wwPDB EM Validation Summary Report

Sep 23, 2026 – 12:20 AM JST

PDB ID	:	8HJV / pdb_00008hjv
EMDB ID	:	EMD-34839
Title	:	Cryo-EM structure of carotenoid-depleted RC-LH complex from Roseiflexus castenholzii at 10,000 lux
Authors	:	Xu, X.; Xin, J.
Deposited on	:	2022-11-23
Resolution	:	3.10 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:

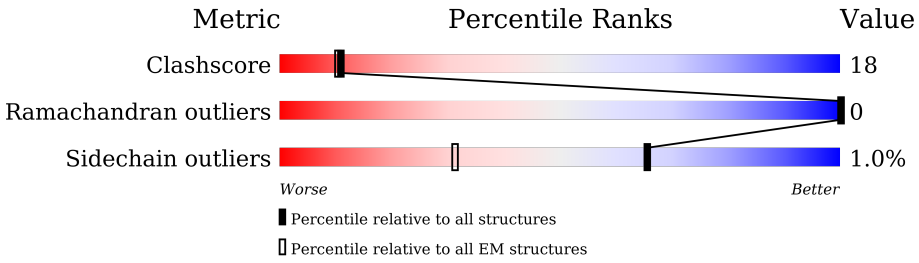
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

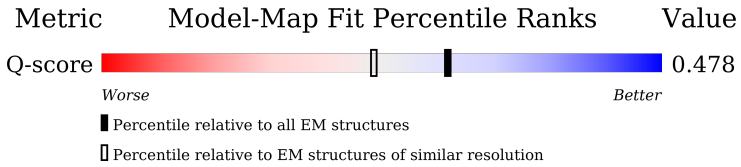
1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	56% 31% • 11%
1	2	55	38% 67% 22% 11%
1	4	55	11% 58% 31% 11%
1	6	55	5% 60% 27% • 11%

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

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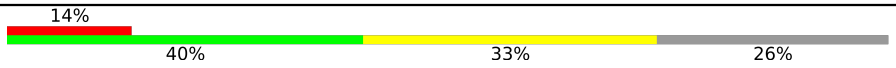
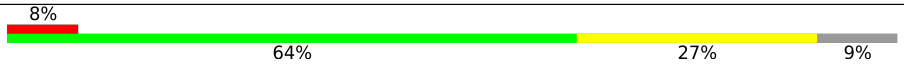
Mol	Chain	Length	Quality of chain
2	V	42	
3	L	315	
4	M	307	
5	Y	39	
6	C	320	
7	Z	63	

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

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 22193 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
1	0	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	2	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	4	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	6	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	8	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	B	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	E	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	G	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	I	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	K	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	O	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	Q	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	S	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	U	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	W	49	Total	C	N	O	S	0	0
			407	275	68	63	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	35	Total	C	N	O	S	0	0
			271	181	45	44	1		
2	3	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	5	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	7	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	D	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	H	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	J	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	N	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	P	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	R	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	V	31	Total	C	N	O	S	0	0
			232	156	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	294	Total	C	N	O	S	0	0
			2337	1565	377	387	8		

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

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

- Molecule 5 is a protein called SUBUNIT Y.

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

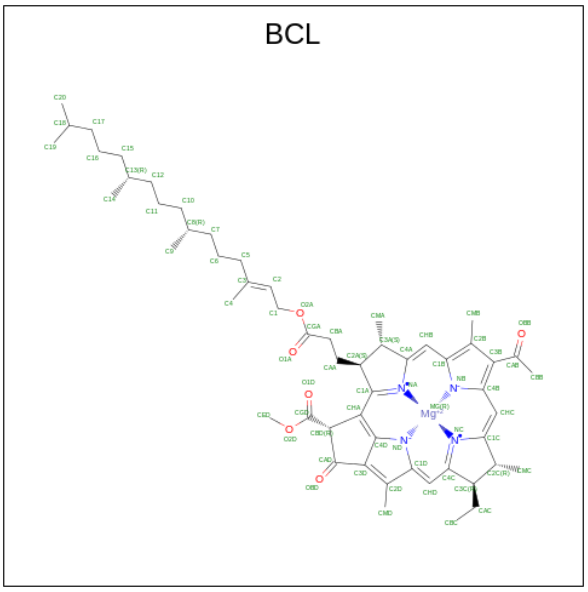
- Molecule 6 is a protein called MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	291	Total	C	N	O	S	0	0
			2216	1407	376	411	22		

- Molecule 7 is a protein called SUBUNIT Z.

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

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
8	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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

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Mol	Chain	Residues	Atoms					AltConf
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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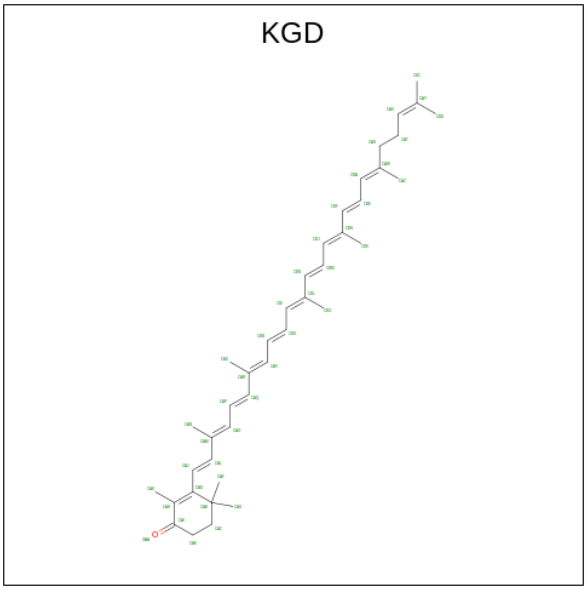
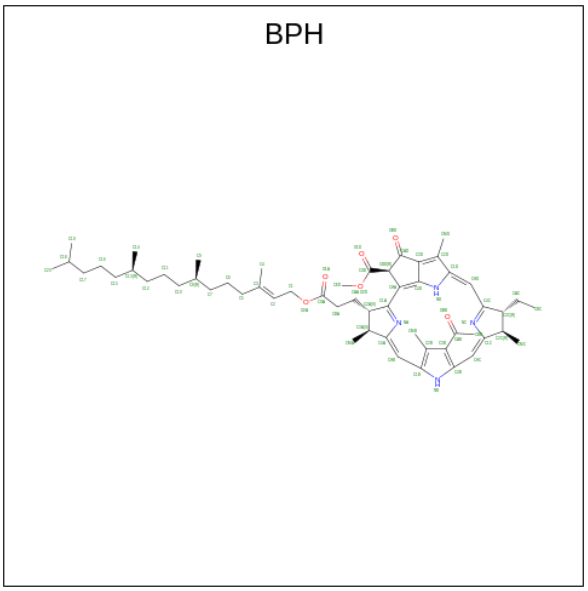
Mol	Chain	Residues	Atoms					AltConf
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is beta,psi-caroten-4-one (CCD ID: KGD) (formula: $C_{40}H_{54}O$).



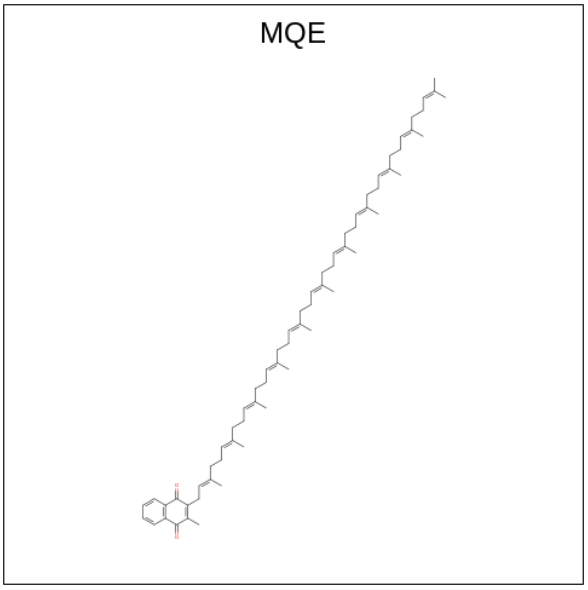
Mol	Chain	Residues	Atoms			AltConf
9	9	1	Total	C	O	0
			41	40	1	
9	D	1	Total	C	O	0
			41	40	1	
9	I	1	Total	C	O	0
			41	40	1	
9	J	1	Total	C	O	0
			41	40	1	
9	N	1	Total	C	O	0
			41	40	1	

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 11 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: $C_{66}H_{96}O_2$).

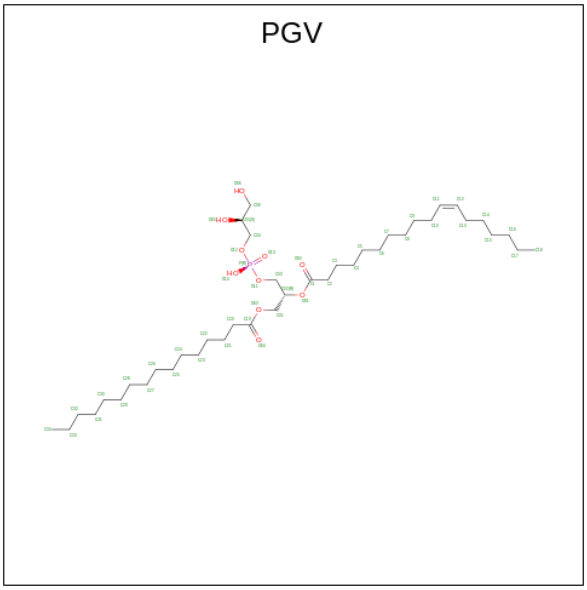


Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total 68	C 66	O 2	0
11	M	1	Total 68	C 66	O 2	0
11	M	1	Total 25	C 23	O 2	0

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

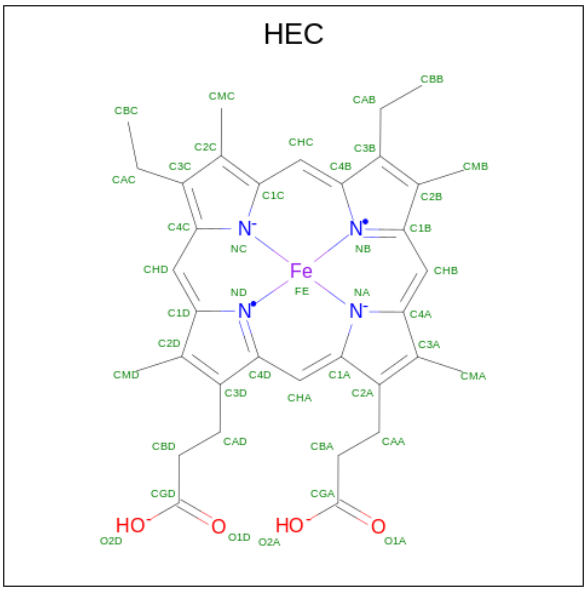
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total 1	Fe 1	0

- Molecule 13 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
13	M	1	Total 45	C 34	O 10	P 1	0
13	M	1	Total 42	C 31	O 10	P 1	0
13	M	1	Total 34	C 23	O 10	P 1	0

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

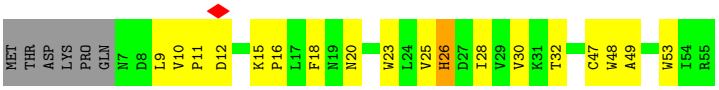
3 Residue-property plots (i)

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:

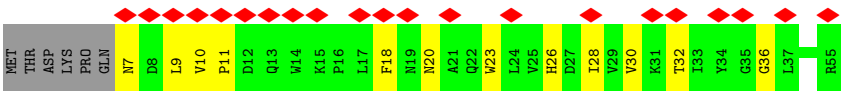




• Molecule 1: Beta subunit of light-harvesting 1

Chain 2:

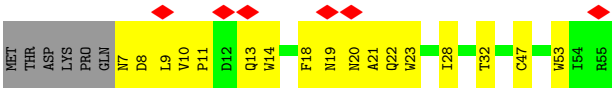




• Molecule 1: Beta subunit of light-harvesting 1

Chain 4:

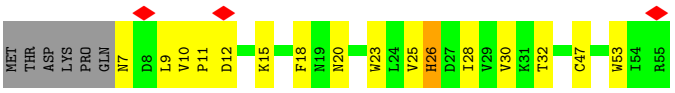




• Molecule 1: Beta subunit of light-harvesting 1

Chain 6:

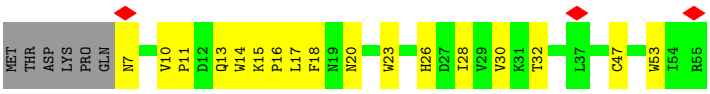




• Molecule 1: Beta subunit of light-harvesting 1

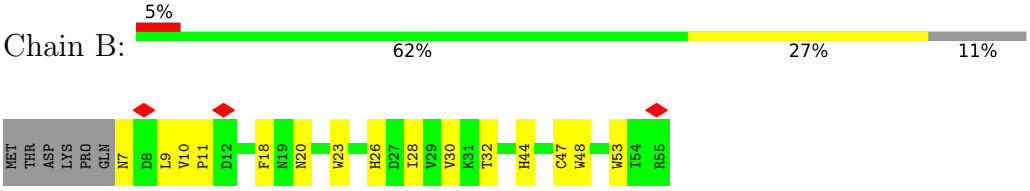
Chain 8:





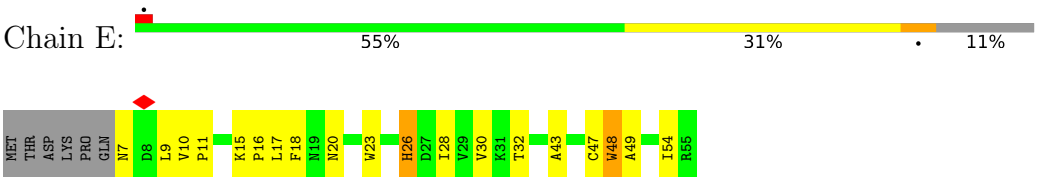
• Molecule 1: Beta subunit of light-harvesting 1

Chain B:



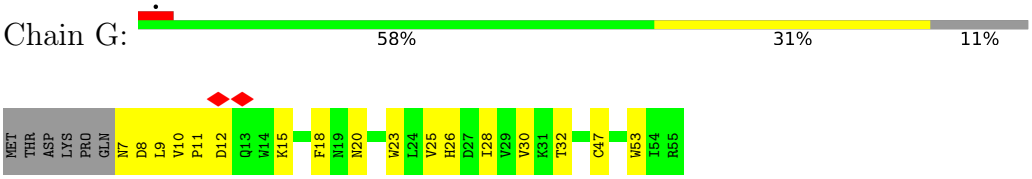
• Molecule 1: Beta subunit of light-harvesting 1

Chain E:



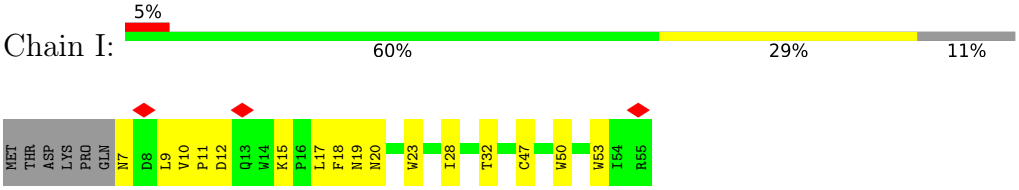
• Molecule 1: Beta subunit of light-harvesting 1

Chain G:



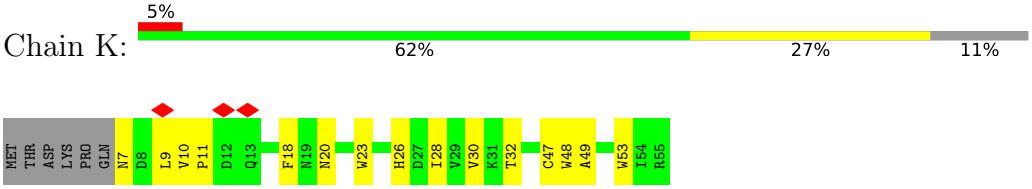
• Molecule 1: Beta subunit of light-harvesting 1

Chain I:



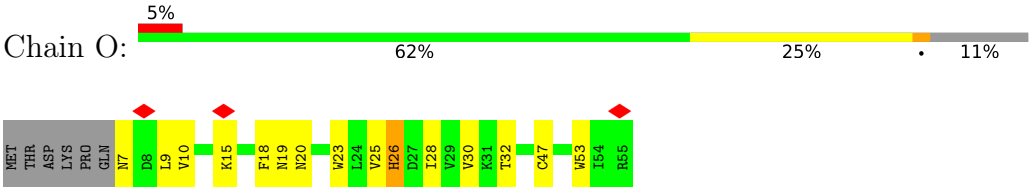
• Molecule 1: Beta subunit of light-harvesting 1

Chain K:



• Molecule 1: Beta subunit of light-harvesting 1

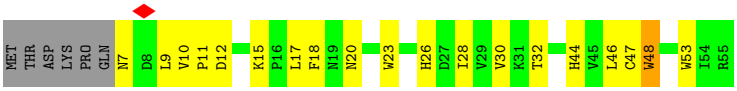
Chain O:



• Molecule 1: Beta subunit of light-harvesting 1

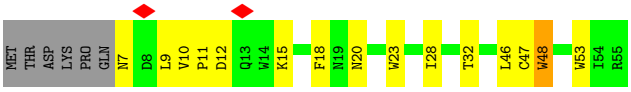
Chain Q:





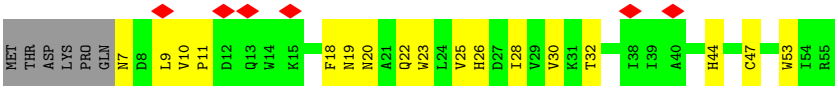
• Molecule 1: Beta subunit of light-harvesting 1





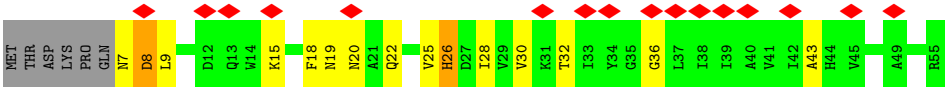
• Molecule 1: Beta subunit of light-harvesting 1





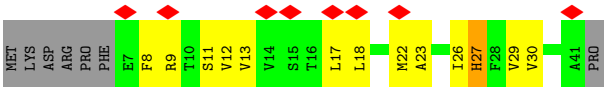
• Molecule 1: Beta subunit of light-harvesting 1





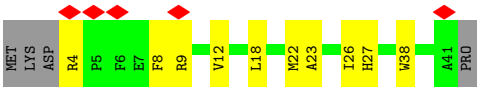
• Molecule 2: Alpha subunit of light-harvesting 1





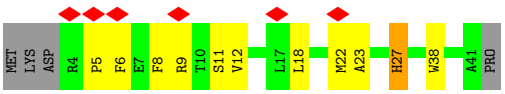
• Molecule 2: Alpha subunit of light-harvesting 1





• Molecule 2: Alpha subunit of light-harvesting 1

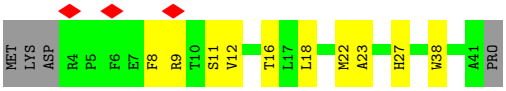




• Molecule 2: Alpha subunit of light-harvesting 1

Chain 7:

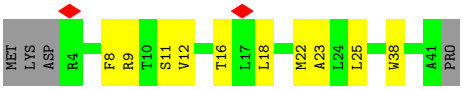




• Molecule 2: Alpha subunit of light-harvesting 1

Chain 9:

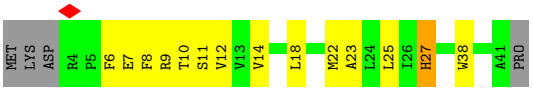




• Molecule 2: Alpha subunit of light-harvesting 1

Chain A:





• Molecule 2: Alpha subunit of light-harvesting 1

Chain D:

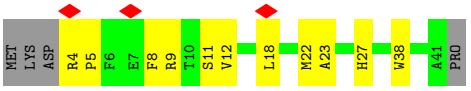




• Molecule 2: Alpha subunit of light-harvesting 1

Chain F:

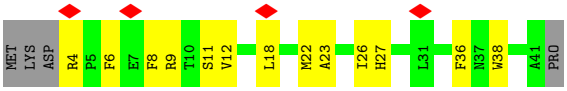




• Molecule 2: Alpha subunit of light-harvesting 1

Chain H:

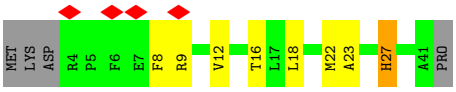




• Molecule 2: Alpha subunit of light-harvesting 1

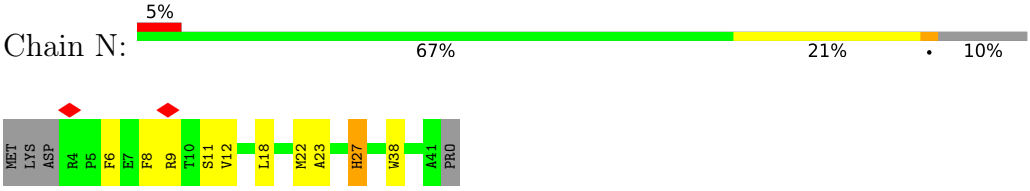
Chain J:





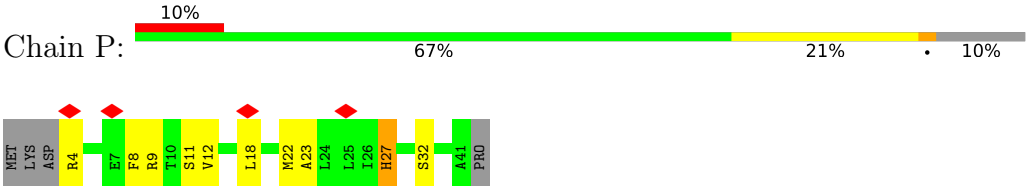
• Molecule 2: Alpha subunit of light-harvesting 1

Chain N:



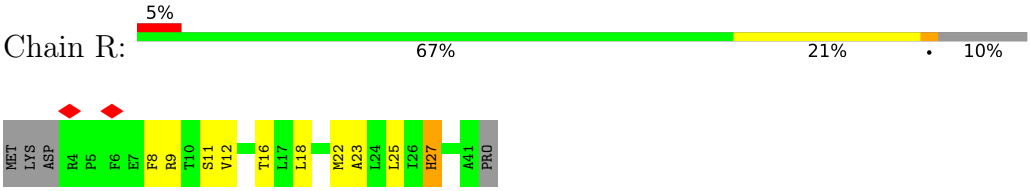
• Molecule 2: Alpha subunit of light-harvesting 1

Chain P:



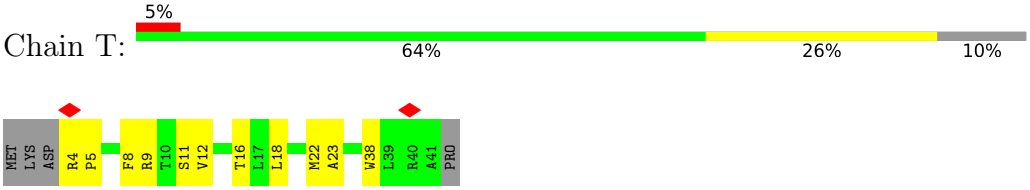
• Molecule 2: Alpha subunit of light-harvesting 1

Chain R:



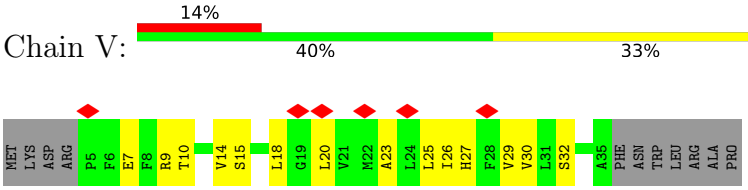
• Molecule 2: Alpha subunit of light-harvesting 1

Chain T:



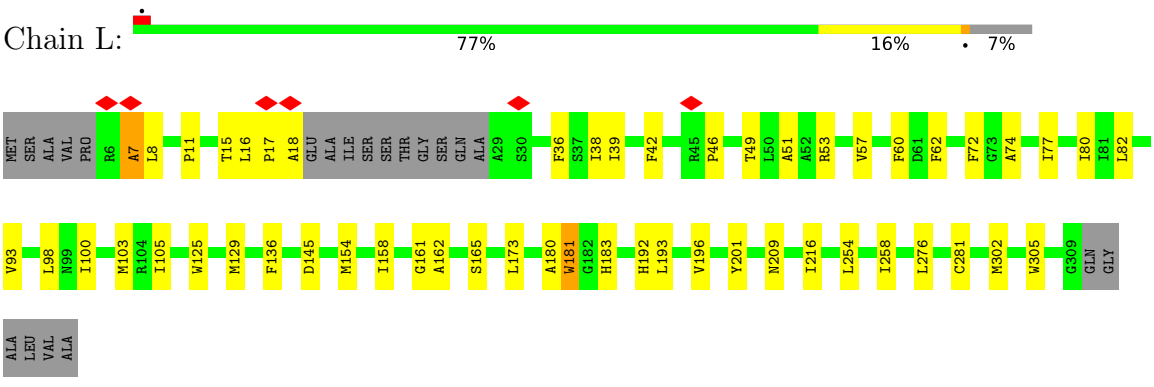
• Molecule 2: Alpha subunit of light-harvesting 1

Chain V:



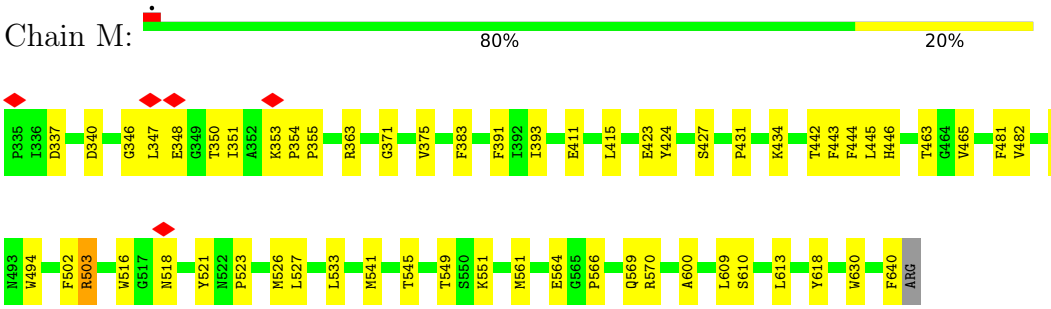
• Molecule 3: Reaction center protein L chain

Chain L:



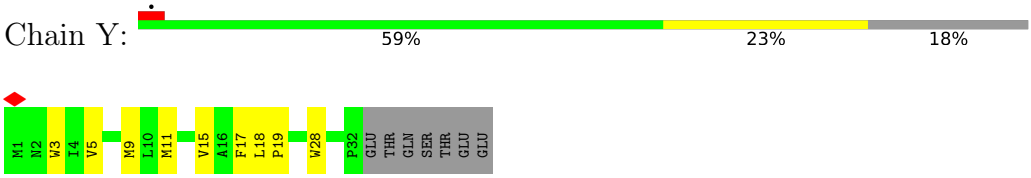
• Molecule 4: Reaction center protein M chain

Chain M:



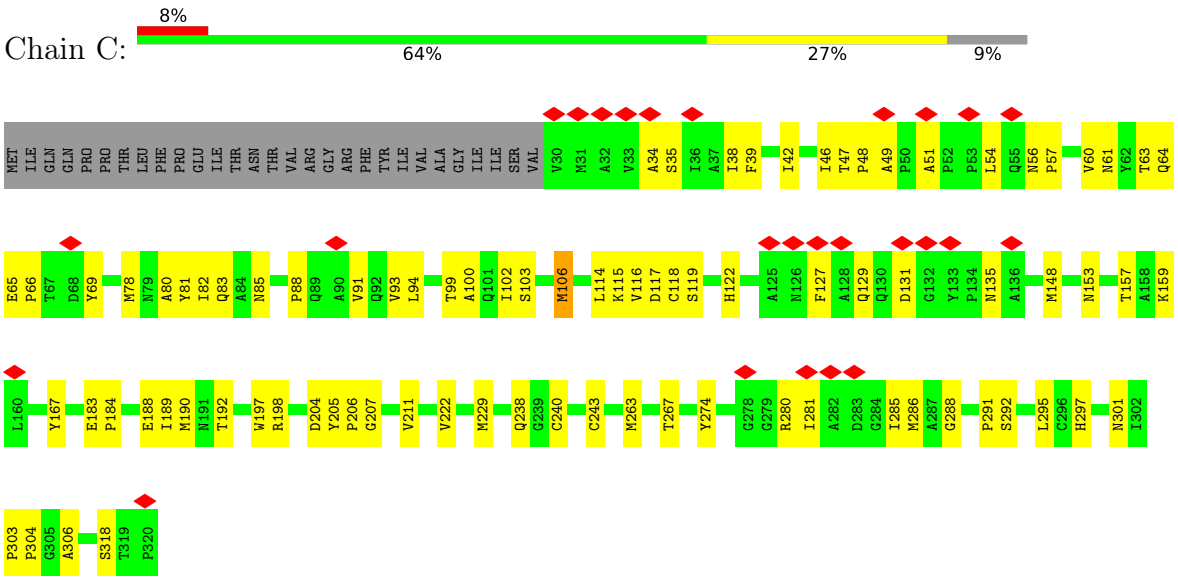
• Molecule 5: SUBUNIT Y

Chain Y:



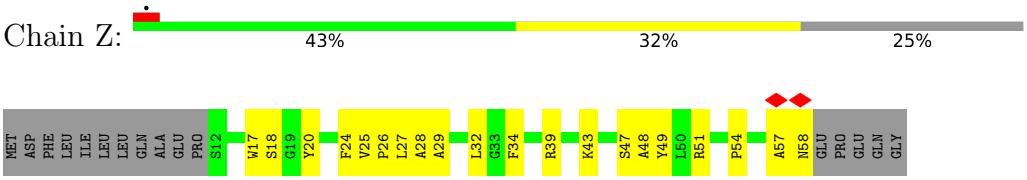
• Molecule 6: MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN

Chain C:



• Molecule 7: SUBUNIT Z

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT,

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Property	Value	Source
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF,

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Property	Value	Source
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	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: FE, HEC, MQE, PGV, BCL, KGD, BPH

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	0.69	2/423 (0.5%)	0.58	0/585
1	2	0.36	0/423	0.45	0/585
1	4	0.40	0/423	0.50	0/585
1	6	0.54	1/423 (0.2%)	0.64	0/585
1	8	0.53	0/423	0.64	0/585
1	B	0.60	1/423 (0.2%)	0.65	1/585 (0.2%)
1	E	0.65	2/423 (0.5%)	0.73	2/585 (0.3%)
1	G	0.46	0/423	0.65	1/585 (0.2%)
1	I	0.58	0/423	0.61	0/585
1	K	0.46	0/423	0.57	0/585
1	O	0.58	1/423 (0.2%)	0.61	0/585
1	Q	0.76	2/423 (0.5%)	0.69	1/585 (0.2%)
1	S	0.52	0/423	0.64	1/585 (0.2%)
1	U	0.59	1/423 (0.2%)	0.51	0/585
1	W	0.77	3/423 (0.7%)	0.69	1/585 (0.2%)
2	1	0.72	2/276 (0.7%)	0.59	0/375
2	3	0.62	1/307 (0.3%)	0.60	2/417 (0.5%)
2	5	0.55	1/307 (0.3%)	0.57	0/417
2	7	0.41	0/307	0.52	0/417
2	9	0.41	0/307	0.50	0/417
2	A	0.58	1/307 (0.3%)	0.54	0/417
2	D	0.49	1/307 (0.3%)	0.47	0/417
2	F	0.46	0/307	0.54	0/417
2	H	0.47	1/307 (0.3%)	0.52	0/417
2	J	0.57	1/307 (0.3%)	0.46	0/417
2	N	0.56	1/307 (0.3%)	0.44	0/417
2	P	0.60	1/307 (0.3%)	0.53	0/417
2	R	0.56	1/307 (0.3%)	0.48	0/417
2	T	0.42	0/307	0.86	0/417
2	V	0.34	0/236	0.53	0/320
3	L	0.39	0/2421	0.59	3/3304 (0.1%)
4	M	0.37	0/2597	0.55	3/3566 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	Y	0.29	0/268	0.46	0/370
6	C	0.38	0/2276	0.57	2/3107 (0.1%)
7	Z	0.27	0/374	0.52	0/513
All	All	0.49	24/18784 (0.1%)	0.58	17/25751 (0.1%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	26	HIS	C-N	-8.89	1.22	1.33
1	U	44	HIS	C-N	8.49	1.44	1.33
1	0	25	VAL	C-N	8.43	1.45	1.33
2	3	26	ILE	C-N	-8.37	1.23	1.33
2	1	27	HIS	C-N	8.06	1.44	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	48	TRP	N-CA-C	-8.33	100.96	112.12
6	C	51	ALA	N-CA-C	8.16	119.92	109.72
1	S	48	TRP	N-CA-C	-7.12	103.45	112.93
1	B	48	TRP	N-CA-C	-6.90	104.50	113.12
1	W	8	ASP	N-CA-C	6.83	120.17	110.68

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	16	0
1	2	407	0	407	9	0
1	4	407	0	407	26	0
1	6	407	0	407	19	0
1	8	407	0	407	13	0
1	B	407	0	407	14	0
1	E	407	0	407	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	407	0	407	23	0
1	I	407	0	407	19	0
1	K	407	0	407	16	0
1	O	407	0	407	17	0
1	Q	407	0	407	19	0
1	S	407	0	407	17	0
1	U	407	0	407	21	0
1	W	407	0	407	14	0
2	1	271	0	287	12	0
2	3	300	0	316	9	0
2	5	300	0	316	11	0
2	7	300	0	316	11	0
2	9	300	0	316	13	0
2	A	300	0	316	23	0
2	D	300	0	316	19	0
2	F	300	0	316	12	0
2	H	300	0	316	19	0
2	J	300	0	316	15	0
2	N	300	0	316	13	0
2	P	300	0	316	10	0
2	R	300	0	316	18	0
2	T	300	0	316	12	0
2	V	232	0	250	19	0
3	L	2337	0	2296	50	0
4	M	2488	0	2373	99	0
5	Y	259	0	272	8	0
6	C	2216	0	2163	88	0
7	Z	362	0	366	41	0
8	0	132	0	148	12	0
8	1	66	0	74	3	0
8	2	132	0	144	6	0
8	3	66	0	74	4	0
8	4	132	0	148	15	0
8	5	66	0	74	4	0
8	6	132	0	148	17	0
8	7	66	0	74	5	0
8	8	132	0	148	12	0
8	9	66	0	74	7	0
8	A	66	0	74	5	0
8	B	132	0	148	16	0
8	D	66	0	74	7	0
8	E	132	0	148	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	66	0	74	4	0
8	G	132	0	148	20	0
8	H	66	0	74	3	0
8	I	132	0	148	16	0
8	J	66	0	74	9	0
8	K	132	0	148	16	0
8	L	66	0	74	11	0
8	M	132	0	148	9	0
8	N	66	0	74	4	0
8	O	132	0	148	15	0
8	P	66	0	74	3	0
8	Q	132	0	148	16	0
8	R	66	0	74	8	0
8	S	132	0	148	14	0
8	T	66	0	74	10	0
8	U	132	0	148	14	0
8	V	66	0	74	10	0
8	W	132	0	144	14	0
9	9	41	0	0	3	0
9	D	41	0	0	4	0
9	I	41	0	0	2	0
9	J	41	0	0	1	0
9	N	41	0	0	1	0
10	L	195	0	228	21	0
11	L	68	0	0	1	0
11	M	93	0	0	11	0
12	M	1	0	0	0	0
13	M	121	0	153	17	0
14	C	172	0	122	17	0
All	All	22193	0	22267	818	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 18.

The worst 5 of 818 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)
6:C:240:CYS:SG	14:C:503:HEC:HAB	1.33	1.68
7:Z:39:ARG:HH12	7:Z:43:LYS:CG	1.14	1.60
7:Z:39:ARG:NH1	7:Z:43:LYS:HG3	1.20	1.46
6:C:240:CYS:SG	14:C:503:HEC:CAB	2.19	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:243:CYS:SG	14:C:503:HEC:HAC	1.74	1.28

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%)	45 (96%)	2 (4%)	0	100	100
1	2	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	4	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	6	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	8	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	B	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	E	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	G	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	I	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	K	47/55 (86%)	43 (92%)	4 (8%)	0	100	100
1	O	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
1	Q	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	S	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	U	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
1	W	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
2	1	33/42 (79%)	31 (94%)	2 (6%)	0	100	100
2	3	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	5	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	7	36/42 (86%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	9	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	A	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	D	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	F	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	H	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	J	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	N	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	P	36/42 (86%)	34 (94%)	2 (6%)	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	29/42 (69%)	26 (90%)	3 (10%)	0	100	100
3	L	290/315 (92%)	282 (97%)	8 (3%)	0	100	100
4	M	304/307 (99%)	291 (96%)	13 (4%)	0	100	100
5	Y	30/39 (77%)	30 (100%)	0	0	100	100
6	C	289/320 (90%)	260 (90%)	29 (10%)	0	100	100
7	Z	45/63 (71%)	42 (93%)	3 (7%)	0	100	100
All	All	2193/2499 (88%)	2068 (94%)	125 (6%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	29 (97%)	1 (3%)	33	63
2	3	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	5	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	7	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	9	33/37 (89%)	33 (100%)	0	100	100
2	A	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	D	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	F	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	H	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	J	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	N	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	P	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	R	33/37 (89%)	32 (97%)	1 (3%)	36	65
2	T	33/37 (89%)	33 (100%)	0	100	100
2	V	27/37 (73%)	27 (100%)	0	100	100
3	L	239/253 (94%)	236 (99%)	3 (1%)	61	77
4	M	244/245 (100%)	242 (99%)	2 (1%)	73	81
5	Y	29/36 (81%)	29 (100%)	0	100	100
6	C	236/262 (90%)	234 (99%)	2 (1%)	73	81
7	Z	36/50 (72%)	36 (100%)	0	100	100
All	All	1915/2136 (90%)	1896 (99%)	19 (1%)	65	79

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	27	HIS
6	C	106	MET
6	C	263	MET
2	R	27	HIS
2	J	27	HIS

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

Mol	Chain	Res	Type
4	M	525	HIS
2	V	27	HIS
7	Z	58	ASN
5	Y	31	ASN
6	C	83	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 1 is monoatomic - leaving 66 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	$\#\|Z\|>2$
13	PGV	M	1008	-	33,33,50	1.16	3 (9%)	36,39,56	1.02	2 (5%)
13	PGV	M	1007	-	41,41,50	0.80	1 (2%)	44,47,56	1.04	3 (6%)
8	BCL	T	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.24	32 (38%)
8	BCL	I	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.16	28 (33%)
8	BCL	M	1005	-	69,74,74	1.80	17 (24%)	83,115,115	2.20	28 (33%)
8	BCL	4	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.16	28 (33%)
8	BCL	0	101	1	69,74,74	1.80	15 (21%)	83,115,115	2.14	28 (33%)
14	HEC	C	503	6	50,50,50	1.67	8 (16%)	68,82,82	2.17	18 (26%)
8	BCL	L	401	3	69,74,74	1.82	17 (24%)	83,115,115	2.26	31 (37%)
9	KGD	N	102	-	41,41,41	0.92	1 (2%)	49,53,53	2.48	14 (28%)
10	BPH	L	405	-	59,70,70	1.61	9 (15%)	61,101,101	1.47	8 (13%)
8	BCL	S	102	1	69,74,74	1.81	15 (21%)	83,115,115	2.15	28 (33%)
8	BCL	H	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.18	31 (37%)
8	BCL	2	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.14	27 (32%)
8	BCL	I	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.14	28 (33%)
8	BCL	4	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.14	27 (32%)
8	BCL	0	102	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)
9	KGD	D	102	-	41,41,41	1.26	5 (12%)	49,53,53	2.47	16 (32%)
8	BCL	9	102	2	69,74,74	1.85	16 (23%)	83,115,115	2.18	31 (37%)
8	BCL	B	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)
8	BCL	W	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.14	28 (33%)
10	BPH	L	402	-	59,70,70	1.60	9 (15%)	61,101,101	1.62	13 (21%)
8	BCL	7	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.19	31 (37%)
14	HEC	C	502	6	50,50,50	1.55	9 (18%)	68,82,82	1.99	17 (25%)
14	HEC	C	501	6	50,50,50	1.53	9 (18%)	68,82,82	1.89	13 (19%)
8	BCL	B	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.14	28 (33%)
11	MQE	L	403	-	69,69,69	0.58	0	84,87,87	1.31	12 (14%)
8	BCL	K	102	1	69,74,74	1.80	15 (21%)	83,115,115	2.14	28 (33%)
8	BCL	6	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)
8	BCL	R	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.19	31 (37%)
8	BCL	D	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.18	31 (37%)
8	BCL	O	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)
14	HEC	C	504	6	50,50,50	1.56	7 (14%)	68,82,82	2.05	19 (27%)
8	BCL	F	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.19	31 (37%)
8	BCL	S	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	BCL	3	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.18	31 (37%)
8	BCL	O	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.14	27 (32%)
8	BCL	V	101	-	69,74,74	1.80	15 (21%)	83,115,115	2.30	30 (36%)
11	MQE	M	1003	-	26,26,69	1.21	4 (15%)	32,35,87	1.52	3 (9%)
9	KGD	I	103	-	41,41,41	1.09	3 (7%)	49,53,53	2.44	15 (30%)
8	BCL	E	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)
8	BCL	M	1001	3	69,74,74	1.83	16 (23%)	83,115,115	2.20	27 (32%)
8	BCL	P	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.19	31 (37%)
8	BCL	A	101	2	69,74,74	1.86	16 (23%)	83,115,115	2.27	31 (37%)
8	BCL	J	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.19	31 (37%)
8	BCL	U	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)
8	BCL	W	101	1	69,74,74	1.89	16 (23%)	83,115,115	2.38	31 (37%)
9	KGD	J	102	-	41,41,41	0.98	3 (7%)	49,53,53	2.20	16 (32%)
8	BCL	G	102	1	69,74,74	1.81	16 (23%)	83,115,115	2.14	28 (33%)
11	MQE	M	1002	-	69,69,69	0.82	1 (1%)	84,87,87	1.53	14 (16%)
8	BCL	E	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.14	28 (33%)
8	BCL	K	101	1	69,74,74	1.84	16 (23%)	83,115,115	2.15	28 (33%)
8	BCL	5	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.19	31 (37%)
8	BCL	Q	101	1	69,74,74	1.84	16 (23%)	83,115,115	2.15	28 (33%)
8	BCL	G	101	1	69,74,74	1.84	17 (24%)	83,115,115	2.15	28 (33%)
8	BCL	2	101	1	69,74,74	1.90	17 (24%)	83,115,115	2.33	33 (39%)
10	BPH	L	404	-	59,70,70	1.58	9 (15%)	61,101,101	1.53	11 (18%)
8	BCL	Q	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.15	27 (32%)
8	BCL	U	102	1	69,74,74	1.81	16 (23%)	83,115,115	2.14	27 (32%)
8	BCL	8	101	1	69,74,74	1.84	16 (23%)	83,115,115	2.15	28 (33%)
8	BCL	N	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.18	31 (37%)
8	BCL	1	101	2	69,74,74	1.85	16 (23%)	83,115,115	2.18	31 (37%)
8	BCL	8	102	1	69,74,74	1.80	16 (23%)	83,115,115	2.16	28 (33%)
13	PGV	M	1006	-	44,44,50	0.72	0	47,50,56	1.00	3 (6%)
8	BCL	6	102	1	69,74,74	1.81	16 (23%)	83,115,115	2.14	27 (32%)
9	KGD	9	101	-	41,41,41	1.08	2 (4%)	49,53,53	2.37	13 (26%)

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
13	PGV	M	1008	-	-	12/38/38/55	-
13	PGV	M	1007	-	-	14/46/46/55	-
8	BCL	T	101	2	-	19/41/137/137	-
8	BCL	I	101	1	-	20/41/137/137	-
8	BCL	M	1005	-	-	15/41/137/137	-
14	HEC	C	503	6	1/1/3/7	4/14/54/54	-
8	BCL	0	101	1	-	18/41/137/137	-
8	BCL	4	101	1	-	20/41/137/137	-
8	BCL	L	401	3	-	18/41/137/137	-
9	KGD	N	102	-	-	10/36/56/56	0/1/1/1
10	BPH	L	405	-	-	14/37/105/105	0/5/6/6
8	BCL	S	102	1	-	18/41/137/137	-
8	BCL	H	101	2	-	17/41/137/137	-
8	BCL	2	102	1	-	18/41/137/137	-
8	BCL	I	102	1	-	18/41/137/137	-
8	BCL	4	102	1	-	19/41/137/137	-
8	BCL	0	102	1	-	20/41/137/137	-
9	KGD	D	102	-	-	17/36/56/56	0/1/1/1
8	BCL	9	102	2	-	17/41/137/137	-
8	BCL	B	101	1	-	20/41/137/137	-
14	HEC	C	502	6	1/1/3/7	4/14/54/54	-
8	BCL	W	102	1	-	18/41/137/137	-
8	BCL	7	101	2	-	20/41/137/137	-
10	BPH	L	402	-	-	17/37/105/105	0/5/6/6
14	HEC	C	501	6	1/1/3/7	4/14/54/54	-
8	BCL	B	102	1	-	18/41/137/137	-
11	MQE	L	403	-	-	16/65/85/85	0/2/2/2
8	BCL	K	102	1	-	18/41/137/137	-
8	BCL	6	101	1	-	20/41/137/137	-
8	BCL	R	101	2	-	20/41/137/137	-
14	HEC	C	504	6	1/1/3/7	6/14/54/54	-
8	BCL	D	101	2	-	20/41/137/137	-
8	BCL	O	101	1	-	20/41/137/137	-
8	BCL	F	101	2	-	19/41/137/137	-
8	BCL	S	101	1	-	20/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	3	101	2	-	19/41/137/137	-
8	BCL	O	102	1	-	18/41/137/137	-
8	BCL	V	101	-	-	21/41/137/137	-
11	MQE	M	1003	-	-	7/14/34/85	0/2/2/2
9	KGD	I	103	-	-	14/36/56/56	0/1/1/1
8	BCL	E	101	1	-	20/41/137/137	-
8	BCL	M	1001	3	-	18/41/137/137	-
8	BCL	P	101	2	-	18/41/137/137	-
8	BCL	A	101	2	-	19/41/137/137	-
8	BCL	J	101	2	-	20/41/137/137	-
8	BCL	U	101	1	-	20/41/137/137	-
8	BCL	W	101	1	-	29/41/137/137	-
9	KGD	J	102	-	-	13/36/56/56	0/1/1/1
8	BCL	G	102	1	-	18/41/137/137	-
11	MQE	M	1002	-	-	21/65/85/85	0/2/2/2
8	BCL	E	102	1	-	18/41/137/137	-
8	BCL	K	101	1	-	20/41/137/137	-
8	BCL	5	101	2	-	20/41/137/137	-
8	BCL	Q	101	1	-	20/41/137/137	-
8	BCL	G	101	1	-	20/41/137/137	-
8	BCL	2	101	1	-	29/41/137/137	-
10	BPH	L	404	-	-	15/37/105/105	0/5/6/6
8	BCL	Q	102	1	-	18/41/137/137	-
8	BCL	U	102	1	-	19/41/137/137	-
8	BCL	8	101	1	-	20/41/137/137	-
8	BCL	N	101	2	-	19/41/137/137	-
8	BCL	1	101	2	-	19/41/137/137	-
8	BCL	8	102	1	-	18/41/137/137	-
13	PGV	M	1006	-	-	11/49/49/55	-
8	BCL	6	102	1	-	18/41/137/137	-
9	KGD	9	101	-	-	15/36/56/56	0/1/1/1

The worst 5 of 860 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	402	BPH	C1D-C2D	6.98	1.47	1.39
8	W	101	BCL	MG-ND	-6.67	1.92	2.05
8	2	101	BCL	MG-ND	-6.64	1.92	2.05
10	L	404	BPH	C1D-C2D	6.62	1.46	1.39
10	L	405	BPH	C1D-C2D	6.55	1.46	1.39

The worst 5 of 1603 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	103	KGD	CBG-CBI-CBL	-8.14	115.69	127.31
8	W	101	BCL	C1C-NC-C4C	-7.99	103.11	106.71
9	I	103	KGD	CAP-CAO-CAM	-7.88	116.06	127.31
9	N	102	KGD	CAP-CAO-CAM	-7.58	116.49	127.31
8	2	101	BCL	C1C-NC-C4C	-7.49	103.34	106.71

All (4) chirality outliers are listed below:

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

5 of 1142 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	0	101	BCL	CHA-CBD-CGD-O1D
8	0	101	BCL	C1-C2-C3-C5
8	0	102	BCL	C1A-C2A-CAA-CBA
8	0	102	BCL	C3A-C2A-CAA-CBA
8	0	102	BCL	C2B-C3B-CAB-CBB

There are no ring outliers.

66 monomers are involved in 385 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1008	PGV	5	0
13	M	1007	PGV	11	0
8	T	101	BCL	10	0
8	I	101	BCL	13	0
8	M	1005	BCL	5	0
8	4	101	BCL	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	0	101	BCL	3	0
14	C	503	HEC	8	0
8	L	401	BCL	11	0
9	N	102	KGD	1	0
10	L	405	BPH	11	0
8	S	102	BCL	3	0
8	H	101	BCL	3	0
8	2	102	BCL	3	0
8	I	102	BCL	3	0
8	4	102	BCL	3	0
8	0	102	BCL	9	0
9	D	102	KGD	4	0
8	9	102	BCL	7	0
8	B	101	BCL	14	0
8	W	102	BCL	2	0
10	L	402	BPH	5	0
8	7	101	BCL	5	0
14	C	502	HEC	2	0
14	C	501	HEC	5	0
8	B	102	BCL	2	0
11	L	403	MQE	1	0
8	K	102	BCL	4	0
8	6	101	BCL	14	0
8	R	101	BCL	8	0
8	D	101	BCL	7	0
8	O	101	BCL	12	0
14	C	504	HEC	2	0
8	F	101	BCL	4	0
8	S	101	BCL	11	0
8	3	101	BCL	4	0
8	O	102	BCL	3	0
8	V	101	BCL	10	0
11	M	1003	MQE	6	0
9	I	103	KGD	2	0
8	E	101	BCL	9	0
8	M	1001	BCL	4	0
8	P	101	BCL	3	0
8	A	101	BCL	5	0
8	J	101	BCL	9	0
8	U	101	BCL	12	0
8	W	101	BCL	12	0
9	J	102	KGD	1	0

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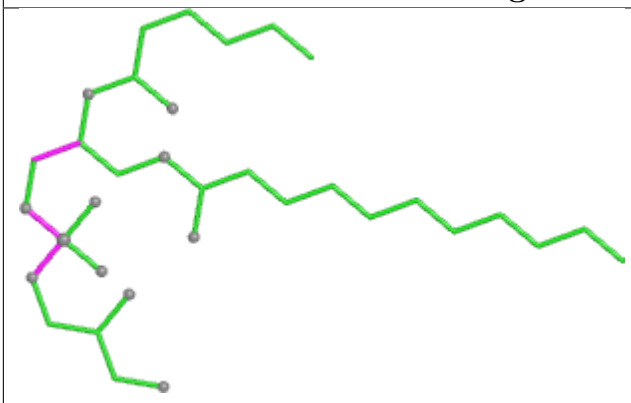
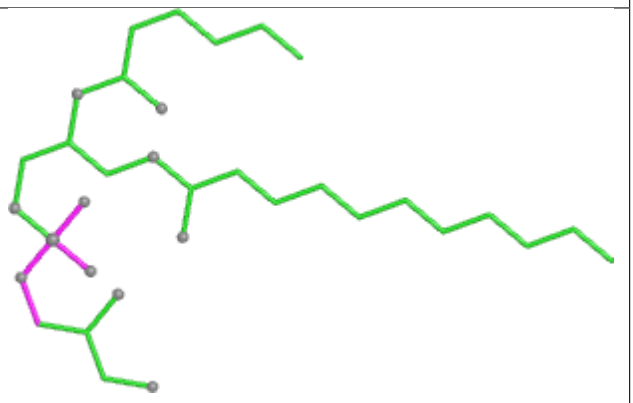
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	102	BCL	6	0
11	M	1002	MQE	5	0
8	E	102	BCL	5	0
8	K	101	BCL	12	0
8	5	101	BCL	4	0
8	Q	101	BCL	13	0
8	G	101	BCL	14	0
8	2	101	BCL	3	0
10	L	404	BPH	6	0
8	Q	102	BCL	3	0
8	U	102	BCL	2	0
8	8	101	BCL	9	0
8	N	101	BCL	4	0
8	1	101	BCL	3	0
8	8	102	BCL	3	0
13	M	1006	PGV	1	0
8	6	102	BCL	3	0
9	9	101	KGD	3	0

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

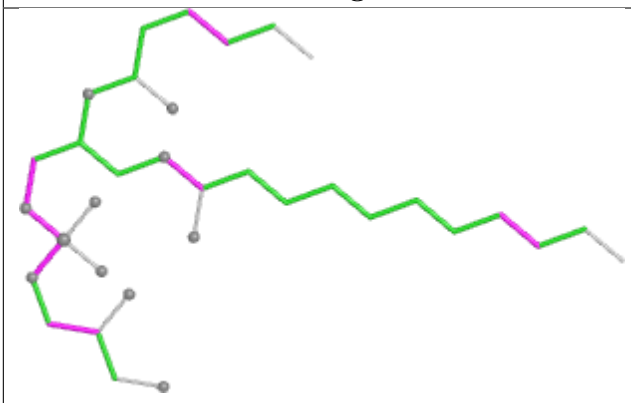
Ligand PGV M 1008



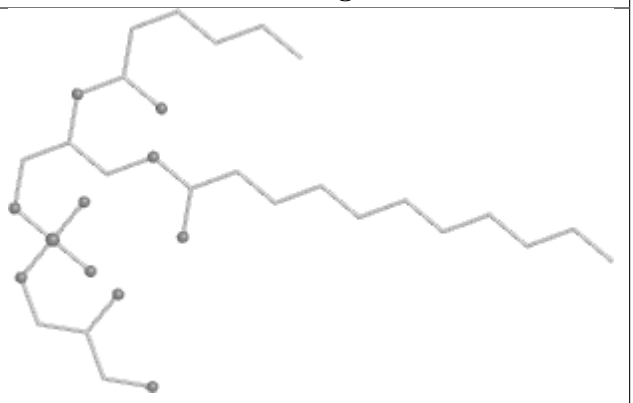
Bond lengths



Bond angles

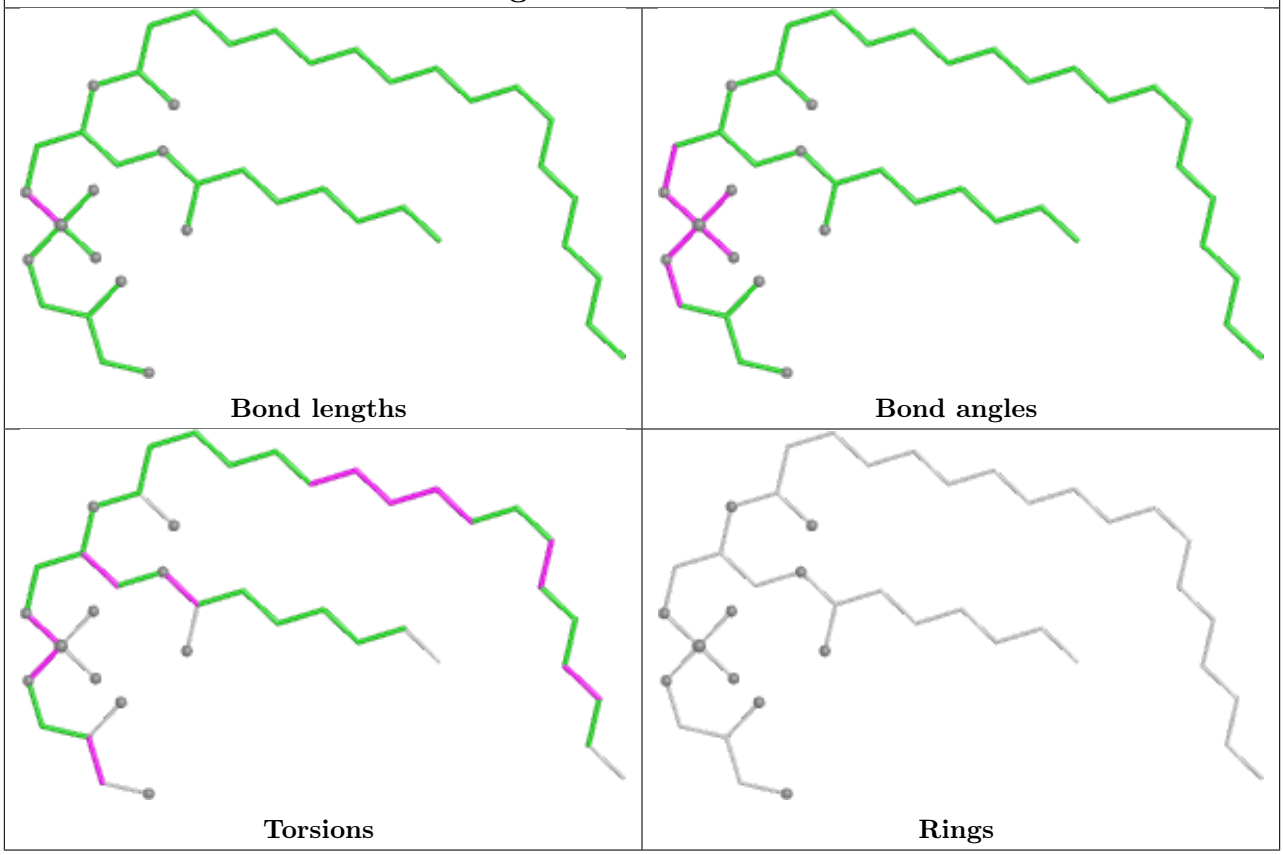


Torsions

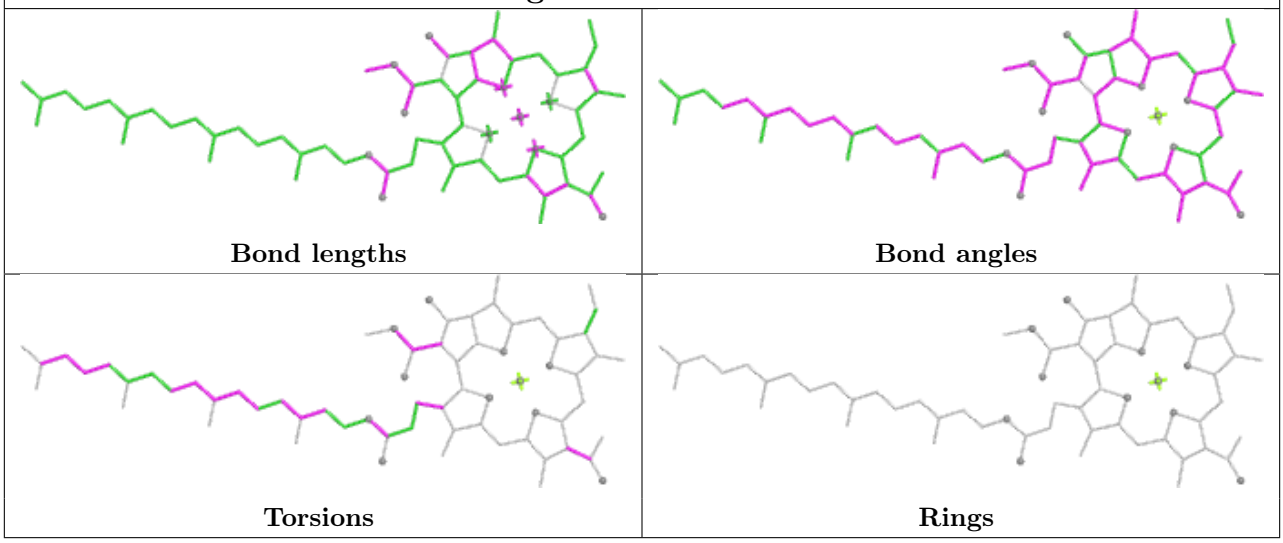


Rings

Ligand PGV M 1007



Ligand BCL T 101



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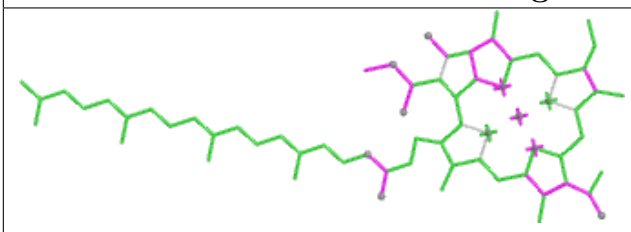

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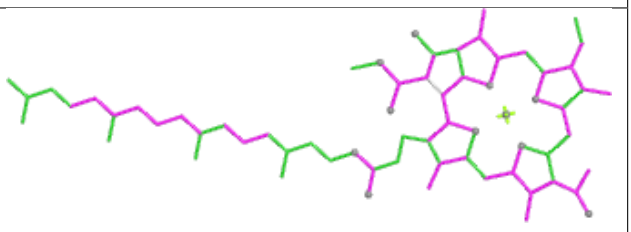
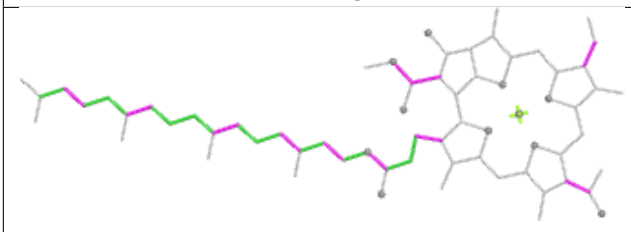
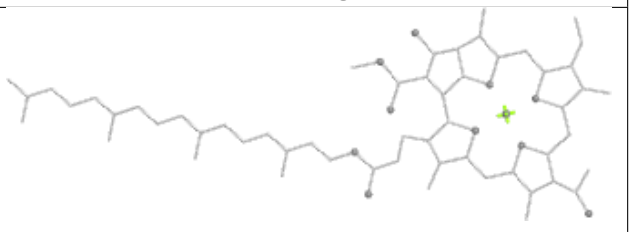


Bond angles



Torsions



Rings

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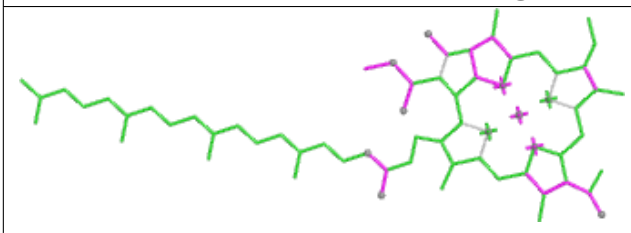
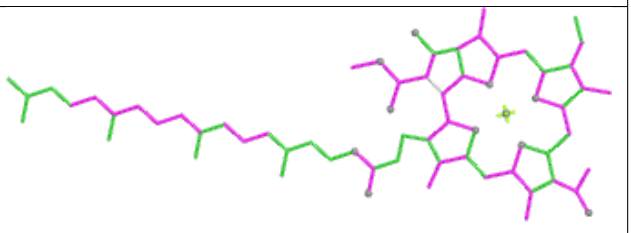
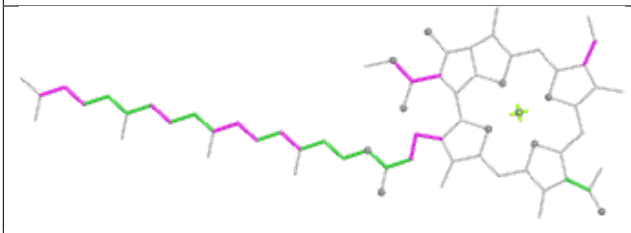


Bond lengths



Bond angles



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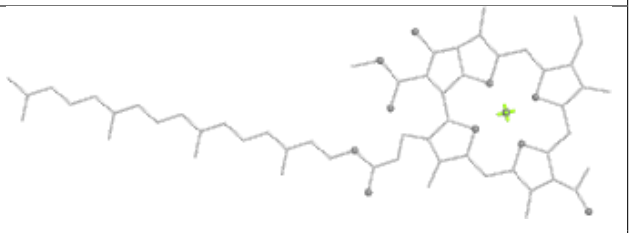
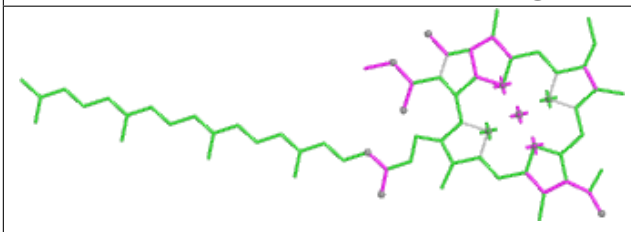


Rings

Ligand BCL 4 101



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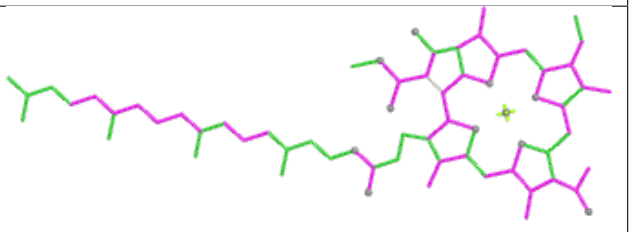

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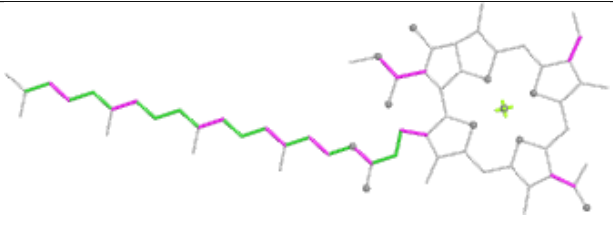

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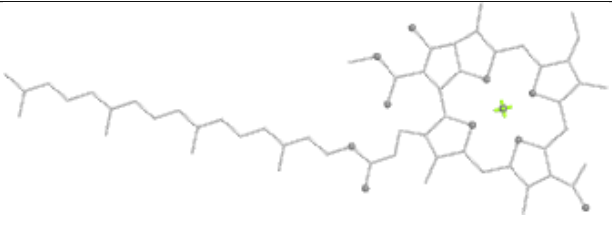

Rings

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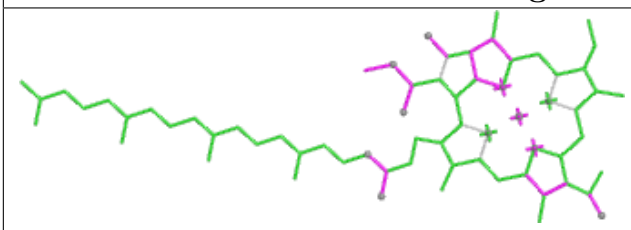

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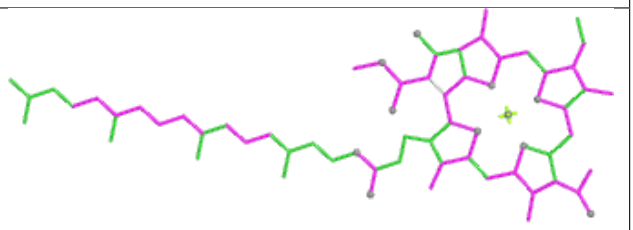

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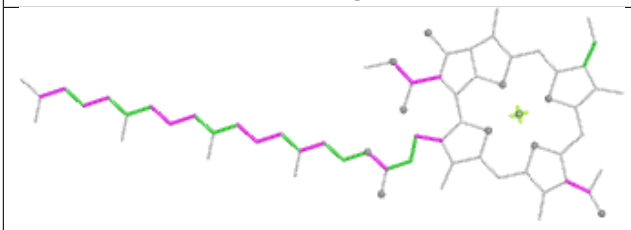

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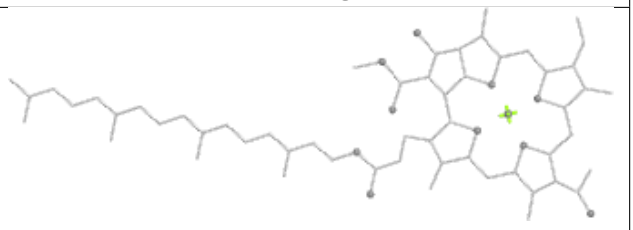
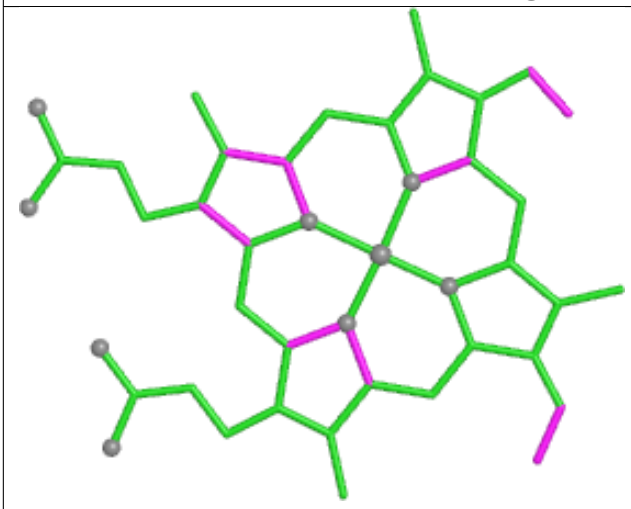


Rings

Ligand HEC C 503



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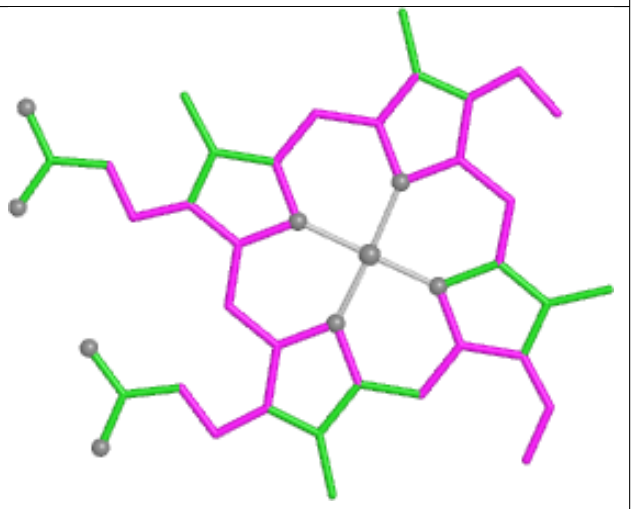

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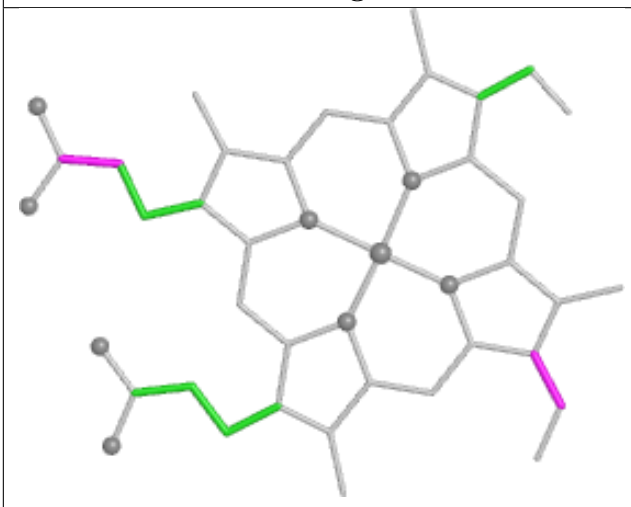

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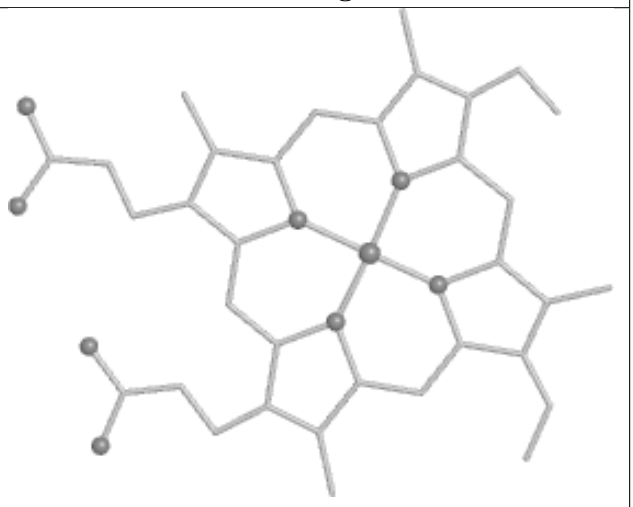

Rings

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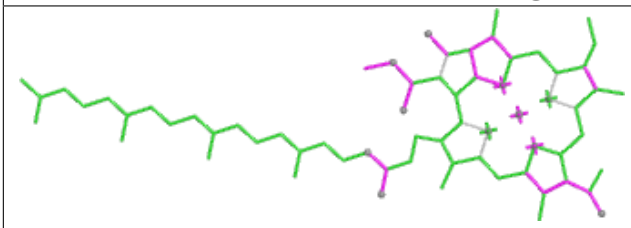
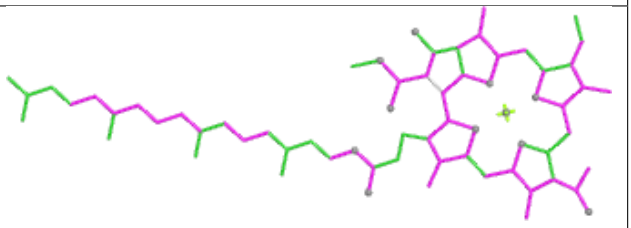
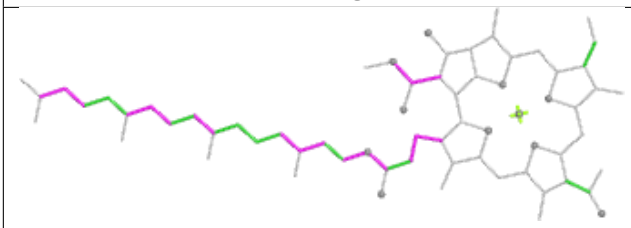
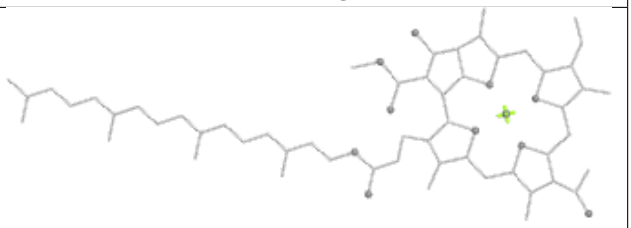
 Bond lengths	 Bond angles
 Torsions	 Rings

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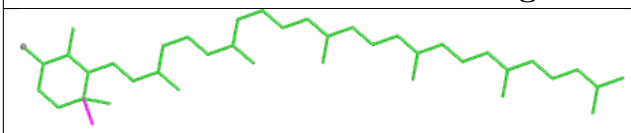
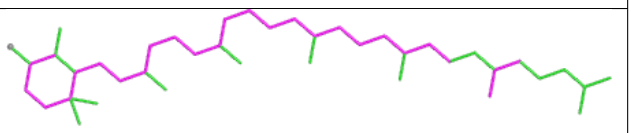
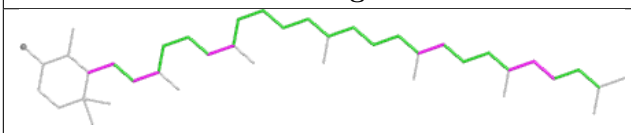
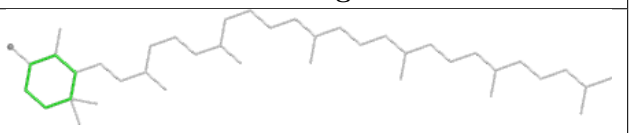
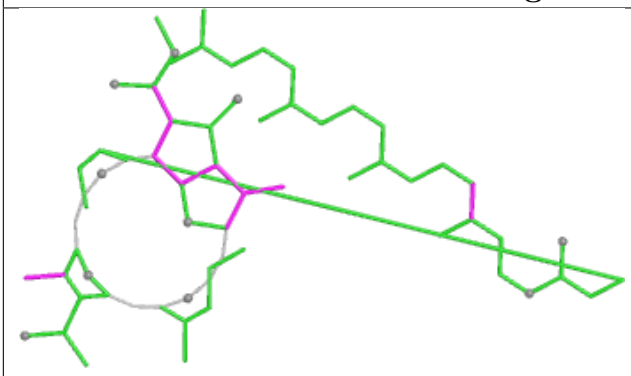
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH L 405



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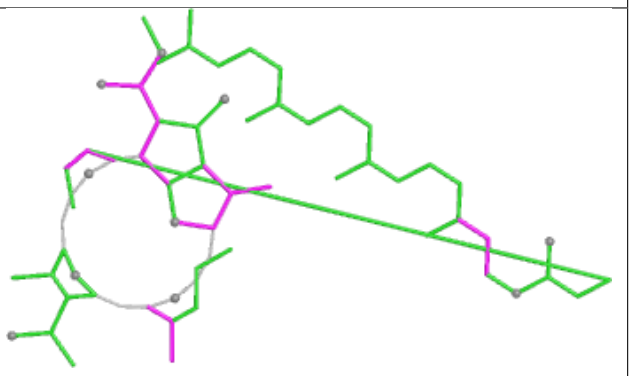

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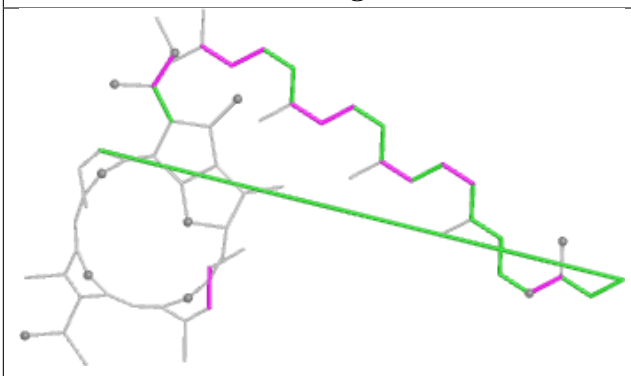

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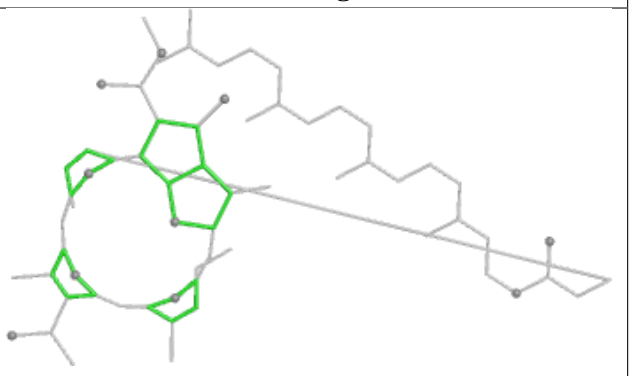
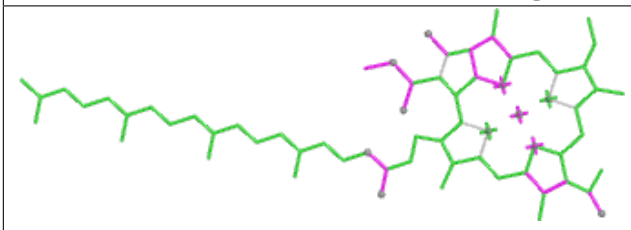


Rings

Ligand BCL S 102



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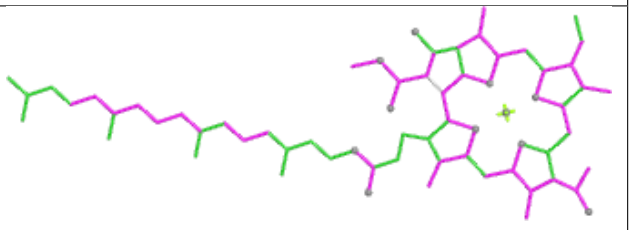

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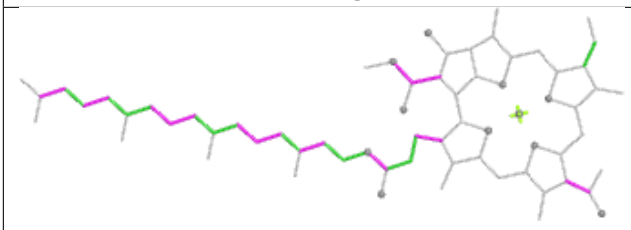

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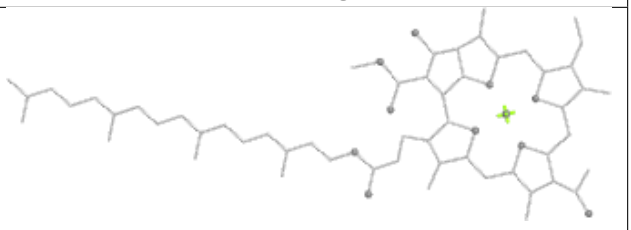

Rings

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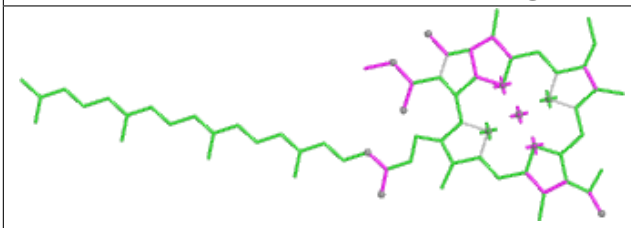

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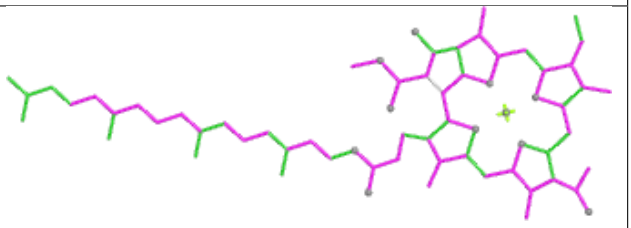

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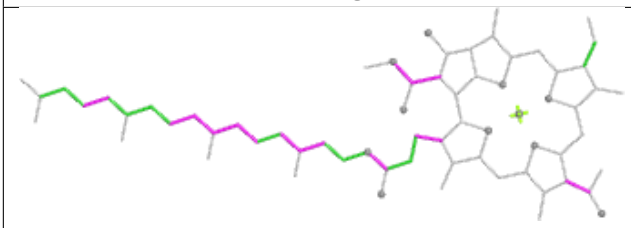

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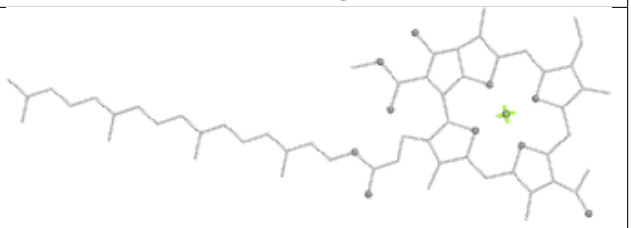
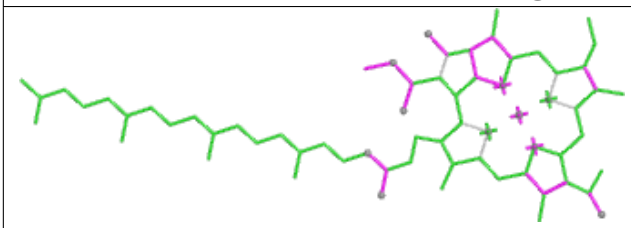


Rings

Ligand BCL 2 102



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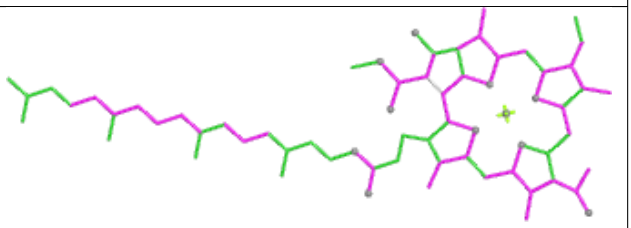
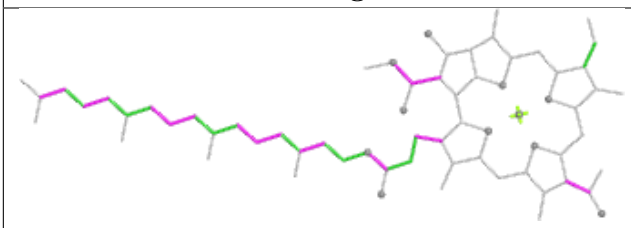


Bond angles



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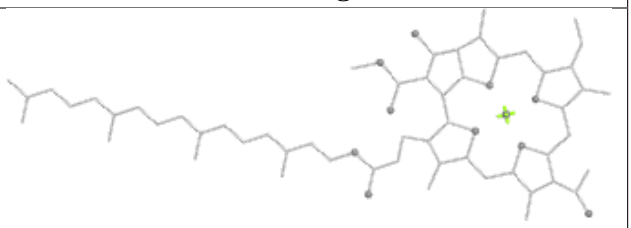
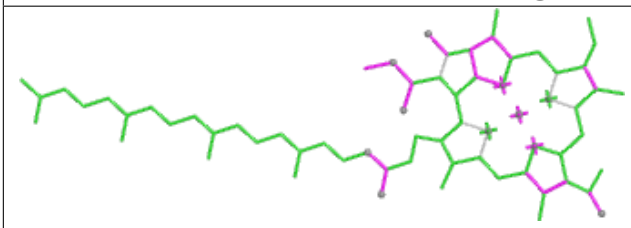


Rings

Ligand BCL I 102



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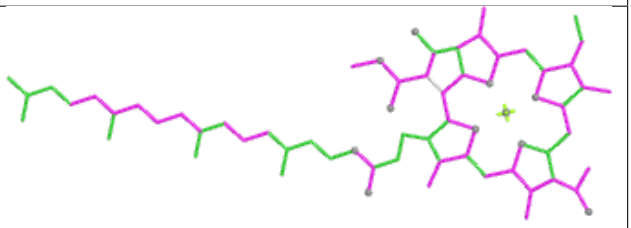
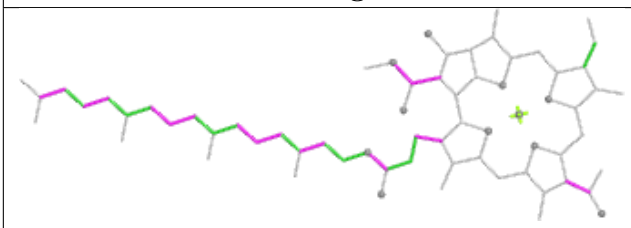


Bond angles



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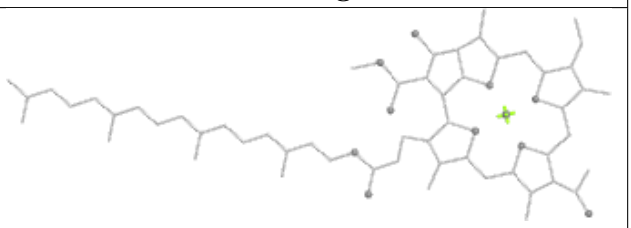
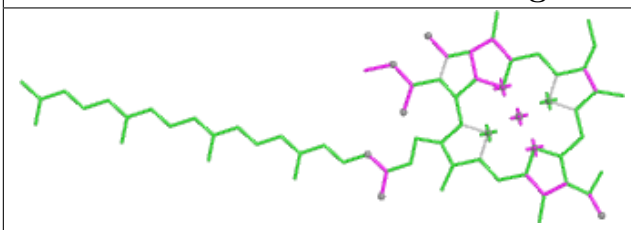


Rings

Ligand BCL 4 102



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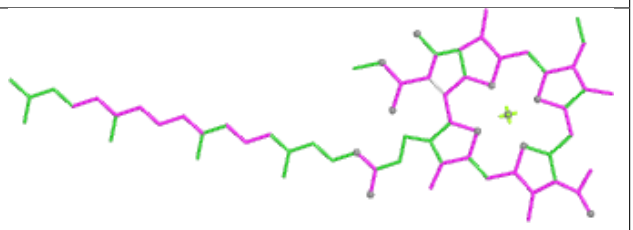

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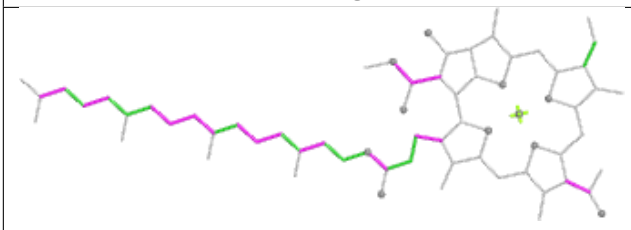

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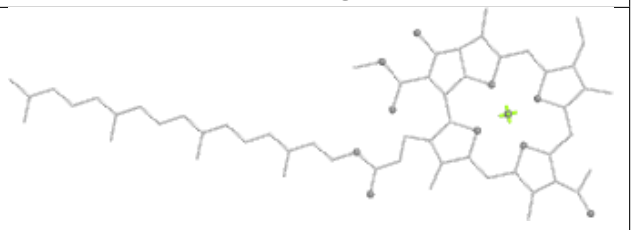
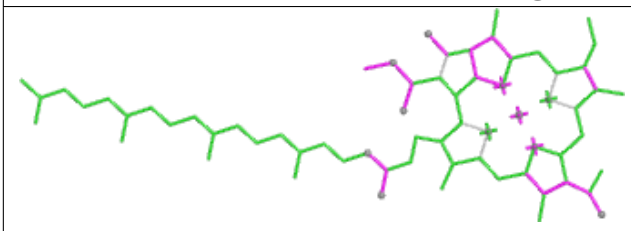


Rings

Ligand BCL 0 102



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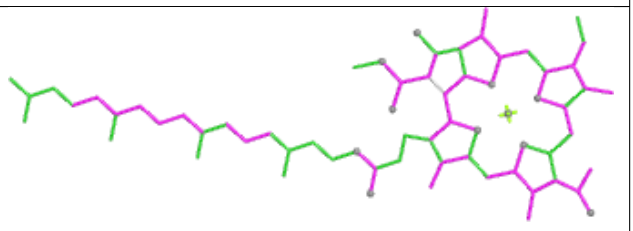

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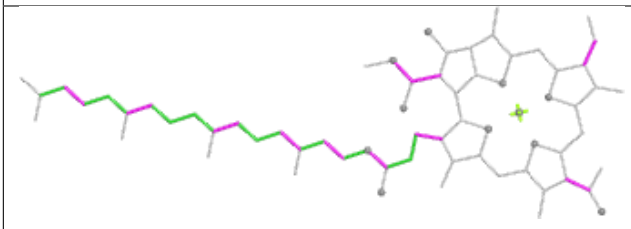

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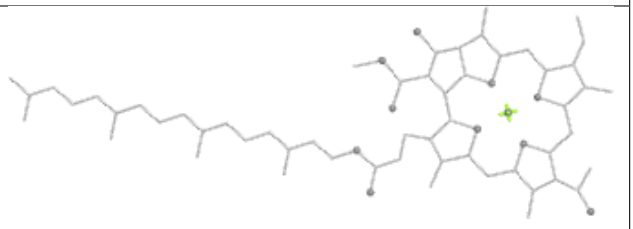
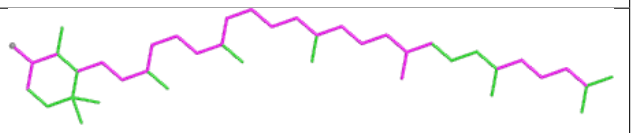


Rings

Ligand KGD D 102



Bond lengths



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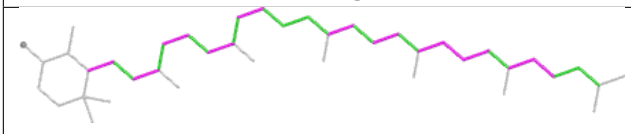

Torsions



Rings

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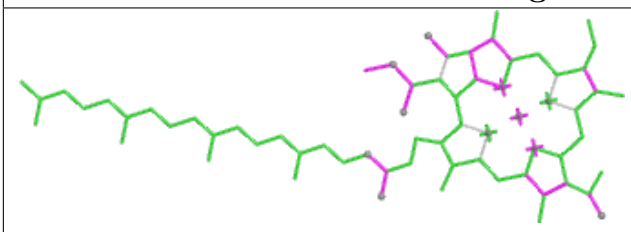

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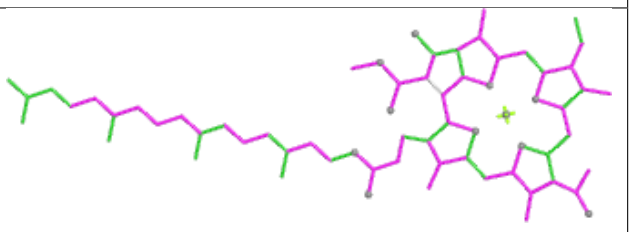

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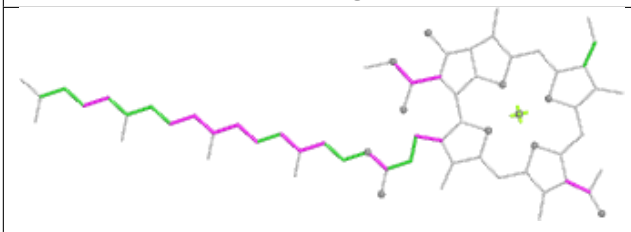

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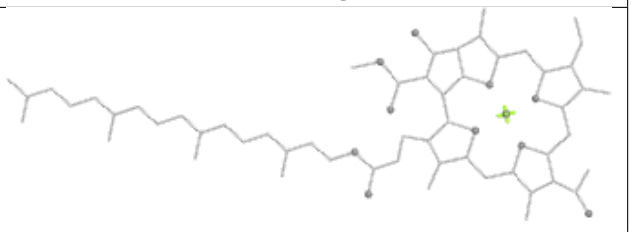

Rings

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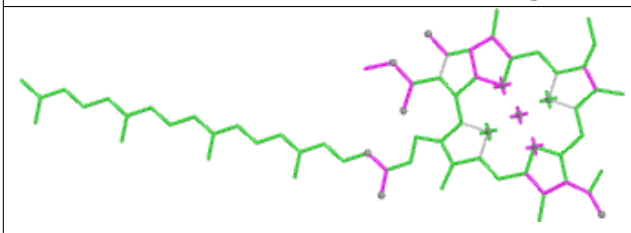

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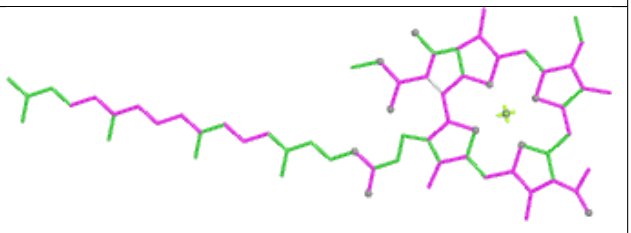

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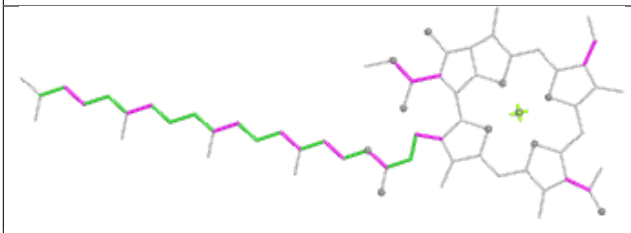

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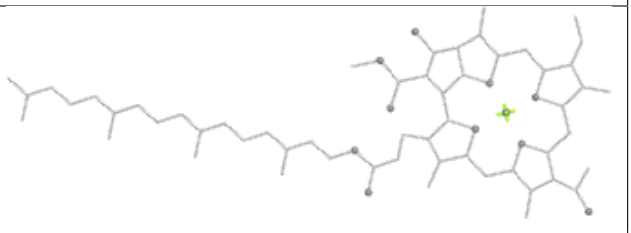

Rings

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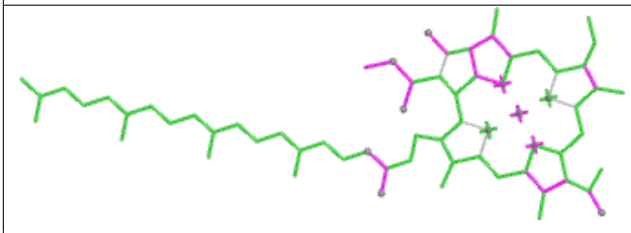

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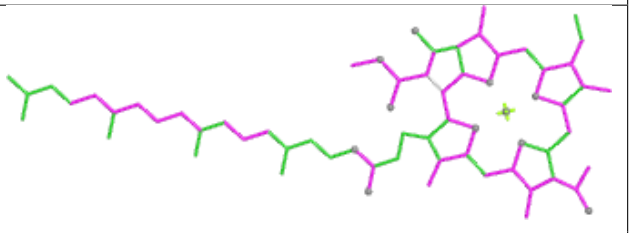

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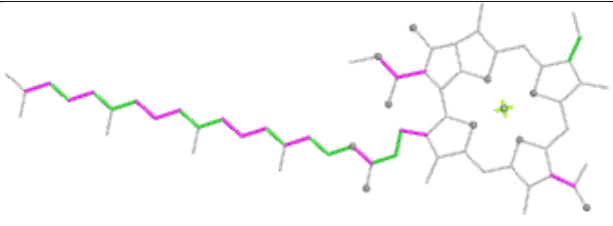

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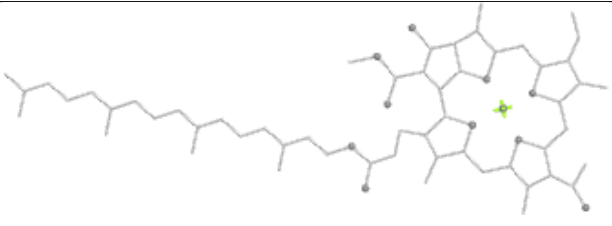
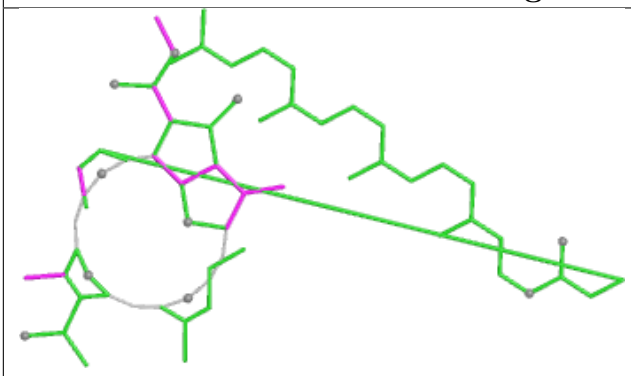


Rings

Ligand BPH L 402



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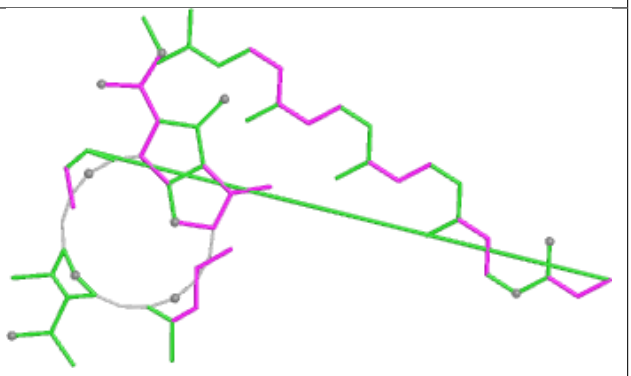

Bond angles



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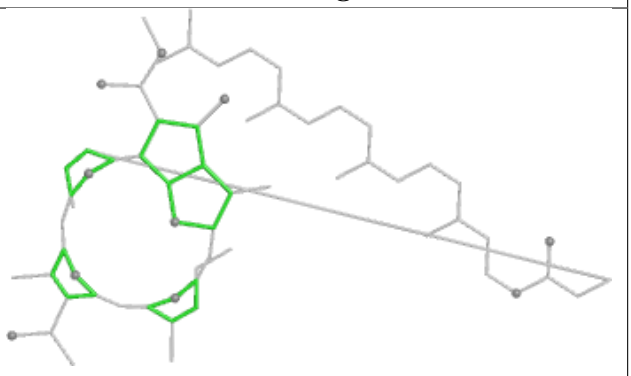
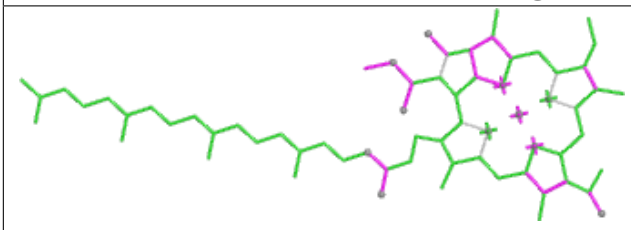


Rings

Ligand BCL 7 101



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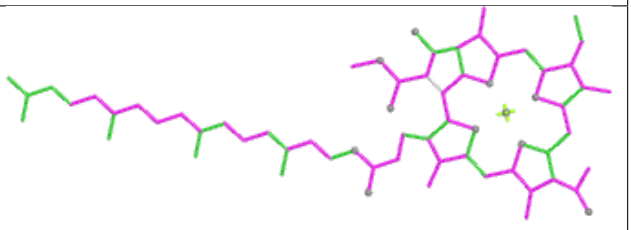

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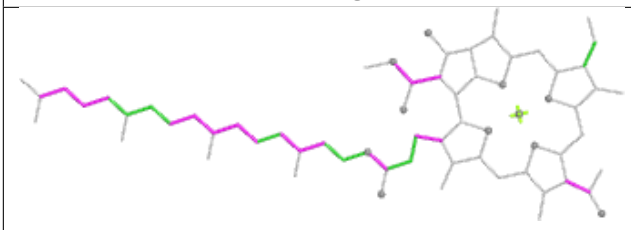

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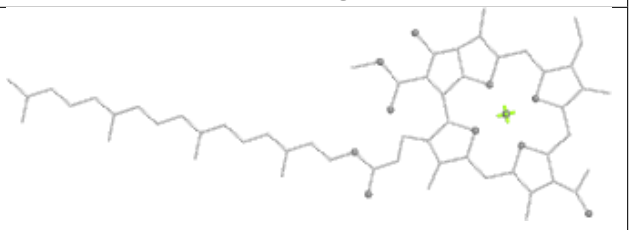
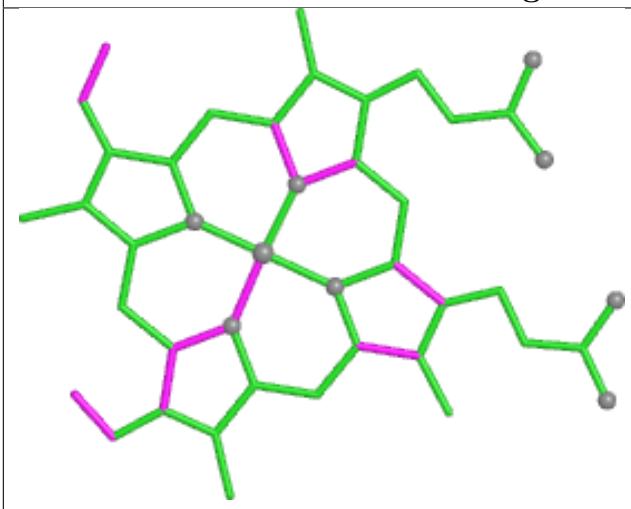


Rings

Ligand HEC C 502



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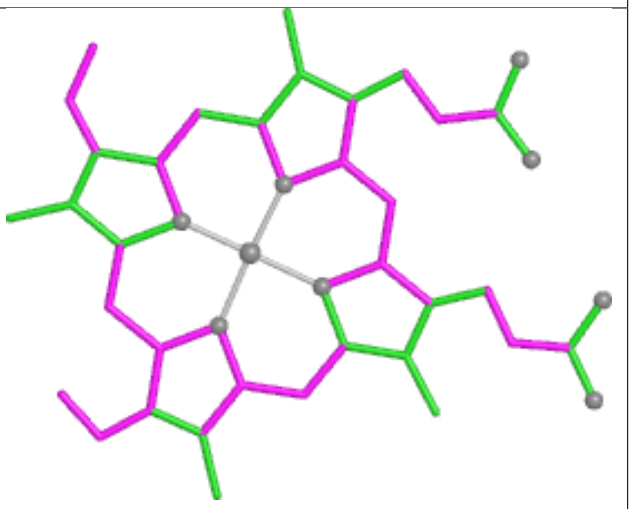

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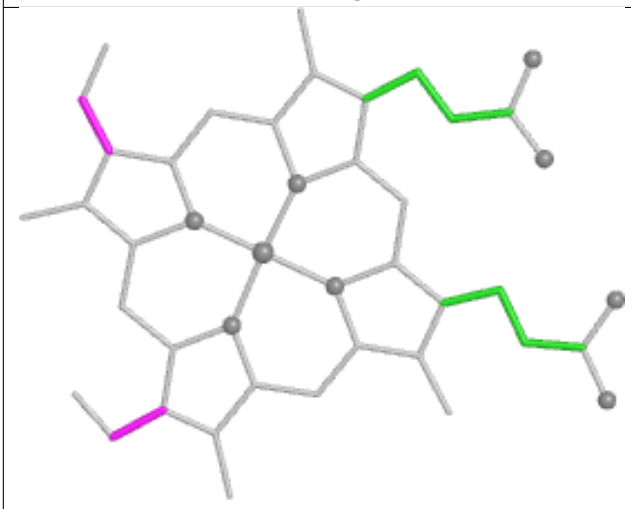

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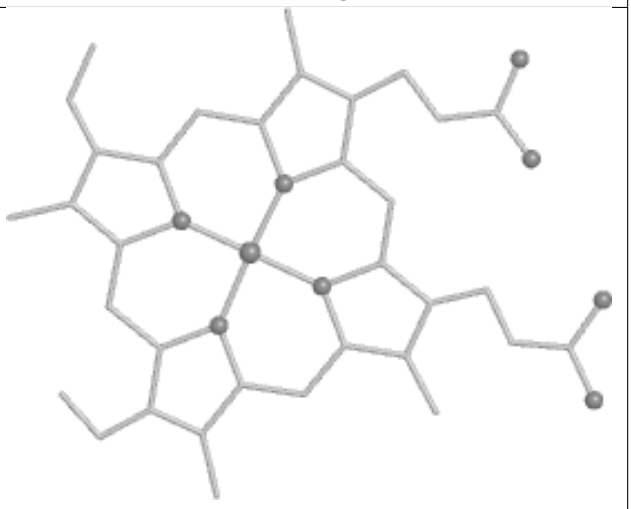

Rings

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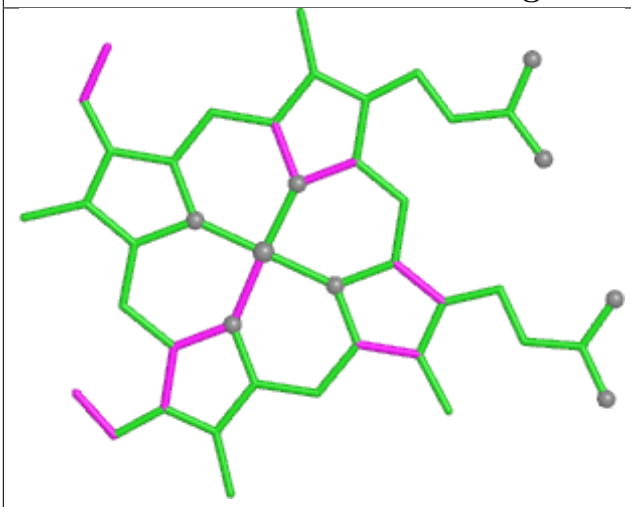

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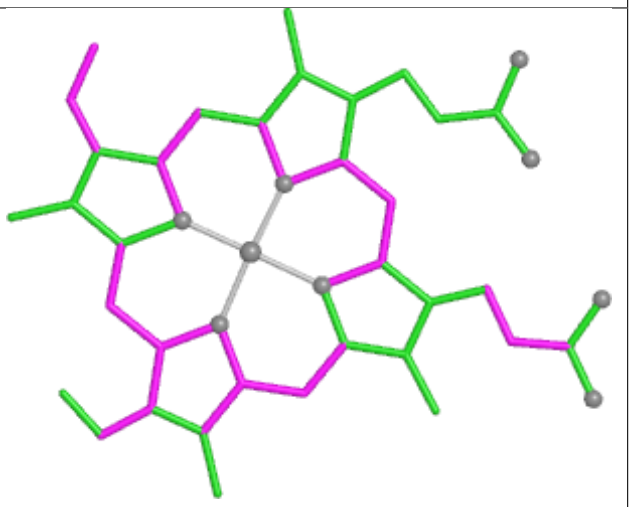

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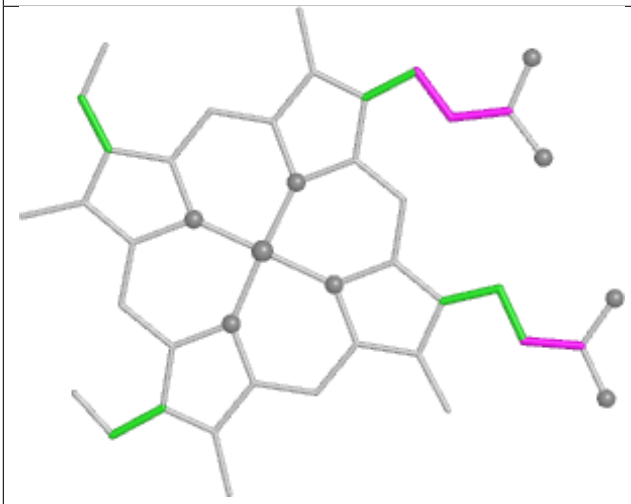

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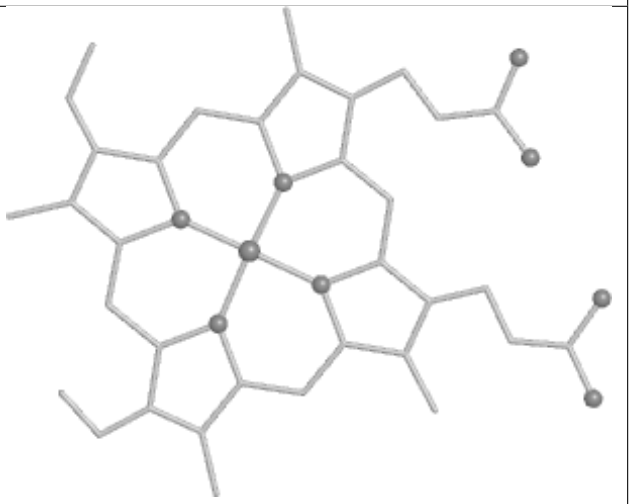
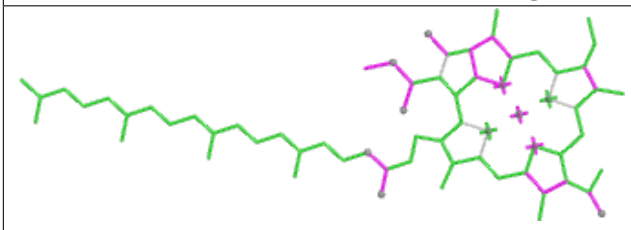


Rings

Ligand BCL B 102



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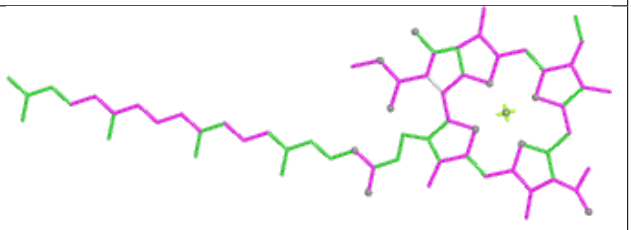

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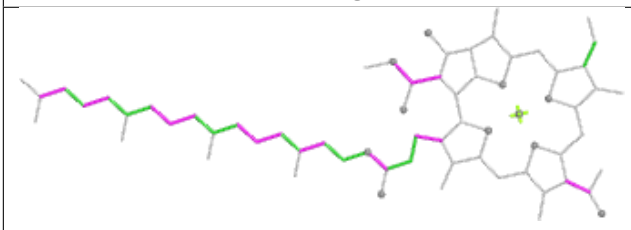

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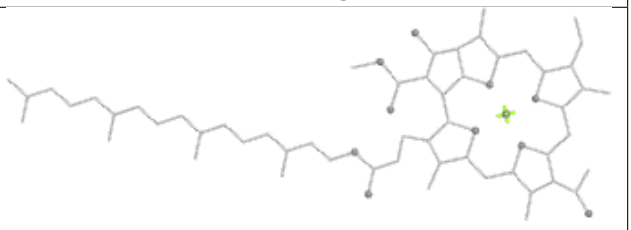
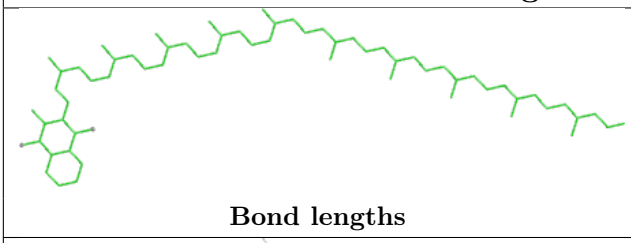


Rings

Ligand MQE L 403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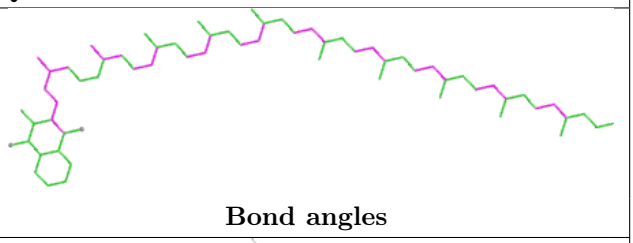
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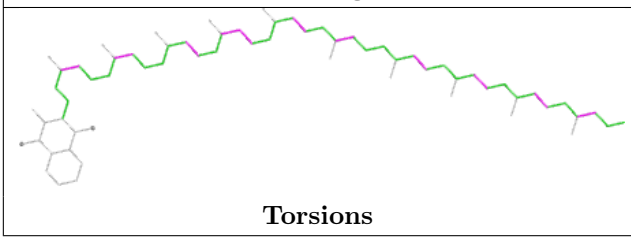
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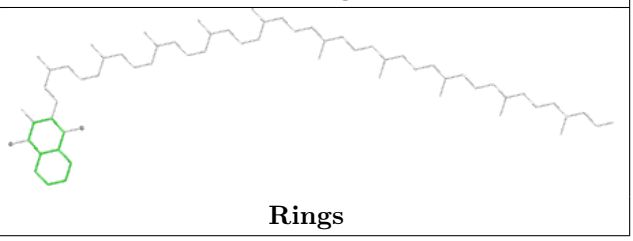
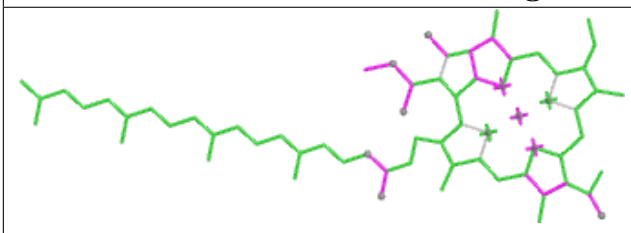

Rings

Ligand BCL K 102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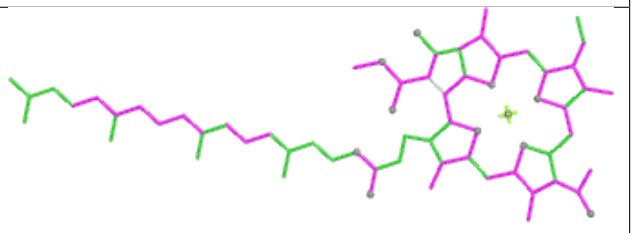
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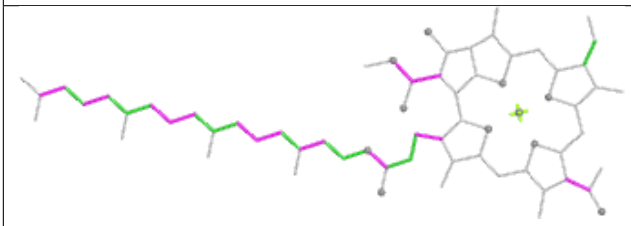
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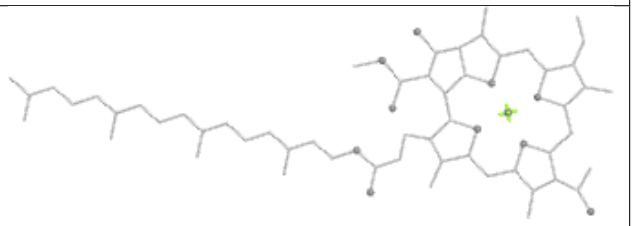
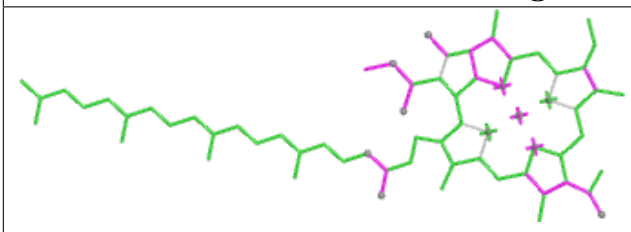

Rings

Ligand BCL 6 101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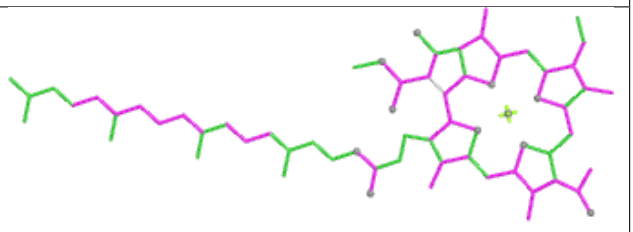
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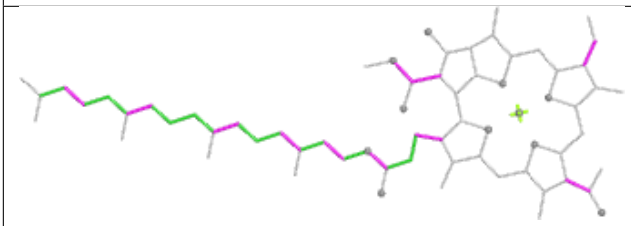
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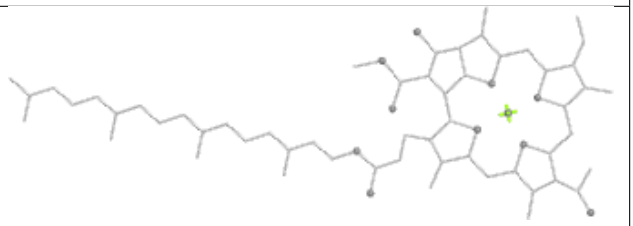
Rings

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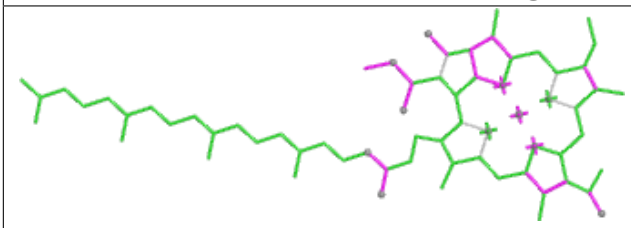

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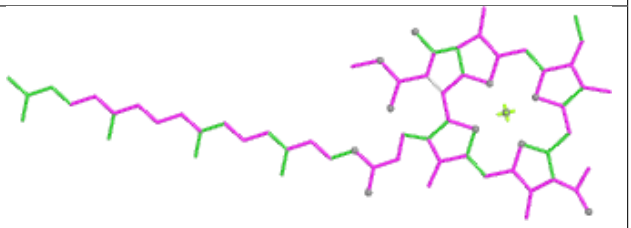

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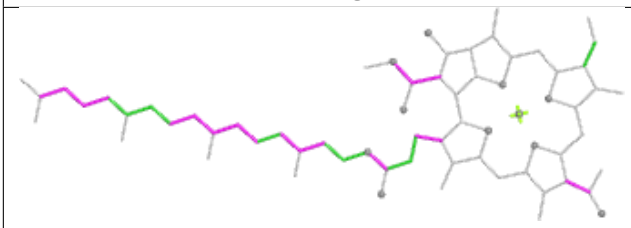

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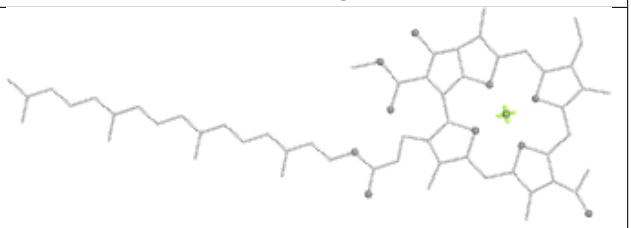

Rings

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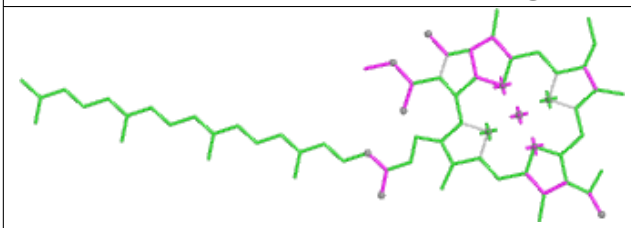

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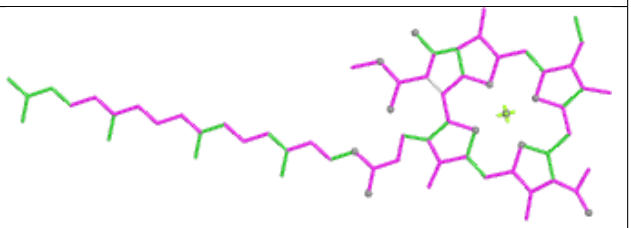
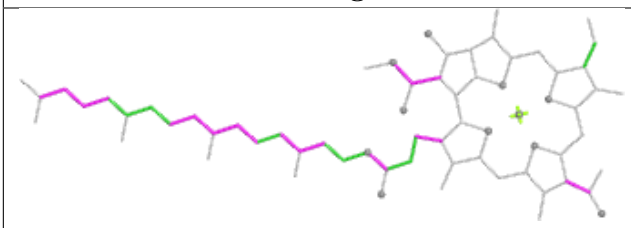
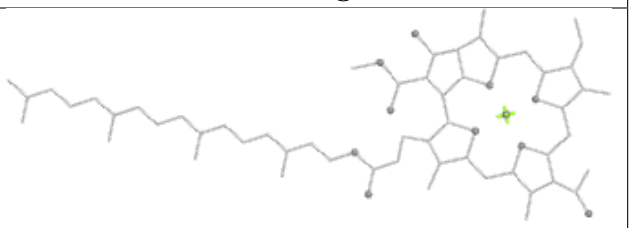


Bond angles

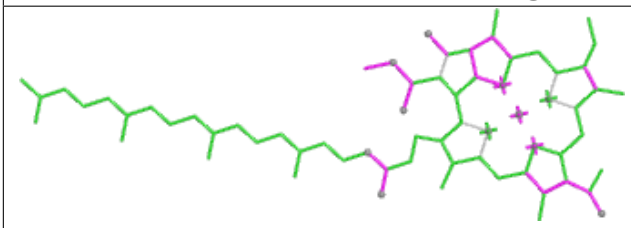


Torsions



Rings

Ligand BCL O 101



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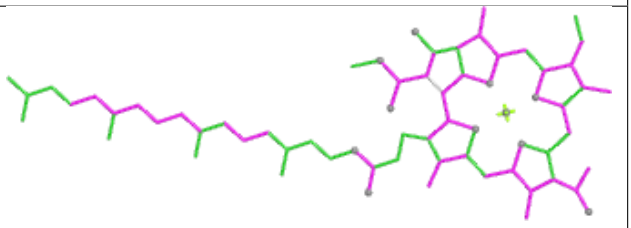

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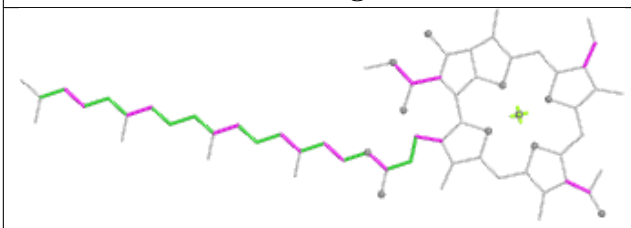

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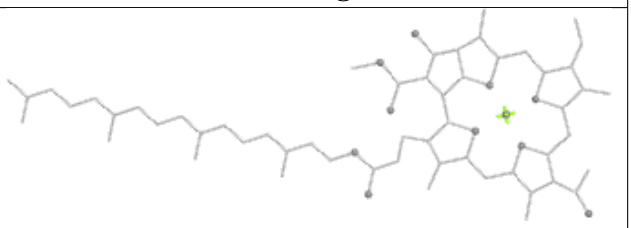
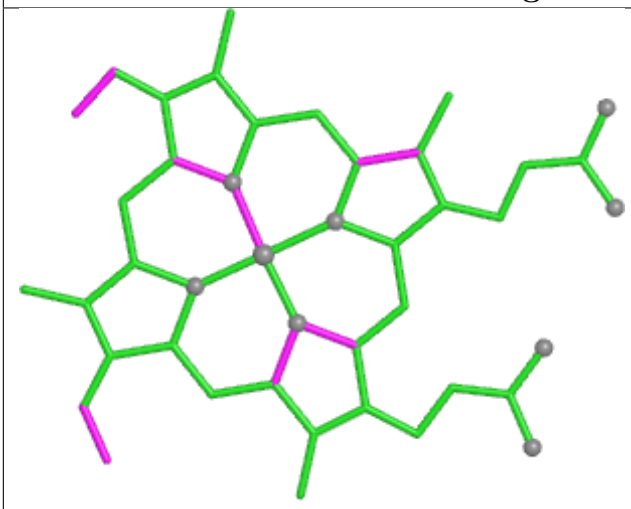


Rings

Ligand HEC C 504



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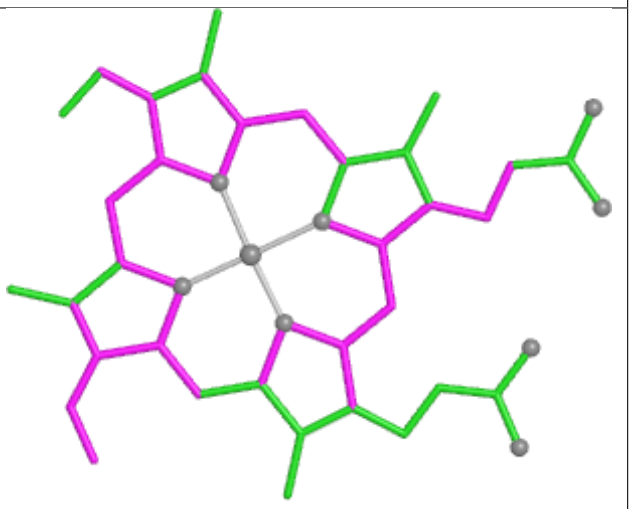

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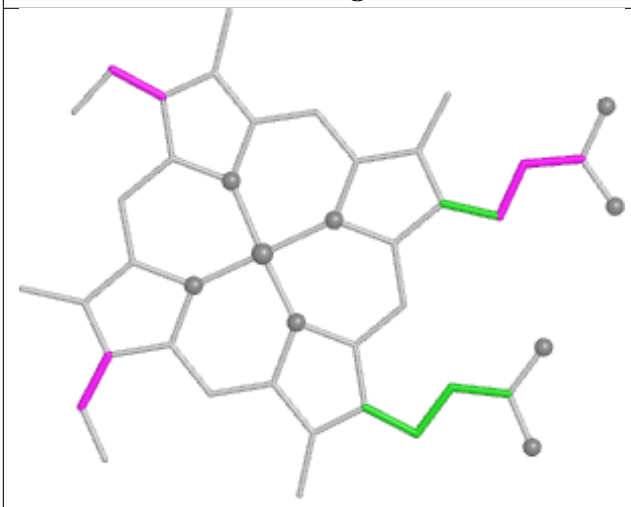

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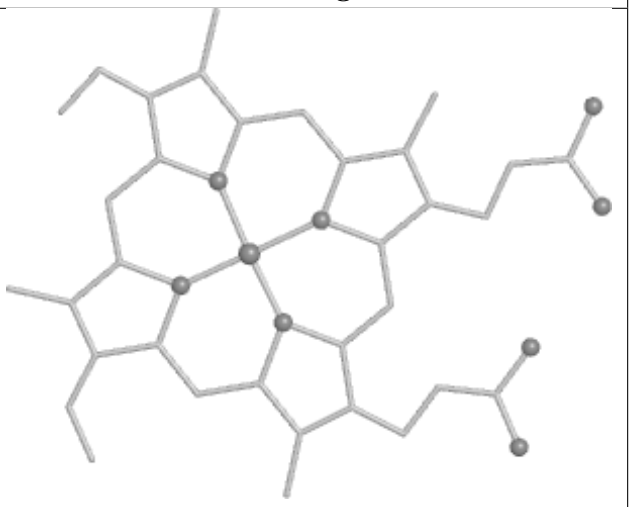
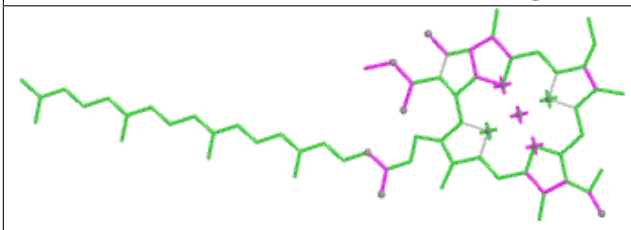


Rings

Ligand BCL F 101



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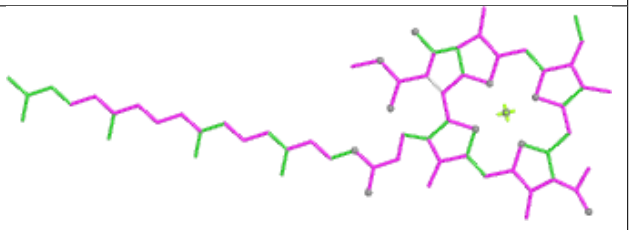

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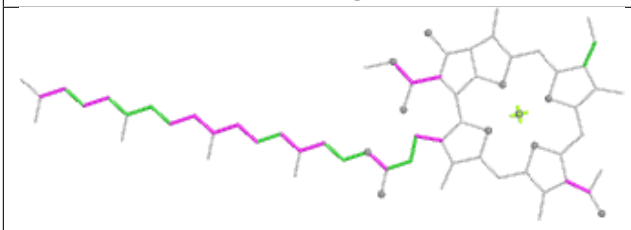

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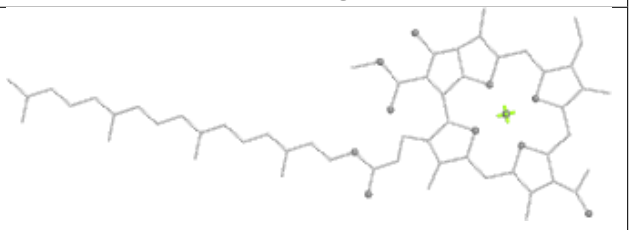

Rings

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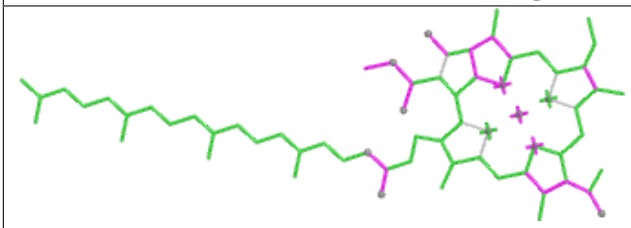

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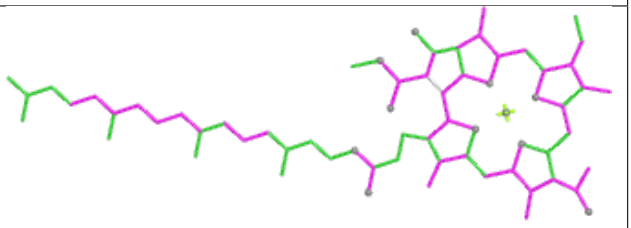

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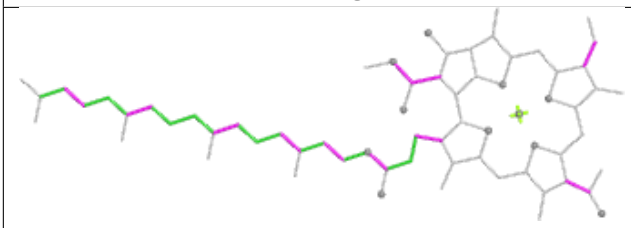

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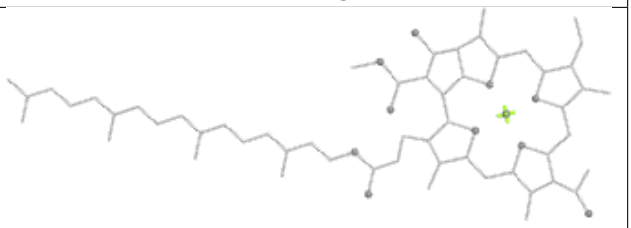

Rings

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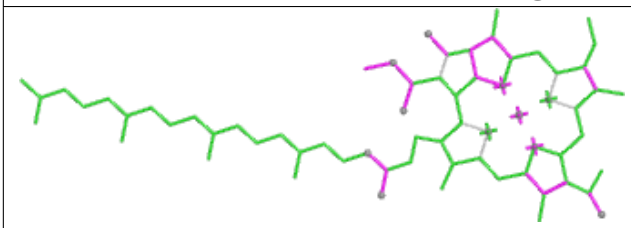

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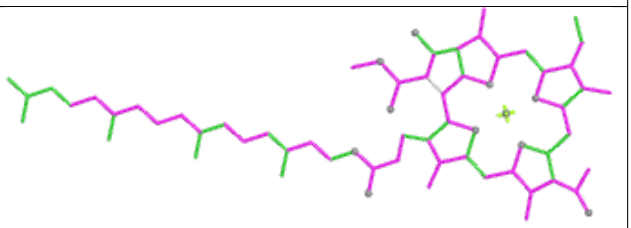

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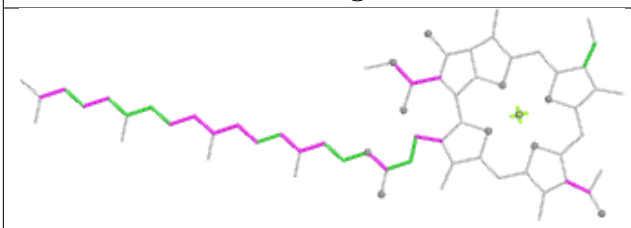

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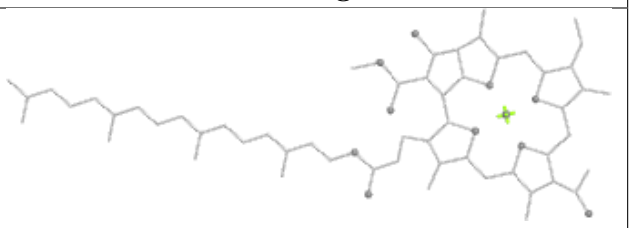

Rings

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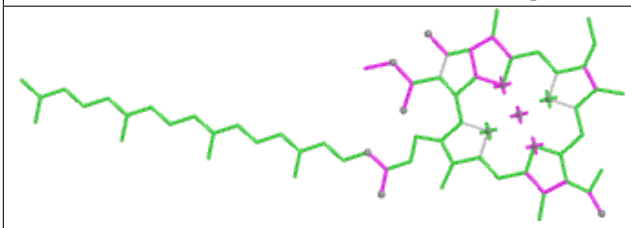

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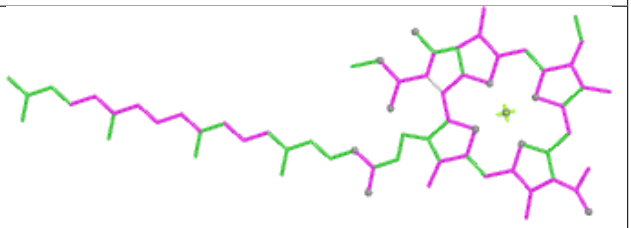

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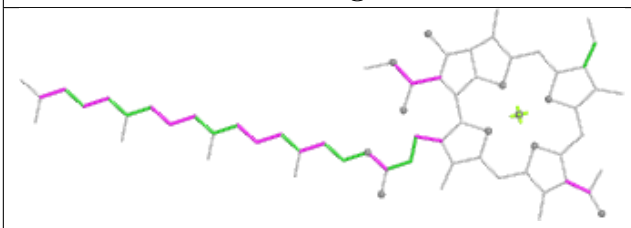

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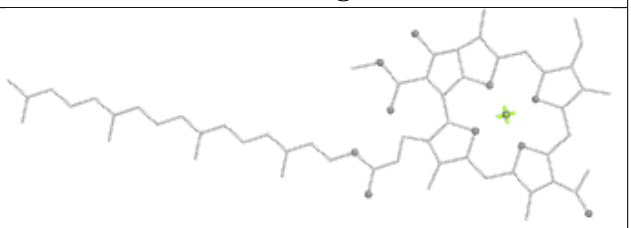

Rings

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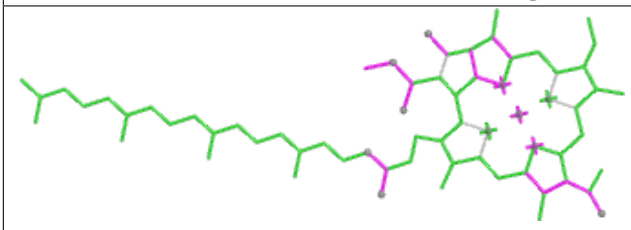

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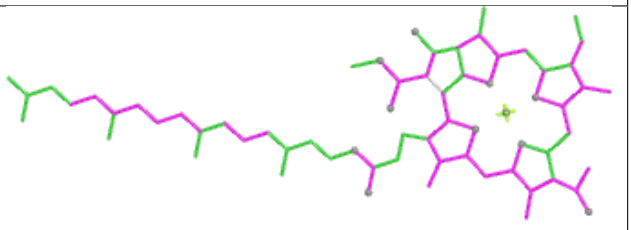

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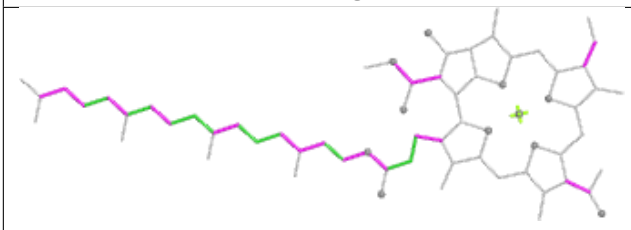

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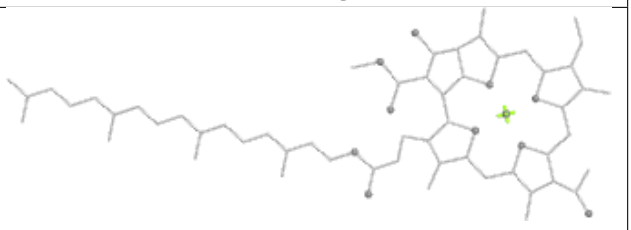
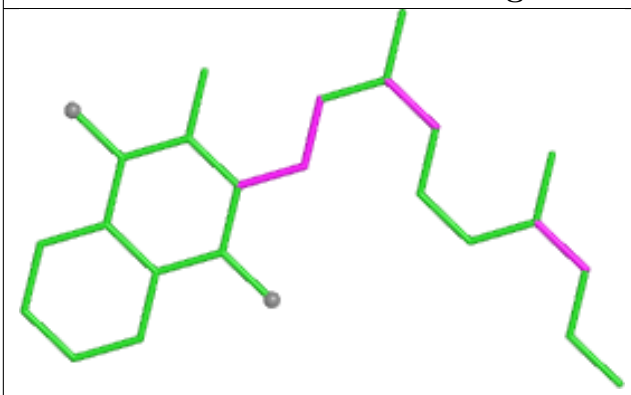


Rings

Ligand MQE M 1003



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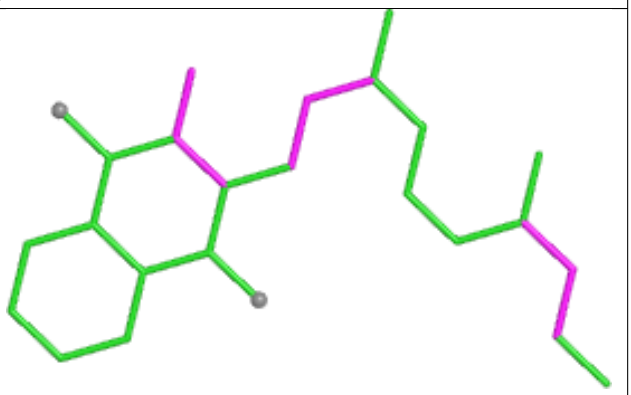

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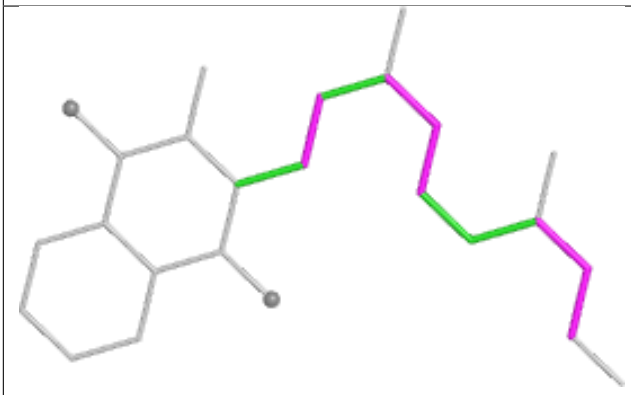

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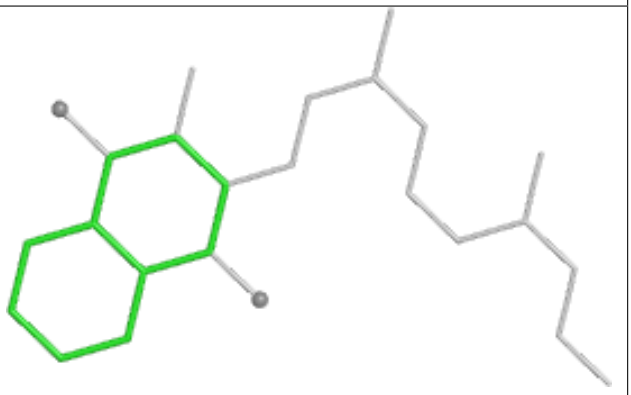
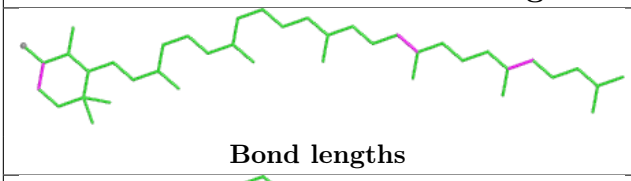


Rings

Ligand KGD I 103



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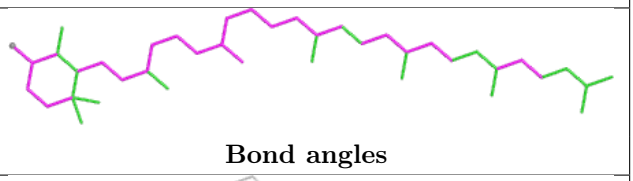

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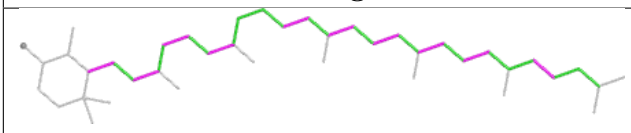
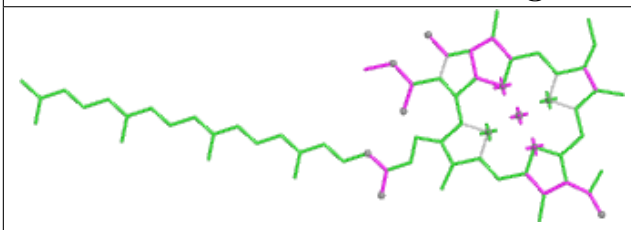


Torsions



Rings

Ligand BCL E 101



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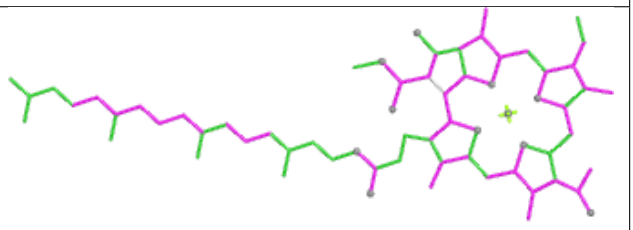

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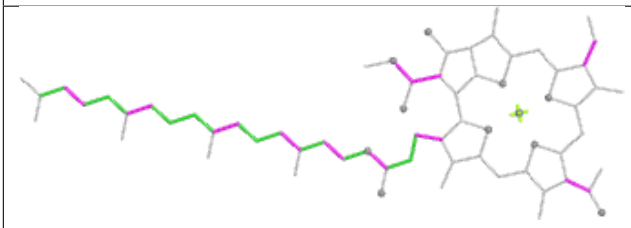

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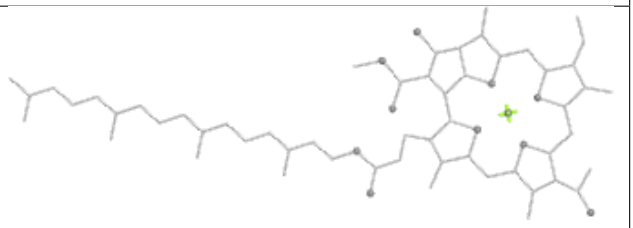
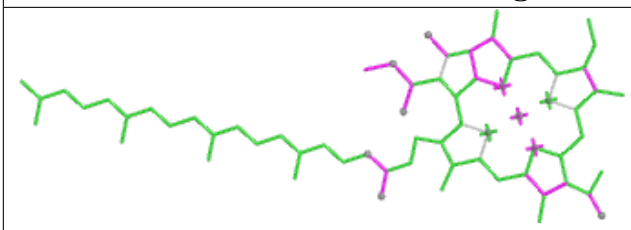


Rings

Ligand BCL M 1001



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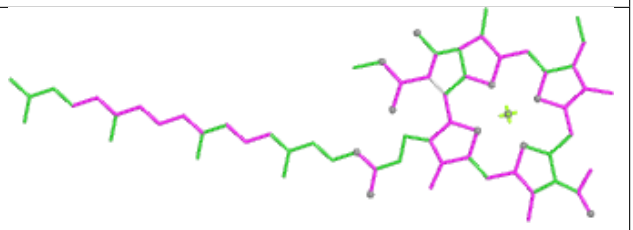

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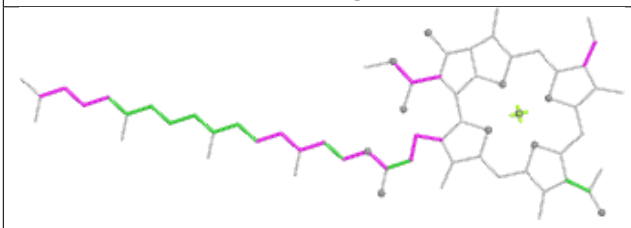

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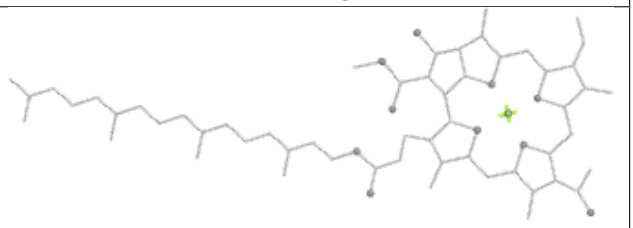
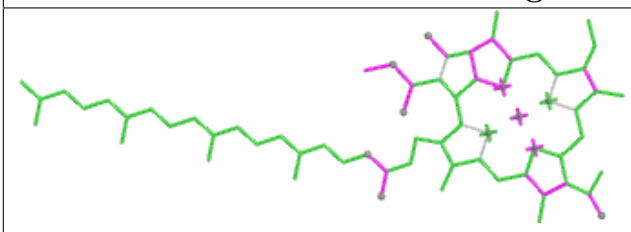


Rings

Ligand BCL P 101



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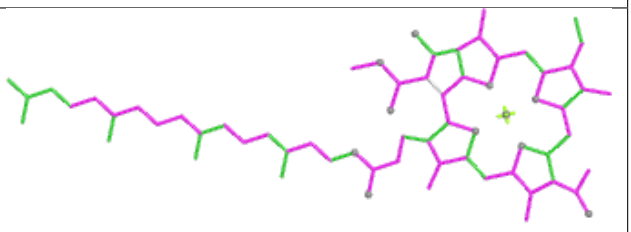
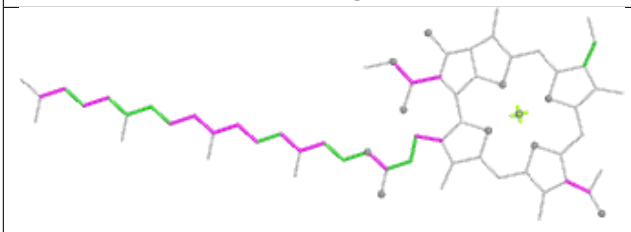


Bond angles



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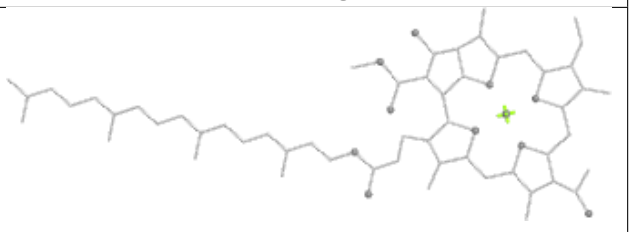
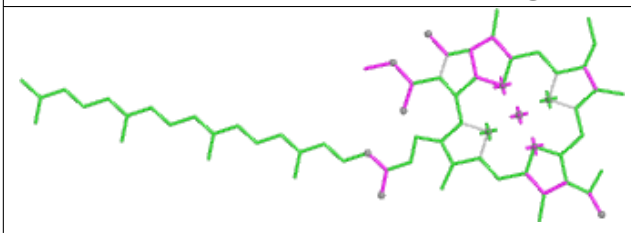


Rings

Ligand BCL A 101



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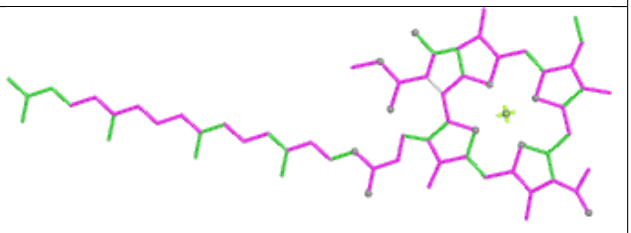
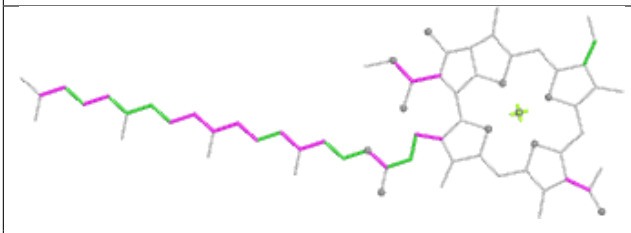


Bond angles



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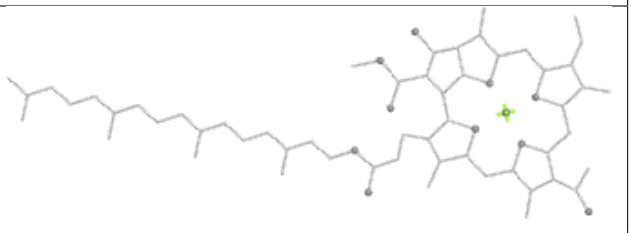

Rings

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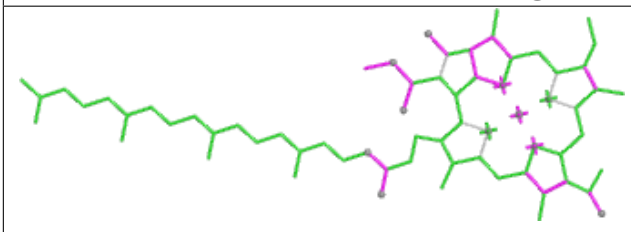

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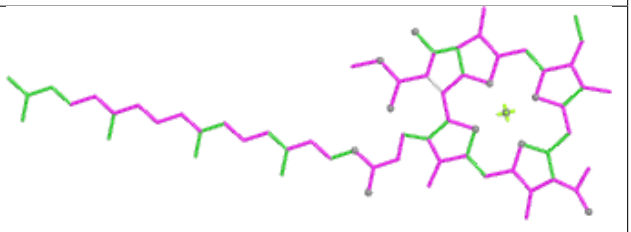
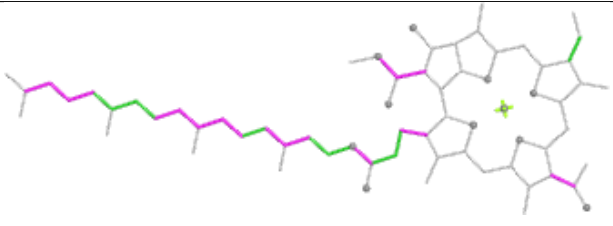


Bond angles



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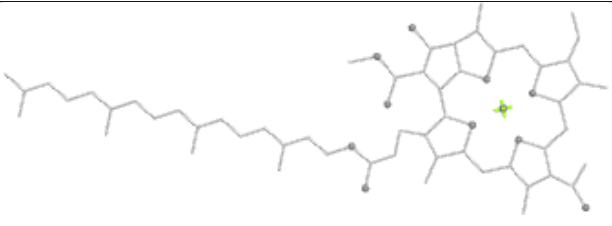
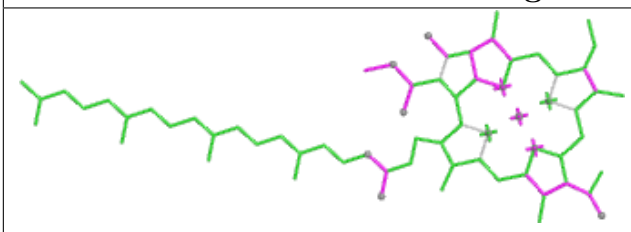
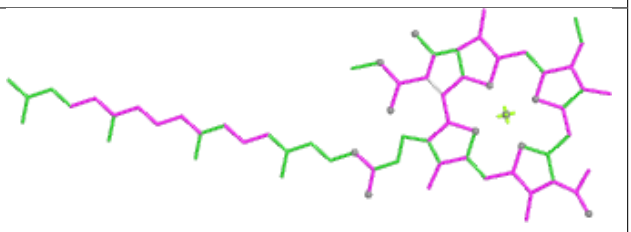


Rings

Ligand BCL U 101



Bond lengths



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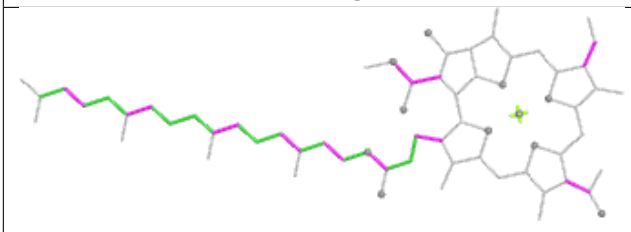

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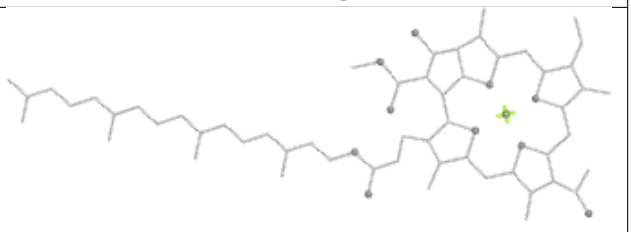
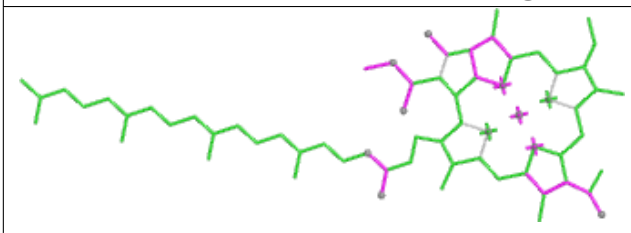


Rings

Ligand BCL W 101



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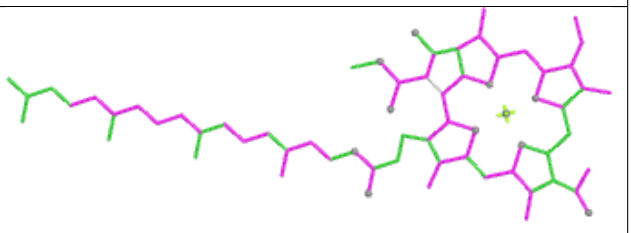

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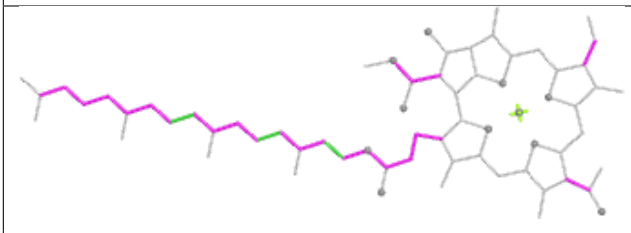

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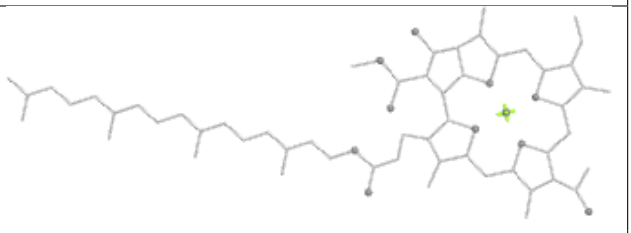

Rings

Ligand KGD J 102



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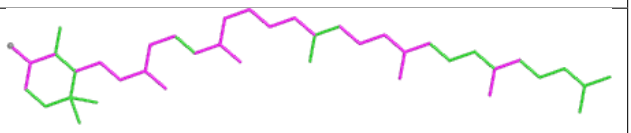

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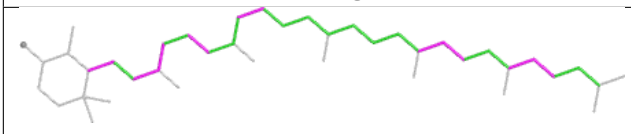

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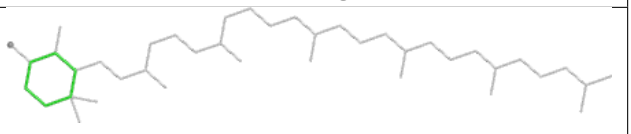

Rings

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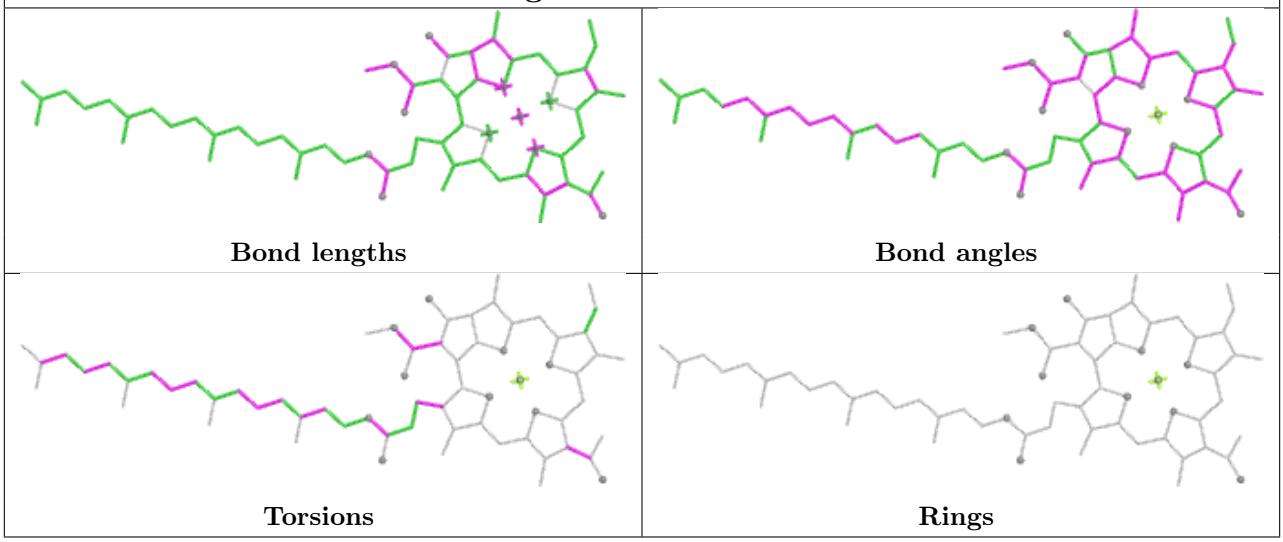

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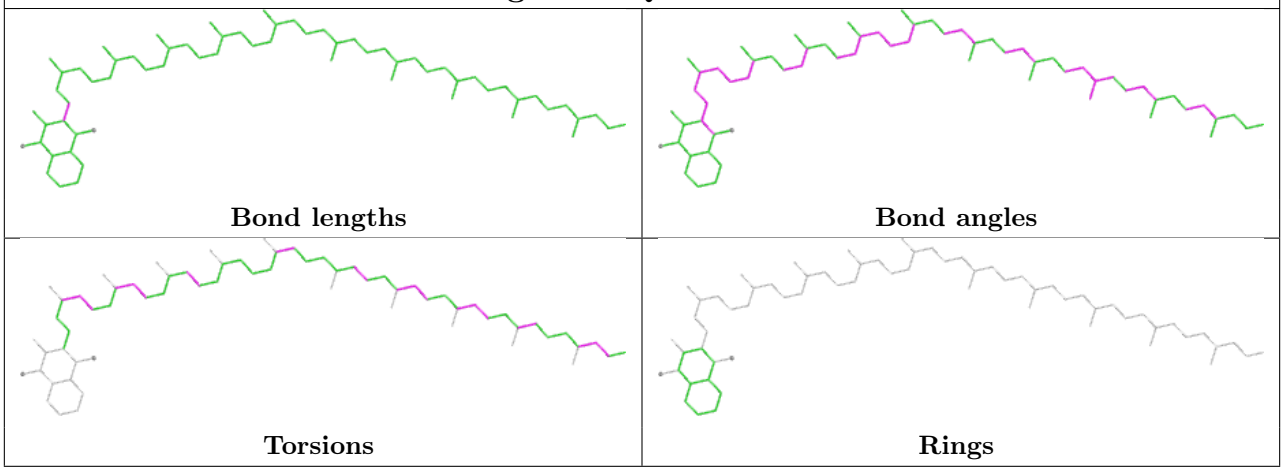

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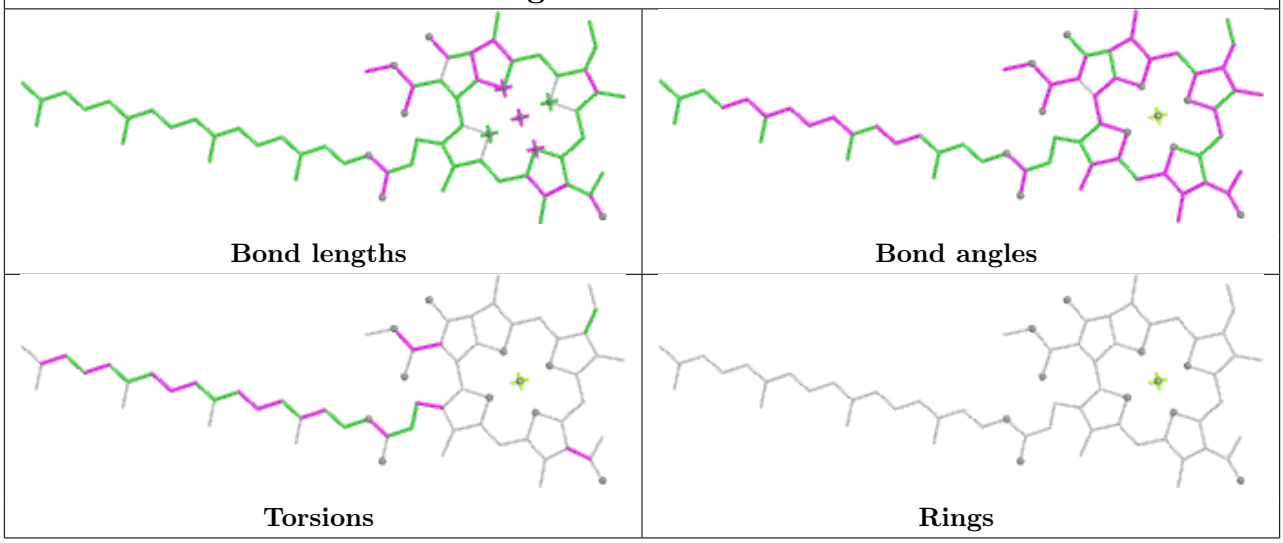

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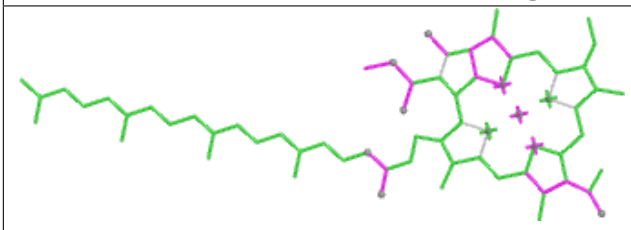

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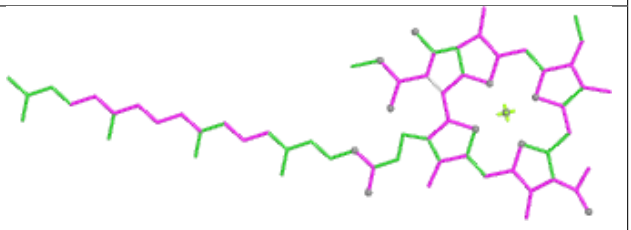
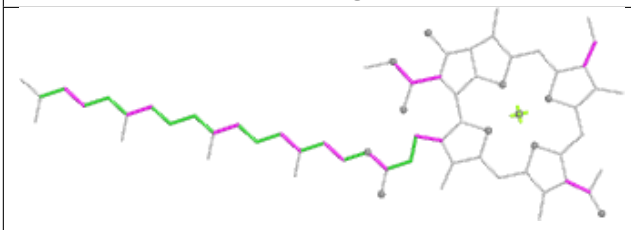


Bond angles



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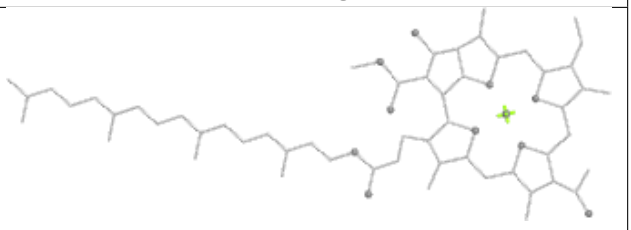

Rings

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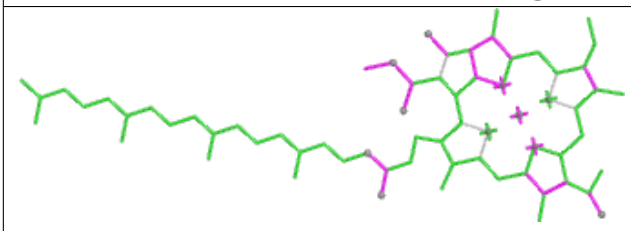

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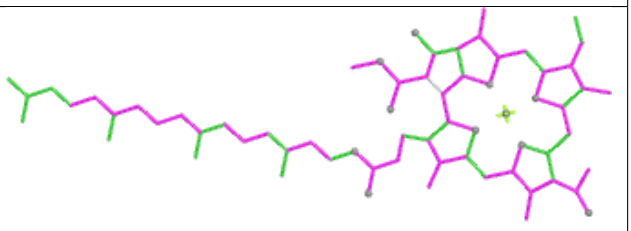

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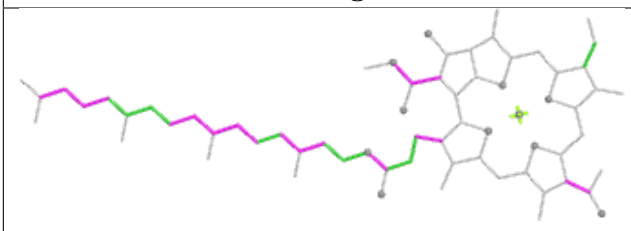

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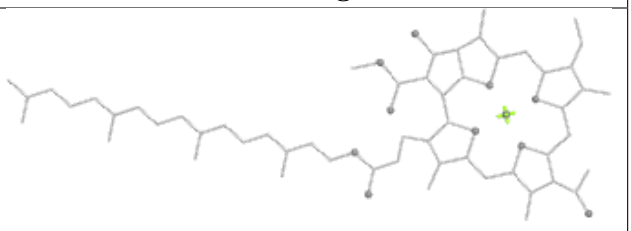

Rings

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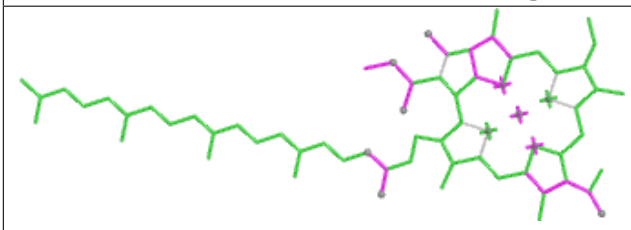

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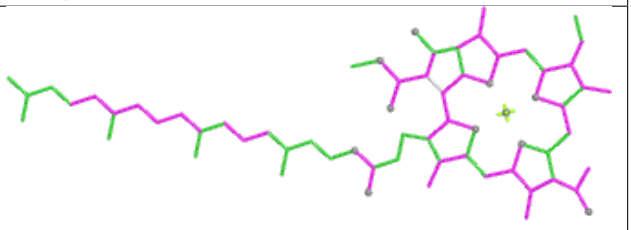

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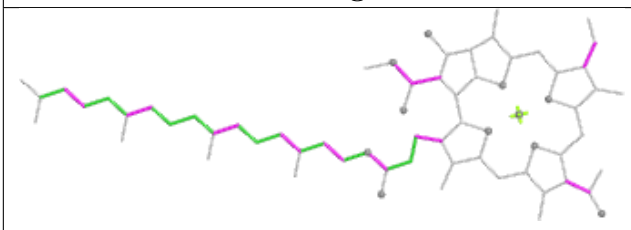

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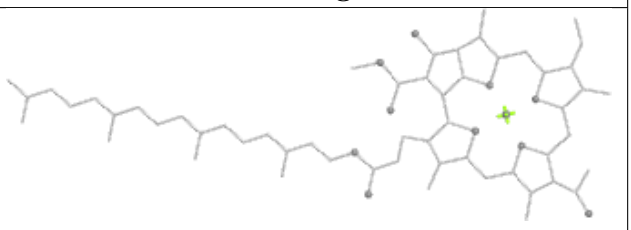

Rings

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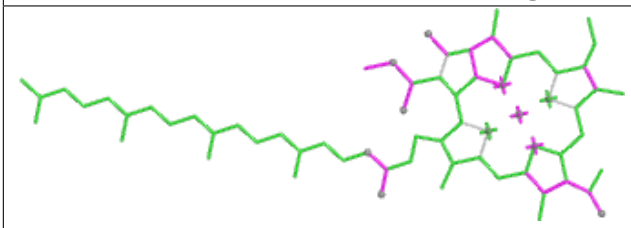
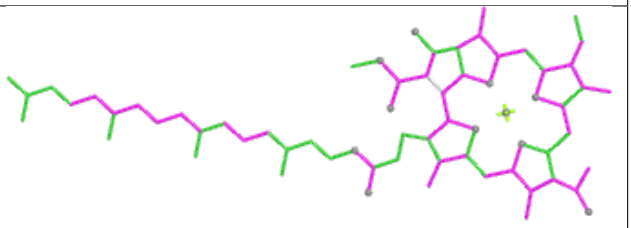
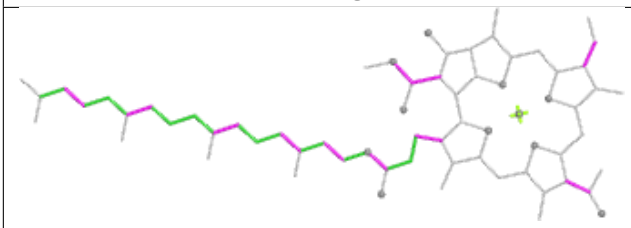
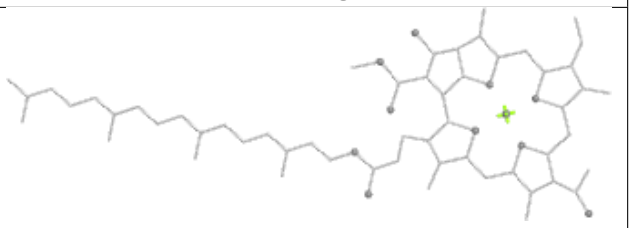
 Bond lengths	 Bond angles
 Torsions	 Rings

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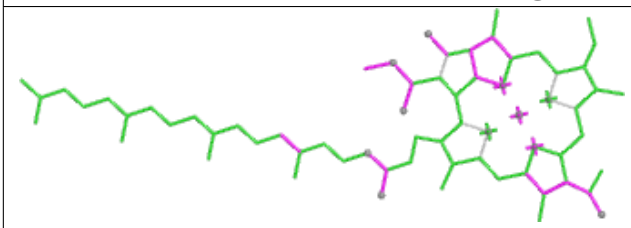
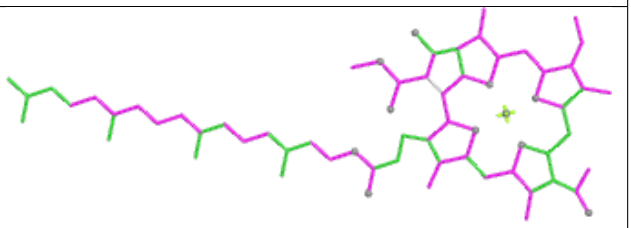
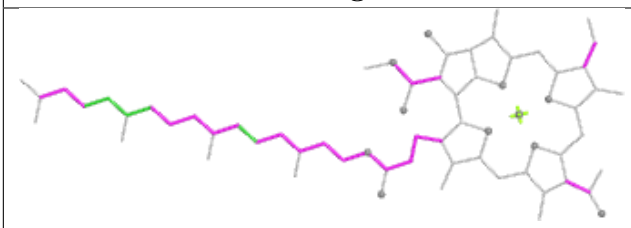
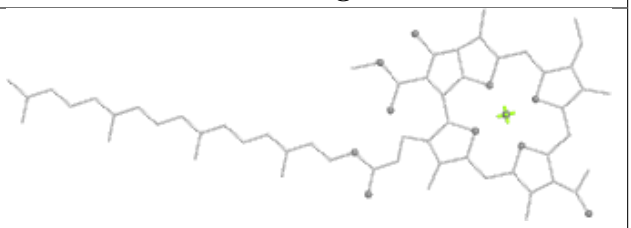
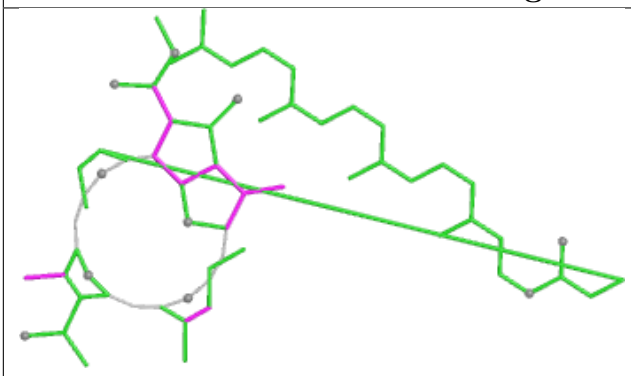
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPH L 404



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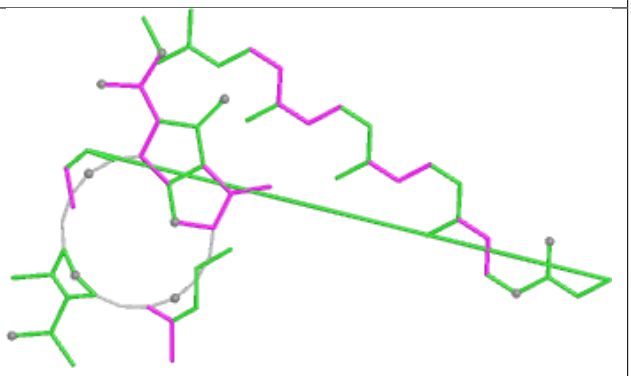
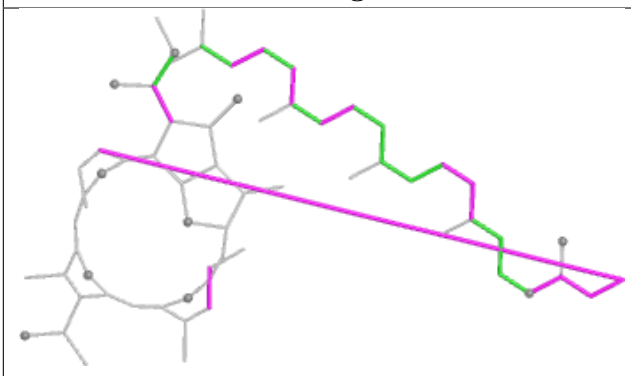


Bond angles



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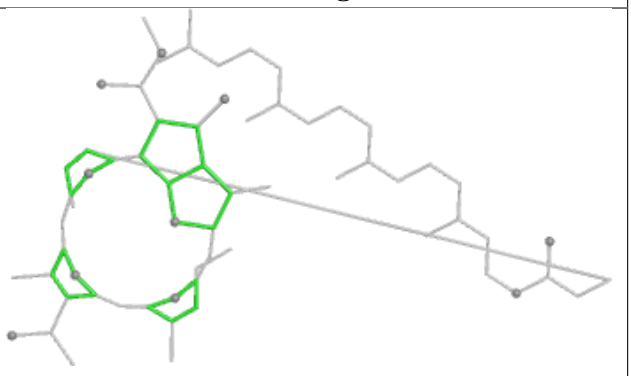

Rings

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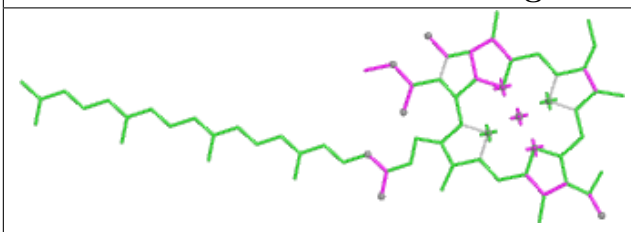

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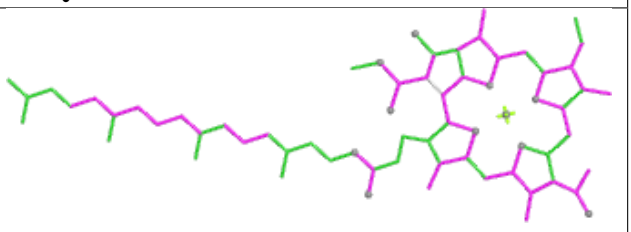

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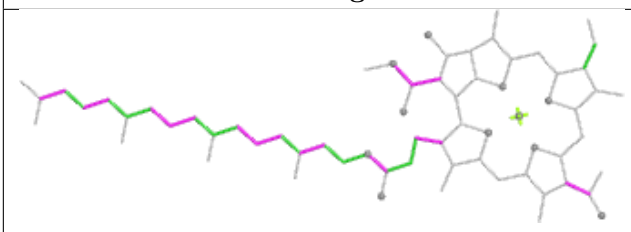

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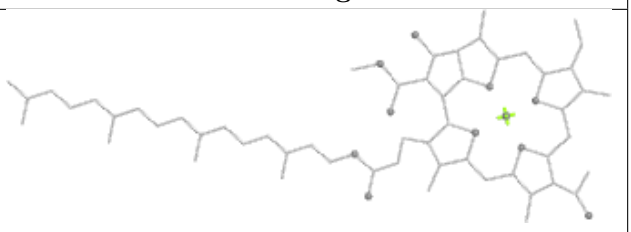
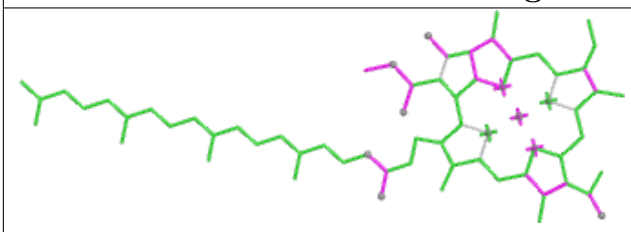


Rings

Ligand BCL U 102



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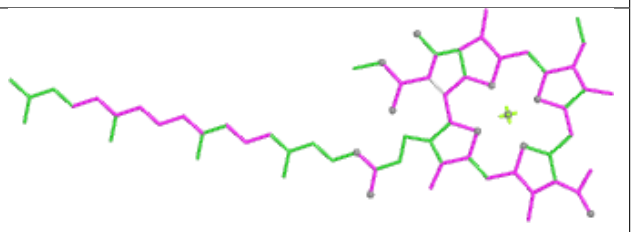

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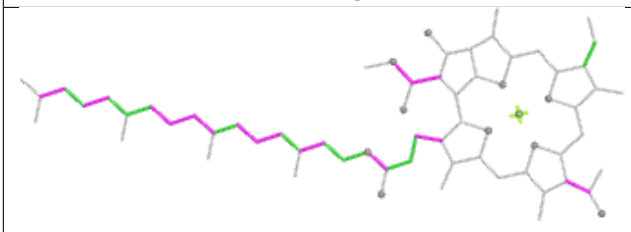

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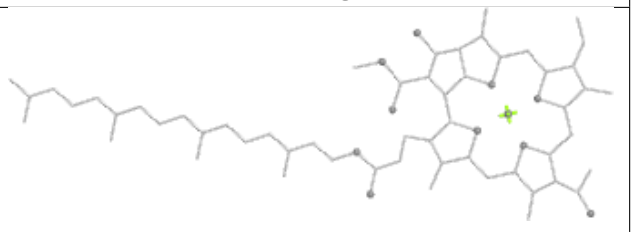

Rings

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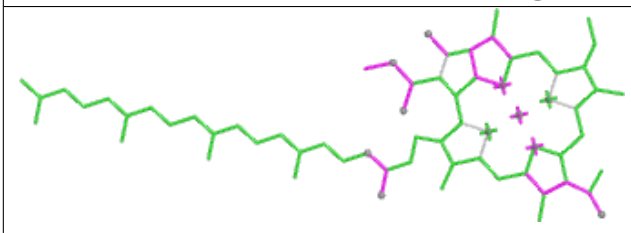

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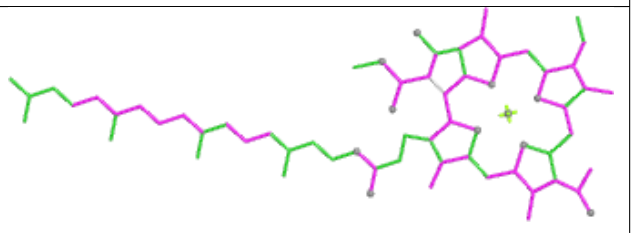

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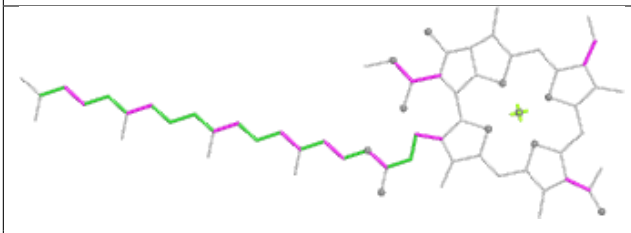

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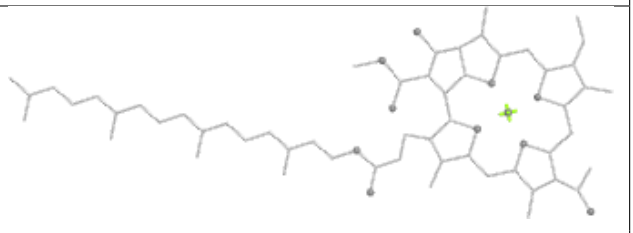

Rings

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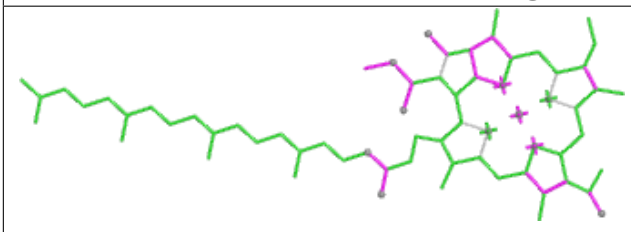

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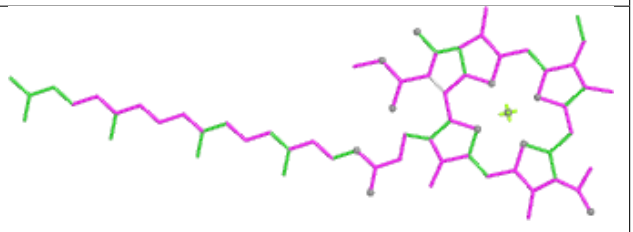

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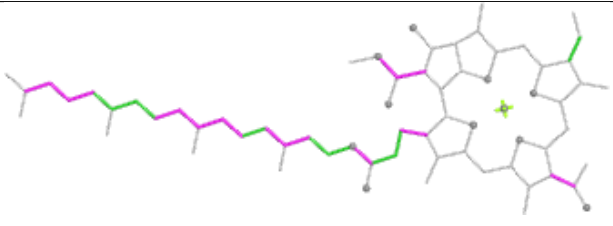

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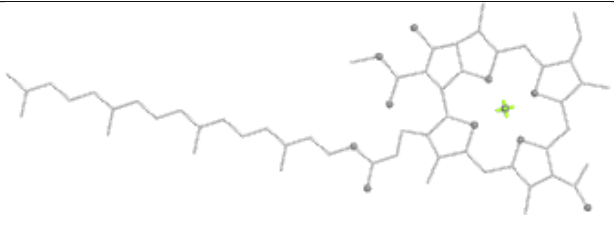

Rings

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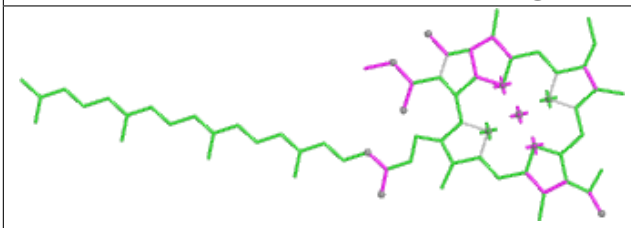
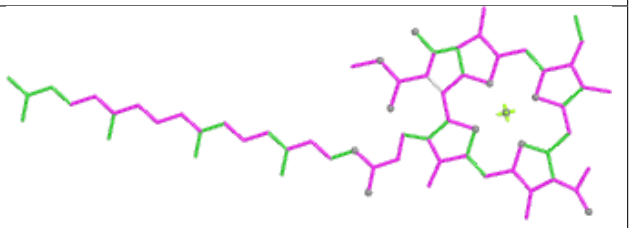
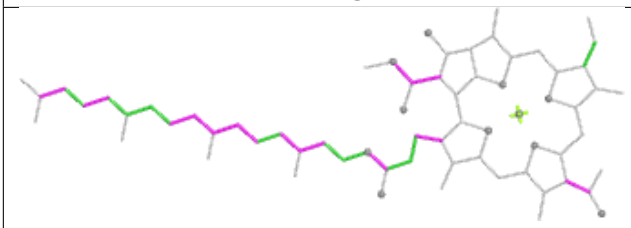
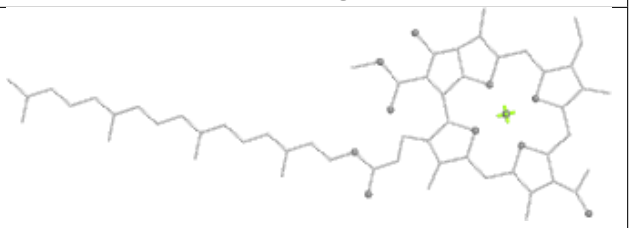
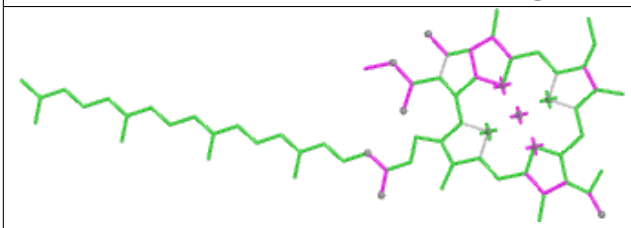
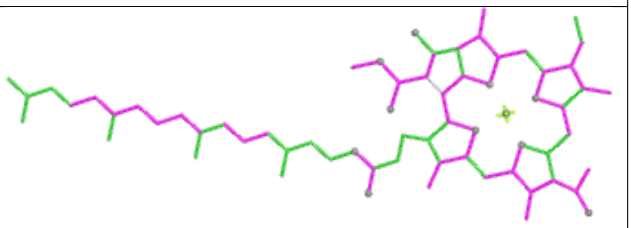
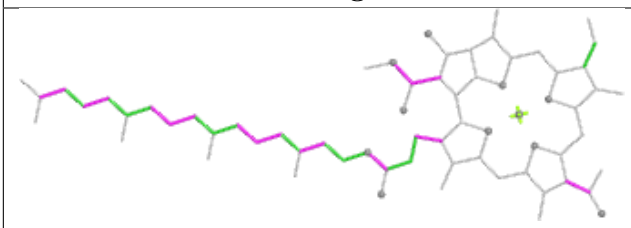
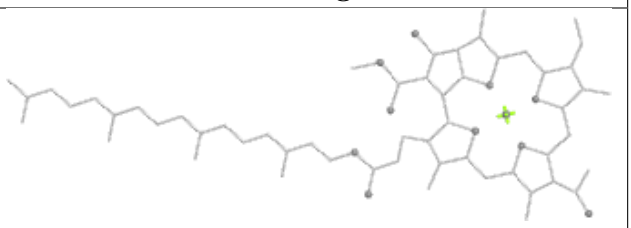
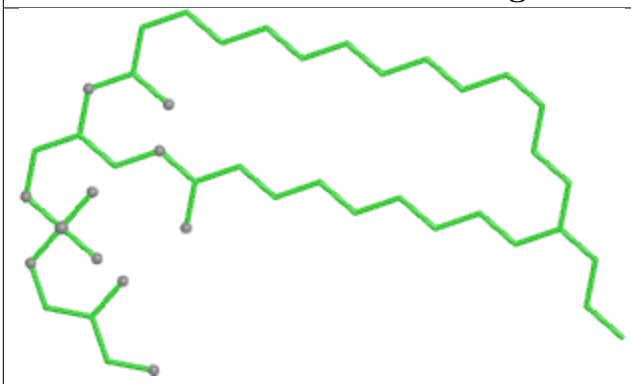
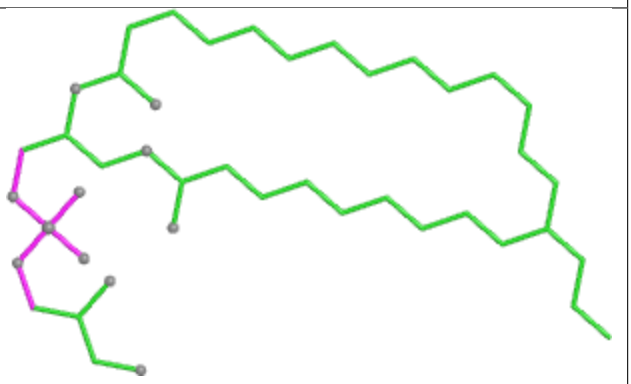
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL 8 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

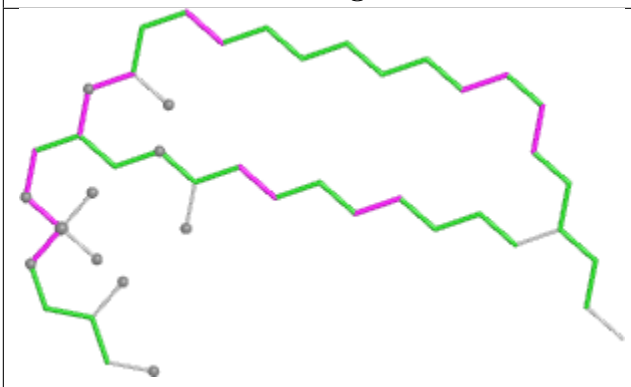
Ligand PGV M 1006



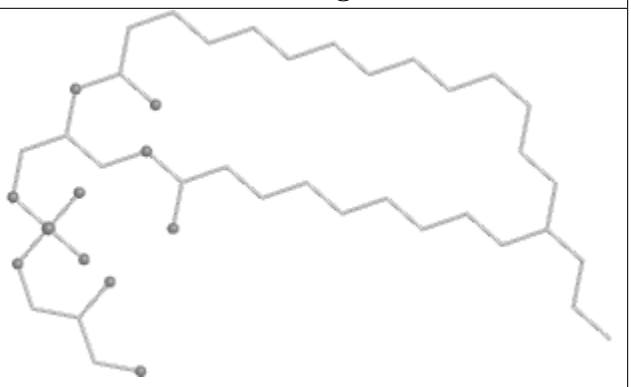
Bond lengths



Bond angles

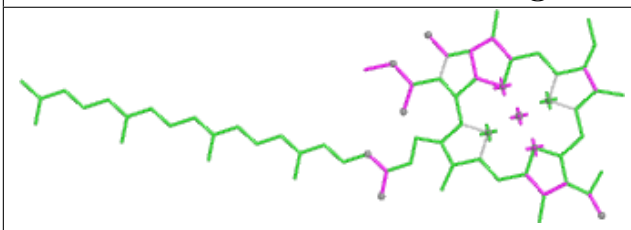


Torsions

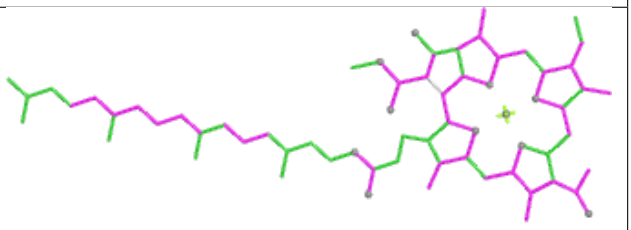


Rings

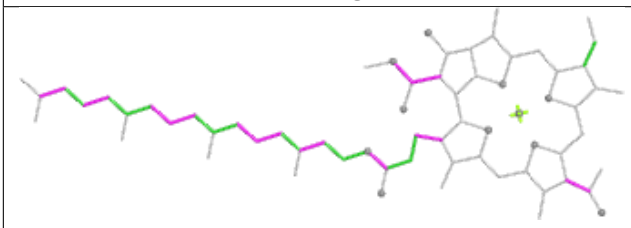
Ligand BCL 6 102



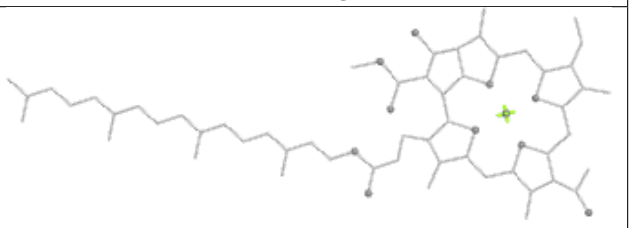
Bond lengths



Bond angles

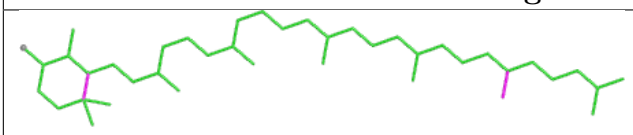


Torsions

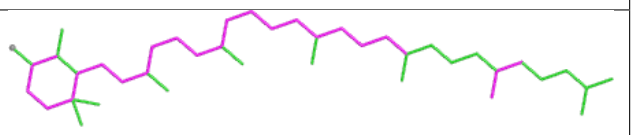


Rings

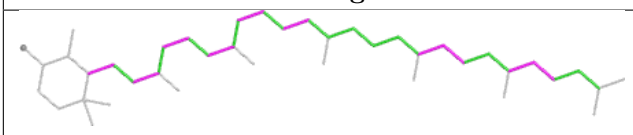
Ligand KGD 9 101



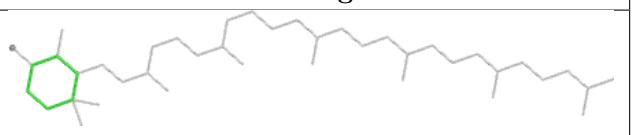
Bond lengths



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.

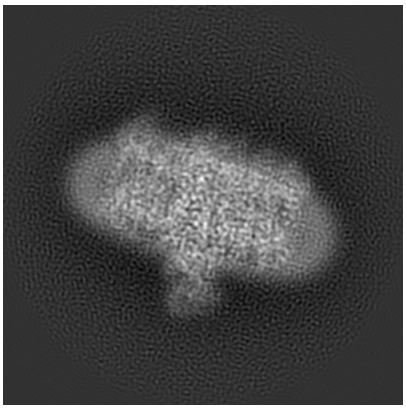
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34839. These allow visual inspection of the internal detail of the map and identification of artifacts.

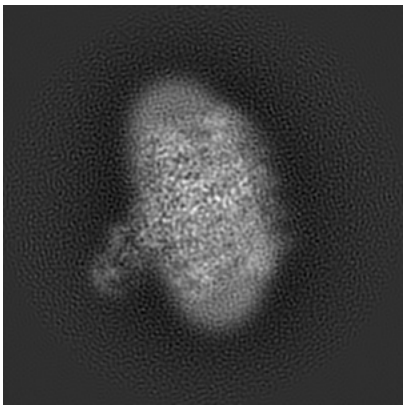
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

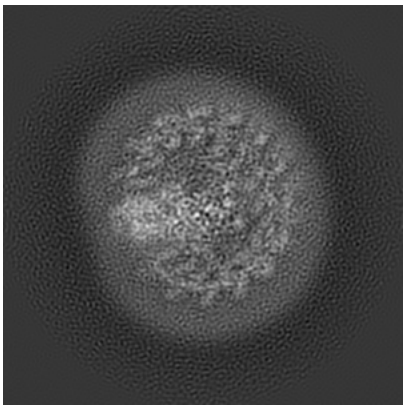
6.1.1 Primary map



X

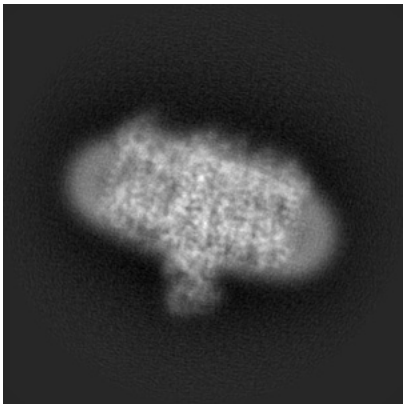


Y

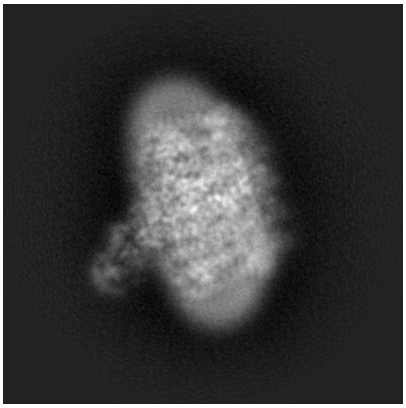


Z

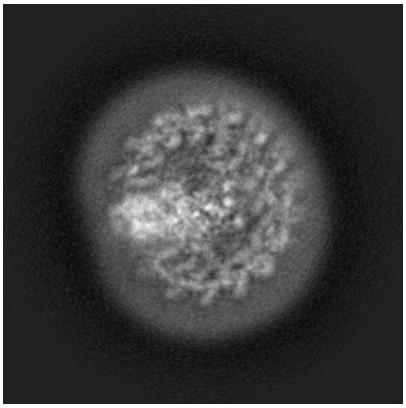
6.1.2 Raw map



X



Y

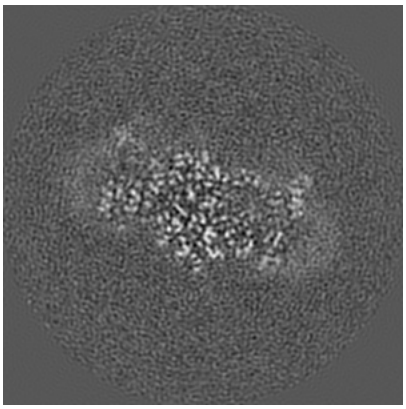


Z

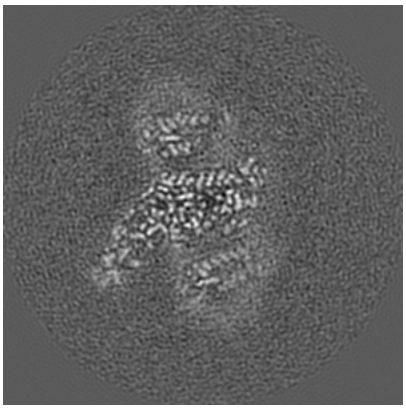
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

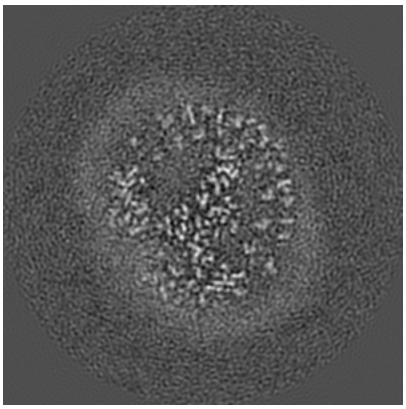
6.2.1 Primary map



X Index: 132

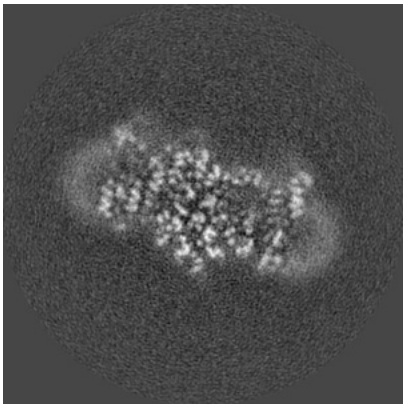


Y Index: 132

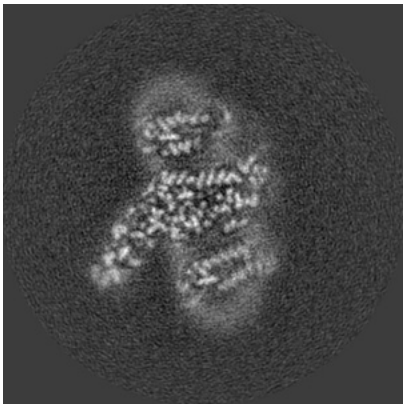


Z Index: 132

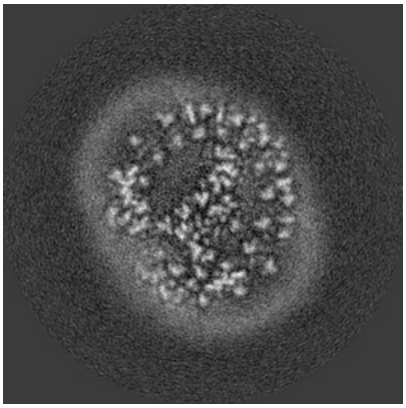
6.2.2 Raw map



X Index: 132



Y Index: 132

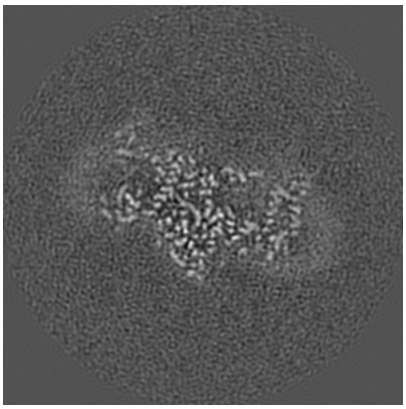


Z Index: 132

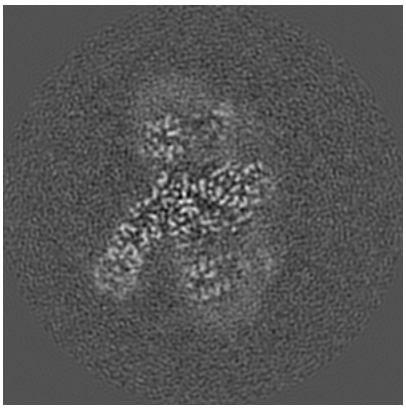
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

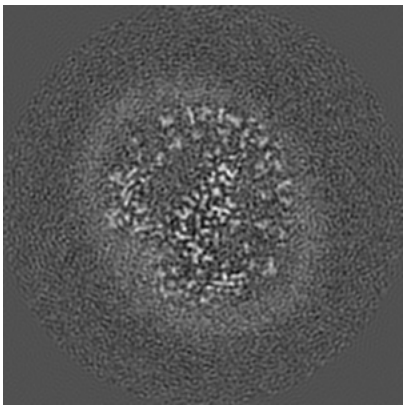
6.3.1 Primary map



X Index: 129

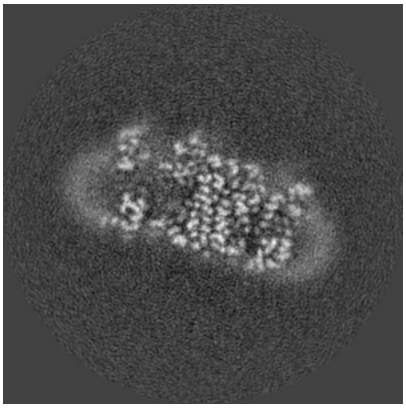


Y Index: 128

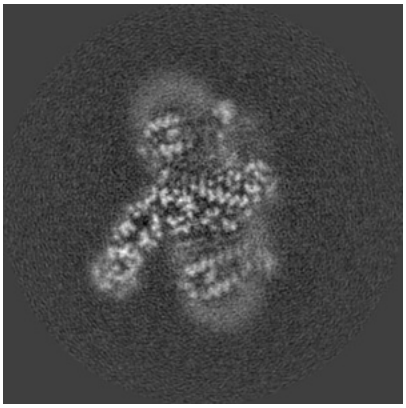


Z Index: 131

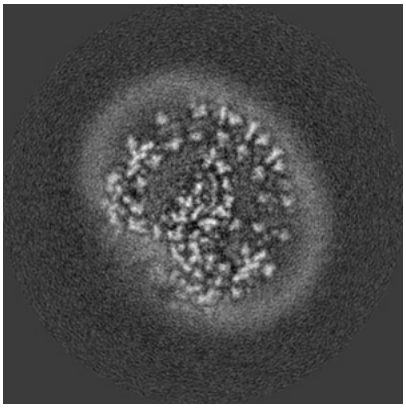
6.3.2 Raw map



X Index: 146



Y Index: 129

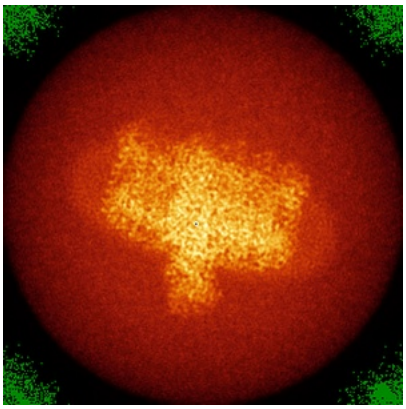


Z Index: 125

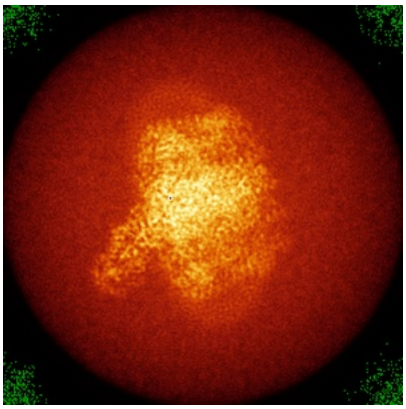
The images above show the largest variance slices of the map in three orthogonal directions.

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

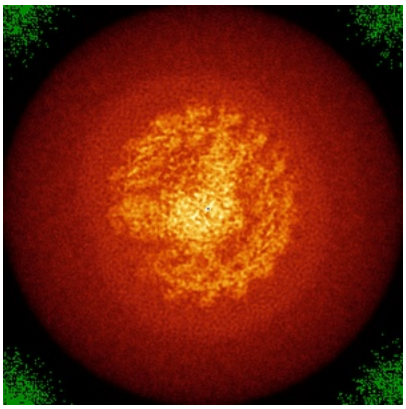
6.4.1 Primary map



X

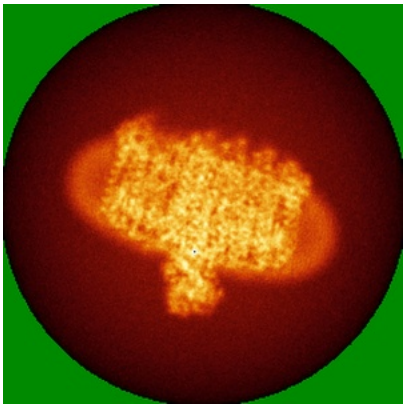


Y

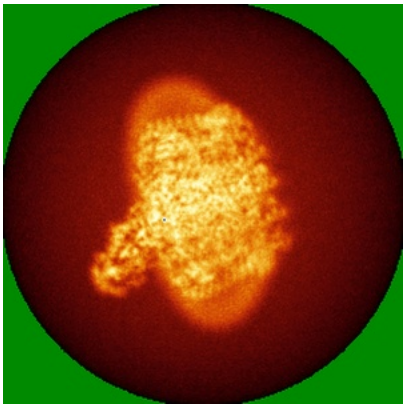


Z

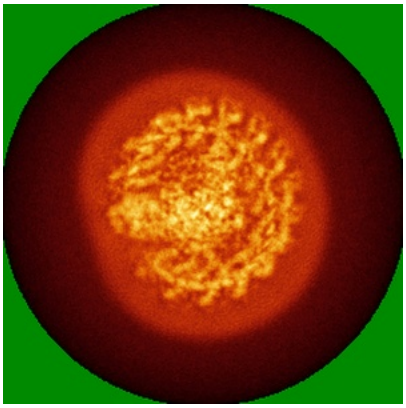
6.4.2 Raw map



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 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

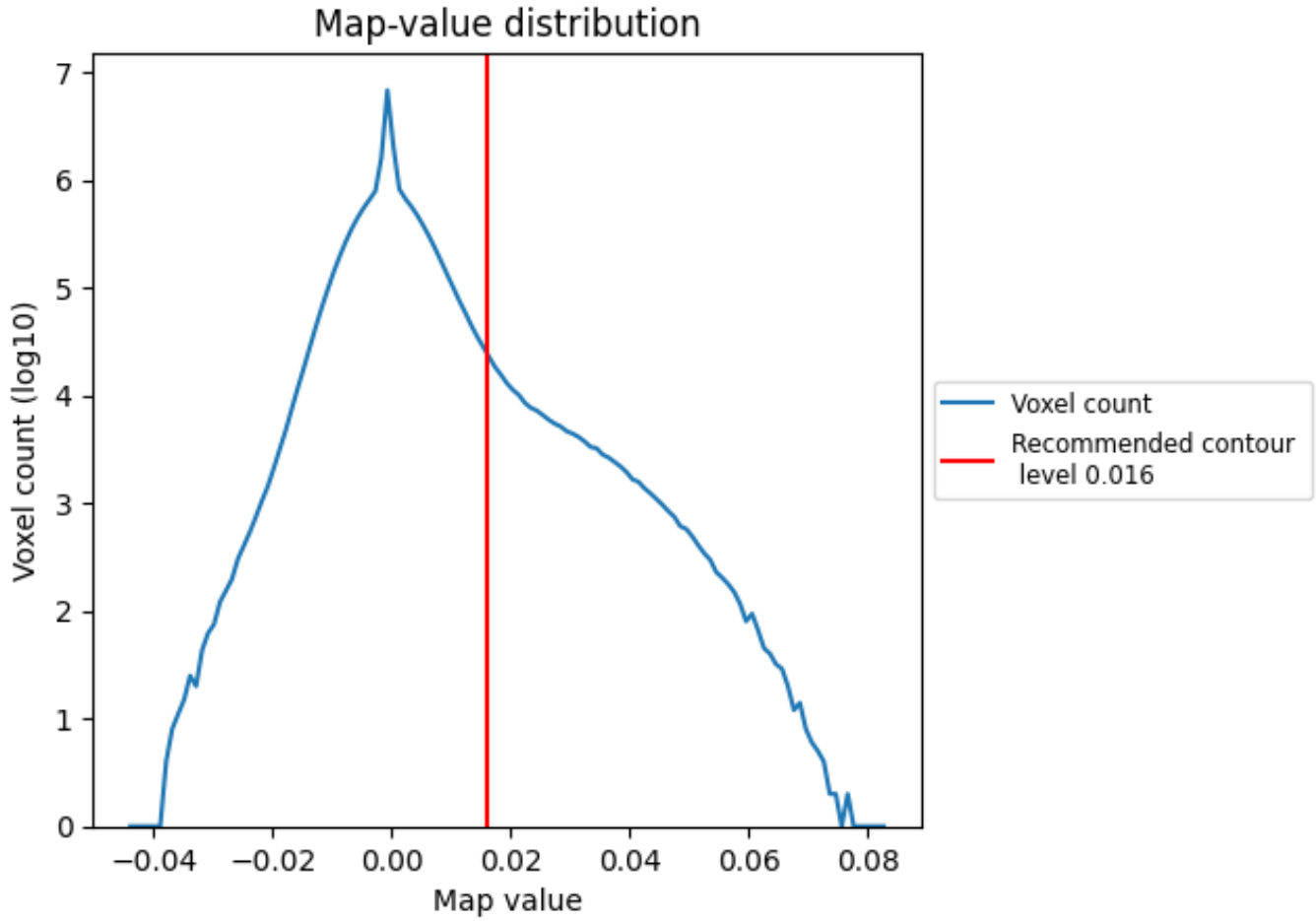
6.6 Mask visualisation (i)

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

7 Map analysis

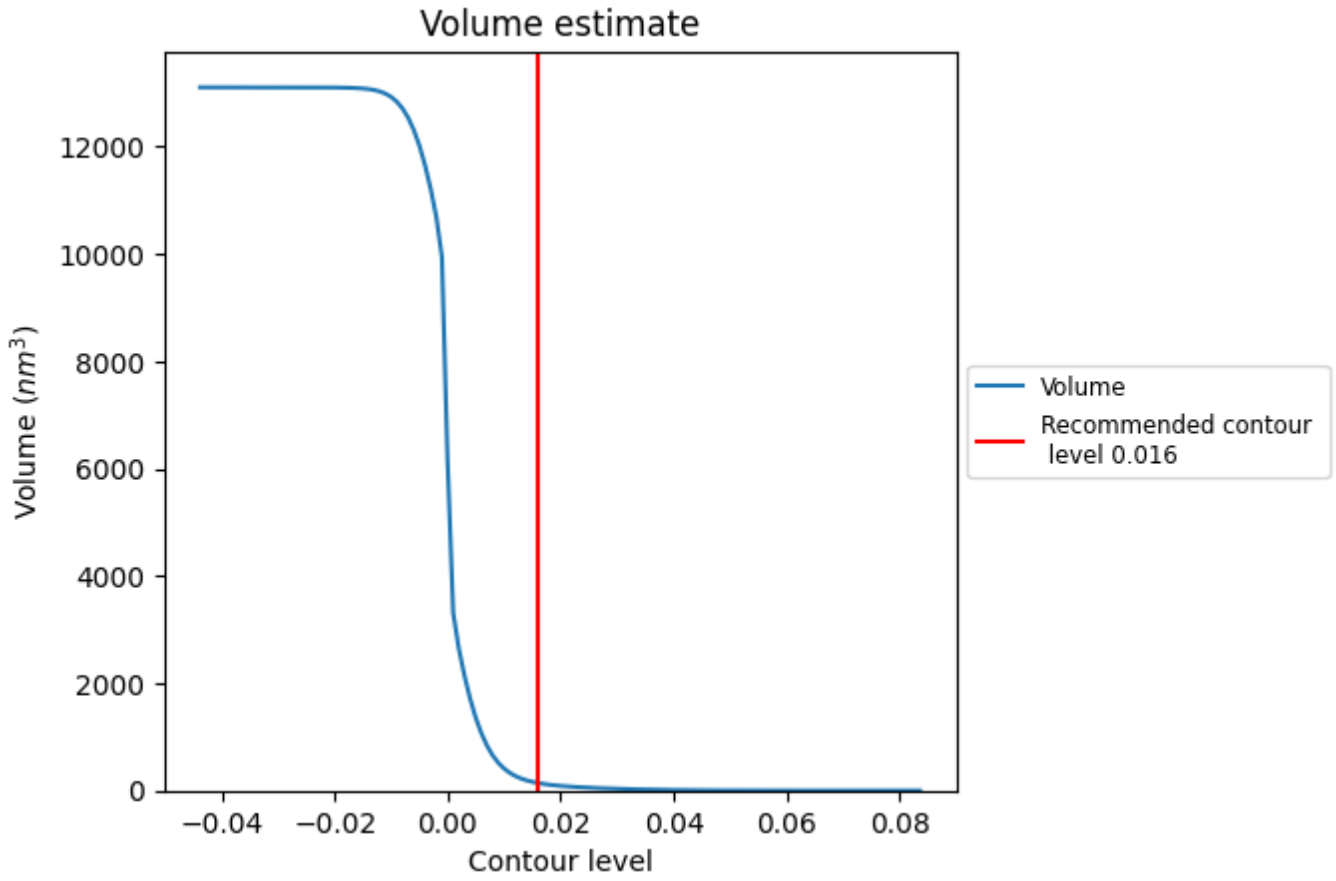
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

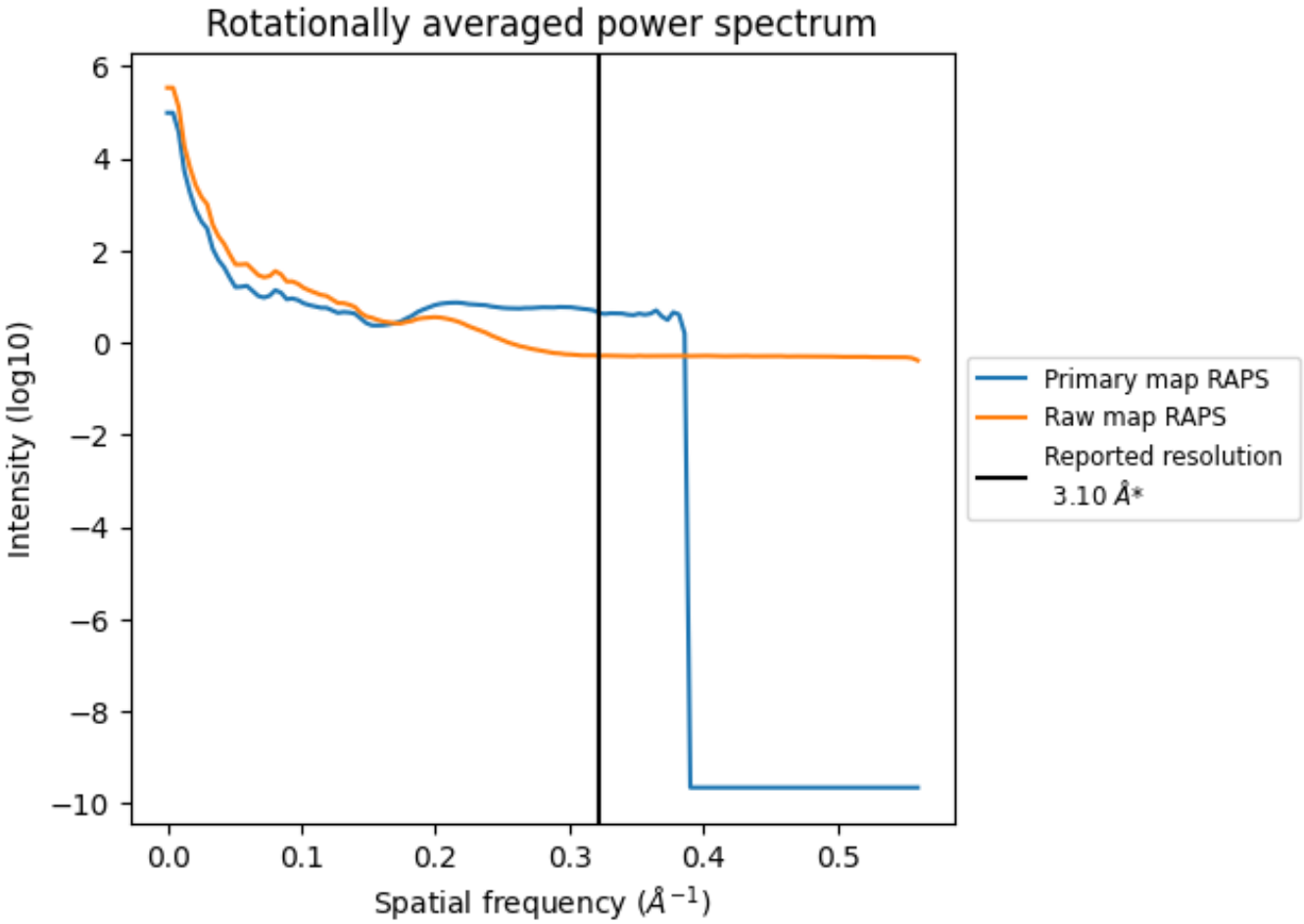
7.2 Volume estimate (i)



The volume at the recommended contour level is 140 nm^3; this corresponds to an approximate mass of 127 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)

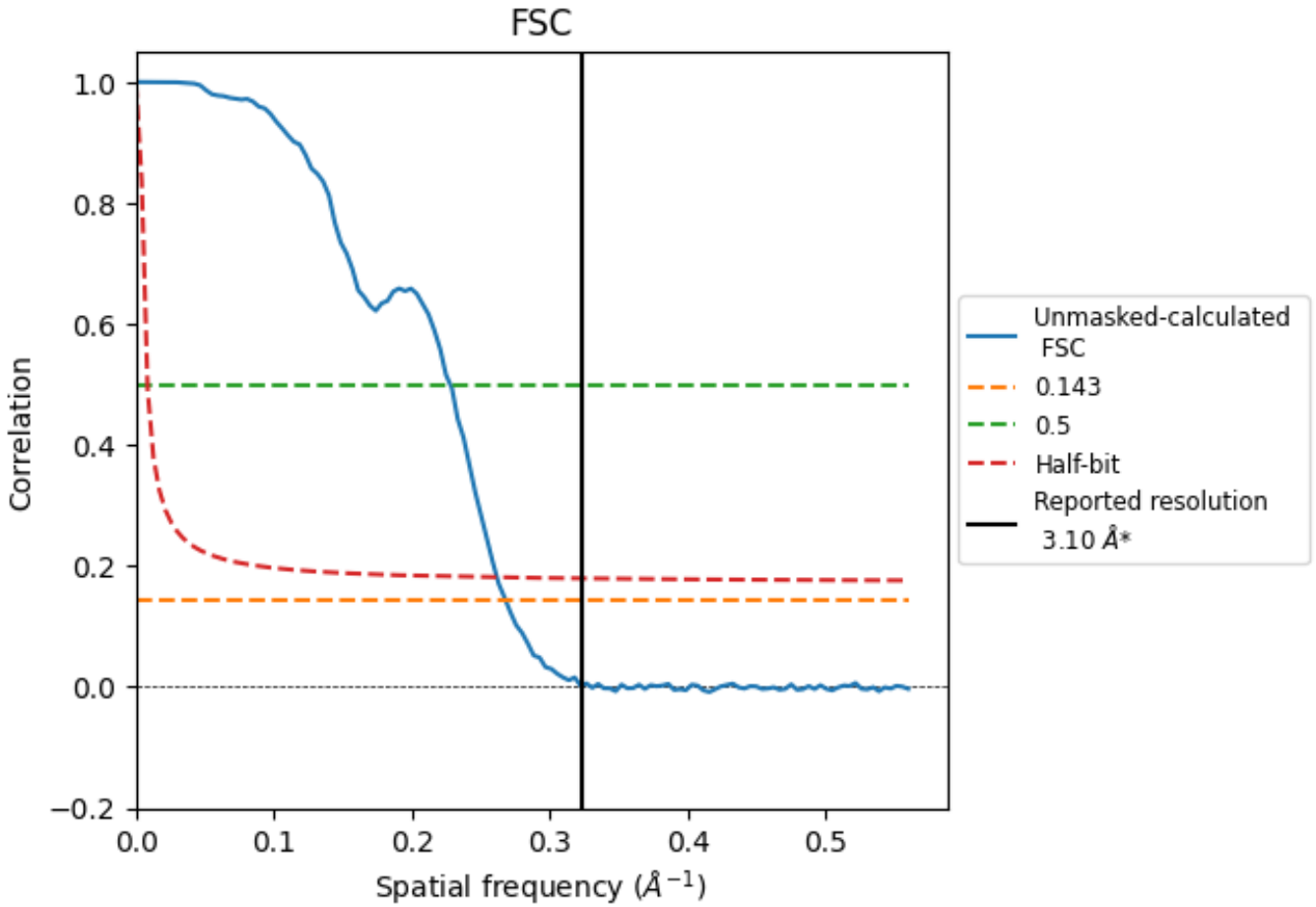


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	4.39	3.82

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

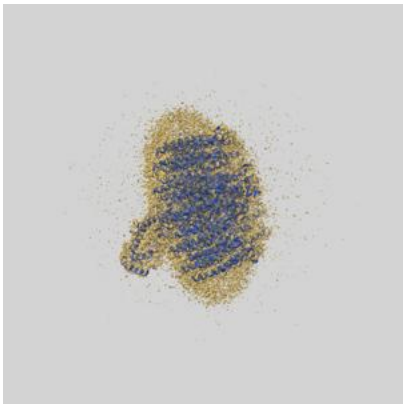
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34839 and PDB model 8HJV. Per-residue inclusion information can be found in section 3 on page 14.

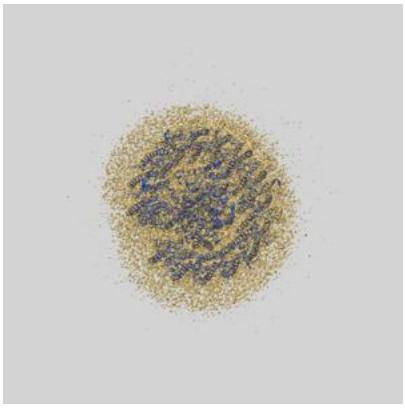
9.1 Map-model overlay



X



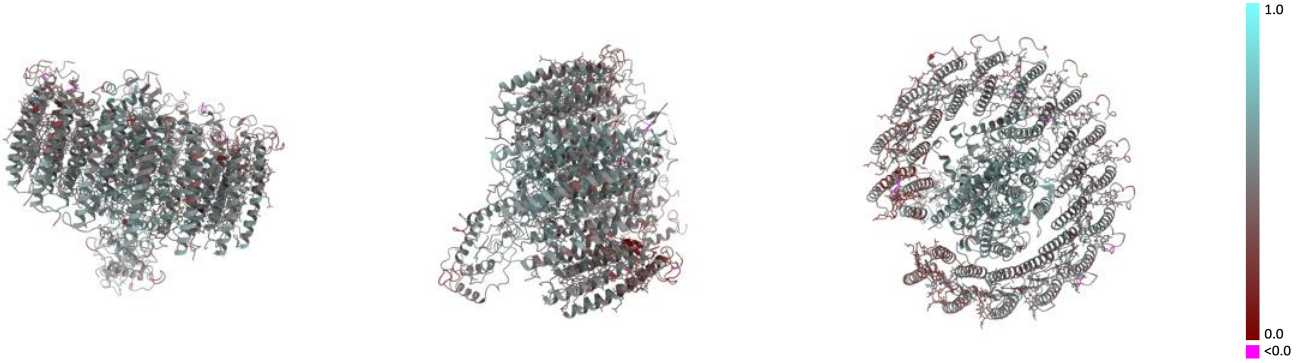
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 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.

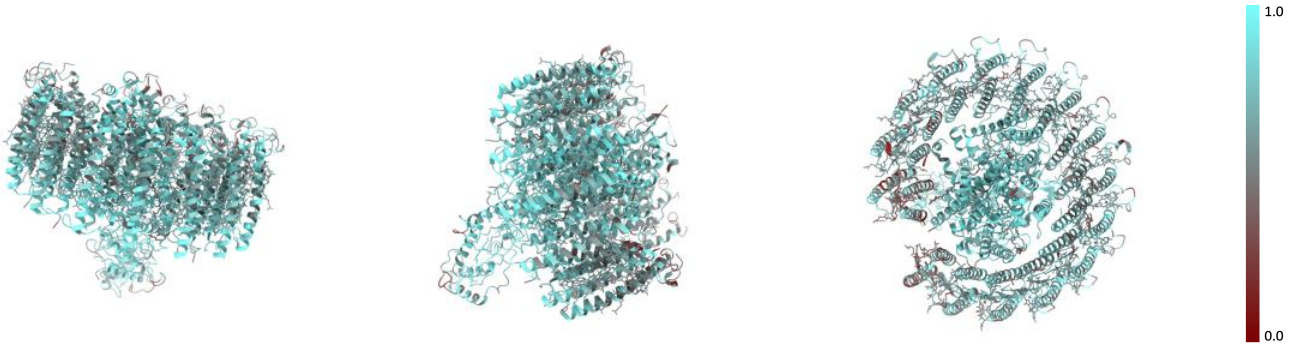
9.2 Q-score mapped to coordinate model (i)



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.

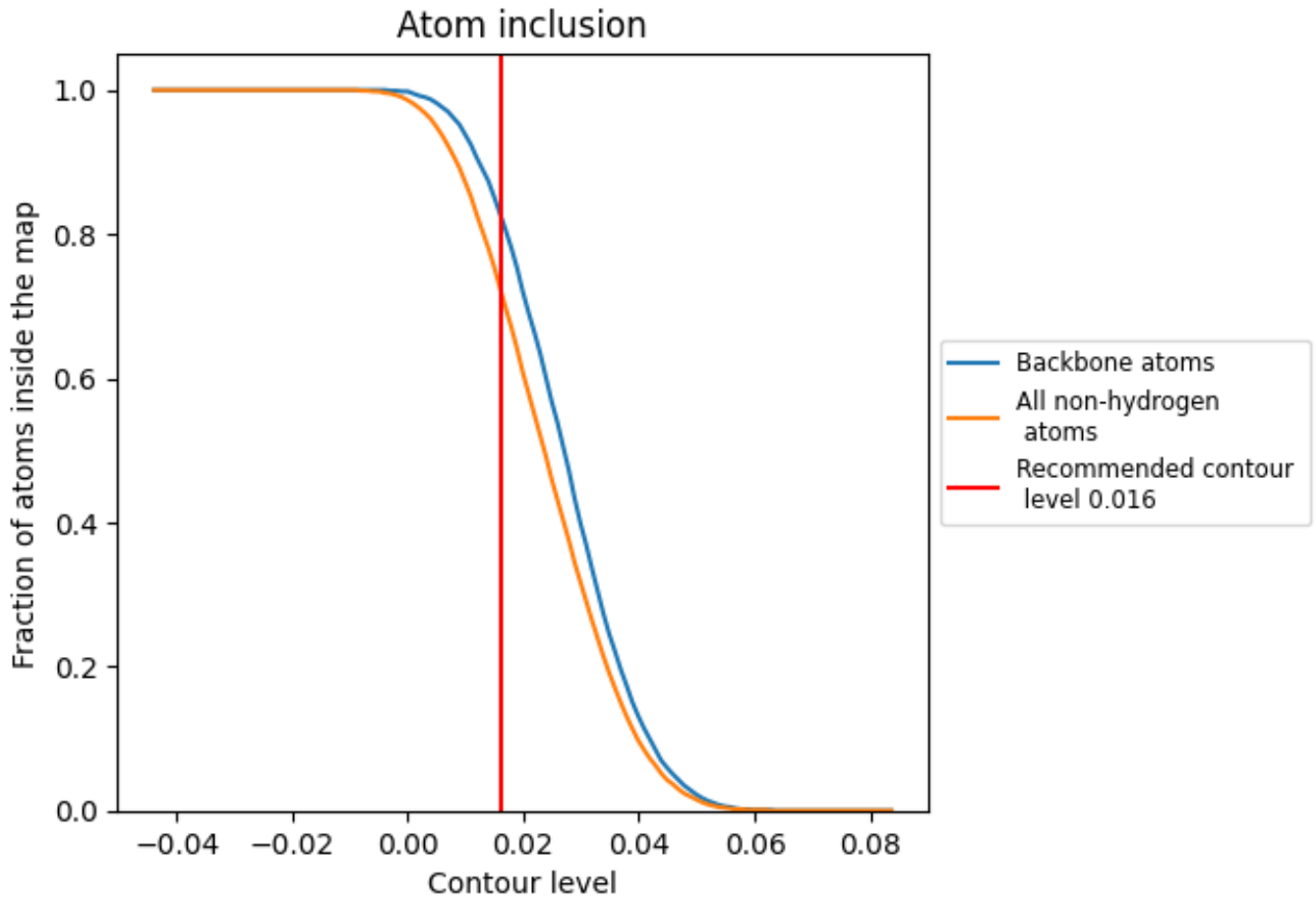
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7240	0.4780
0	0.7440	0.4750
1	0.6250	0.4370
2	0.4760	0.3260
3	0.6110	0.4170
4	0.6180	0.4030
5	0.6560	0.4360
6	0.6630	0.4360
7	0.7240	0.4890
8	0.6730	0.4480
9	0.6550	0.4520
A	0.7630	0.4950
B	0.7380	0.4830
C	0.7700	0.4790
D	0.6780	0.4480
E	0.7210	0.4690
F	0.6840	0.4710
G	0.6900	0.4610
H	0.6760	0.4500
I	0.6810	0.4590
J	0.6830	0.4900
K	0.7400	0.4670
L	0.8230	0.5480
M	0.8440	0.5500
N	0.7110	0.4840
O	0.6980	0.4550
P	0.6960	0.4610
Q	0.7190	0.4580
R	0.6900	0.4560
S	0.7150	0.4810
T	0.6840	0.4670
U	0.6400	0.4210
V	0.4830	0.3520
W	0.4990	0.3560
Y	0.7930	0.5540
Z	0.7880	0.5300

