wwPDB EM Validation Summary Report (i)

Sep 23, 2026 – 12:22 AM JST

PDB ID	:	8J5O / pdb_00008j5o
EMDB ID	:	EMD-35988
Title	:	Cryo-EM structure of native RC-LH complex from Roseiflexus castenholzii at 100lux
Authors	:	Xu, X.; Xin, J.
Deposited on	:	2023-04-24
Resolution	:	2.90 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:

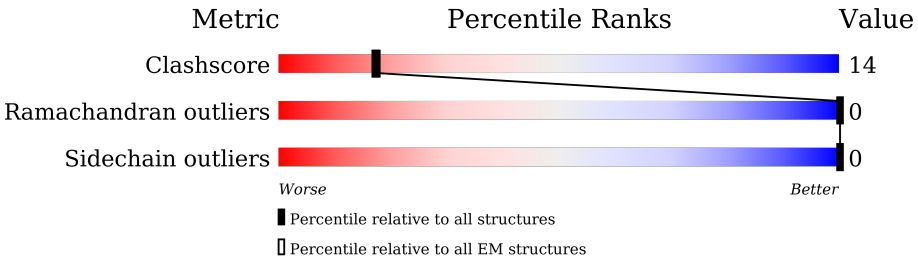
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

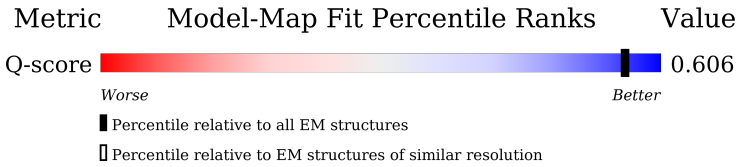
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	0	55	62% 27% 11%
1	2	55	78% 11% 11%
1	4	55	69% 20% 11%
1	6	55	65% 24% 11%

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Mol	Chain	Length	Quality of chain
1	8	55	65% 24% 11%
1	B	55	75% 15% 11%
1	E	55	65% 24% 11%
1	G	55	69% 20% 11%
1	I	55	69% 20% 11%
1	K	55	71% 18% 11%
1	O	55	64% 25% 11%
1	Q	55	65% 24% 11%
1	S	55	64% 25% 11%
1	U	55	58% 31% 11%
1	W	55	62% 27% 11%
2	1	42	67% 14% 19%
2	3	42	67% 21% 12%
2	5	42	55% 36% 10%
2	7	42	55% 33% 12%
2	9	42	71% 17% 12%
2	A	42	62% 29% 10%
2	D	42	52% 38% 10%
2	F	42	62% 26% 12%
2	H	42	71% 19% 10%
2	J	42	57% 31% 12%
2	N	42	60% 29% 12%
2	P	42	81% 7% 12%
2	R	42	62% 29% 10%
2	T	42	71% 19% 10%

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Mol	Chain	Length	Quality of chain
2	V	42	57% 31% 12%
3	C	320	74% 24%
4	L	315	65% 30% 5%
5	M	307	75% 24%
6	X	32	69% 12% 19%
7	Y	39	56% 23% 18%
8	Z	63	56% 19% 25%

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
11	HEC	C	501	X	-	-	-
11	HEC	C	502	X	-	-	-
11	HEC	C	503	X	-	-	-
11	HEC	C	504	X	-	-	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 23692 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 Beta subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	49	407	275	68	63	1	0	0
1	2	49	407	275	68	63	1	0	0
1	4	49	407	275	68	63	1	0	0
1	6	49	407	275	68	63	1	0	0
1	8	49	407	275	68	63	1	0	0
1	B	49	407	275	68	63	1	0	0
1	E	49	407	275	68	63	1	0	0
1	G	49	407	275	68	63	1	0	0
1	I	49	407	275	68	63	1	0	0
1	K	49	407	275	68	63	1	0	0
1	O	49	407	275	68	63	1	0	0
1	Q	49	407	275	68	63	1	0	0
1	S	49	407	275	68	63	1	0	0
1	U	49	407	275	68	63	1	0	0
1	W	49	407	275	68	63	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	34	266	178	44	43	1	0	0
2	3	37	295	198	50	46	1	0	0
2	5	38	300	201	51	47	1	0	0
2	7	37	295	198	50	46	1	0	0
2	9	37	295	198	50	46	1	0	0
2	A	38	300	201	51	47	1	0	0
2	D	38	300	201	51	47	1	0	0
2	F	37	295	198	50	46	1	0	0
2	H	38	300	201	51	47	1	0	0
2	J	37	295	198	50	46	1	0	0
2	N	37	295	198	50	46	1	0	0
2	P	37	295	198	50	46	1	0	0
2	R	38	300	201	51	47	1	0	0
2	T	38	300	201	51	47	1	0	0
2	V	37	295	198	50	46	1	0	0

- Molecule 3 is a protein called MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	315	2404	1532	407	443	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	299	2364	1583	380	393	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	306	2488	1673	399	409	7	0	0

- Molecule 6 is a protein called Subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	X	26	206	145	26	31	4	0	0

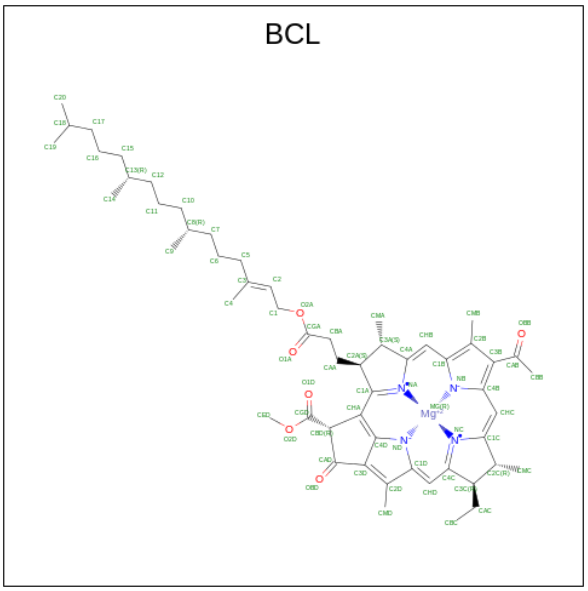
- Molecule 7 is a protein called Subunit Y.

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

- Molecule 8 is a protein called Subunit Z.

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

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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

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

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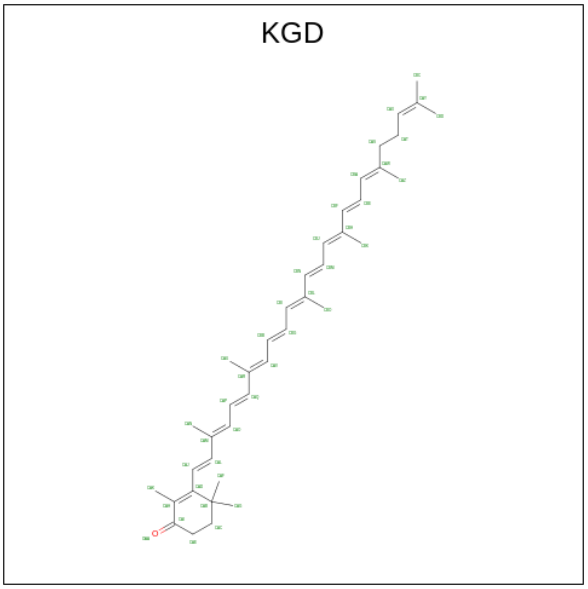
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	U	1	66	55	1	4	6	0
9	U	1	66	55	1	4	6	0
9	V	1	66	55	1	4	6	0
9	W	1	66	55	1	4	6	0
9	W	1	66	55	1	4	6	0

- Molecule 10 is beta,psi-caroten-4-one (CCD ID: KGD) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	0	1	41	40	1	0
10	0	1	41	40	1	0
10	1	1	41	40	1	0
10	1	1	41	40	1	0
10	2	1	41	40	1	0
10	4	1	41	40	1	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	5	1	41	40	1	0
10	6	1	41	40	1	0
10	7	1	41	40	1	0
10	8	1	41	40	1	0
10	A	1	41	40	1	0
10	B	1	41	40	1	0
10	C	1	41	40	1	0
10	C	1	41	40	1	0
10	D	1	41	40	1	0
10	D	1	41	40	1	0
10	E	1	41	40	1	0
10	G	1	41	40	1	0
10	H	1	41	40	1	0
10	I	1	41	40	1	0
10	J	1	41	40	1	0
10	J	1	41	40	1	0
10	K	1	41	40	1	0
10	O	1	41	40	1	0
10	P	1	41	40	1	0
10	Q	1	41	40	1	0
10	R	1	41	40	1	0

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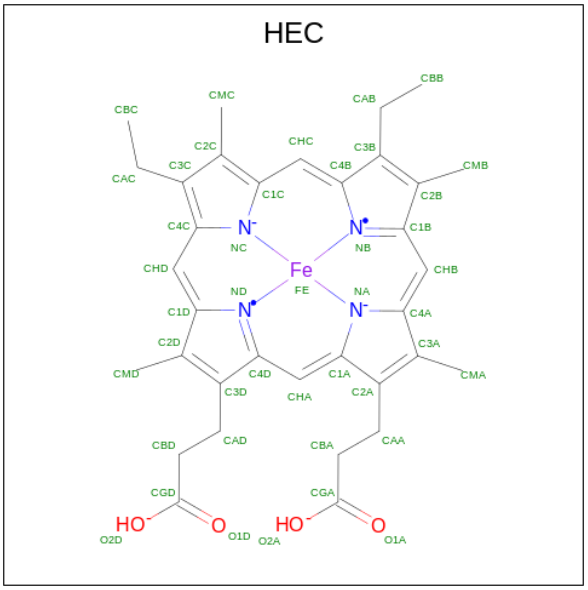
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	S	1	41	40	1	0
			Total	C	O	
10	S	1	41	40	1	0
			Total	C	O	
10	U	1	41	40	1	0

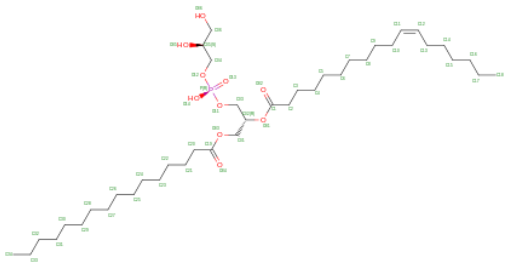
- Molecule 11 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 12 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).

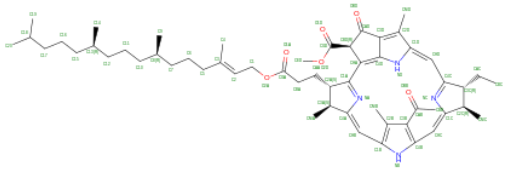
PGV



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	C	1	45	34	10	1	0
			Total	C	O	P	
12	L	1	30	19	10	1	0
			Total	C	O	P	
12	L	1	42	31	10	1	0
			Total	C	O	P	
12	L	1	35	24	10	1	0

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

BPH

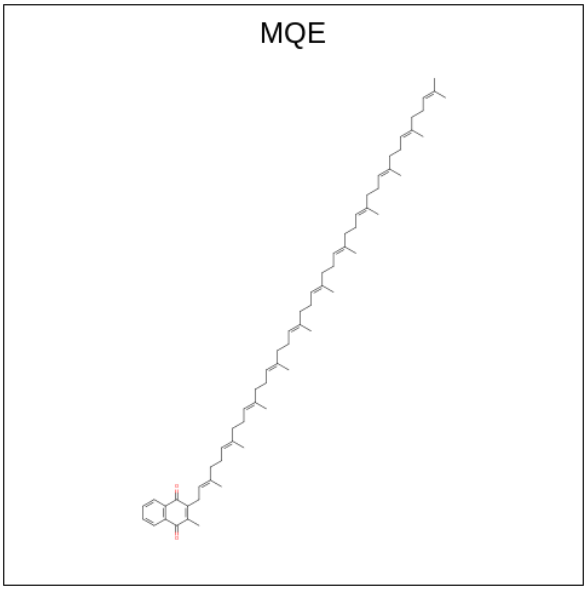


Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	N	O	0
			65	55	4	6	
13	L	1	Total	C	N	O	0
			65	55	4	6	
13	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 14 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 15 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetratetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (CCD ID: MQE) (formula: $C_{66}H_{96}O_2$).



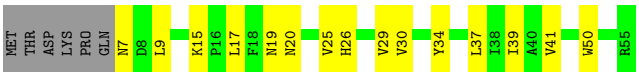
Mol	Chain	Residues	Atoms			AltConf
15	L	1	Total	C	O	0
			68	66	2	
15	M	1	Total	C	O	0
			68	66	2	
15	M	1	Total	C	O	0
			24	22	2	

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.

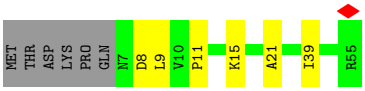
• Molecule 1: Beta subunit of light-harvesting 1

Chain 0:



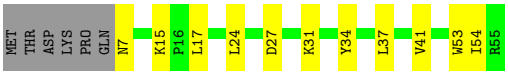
• Molecule 1: Beta subunit of light-harvesting 1

Chain 2:



• Molecule 1: Beta subunit of light-harvesting 1

Chain 4:

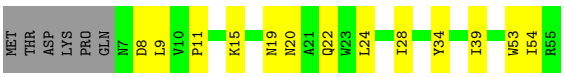


• Molecule 1: Beta subunit of light-harvesting 1

Chain 6:

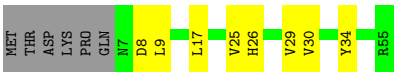
• Molecule 1: Beta subunit of light-harvesting 1

Chain 8:



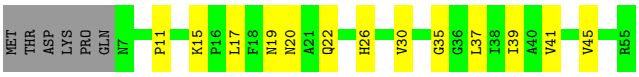
• Molecule 1: Beta subunit of light-harvesting 1

Chain B: 75% 15% 11%



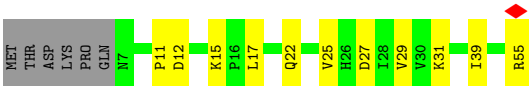
• Molecule 1: Beta subunit of light-harvesting 1

Chain E: 65% 24% 11%



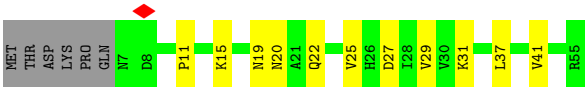
• Molecule 1: Beta subunit of light-harvesting 1

Chain G: 69% 20% 11%



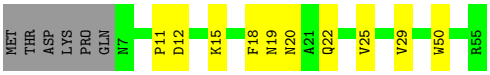
• Molecule 1: Beta subunit of light-harvesting 1

Chain I: 69% 20% 11%



• Molecule 1: Beta subunit of light-harvesting 1

Chain K: 71% 18% 11%

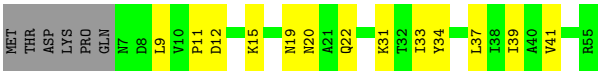


• Molecule 1: Beta subunit of light-harvesting 1

Chain O: 64% 25% 11%

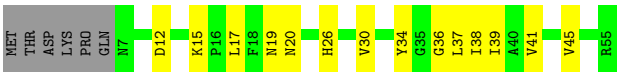
• Molecule 1: Beta subunit of light-harvesting 1

Chain Q: 65% 24% 11%



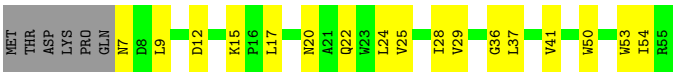
• Molecule 1: Beta subunit of light-harvesting 1

Chain S: 64% 25% 11%



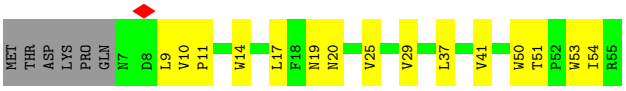
• Molecule 1: Beta subunit of light-harvesting 1

Chain U: 58% 31% 11%



• Molecule 1: Beta subunit of light-harvesting 1

Chain W: 62% 27% 11%

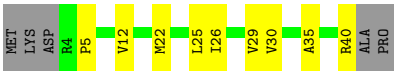


• Molecule 2: Alpha subunit of light-harvesting 1

Chain 1: 67% 14% 19%

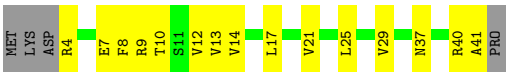
• Molecule 2: Alpha subunit of light-harvesting 1

Chain 3: 67% 21% 12%



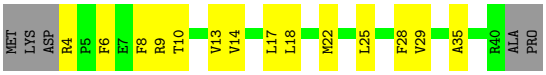
• Molecule 2: Alpha subunit of light-harvesting 1

Chain 5: 55% 36% 10%



• Molecule 2: Alpha subunit of light-harvesting 1

Chain 7: 55% 33% 12%

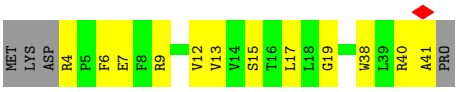


• Molecule 2: Alpha subunit of light-harvesting 1

Chain 9:

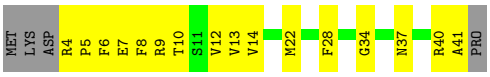
- Molecule 2: Alpha subunit of light-harvesting 1

Chain A:



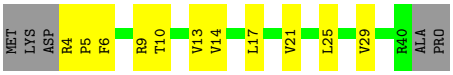
- Molecule 2: Alpha subunit of light-harvesting 1

Chain D:



- Molecule 2: Alpha subunit of light-harvesting 1

Chain F:

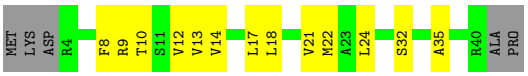


- Molecule 2: Alpha subunit of light-harvesting 1

Chain H:

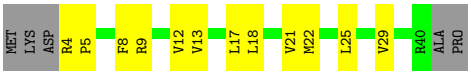
- Molecule 2: Alpha subunit of light-harvesting 1

Chain J:



- Molecule 2: Alpha subunit of light-harvesting 1

Chain N:

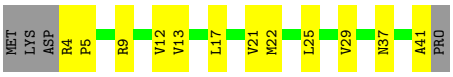


- Molecule 2: Alpha subunit of light-harvesting 1

Chain P: 81% 7% 12%

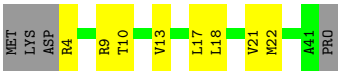
• Molecule 2: Alpha subunit of light-harvesting 1

Chain R: 62% 29% 10%



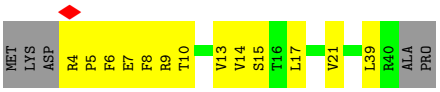
• Molecule 2: Alpha subunit of light-harvesting 1

Chain T: 71% 19% 10%



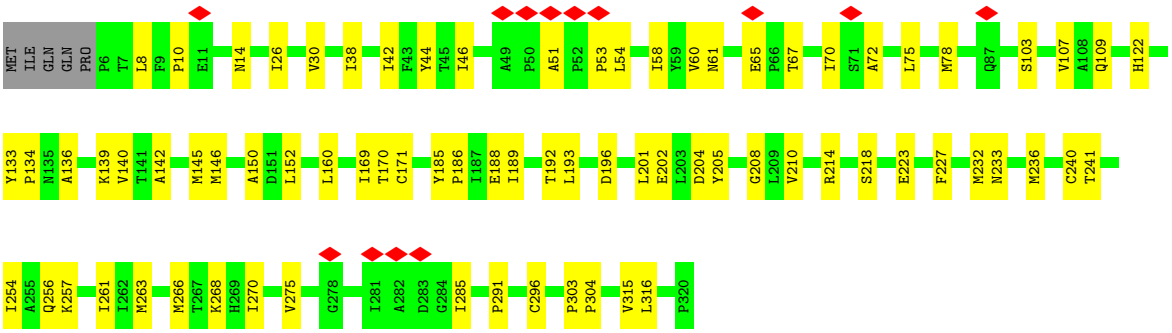
• Molecule 2: Alpha subunit of light-harvesting 1

Chain V: 57% 31% 12%



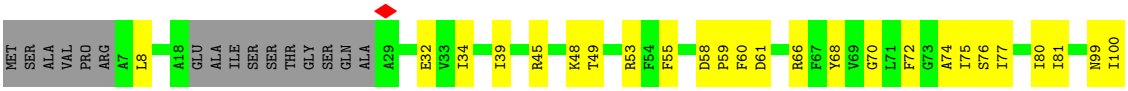
• Molecule 3: MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN

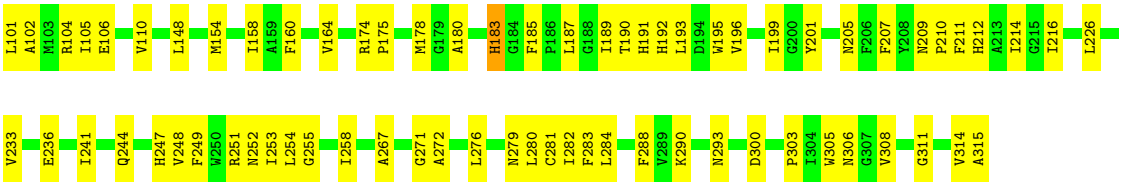
Chain C: 74% 24%



• Molecule 4: Reaction center protein L chain

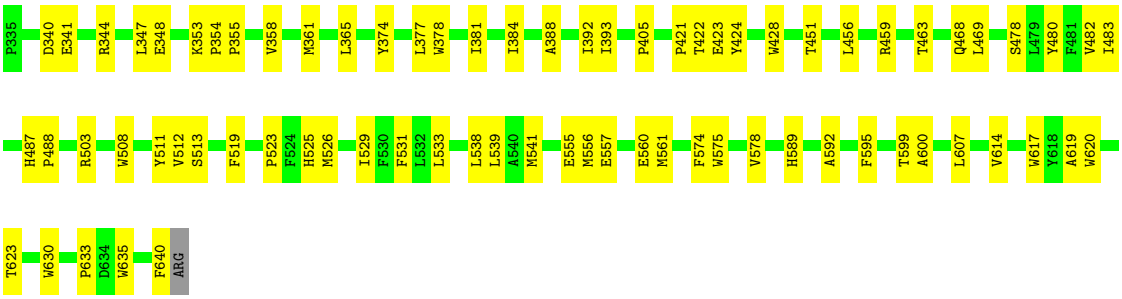
Chain L: 65% 30% 5%





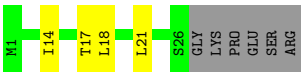
- Molecule 5: Reaction center protein M chain

Chain M:



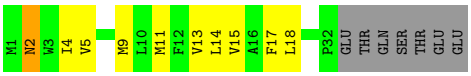
- Molecule 6: Subunit X

Chain X:



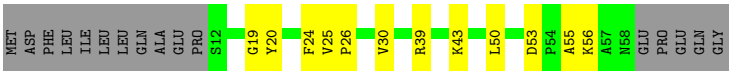
- Molecule 7: Subunit Y

Chain Y:



- Molecule 8: Subunit Z

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	322595	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.237	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	235.752, 235.752, 235.752	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.893, 0.893, 0.893	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: BCL, FE, MQE, BPH, PGV, HEC, KGD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.14	0/423	0.28	0/585
1	2	0.14	0/423	0.25	0/585
1	4	0.16	0/423	0.28	0/585
1	6	0.13	0/423	0.25	0/585
1	8	0.17	0/423	0.29	0/585
1	B	0.16	0/423	0.28	0/585
1	E	0.23	0/423	0.35	0/585
1	G	0.22	0/423	0.33	0/585
1	I	0.12	0/423	0.26	0/585
1	K	0.12	0/423	0.22	0/585
1	O	0.14	0/423	0.25	0/585
1	Q	0.12	0/423	0.27	0/585
1	S	0.12	0/423	0.27	0/585
1	U	0.13	0/423	0.30	0/585
1	W	0.14	0/423	0.29	0/585
2	1	0.19	0/271	0.40	0/368
2	3	0.14	0/302	0.29	0/410
2	5	0.11	0/307	0.24	0/417
2	7	0.11	0/302	0.24	0/410
2	9	0.13	0/302	0.26	0/410
2	A	0.14	0/307	0.28	0/417
2	D	0.12	0/307	0.27	0/417
2	F	0.12	0/302	0.26	0/410
2	H	0.11	0/307	0.25	0/417
2	J	0.13	0/302	0.28	0/410
2	N	0.10	0/302	0.23	0/410
2	P	0.13	0/302	0.23	0/410
2	R	0.12	0/307	0.23	0/417
2	T	0.13	0/307	0.27	0/417
2	V	0.13	0/302	0.24	0/410
3	C	0.14	0/2469	0.33	0/3371
4	L	0.24	0/2448	0.48	3/3342 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	M	0.19	0/2597	0.37	0/3566
6	X	0.11	0/211	0.23	0/285
7	Y	0.39	0/268	0.47	1/370 (0.3%)
8	Z	0.14	0/374	0.36	0/513
All	All	0.17	0/19241	0.33	4/26372 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	185	PHE	N-CA-C	8.98	121.06	109.93
4	L	183	HIS	N-CA-CB	-5.47	102.27	110.91
4	L	308	VAL	N-CA-C	5.44	118.12	112.90
7	Y	2	ASN	N-CA-C	-5.10	100.85	108.96

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	0	407	0	407	12	0
1	2	407	0	407	4	0
1	4	407	0	407	8	0
1	6	407	0	407	11	0
1	8	407	0	407	8	0
1	B	407	0	407	5	0
1	E	407	0	407	9	0
1	G	407	0	407	8	0
1	I	407	0	407	6	0
1	K	407	0	407	7	0
1	O	407	0	407	12	0
1	Q	407	0	407	11	0
1	S	407	0	407	14	0
1	U	407	0	407	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	407	0	407	10	0
2	1	266	0	282	4	0
2	3	295	0	311	8	0
2	5	300	0	316	10	0
2	7	295	0	311	14	0
2	9	295	0	311	11	0
2	A	300	0	316	21	0
2	D	300	0	316	17	0
2	F	295	0	311	10	0
2	H	300	0	316	12	0
2	J	295	0	311	13	0
2	N	295	0	311	12	0
2	P	295	0	311	2	0
2	R	300	0	316	14	0
2	T	300	0	316	10	0
2	V	295	0	311	15	0
3	C	2404	0	2360	65	0
4	L	2364	0	2324	79	0
5	M	2488	0	2373	67	0
6	X	206	0	224	2	0
7	Y	259	0	272	12	0
8	Z	362	0	366	13	0
9	0	132	0	148	11	0
9	1	66	0	74	0	0
9	2	132	0	148	3	0
9	3	66	0	74	5	0
9	4	132	0	148	11	0
9	5	66	0	74	1	0
9	6	132	0	148	12	0
9	7	66	0	74	3	0
9	8	132	0	148	9	0
9	9	66	0	74	5	0
9	A	66	0	74	7	0
9	B	132	0	148	10	0
9	D	66	0	74	3	0
9	E	132	0	148	11	0
9	F	132	0	148	2	0
9	G	66	0	74	4	0
9	H	66	0	74	1	0
9	I	132	0	148	10	0
9	J	66	0	74	2	0
9	K	132	0	148	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	132	0	148	6	0
9	M	66	0	74	4	0
9	N	66	0	74	5	0
9	O	132	0	148	12	0
9	P	66	0	74	4	0
9	Q	132	0	148	9	0
9	R	66	0	74	5	0
9	S	132	0	148	17	0
9	T	66	0	74	8	0
9	U	132	0	148	14	0
9	V	66	0	74	3	0
9	W	132	0	148	8	0
10	0	82	0	0	1	0
10	1	82	0	0	2	0
10	2	41	0	0	3	0
10	4	41	0	0	3	0
10	5	41	0	0	1	0
10	6	41	0	0	4	0
10	7	41	0	0	1	0
10	8	41	0	0	1	0
10	A	41	0	0	2	0
10	B	41	0	0	4	0
10	C	82	0	0	3	0
10	D	82	0	0	10	0
10	E	41	0	0	3	0
10	G	41	0	0	5	0
10	H	41	0	0	2	0
10	I	41	0	0	3	0
10	J	82	0	0	3	0
10	K	41	0	0	2	0
10	O	41	0	0	1	0
10	P	41	0	0	3	0
10	Q	41	0	0	1	0
10	R	41	0	0	1	0
10	S	82	0	0	8	0
10	U	41	0	0	9	0
11	C	172	0	120	14	0
12	C	45	0	61	2	0
12	L	107	0	122	2	0
13	L	130	0	152	12	0
13	M	65	0	76	4	0
14	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	68	0	0	1	0
15	M	92	0	0	5	0
All	All	23692	0	22773	637	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 14.

The worst 5 of 637 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)
10:U:103:KGD:CAF	9:W:102:BCL:H62	1.72	1.19
3:C:232:MET:HE2	11:C:503:HEC:HBC2	1.35	1.08
4:L:211:PHE:HB2	4:L:281:CYS:HB3	1.28	1.07
10:S:104:KGD:CAG	9:U:102:BCL:H62	1.85	1.06
10:H:102:KGD:CAE	9:K:102:BCL:HBB3	1.94	0.98

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	0	47/55 (86%)	47 (100%)	0	0	100	100
1	2	47/55 (86%)	47 (100%)	0	0	100	100
1	4	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
1	6	47/55 (86%)	47 (100%)	0	0	100	100
1	8	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
1	B	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
1	E	47/55 (86%)	47 (100%)	0	0	100	100
1	G	47/55 (86%)	47 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	47/55 (86%)	47 (100%)	0	0	100	100
1	K	47/55 (86%)	47 (100%)	0	0	100	100
1	O	47/55 (86%)	47 (100%)	0	0	100	100
1	Q	47/55 (86%)	47 (100%)	0	0	100	100
1	S	47/55 (86%)	47 (100%)	0	0	100	100
1	U	47/55 (86%)	47 (100%)	0	0	100	100
1	W	47/55 (86%)	46 (98%)	1 (2%)	0	100	100
2	1	32/42 (76%)	30 (94%)	2 (6%)	0	100	100
2	3	35/42 (83%)	33 (94%)	2 (6%)	0	100	100
2	5	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	7	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	9	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	A	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	D	36/42 (86%)	32 (89%)	4 (11%)	0	100	100
2	F	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	H	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	J	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	N	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	P	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
2	R	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	T	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	V	35/42 (83%)	35 (100%)	0	0	100	100
3	C	313/320 (98%)	296 (95%)	17 (5%)	0	100	100
4	L	295/315 (94%)	283 (96%)	12 (4%)	0	100	100
5	M	304/307 (99%)	293 (96%)	11 (4%)	0	100	100
6	X	24/32 (75%)	23 (96%)	1 (4%)	0	100	100
7	Y	30/39 (77%)	30 (100%)	0	0	100	100
8	Z	45/63 (71%)	43 (96%)	2 (4%)	0	100	100
All	All	2244/2531 (89%)	2172 (97%)	72 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	43/49 (88%)	43 (100%)	0	100	100
1	2	43/49 (88%)	43 (100%)	0	100	100
1	4	43/49 (88%)	43 (100%)	0	100	100
1	6	43/49 (88%)	43 (100%)	0	100	100
1	8	43/49 (88%)	43 (100%)	0	100	100
1	B	43/49 (88%)	43 (100%)	0	100	100
1	E	43/49 (88%)	43 (100%)	0	100	100
1	G	43/49 (88%)	43 (100%)	0	100	100
1	I	43/49 (88%)	43 (100%)	0	100	100
1	K	43/49 (88%)	43 (100%)	0	100	100
1	O	43/49 (88%)	43 (100%)	0	100	100
1	Q	43/49 (88%)	43 (100%)	0	100	100
1	S	43/49 (88%)	43 (100%)	0	100	100
1	U	43/49 (88%)	43 (100%)	0	100	100
1	W	43/49 (88%)	43 (100%)	0	100	100
2	1	30/37 (81%)	30 (100%)	0	100	100
2	3	33/37 (89%)	33 (100%)	0	100	100
2	5	33/37 (89%)	33 (100%)	0	100	100
2	7	33/37 (89%)	33 (100%)	0	100	100
2	9	33/37 (89%)	33 (100%)	0	100	100
2	A	33/37 (89%)	33 (100%)	0	100	100
2	D	33/37 (89%)	33 (100%)	0	100	100
2	F	33/37 (89%)	33 (100%)	0	100	100
2	H	33/37 (89%)	33 (100%)	0	100	100
2	J	33/37 (89%)	33 (100%)	0	100	100
2	N	33/37 (89%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	33/37 (89%)	33 (100%)	0	100	100
2	R	33/37 (89%)	33 (100%)	0	100	100
2	T	33/37 (89%)	33 (100%)	0	100	100
2	V	33/37 (89%)	33 (100%)	0	100	100
3	C	257/262 (98%)	257 (100%)	0	100	100
4	L	241/253 (95%)	241 (100%)	0	100	100
5	M	244/245 (100%)	244 (100%)	0	100	100
6	X	23/28 (82%)	23 (100%)	0	100	100
7	Y	29/36 (81%)	29 (100%)	0	100	100
8	Z	36/50 (72%)	36 (100%)	0	100	100
All	All	1967/2164 (91%)	1967 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	22	GLN
4	L	183	HIS
2	P	37	ASN
5	M	582	ASN
2	P	27	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 93 ligands modelled in this entry, 1 is monoatomic - leaving 92 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BCL	A	101	2	69,74,74	1.13	4 (5%)	83,115,115	1.35	7 (8%)
10	KGD	A	102	-	41,41,41	1.00	2 (4%)	49,53,53	1.49	10 (20%)
15	MQE	M	704	-	25,25,69	0.49	0	31,34,87	0.94	2 (6%)
10	KGD	8	103	-	41,41,41	1.16	4 (9%)	49,53,53	1.85	13 (26%)
10	KGD	4	103	-	41,41,41	1.46	2 (4%)	49,53,53	2.06	9 (18%)
9	BCL	B	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.35	9 (10%)
9	BCL	B	102	1	69,74,74	1.13	5 (7%)	83,115,115	1.35	9 (10%)
9	BCL	J	101	2	69,74,74	1.13	5 (7%)	83,115,115	1.40	7 (8%)
9	BCL	3	101	2	69,74,74	1.15	5 (7%)	83,115,115	1.37	8 (9%)
11	HEC	C	501	3	50,50,50	1.28	4 (8%)	68,82,82	1.07	2 (2%)
12	PGV	L	1008	-	41,41,50	0.54	0	44,47,56	0.52	0
9	BCL	E	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.38	9 (10%)
9	BCL	F	102	1	69,74,74	1.14	5 (7%)	83,115,115	1.39	10 (12%)
10	KGD	U	103	-	41,41,41	1.26	3 (7%)	49,53,53	1.96	15 (30%)
9	BCL	O	102	1	69,74,74	1.13	5 (7%)	83,115,115	1.37	9 (10%)
10	KGD	0	103	-	41,41,41	1.03	1 (2%)	49,53,53	1.56	8 (16%)
9	BCL	I	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.42	11 (13%)
9	BCL	D	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.38	7 (8%)
12	PGV	C	507	-	44,44,50	0.51	0	47,50,56	0.69	1 (2%)
10	KGD	5	102	-	41,41,41	1.12	1 (2%)	49,53,53	1.61	9 (18%)
10	KGD	E	103	-	41,41,41	1.05	1 (2%)	49,53,53	1.73	11 (22%)
9	BCL	L	1001	4	69,74,74	1.15	5 (7%)	83,115,115	1.42	6 (7%)
9	BCL	V	101	2	69,74,74	1.16	5 (7%)	83,115,115	1.39	7 (8%)
10	KGD	O	103	-	41,41,41	0.99	1 (2%)	49,53,53	1.68	10 (20%)
9	BCL	T	101	2	69,74,74	1.13	5 (7%)	83,115,115	1.37	8 (9%)
10	KGD	H	102	-	41,41,41	1.04	1 (2%)	49,53,53	1.68	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	KGD	Q	103	-	41,41,41	1.01	2 (4%)	49,53,53	1.61	10 (20%)
10	KGD	P	102	-	41,41,41	1.01	1 (2%)	49,53,53	1.50	10 (20%)
9	BCL	Q	102	1	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
10	KGD	C	505	-	41,41,41	0.96	1 (2%)	49,53,53	1.57	10 (20%)
9	BCL	N	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.39	7 (8%)
10	KGD	I	103	-	41,41,41	1.21	1 (2%)	49,53,53	2.21	15 (30%)
9	BCL	R	101	2	69,74,74	1.13	6 (8%)	83,115,115	1.38	7 (8%)
10	KGD	2	103	-	41,41,41	0.95	2 (4%)	49,53,53	1.58	10 (20%)
10	KGD	S	104	-	41,41,41	1.10	1 (2%)	49,53,53	1.72	14 (28%)
9	BCL	O	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.54	9 (10%)
10	KGD	D	102	-	41,41,41	0.95	1 (2%)	49,53,53	1.48	9 (18%)
13	BPH	L	1006	-	59,70,70	1.00	3 (5%)	61,101,101	1.42	6 (9%)
10	KGD	J	102	-	41,41,41	1.12	1 (2%)	49,53,53	1.66	12 (24%)
9	BCL	S	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.37	8 (9%)
9	BCL	G	101	1	69,74,74	1.12	4 (5%)	83,115,115	1.39	10 (12%)
10	KGD	6	103	-	41,41,41	1.24	2 (4%)	49,53,53	1.99	12 (24%)
9	BCL	L	1002	4	69,74,74	1.14	5 (7%)	83,115,115	1.34	8 (9%)
11	HEC	C	503	3	50,50,50	1.25	5 (10%)	68,82,82	1.09	6 (8%)
10	KGD	C	506	-	41,41,41	1.47	6 (14%)	49,53,53	1.59	7 (14%)
9	BCL	K	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
9	BCL	H	101	2	69,74,74	1.14	5 (7%)	83,115,115	1.41	8 (9%)
10	KGD	0	104	-	41,41,41	1.10	1 (2%)	49,53,53	1.46	7 (14%)
9	BCL	F	101	2	69,74,74	1.13	6 (8%)	83,115,115	1.39	8 (9%)
10	KGD	1	102	-	41,41,41	1.25	1 (2%)	49,53,53	2.03	15 (30%)
9	BCL	U	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.36	8 (9%)
9	BCL	8	101	1	69,74,74	1.12	5 (7%)	83,115,115	1.41	9 (10%)
9	BCL	Q	101	1	69,74,74	1.10	5 (7%)	83,115,115	1.34	7 (8%)
10	KGD	B	103	-	41,41,41	1.16	2 (4%)	49,53,53	2.18	11 (22%)
9	BCL	M	702	5	69,74,74	1.15	5 (7%)	83,115,115	1.43	8 (9%)
15	MQE	M	701	-	69,69,69	0.31	0	84,87,87	0.61	2 (2%)
9	BCL	1	101	2	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
10	KGD	J	103	-	41,41,41	2.15	15 (36%)	49,53,53	1.34	6 (12%)
11	HEC	C	502	3	50,50,50	1.33	3 (6%)	68,82,82	1.16	4 (5%)
9	BCL	I	102	1	69,74,74	1.11	5 (7%)	83,115,115	1.36	9 (10%)
9	BCL	S	102	1	69,74,74	1.11	5 (7%)	83,115,115	1.37	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	BCL	2	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.38	7 (8%)
9	BCL	K	102	1	69,74,74	1.80	19 (27%)	83,115,115	2.42	23 (27%)
15	MQE	L	1005	-	69,69,69	0.30	0	84,87,87	0.48	1 (1%)
9	BCL	6	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.42	9 (10%)
9	BCL	2	102	1	69,74,74	1.12	5 (7%)	83,115,115	1.35	7 (8%)
9	BCL	U	102	1	69,74,74	1.12	5 (7%)	83,115,115	1.38	8 (9%)
9	BCL	7	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.38	7 (8%)
10	KGD	D	103	-	41,41,41	0.91	1 (2%)	49,53,53	1.60	12 (24%)
9	BCL	4	102	1	69,74,74	1.10	4 (5%)	83,115,115	1.39	10 (12%)
9	BCL	0	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.42	8 (9%)
12	PGV	L	1007	-	29,29,50	0.61	0	32,35,56	0.59	0
9	BCL	P	101	2	69,74,74	1.15	5 (7%)	83,115,115	1.32	7 (8%)
9	BCL	W	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.36	7 (8%)
9	BCL	W	102	1	69,74,74	1.79	18 (26%)	83,115,115	2.46	25 (30%)
10	KGD	G	102	-	41,41,41	0.99	2 (4%)	49,53,53	1.93	8 (16%)
11	HEC	C	504	3	50,50,50	1.24	2 (4%)	68,82,82	1.04	0
9	BCL	8	102	1	69,74,74	1.10	6 (8%)	83,115,115	1.41	8 (9%)
9	BCL	4	101	1	69,74,74	1.13	5 (7%)	83,115,115	1.38	8 (9%)
9	BCL	6	102	1	69,74,74	1.13	4 (5%)	83,115,115	1.37	9 (10%)
10	KGD	1	103	-	41,41,41	1.17	3 (7%)	49,53,53	1.81	14 (28%)
9	BCL	9	101	2	69,74,74	1.14	4 (5%)	83,115,115	1.41	7 (8%)
9	BCL	0	102	1	69,74,74	1.11	4 (5%)	83,115,115	1.35	8 (9%)
10	KGD	R	102	-	41,41,41	1.15	1 (2%)	49,53,53	1.76	11 (22%)
10	KGD	S	103	-	41,41,41	1.17	1 (2%)	49,53,53	1.77	10 (20%)
13	BPH	M	703	-	59,70,70	1.00	3 (5%)	61,101,101	1.36	4 (6%)
9	BCL	E	102	1	69,74,74	1.10	5 (7%)	83,115,115	1.35	7 (8%)
10	KGD	7	102	-	41,41,41	1.05	3 (7%)	49,53,53	1.62	10 (20%)
12	PGV	L	1009	-	34,34,50	0.57	0	37,40,56	0.54	0
10	KGD	K	103	-	41,41,41	1.03	1 (2%)	49,53,53	1.80	9 (18%)
13	BPH	L	1003	-	59,70,70	1.01	2 (3%)	61,101,101	1.46	7 (11%)
9	BCL	5	101	2	69,74,74	1.12	4 (5%)	83,115,115	1.42	9 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	A	101	2	-	5/41/137/137	-
10	KGD	A	102	-	-	3/36/56/56	0/1/1/1
15	MQE	M	704	-	-	2/13/33/85	0/2/2/2
10	KGD	8	103	-	-	4/36/56/56	0/1/1/1
10	KGD	4	103	-	-	3/36/56/56	0/1/1/1
9	BCL	B	101	1	-	4/41/137/137	-
9	BCL	B	102	1	-	3/41/137/137	-
9	BCL	J	101	2	-	7/41/137/137	-
9	BCL	3	101	2	-	4/41/137/137	-
11	HEC	C	501	3	1/1/3/7	2/14/54/54	-
12	PGV	L	1008	-	-	18/46/46/55	-
9	BCL	E	101	1	-	8/41/137/137	-
9	BCL	F	102	1	-	2/41/137/137	-
10	KGD	U	103	-	-	4/36/56/56	0/1/1/1
9	BCL	O	102	1	-	4/41/137/137	-
10	KGD	0	103	-	-	0/36/56/56	0/1/1/1
9	BCL	I	101	1	-	6/41/137/137	-
9	BCL	D	101	2	-	6/41/137/137	-
12	PGV	C	507	-	-	18/49/49/55	-
10	KGD	5	102	-	-	4/36/56/56	0/1/1/1
10	KGD	E	103	-	-	5/36/56/56	0/1/1/1
9	BCL	L	1001	4	-	3/41/137/137	-
9	BCL	V	101	2	-	4/41/137/137	-
10	KGD	O	103	-	-	4/36/56/56	0/1/1/1
9	BCL	T	101	2	-	4/41/137/137	-
10	KGD	H	102	-	-	3/36/56/56	0/1/1/1
10	KGD	Q	103	-	-	4/36/56/56	0/1/1/1
10	KGD	P	102	-	-	2/36/56/56	0/1/1/1
9	BCL	Q	102	1	-	4/41/137/137	-
10	KGD	C	505	-	-	4/36/56/56	0/1/1/1
9	BCL	N	101	2	-	6/41/137/137	-
10	KGD	I	103	-	-	4/36/56/56	0/1/1/1
9	BCL	R	101	2	-	7/41/137/137	-
10	KGD	2	103	-	-	8/36/56/56	0/1/1/1
10	KGD	S	104	-	-	7/36/56/56	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	O	101	1	-	6/41/137/137	-
10	KGD	D	102	-	-	6/36/56/56	0/1/1/1
13	BPH	L	1006	-	-	16/37/105/105	0/5/6/6
10	KGD	J	102	-	-	6/36/56/56	0/1/1/1
9	BCL	S	101	1	-	5/41/137/137	-
9	BCL	G	101	1	-	4/41/137/137	-
10	KGD	6	103	-	-	6/36/56/56	0/1/1/1
9	BCL	L	1002	4	-	5/41/137/137	-
11	HEC	C	503	3	1/1/3/7	8/14/54/54	-
10	KGD	C	506	-	-	6/36/56/56	0/1/1/1
9	BCL	K	101	1	-	7/41/137/137	-
9	BCL	H	101	2	-	3/41/137/137	-
10	KGD	0	104	-	-	4/36/56/56	0/1/1/1
9	BCL	F	101	2	-	4/41/137/137	-
10	KGD	1	102	-	-	5/36/56/56	0/1/1/1
9	BCL	U	101	1	-	9/41/137/137	-
9	BCL	8	101	1	-	2/41/137/137	-
9	BCL	Q	101	1	-	5/41/137/137	-
10	KGD	B	103	-	-	9/36/56/56	0/1/1/1
9	BCL	M	702	5	-	4/41/137/137	-
15	MQE	M	701	-	-	19/65/85/85	0/2/2/2
9	BCL	1	101	2	-	8/41/137/137	-
10	KGD	J	103	-	-	4/36/56/56	0/1/1/1
11	HEC	C	502	3	1/1/3/7	2/14/54/54	-
9	BCL	I	102	1	-	4/41/137/137	-
9	BCL	S	102	1	-	4/41/137/137	-
9	BCL	2	101	1	-	4/41/137/137	-
9	BCL	K	102	1	-	22/41/137/137	-
15	MQE	L	1005	-	-	9/65/85/85	0/2/2/2
9	BCL	6	101	1	-	7/41/137/137	-
9	BCL	2	102	1	-	10/41/137/137	-
9	BCL	U	102	1	-	4/41/137/137	-
9	BCL	7	101	2	-	7/41/137/137	-
10	KGD	D	103	-	-	3/36/56/56	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	4	102	1	-	2/41/137/137	-
9	BCL	0	101	1	-	4/41/137/137	-
12	PGV	L	1007	-	-	12/34/34/55	-
9	BCL	P	101	2	-	3/41/137/137	-
9	BCL	W	101	1	-	4/41/137/137	-
9	BCL	W	102	1	-	18/41/137/137	-
10	KGD	G	102	-	-	7/36/56/56	0/1/1/1
11	HEC	C	504	3	1/1/3/7	3/14/54/54	-
9	BCL	8	102	1	-	3/41/137/137	-
9	BCL	4	101	1	-	7/41/137/137	-
9	BCL	6	102	1	-	2/41/137/137	-
10	KGD	1	103	-	-	4/36/56/56	0/1/1/1
9	BCL	9	101	2	-	7/41/137/137	-
9	BCL	0	102	1	-	2/41/137/137	-
10	KGD	R	102	-	-	4/36/56/56	0/1/1/1
10	KGD	S	103	-	-	12/36/56/56	0/1/1/1
13	BPH	M	703	-	-	20/37/105/105	0/5/6/6
9	BCL	E	102	1	-	6/41/137/137	-
10	KGD	7	102	-	-	4/36/56/56	0/1/1/1
12	PGV	L	1009	-	-	15/39/39/55	-
10	KGD	K	103	-	-	7/36/56/56	0/1/1/1
13	BPH	L	1003	-	-	18/37/105/105	0/5/6/6
9	BCL	5	101	2	-	7/41/137/137	-

The worst 5 of 347 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	103	KGD	CAG-CAB	-5.70	1.42	1.53
10	4	103	KGD	CAB-CAD	-5.55	1.46	1.53
9	L	1001	BCL	MG-NA	5.08	2.18	2.06
9	M	702	BCL	MG-NA	5.07	2.18	2.06
9	W	102	BCL	O2D-CGD	5.02	1.45	1.33

The worst 5 of 769 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	102	BCL	C2B-C1B-NB	8.94	116.22	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	K	102	BCL	CHD-C1D-ND	-8.35	116.78	124.45
9	W	102	BCL	CHD-C1D-ND	-8.28	116.85	124.45
9	K	102	BCL	CMD-C2D-C1D	8.20	139.17	124.71
9	K	102	BCL	C2B-C1B-NB	7.90	115.53	110.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	C	501	HEC	NA
11	C	502	HEC	NA
11	C	503	HEC	NA
11	C	504	HEC	NA

5 of 574 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	102	BCL	C4-C3-C5-C6
9	2	102	BCL	C2-C3-C5-C6
9	2	102	BCL	C4-C3-C5-C6
9	4	101	BCL	C2-C3-C5-C6
9	4	101	BCL	C4-C3-C5-C6

There are no ring outliers.

83 monomers are involved in 270 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	101	BCL	7	0
10	A	102	KGD	2	0
15	M	704	MQE	3	0
10	8	103	KGD	1	0
10	4	103	KGD	3	0
9	B	101	BCL	5	0
9	B	102	BCL	5	0
9	J	101	BCL	2	0
9	3	101	BCL	5	0
11	C	501	HEC	1	0
12	L	1008	PGV	1	0
9	E	101	BCL	7	0
9	F	102	BCL	2	0
10	U	103	KGD	9	0
9	O	102	BCL	5	0
9	I	101	BCL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	101	BCL	3	0
12	C	507	PGV	2	0
10	5	102	KGD	1	0
10	E	103	KGD	3	0
9	L	1001	BCL	3	0
9	V	101	BCL	3	0
10	O	103	KGD	1	0
9	T	101	BCL	8	0
10	H	102	KGD	2	0
10	Q	103	KGD	1	0
10	P	102	KGD	3	0
9	Q	102	BCL	4	0
10	C	505	KGD	3	0
9	N	101	BCL	5	0
10	I	103	KGD	3	0
9	R	101	BCL	5	0
10	2	103	KGD	3	0
10	S	104	KGD	5	0
9	O	101	BCL	7	0
10	D	102	KGD	5	0
13	L	1006	BPH	7	0
9	S	101	BCL	9	0
9	G	101	BCL	4	0
10	6	103	KGD	4	0
9	L	1002	BCL	3	0
11	C	503	HEC	5	0
9	K	101	BCL	5	0
9	H	101	BCL	1	0
10	0	104	KGD	1	0
10	1	102	KGD	2	0
9	U	101	BCL	7	0
9	8	101	BCL	3	0
9	Q	101	BCL	5	0
10	B	103	KGD	4	0
9	M	702	BCL	4	0
15	M	701	MQE	2	0
10	J	103	KGD	3	0
9	I	102	BCL	8	0
9	S	102	BCL	8	0
9	K	102	BCL	6	0
15	L	1005	MQE	1	0
9	6	101	BCL	4	0

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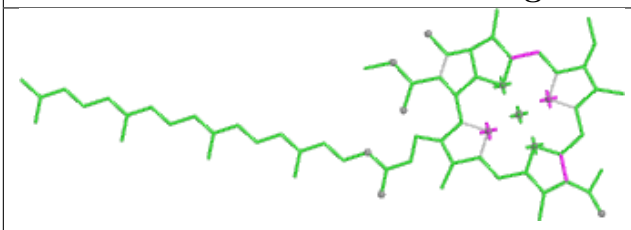
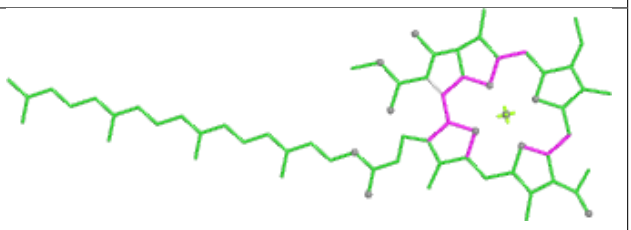
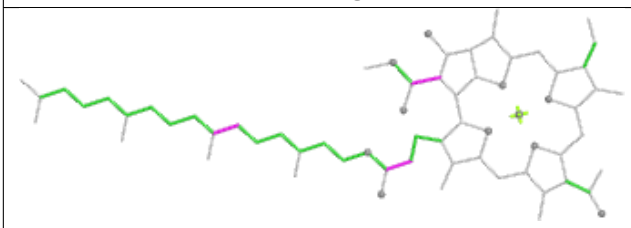
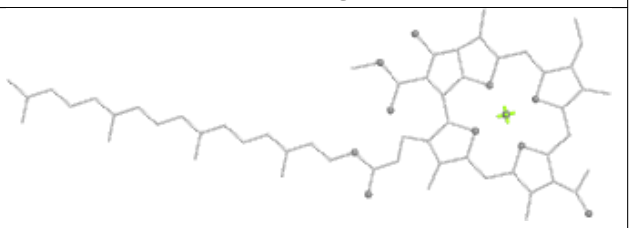
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	2	102	BCL	3	0
9	U	102	BCL	7	0
9	7	101	BCL	3	0
10	D	103	KGD	5	0
9	4	102	BCL	8	0
9	0	101	BCL	6	0
9	P	101	BCL	4	0
9	W	101	BCL	2	0
9	W	102	BCL	6	0
10	G	102	KGD	5	0
11	C	504	HEC	8	0
9	8	102	BCL	6	0
9	4	101	BCL	3	0
9	6	102	BCL	8	0
9	9	101	BCL	5	0
9	0	102	BCL	5	0
10	R	102	KGD	1	0
10	S	103	KGD	3	0
13	M	703	BPH	4	0
9	E	102	BCL	4	0
10	7	102	KGD	1	0
12	L	1009	PGV	1	0
10	K	103	KGD	2	0
13	L	1003	BPH	5	0
9	5	101	BCL	1	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 A 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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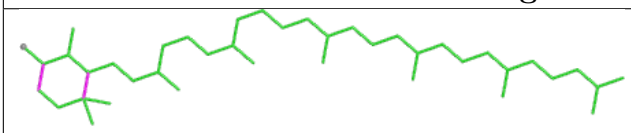
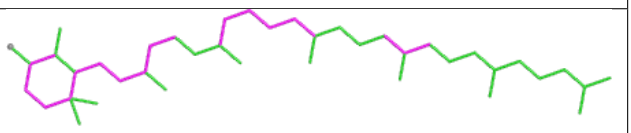
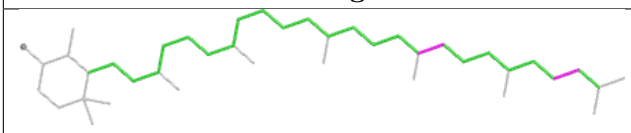
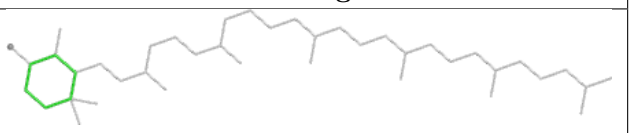
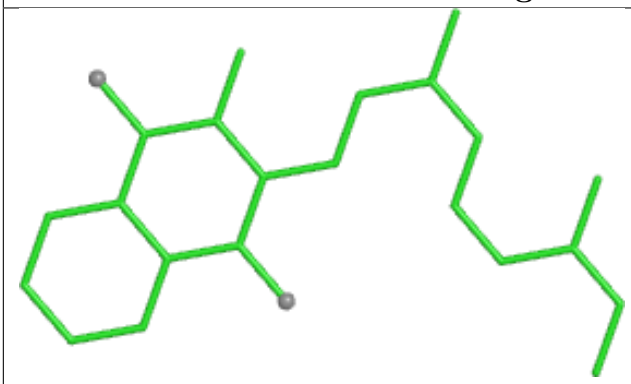
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand MQE M 704



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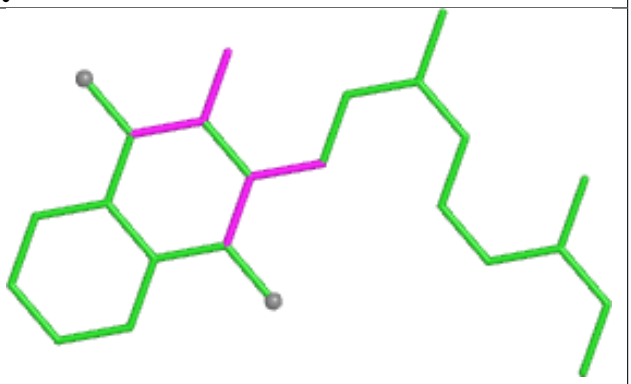

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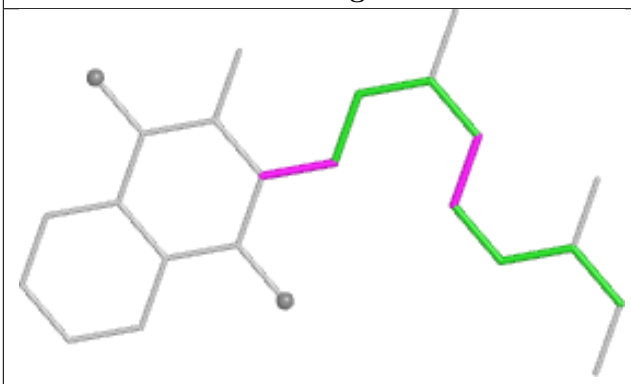

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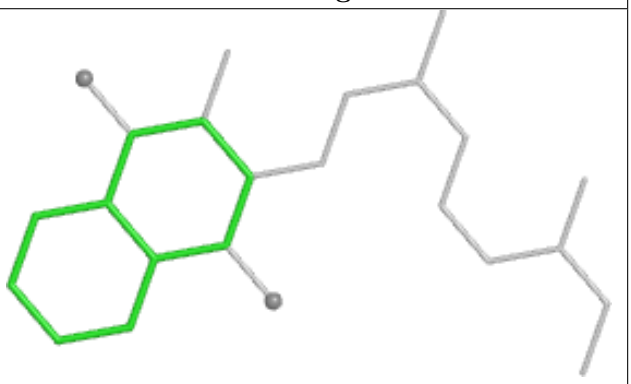
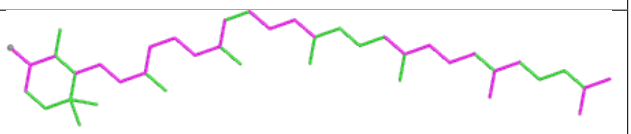


Rings

Ligand KGD 8 103

Bond lengths



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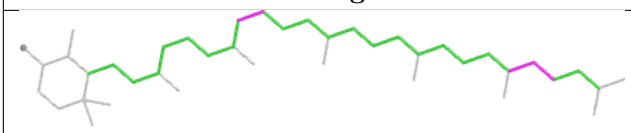
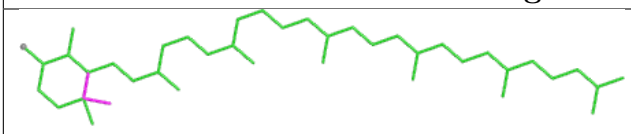


Torsions

Rings

Ligand KGD 4 103



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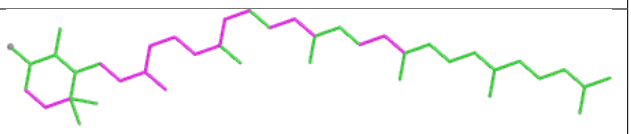

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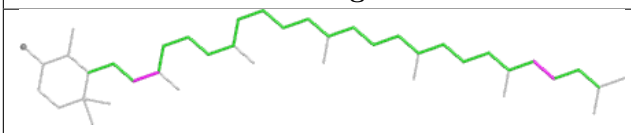

Torsions

Rings

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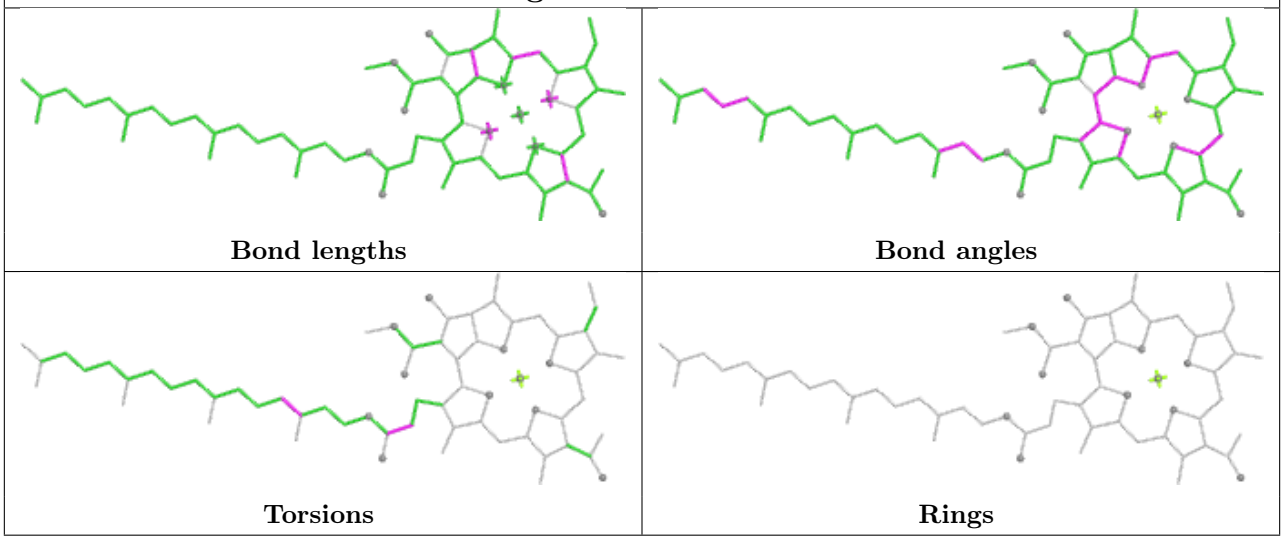

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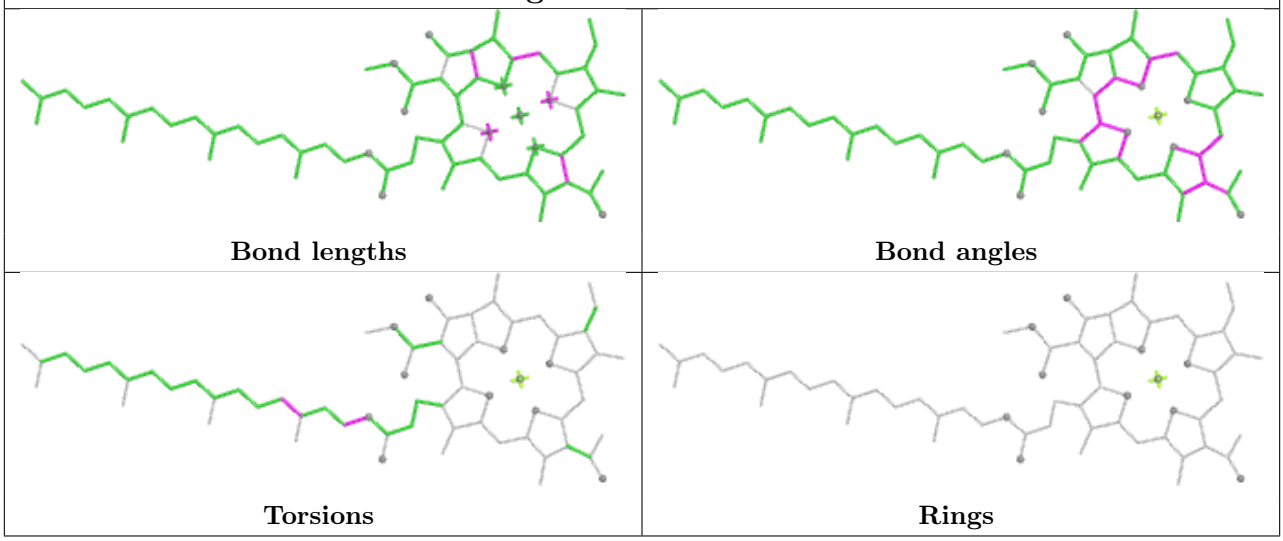

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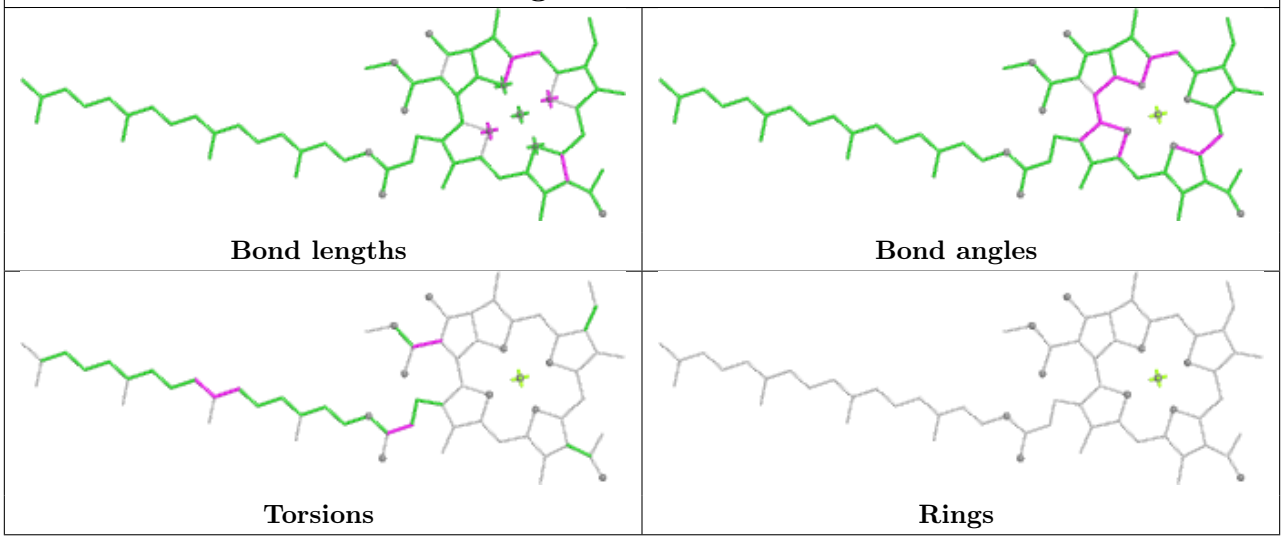

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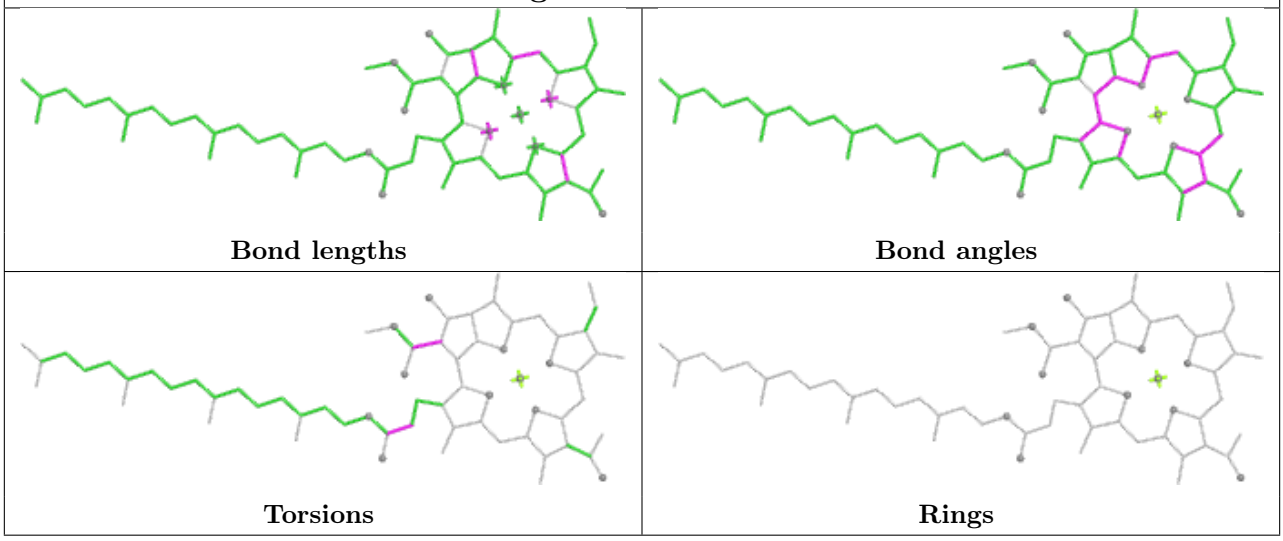

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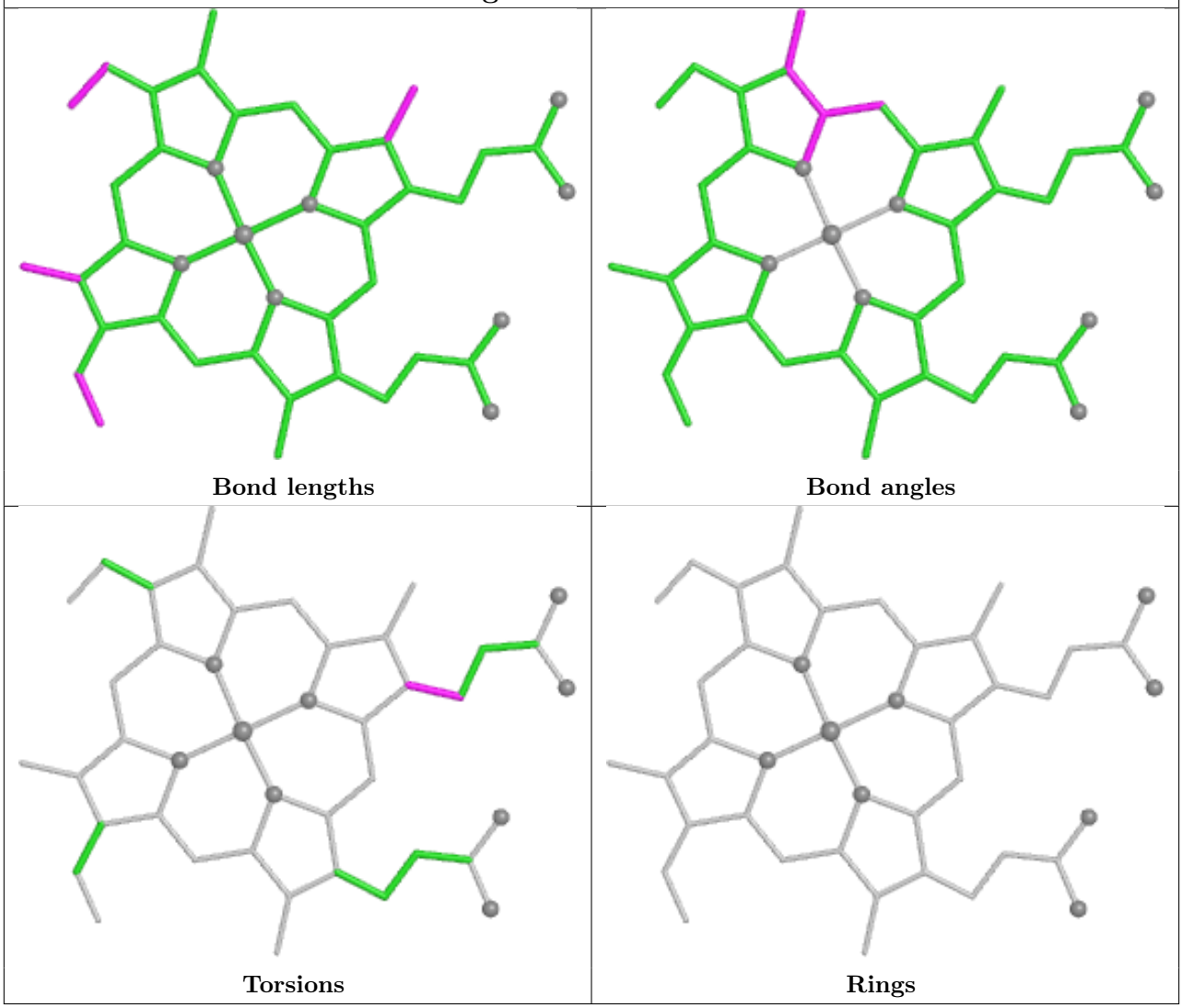

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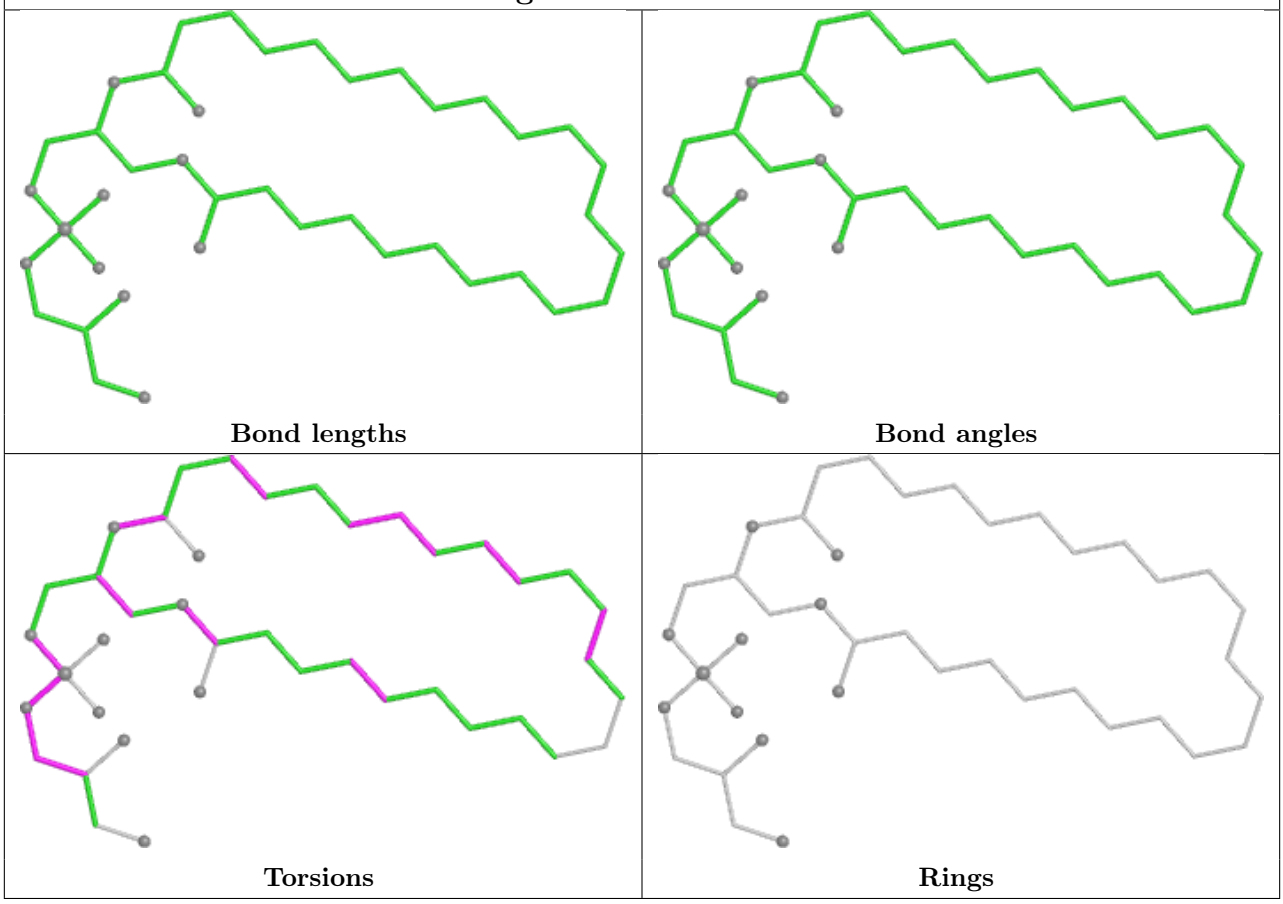

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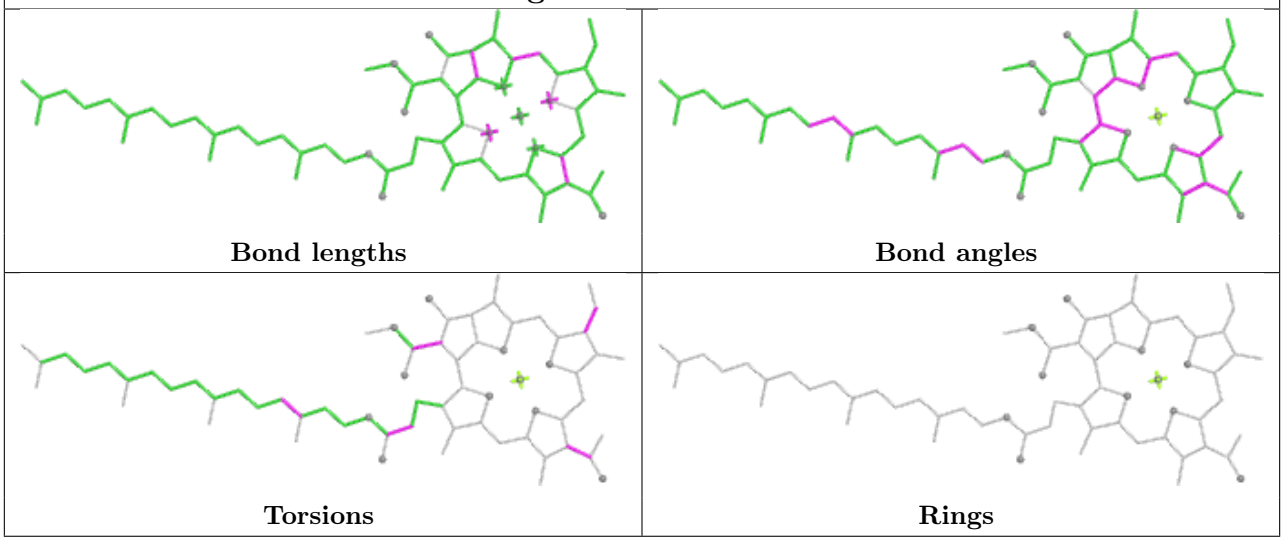

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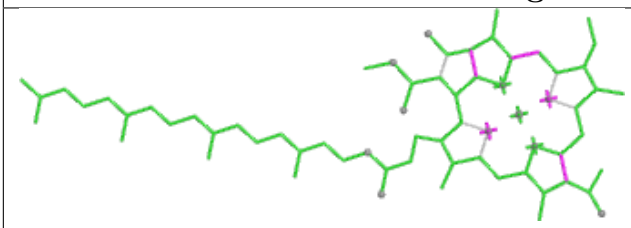
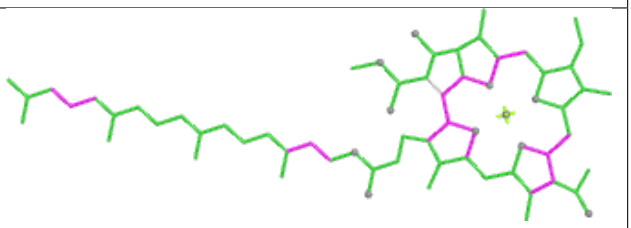
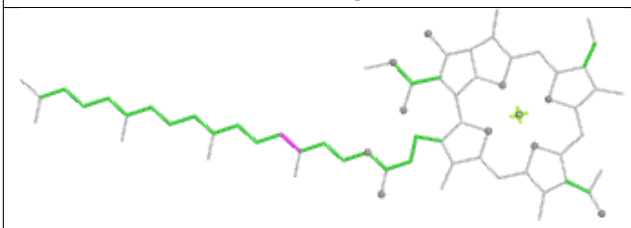
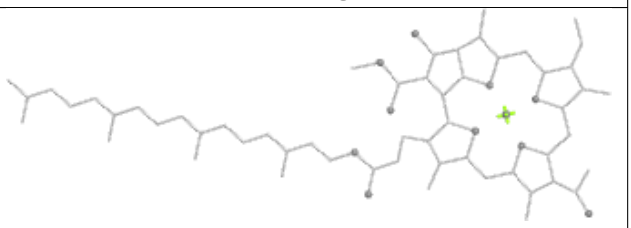
 Bond lengths	 Bond angles
 Torsions	 Rings

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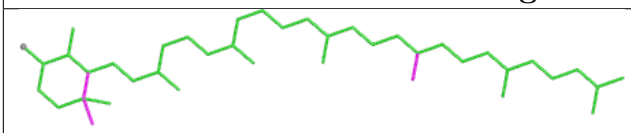
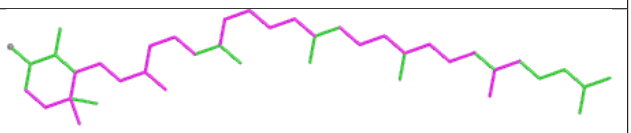
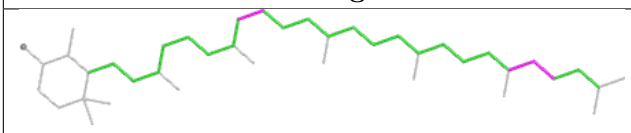
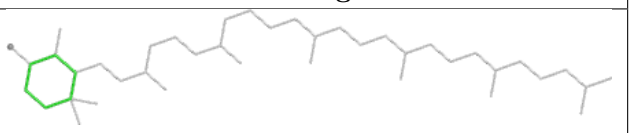
 Bond lengths	 Bond angles
 Torsions	 Rings

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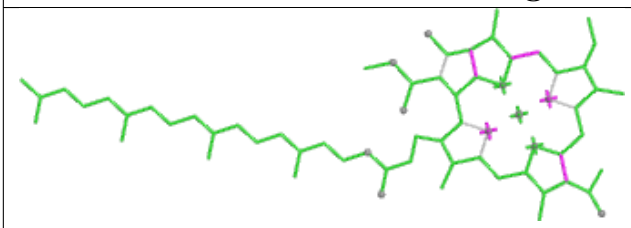
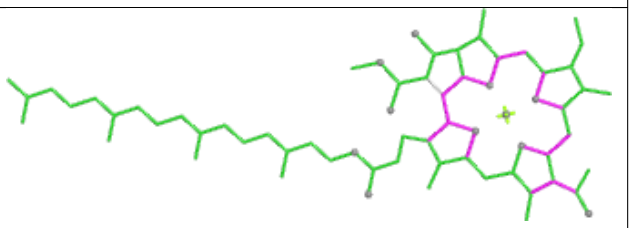
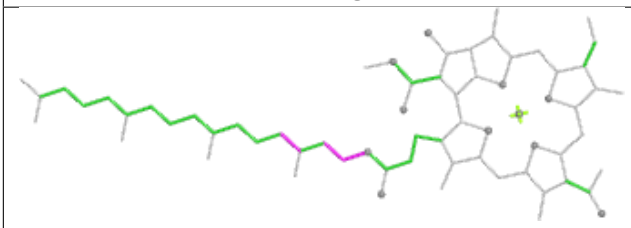
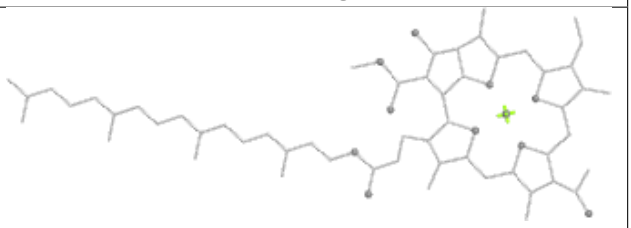
 Bond lengths	 Bond angles
 Torsions	 Rings

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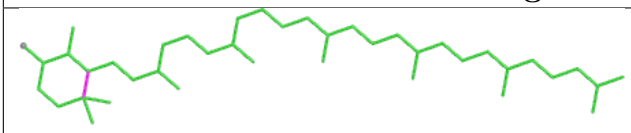
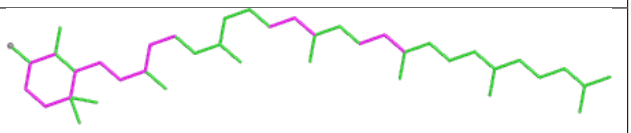
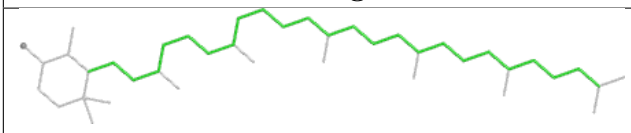
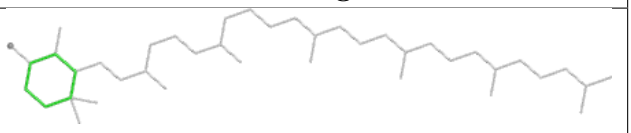
 Bond lengths	 Bond angles
 Torsions	 Rings

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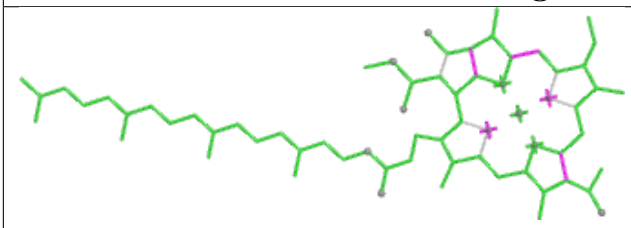
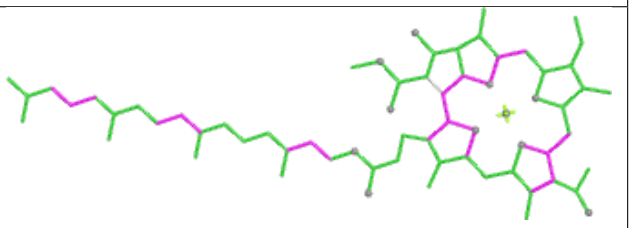
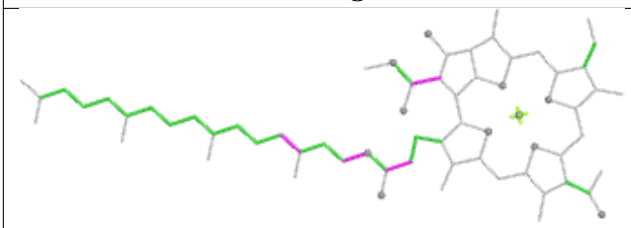
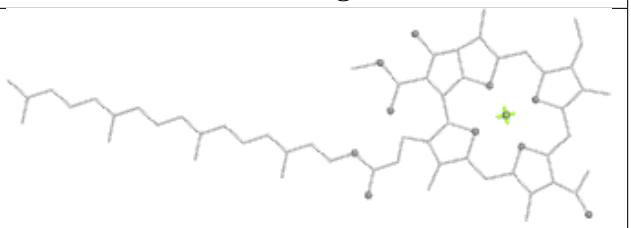
 Bond lengths	 Bond angles
 Torsions	 Rings

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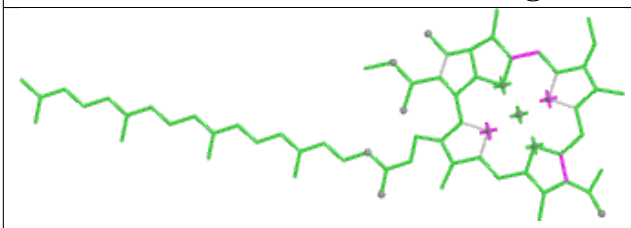
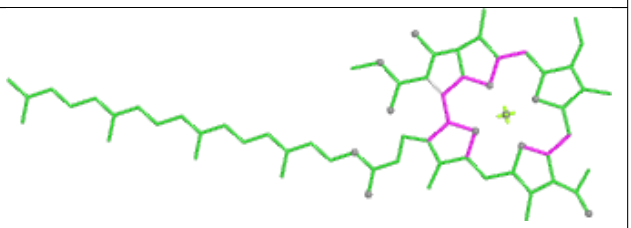
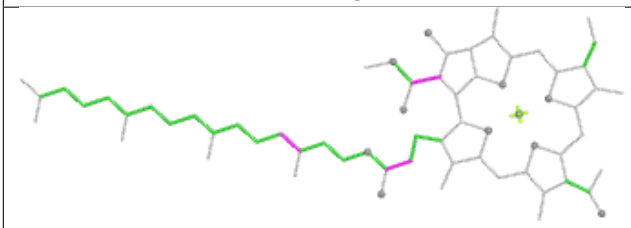
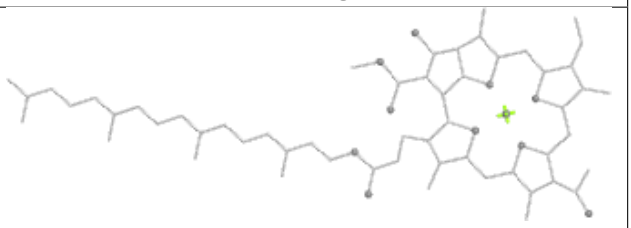
 Bond lengths	 Bond angles
 Torsions	 Rings

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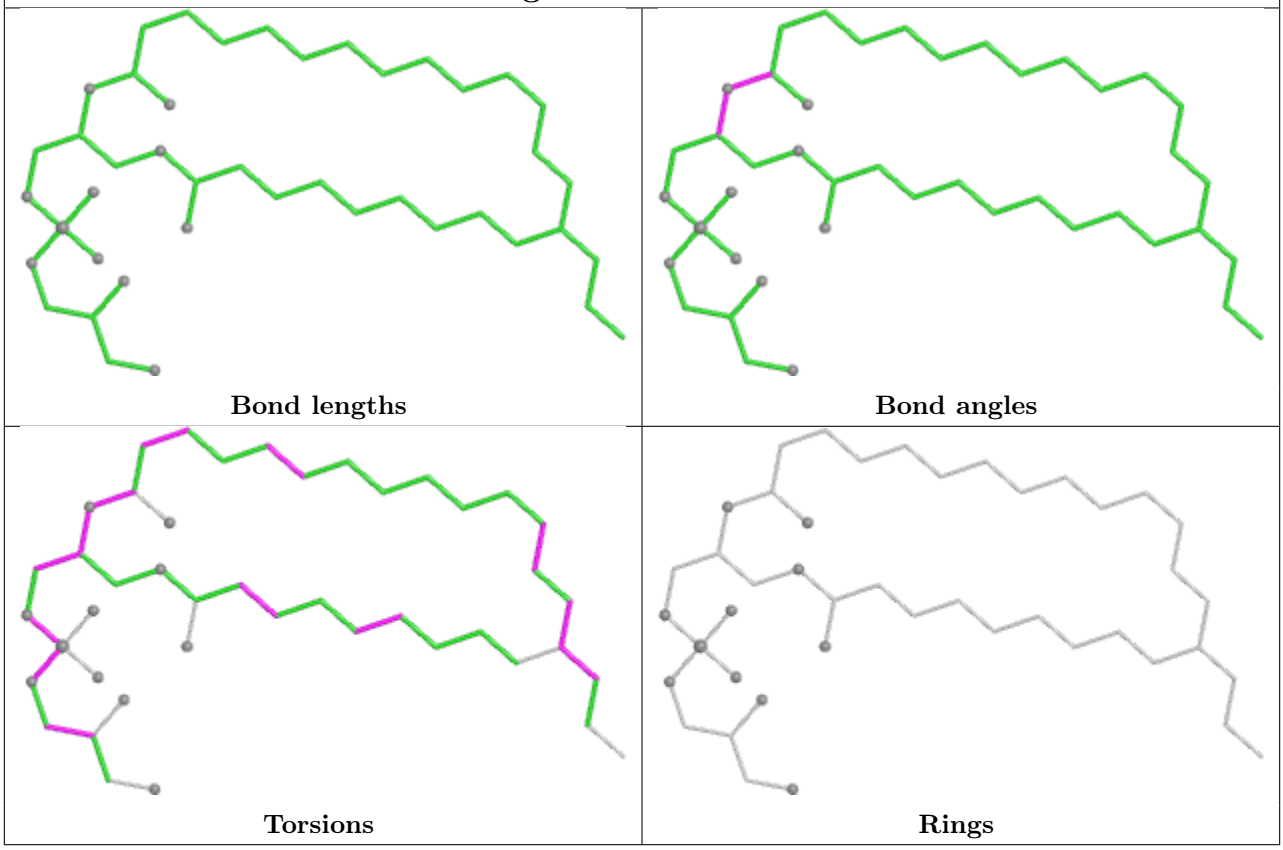

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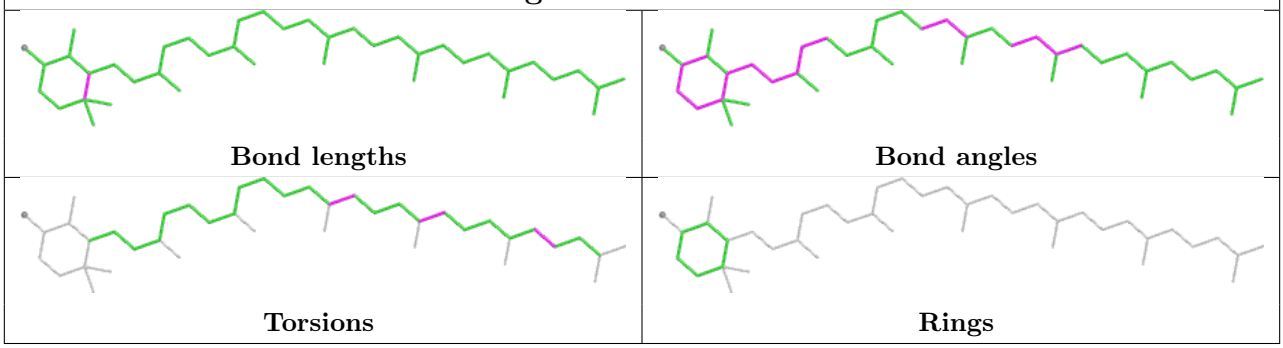

Ligand KGD E 103

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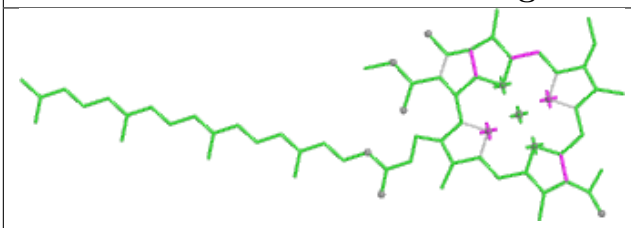
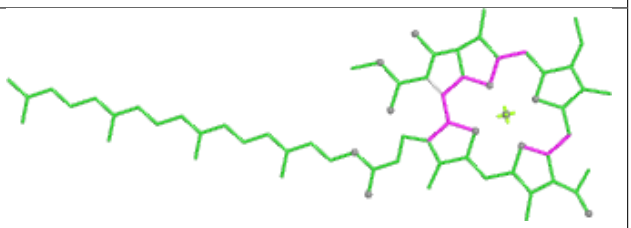
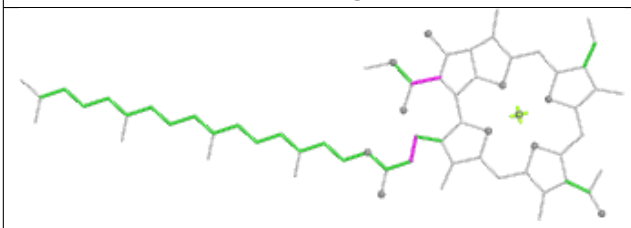


Bond lengths



Bond angles



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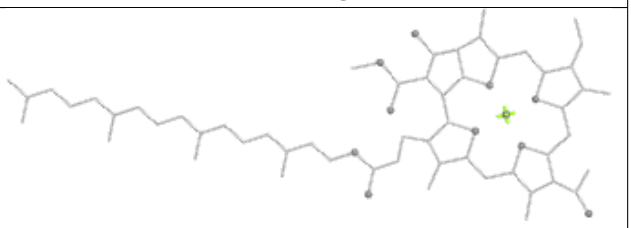

Rings

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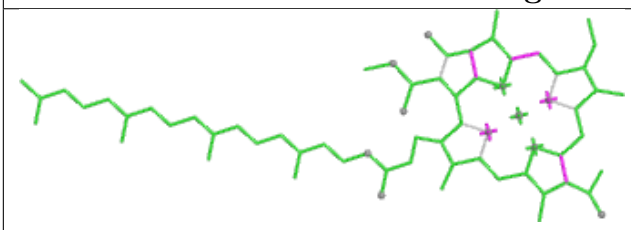

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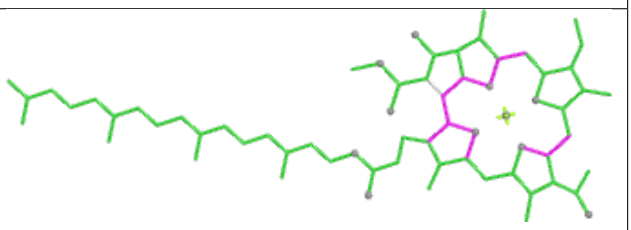

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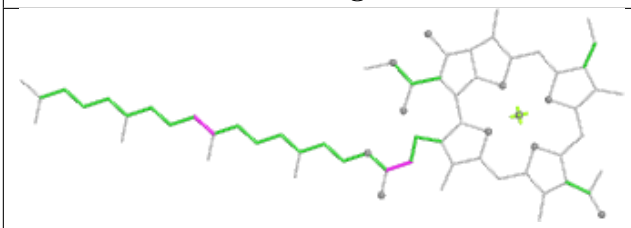

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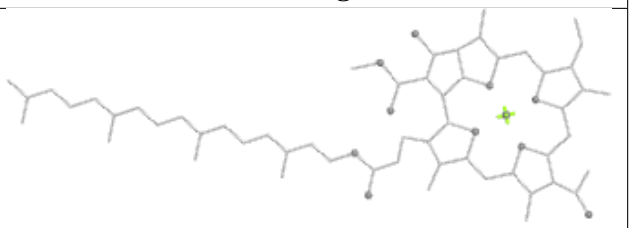

Rings

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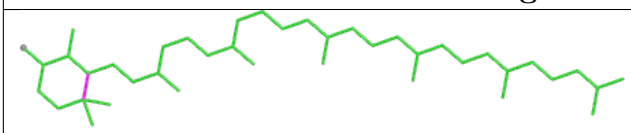

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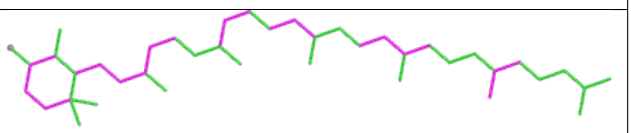

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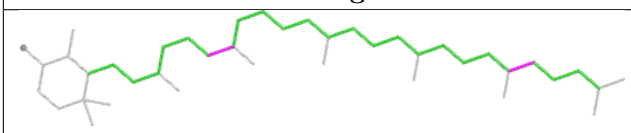

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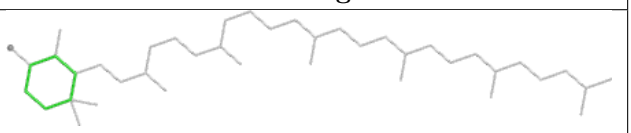

Rings

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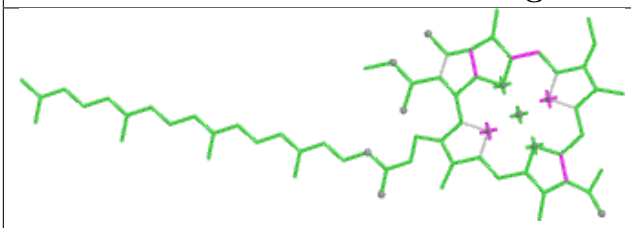

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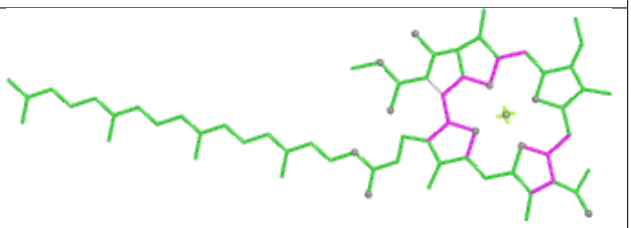

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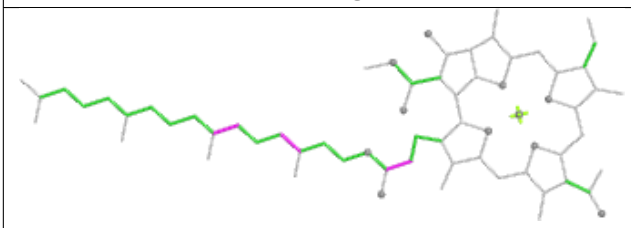

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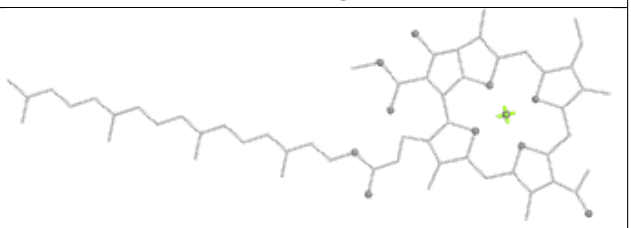

Rings

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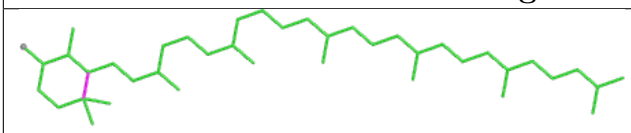

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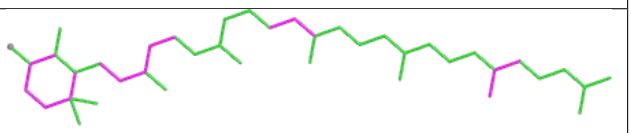

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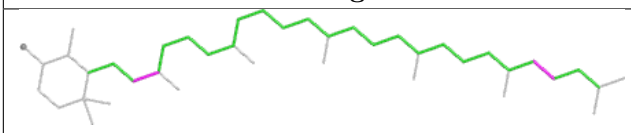

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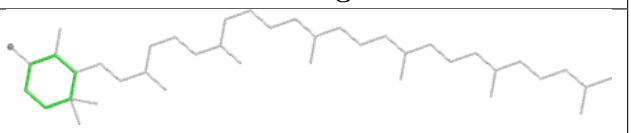
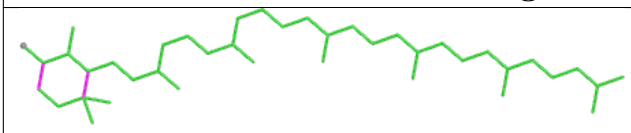


Rings

Ligand KGD Q 103



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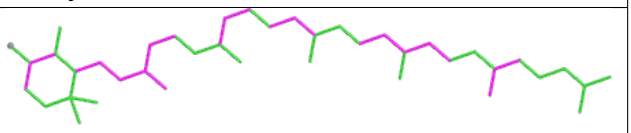

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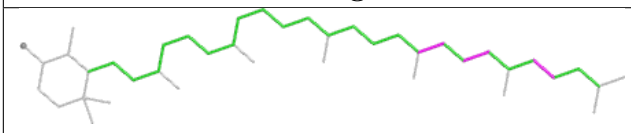

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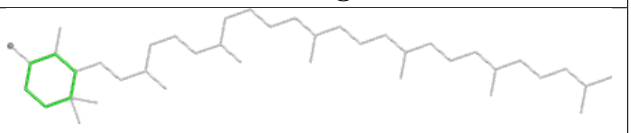
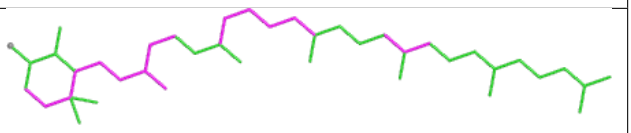


Rings

Ligand KGD P 102

Bond lengths



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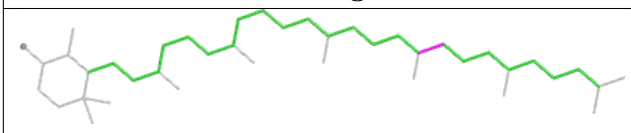

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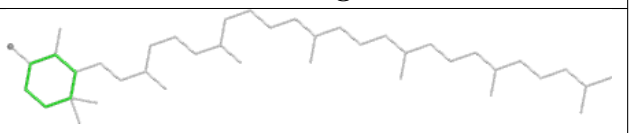

Rings

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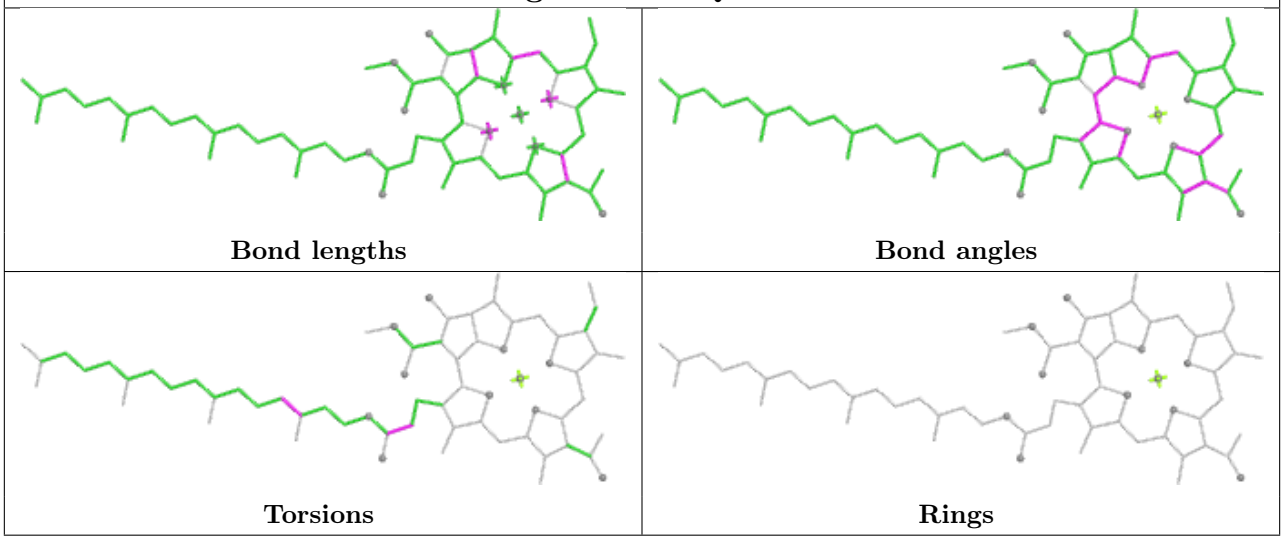

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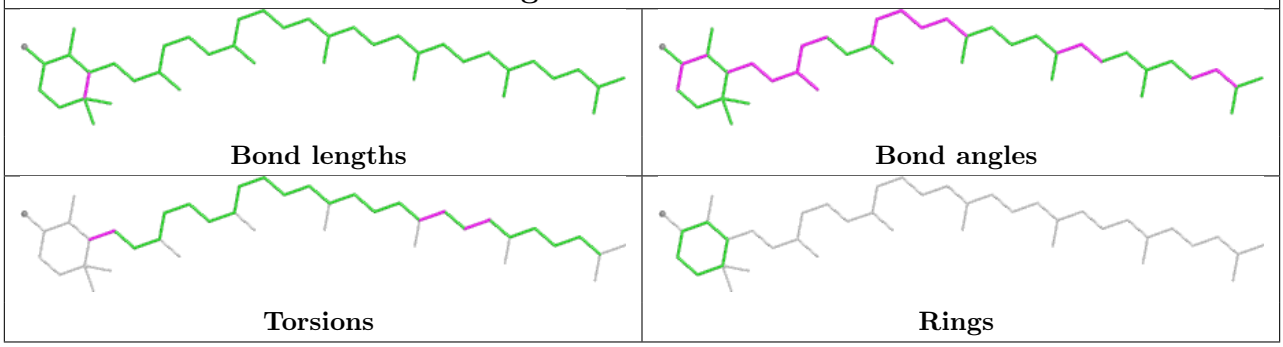

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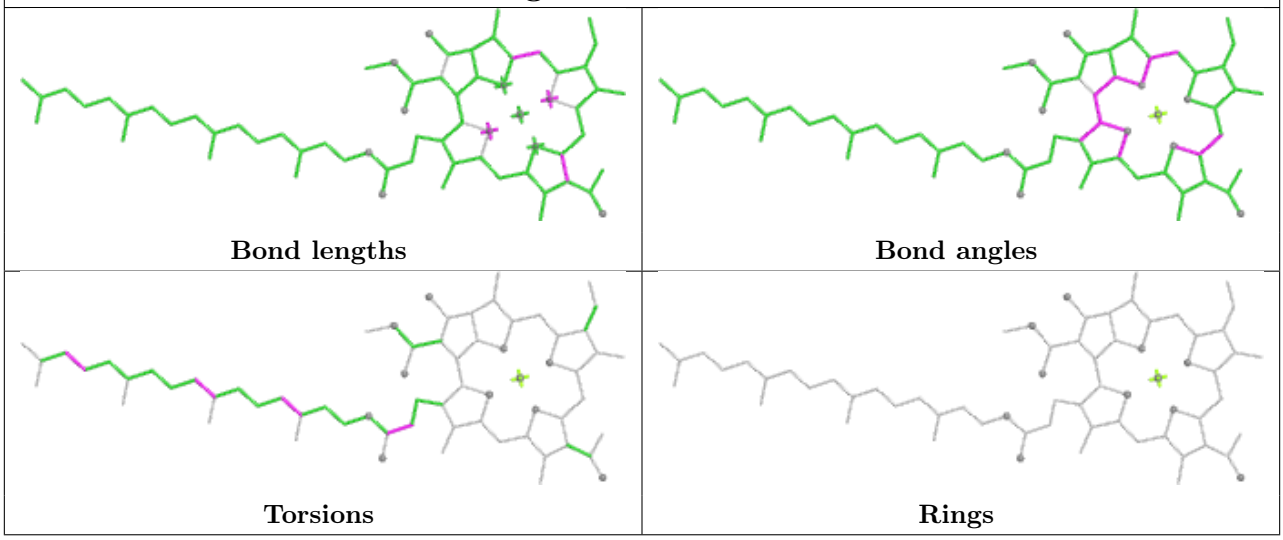

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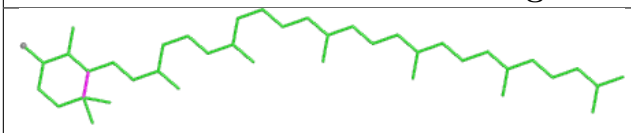

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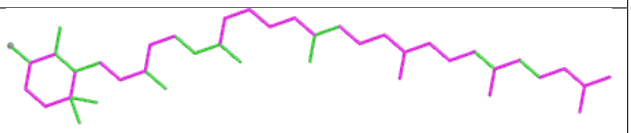

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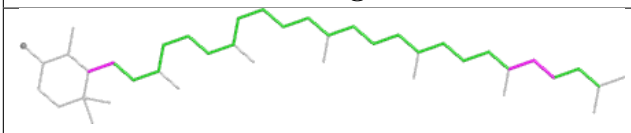

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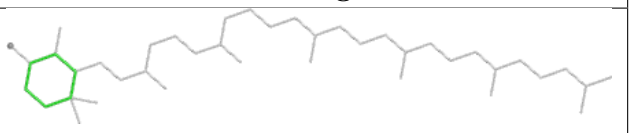
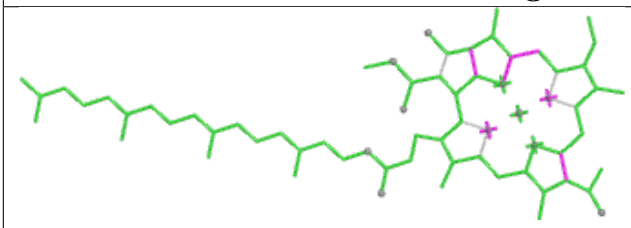


Rings

Ligand BCL R 101



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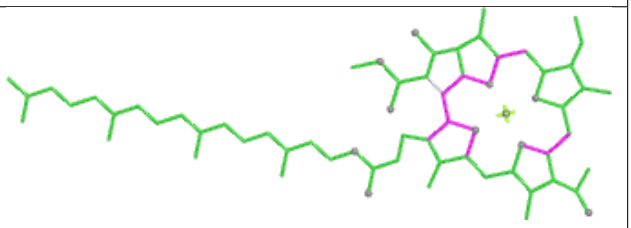

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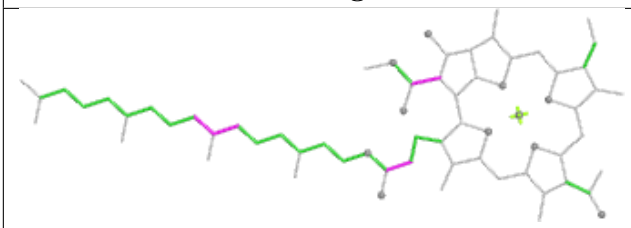

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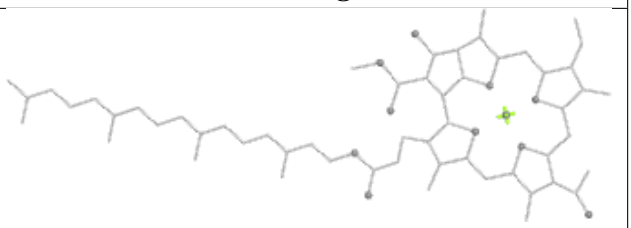
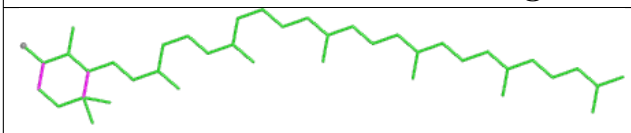


Rings

Ligand KGD 2 103



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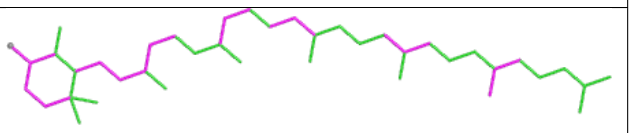
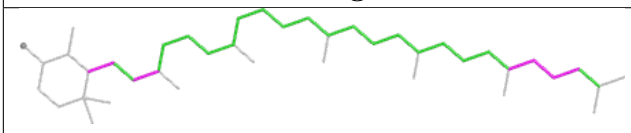
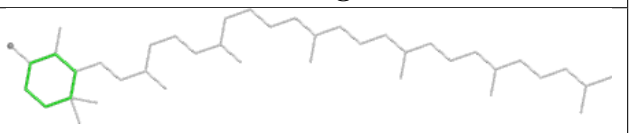


Bond angles



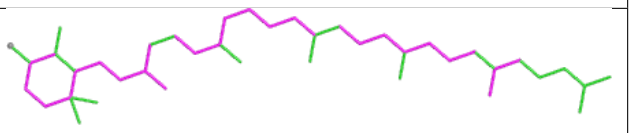
Torsions



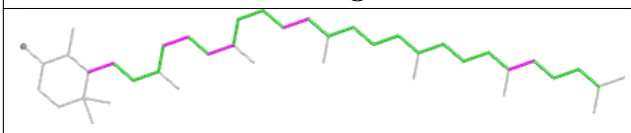
Rings

Ligand KGD S 104

Bond lengths



Bond angles



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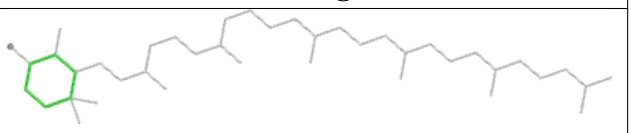
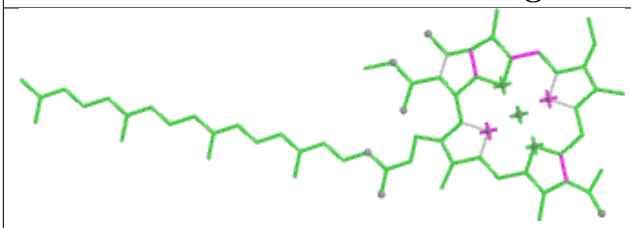
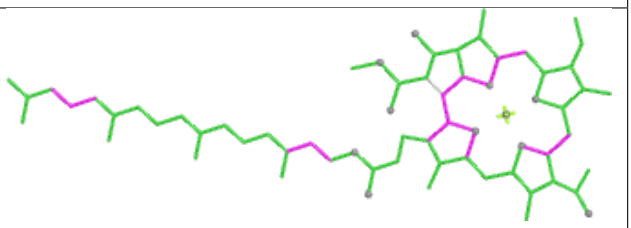
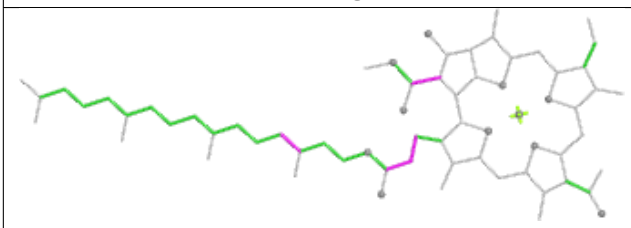
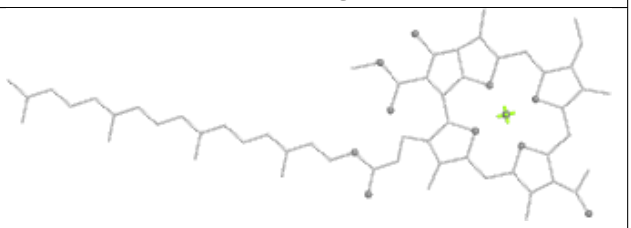
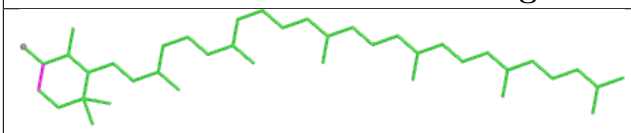
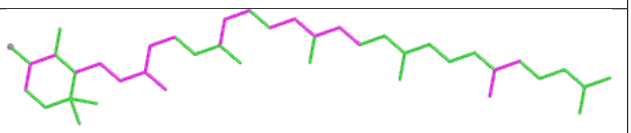
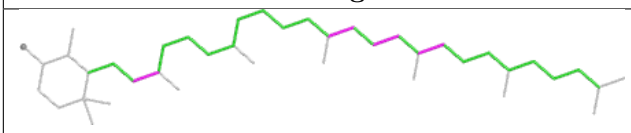
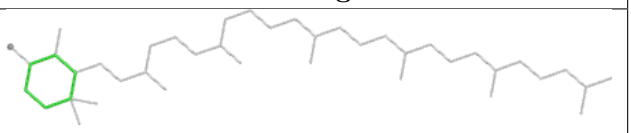


Rings

Ligand BCL O 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KGD D 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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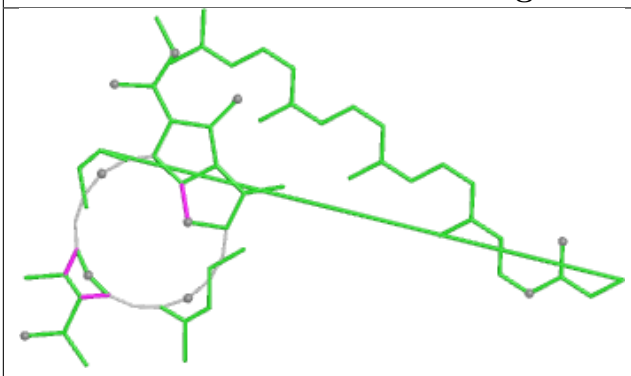
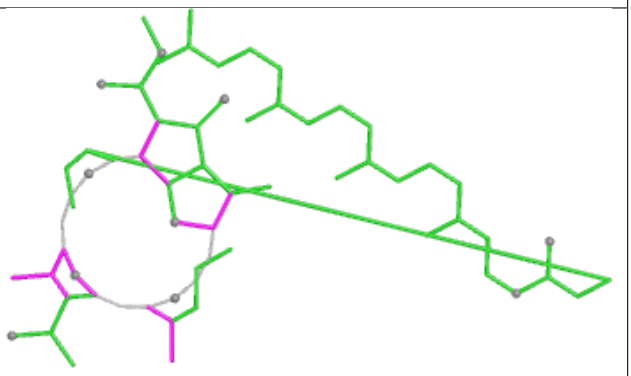
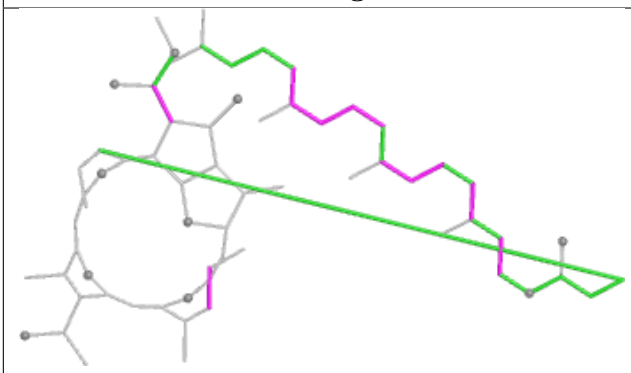
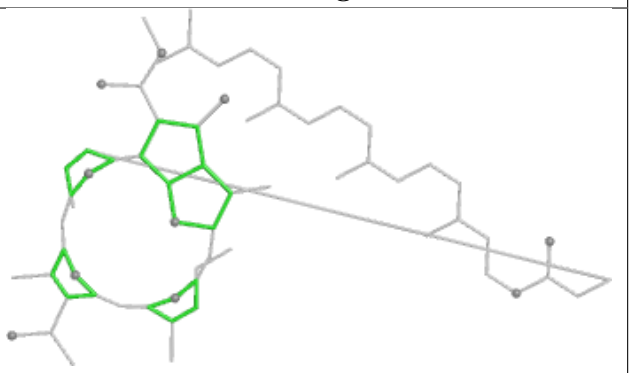
 Bond lengths	 Bond angles
 Torsions	 Rings

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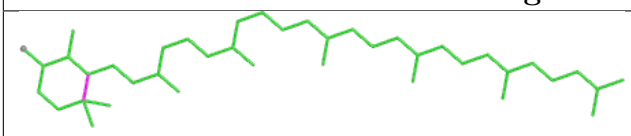
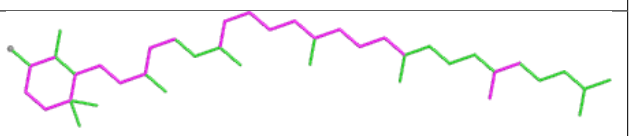
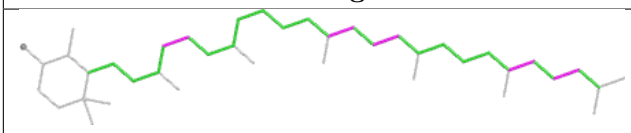
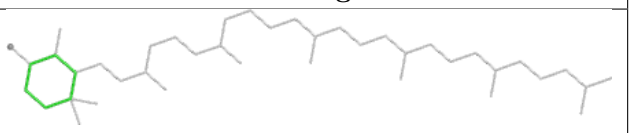
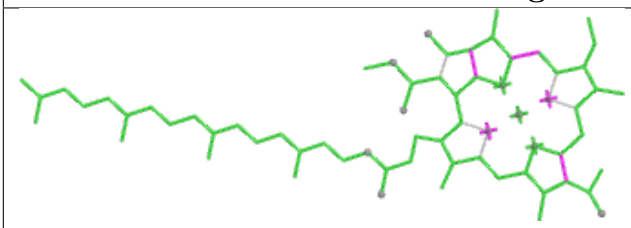
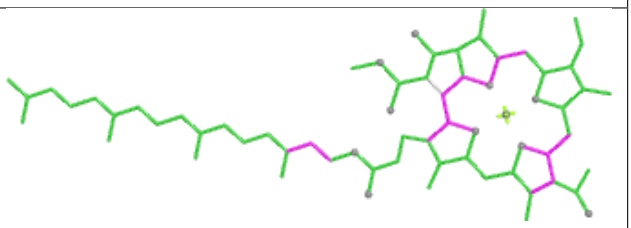
 Bond lengths	 Bond angles
 Torsions	 Rings

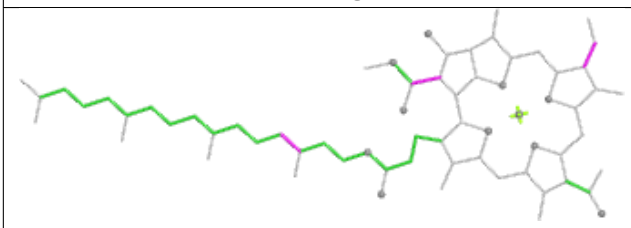
Ligand BCL S 101



Bond lengths



Bond angles



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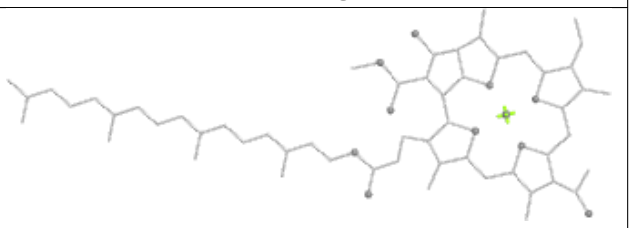
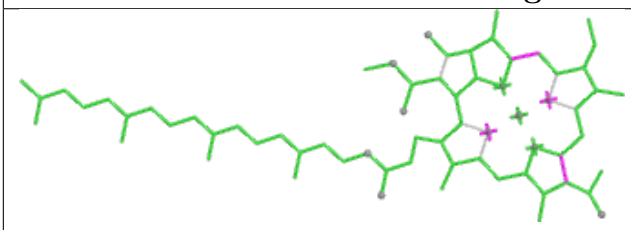


Rings

Ligand BCL G 101



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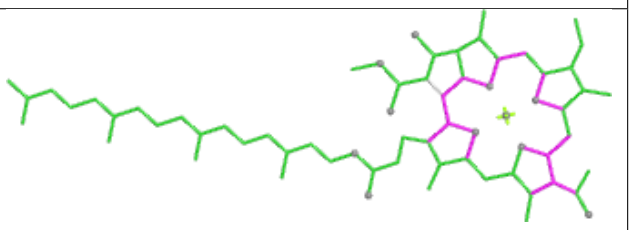
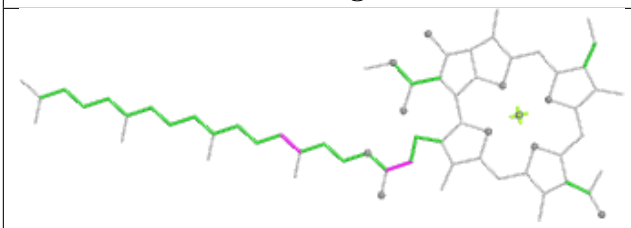


Bond angles



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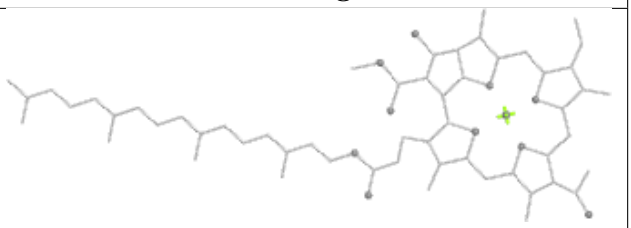
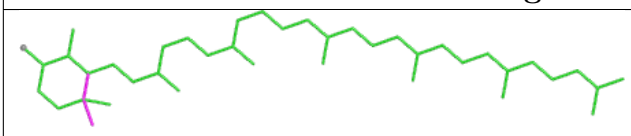


Rings

Ligand KGD 6 103



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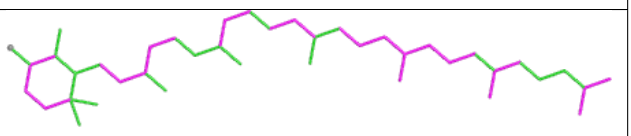
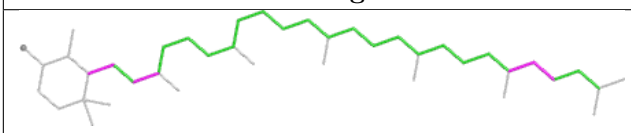


Bond angles



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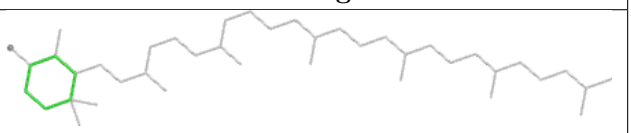
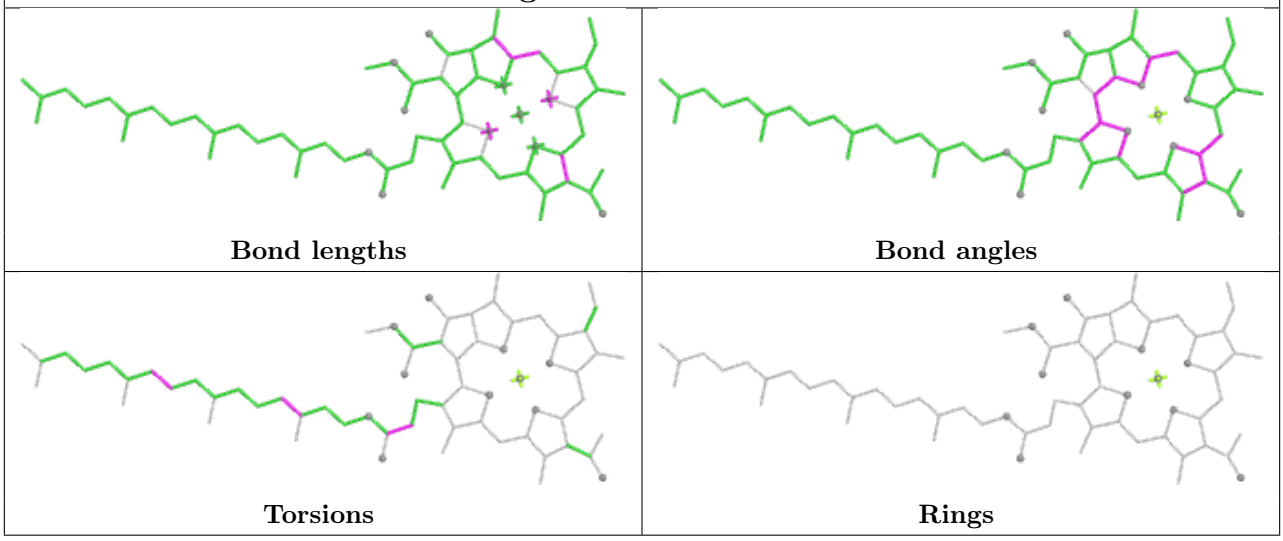
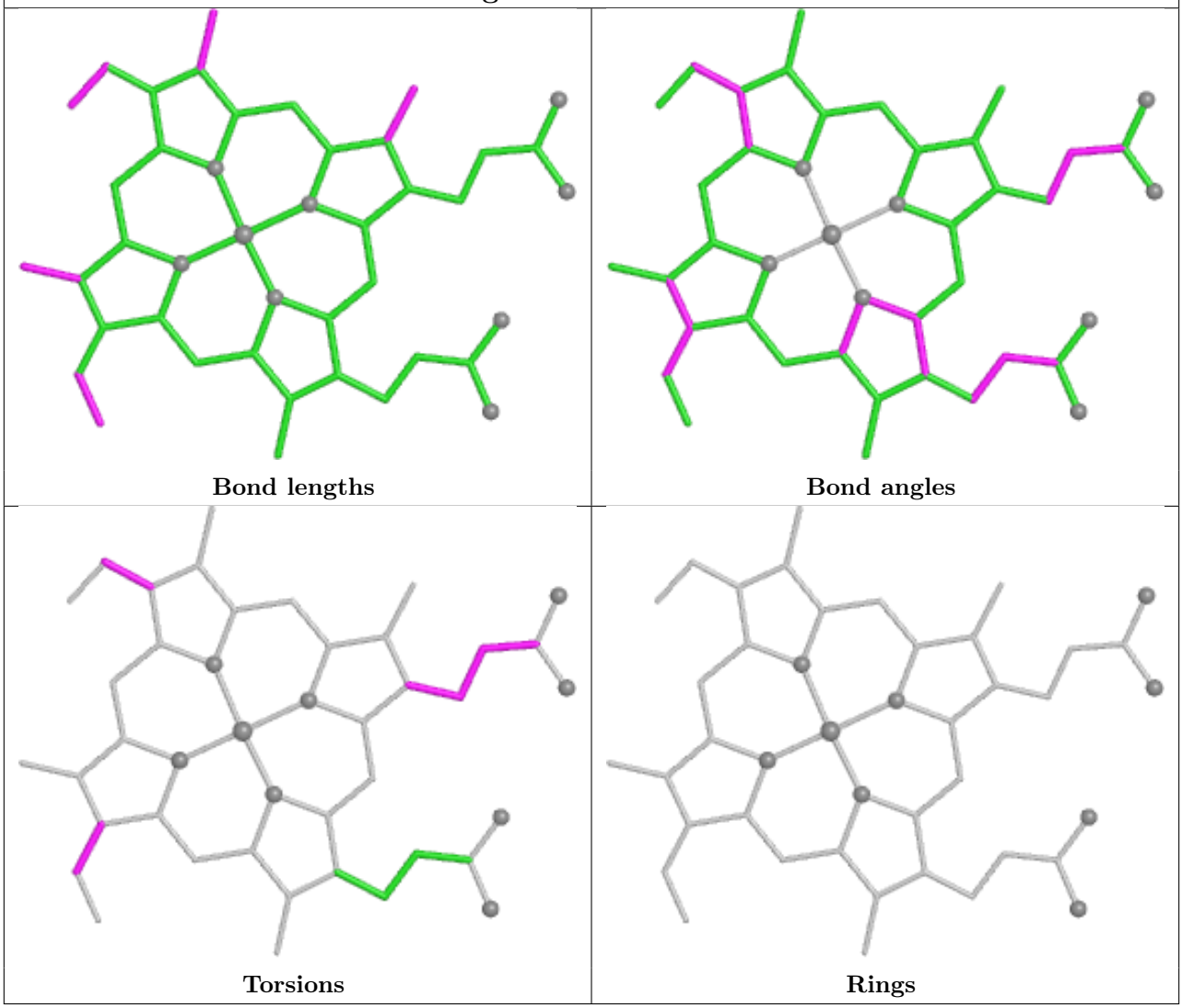


Rings

Ligand BCL L 1002



Ligand HEC C 503



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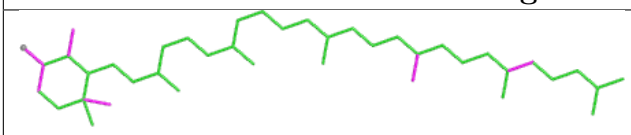
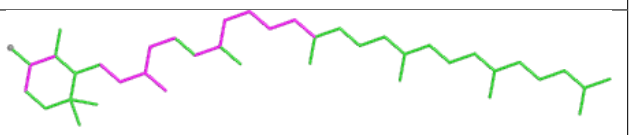
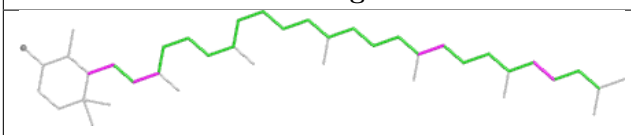
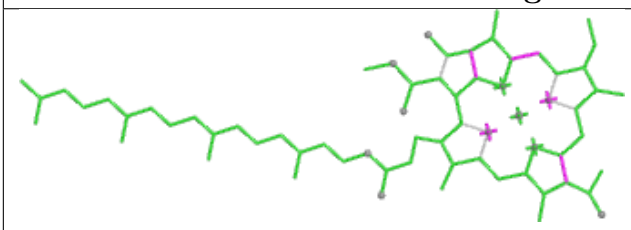
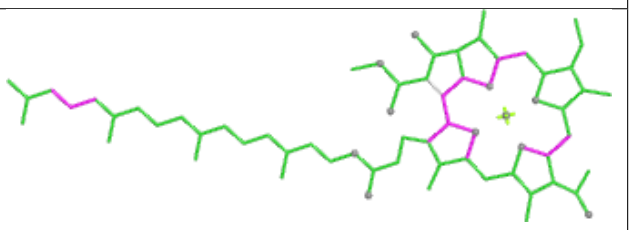
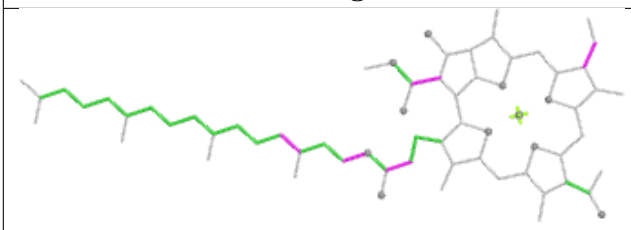
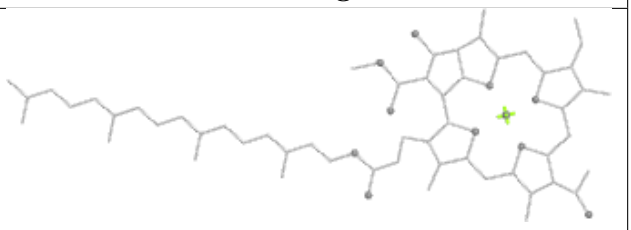
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand BCL K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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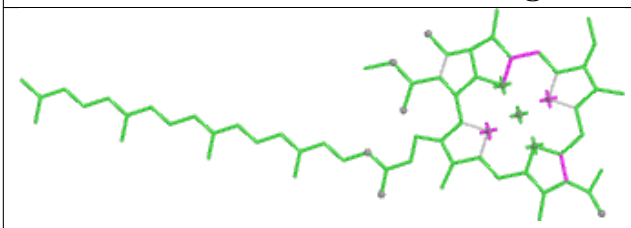
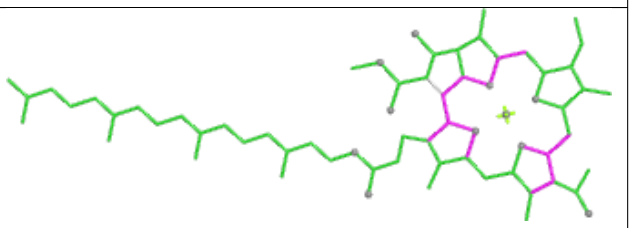
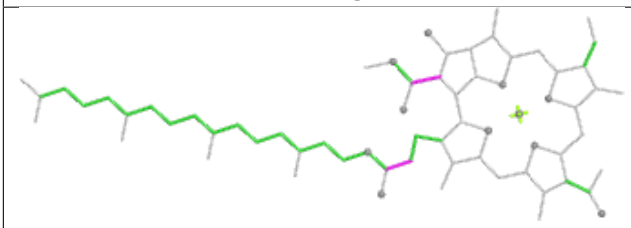
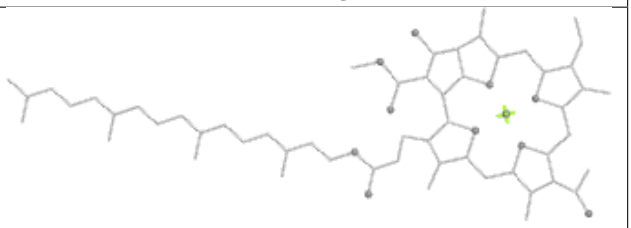
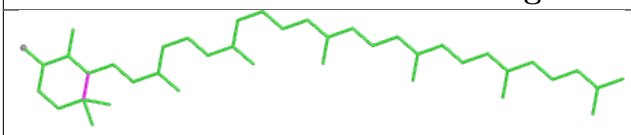
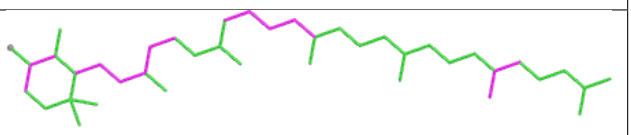
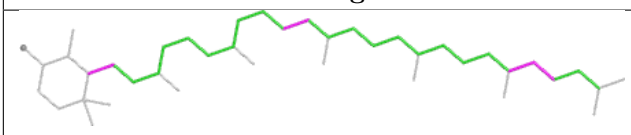
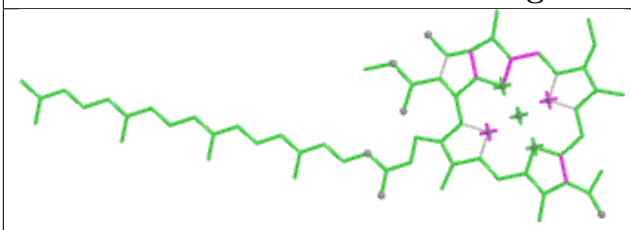
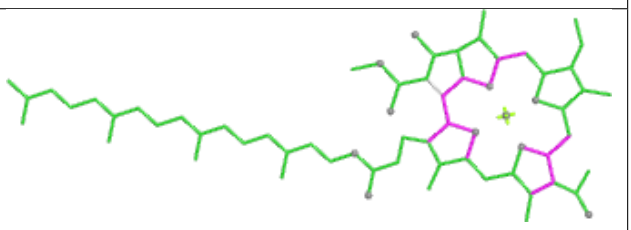
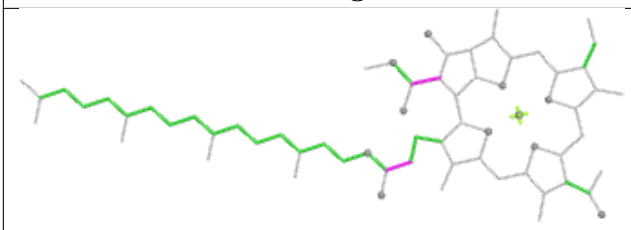
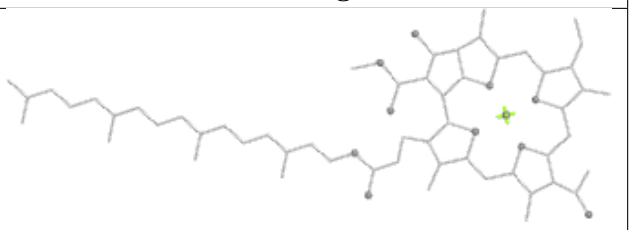
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KGD 0 104	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand BCL F 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

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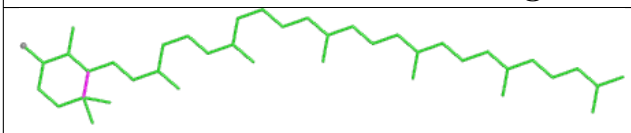
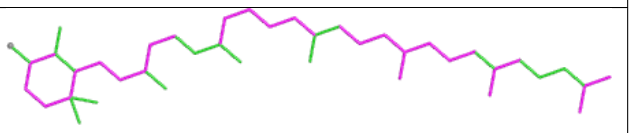
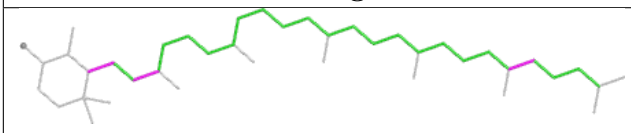
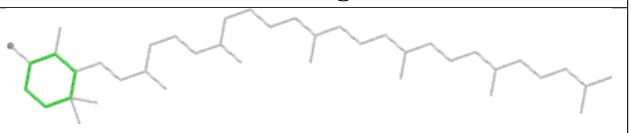
 Bond lengths	 Bond angles
 Torsions	 Rings

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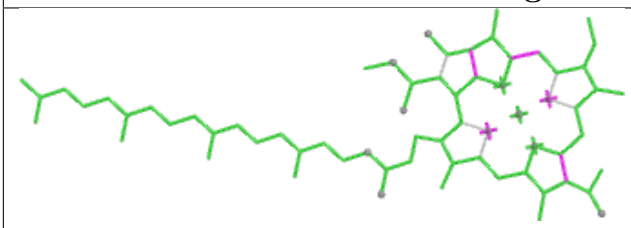
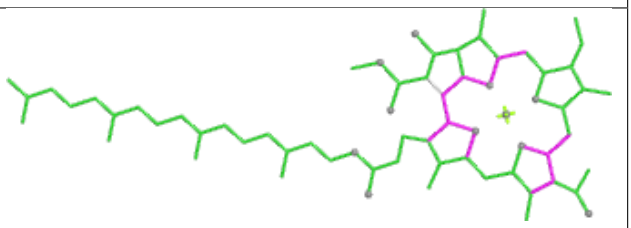
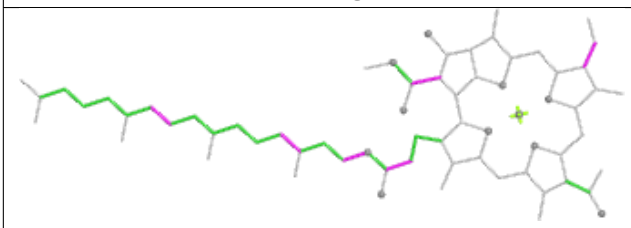
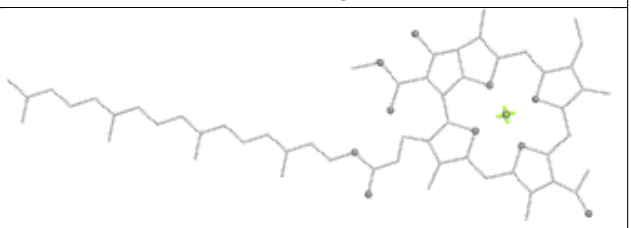
 Bond lengths	 Bond angles
 Torsions	 Rings

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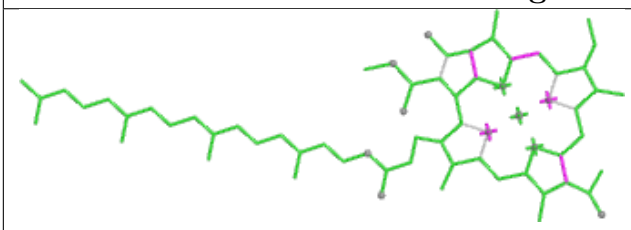
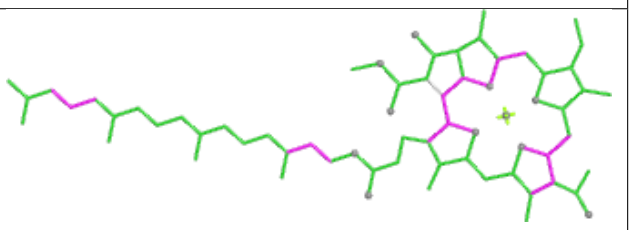
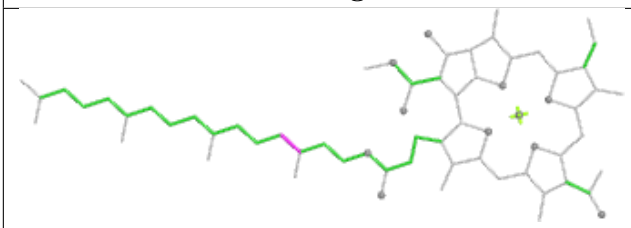
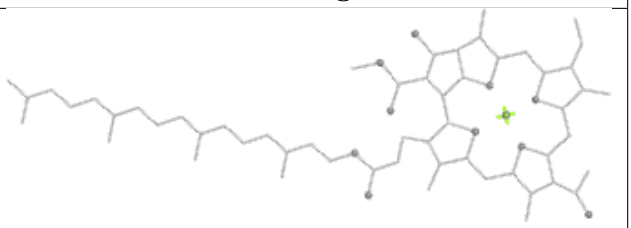
 Bond lengths	 Bond angles
 Torsions	 Rings

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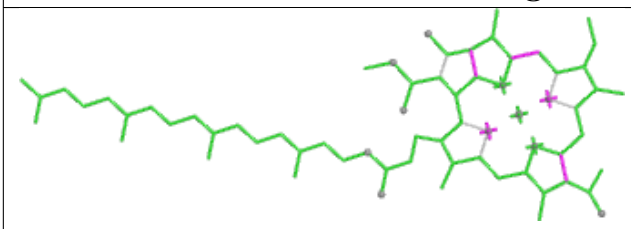
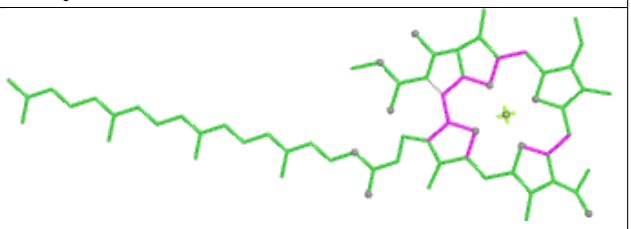
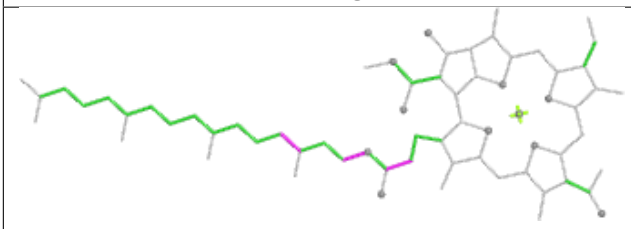
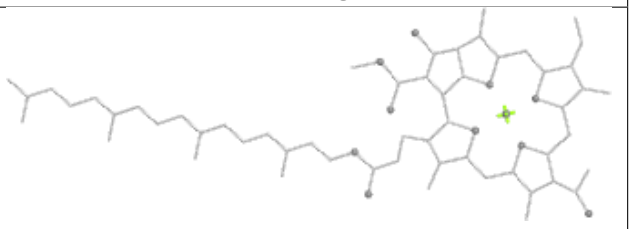
 Bond lengths	 Bond angles
 Torsions	 Rings

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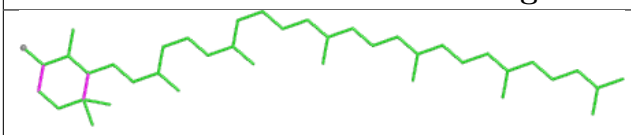
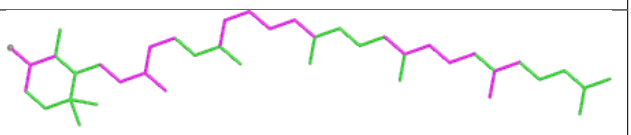
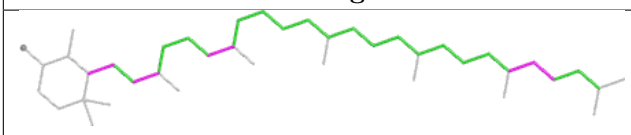
 Bond lengths	 Bond angles
 Torsions	Rings

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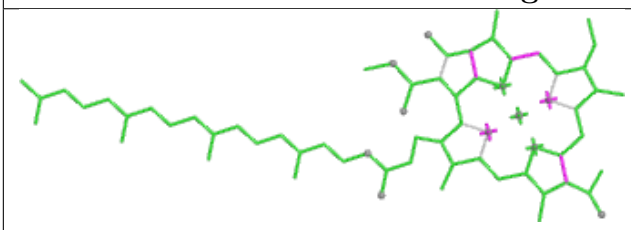
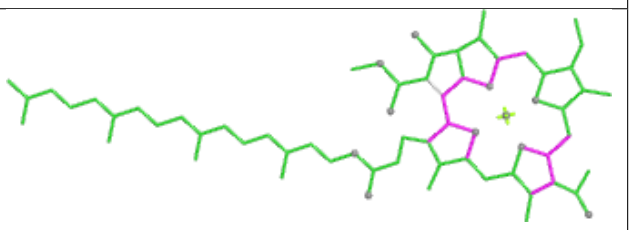
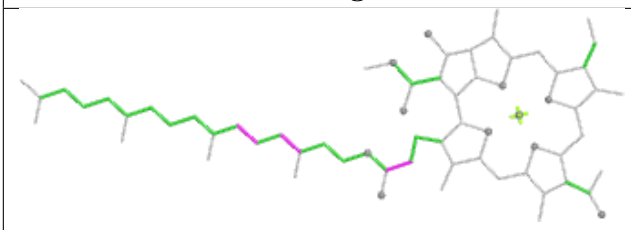
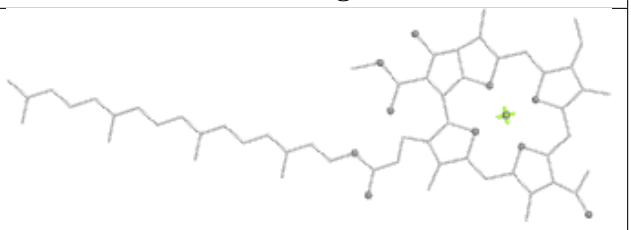
 Bond lengths	 Bond angles
 Torsions	 Rings

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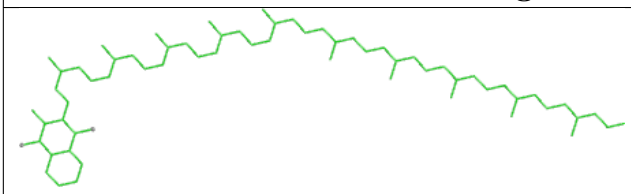
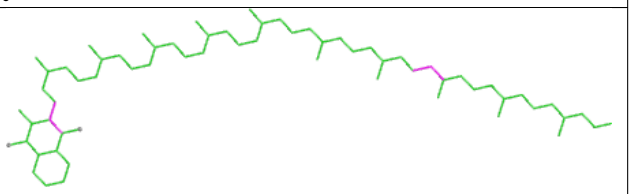
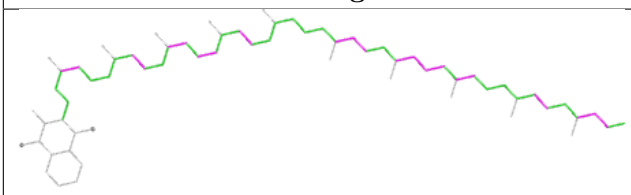
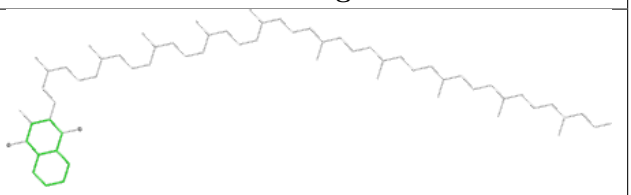
 Bond lengths	 Bond angles
 Torsions	 Rings

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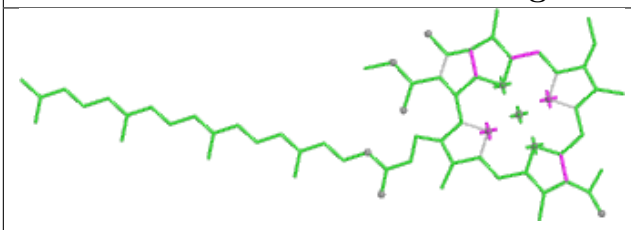
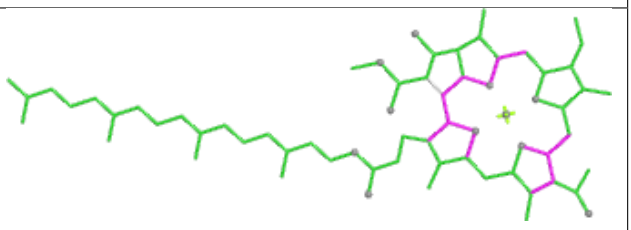
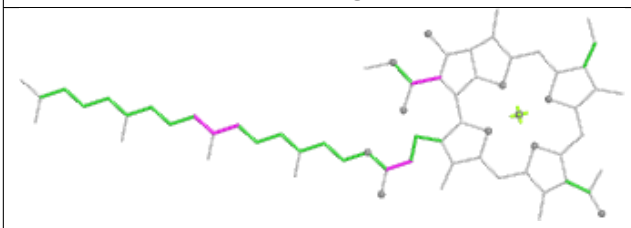
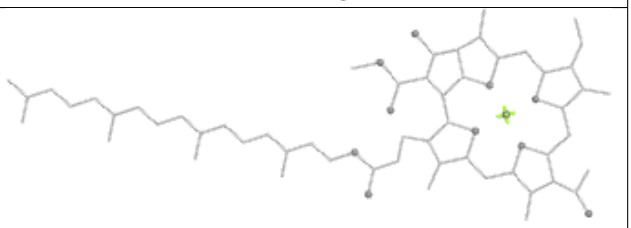
 Bond lengths	 Bond angles
 Torsions	 Rings

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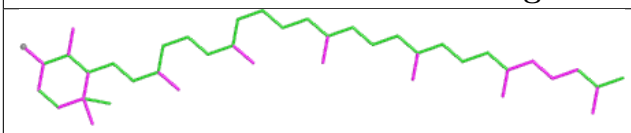
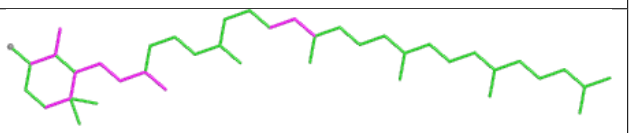
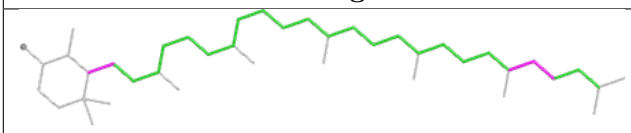
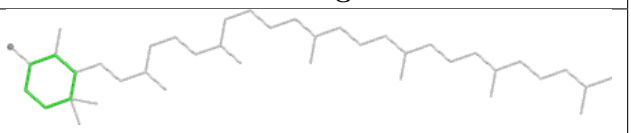
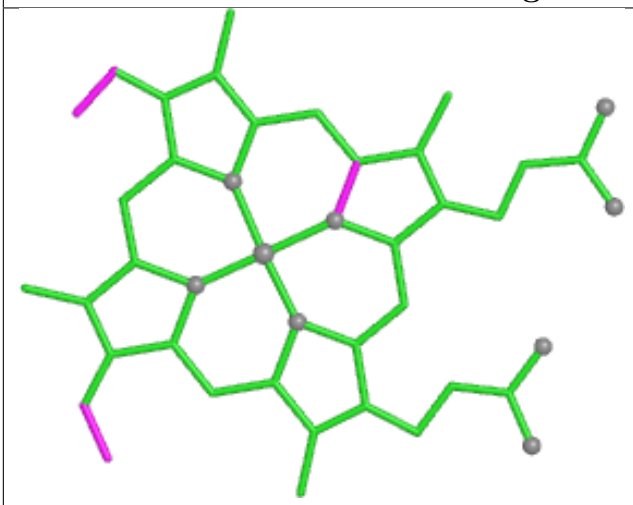
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEC C 502



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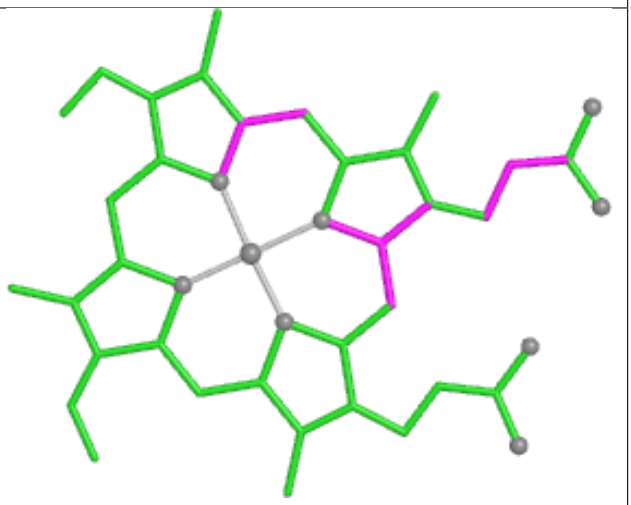

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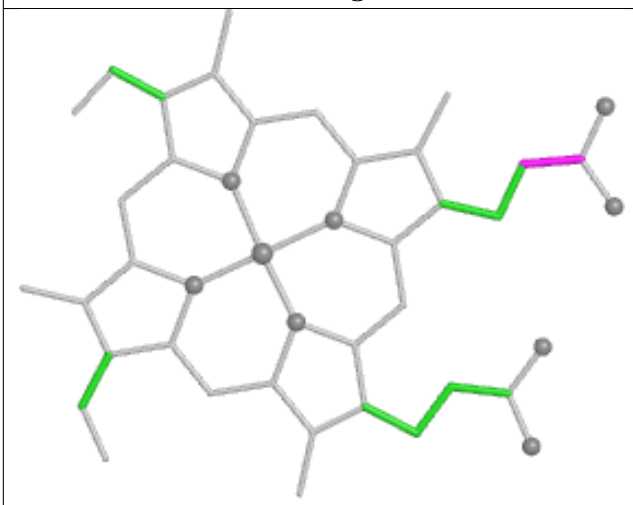

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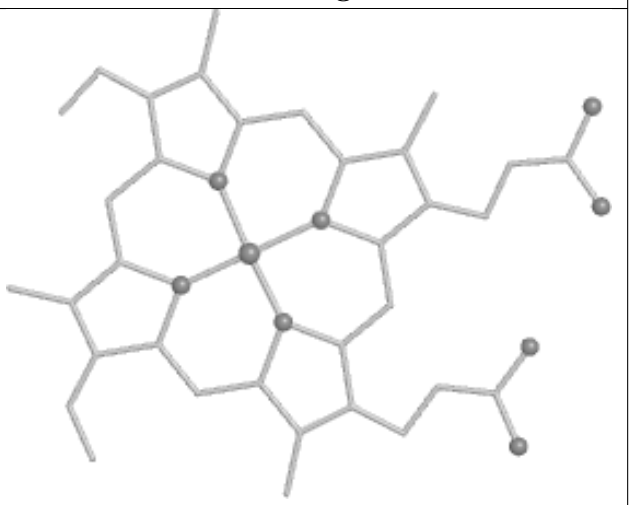
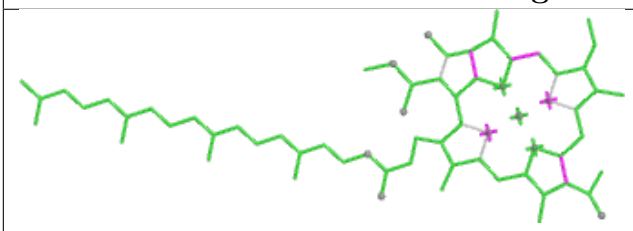


Rings

Ligand BCL I 102



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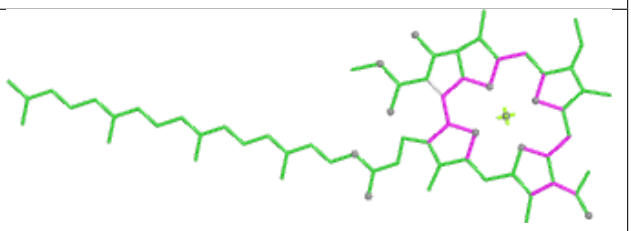

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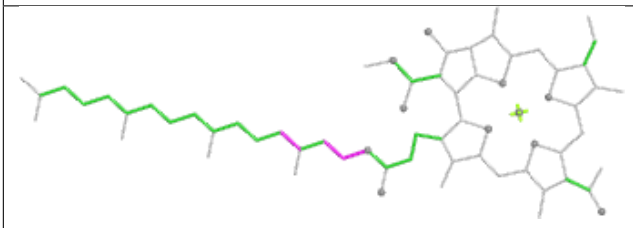

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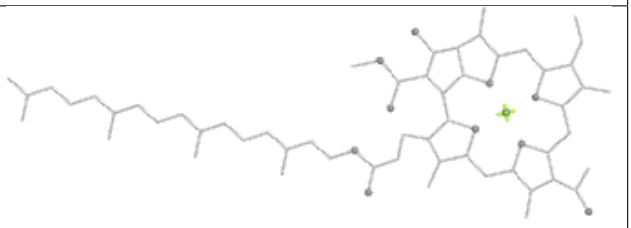

Rings

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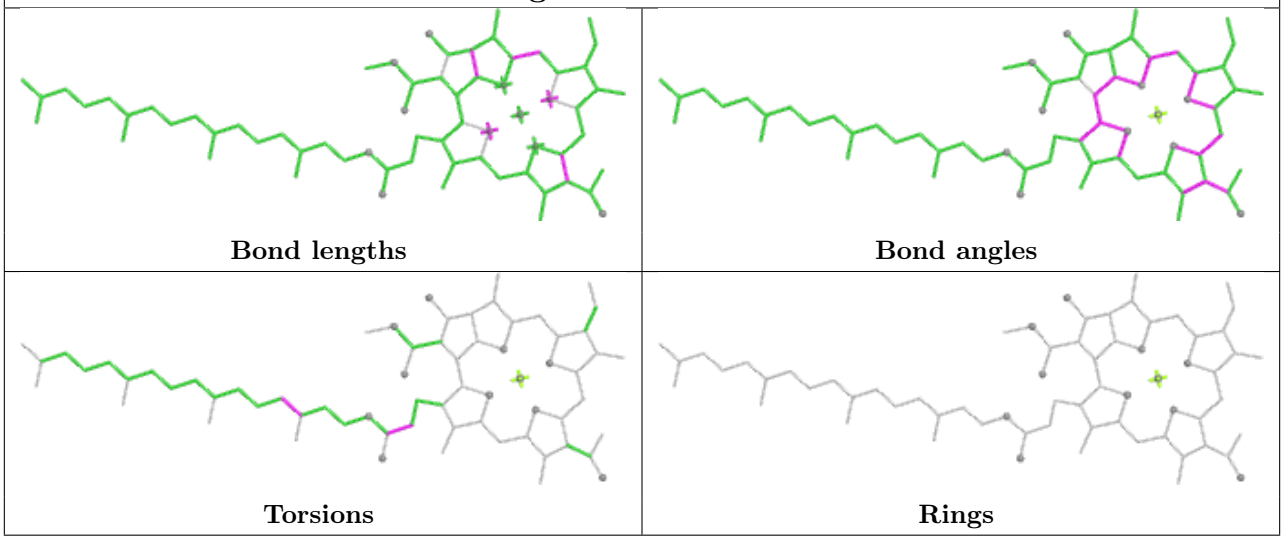

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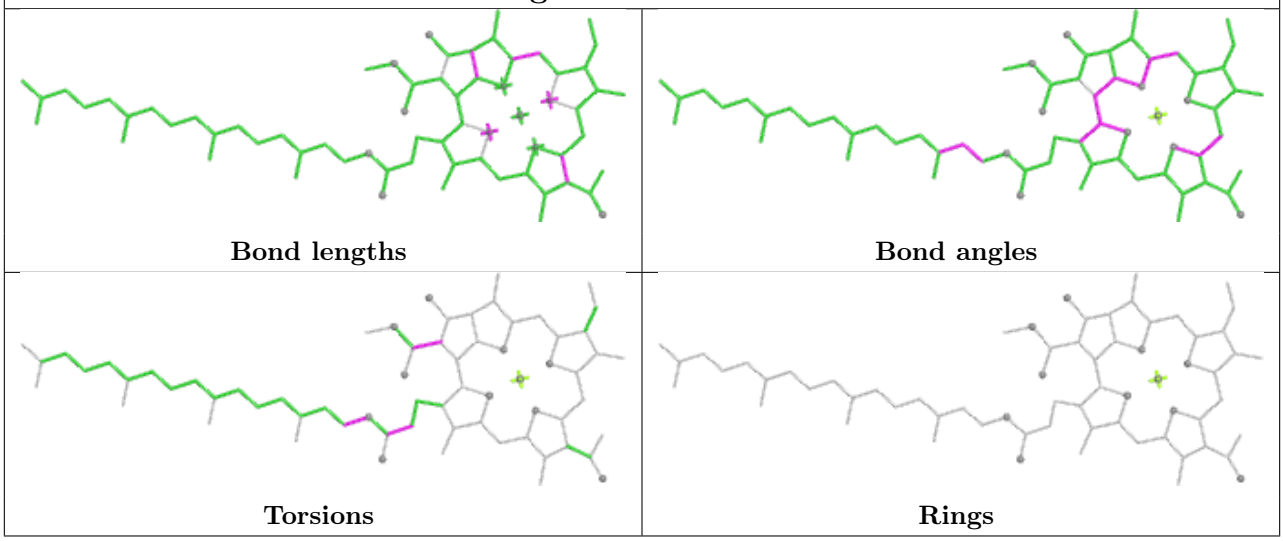

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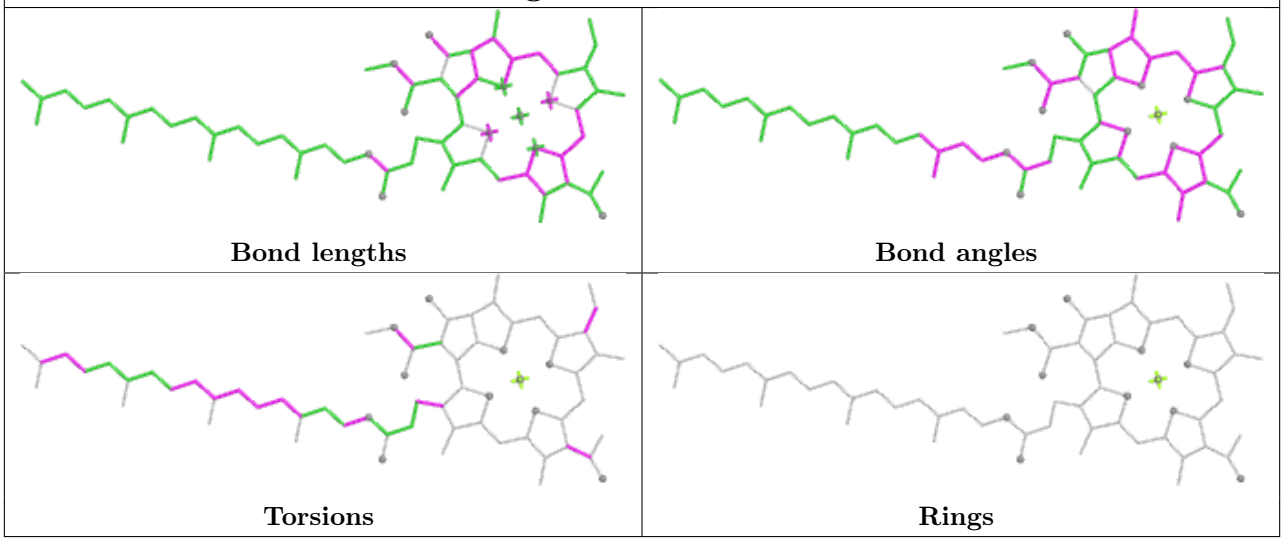
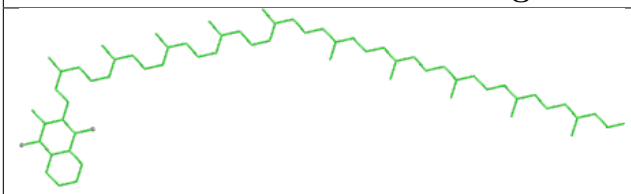
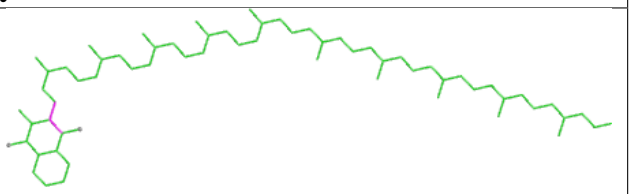


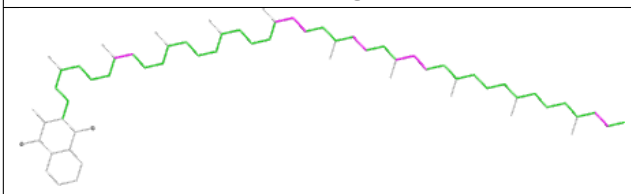
Ligand MQE L 1005



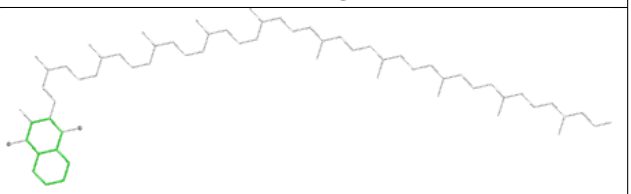
Bond lengths



Bond angles

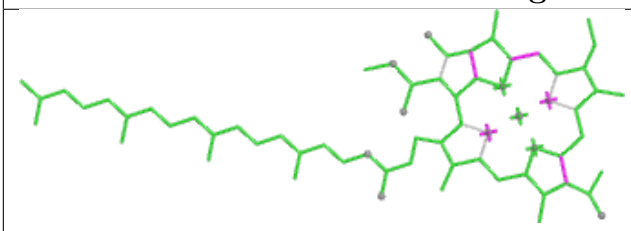


Torsions



Rings

Ligand BCL 6 101



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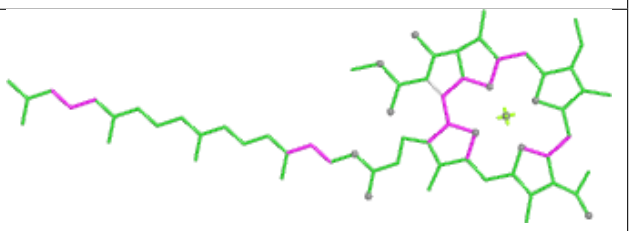

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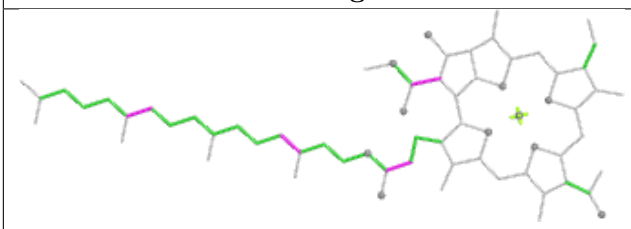

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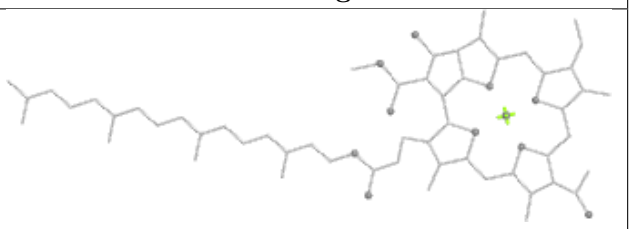
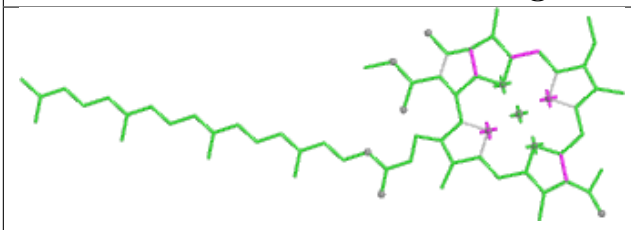


Rings

Ligand BCL 2 102



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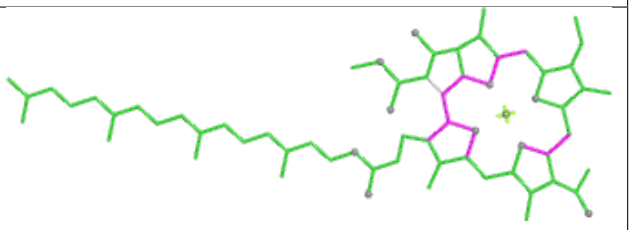
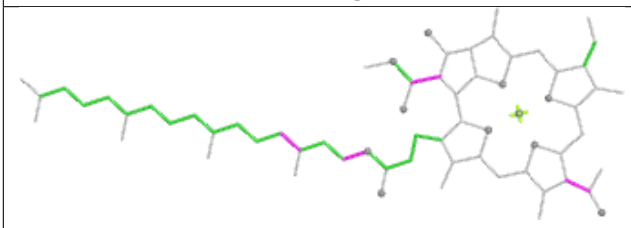
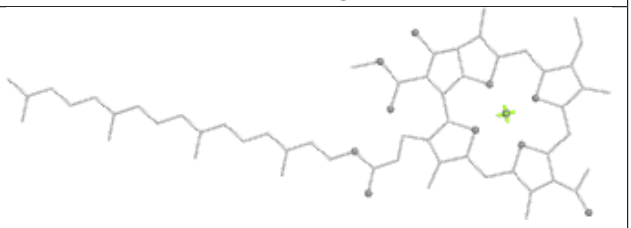


Bond angles

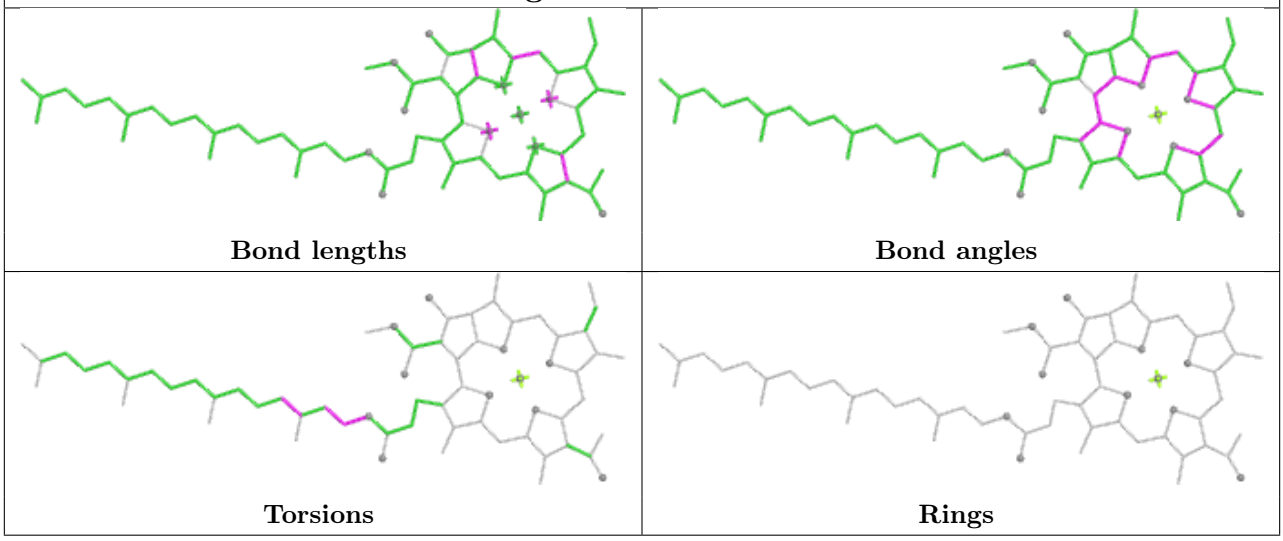


Torsions

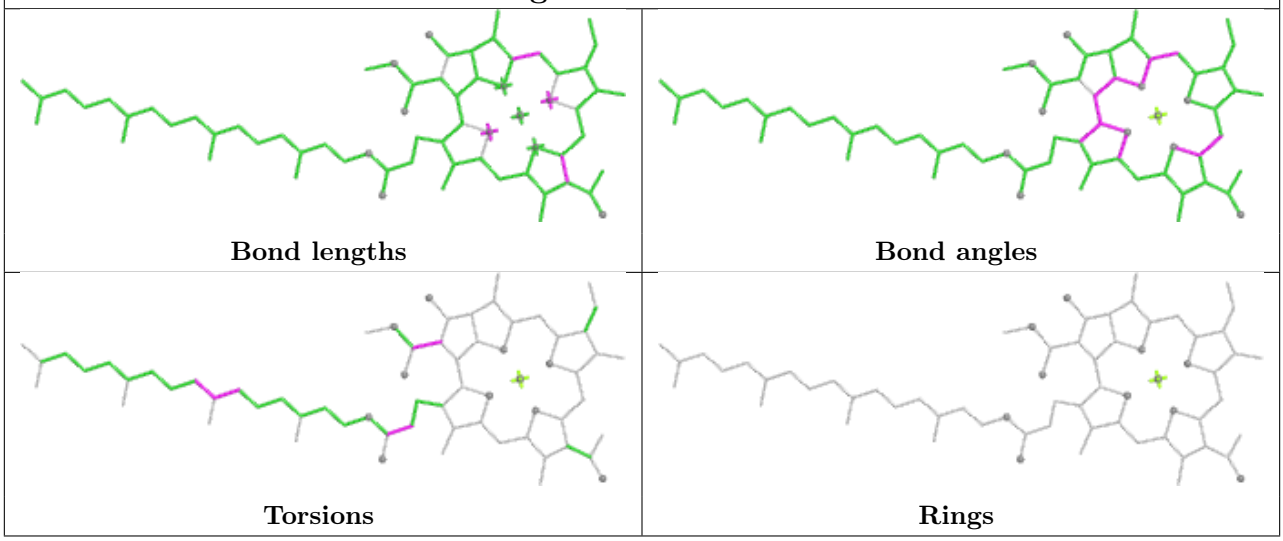


Rings

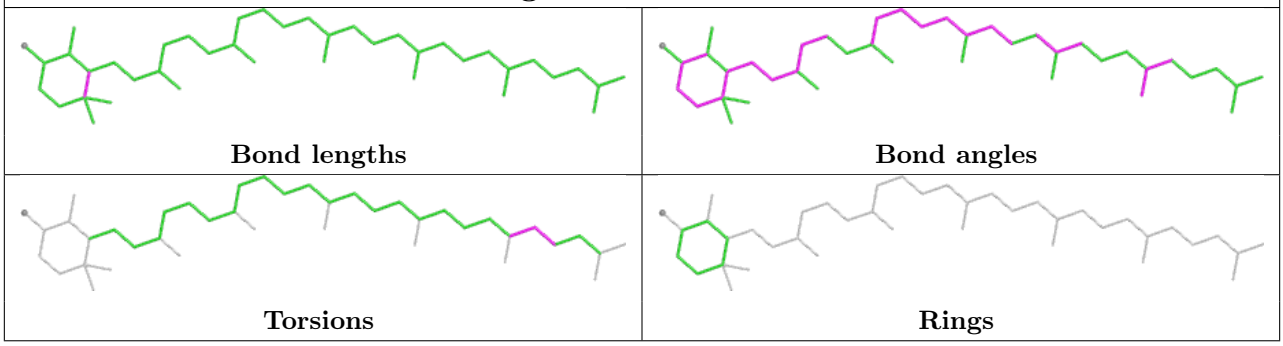
Ligand BCL U 102



Ligand BCL 7 101



Ligand KGD D 103



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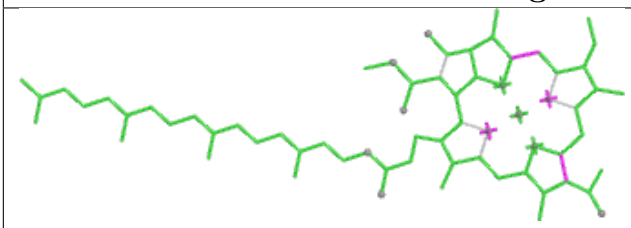
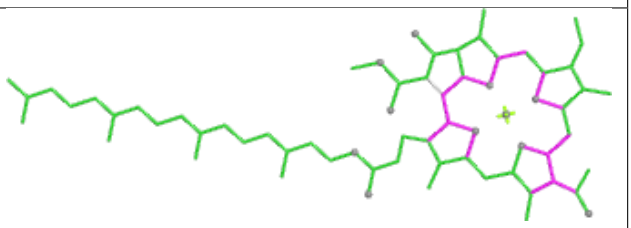
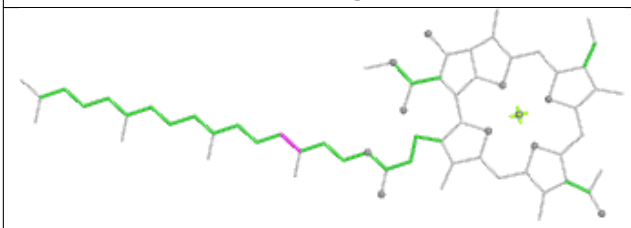
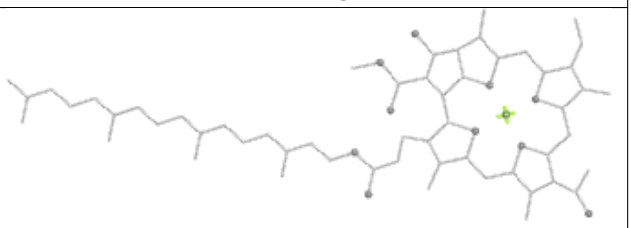
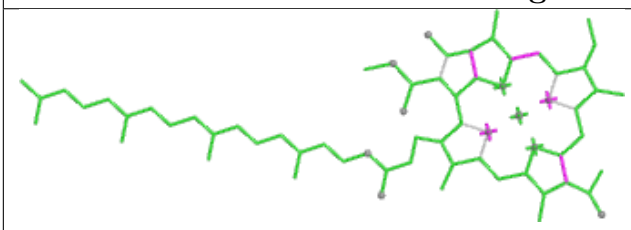
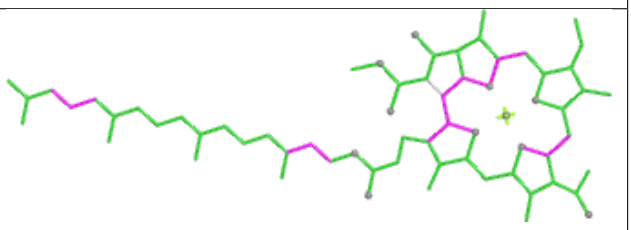
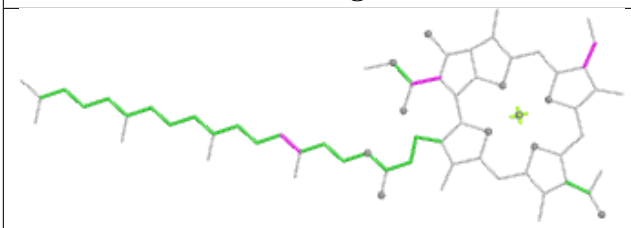
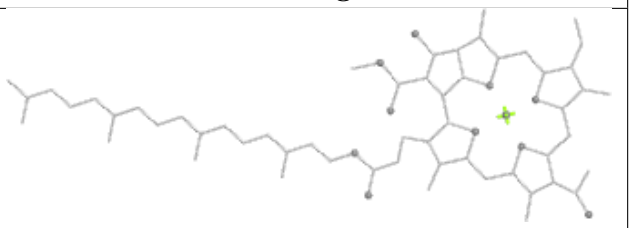
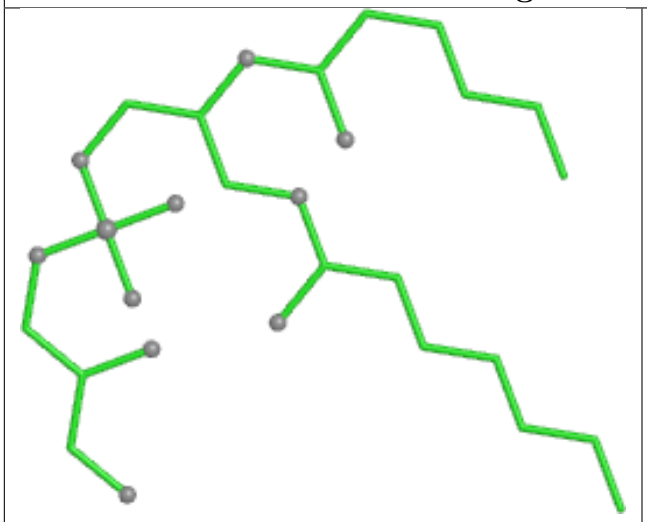
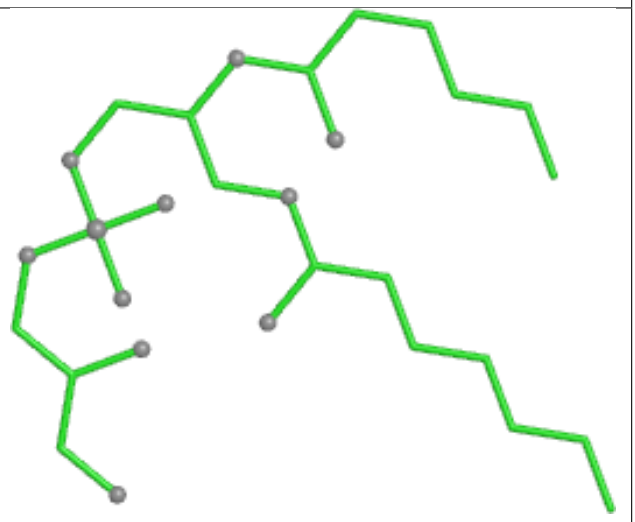
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 0 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV L 1007



Bond lengths



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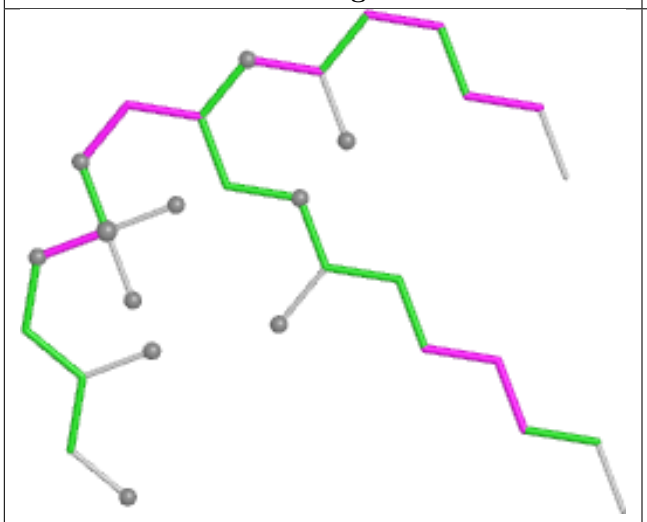

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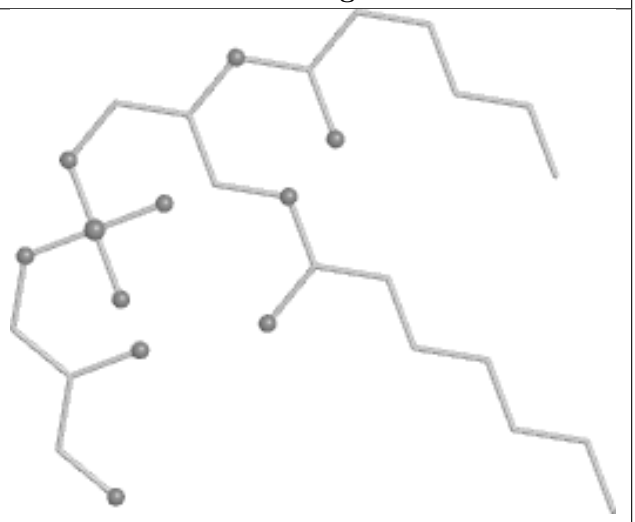
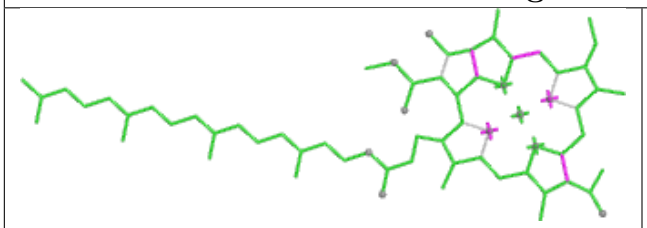


Rings

Ligand BCL P 101



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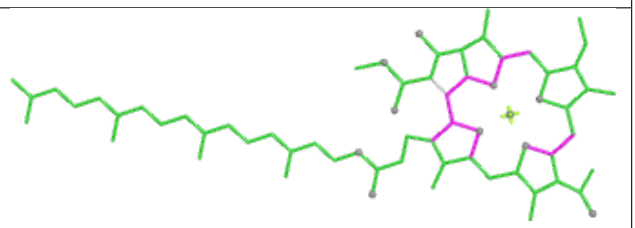

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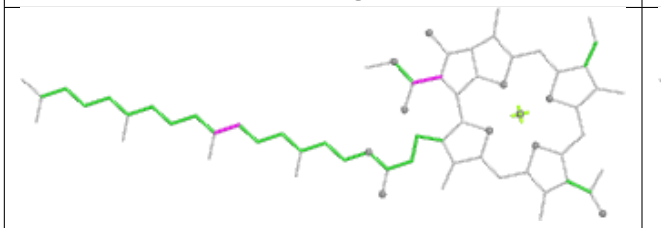

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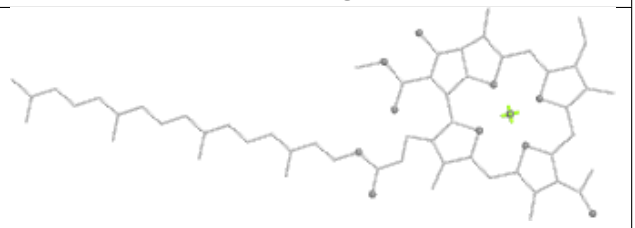
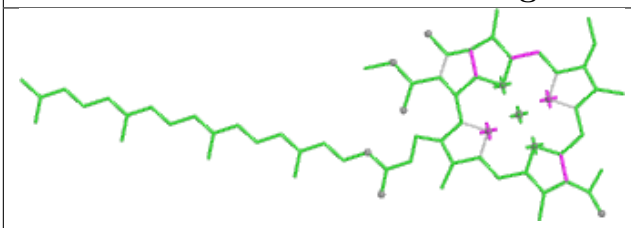


Rings

Ligand BCL W 101



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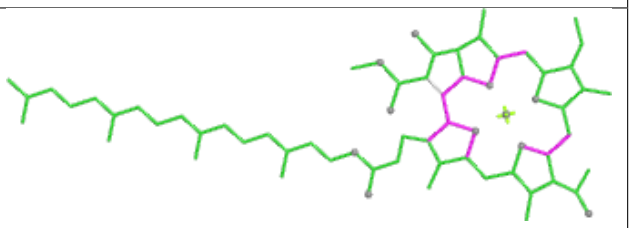

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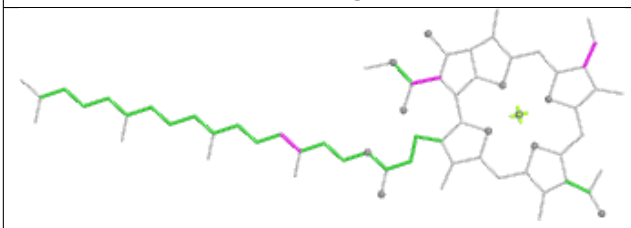

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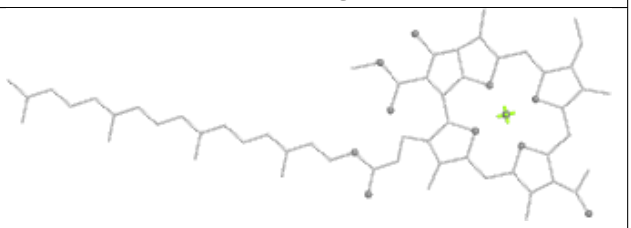

Rings

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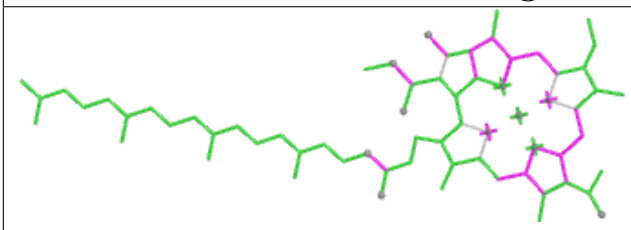

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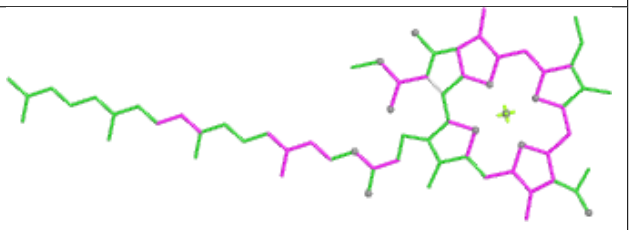

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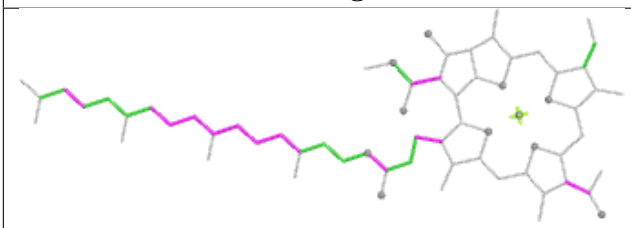

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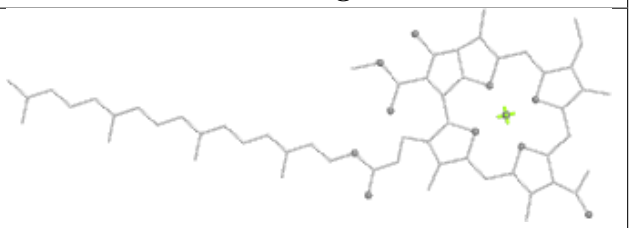
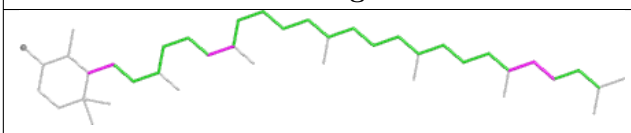


Rings

Ligand KGD G 102

Bond lengths

Bond angles



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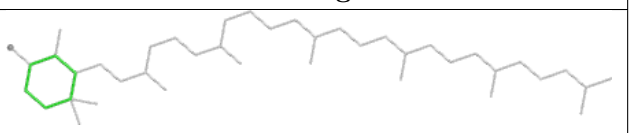
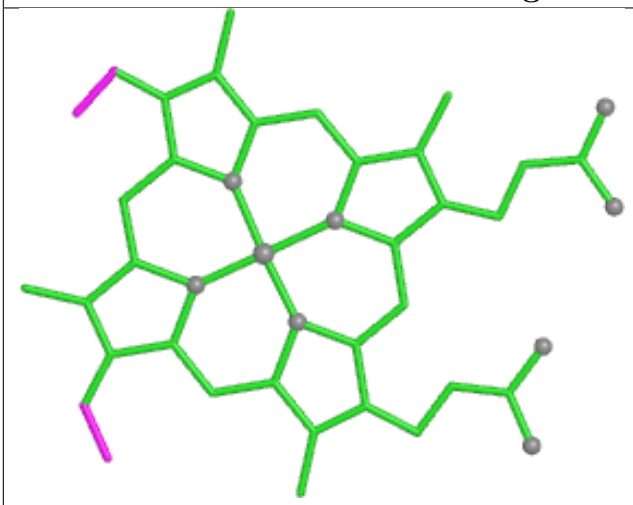


Rings

Ligand HEC C 504



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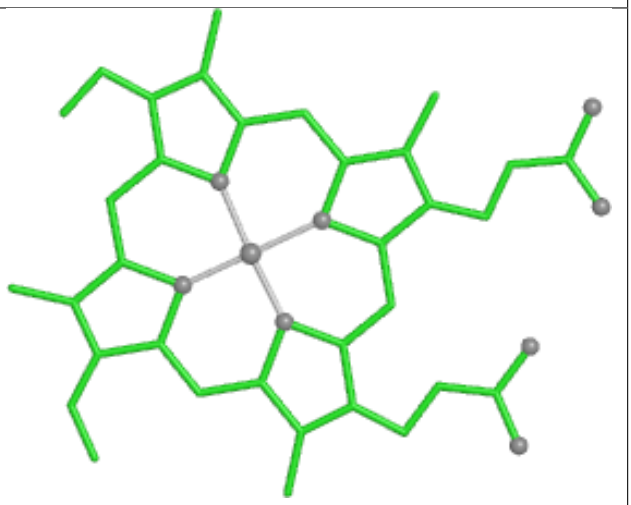
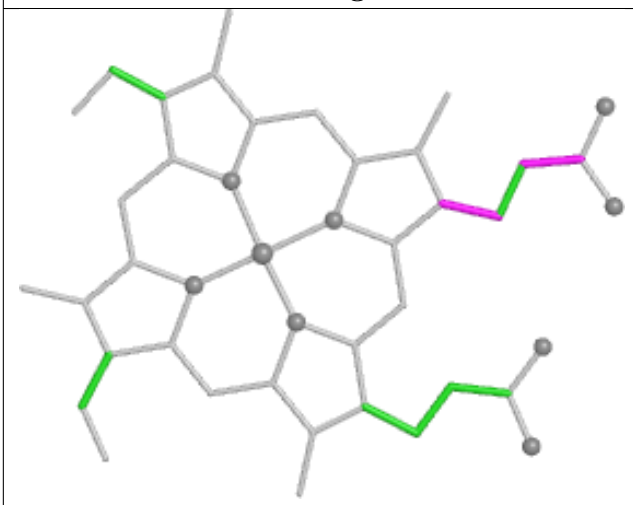


Bond angles



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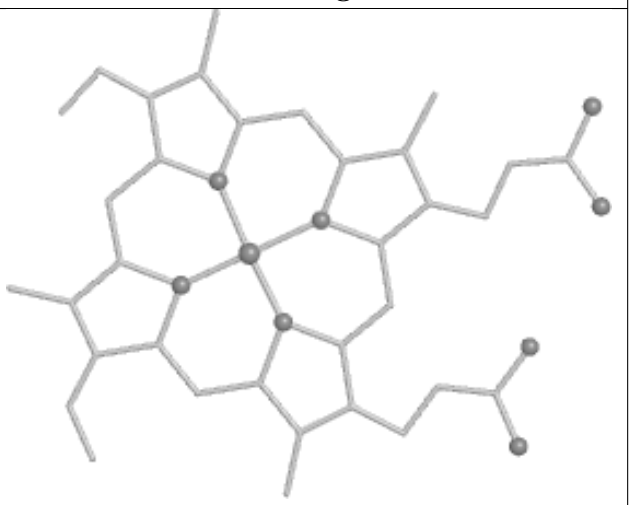
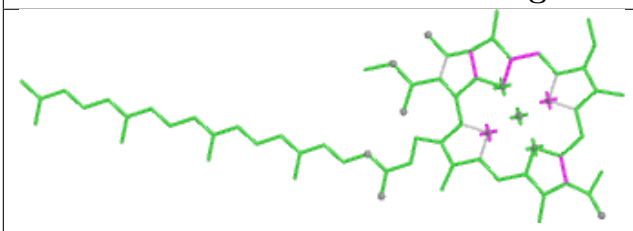


Rings

Ligand BCL 8 102



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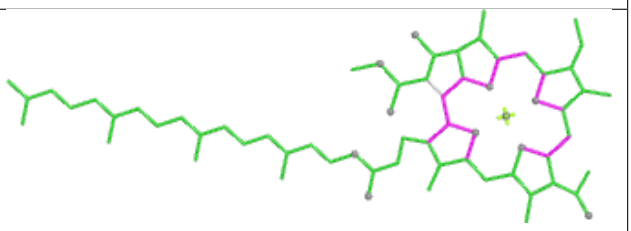

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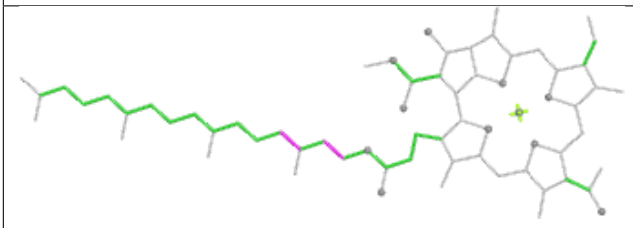

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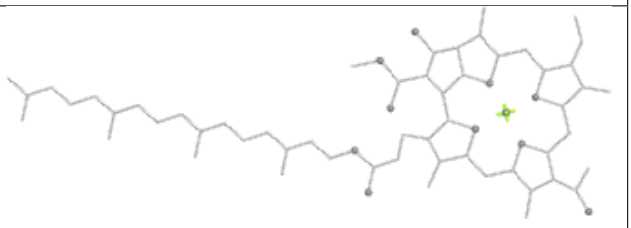

Rings

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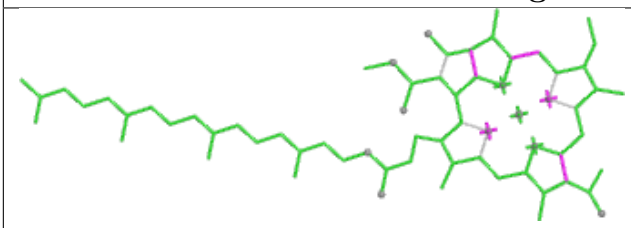

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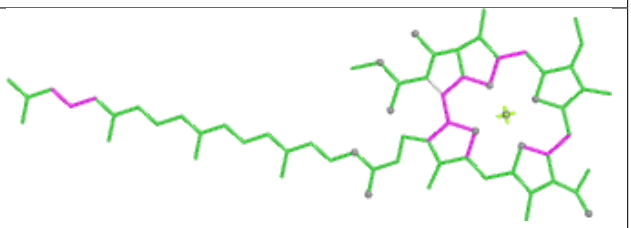

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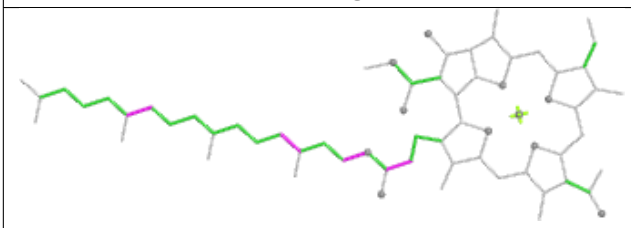

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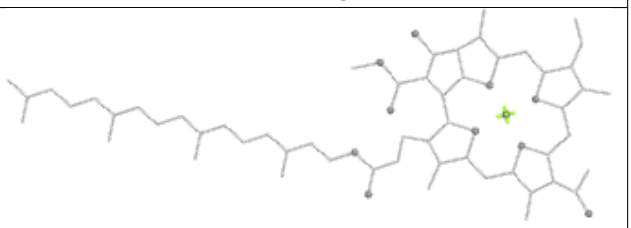

Rings

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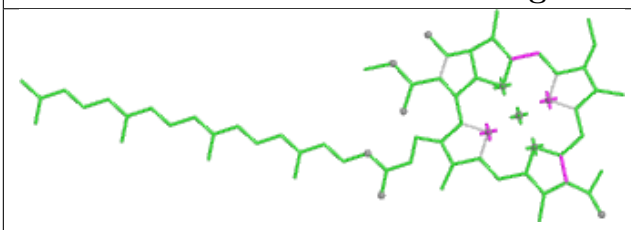

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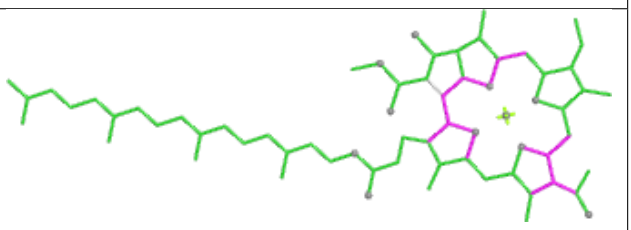

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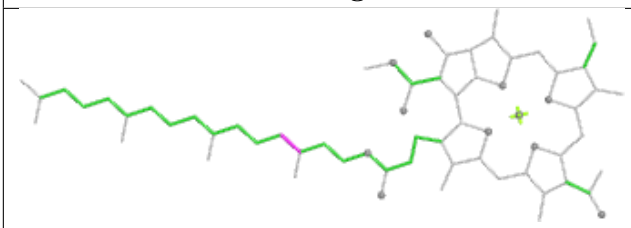

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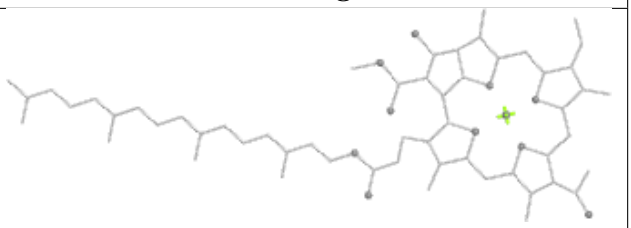
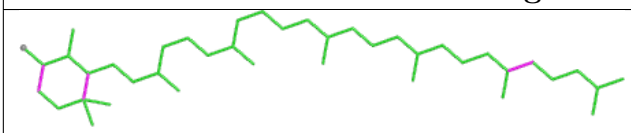


Rings

Ligand KGD 1 103



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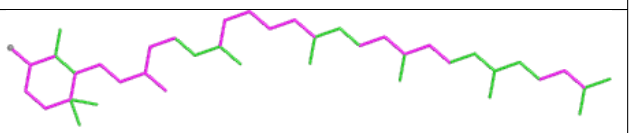

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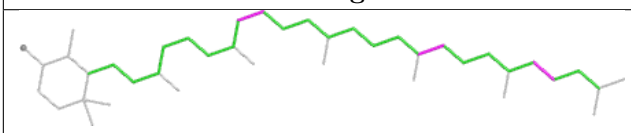

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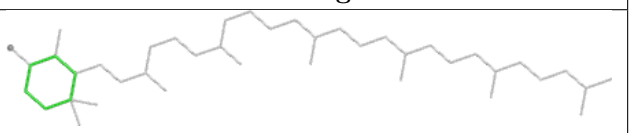
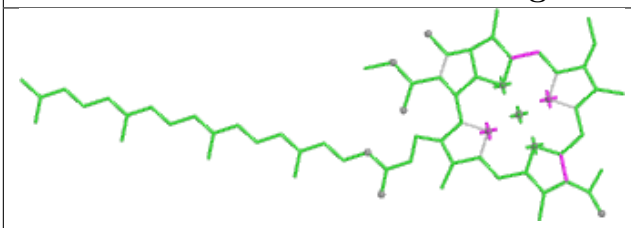
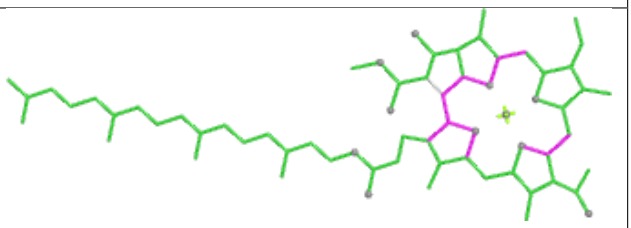
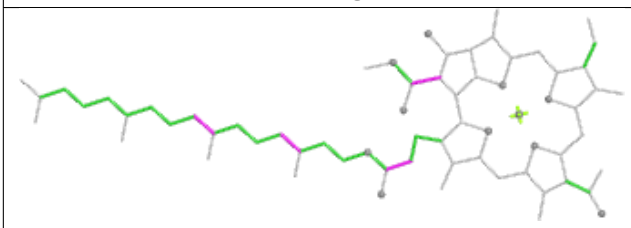
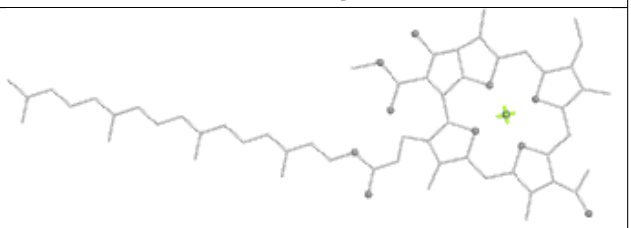
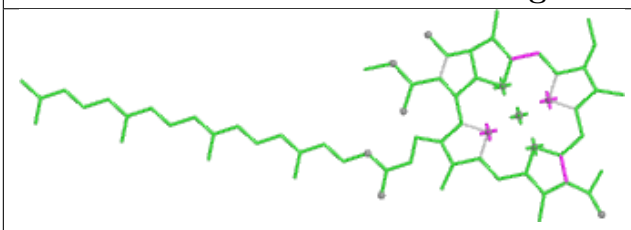
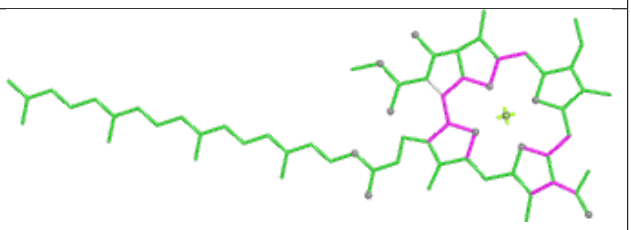
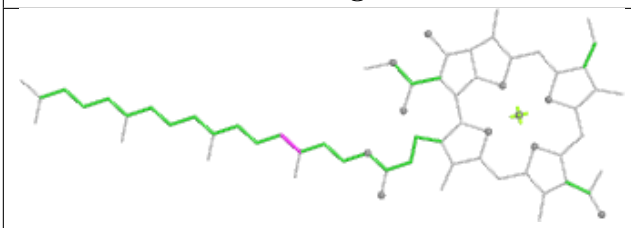
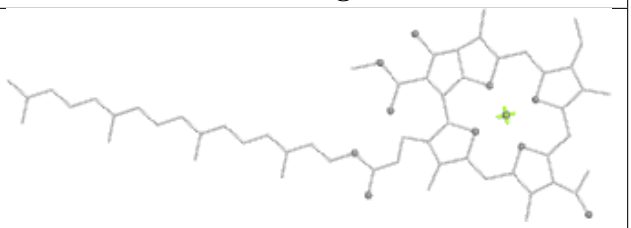


Rings

Ligand BCL 9 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 0 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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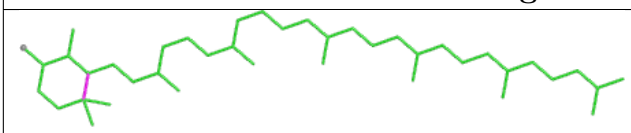
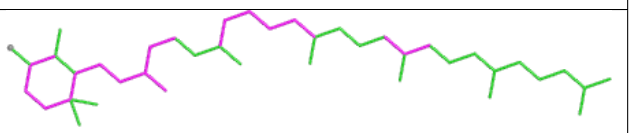
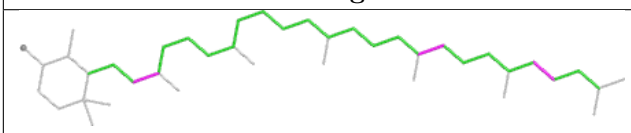
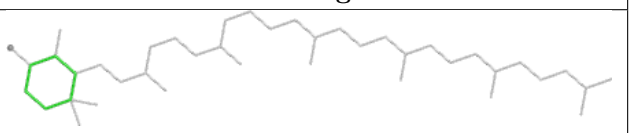
 Bond lengths	 Bond angles
 Torsions	 Rings

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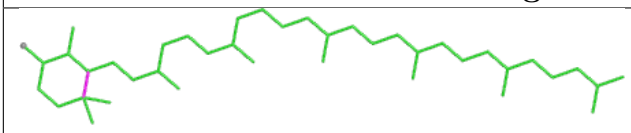
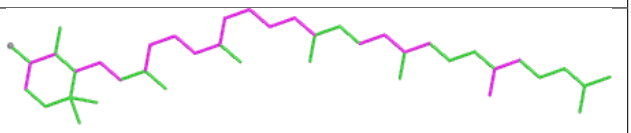
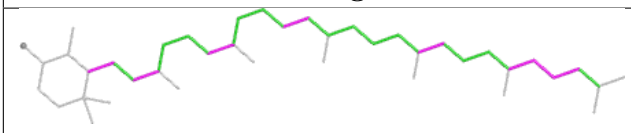
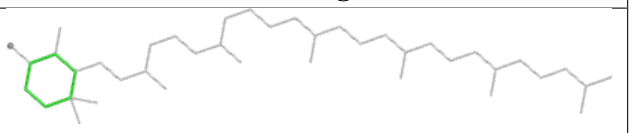
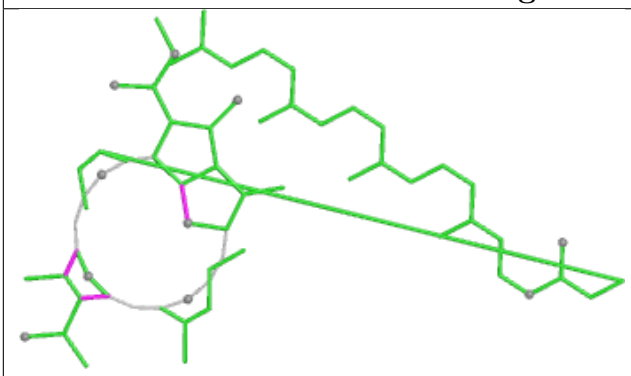
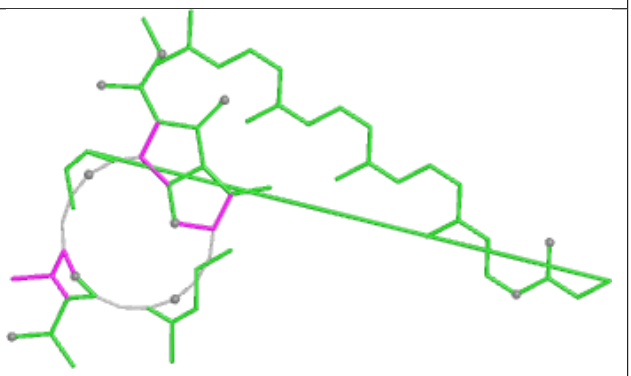
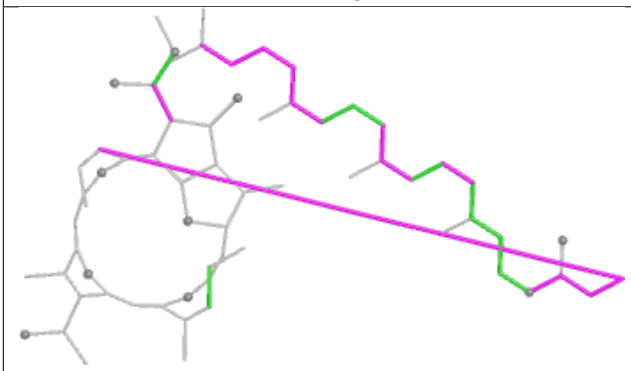
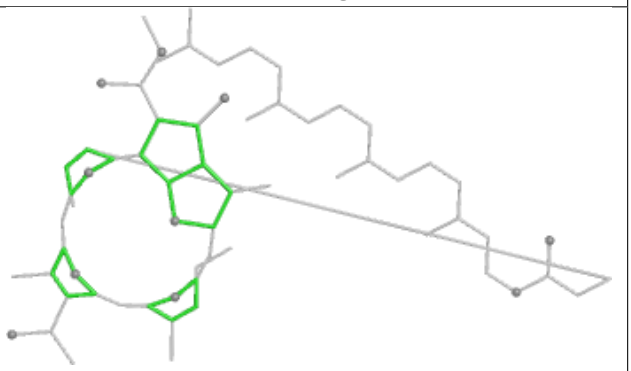
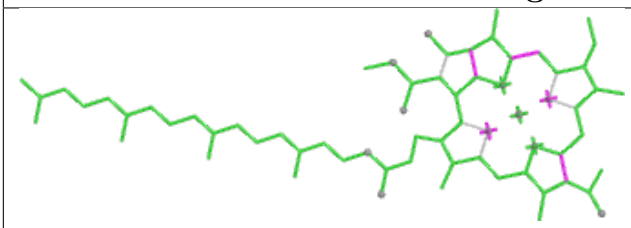
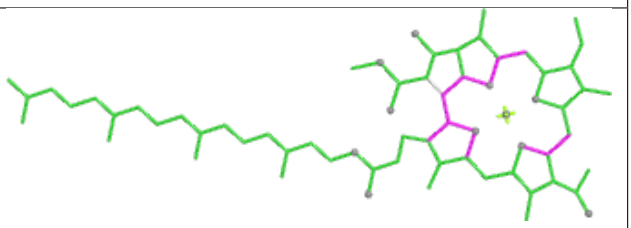
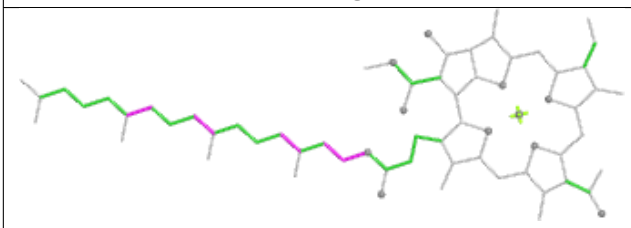
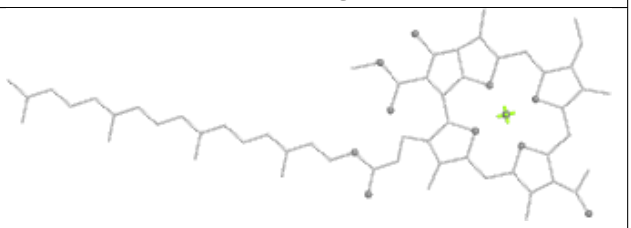
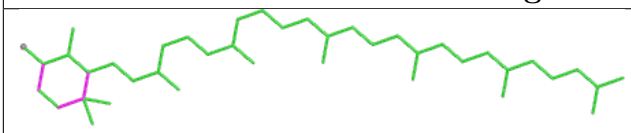
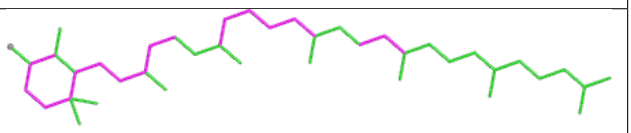
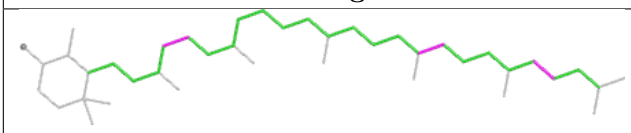
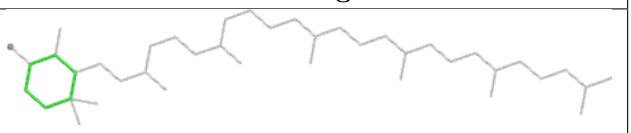
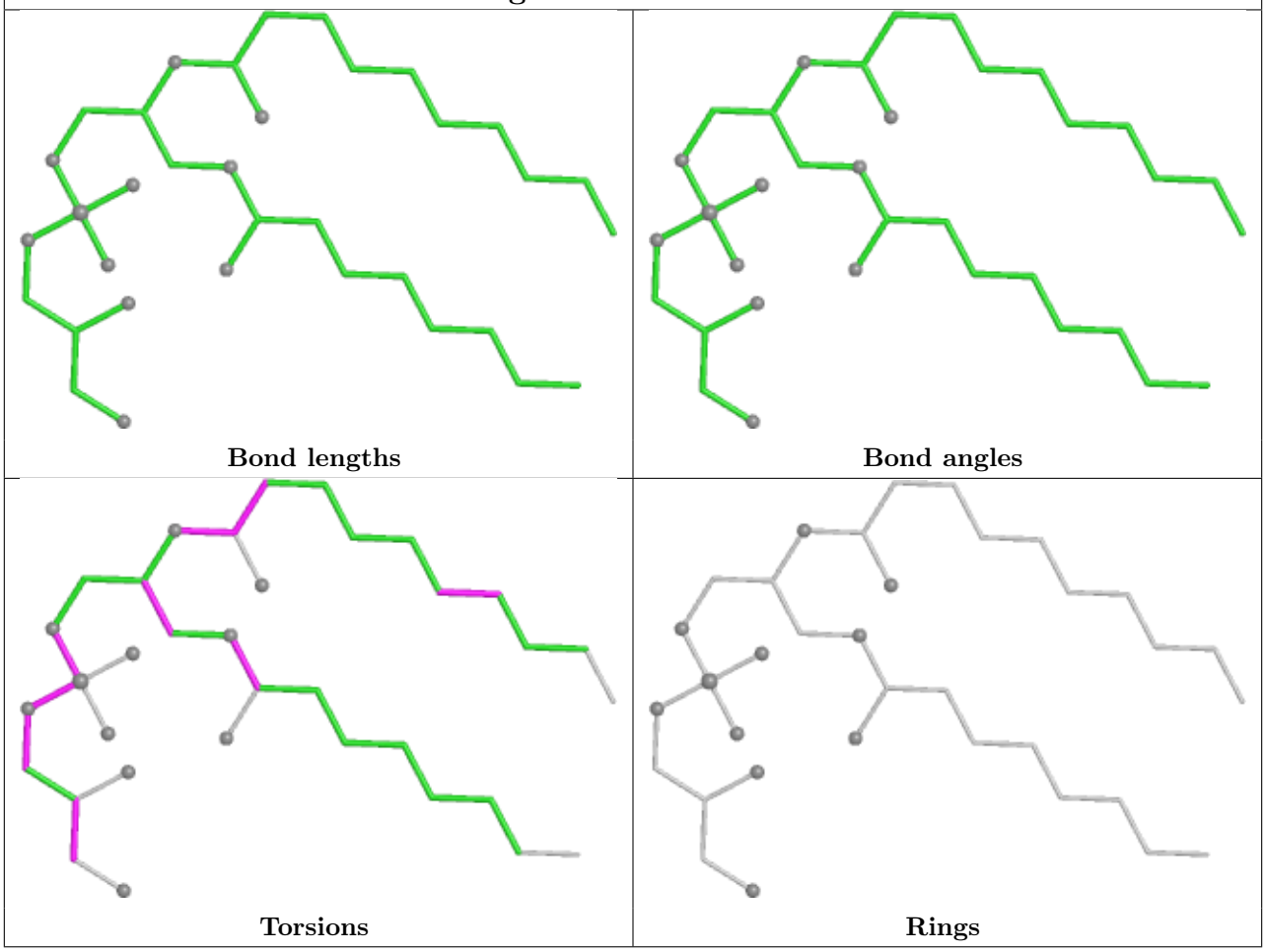
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH M 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL E 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

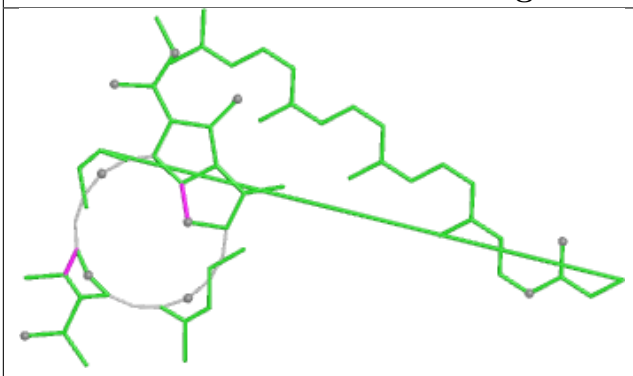
Ligand KGD 7 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGV L 1009

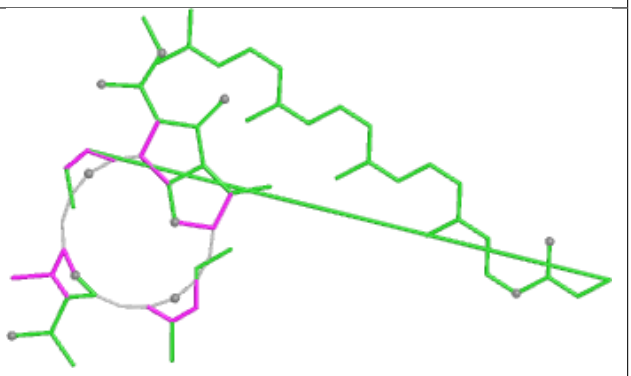


Ligand KGD K 103

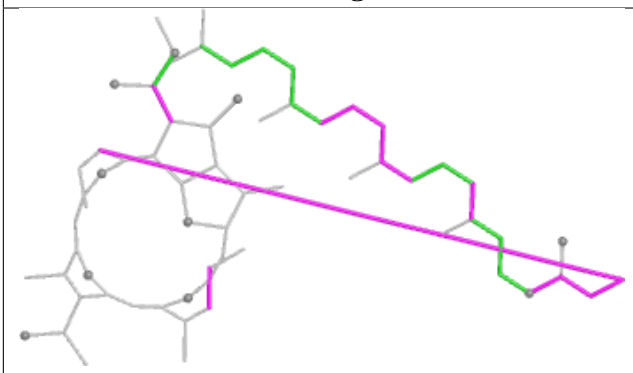
Ligand BPH L 1003



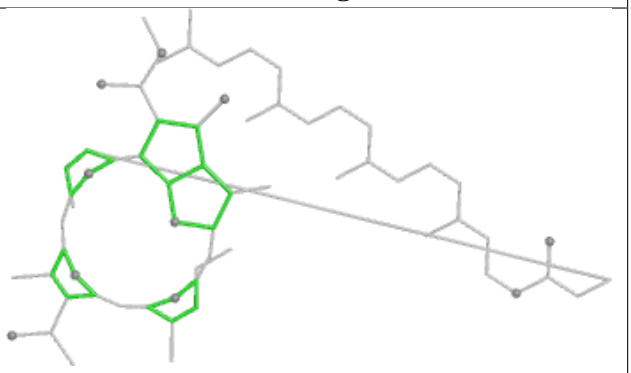
Bond lengths



Bond angles

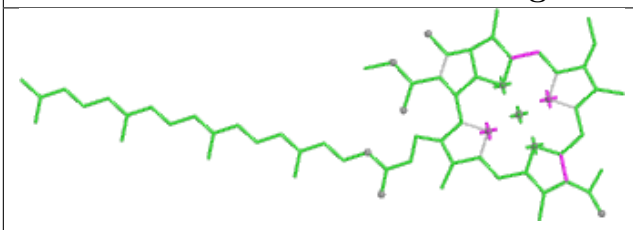


Torsions

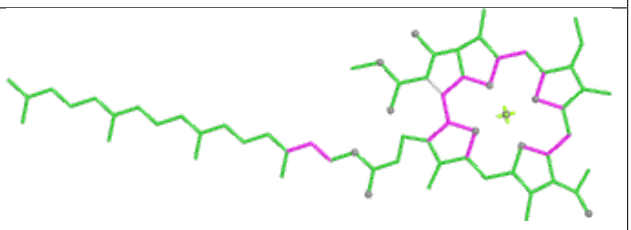


Rings

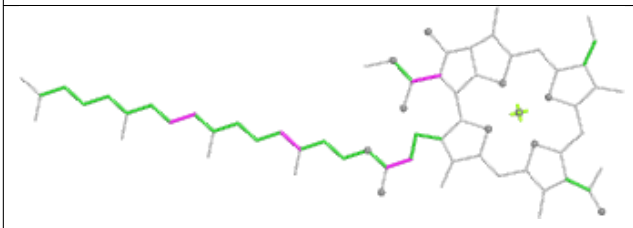
Ligand BCL 5 101



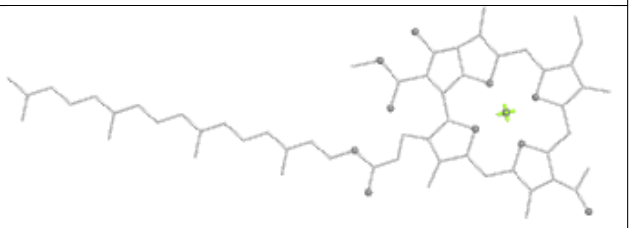
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

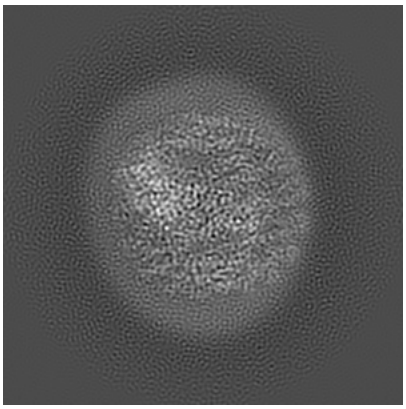
6 Map visualisation (i)

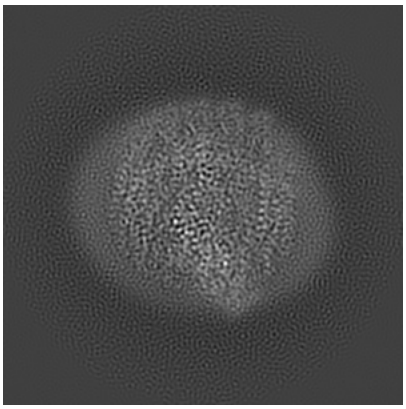
This section contains visualisations of the EMDB entry EMD-35988. These allow visual inspection of the internal detail of the map and identification of artifacts.

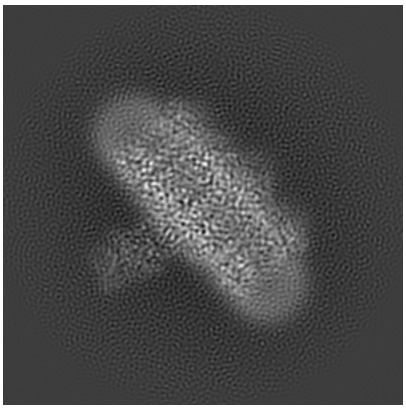
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

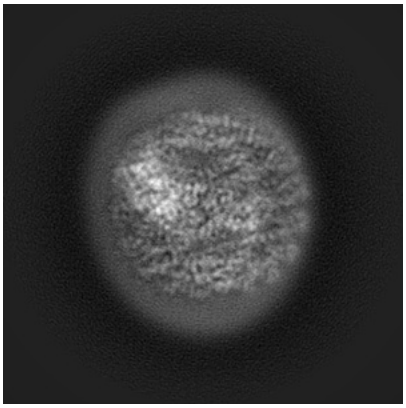
6.1.1 Primary map

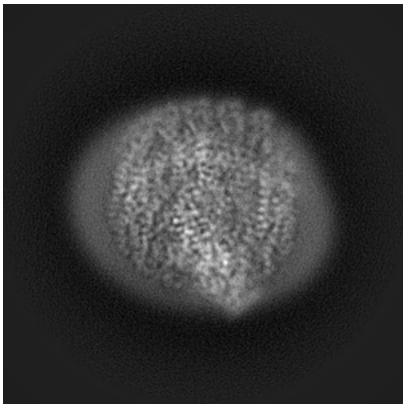

X

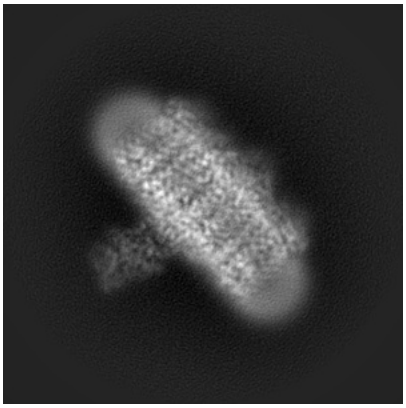

Y


Z

6.1.2 Raw map


X

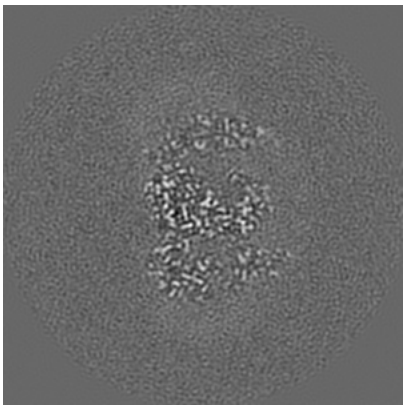

Y

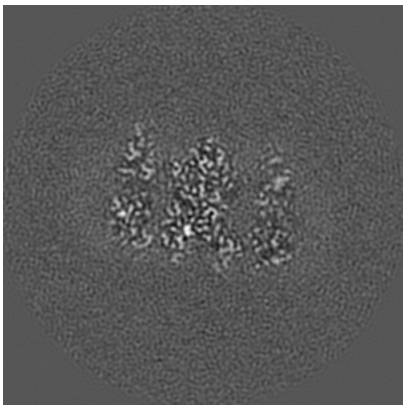

Z

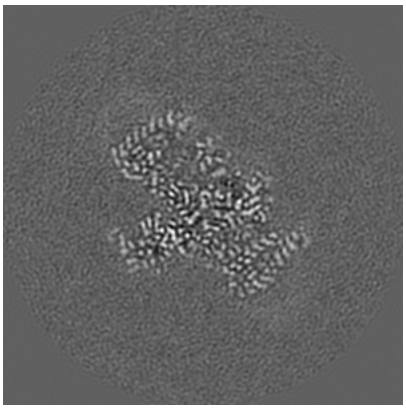
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

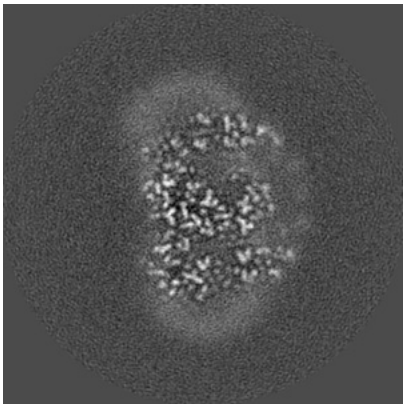
6.2.1 Primary map

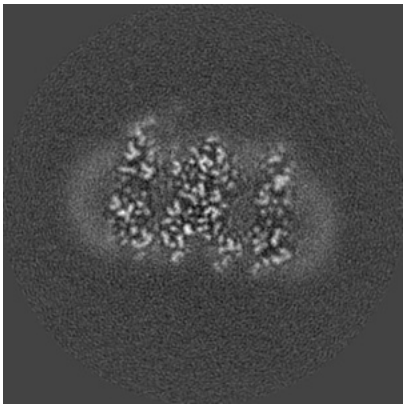

X Index: 132

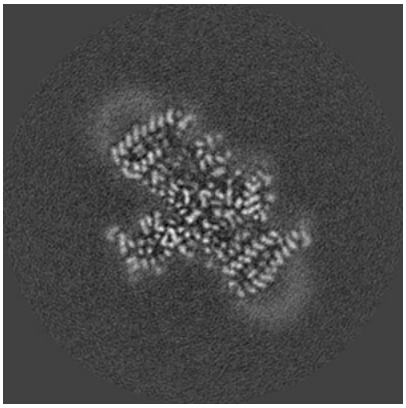

Y Index: 132


Z Index: 132

6.2.2 Raw map


X Index: 132

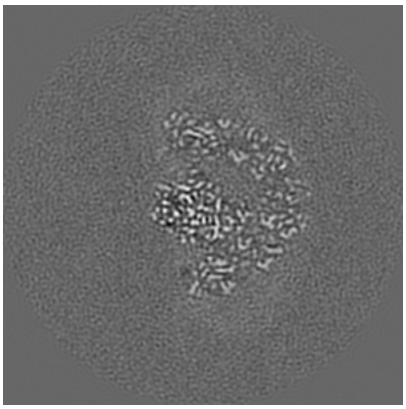

Y Index: 132

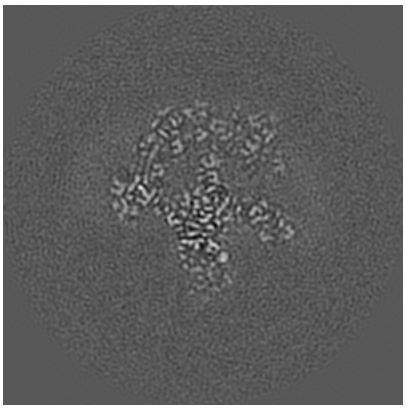

Z Index: 132

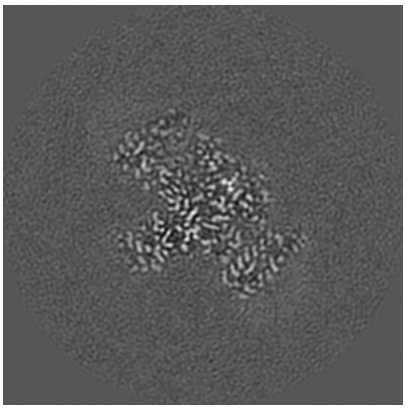
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

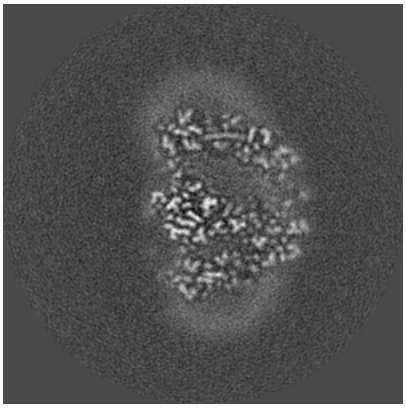
6.3.1 Primary map

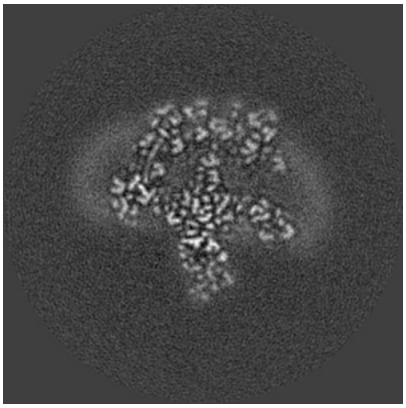

X Index: 114

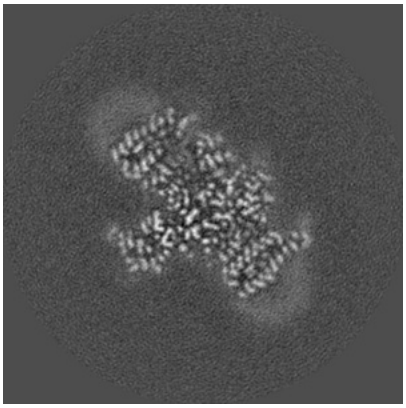

Y Index: 112


Z Index: 130

6.3.2 Raw map


X Index: 121

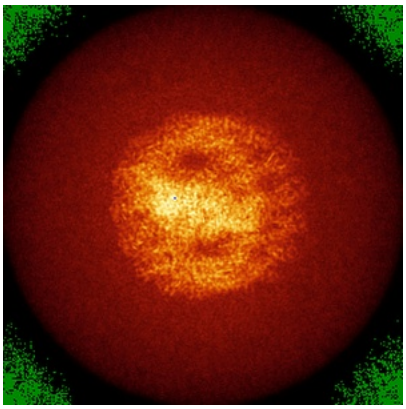

Y Index: 112

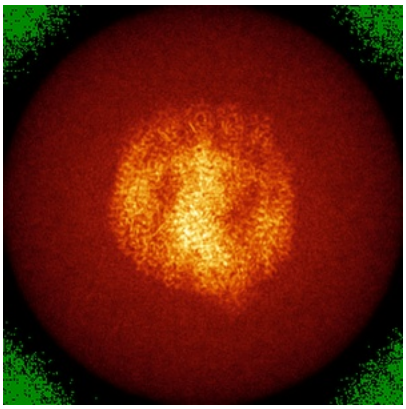

Z Index: 131

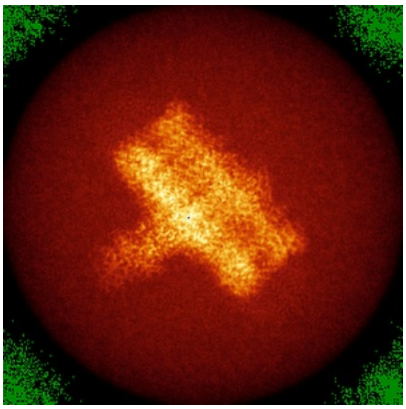
The images above show the largest variance slices of the map in three orthogonal directions.

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

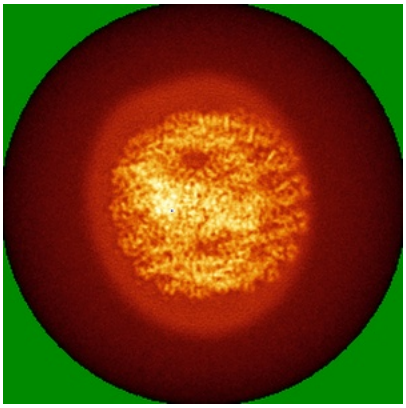
6.4.1 Primary map

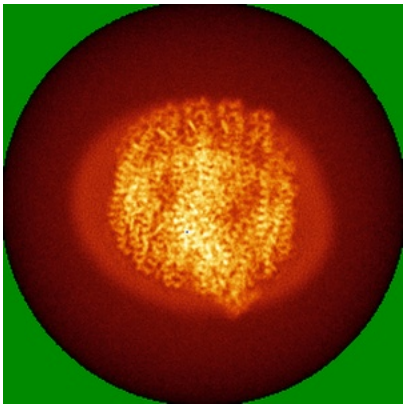

X

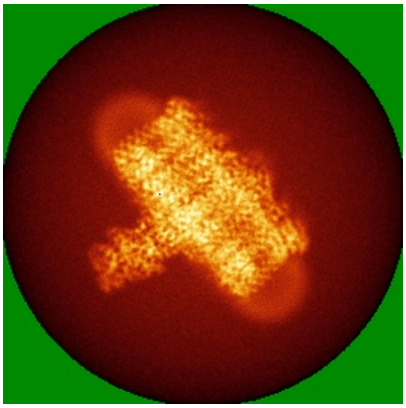

Y


Z

6.4.2 Raw map


X

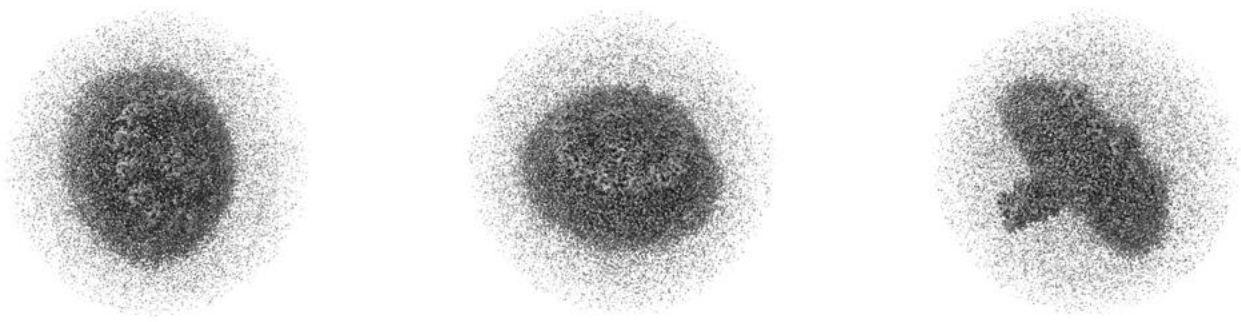

Y


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)

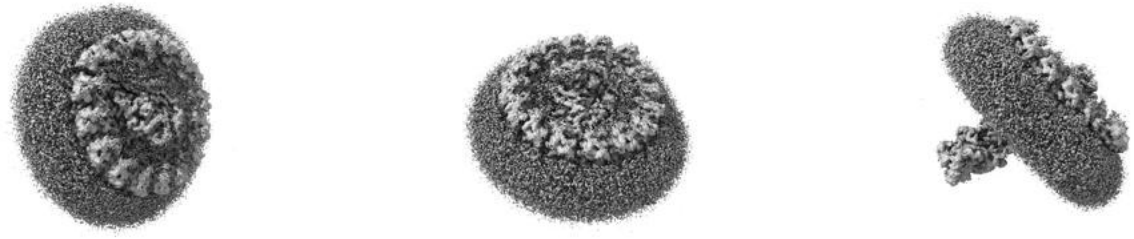
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

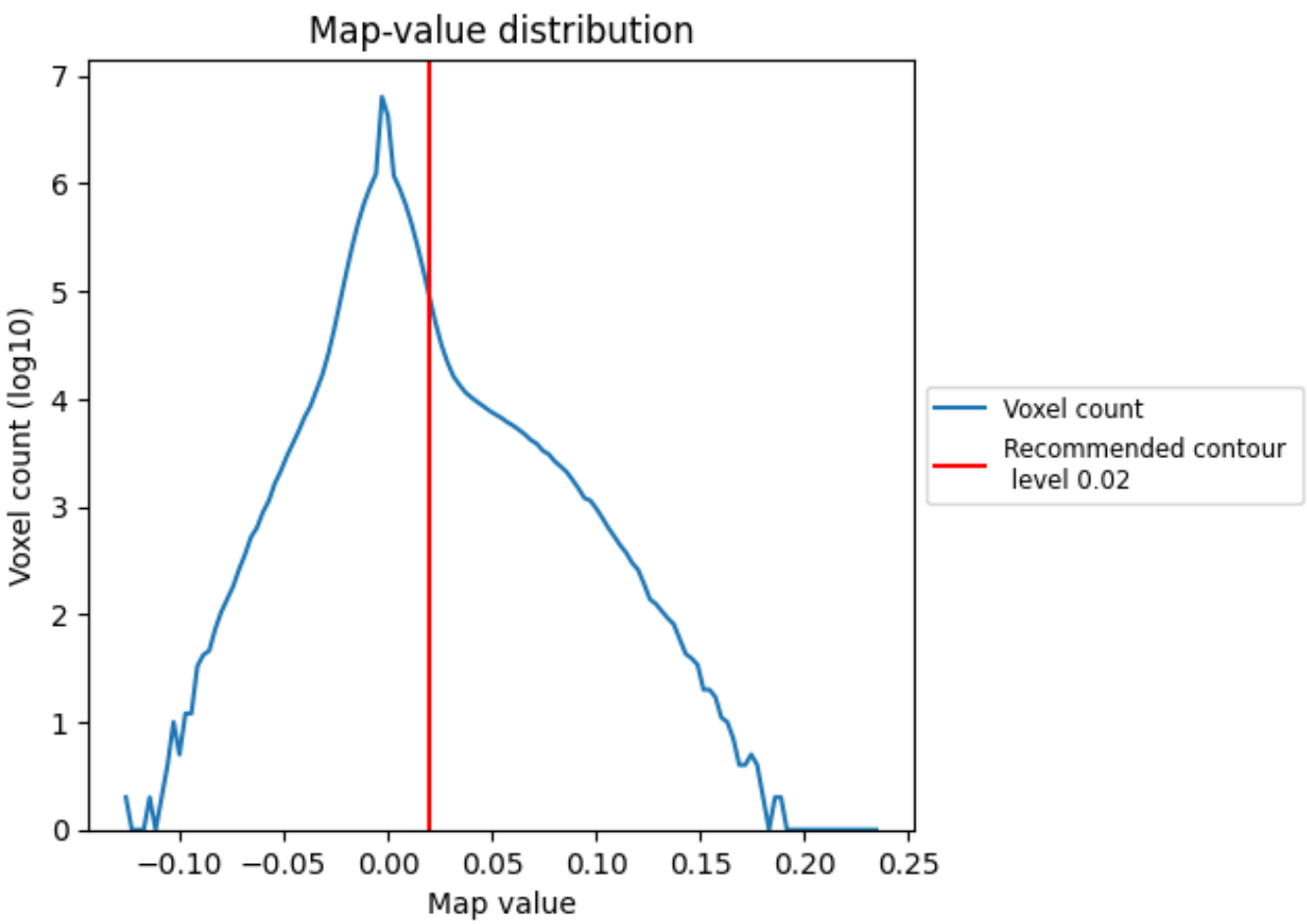
6.6 Mask visualisation (i)

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

7 Map analysis (i)

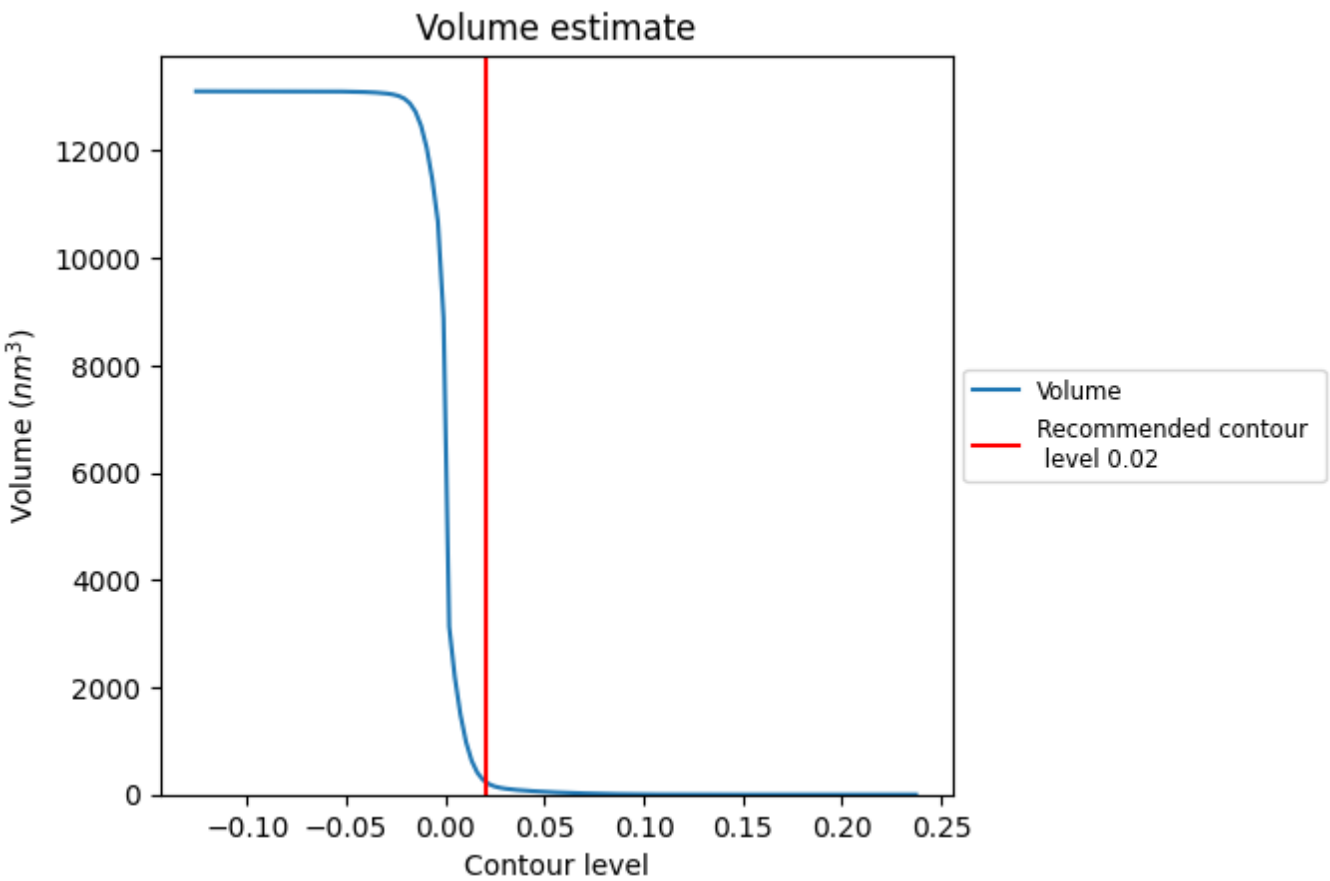
This section contains the results of statistical analysis of the map.

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.

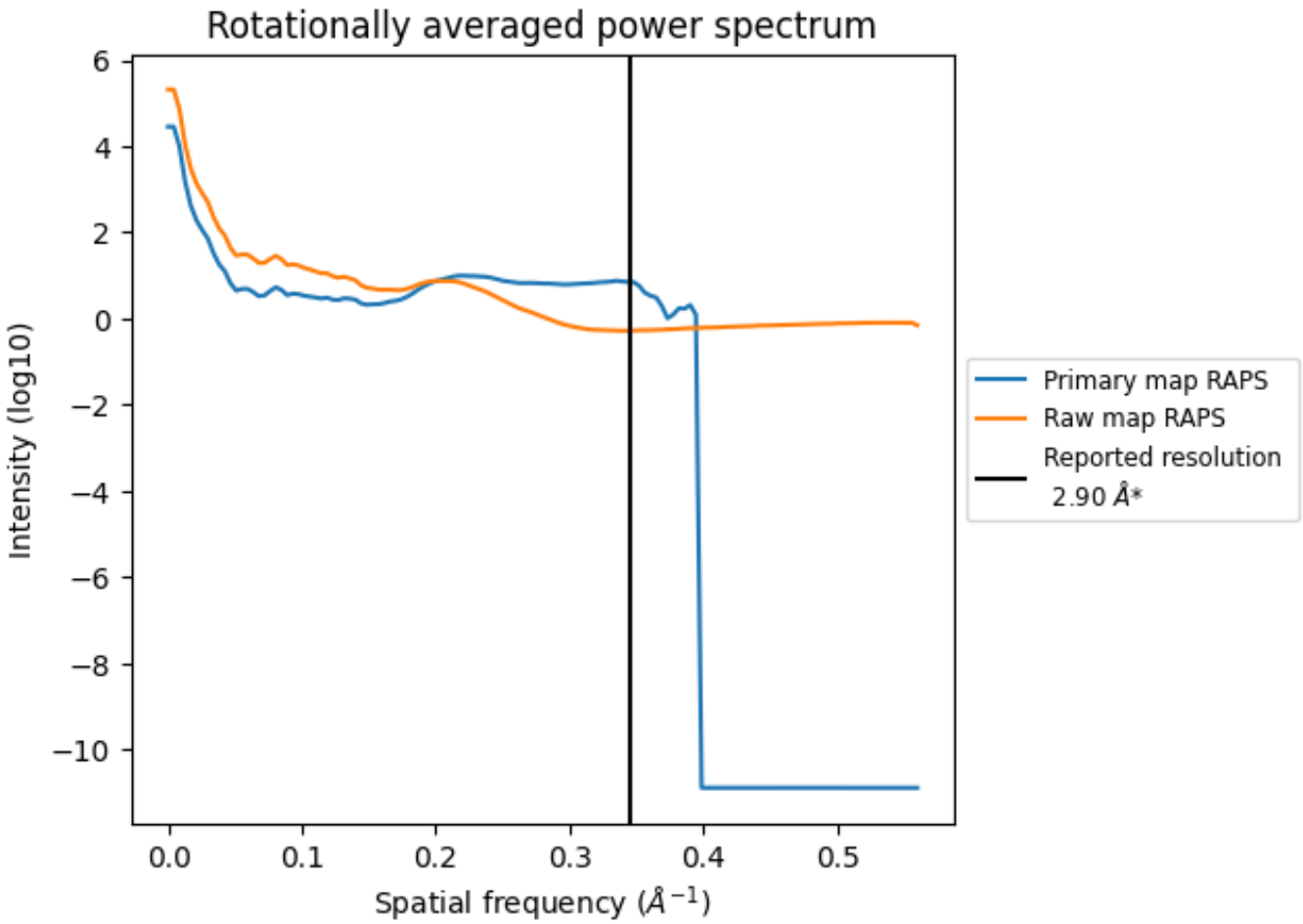
7.2 Volume estimate (i)



The volume at the recommended contour level is 247 nm^3; this corresponds to an approximate mass of 223 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)

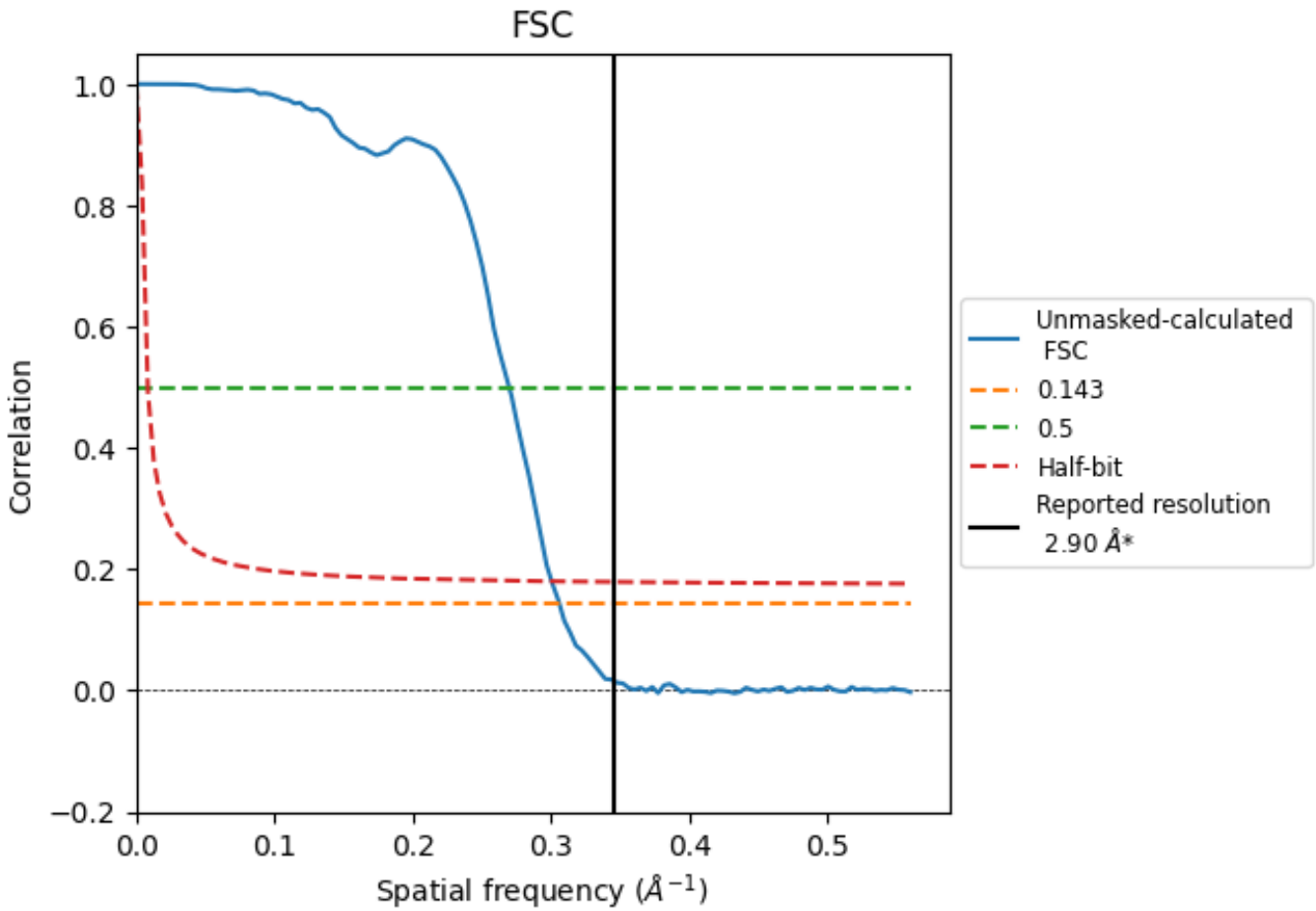


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

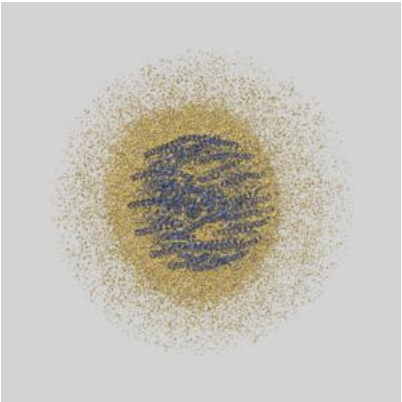
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.27	3.71	3.33

*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 3.27 differs from the reported value 2.9 by more than 10 %

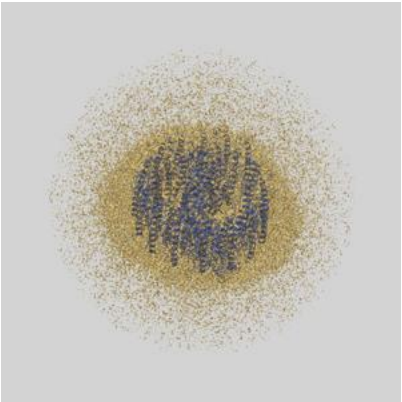
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35988 and PDB model 8J5O. Per-residue inclusion information can be found in section 3 on page 15.

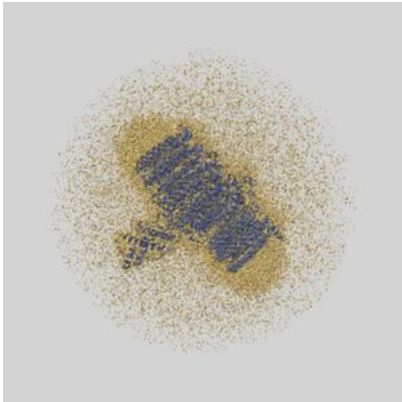
9.1 Map-model overlay (i)



X



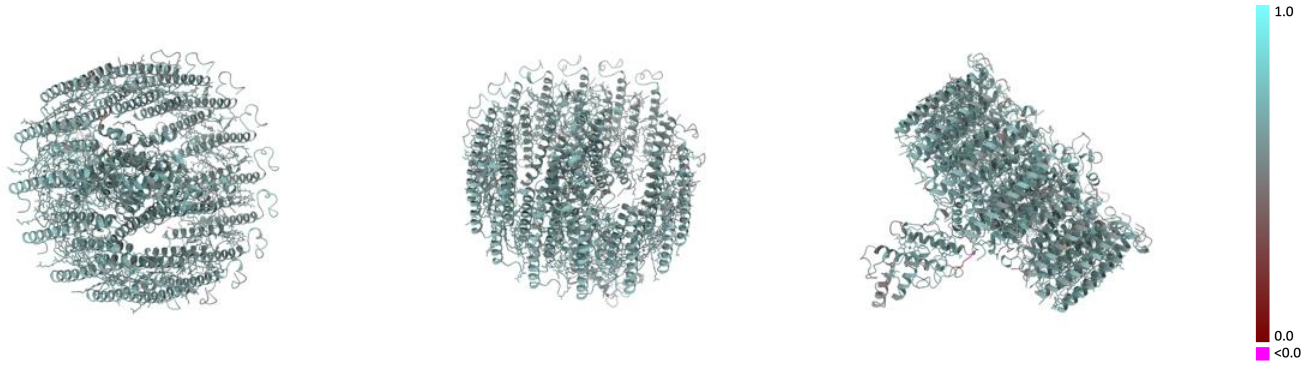
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

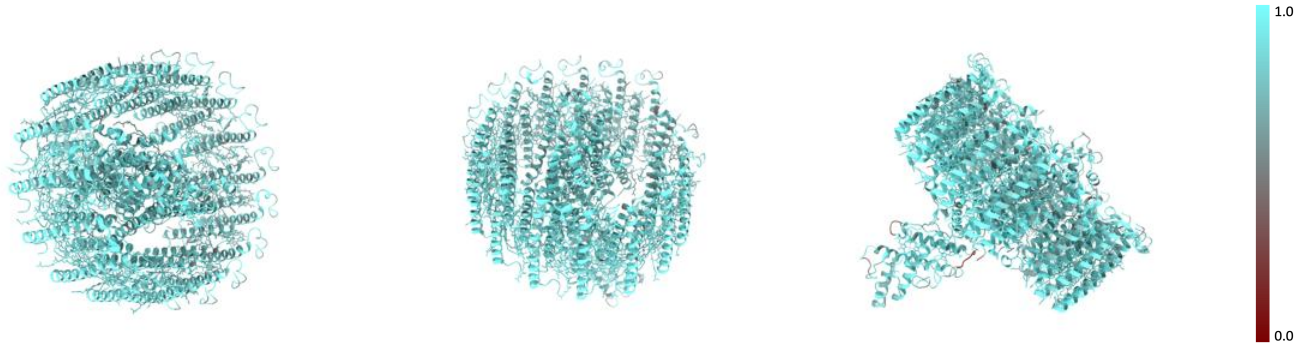
9.2 Q-score mapped to coordinate model (i)



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.

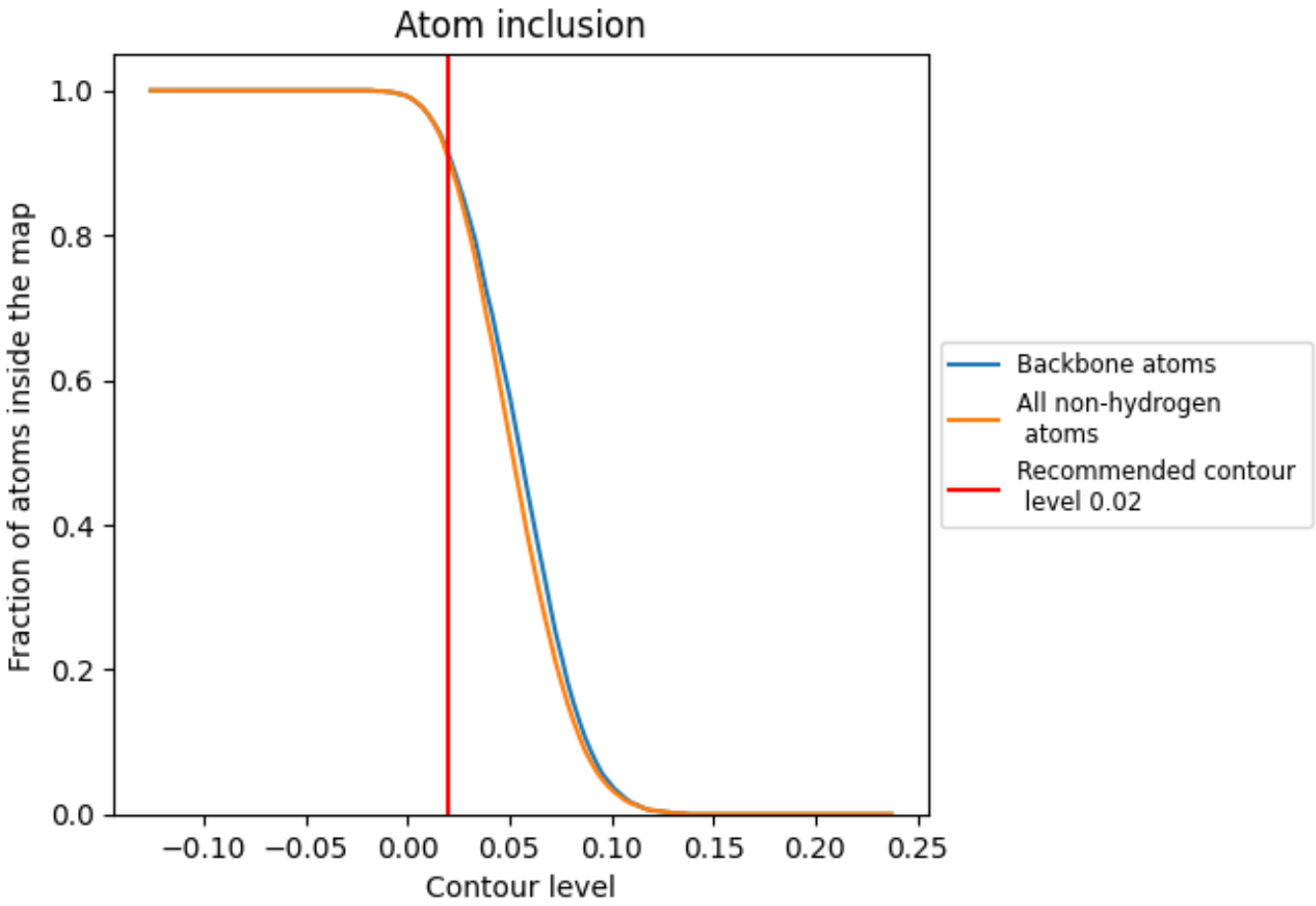
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.6060
0	0.9020	0.6030
1	0.9280	0.6150
2	0.8430	0.5720
3	0.9310	0.6140
4	0.8840	0.5870
5	0.9210	0.6170
6	0.8840	0.5900
7	0.9410	0.6260
8	0.8770	0.5930
9	0.9290	0.6160
A	0.9260	0.6060
B	0.9060	0.6130
C	0.8830	0.5860
D	0.9450	0.6270
E	0.8970	0.6070
F	0.9220	0.6160
G	0.8820	0.5920
H	0.9360	0.6220
I	0.8990	0.5920
J	0.9440	0.6350
K	0.8950	0.6070
L	0.9180	0.6160
M	0.9460	0.6290
N	0.9510	0.6250
O	0.9070	0.6010
P	0.9460	0.6200
Q	0.9000	0.6030
R	0.9260	0.6190
S	0.8980	0.6130
T	0.9210	0.6020
U	0.8830	0.5990
V	0.8740	0.5730
W	0.8510	0.5720
X	0.7460	0.5500

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Chain	Atom inclusion	Q-score
Y	0.9060	0.5970
Z	0.8930	0.5980