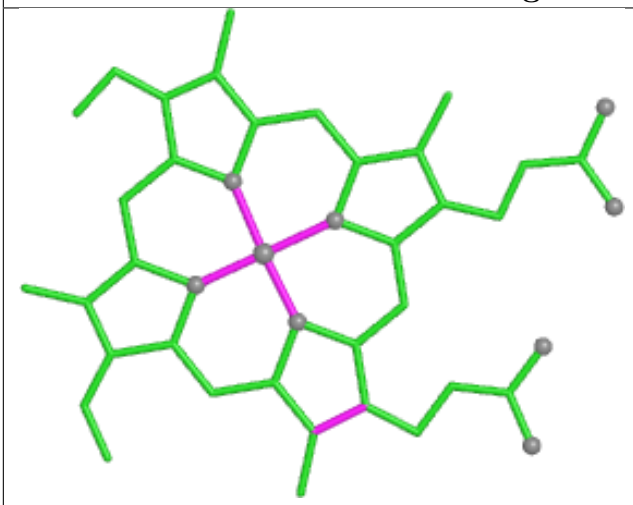
Ligand BCL b 101



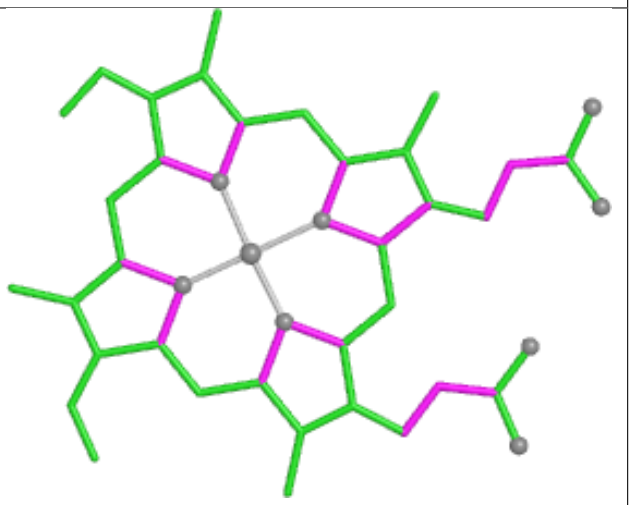
Ligand 8K6 L 407



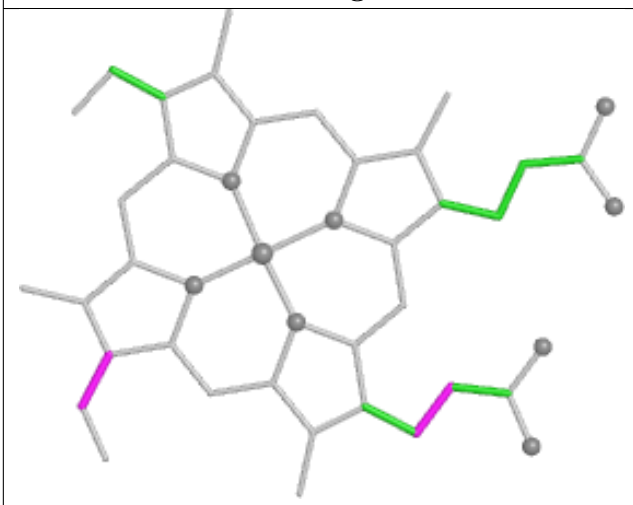
Ligand HEC C 502



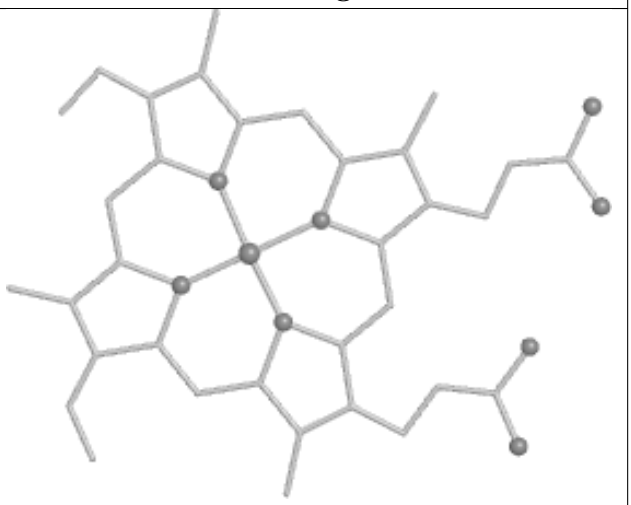
Bond lengths



Bond angles

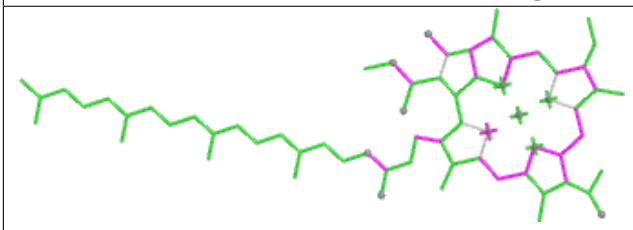


Torsions

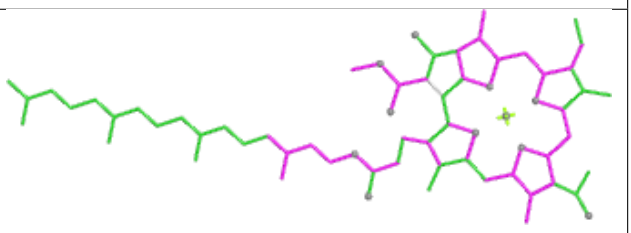


Rings

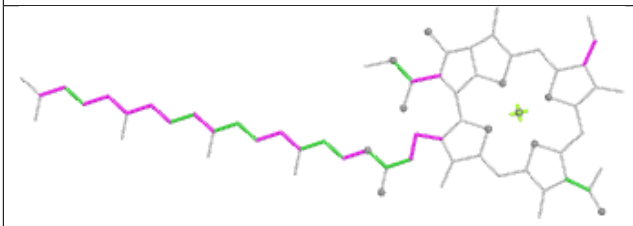
Ligand BCL J 101



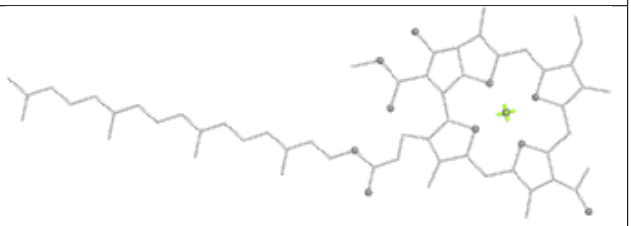
Bond lengths



Bond angles

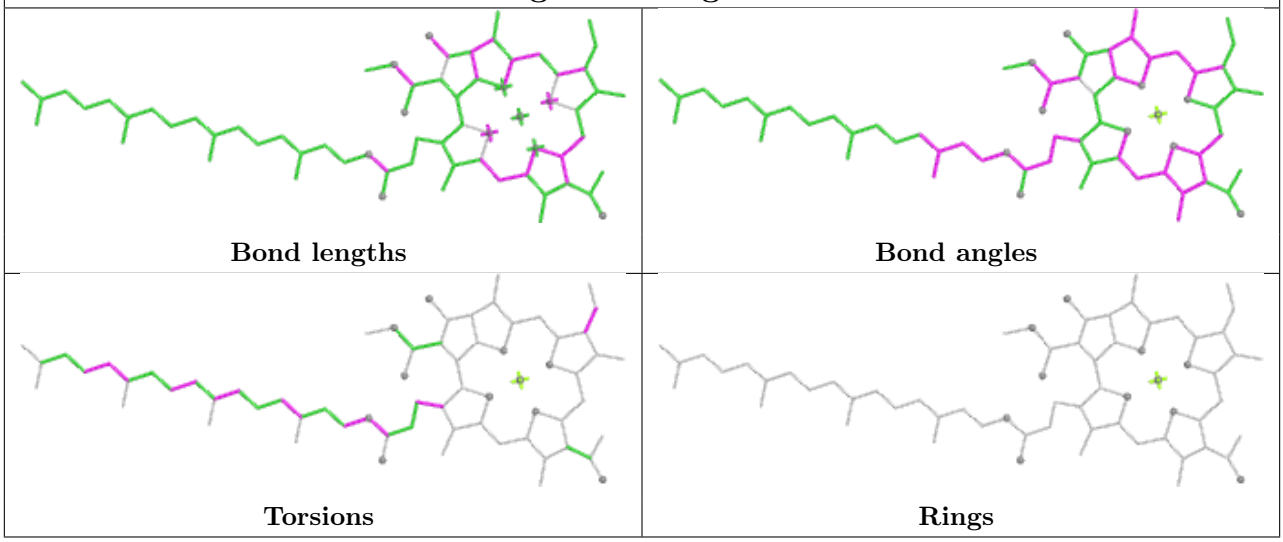


Torsions

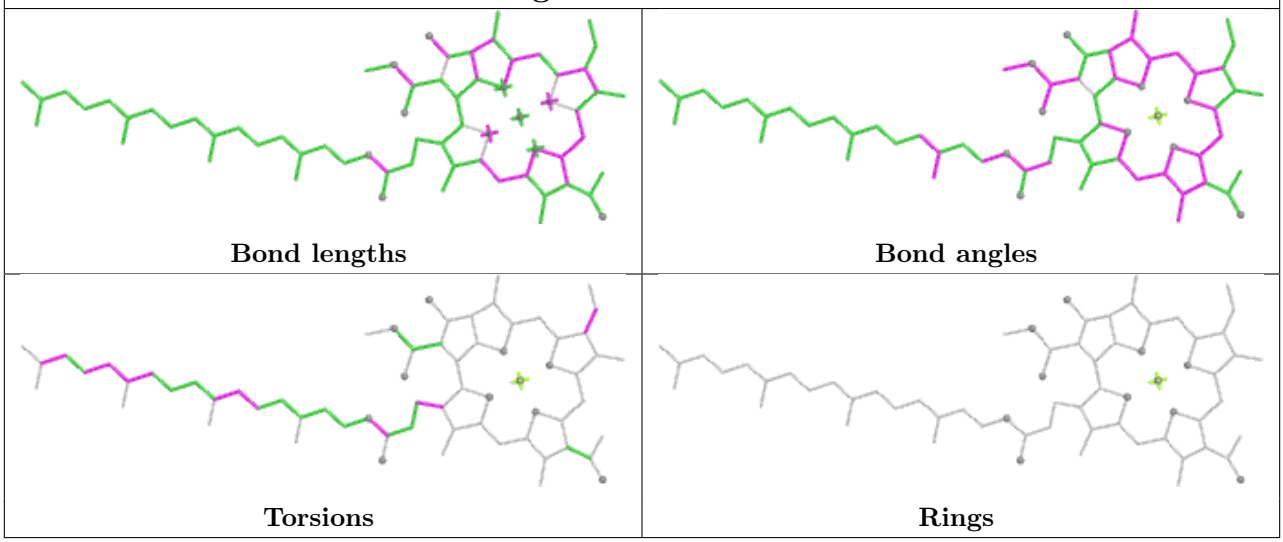


Rings

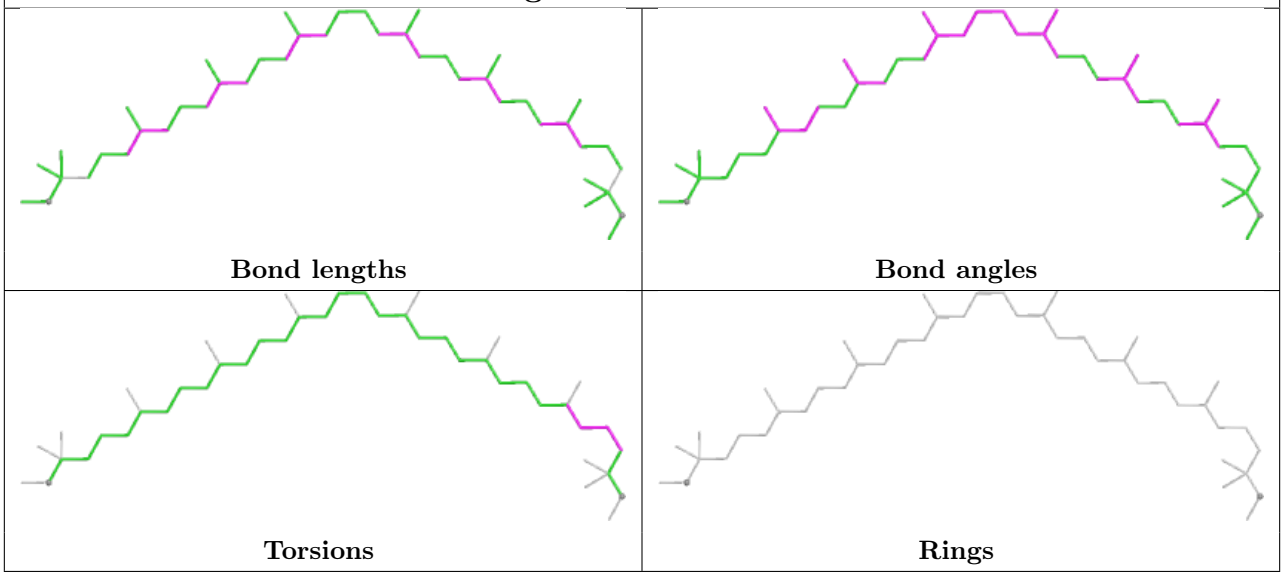
Ligand BCL g 101



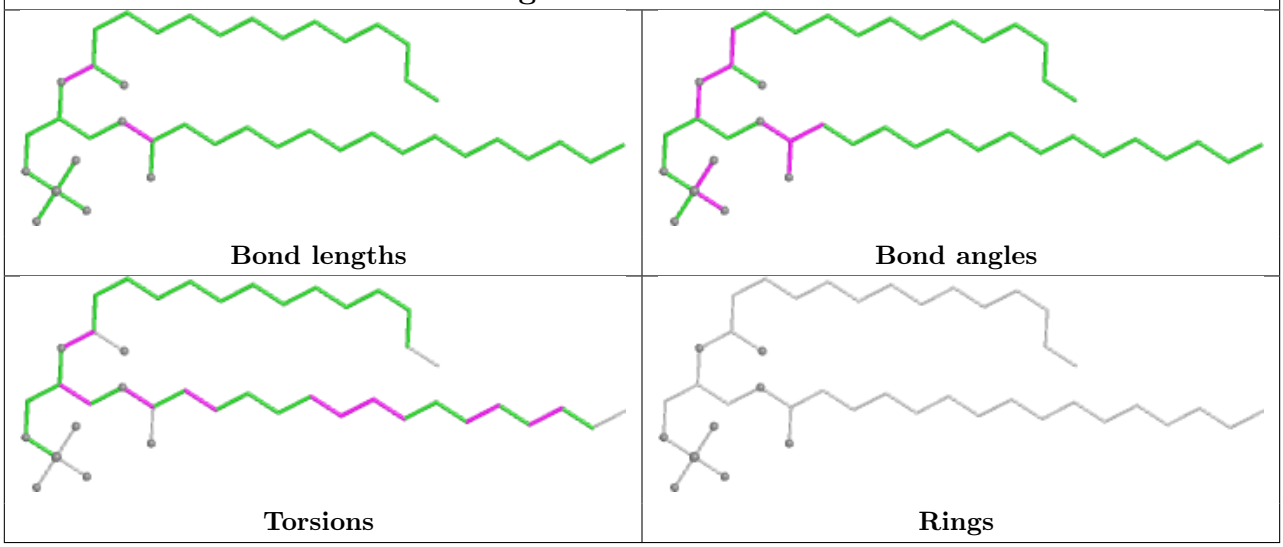
Ligand BCL I 101



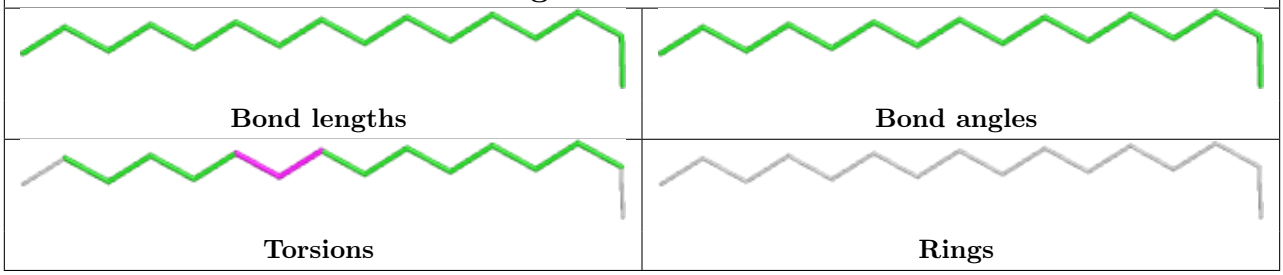
Ligand CRT R 103



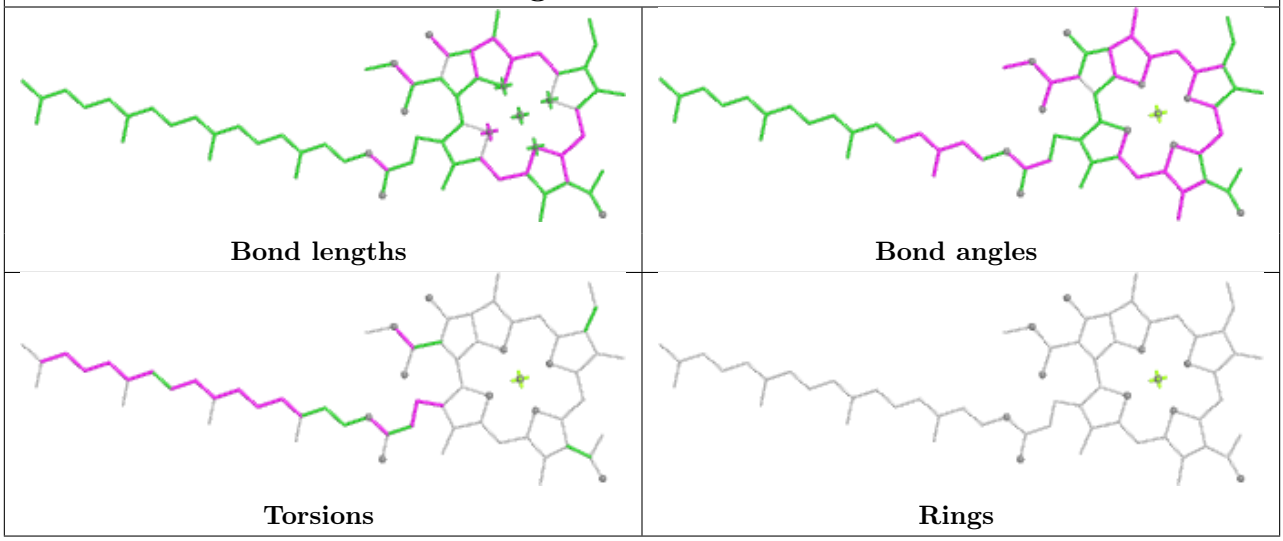
Ligand PGV M 408



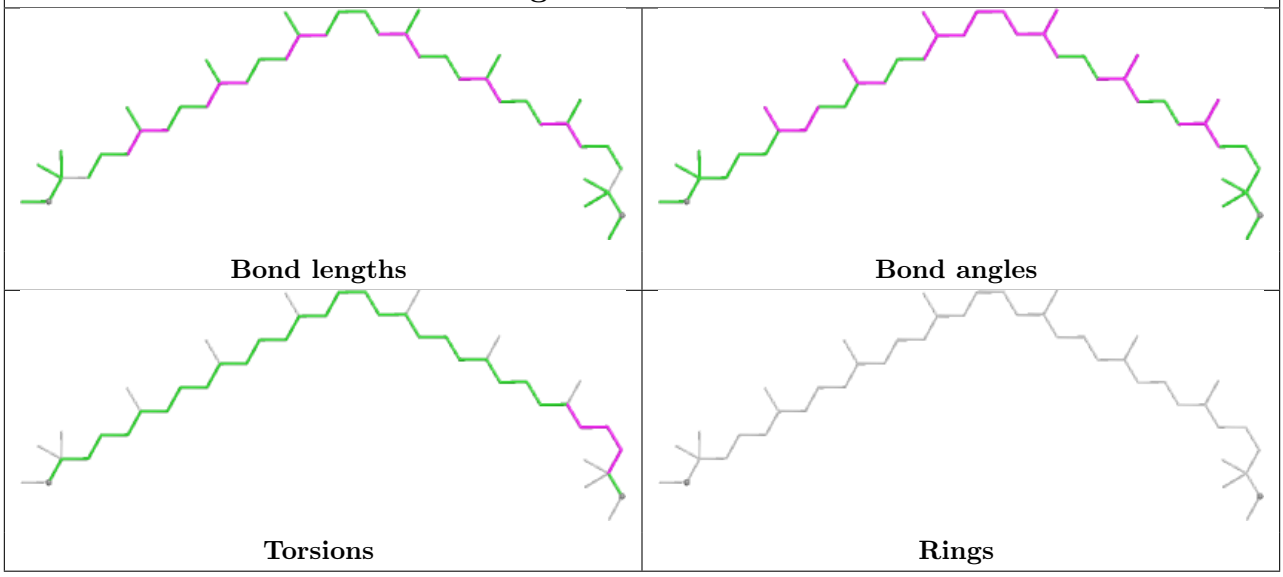
Ligand 8K6 C 509



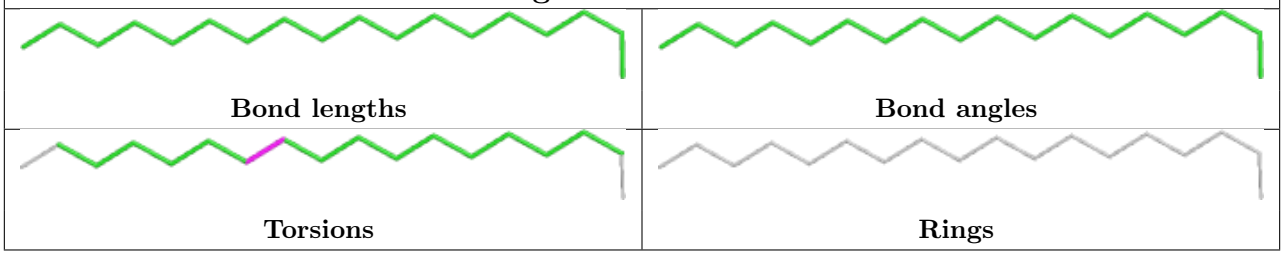
Ligand BCL d 102



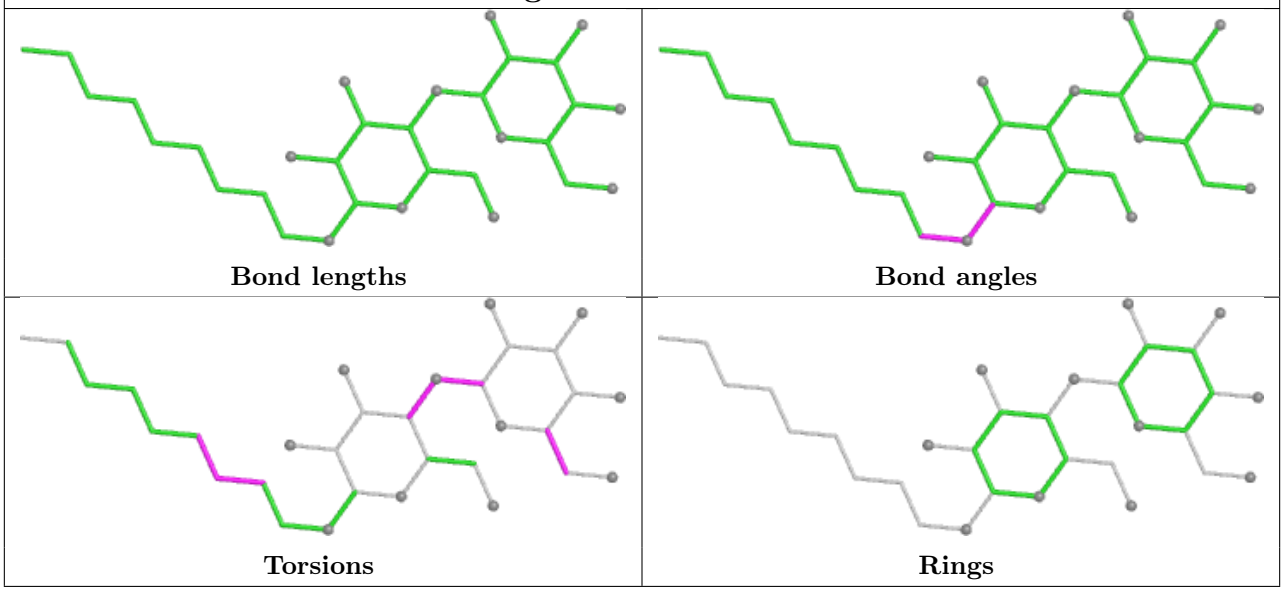
Ligand CRT e 102

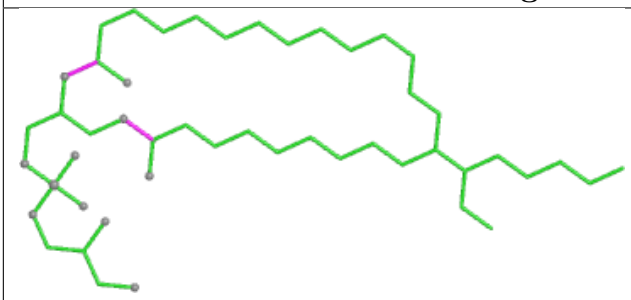
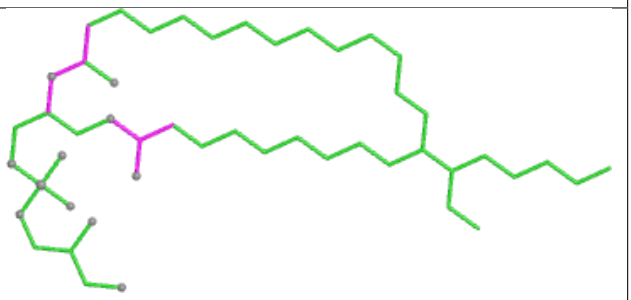
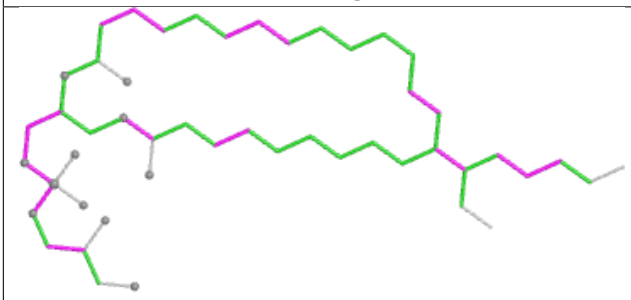
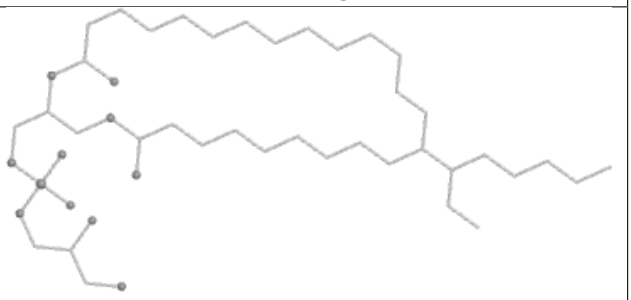


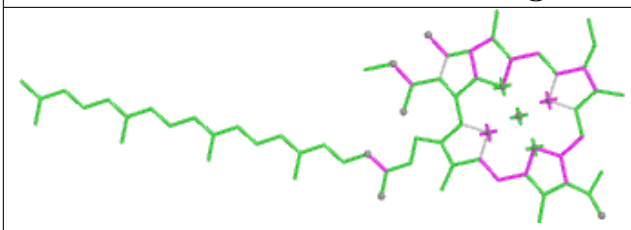
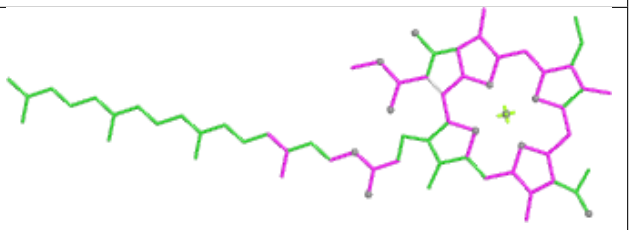
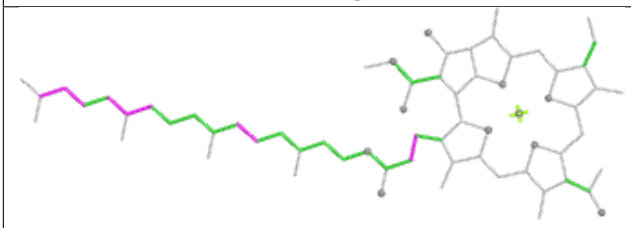
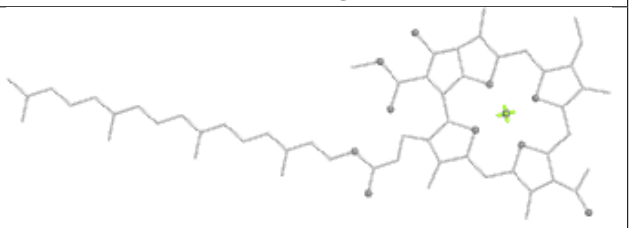
Ligand 8K6 L 405



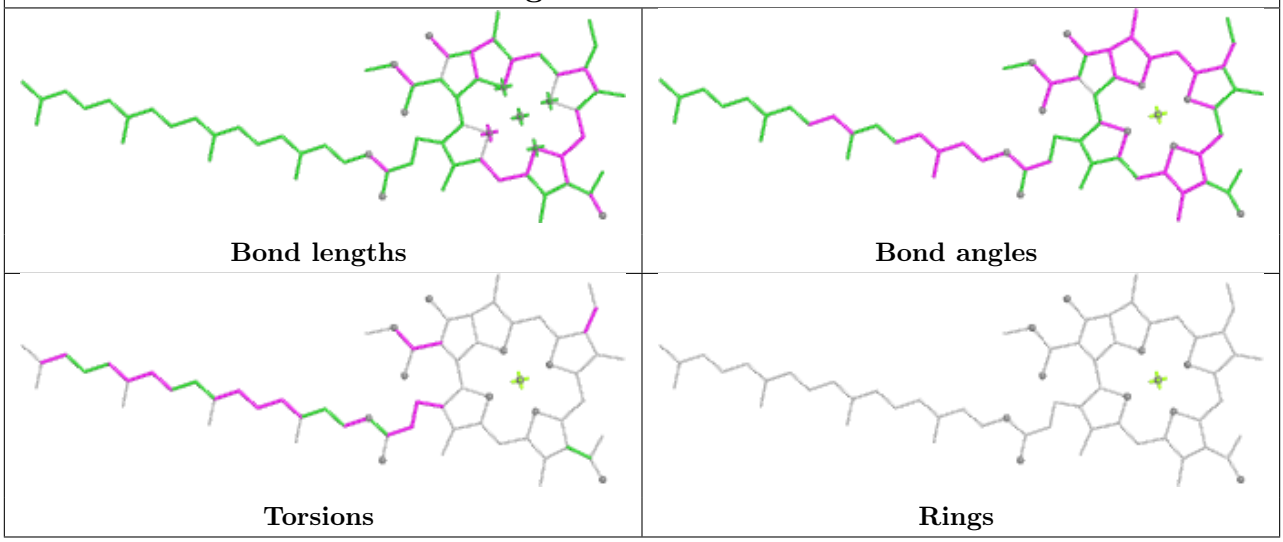
Ligand LMT L 408



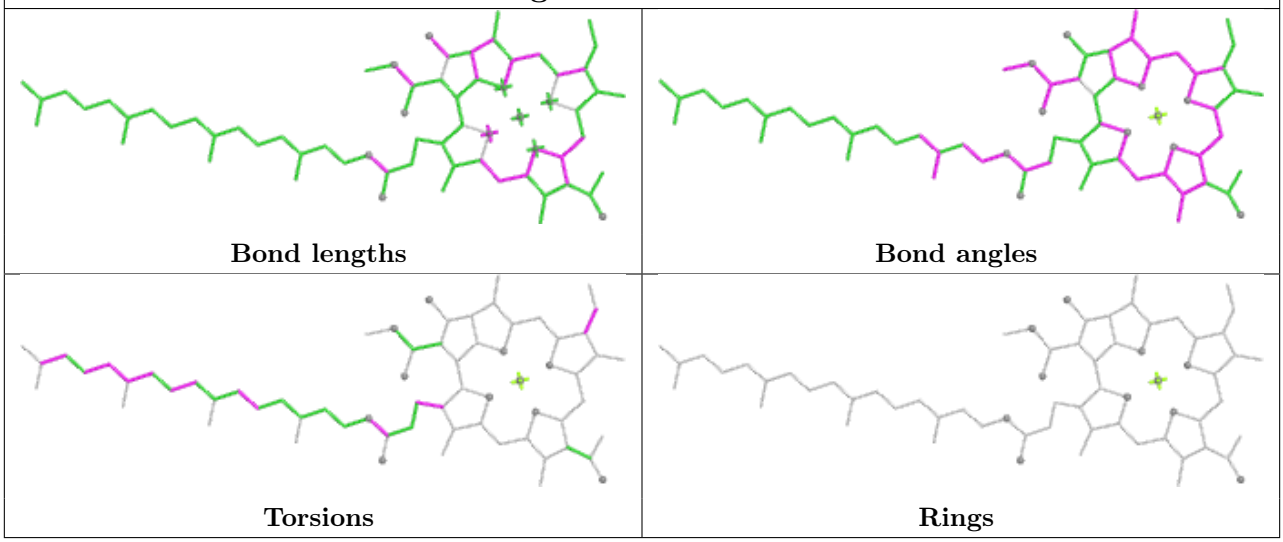
Ligand PGV H 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL L 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

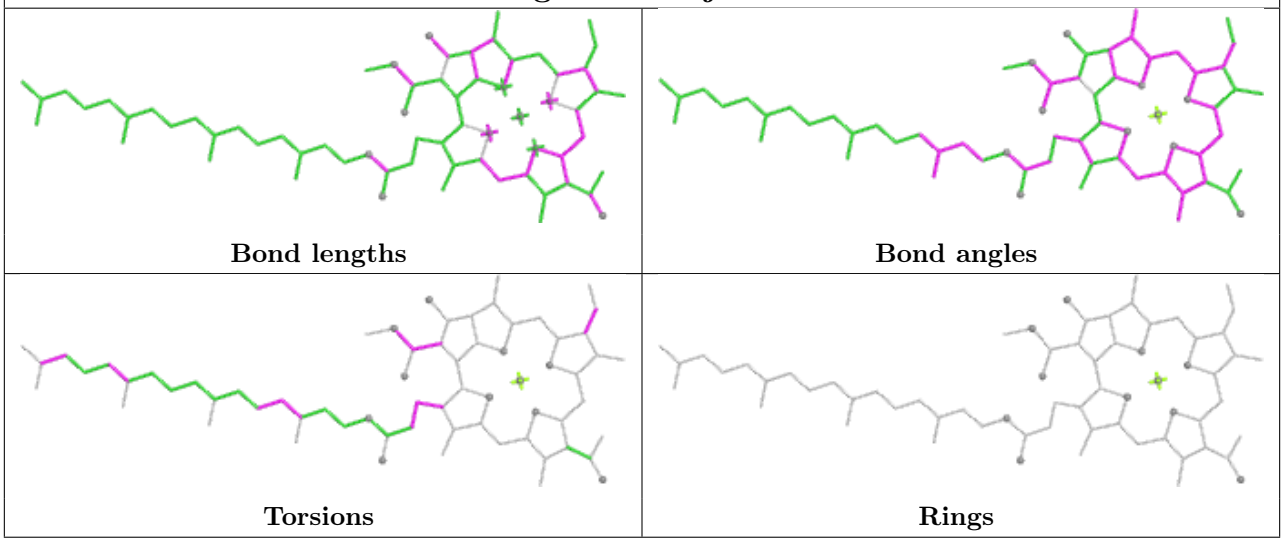
Ligand BCL A 101



Ligand BCL a 101



Ligand BCL j 102



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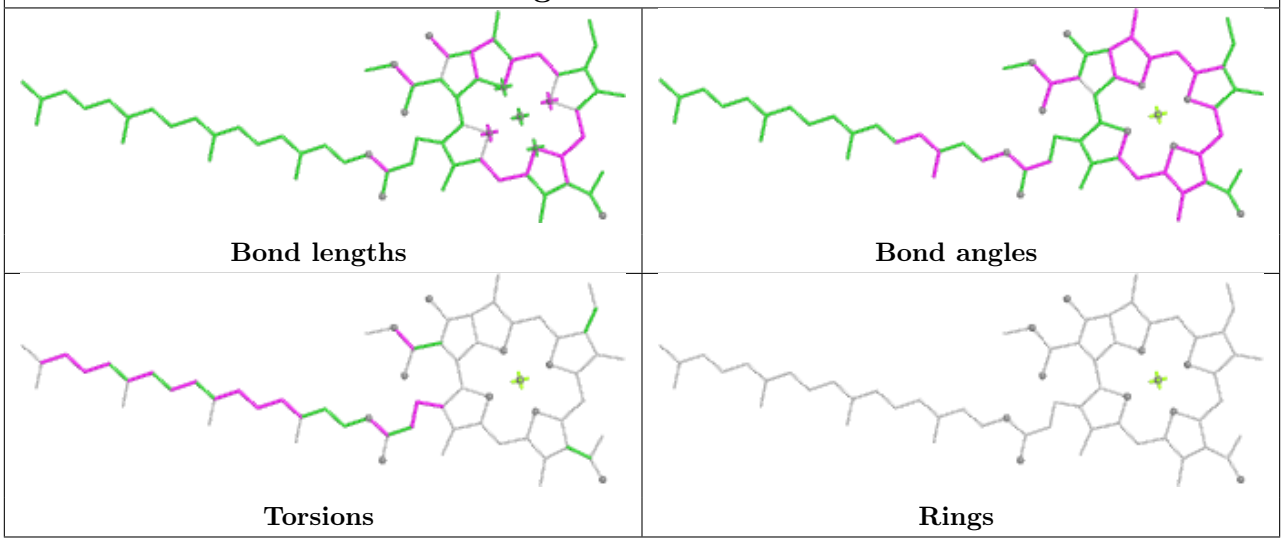

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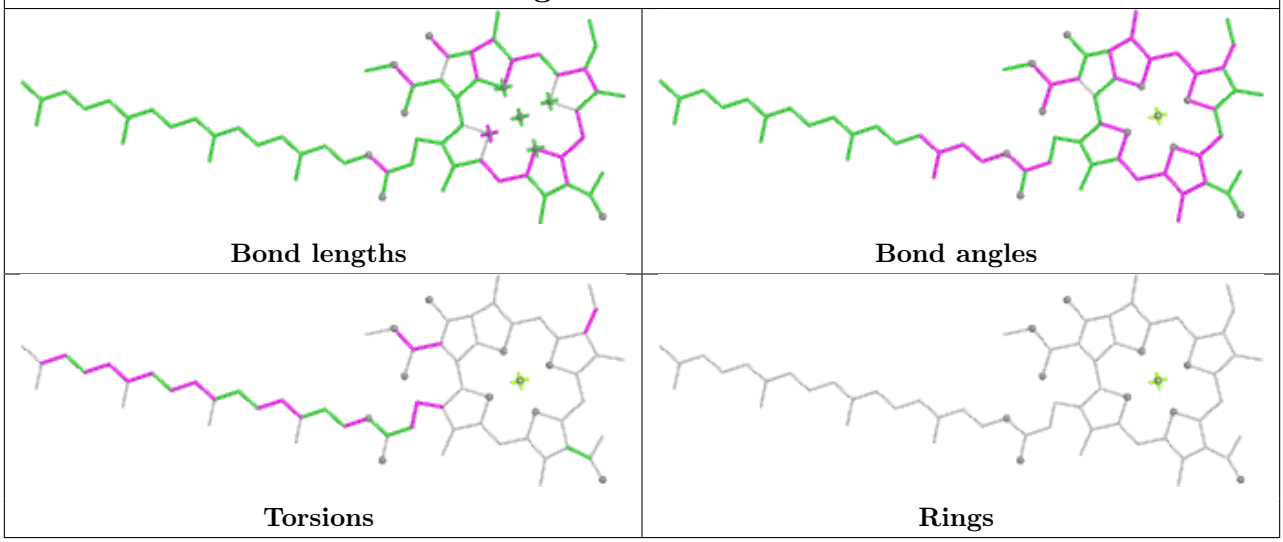
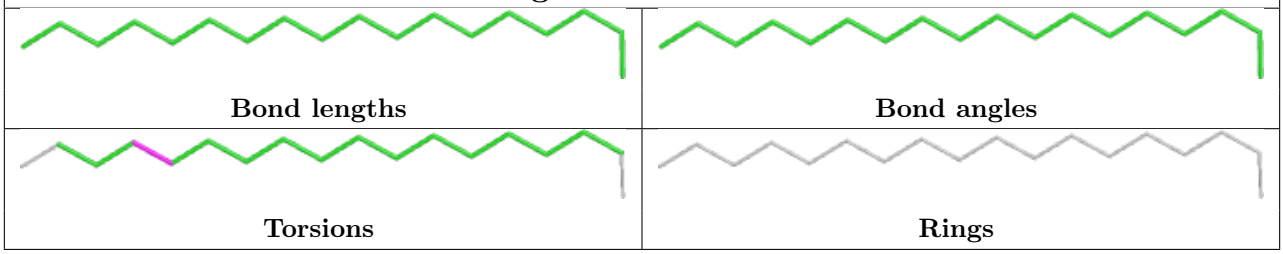
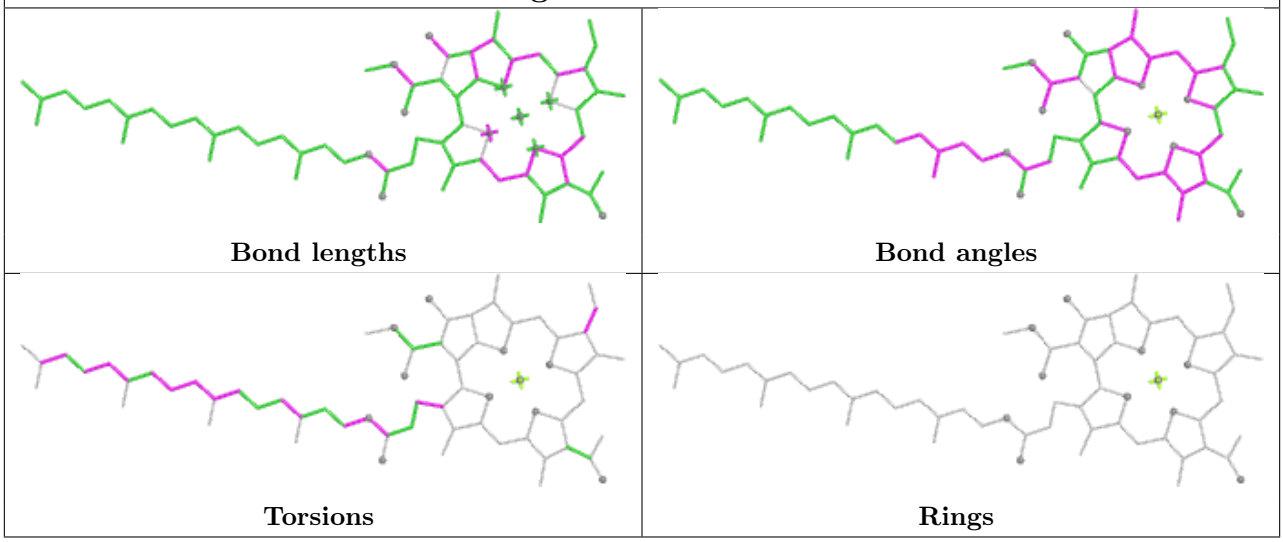


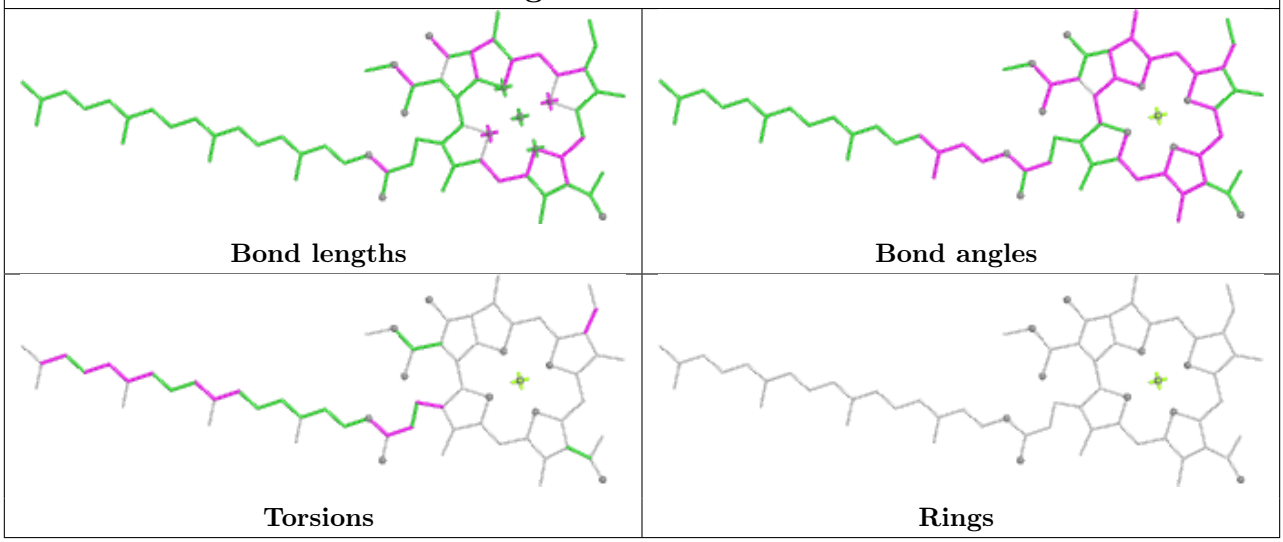
Ligand 8K6 P 104



Ligand BCL e 101



Ligand BCL K 101



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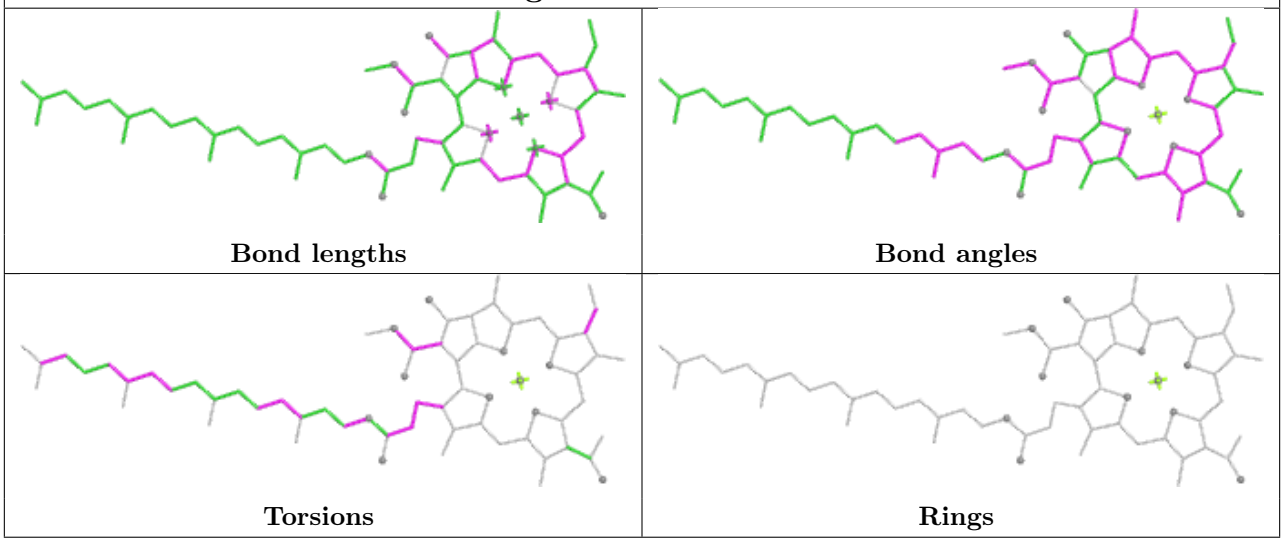

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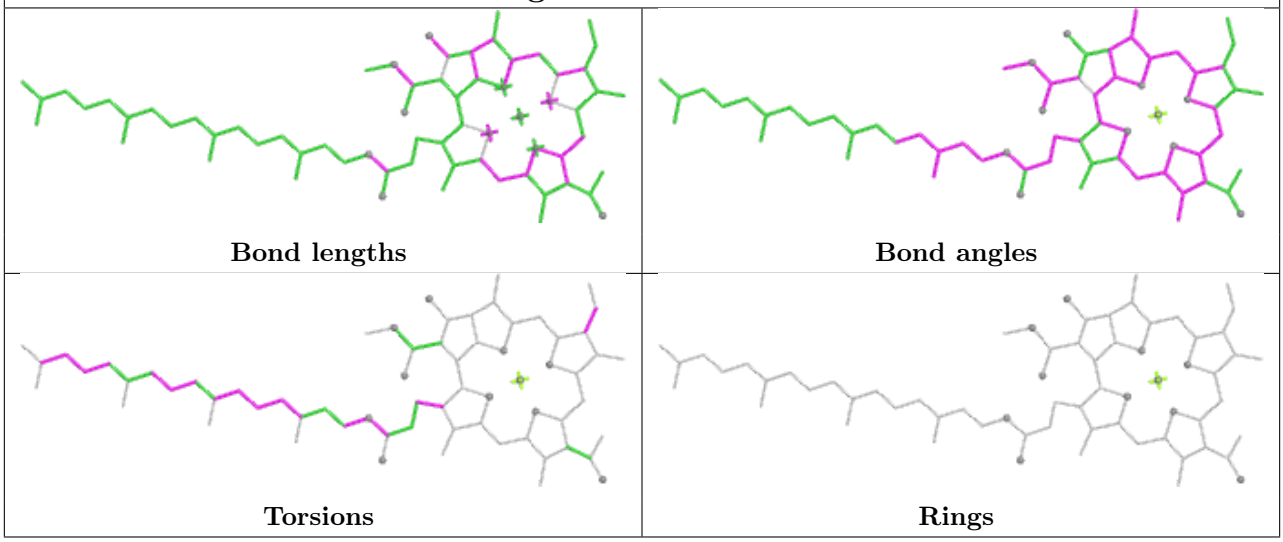
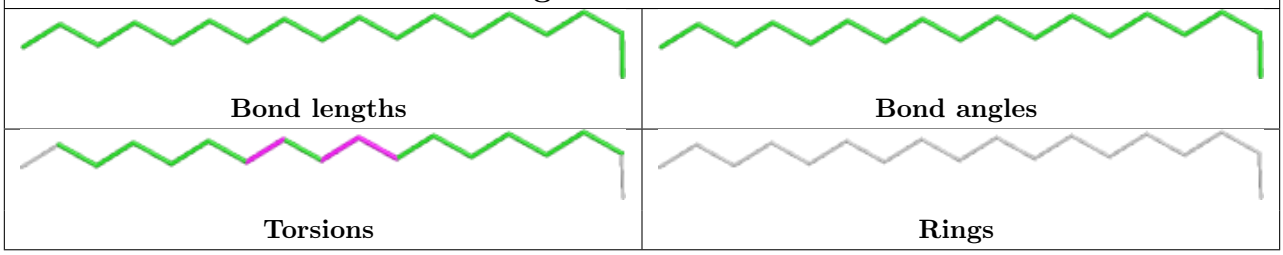


Ligand 8K6 d 103



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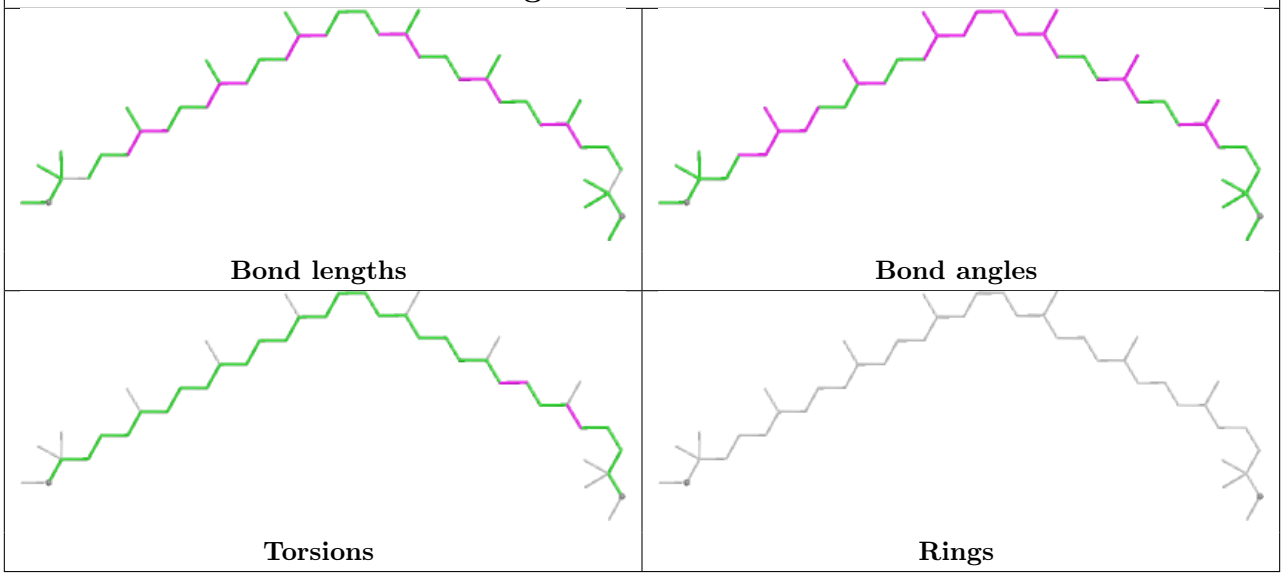
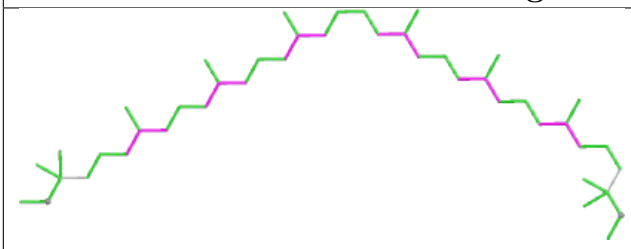
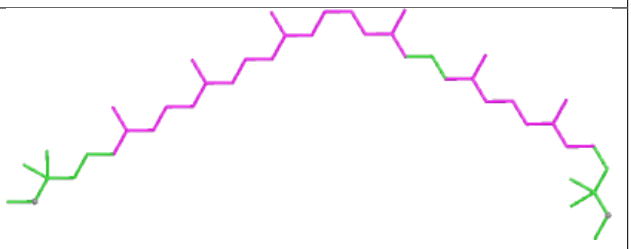


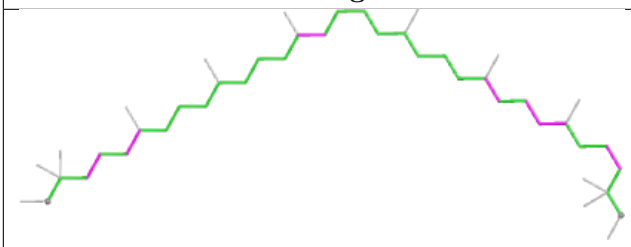
Ligand CRT Z 102



Bond lengths



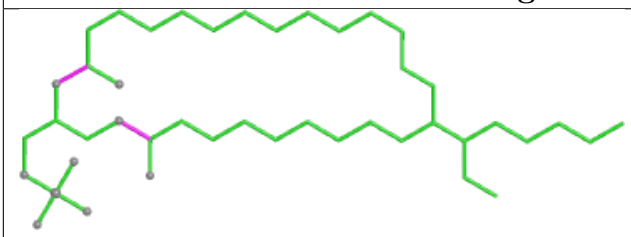
Bond angles



Torsions

Rings

Ligand PGV M 407



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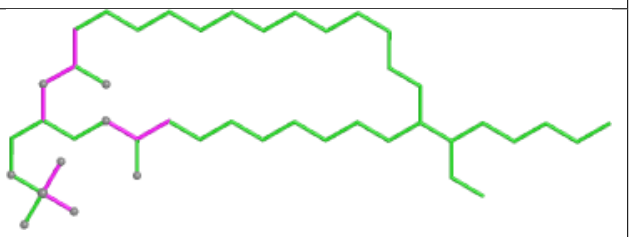
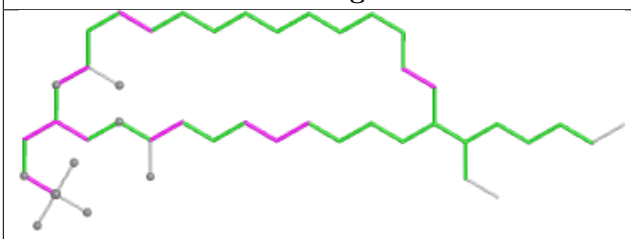
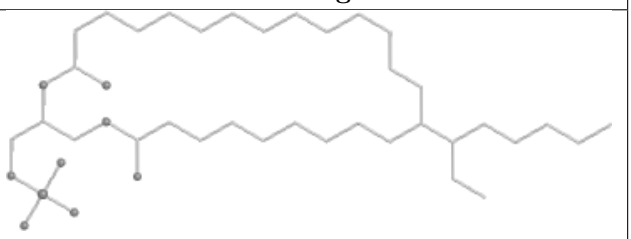


Bond angles

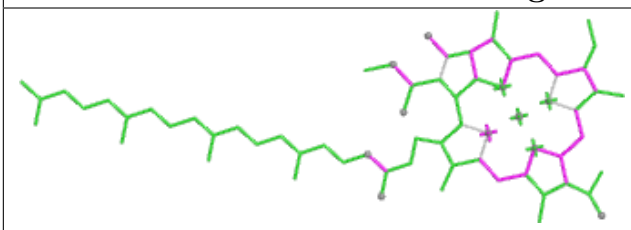


Torsions

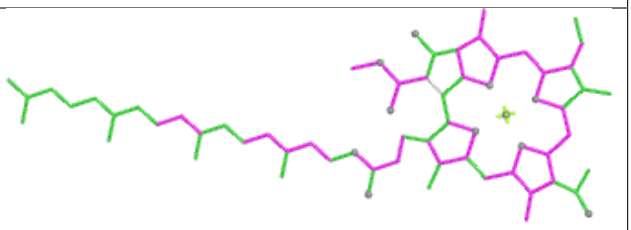


Rings

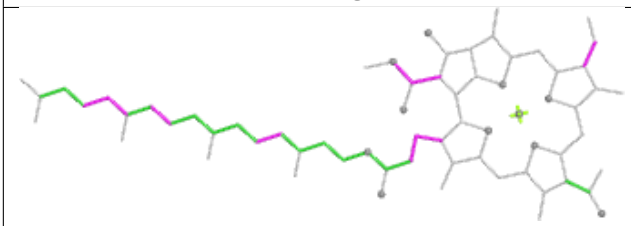
Ligand BCL d 101



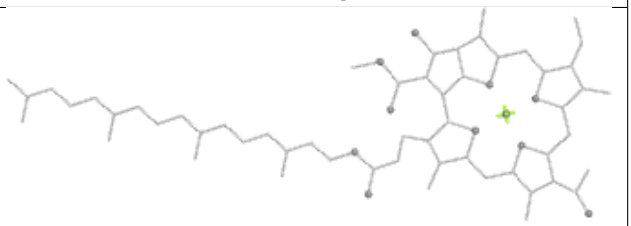
Bond lengths



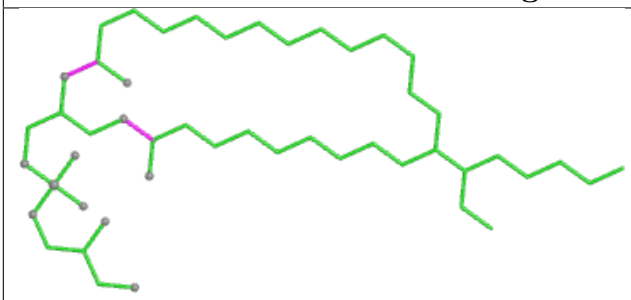
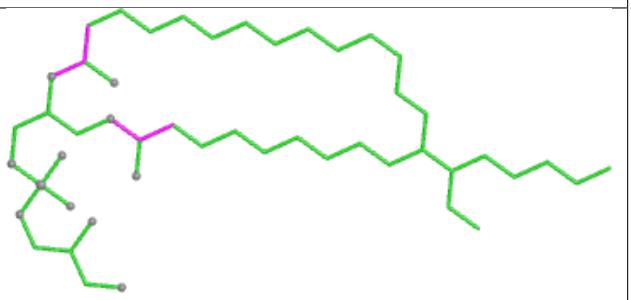
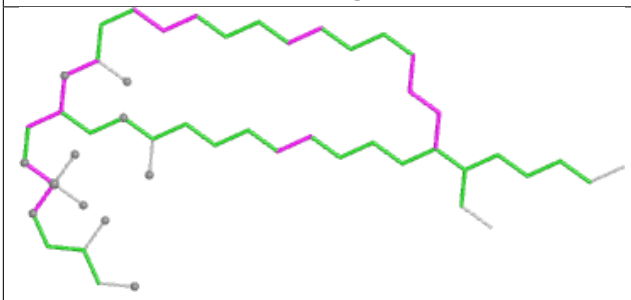
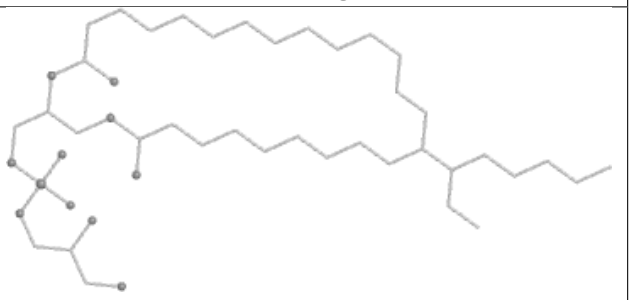
Bond angles

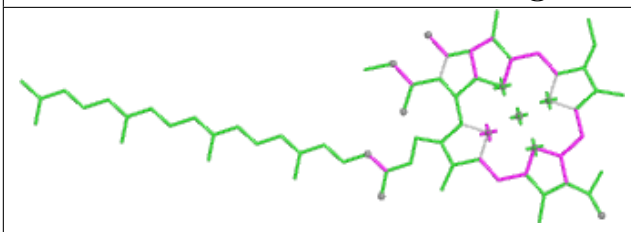
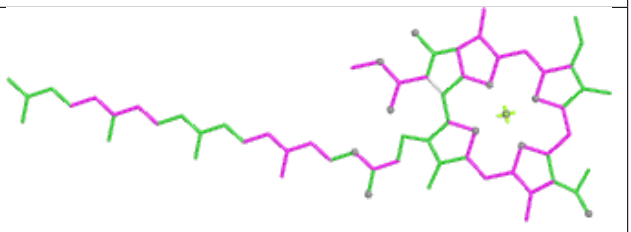
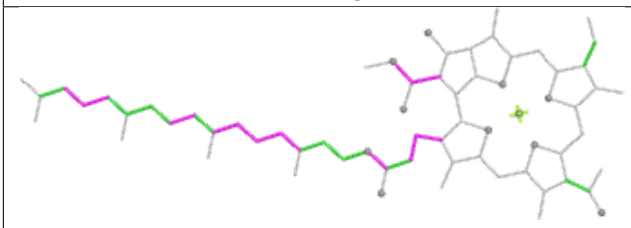
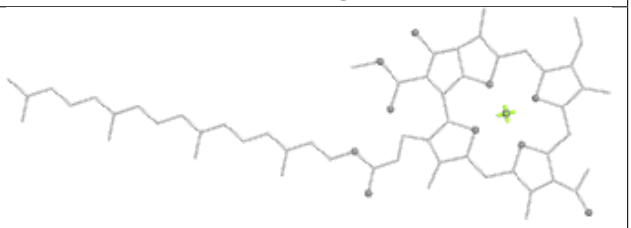


Torsions

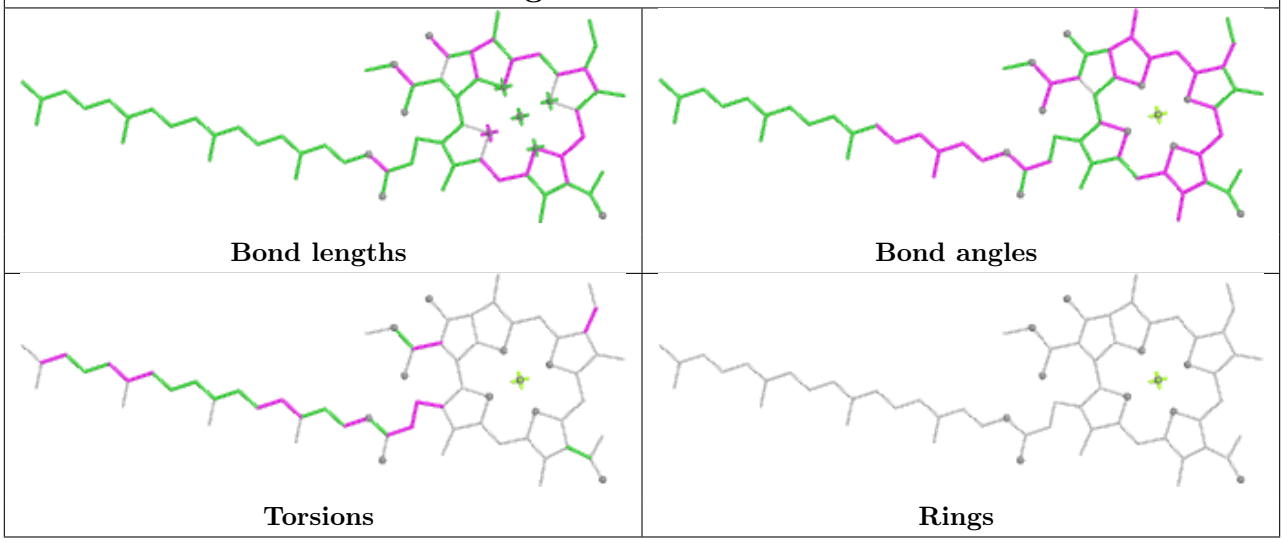


Rings

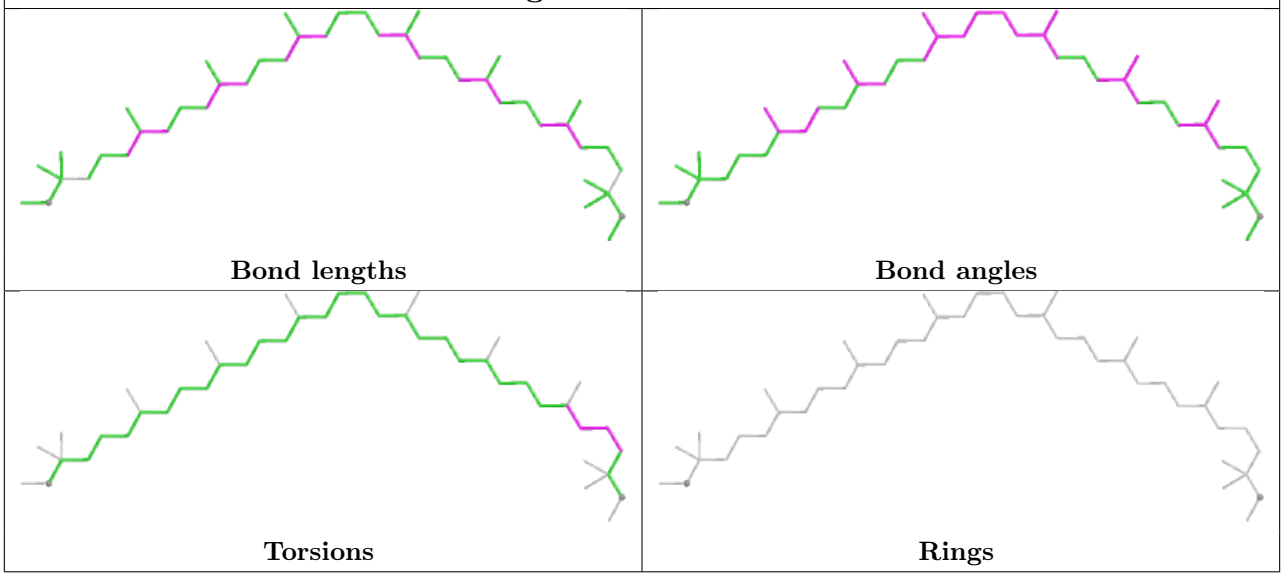
Ligand PGV R 104	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

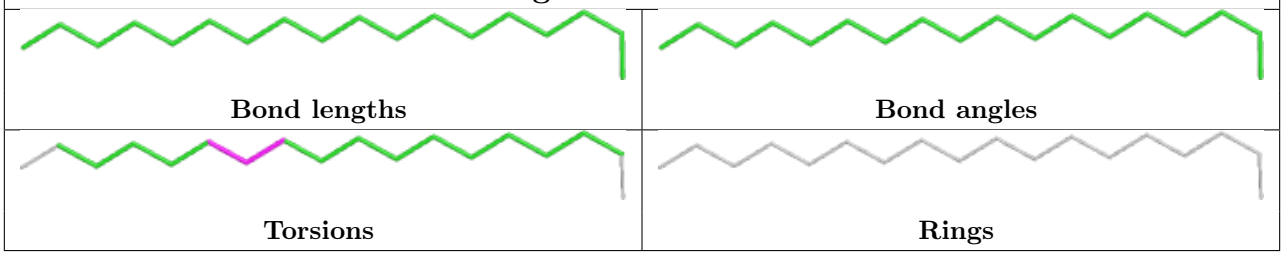
Ligand BCL G 101

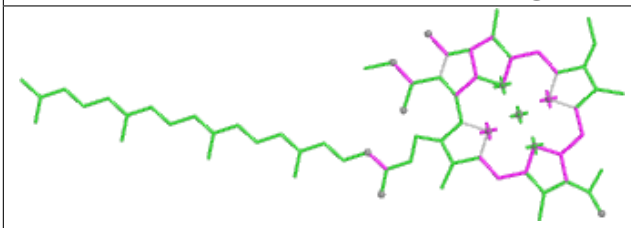
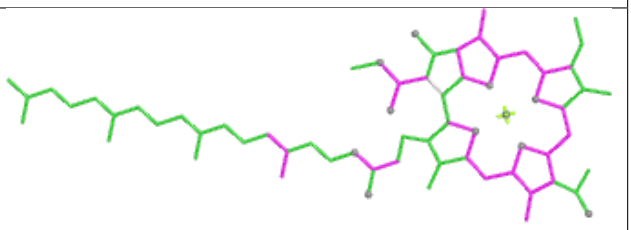
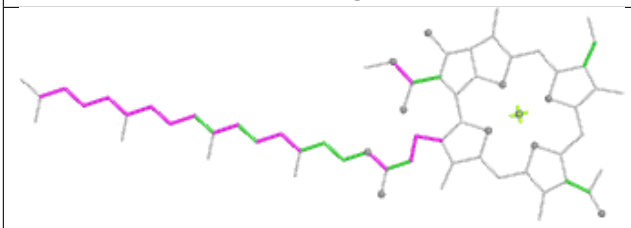
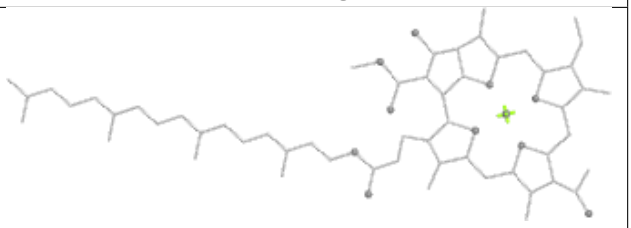


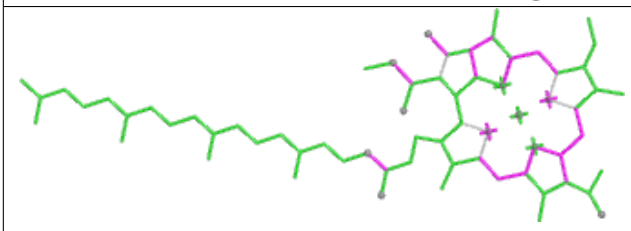
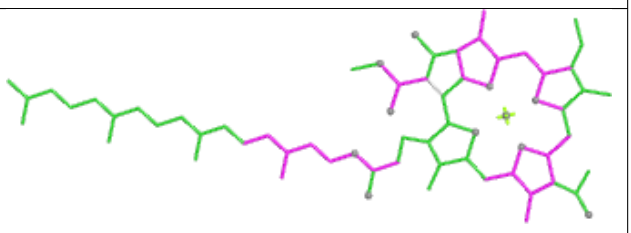
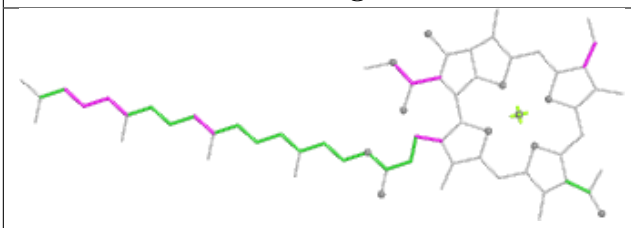
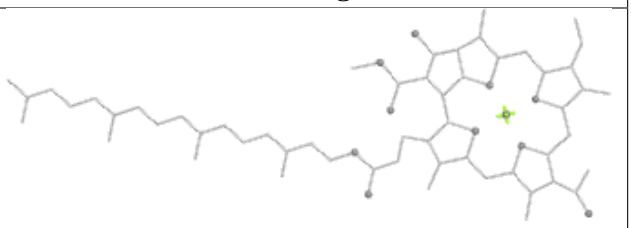
Ligand CRT P 103

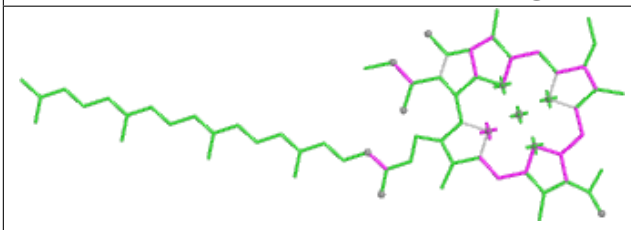
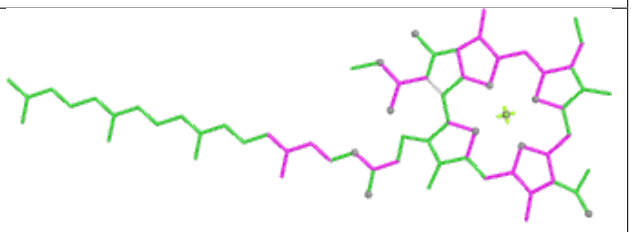
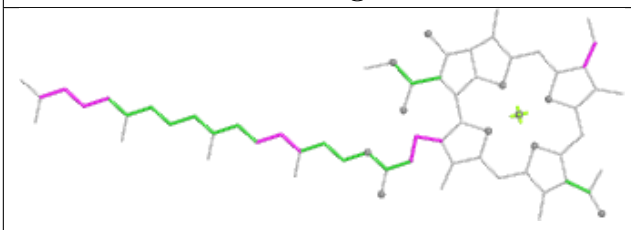
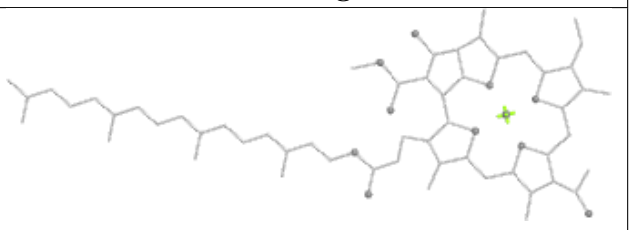


Ligand 8K6 L 406

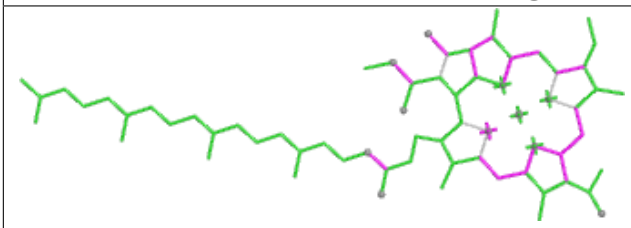


Ligand BCL h 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL L 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL B 101



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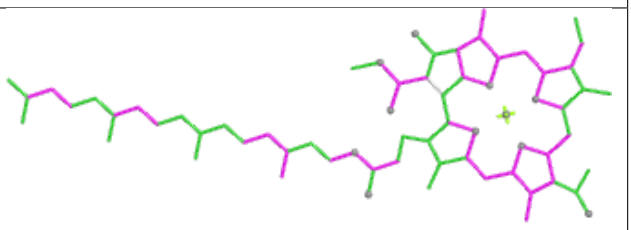

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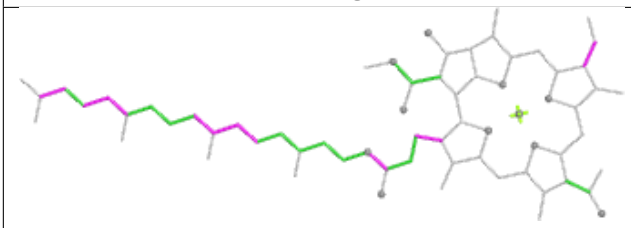

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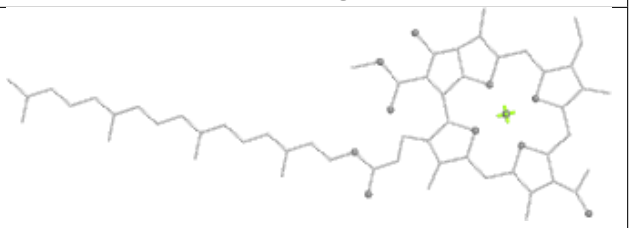
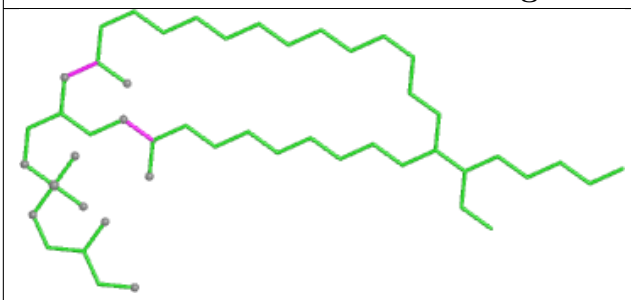


Rings

Ligand PGV H 302



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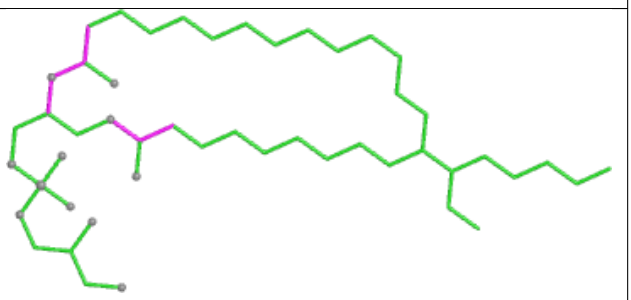

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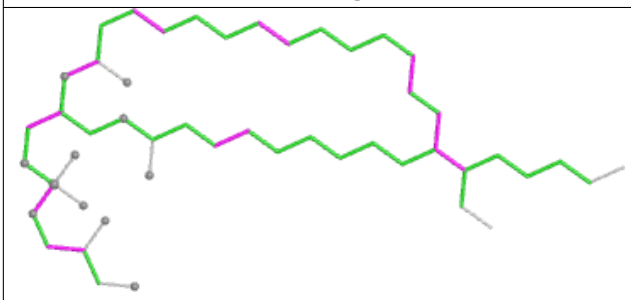

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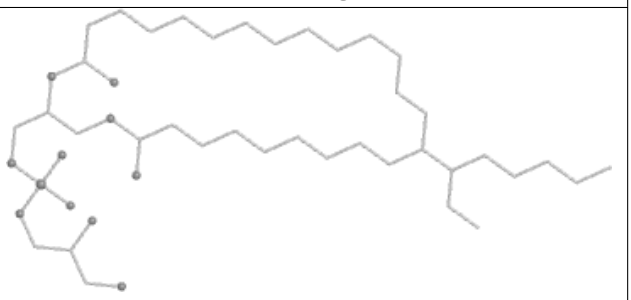

Rings

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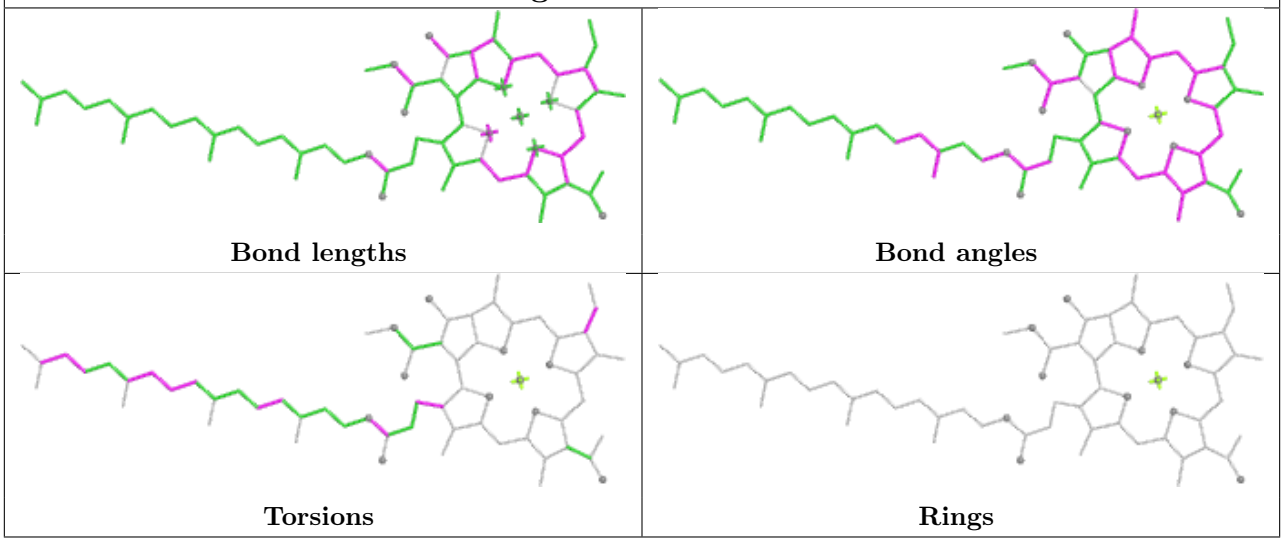

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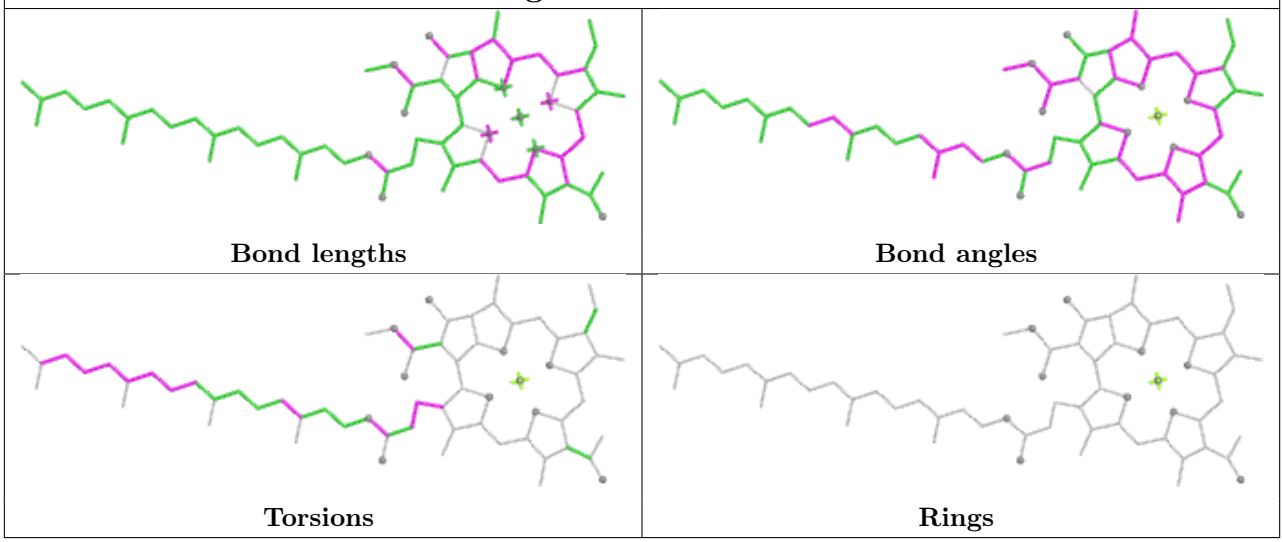

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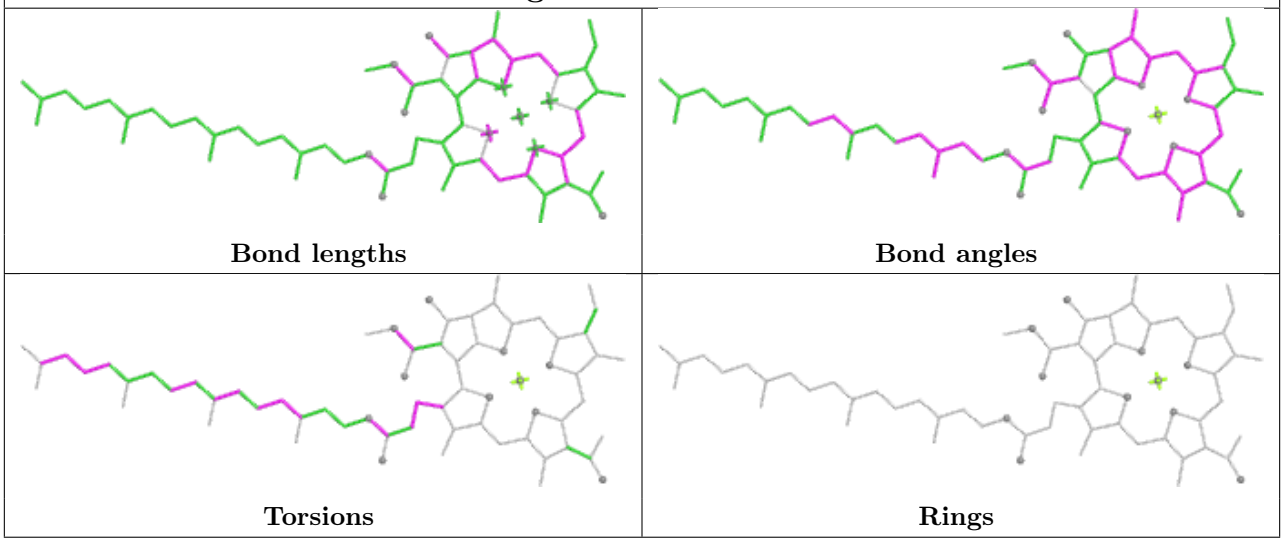

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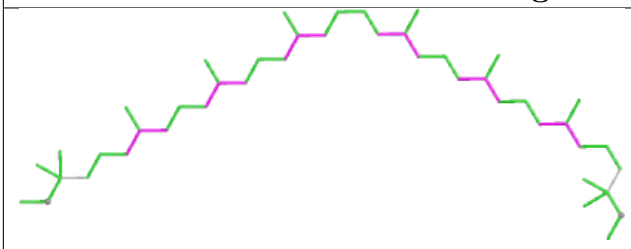
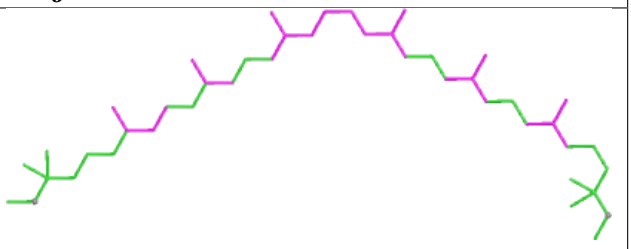
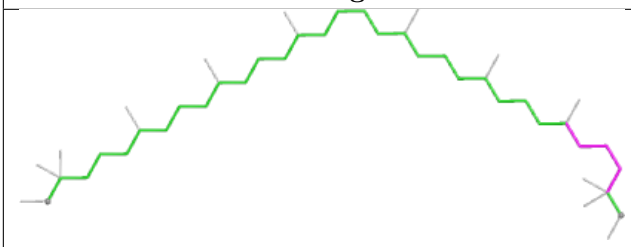
 Bond lengths	 Bond angles
 Torsions	Rings

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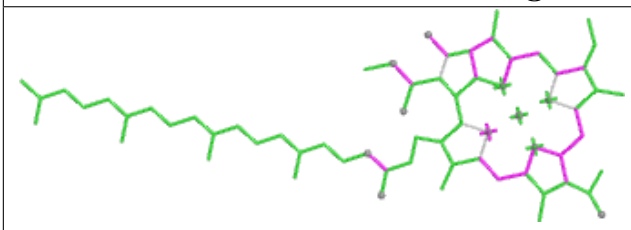
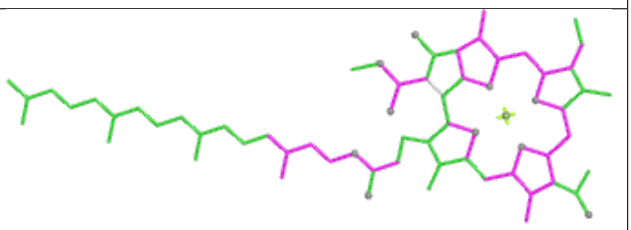
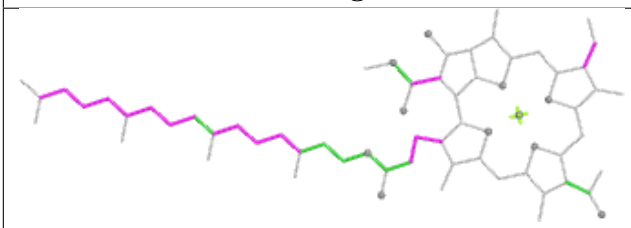
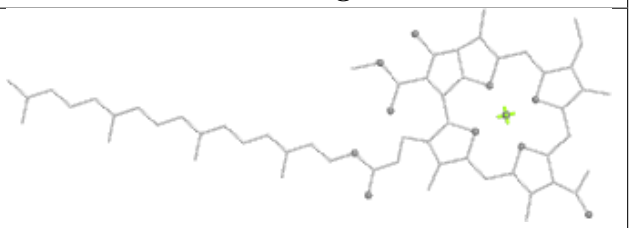
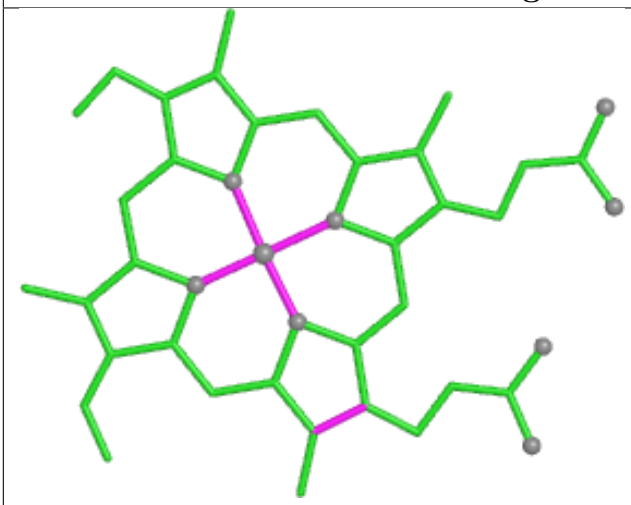
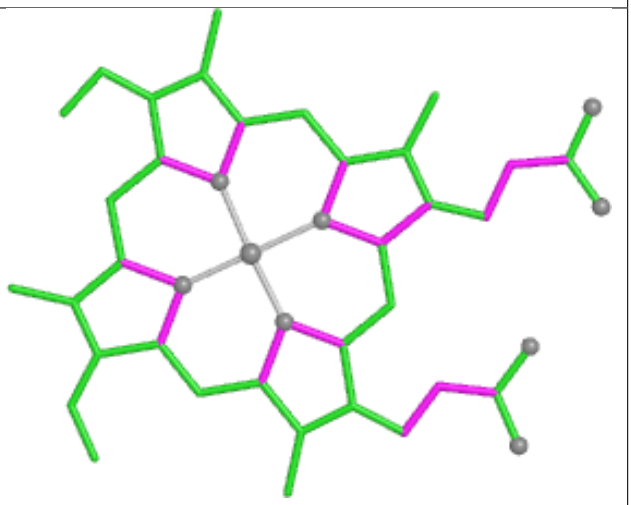
 Bond lengths	 Bond angles
 Torsions	 Rings

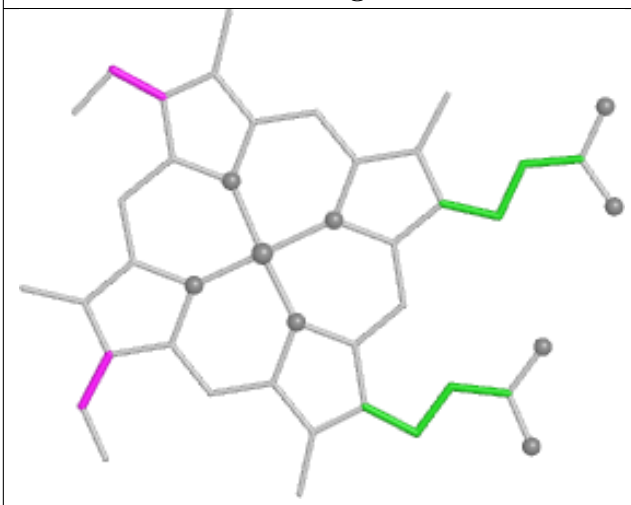
Ligand HEC C 501



Bond lengths



Bond angles



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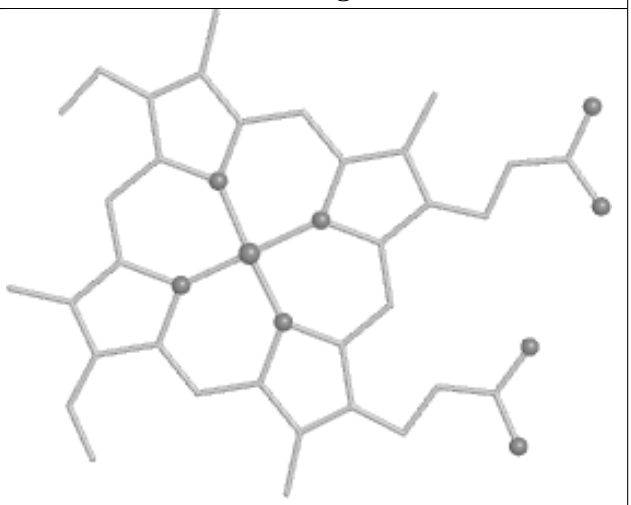
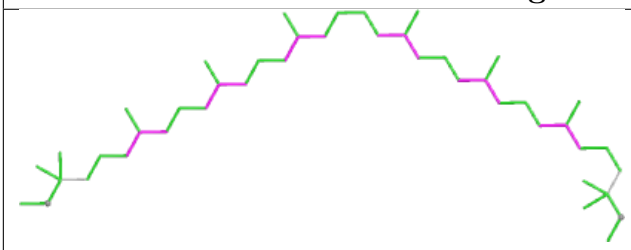
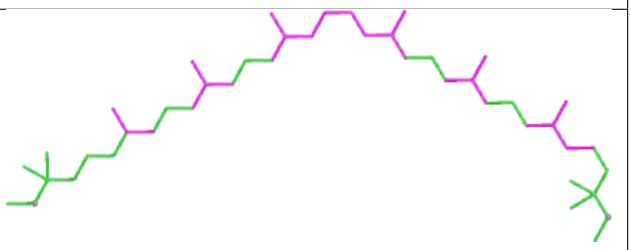


Rings

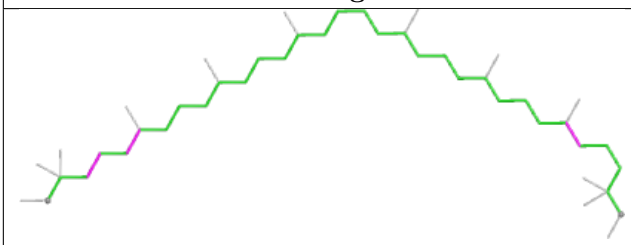
Ligand CRT a 102



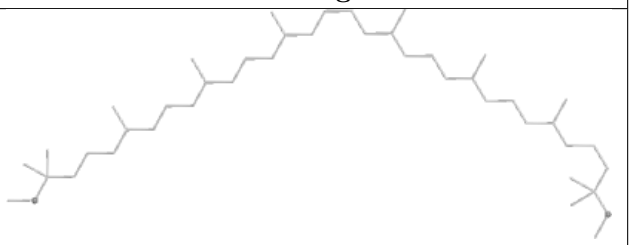
Bond lengths



Bond angles

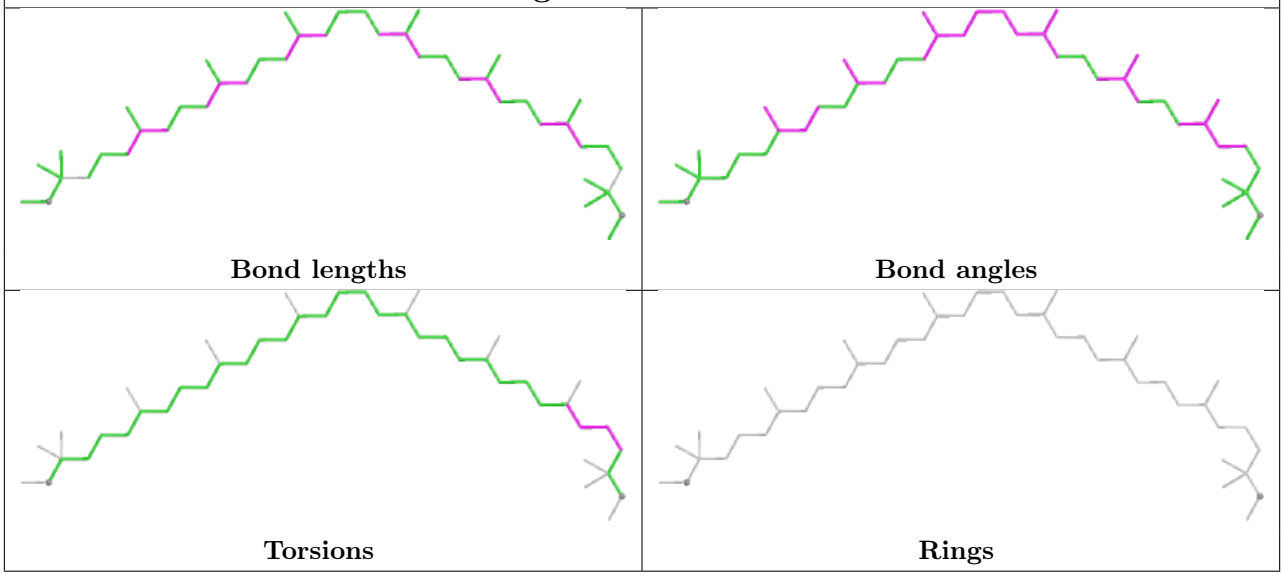


Torsions

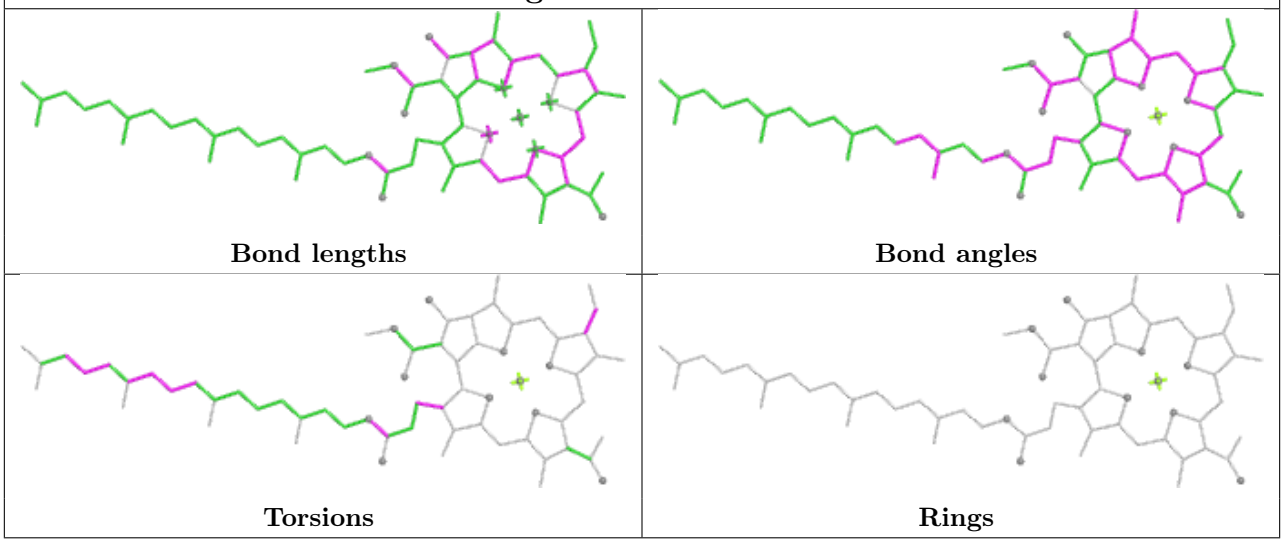


Rings

Ligand CRT i 102



Ligand BCL O 101



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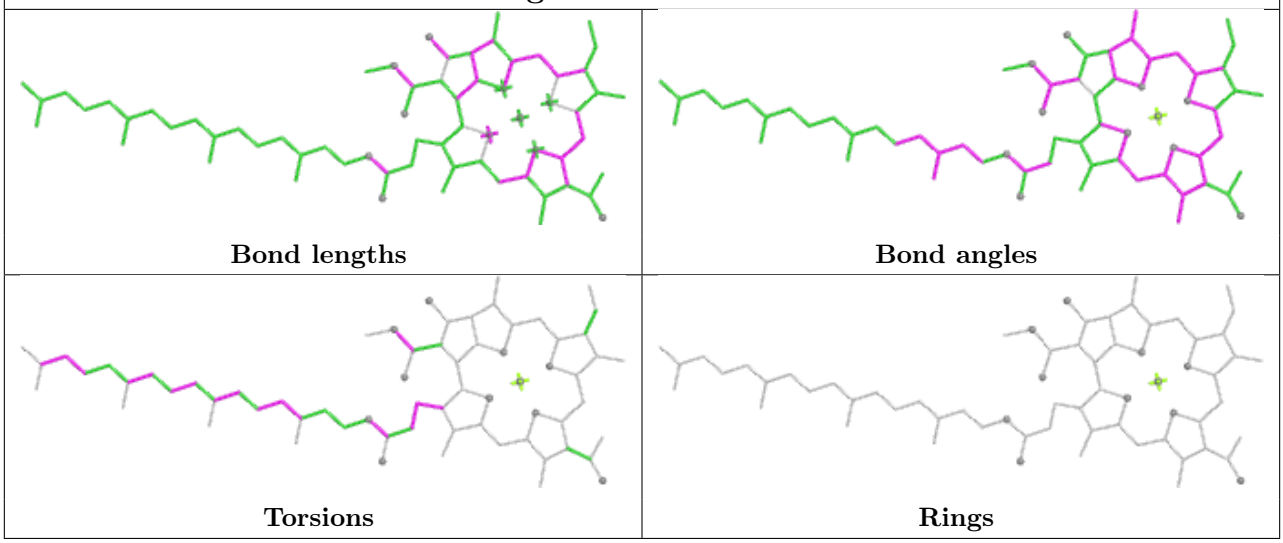

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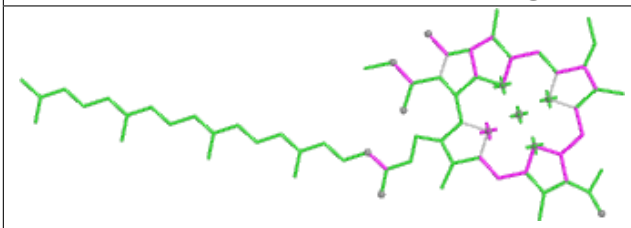
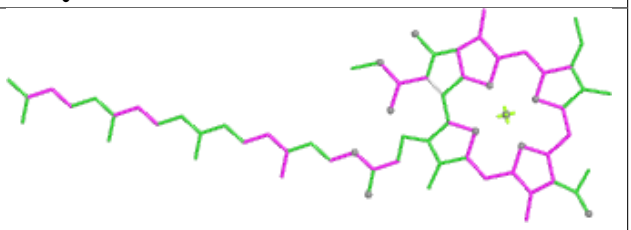
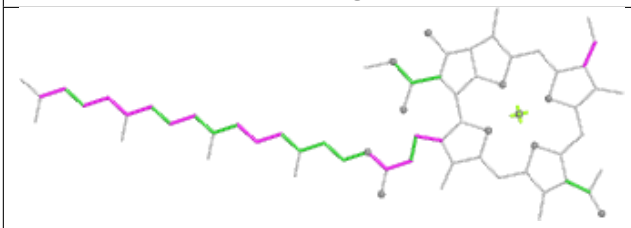
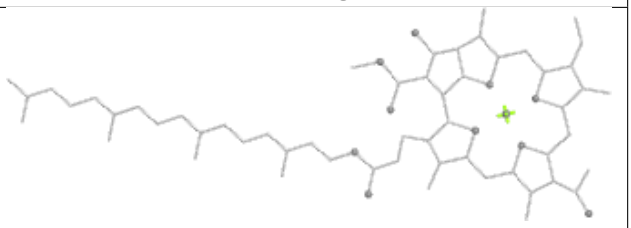
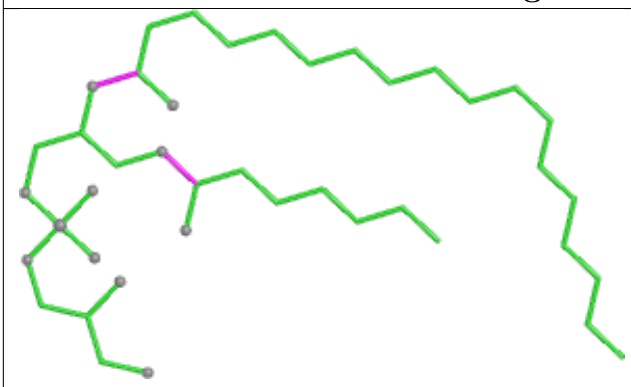
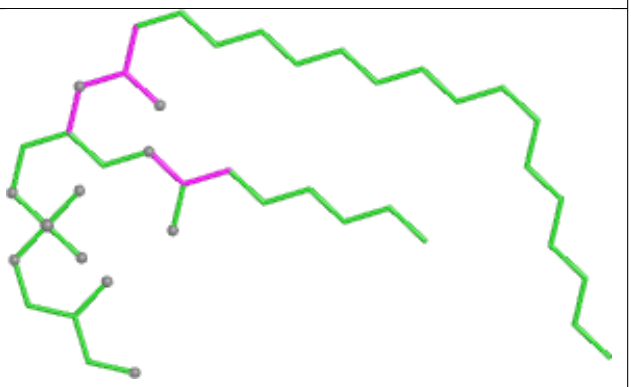
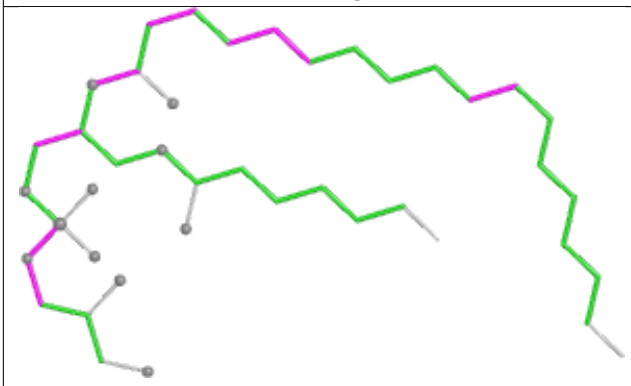
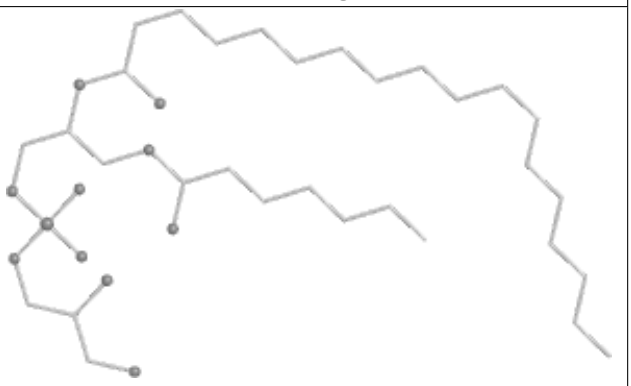
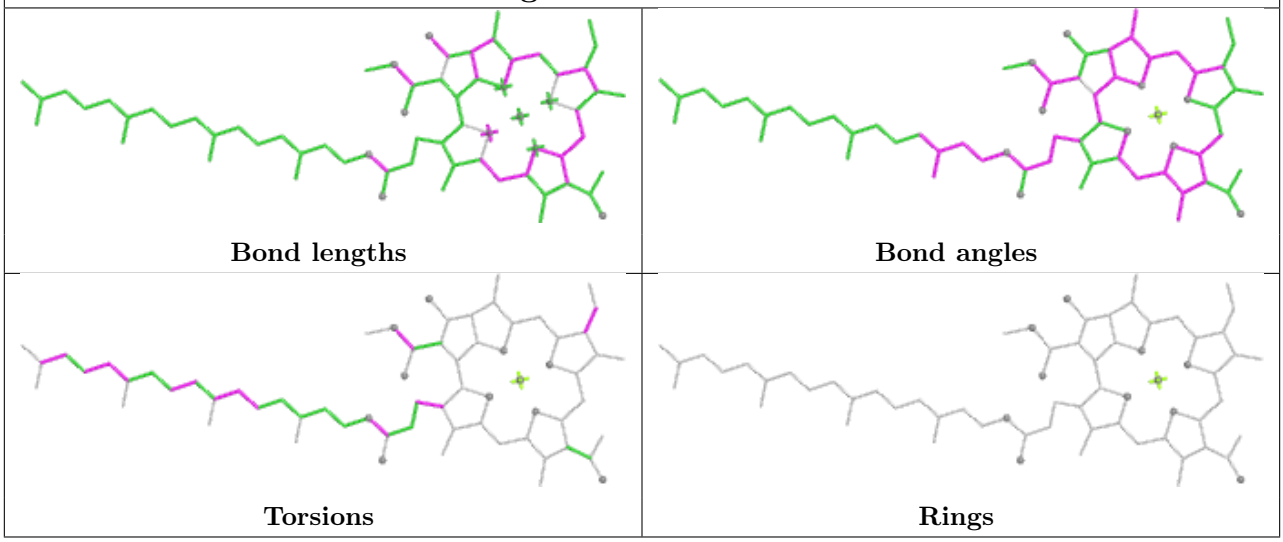
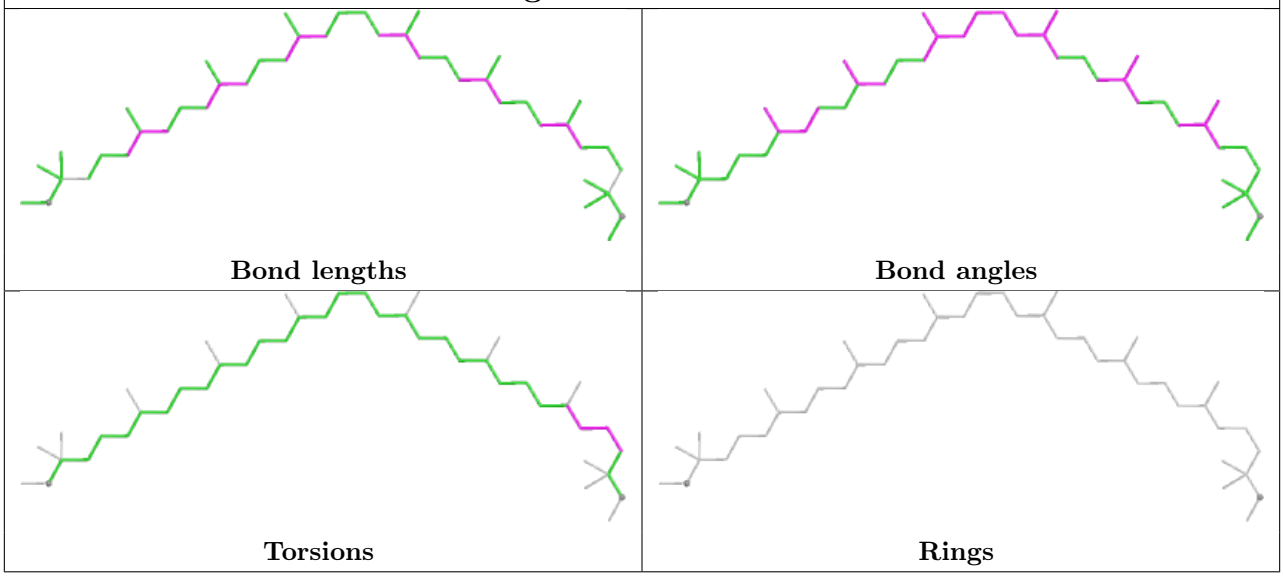
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV Z 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

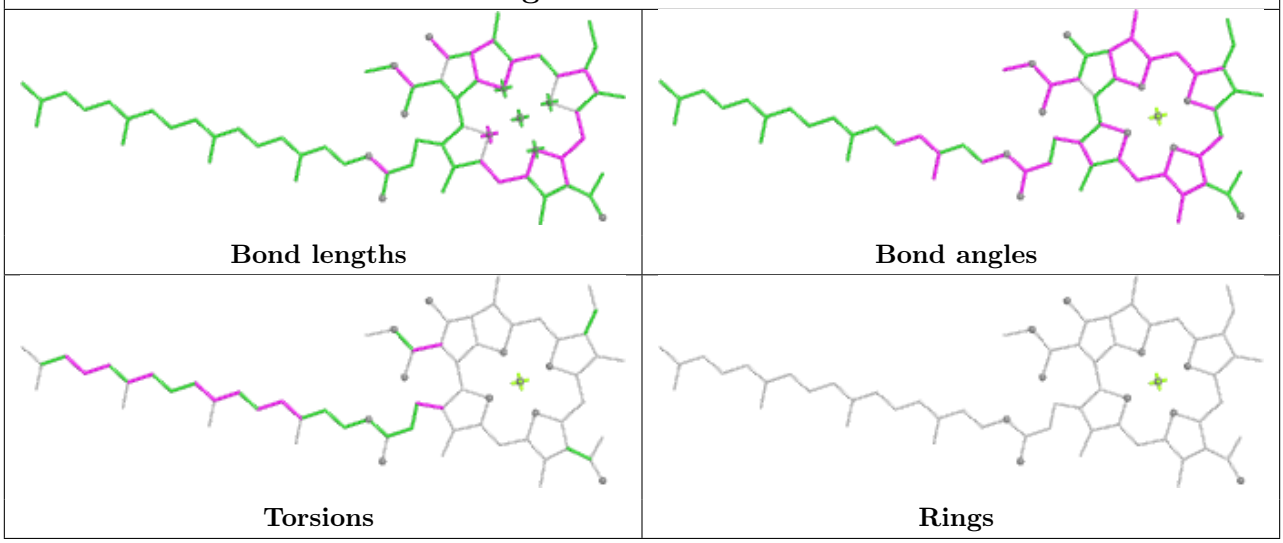
Ligand BCL W 101



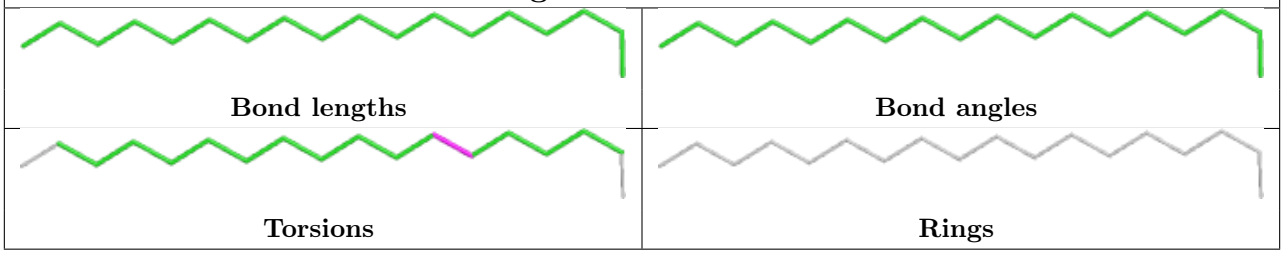
Ligand CRT N 103



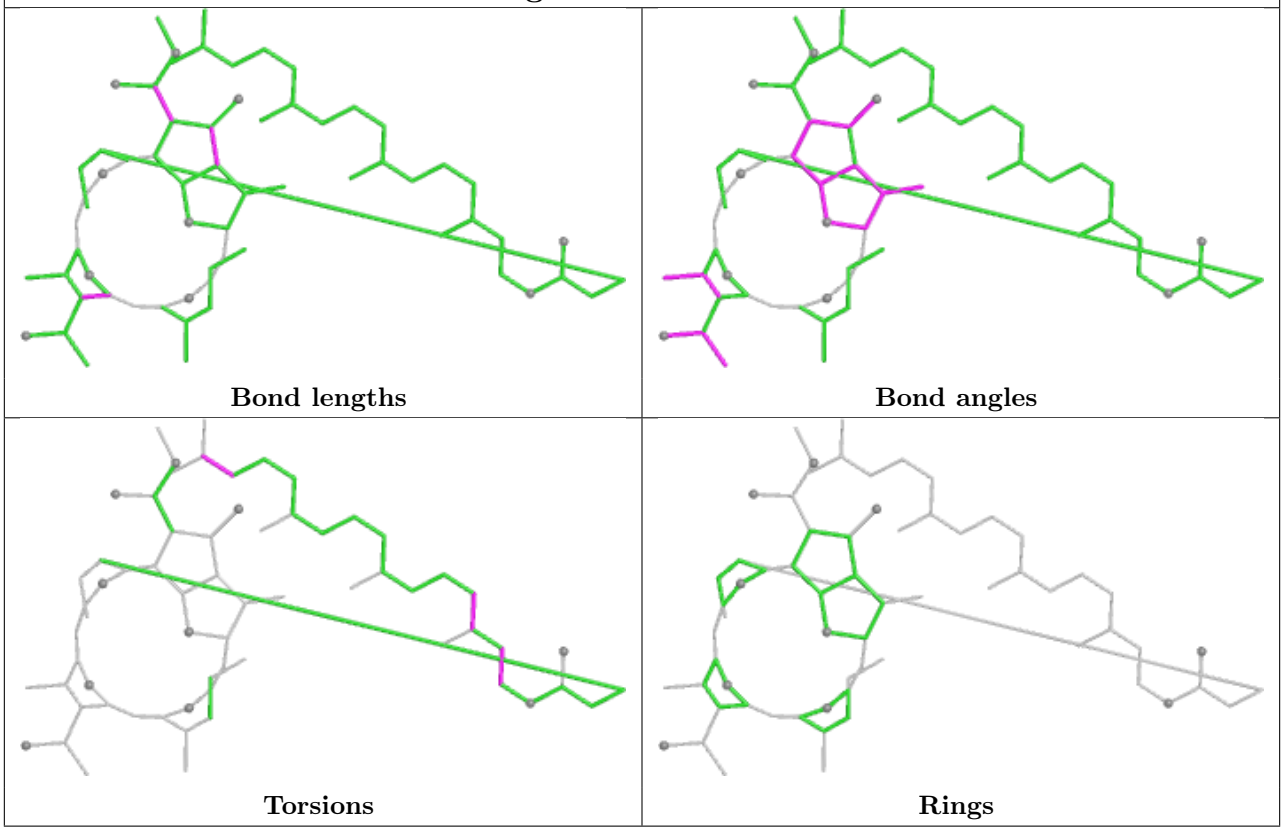
Ligand BCL M 403



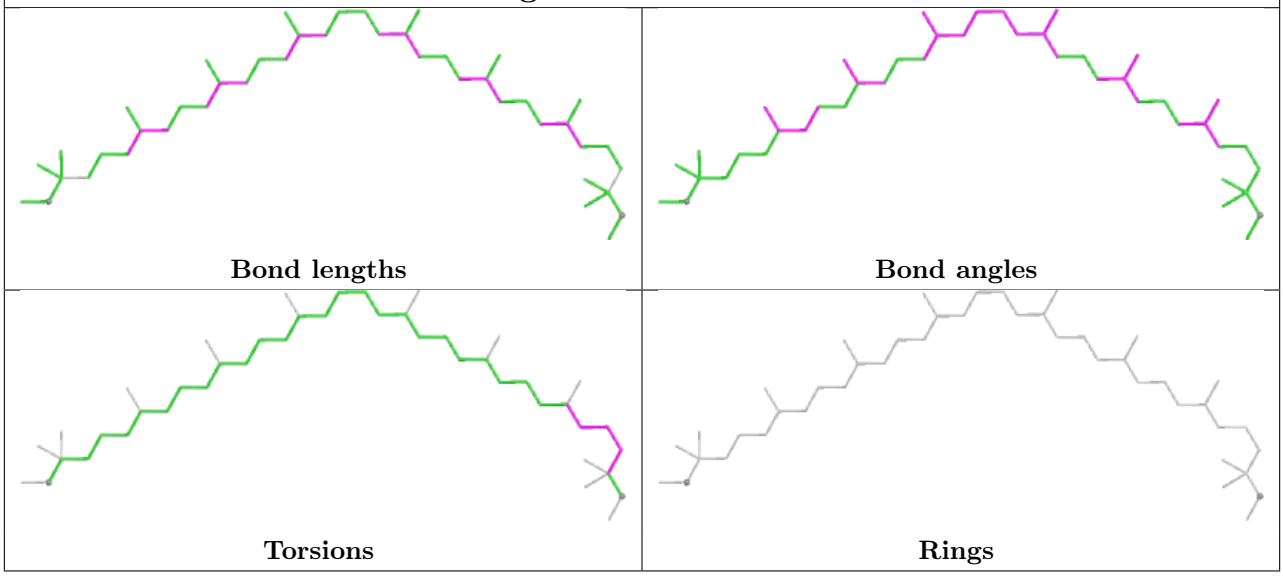
Ligand 8K6 V 103



Ligand BPH L 403



Ligand CRT W 102



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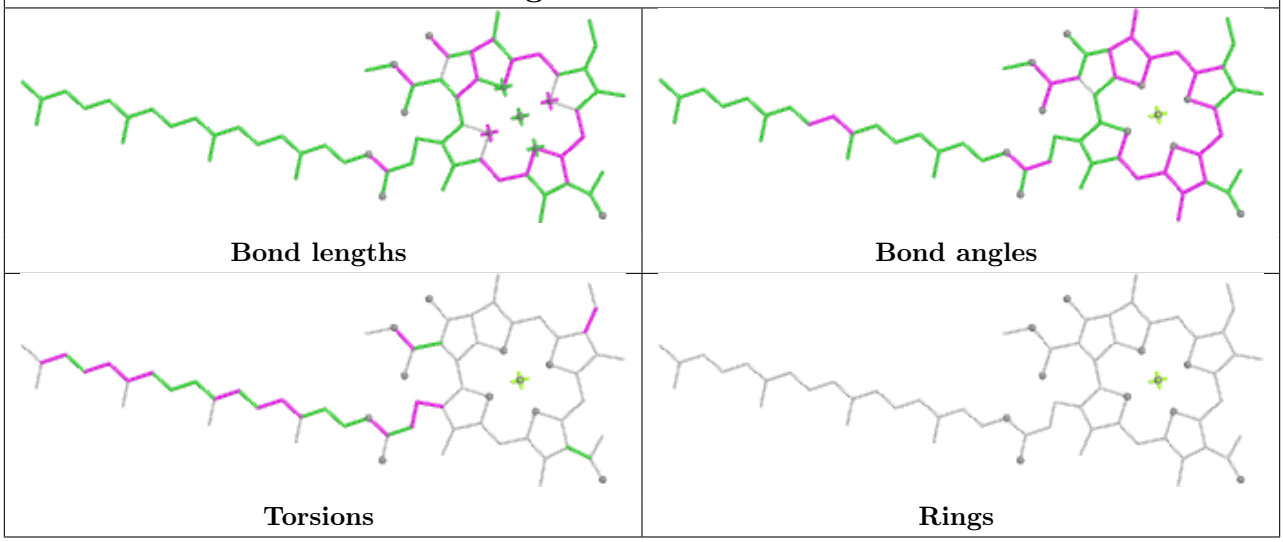

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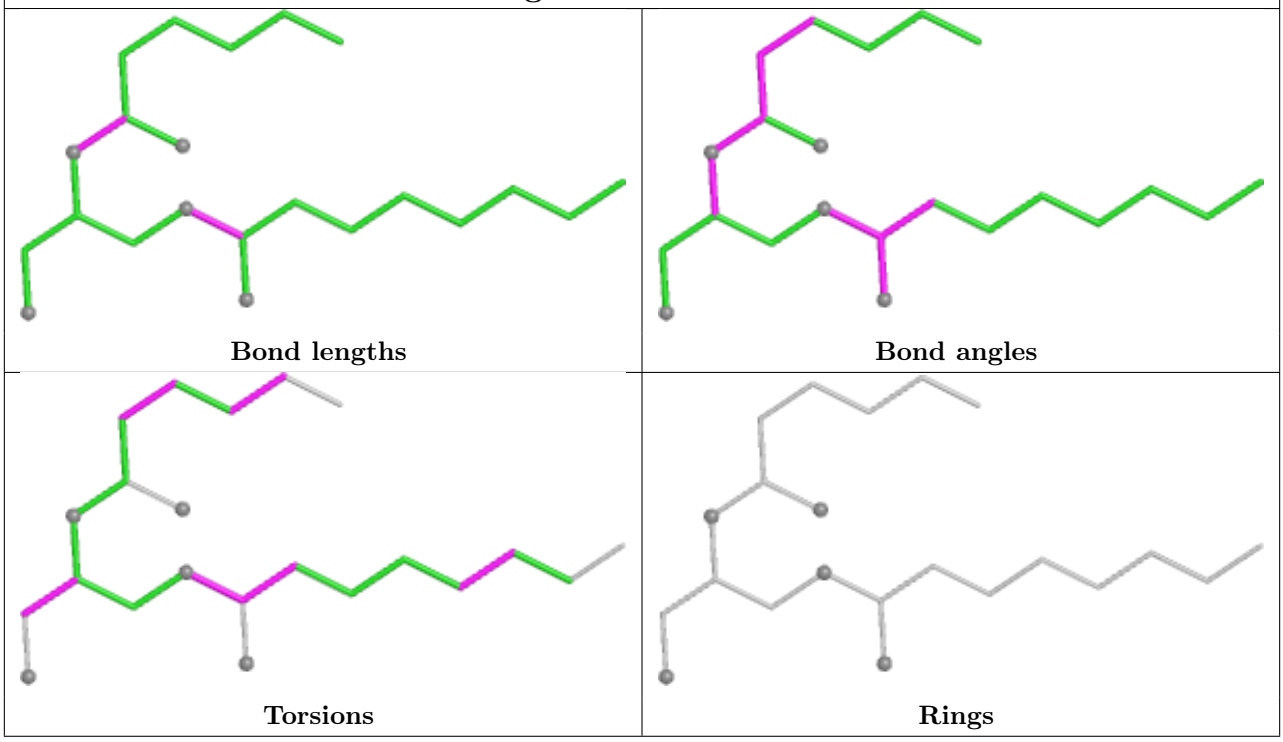
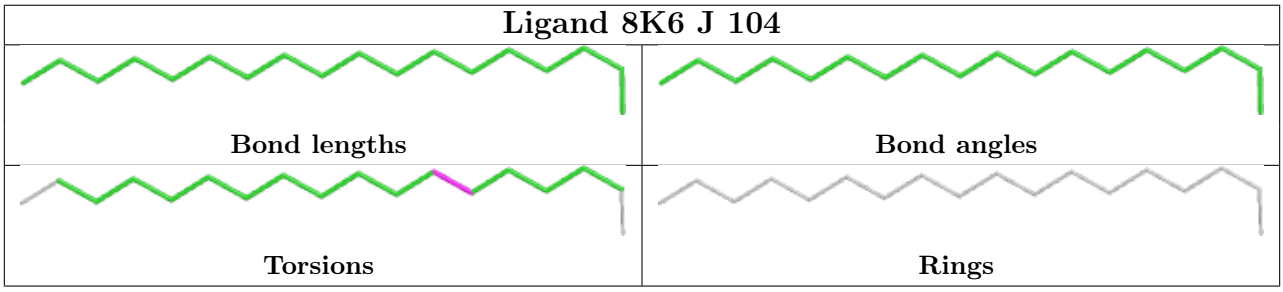
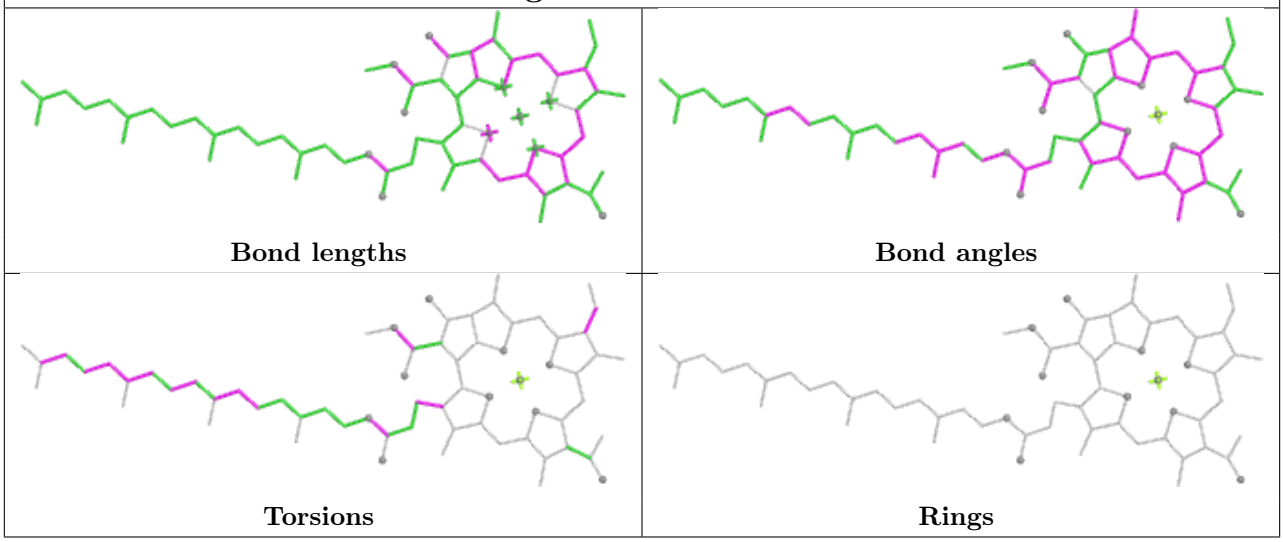


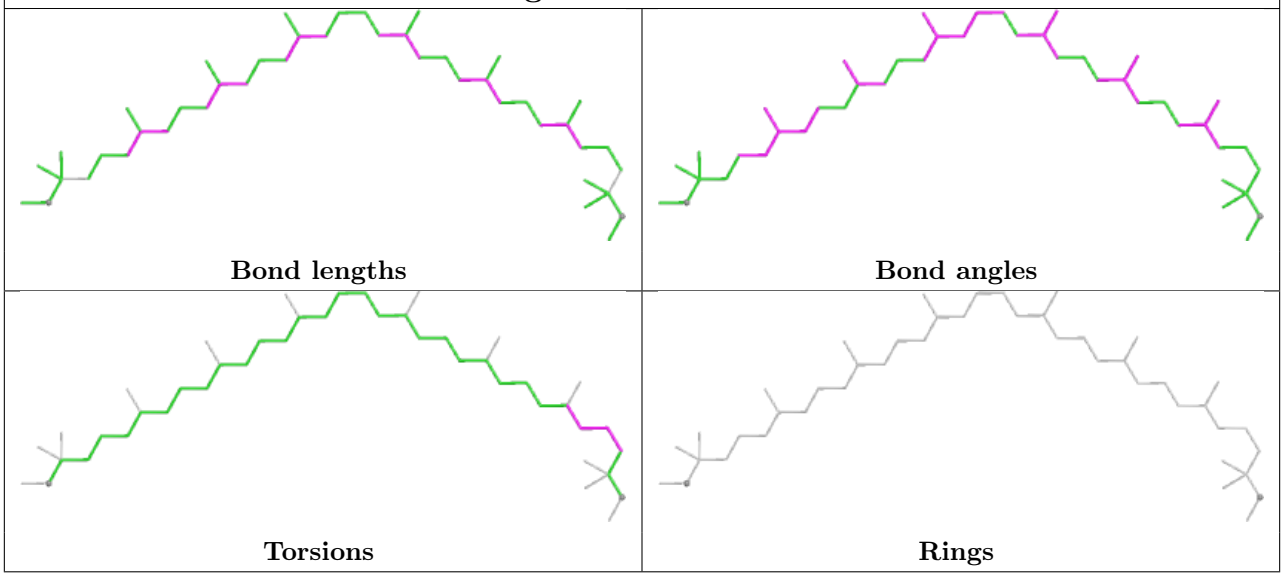
Ligand 8K6 J 104



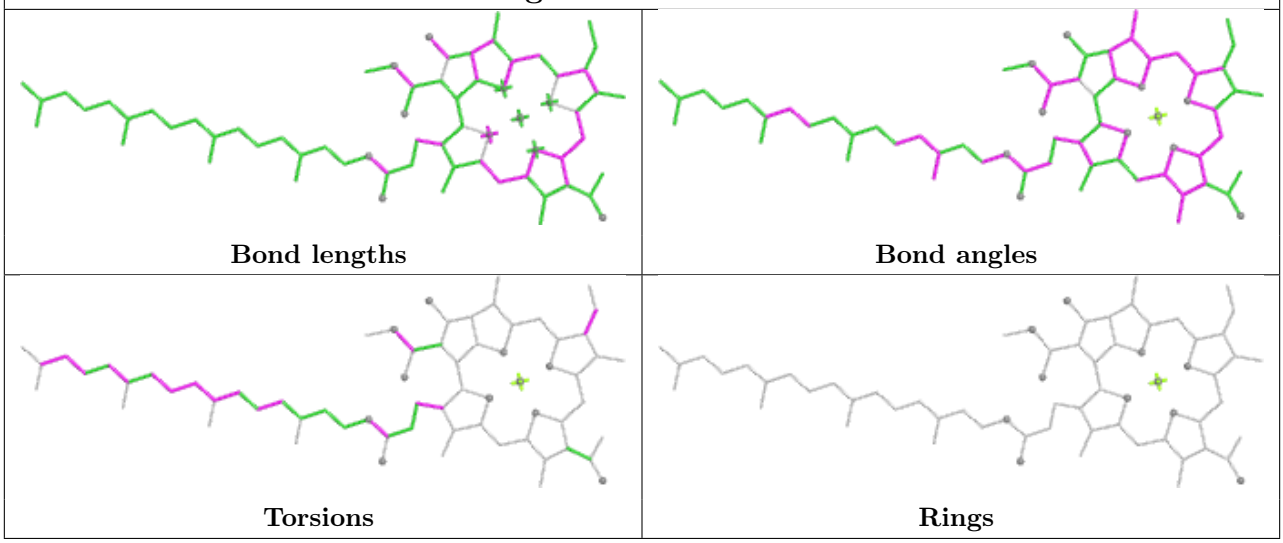
Ligand BCL Y 101



Ligand CRT A 103



Ligand BCL D 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

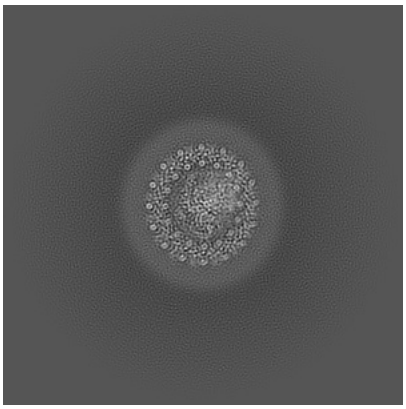
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-60165. These allow visual inspection of the internal detail of the map and identification of artifacts.

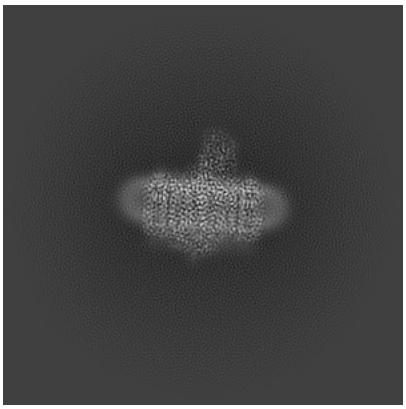
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

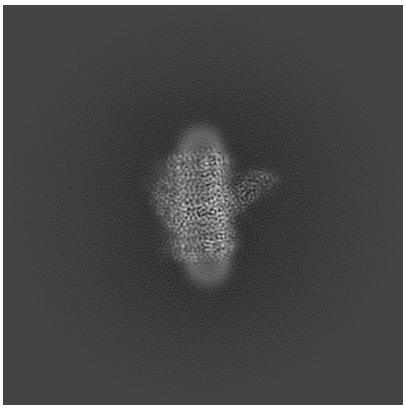
6.1.1 Primary map



X

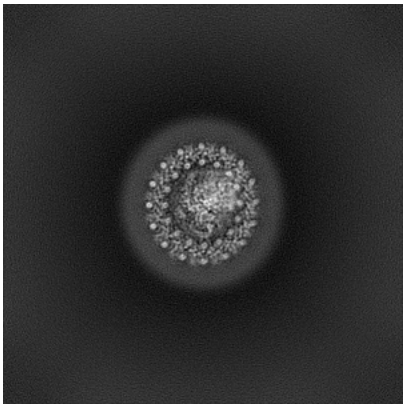


Y

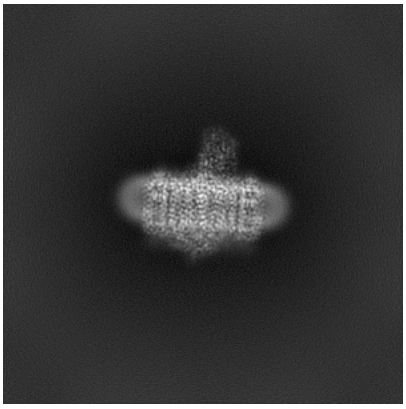


Z

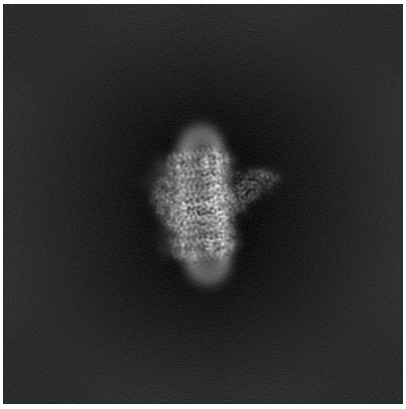
6.1.2 Raw map



X



Y

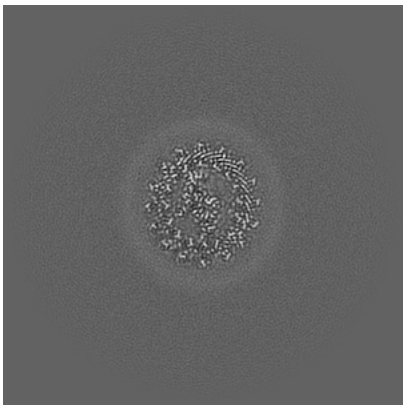


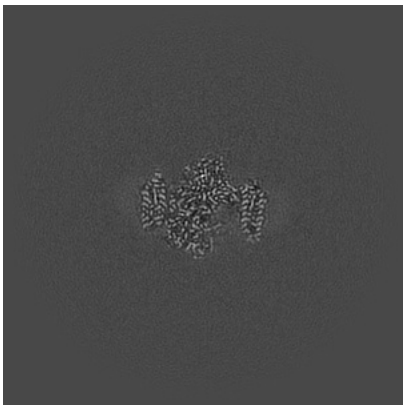
Z

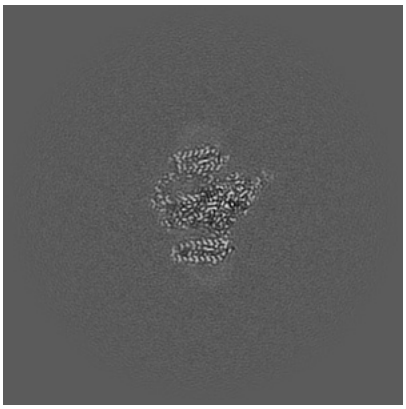
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

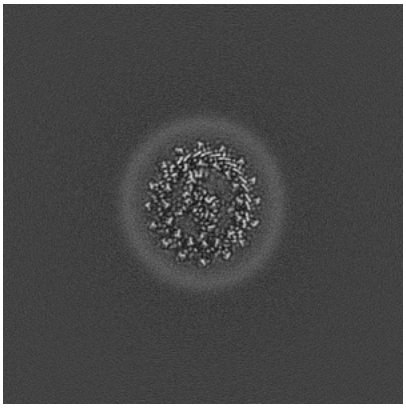
6.2.1 Primary map

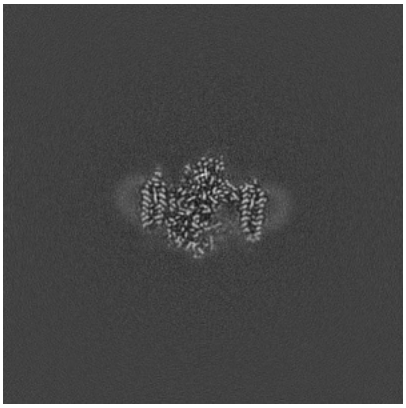

X Index: 180

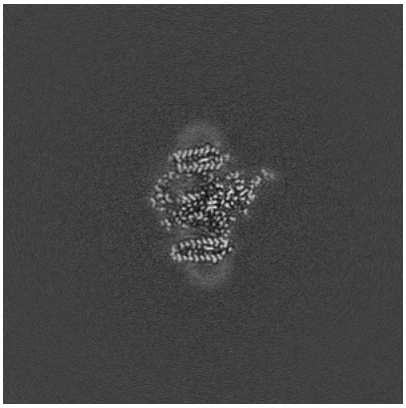

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

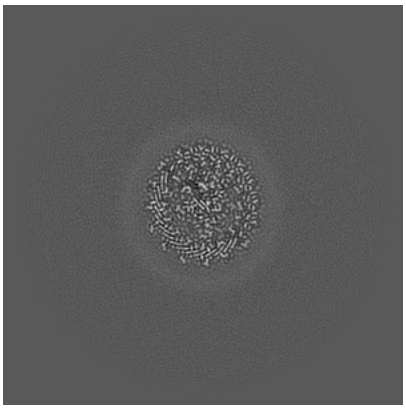

Y Index: 180

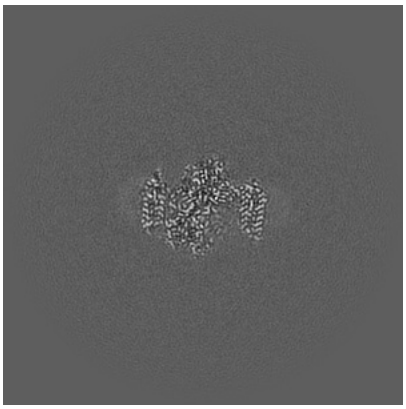

Z Index: 180

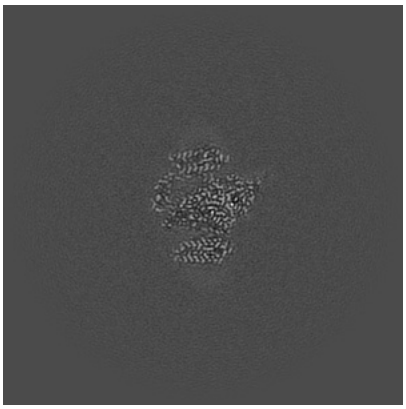
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

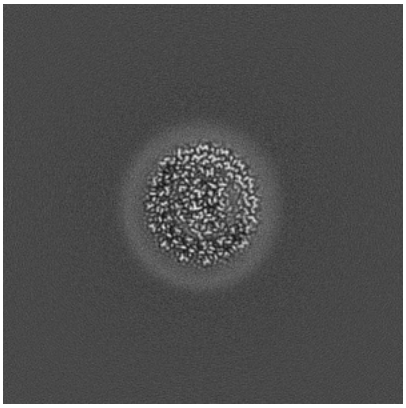
6.3.1 Primary map

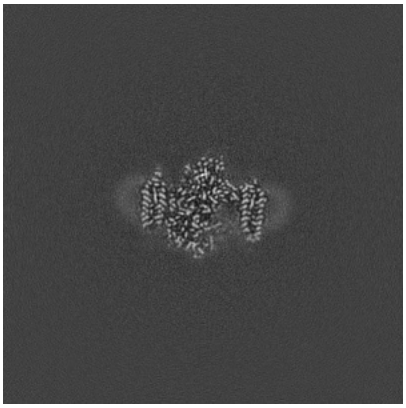

X Index: 187

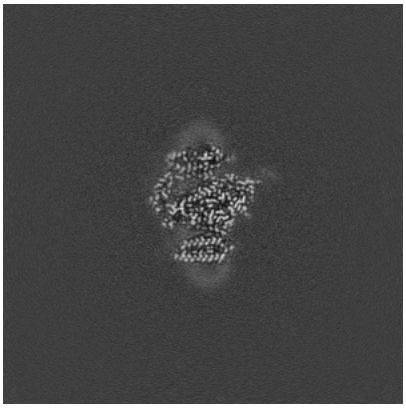

Y Index: 179


Z Index: 179

6.3.2 Raw map


X Index: 192

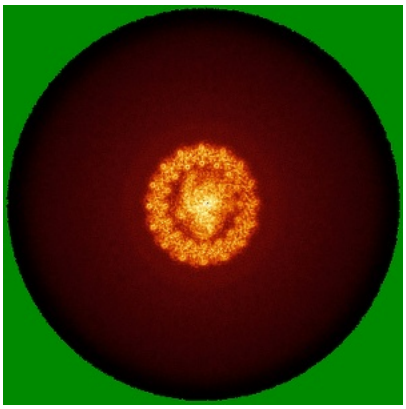

Y Index: 180

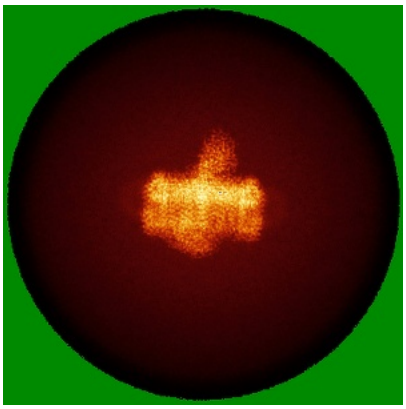

Z Index: 178

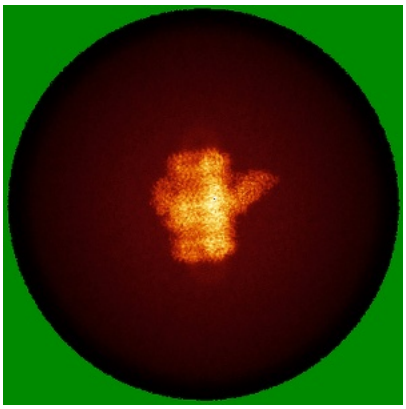
The images above show the largest variance slices of the map in three orthogonal directions.

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

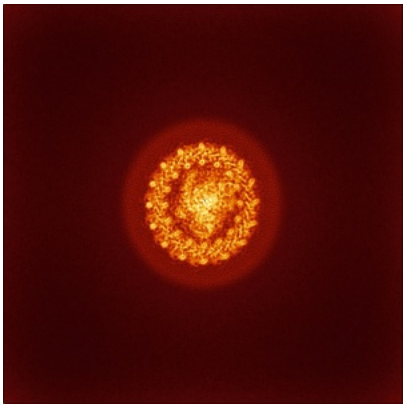
6.4.1 Primary map

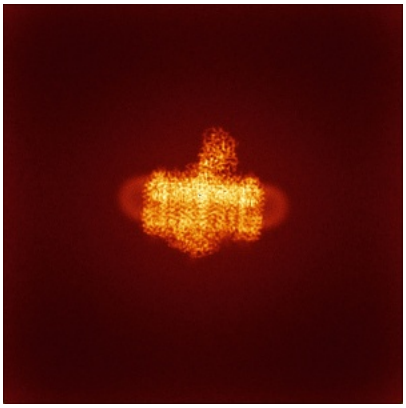

X

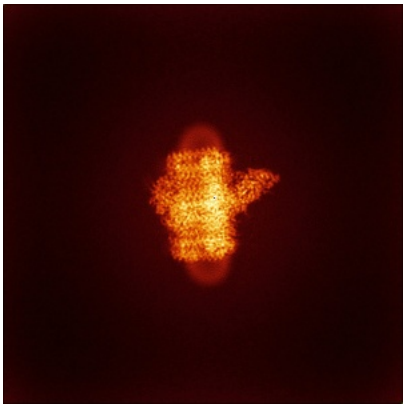

Y


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.

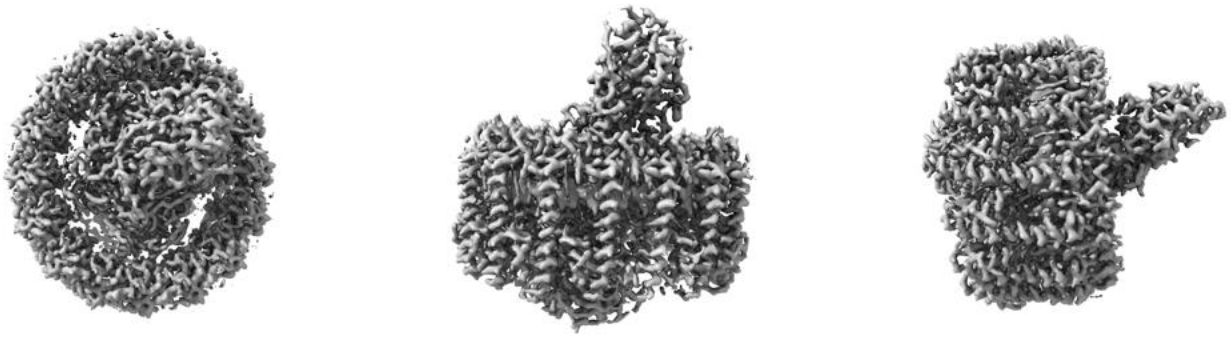
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.562. 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.

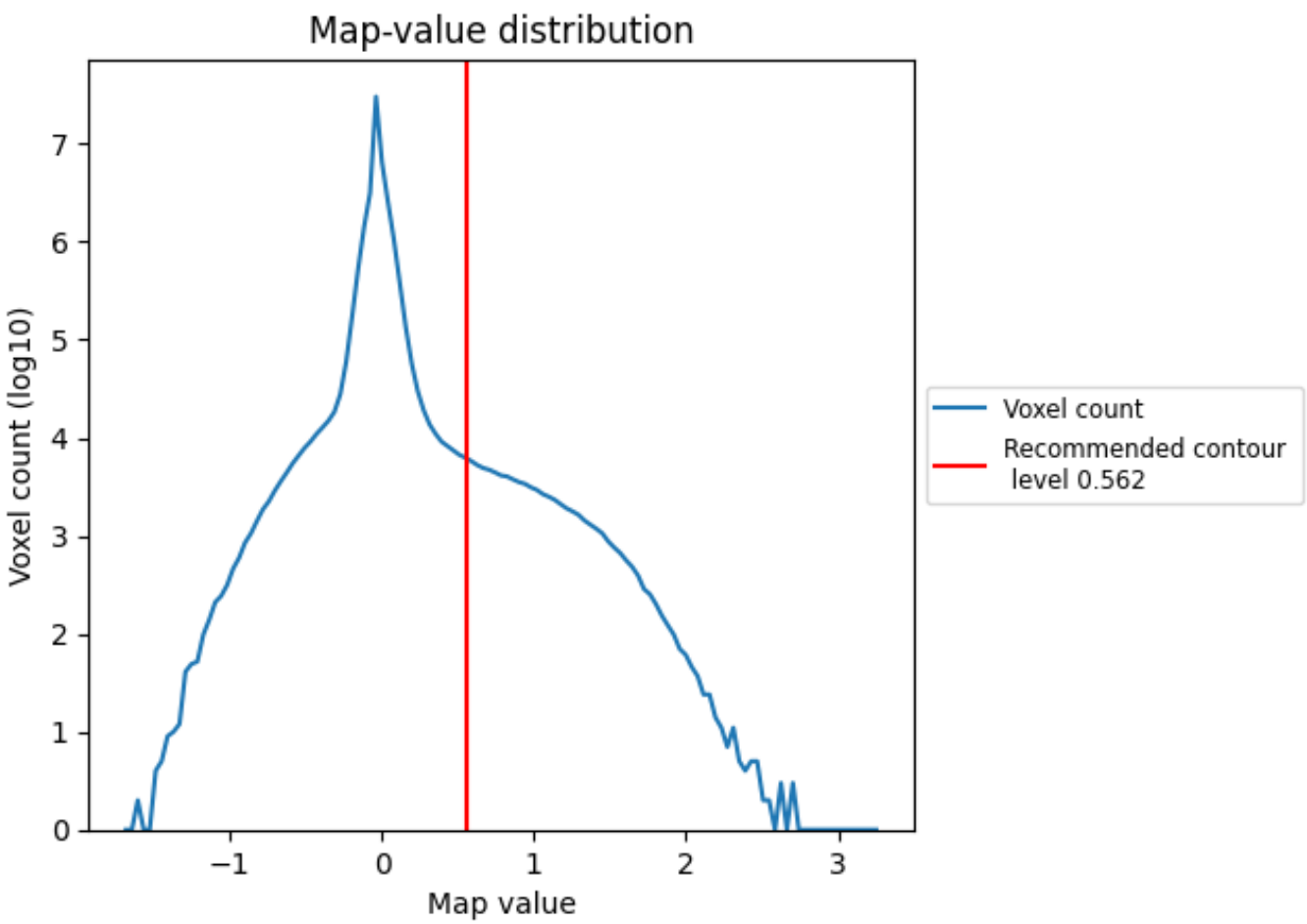
6.6 Mask visualisation (i)

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

7 Map analysis (i)

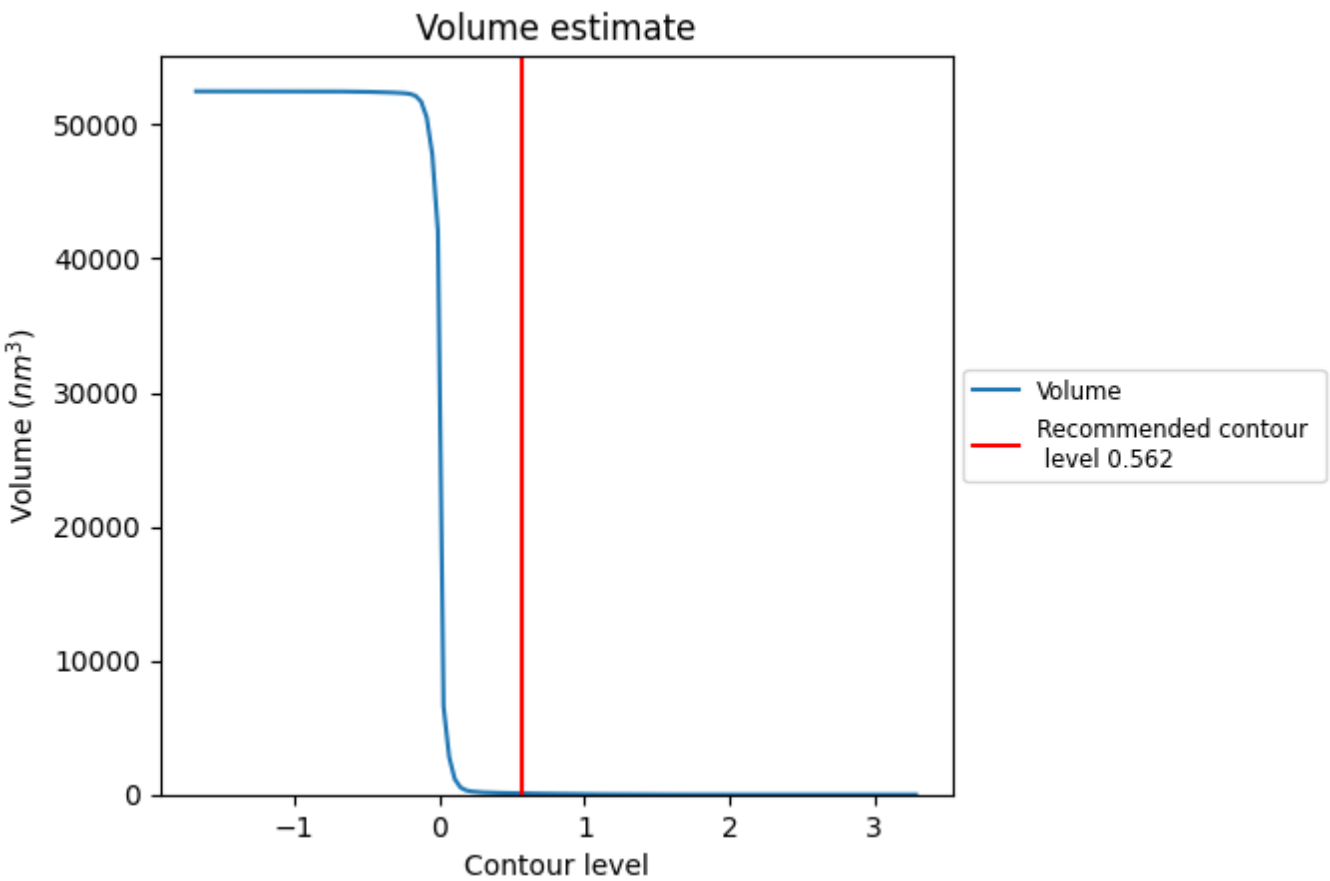
This section contains the results of statistical analysis of the map.

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.

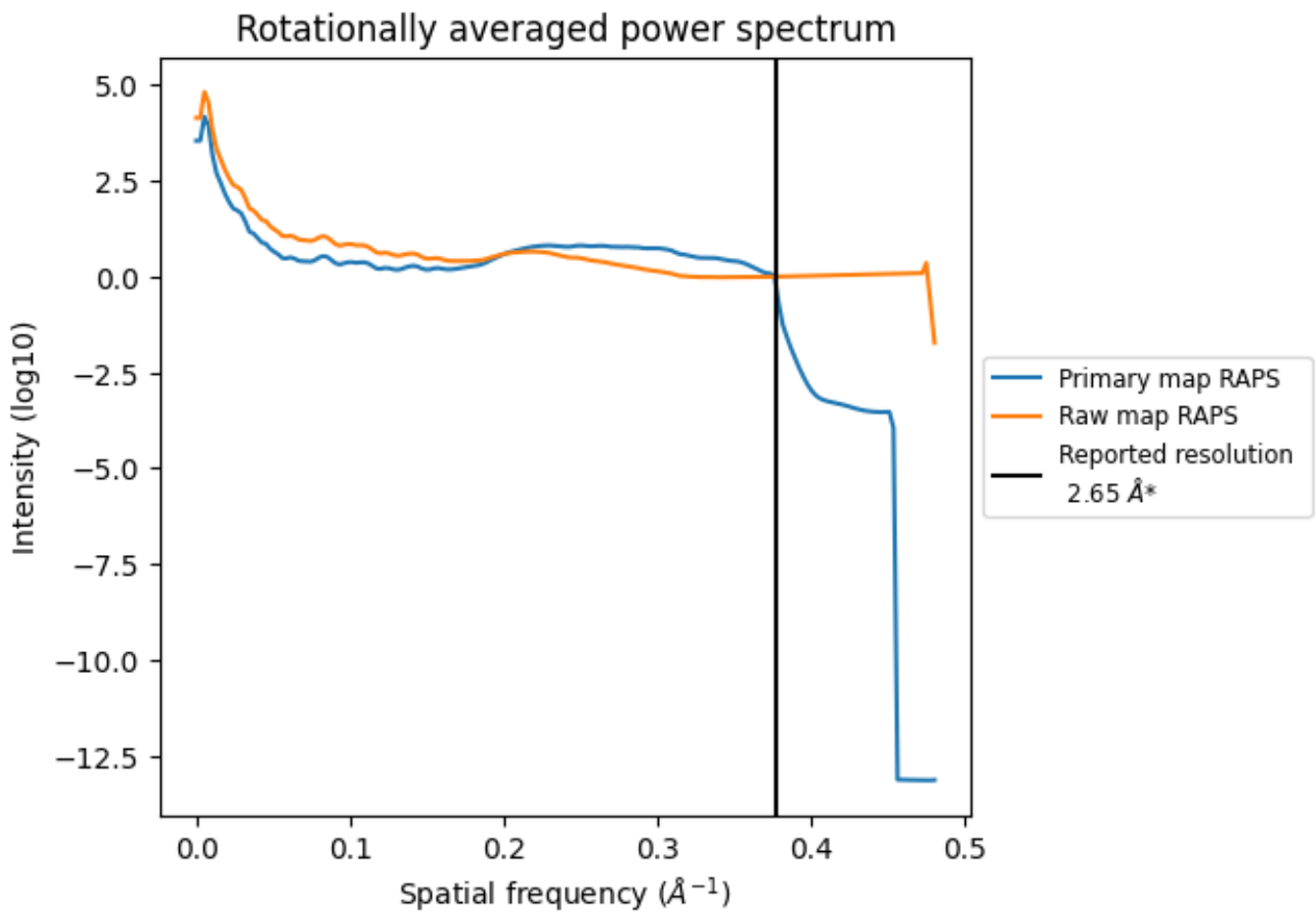
7.2 Volume estimate (i)



The volume at the recommended contour level is 89 nm^3; this corresponds to an approximate mass of 81 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)

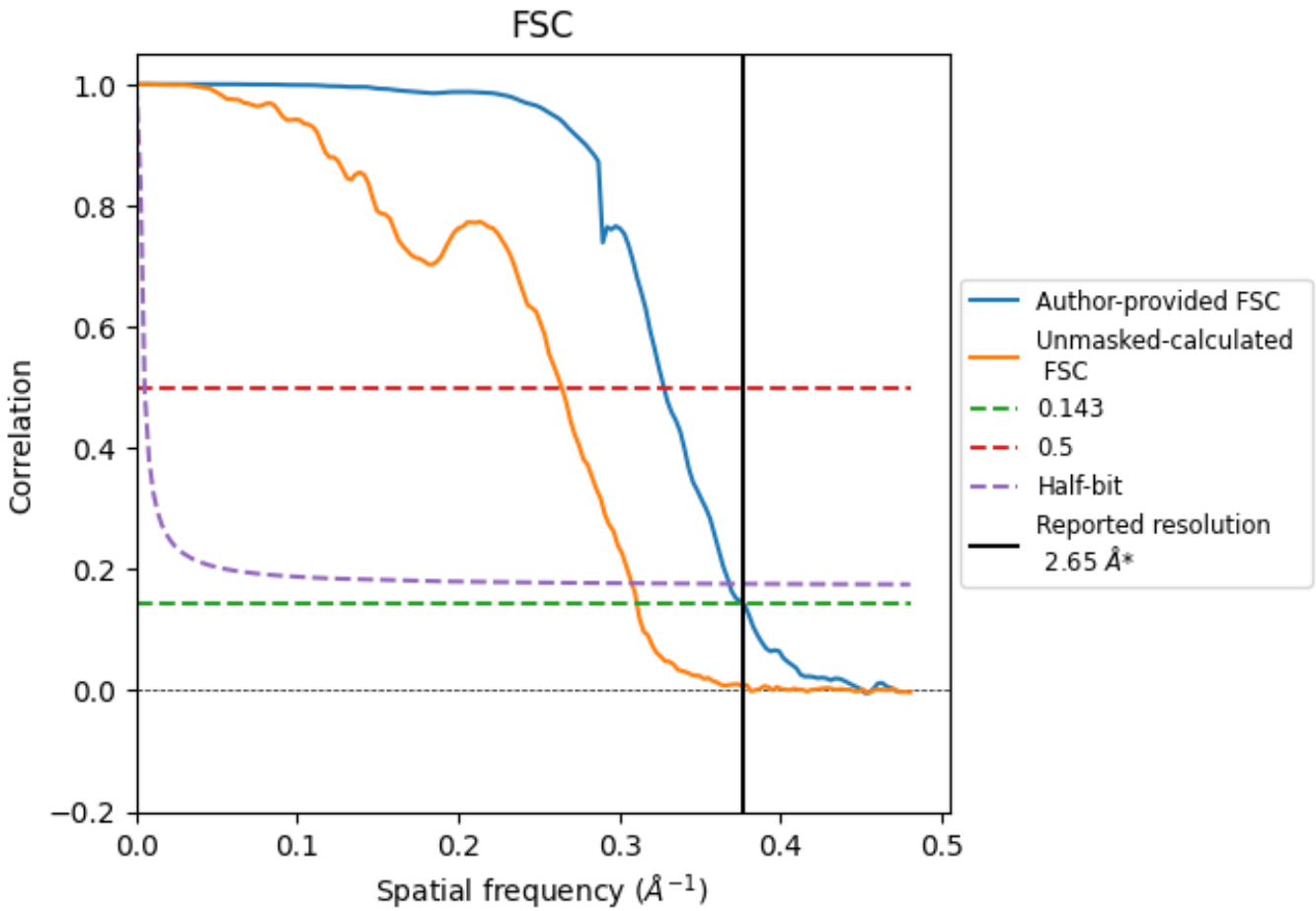


*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

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 0.377 Å^{-1}

8.2 Resolution estimates (i)

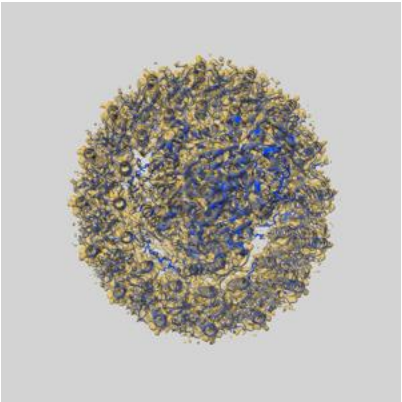
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.05	2.71
Unmasked-calculated*	3.22	3.79	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.65 by more than 10 %

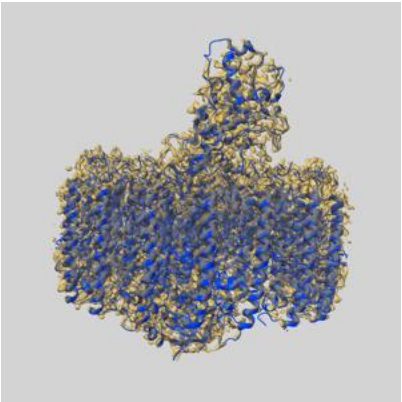
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-60165 and PDB model 8ZK2. Per-residue inclusion information can be found in section 3 on page 18.

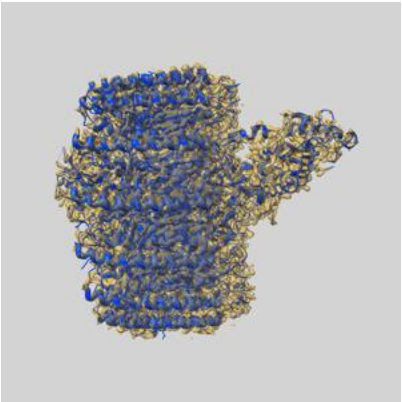
9.1 Map-model overlay (i)



X



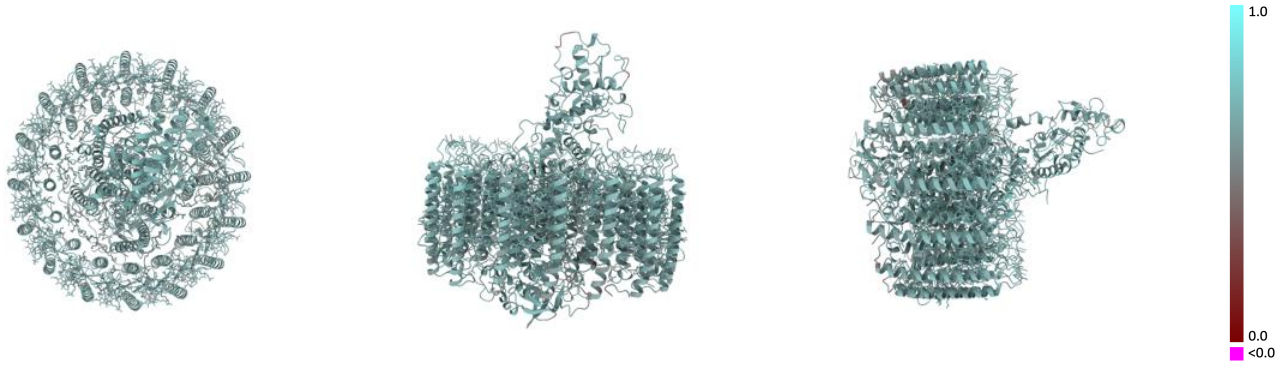
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.562 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.

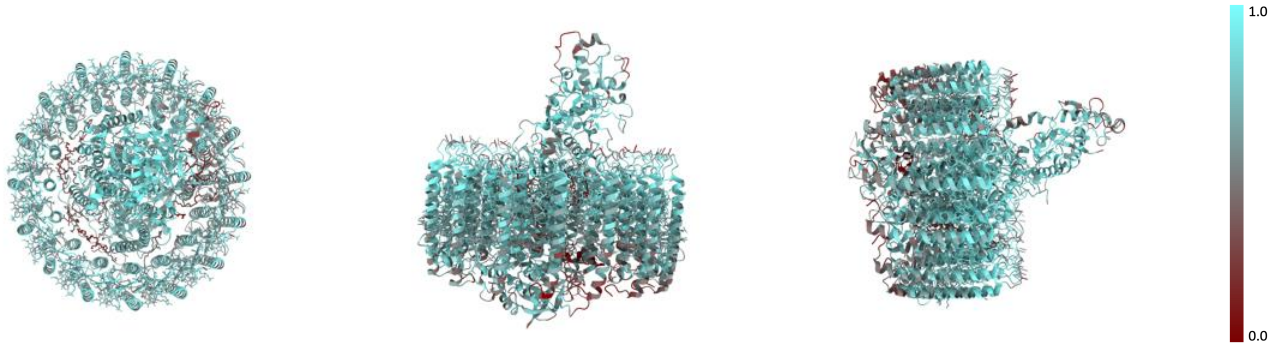
9.2 Q-score mapped to coordinate model (i)



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.

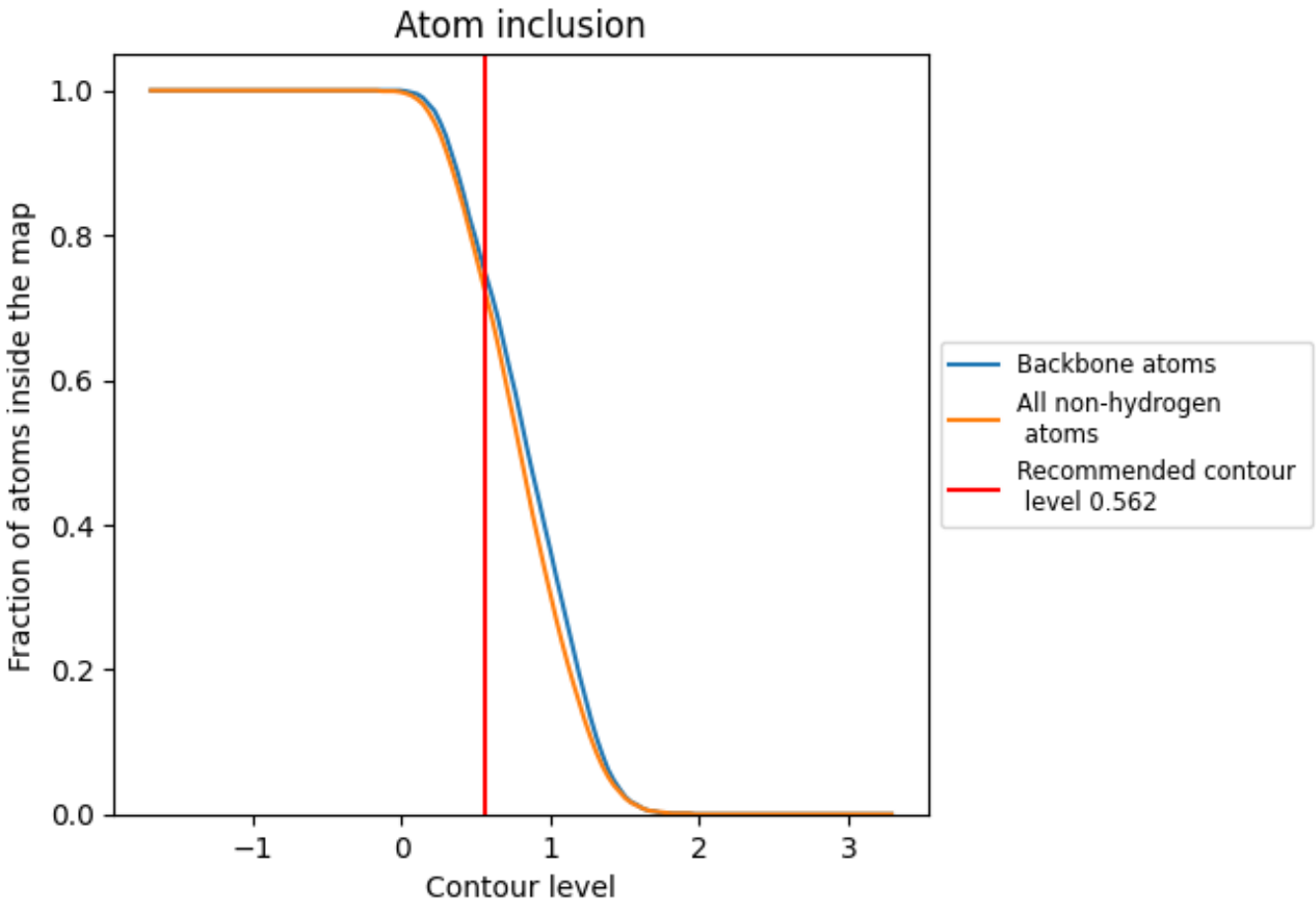
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.562).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.562) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.6360
A	0.6740	0.6380
B	0.6430	0.6190
C	0.7380	0.6320
D	0.6850	0.6350
E	0.7510	0.6440
F	0.7150	0.6240
G	0.7620	0.6460
H	0.6530	0.6250
I	0.7250	0.6320
J	0.7380	0.6410
K	0.7160	0.6300
L	0.7920	0.6510
M	0.7740	0.6520
N	0.7220	0.6390
O	0.6990	0.6220
P	0.6970	0.6340
Q	0.7180	0.6290
R	0.7320	0.6390
S	0.7200	0.6370
T	0.7490	0.6480
U	0.7290	0.6330
V	0.7020	0.6410
W	0.7650	0.6340
X	0.7700	0.6490
Y	0.6090	0.6110
Z	0.5700	0.5990
a	0.7580	0.6360
b	0.7640	0.6480
c	0.6410	0.6220
d	0.6320	0.6290
e	0.7080	0.6340
f	0.7020	0.6390
g	0.7010	0.6400
h	0.7140	0.6350

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Chain	Atom inclusion	Q-score
i	0.7580	0.6340
j	0.7150	0.6350