



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 06:49 PM UTC

PDB ID : 5YQ7 / pdb_00005yq7
EMDB ID : EMD-6828
Title : Cryo-EM structure of the RC-LH core complex from *Roseiflexus castenholzii*
Authors : Shi, Y.; Xin, Y.Y.; Niu, T.X.; Wang, Q.Q.; Niu, W.Q.; Huang, X.J.; Ding, W.; Blankenship, R.E.; Xu, X.L.; Sun, F.
Deposited on : 2017-11-05
Resolution : 4.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

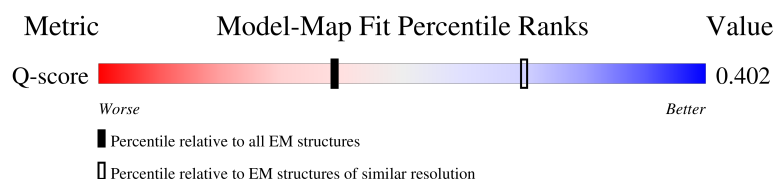
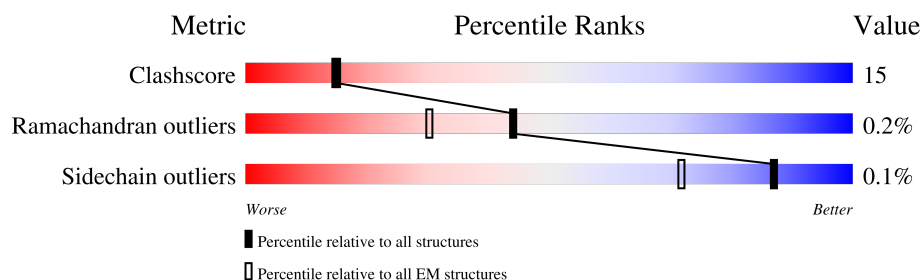
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 4.10 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	6458 (3.60 - 4.60)

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 $\leq 5\%$. 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	9% 64% 16% 20%
1	2	55	18% 65% 15% 20%
1	4	55	15% 62% 18% 20%
1	6	55	15% 69% 11% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8	55	
1	B	55	
1	E	55	
1	G	55	
1	I	55	
1	K	55	
1	O	55	
1	Q	55	
1	S	55	
1	U	55	
1	W	55	
2	L	310	
3	C	320	
4	1	42	
4	3	42	
4	5	42	
4	7	42	
4	9	42	
4	A	42	
4	D	42	
4	F	42	
4	H	42	
4	J	42	
4	N	42	
4	P	42	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	R	42	
4	T	42	
4	V	42	
5	Y	25	
6	X	23	
7	M	306	

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
8	BCL	B	102	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 20009 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	E	44	Total	C	N	O	S	0	0
			325	220	54	50	1		
1	B	44	Total	C	N	O	S	0	0
			325	220	54	50	1		
1	0	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	8	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	6	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	4	44	Total	C	N	O	S	0	0
			319	216	54	48	1		
1	2	44	Total	C	N	O	S	0	0
			326	220	55	50	1		
1	K	44	Total	C	N	O	S	0	0
			325	220	54	50	1		
1	I	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	G	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	W	44	Total	C	N	O	S	0	0
			312	208	54	49	1		
1	U	44	Total	C	N	O	S	0	0
			329	223	55	50	1		
1	S	44	Total	C	N	O	S	0	0
			326	220	55	50	1		
1	Q	44	Total	C	N	O	S	0	0
			318	214	54	49	1		
1	O	44	Total	C	N	O	S	0	0
			325	220	54	50	1		

- Molecule 2 is a protein called Precursor for L subunits of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	309	Total	C	N	O	S	0	0
			2292	1526	372	389	5		

- Molecule 3 is a protein called Cytochrome subunit of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	293	Total	C	N	O	S	0	0
			2041	1294	352	382	13		

- Molecule 4 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	V	36	Total	C	N	O	S	0	0
			263	179	40	43	1		
4	R	36	Total	C	N	O		0	0
			257	174	40	43			
4	P	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	N	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	J	36	Total	C	N	O	S	0	0
			263	179	40	43	1		
4	H	36	Total	C	N	O	S	0	0
			260	176	40	43	1		
4	F	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	D	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	A	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	9	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	7	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	5	36	Total	C	N	O	S	0	0
			266	182	40	43	1		
4	3	36	Total	C	N	O	S	0	0
			260	176	40	43	1		
4	1	36	Total	C	N	O	S	0	0
			245	161	40	43	1		

- Molecule 5 is a protein called Peptide from Precursor for L and M subunits of photosynthetic

reaction center.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	25	Total	C	N	O	0	0
			125	75	25	25		

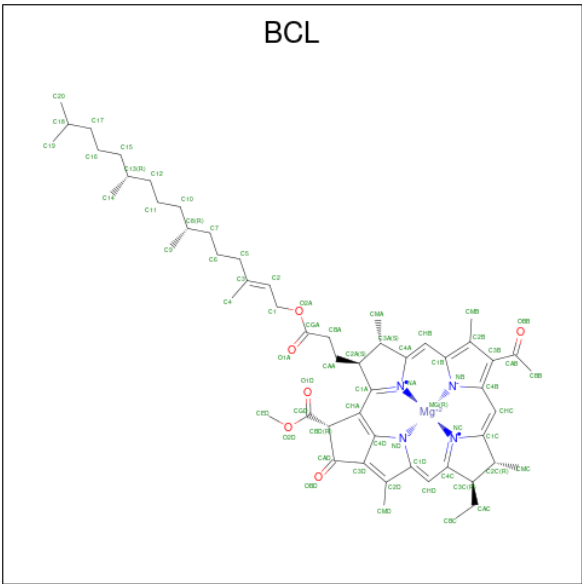
- Molecule 6 is a protein called Subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	X	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 7 is a protein called Precursor for M subunits of photosynthetic reaction center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	305	Total	C	N	O	S	0	0
			2373	1603	381	385	4		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
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	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	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

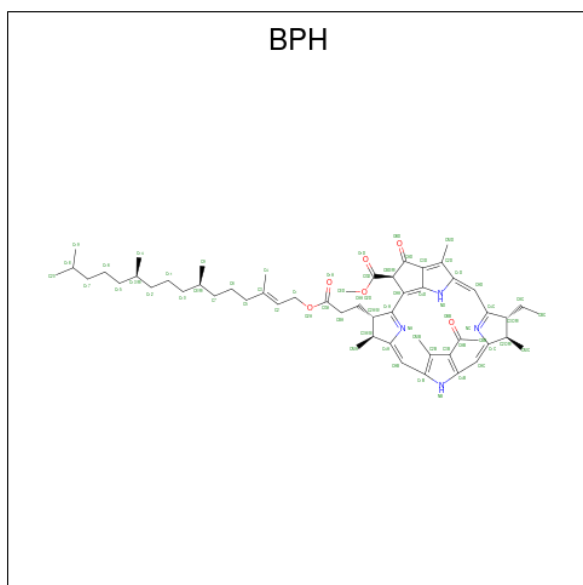
Mol	Chain	Residues	Atoms					AltConf
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

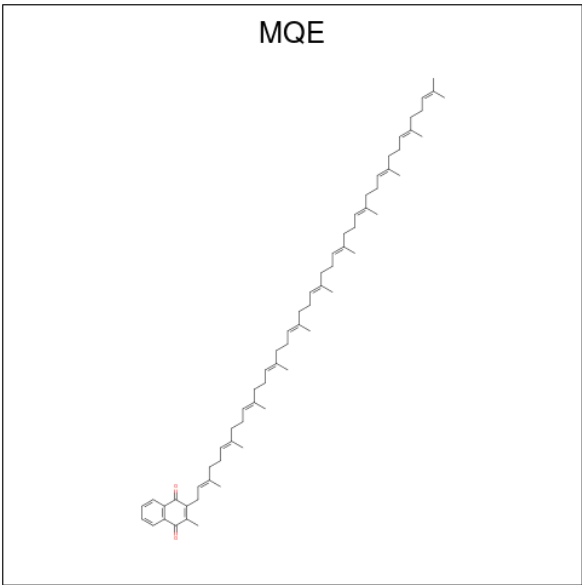
Mol	Chain	Residues	Atoms					AltConf
8	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



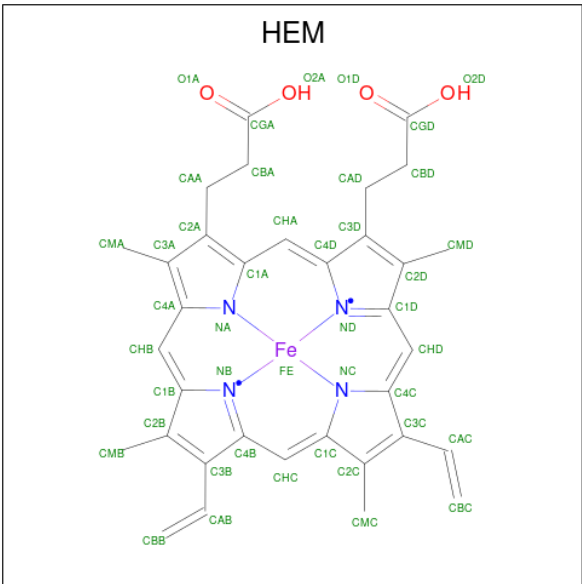
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 10 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
10	L	1	Total	C	O	0
			68	66	2	
10	M	1	Total	C	O	0
			68	66	2	

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



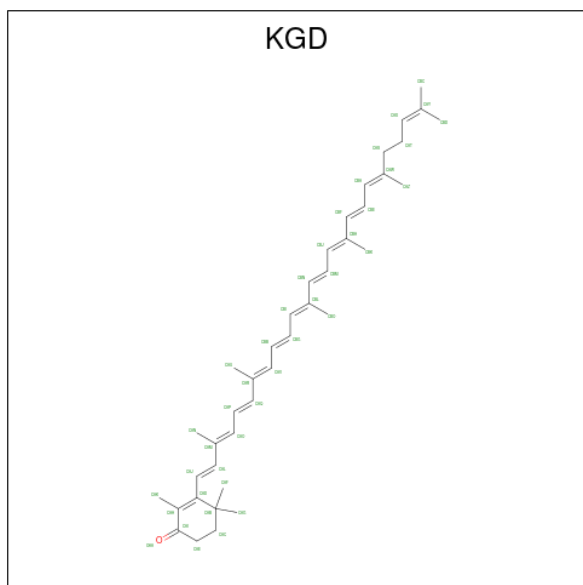
Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

Continued on next page...

Continued from previous page...

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

- Molecule 12 is beta,psi-caroten-4-one (CCD ID: KGD) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			AltConf
12	T	1	Total	C	O	0
			41	40	1	
12	T	1	Total	C	O	0
			41	40	1	
12	R	1	Total	C	O	0
			41	40	1	
12	N	1	Total	C	O	0
			41	40	1	
12	N	1	Total	C	O	0
			41	40	1	
12	J	1	Total	C	O	0
			41	40	1	
12	H	1	Total	C	O	0
			41	40	1	
12	F	1	Total	C	O	0
			41	40	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			41	40	1	
12	9	1	Total	C	O	0
			41	40	1	
12	9	1	Total	C	O	0
			41	40	1	
12	5	1	Total	C	O	0
			41	40	1	
12	3	1	Total	C	O	0
			41	40	1	
12	3	1	Total	C	O	0
			41	40	1	

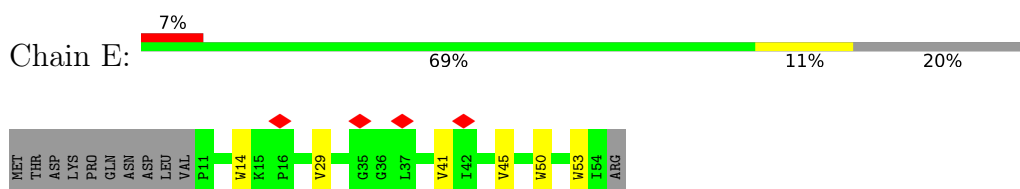
- Molecule 13 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

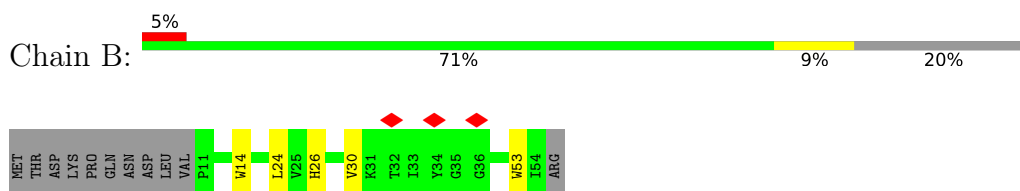
3 Residue-property plots [i](#)

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.

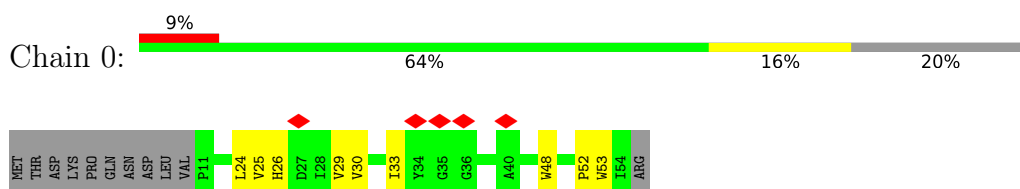
- Molecule 1: Beta subunit of light-harvesting 1



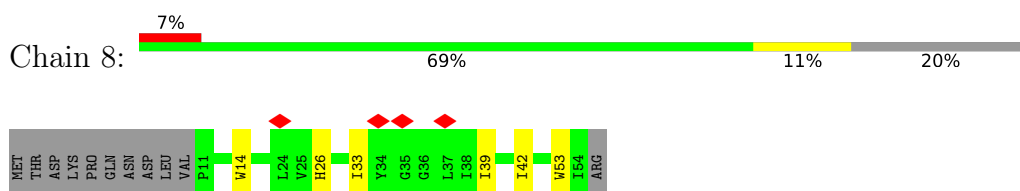
- Molecule 1: Beta subunit of light-harvesting 1



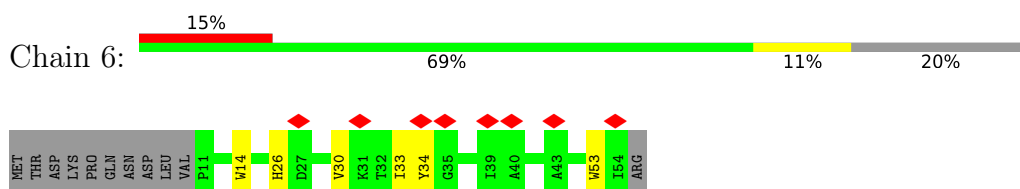
- Molecule 1: Beta subunit of light-harvesting 1



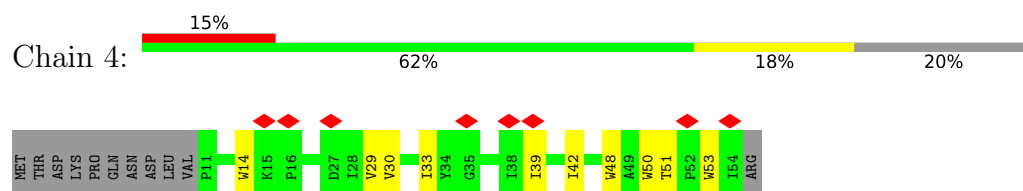
- Molecule 1: Beta subunit of light-harvesting 1



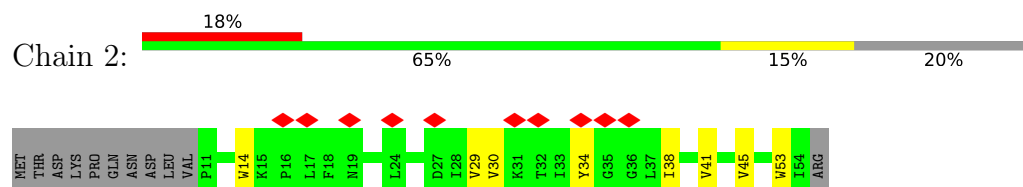
- Molecule 1: Beta subunit of light-harvesting 1



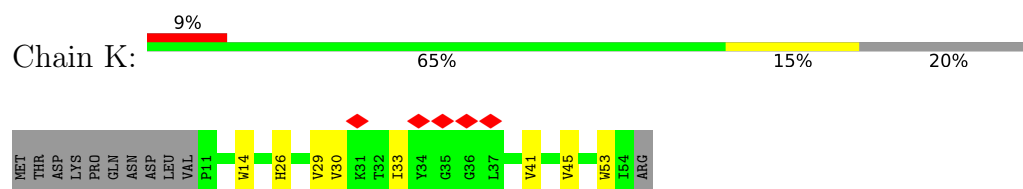
- Molecule 1: Beta subunit of light-harvesting 1



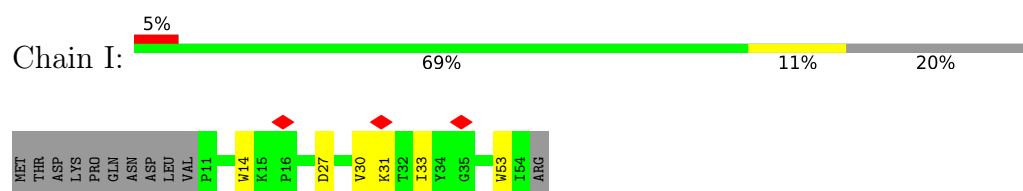
- Molecule 1: Beta subunit of light-harvesting 1



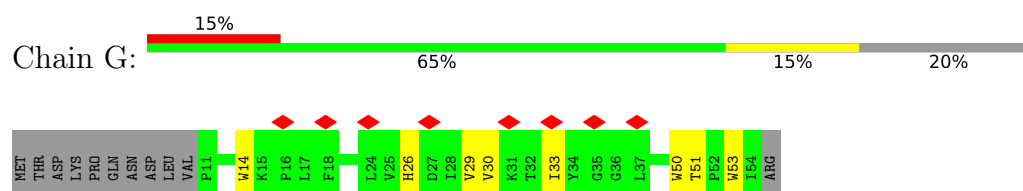
- Molecule 1: Beta subunit of light-harvesting 1



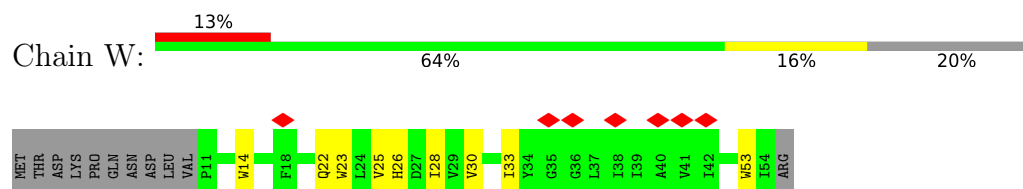
- Molecule 1: Beta subunit of light-harvesting 1



- Molecule 1: Beta subunit of light-harvesting 1



- Molecule 1: Beta subunit of light-harvesting 1

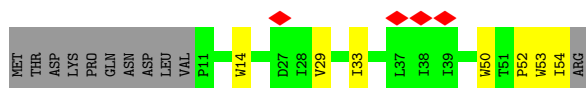


- Molecule 1: Beta subunit of light-harvesting 1





- Molecule 1: Beta subunit of light-harvesting 1



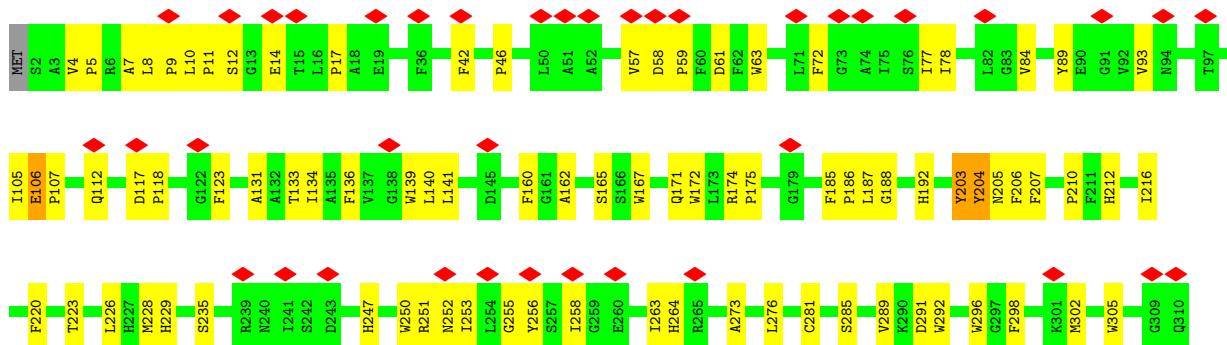
- Molecule 1: Beta subunit of light-harvesting 1



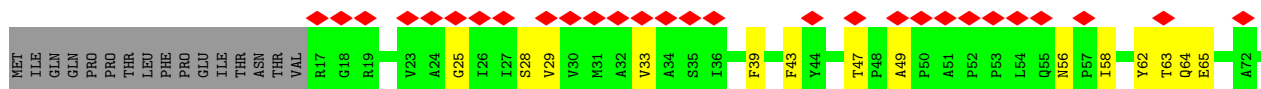
- Molecule 1: Beta subunit of light-harvesting 1

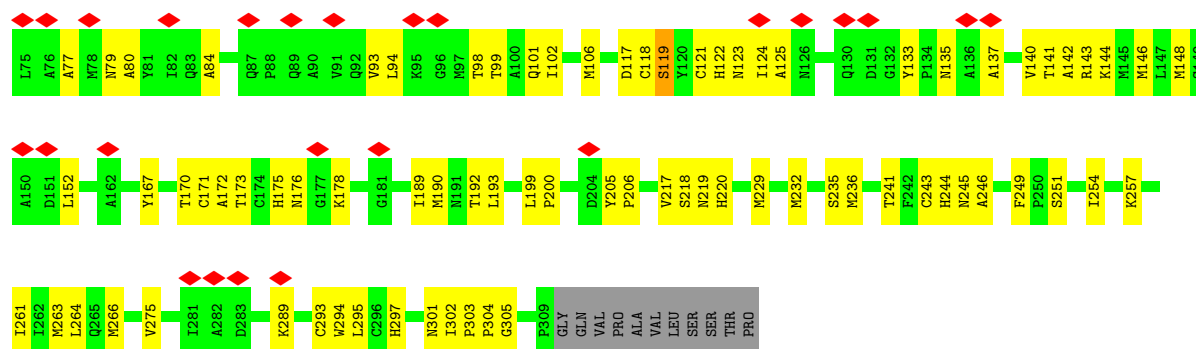


- Molecule 2: Precursor for L subunits of photosynthetic reaction center

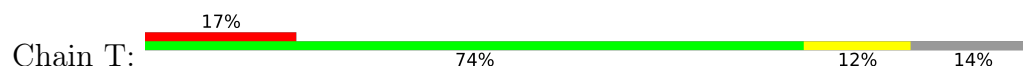


- Molecule 3: Cytochrome subunit of photosynthetic reaction center

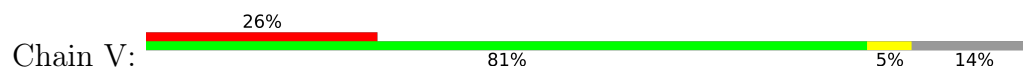




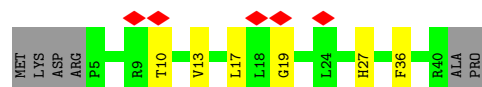
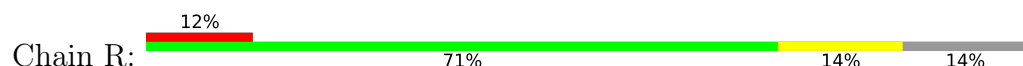
- Molecule 4: Alpha subunit of light-harvesting 1



- Molecule 4: Alpha subunit of light-harvesting 1



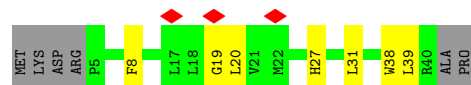
- Molecule 4: Alpha subunit of light-harvesting 1



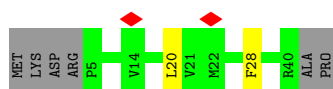
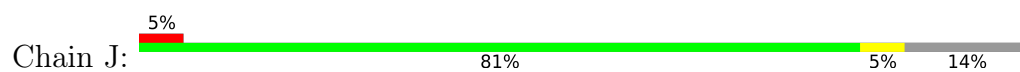
- Molecule 4: Alpha subunit of light-harvesting 1



- Molecule 4: Alpha subunit of light-harvesting 1



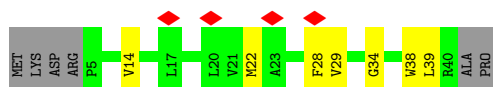
- Molecule 4: Alpha subunit of light-harvesting 1



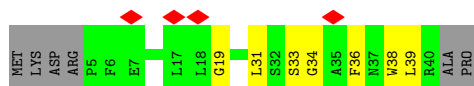
- Molecule 4: Alpha subunit of light-harvesting 1



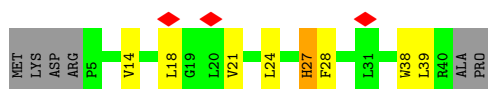
- Molecule 4: Alpha subunit of light-harvesting 1



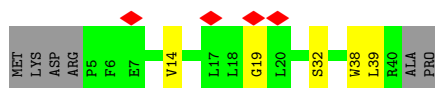
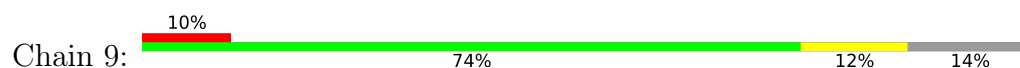
- Molecule 4: Alpha subunit of light-harvesting 1



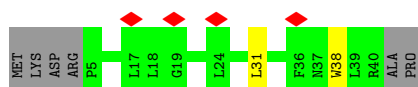
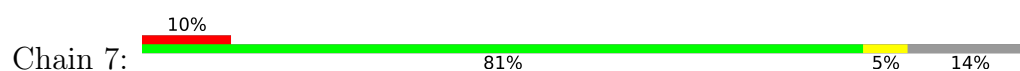
- Molecule 4: Alpha subunit of light-harvesting 1



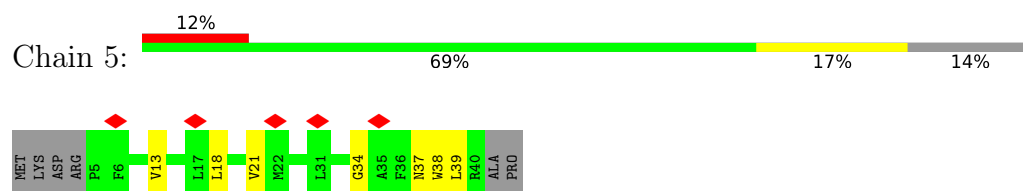
- Molecule 4: Alpha subunit of light-harvesting 1



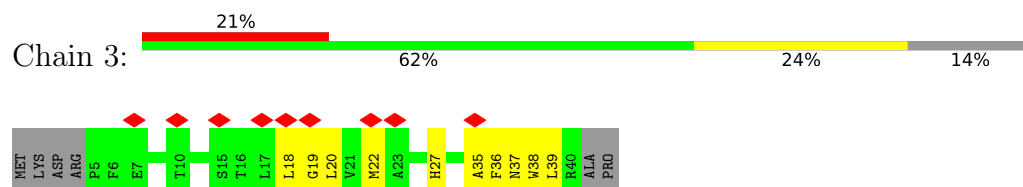
- Molecule 4: Alpha subunit of light-harvesting 1



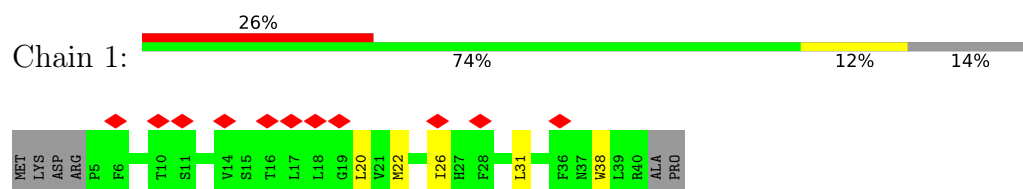
- Molecule 4: Alpha subunit of light-harvesting 1



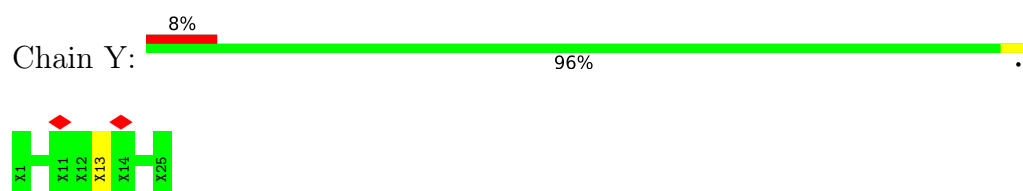
- Molecule 4: Alpha subunit of light-harvesting 1



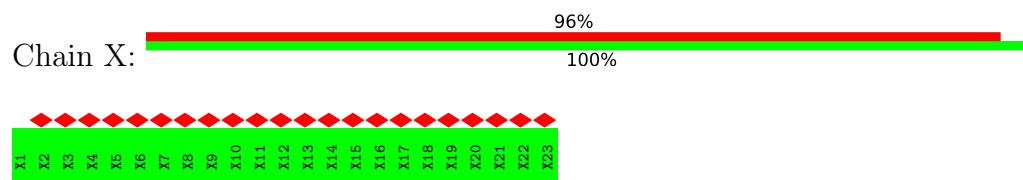
- Molecule 4: Alpha subunit of light-harvesting 1



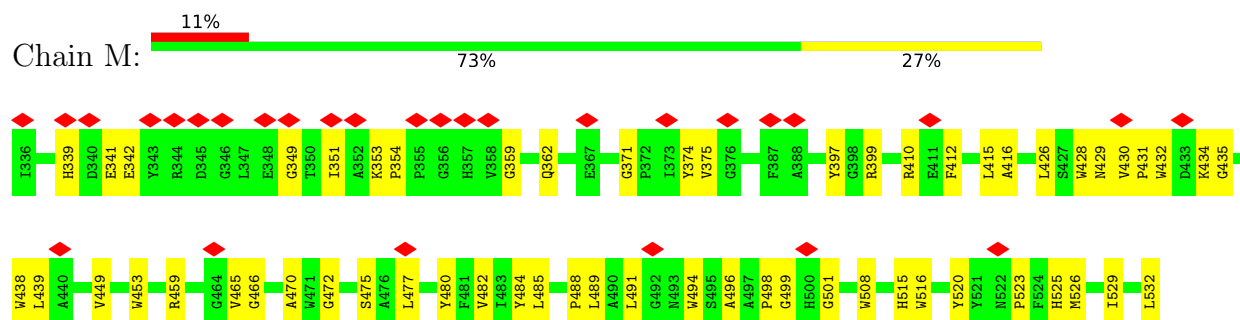
- Molecule 5: Peptide from Precursor for L and M subunits of photosynthetic reaction center



- Molecule 6: Subunit X



- Molecule 7: Precursor for M subunits of photosynthetic reaction center





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	256903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	215.04001, 215.04001, 215.04001	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, BCL, MQE, KGD, BPH, FE

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	0.23	0/341	0.56	0/474
1	2	0.17	0/338	0.43	0/470
1	4	0.20	0/331	0.47	0/462
1	6	0.17	0/341	0.39	0/474
1	8	0.20	0/341	0.54	0/474
1	B	0.20	0/337	0.44	0/470
1	E	0.22	0/337	0.46	0/470
1	G	0.22	0/341	0.50	0/474
1	I	0.19	0/341	0.41	0/474
1	K	0.22	0/337	0.59	0/470
1	O	0.20	0/337	0.49	0/470
1	Q	0.19	0/329	0.48	0/459
1	S	0.19	0/338	0.46	0/470
1	U	0.20	0/341	0.52	0/474
1	W	0.19	0/323	0.43	0/451
2	L	0.24	0/2374	0.55	2/3262 (0.1%)
3	C	0.23	0/2093	0.67	2/2880 (0.1%)
4	1	0.20	0/248	0.45	0/341
4	3	0.22	0/265	0.61	0/363
4	5	0.24	0/272	0.53	0/372
4	7	0.24	0/272	0.48	0/372
4	9	0.21	0/272	0.55	0/372
4	A	0.24	0/272	0.55	0/372
4	D	0.23	0/272	0.59	0/372
4	F	0.18	0/272	0.55	0/372
4	H	0.26	0/265	0.80	1/363 (0.3%)
4	J	0.20	0/269	0.56	0/368
4	N	0.21	0/272	0.44	0/372
4	P	0.21	0/272	0.45	0/372
4	R	0.23	0/262	0.47	0/360
4	T	0.22	0/272	0.46	0/372
4	V	0.19	0/269	0.53	0/368

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	M	0.26	0/2478	0.52	0/3417
All	All	0.23	0/16024	0.54	5/22106 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	2
3	C	0	1
4	5	0	1
7	M	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	8	PHE	N-CA-C	8.54	120.67	111.36
3	C	295	LEU	N-CA-C	-6.07	105.42	114.64
3	C	119	SER	N-CA-C	-5.52	100.33	107.73
2	L	204	TYR	CA-C-N	5.21	131.49	121.54
2	L	204	TYR	C-N-CA	5.21	131.49	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	5	37	ASN	Peptide
3	C	62	TYR	Peptide
2	L	106	GLU	Peptide
2	L	203	TYR	Peptide
7	M	374	TYR	Peptide

5.2 Too-close contacts

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	329	0	293	11	0
1	2	326	0	284	10	0
1	4	319	0	271	16	0
1	6	329	0	293	11	0
1	8	329	0	293	12	0
1	B	325	0	282	25	0
1	E	325	0	282	9	0
1	G	329	0	293	10	0
1	I	329	0	293	17	0
1	K	325	0	282	18	0
1	O	325	0	282	8	0
1	Q	318	0	275	10	0
1	S	326	0	284	8	0
1	U	329	0	293	9	0
1	W	312	0	257	18	0
2	L	2292	0	2129	81	0
3	C	2041	0	1834	81	0
4	1	245	0	237	4	0
4	3	260	0	260	10	0
4	5	266	0	267	4	0
4	7	266	0	267	4	0
4	9	266	0	267	5	0
4	A	266	0	267	11	0
4	D	266	0	267	6	0
4	F	266	0	267	6	0
4	H	260	0	260	12	0
4	J	263	0	258	2	0
4	N	266	0	267	6	0
4	P	266	0	267	7	0
4	R	257	0	253	10	0
4	T	266	0	267	7	0
4	V	263	0	258	3	0
5	Y	125	0	27	1	0
6	X	115	0	26	0	0
7	M	2373	0	2192	60	0
8	0	132	0	148	11	0
8	1	66	0	74	4	0
8	2	132	0	148	12	0
8	3	66	0	72	4	0
8	4	132	0	147	11	0
8	5	66	0	74	3	0
8	6	132	0	148	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	7	66	0	74	7	0
8	8	132	0	148	14	0
8	9	66	0	74	2	0
8	A	66	0	74	5	0
8	B	132	0	148	30	0
8	D	66	0	74	2	0
8	E	132	0	148	8	0
8	F	66	0	74	4	0
8	G	132	0	148	12	0
8	H	66	0	74	7	0
8	I	132	0	148	19	0
8	J	66	0	74	4	0
8	K	132	0	148	19	0
8	L	132	0	148	18	0
8	M	66	0	74	5	0
8	N	66	0	74	3	0
8	O	132	0	148	11	0
8	P	66	0	74	1	0
8	Q	132	0	148	14	0
8	R	66	0	72	6	0
8	S	132	0	145	11	0
8	T	66	0	74	3	0
8	U	132	0	146	12	0
8	V	66	0	74	4	0
8	W	132	0	146	17	0
9	L	65	0	76	7	0
9	M	130	0	152	2	0
10	L	68	0	0	0	0
10	M	68	0	0	3	0
11	C	172	0	120	31	0
12	3	82	0	0	6	0
12	5	41	0	0	0	0
12	9	82	0	0	1	0
12	A	41	0	0	1	0
12	F	41	0	0	3	0
12	H	41	0	0	5	0
12	J	41	0	0	0	0
12	N	82	0	0	3	0
12	R	41	0	0	1	0
12	T	82	0	0	1	0
13	M	1	0	0	0	0
All	All	20009	0	18282	576	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 15.

The worst 5 of 576 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)
1:I:33:ILE:HG13	8:I:102:BCL:CED	1.49	1.40
1:W:33:ILE:CG1	8:W:102:BCL:HED1	1.50	1.39
1:B:30:VAL:CB	8:B:102:BCL:O1D	1.78	1.32
1:B:30:VAL:CA	8:B:102:BCL:O1D	1.77	1.32
1:B:30:VAL:HA	8:B:102:BCL:O1D	1.25	1.30

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	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	2	42/55 (76%)	36 (86%)	6 (14%)	0	100	100
1	4	42/55 (76%)	40 (95%)	2 (5%)	0	100	100
1	6	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	8	42/55 (76%)	34 (81%)	8 (19%)	0	100	100
1	B	42/55 (76%)	39 (93%)	3 (7%)	0	100	100
1	E	42/55 (76%)	39 (93%)	3 (7%)	0	100	100
1	G	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	I	42/55 (76%)	35 (83%)	7 (17%)	0	100	100
1	K	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	O	42/55 (76%)	37 (88%)	5 (12%)	0	100	100
1	Q	42/55 (76%)	38 (90%)	4 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
1	U	42/55 (76%)	36 (86%)	6 (14%)	0	100	100
1	W	42/55 (76%)	38 (90%)	4 (10%)	0	100	100
2	L	307/310 (99%)	253 (82%)	53 (17%)	1 (0%)	36	70
3	C	291/320 (91%)	213 (73%)	76 (26%)	2 (1%)	18	55
4	1	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	3	34/42 (81%)	28 (82%)	6 (18%)	0	100	100
4	5	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
4	7	34/42 (81%)	26 (76%)	8 (24%)	0	100	100
4	9	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
4	A	34/42 (81%)	27 (79%)	7 (21%)	0	100	100
4	D	34/42 (81%)	31 (91%)	3 (9%)	0	100	100
4	F	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	H	34/42 (81%)	31 (91%)	3 (9%)	0	100	100
4	J	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
4	N	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
4	P	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	R	34/42 (81%)	30 (88%)	4 (12%)	0	100	100
4	T	34/42 (81%)	33 (97%)	1 (3%)	0	100	100
4	V	34/42 (81%)	32 (94%)	2 (6%)	0	100	100
7	M	303/306 (99%)	253 (84%)	49 (16%)	1 (0%)	36	70
All	All	2041/2391 (85%)	1738 (85%)	299 (15%)	4 (0%)	44	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	206	PHE
3	C	118	CYS
3	C	124	ILE
7	M	349	GLY

5.3.2 Protein sidechains ⓘ

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	27/49 (55%)	27 (100%)	0	100	100
1	2	26/49 (53%)	26 (100%)	0	100	100
1	4	24/49 (49%)	24 (100%)	0	100	100
1	6	27/49 (55%)	27 (100%)	0	100	100
1	8	27/49 (55%)	27 (100%)	0	100	100
1	B	26/49 (53%)	26 (100%)	0	100	100
1	E	26/49 (53%)	26 (100%)	0	100	100
1	G	27/49 (55%)	27 (100%)	0	100	100
1	I	27/49 (55%)	27 (100%)	0	100	100
1	K	26/49 (53%)	26 (100%)	0	100	100
1	O	26/49 (53%)	26 (100%)	0	100	100
1	Q	25/49 (51%)	25 (100%)	0	100	100
1	S	26/49 (53%)	26 (100%)	0	100	100
1	U	27/49 (55%)	27 (100%)	0	100	100
1	W	23/49 (47%)	23 (100%)	0	100	100
2	L	214/251 (85%)	214 (100%)	0	100	100
3	C	183/262 (70%)	183 (100%)	0	100	100
4	1	24/37 (65%)	24 (100%)	0	100	100
4	3	27/37 (73%)	27 (100%)	0	100	100
4	5	28/37 (76%)	28 (100%)	0	100	100
4	7	28/37 (76%)	28 (100%)	0	100	100
4	9	28/37 (76%)	28 (100%)	0	100	100
4	A	28/37 (76%)	27 (96%)	1 (4%)	31	53
4	D	28/37 (76%)	28 (100%)	0	100	100
4	F	28/37 (76%)	28 (100%)	0	100	100
4	H	27/37 (73%)	27 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	27/37 (73%)	27 (100%)	0	100	100
4	N	28/37 (76%)	27 (96%)	1 (4%)	31	53
4	P	28/37 (76%)	28 (100%)	0	100	100
4	R	26/37 (70%)	26 (100%)	0	100	100
4	T	28/37 (76%)	28 (100%)	0	100	100
4	V	27/37 (73%)	27 (100%)	0	100	100
7	M	216/244 (88%)	216 (100%)	0	100	100
All	All	1413/2047 (69%)	1411 (100%)	2 (0%)	87	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	31	LEU
4	A	27	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	44	HIS
4	A	27	HIS
4	R	27	HIS
4	9	27	HIS
3	C	101	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

Of 72 ligands modelled in this entry, 1 is monoatomic - leaving 71 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	BCL	E	101	-	69,74,74	1.07	4 (5%)	79,115,115	1.46	10 (12%)
8	BCL	B	102	1	69,74,74	1.11	6 (8%)	79,115,115	1.51	10 (12%)
8	BCL	0	101	1	69,74,74	1.07	5 (7%)	79,115,115	1.35	8 (10%)
8	BCL	Q	102	1	69,74,74	1.10	6 (8%)	79,115,115	1.50	11 (13%)
8	BCL	R	102	4,8	69,74,74	1.09	5 (7%)	79,115,115	1.50	11 (13%)
8	BCL	W	102	1	69,74,74	1.07	5 (7%)	79,115,115	1.36	8 (10%)
8	BCL	T	103	4	69,74,74	1.10	5 (7%)	79,115,115	1.34	7 (8%)
8	BCL	W	101	1	69,74,74	1.10	5 (7%)	79,115,115	4.09	11 (13%)
8	BCL	F	102	4	69,74,74	1.07	6 (8%)	79,115,115	1.54	10 (12%)
10	MQE	L	1004	-	69,69,69	3.94	19 (27%)	85,87,87	2.34	23 (27%)
8	BCL	Q	101	1	69,74,74	1.10	7 (10%)	79,115,115	1.38	9 (11%)
8	BCL	O	101	1	69,74,74	1.11	5 (7%)	79,115,115	1.45	10 (12%)
8	BCL	7	101	4	69,74,74	1.08	6 (8%)	79,115,115	1.39	9 (11%)
8	BCL	5	102	4	69,74,74	1.10	5 (7%)	79,115,115	1.43	8 (10%)
8	BCL	I	102	1	69,74,74	1.07	5 (7%)	79,115,115	1.39	8 (10%)
8	BCL	G	101	1	69,74,74	1.13	5 (7%)	79,115,115	1.47	11 (13%)
8	BCL	K	102	1	69,74,74	1.10	5 (7%)	79,115,115	1.41	9 (11%)
8	BCL	4	102	1	69,74,74	1.09	4 (5%)	79,115,115	1.30	6 (7%)
11	HEM	C	504	3	50,50,50	1.30	5 (10%)	67,82,82	1.30	8 (11%)
8	BCL	P	101	4	69,74,74	1.08	6 (8%)	79,115,115	1.40	8 (10%)
8	BCL	M	703	7	69,74,74	1.10	6 (8%)	79,115,115	1.57	9 (11%)
8	BCL	V	101	4	69,74,74	1.09	6 (8%)	79,115,115	1.54	10 (12%)
12	KGD	5	101	-	41,41,41	4.74	25 (60%)	50,53,53	4.29	24 (48%)
8	BCL	L	1001	2	69,74,74	1.10	6 (8%)	79,115,115	1.40	7 (8%)
8	BCL	U	101	1	69,74,74	1.09	5 (7%)	79,115,115	4.11	14 (17%)
8	BCL	L	1002	2	69,74,74	1.12	5 (7%)	79,115,115	1.38	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BPH	M	704	-	59,70,70	1.17	3 (5%)	59,101,101	1.99	11 (18%)
12	KGD	H	102	-	41,41,41	4.40	25 (60%)	50,53,53	3.38	23 (46%)
8	BCL	S	102	1	69,74,74	1.08	5 (7%)	79,115,115	1.30	7 (8%)
8	BCL	8	102	1	69,74,74	1.10	5 (7%)	79,115,115	1.39	8 (10%)
8	BCL	K	101	1	69,74,74	1.08	4 (5%)	79,115,115	1.35	8 (10%)
8	BCL	N	103	4	69,74,74	1.09	6 (8%)	79,115,115	1.40	9 (11%)
8	BCL	S	101	1,8	69,74,74	1.08	5 (7%)	79,115,115	1.39	8 (10%)
8	BCL	9	103	4	69,74,74	1.09	5 (7%)	79,115,115	1.41	8 (10%)
8	BCL	0	102	1	69,74,74	1.11	6 (8%)	79,115,115	1.47	10 (12%)
8	BCL	A	102	4	69,74,74	1.08	7 (10%)	79,115,115	1.38	9 (11%)
8	BCL	D	101	4	69,74,74	1.07	6 (8%)	79,115,115	1.49	10 (12%)
12	KGD	F	101	-	41,41,41	4.43	26 (63%)	50,53,53	4.01	23 (46%)
9	BPH	M	705	-	59,70,70	1.17	3 (5%)	59,101,101	1.85	10 (16%)
8	BCL	E	102	-	69,74,74	1.11	5 (7%)	79,115,115	1.47	10 (12%)
8	BCL	6	102	1	69,74,74	1.08	6 (8%)	79,115,115	1.38	7 (8%)
8	BCL	O	102	1	69,74,74	1.09	6 (8%)	79,115,115	1.32	6 (7%)
8	BCL	J	102	4	69,74,74	1.11	5 (7%)	79,115,115	1.44	8 (10%)
11	HEM	C	501	3	50,50,50	1.28	6 (12%)	67,82,82	0.98	1 (1%)
8	BCL	2	102	1	69,74,74	1.11	6 (8%)	79,115,115	1.36	9 (11%)
8	BCL	B	101	1	69,74,74	1.12	4 (5%)	79,115,115	1.41	8 (10%)
11	HEM	C	502	3	50,50,50	1.29	6 (12%)	67,82,82	1.06	5 (7%)
11	HEM	C	503	3	50,50,50	1.28	5 (10%)	67,82,82	0.98	2 (2%)
12	KGD	N	102	-	41,41,41	4.50	25 (60%)	50,53,53	4.61	23 (46%)
12	KGD	T	101	-	41,41,41	4.58	25 (60%)	50,53,53	4.11	22 (44%)
12	KGD	9	102	-	41,41,41	4.54	26 (63%)	50,53,53	4.11	23 (46%)
8	BCL	6	101	1	69,74,74	1.10	6 (8%)	79,115,115	1.47	11 (13%)
9	BPH	L	1003	-	59,70,70	1.16	3 (5%)	59,101,101	1.92	10 (16%)
12	KGD	N	101	-	41,41,41	4.47	26 (63%)	50,53,53	4.11	23 (46%)
12	KGD	9	101	-	41,41,41	4.30	25 (60%)	50,53,53	4.15	20 (40%)
12	KGD	J	101	-	41,41,41	4.36	25 (60%)	50,53,53	4.08	23 (46%)
8	BCL	G	102	1	69,74,74	1.08	5 (7%)	79,115,115	1.38	7 (8%)
8	BCL	U	102	1	69,74,74	1.10	6 (8%)	79,115,115	1.41	7 (8%)
12	KGD	T	102	-	41,41,41	4.61	25 (60%)	50,53,53	4.30	23 (46%)
8	BCL	2	101	1	69,74,74	1.09	6 (8%)	79,115,115	1.39	7 (8%)
8	BCL	4	101	1,8	69,74,74	1.12	6 (8%)	79,115,115	1.48	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	KGD	R	101	-	41,41,41	4.21	25 (60%)	50,53,53	4.04	24 (48%)
12	KGD	A	101	-	41,41,41	4.35	25 (60%)	50,53,53	3.69	20 (40%)
8	BCL	3	102	4,8	69,74,74	1.10	6 (8%)	79,115,115	1.51	11 (13%)
8	BCL	H	101	4	69,74,74	1.11	7 (10%)	79,115,115	1.45	8 (10%)
8	BCL	1	101	4	69,74,74	1.09	5 (7%)	79,115,115	1.37	7 (8%)
8	BCL	8	101	1	69,74,74	1.07	5 (7%)	79,115,115	1.45	8 (10%)
10	MQE	M	702	-	69,69,69	3.81	19 (27%)	85,87,87	2.85	30 (35%)
12	KGD	3	101	-	41,41,41	4.40	25 (60%)	50,53,53	4.20	23 (46%)
8	BCL	I	101	1	69,74,74	1.09	6 (8%)	79,115,115	1.44	9 (11%)
12	KGD	3	103	-	41,41,41	4.53	26 (63%)	50,53,53	3.61	25 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	E	101	-	-	5/41/137/137	-
8	BCL	B	102	1	-	7/41/137/137	-
8	BCL	0	101	1	-	7/41/137/137	-
8	BCL	Q	102	1	-	12/41/137/137	-
8	BCL	R	102	4,8	-	8/41/137/137	-
8	BCL	W	102	1	-	10/41/137/137	-
8	BCL	T	103	4	-	4/41/137/137	-
8	BCL	W	101	1	-	3/41/137/137	-
8	BCL	F	102	4	-	11/41/137/137	-
10	MQE	L	1004	-	-	12/65/85/85	0/2/2/2
8	BCL	Q	101	1	-	5/41/137/137	-
8	BCL	O	101	1	-	2/41/137/137	-
8	BCL	7	101	4	-	4/41/137/137	-
8	BCL	5	102	4	-	6/41/137/137	-
8	BCL	I	102	1	-	12/41/137/137	-
8	BCL	G	101	1	-	5/41/137/137	-
8	BCL	K	102	1	-	8/41/137/137	-
8	BCL	4	102	1	-	12/41/137/137	-
11	HEM	C	504	3	-	2/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	P	101	4	-	2/41/137/137	-
8	BCL	M	703	7	-	4/41/137/137	-
8	BCL	V	101	4	-	3/41/137/137	-
12	KGD	5	101	-	-	2/36/56/56	0/1/1/1
8	BCL	L	1001	2	-	13/41/137/137	-
8	BCL	U	101	1	-	3/41/137/137	-
8	BCL	L	1002	2	-	5/41/137/137	-
9	BPH	M	704	-	-	5/37/105/105	0/5/6/6
12	KGD	H	102	-	-	2/36/56/56	0/1/1/1
8	BCL	S	102	1	-	5/41/137/137	-
8	BCL	8	102	1	-	12/41/137/137	-
8	BCL	K	101	1	-	4/41/137/137	-
8	BCL	N	103	4	-	6/41/137/137	-
8	BCL	S	101	1,8	-	7/41/137/137	-
8	BCL	9	103	4	-	6/41/137/137	-
8	BCL	0	102	1	-	7/41/137/137	-
8	BCL	A	102	4	-	8/41/137/137	-
8	BCL	D	101	4	-	6/41/137/137	-
12	KGD	F	101	-	-	0/36/56/56	0/1/1/1
9	BPH	M	705	-	-	2/37/105/105	0/5/6/6
8	BCL	E	102	-	-	11/41/137/137	-
8	BCL	6	102	1	-	5/41/137/137	-
8	BCL	O	102	1	-	7/41/137/137	-
8	BCL	J	102	4	-	2/41/137/137	-
11	HEM	C	501	3	-	2/14/54/54	-
8	BCL	2	102	1	-	14/41/137/137	-
8	BCL	B	101	1	-	7/41/137/137	-
11	HEM	C	502	3	-	2/14/54/54	-
11	HEM	C	503	3	-	0/14/54/54	-
12	KGD	N	102	-	-	1/36/56/56	0/1/1/1
12	KGD	T	101	-	-	0/36/56/56	0/1/1/1
12	KGD	9	102	-	-	2/36/56/56	0/1/1/1
8	BCL	6	101	1	-	5/41/137/137	-
9	BPH	L	1003	-	-	7/37/105/105	0/5/6/6
12	KGD	N	101	-	-	0/36/56/56	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	KGD	9	101	-	-	1/36/56/56	0/1/1/1
12	KGD	J	101	-	-	0/36/56/56	0/1/1/1
8	BCL	G	102	1	-	10/41/137/137	-
8	BCL	U	102	1	-	8/41/137/137	-
12	KGD	T	102	-	-	1/36/56/56	0/1/1/1
8	BCL	2	101	1	-	3/41/137/137	-
8	BCL	4	101	1,8	-	9/41/137/137	-
12	KGD	R	101	-	-	2/36/56/56	0/1/1/1
12	KGD	A	101	-	-	2/36/56/56	0/1/1/1
8	BCL	3	102	4,8	-	4/41/137/137	-
8	BCL	H	101	4	-	5/41/137/137	-
8	BCL	1	101	4	-	4/41/137/137	-
8	BCL	8	101	1	-	4/41/137/137	-
10	MQE	M	702	-	-	17/65/85/85	0/2/2/2
12	KGD	3	101	-	-	2/36/56/56	0/1/1/1
8	BCL	I	101	1	-	0/41/137/137	-
12	KGD	3	103	-	-	1/36/56/56	0/1/1/1

The worst 5 of 685 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	3	103	KGD	CAE-CAI	-10.12	1.37	1.50
12	9	102	KGD	CAE-CAI	-10.05	1.37	1.50
12	5	101	KGD	CAE-CAI	-10.00	1.37	1.50
12	N	102	KGD	CAE-CAI	-9.92	1.37	1.50
12	A	101	KGD	CAE-CAI	-9.87	1.37	1.50

The worst 5 of 841 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	101	BCL	C4-C3-C5	-26.98	68.40	115.23
8	U	101	BCL	C4-C3-C5	-26.66	68.96	115.23
8	U	101	BCL	C5-C3-C2	17.69	160.88	121.17
8	W	101	BCL	C5-C3-C2	17.47	160.40	121.17
12	N	102	KGD	CBM-CBJ-CBH	-14.47	106.98	127.28

There are no chirality outliers.

5 of 375 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	102	BCL	CAD-CBD-CGD-O1D
8	E	102	BCL	CAD-CBD-CGD-O2D
8	B	101	BCL	C2C-C3C-CAC-CBC
8	B	101	BCL	C4C-C3C-CAC-CBC
8	0	101	BCL	C2C-C3C-CAC-CBC

There are no ring outliers.

64 monomers are involved in 335 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	101	BCL	4	0
8	B	102	BCL	24	0
8	0	101	BCL	7	0
8	Q	102	BCL	10	0
8	R	102	BCL	6	0
8	W	102	BCL	13	0
8	T	103	BCL	3	0
8	W	101	BCL	4	0
8	F	102	BCL	4	0
8	Q	101	BCL	4	0
8	O	101	BCL	6	0
8	7	101	BCL	7	0
8	5	102	BCL	3	0
8	I	102	BCL	15	0
8	G	101	BCL	7	0
8	K	102	BCL	15	0
8	4	102	BCL	5	0
11	C	504	HEM	11	0
8	P	101	BCL	1	0
8	M	703	BCL	5	0
8	V	101	BCL	4	0
8	L	1001	BCL	12	0
8	U	101	BCL	3	0
8	L	1002	BCL	8	0
9	M	704	BPH	2	0
12	H	102	KGD	5	0
8	S	102	BCL	5	0
8	8	102	BCL	9	0
8	K	101	BCL	4	0
8	N	103	BCL	3	0
8	S	101	BCL	6	0
8	9	103	BCL	2	0
8	0	102	BCL	4	0

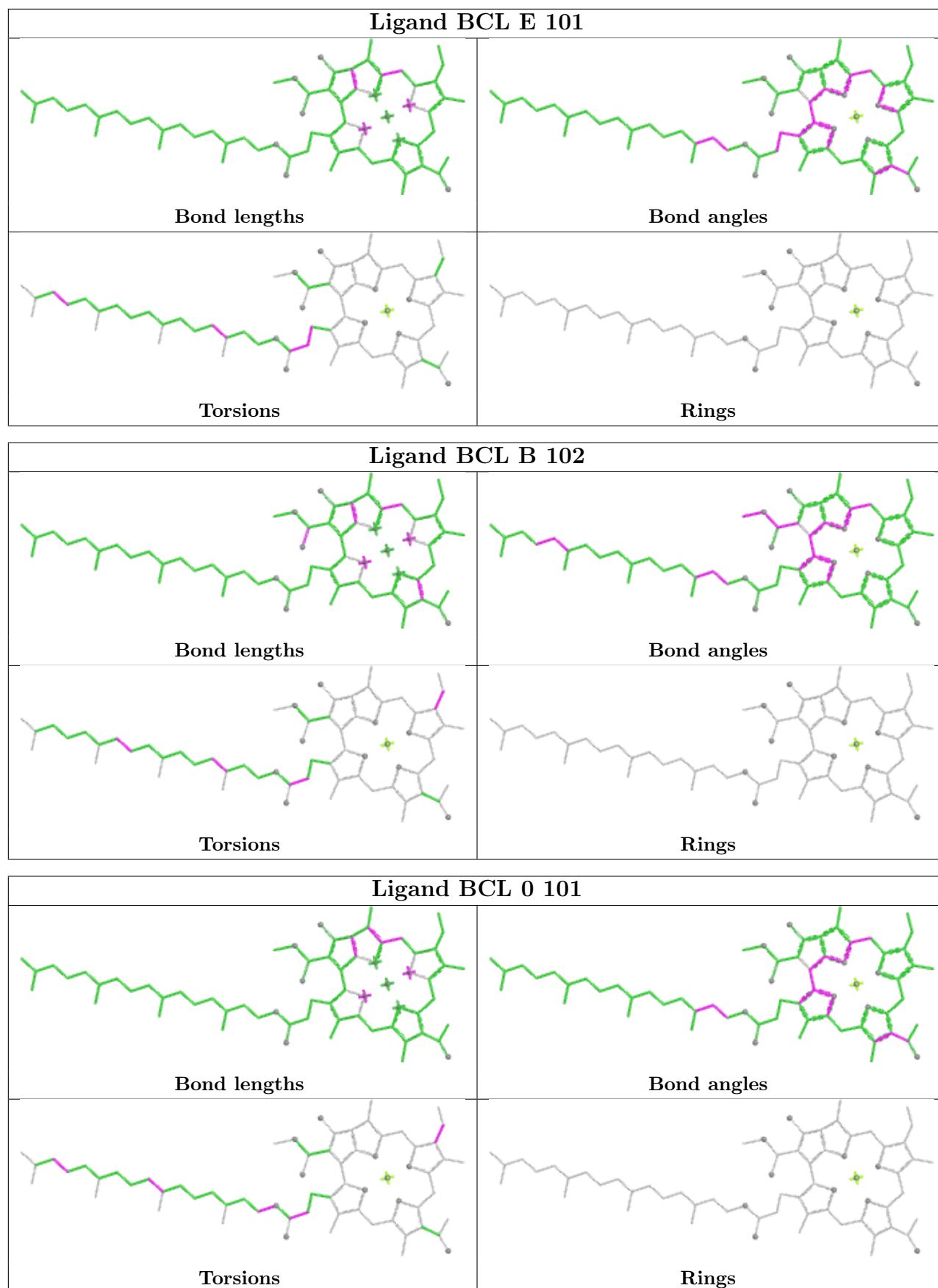
Continued on next page...

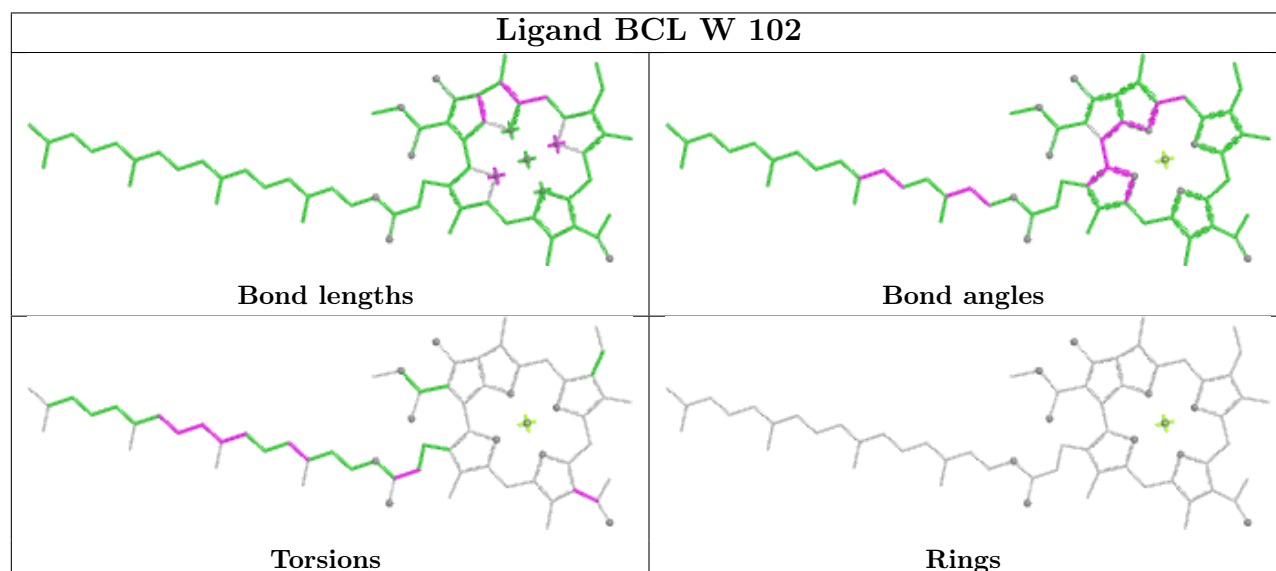
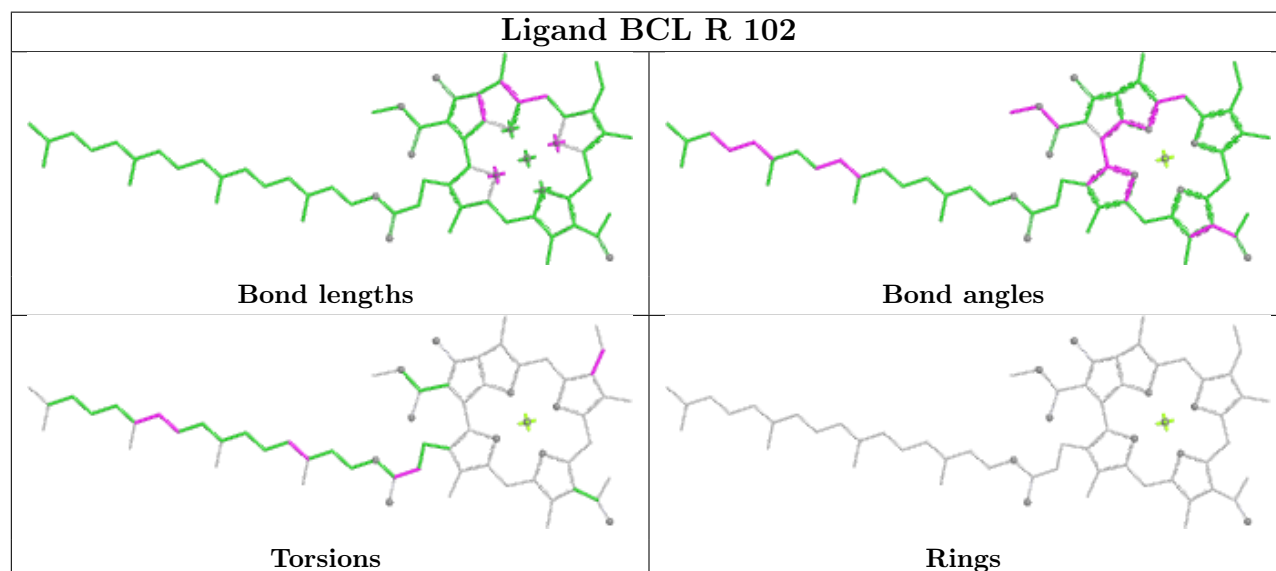
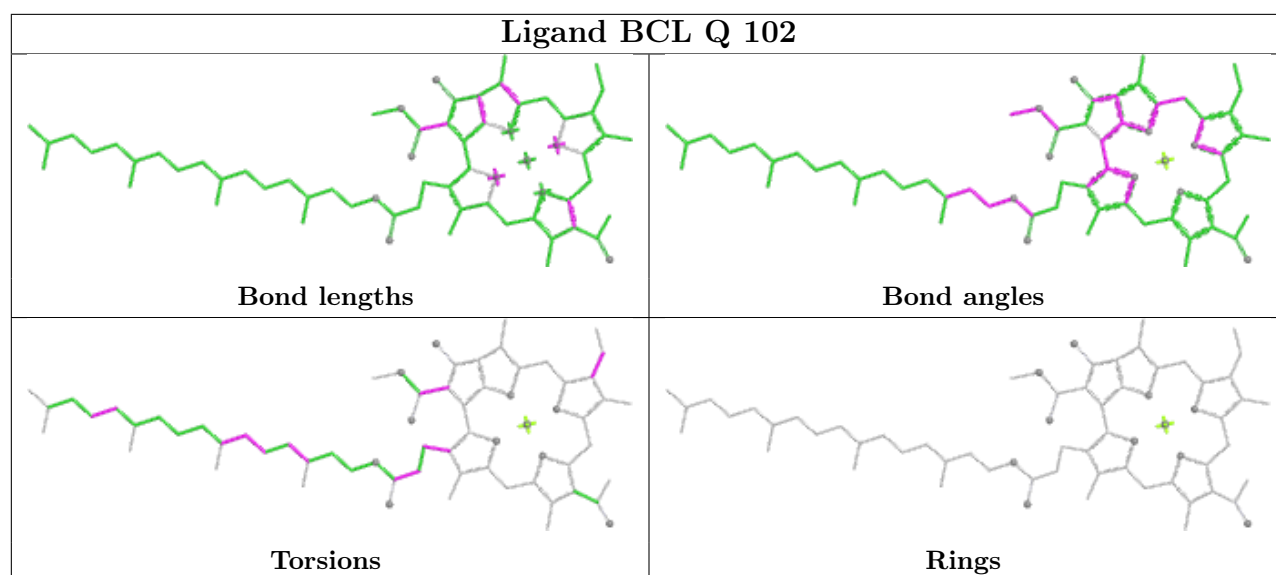
Continued from previous page...

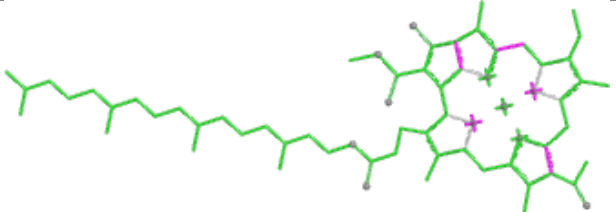
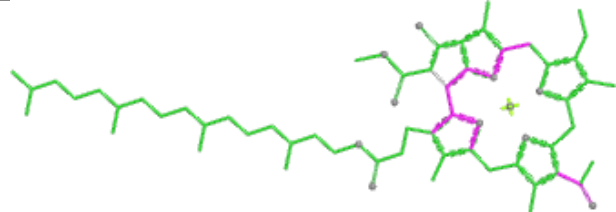
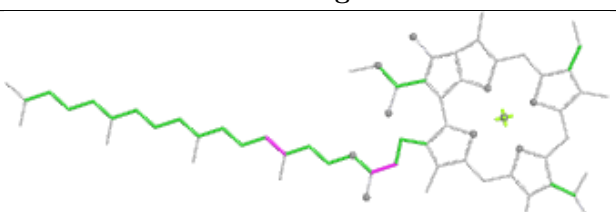
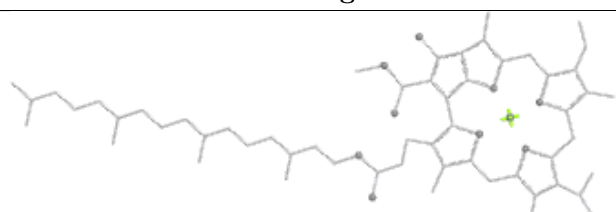
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	102	BCL	5	0
8	D	101	BCL	2	0
12	F	101	KGD	3	0
8	E	102	BCL	4	0
8	6	102	BCL	11	0
8	O	102	BCL	5	0
8	J	102	BCL	4	0
11	C	501	HEM	10	0
8	2	102	BCL	6	0
8	B	101	BCL	6	0
11	C	502	HEM	5	0
11	C	503	HEM	5	0
12	N	102	KGD	1	0
12	T	101	KGD	1	0
12	9	102	KGD	1	0
8	6	101	BCL	7	0
9	L	1003	BPH	7	0
12	N	101	KGD	2	0
8	G	102	BCL	5	0
8	U	102	BCL	9	0
8	2	101	BCL	6	0
8	4	101	BCL	6	0
12	R	101	KGD	1	0
12	A	101	KGD	1	0
8	3	102	BCL	4	0
8	H	101	BCL	7	0
8	1	101	BCL	4	0
8	8	101	BCL	5	0
10	M	702	MQE	3	0
8	I	101	BCL	4	0
12	3	103	KGD	6	0

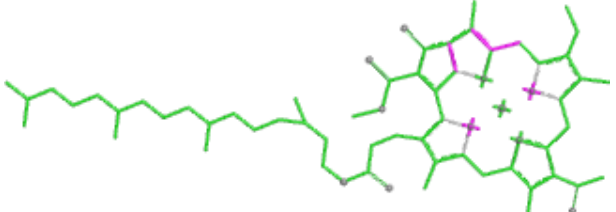
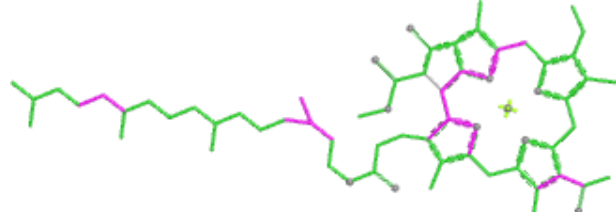
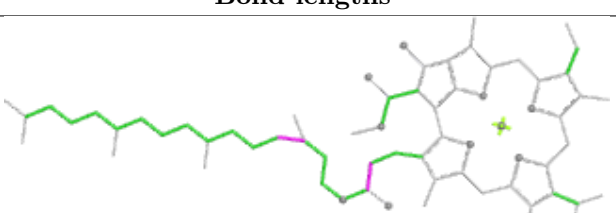
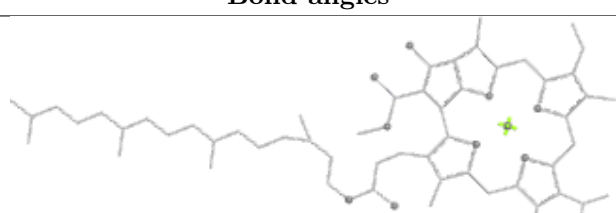
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

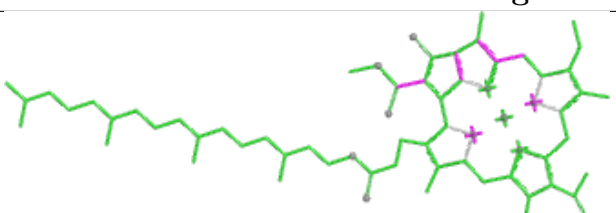
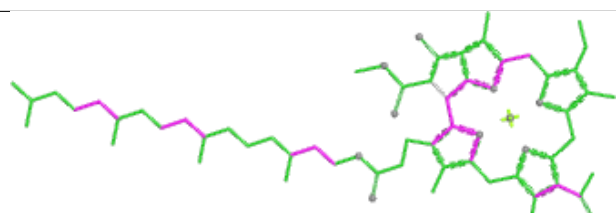
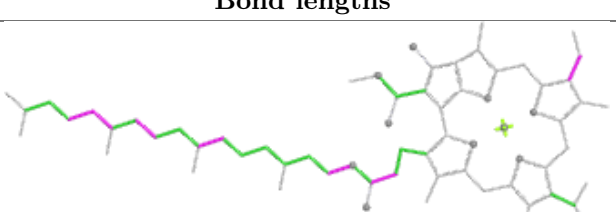
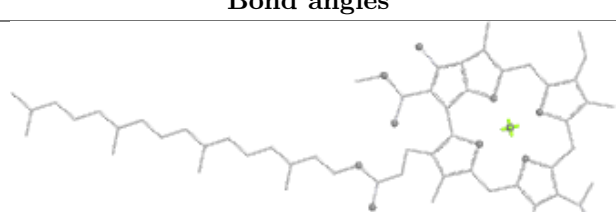
equivalents in the CSD to analyse the geometry.

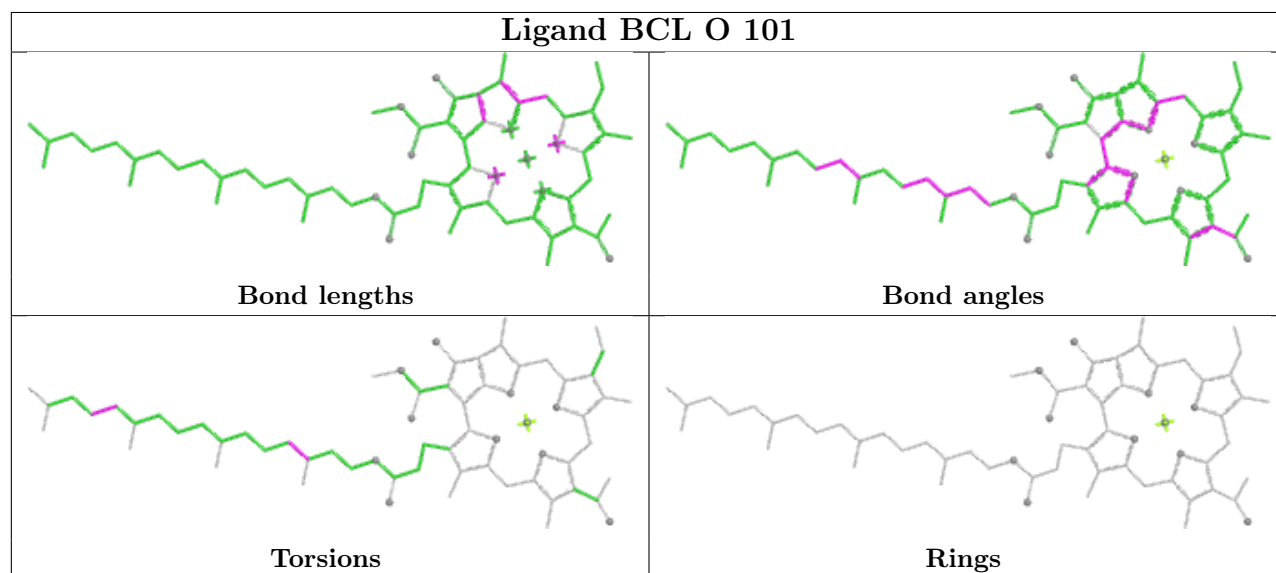
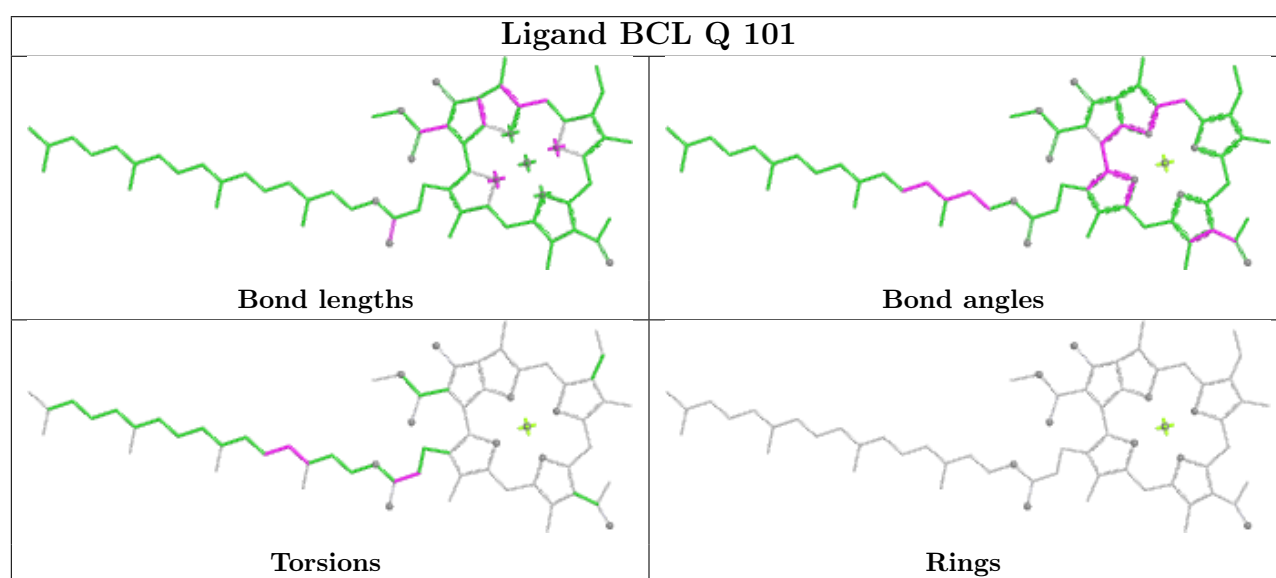
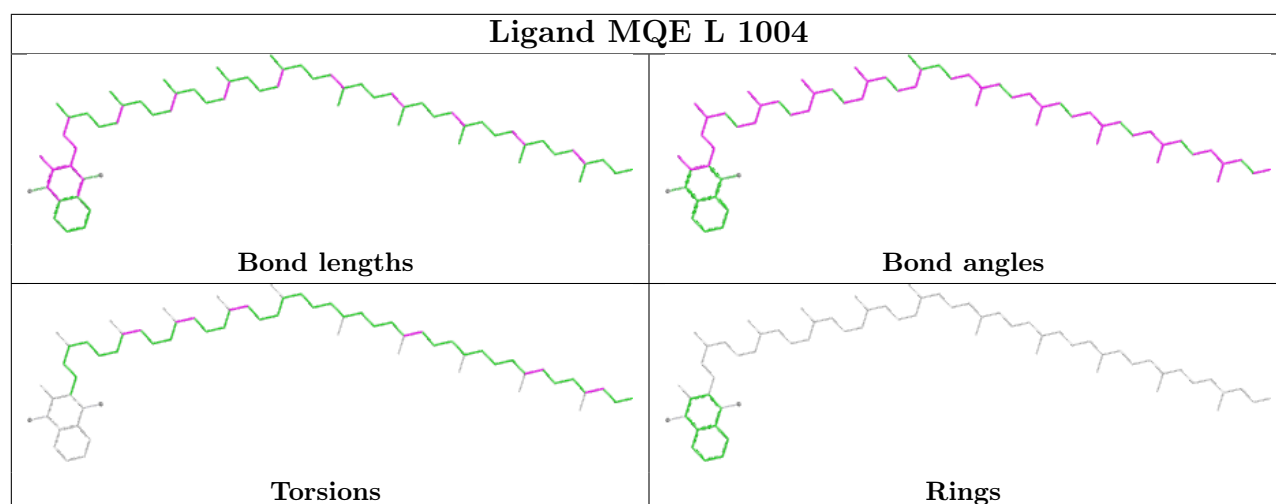


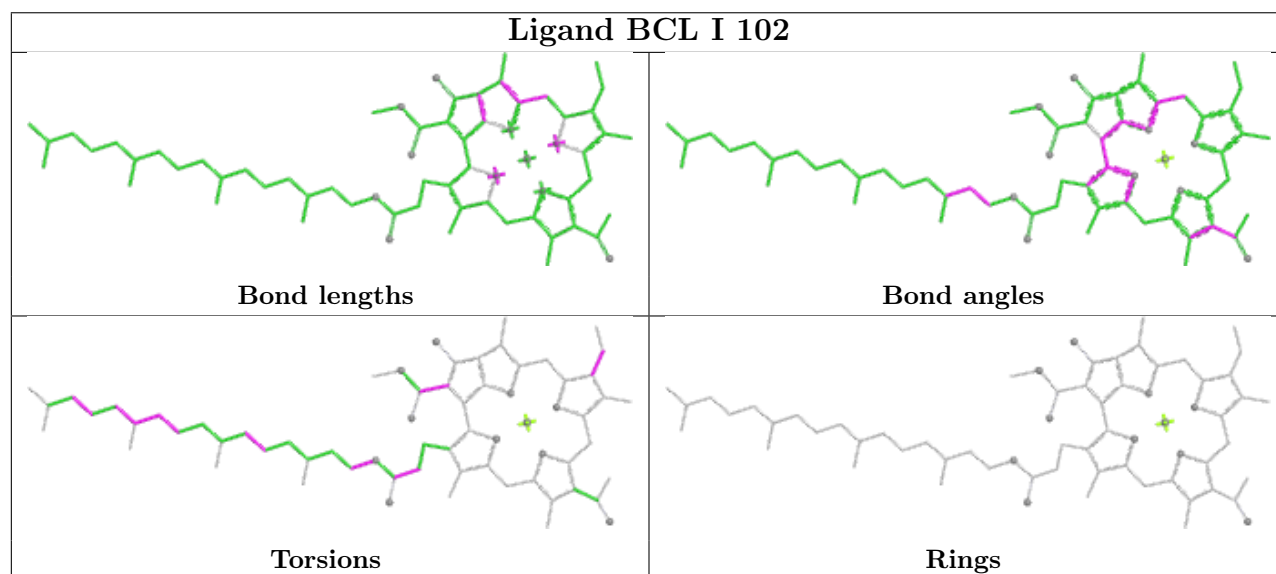
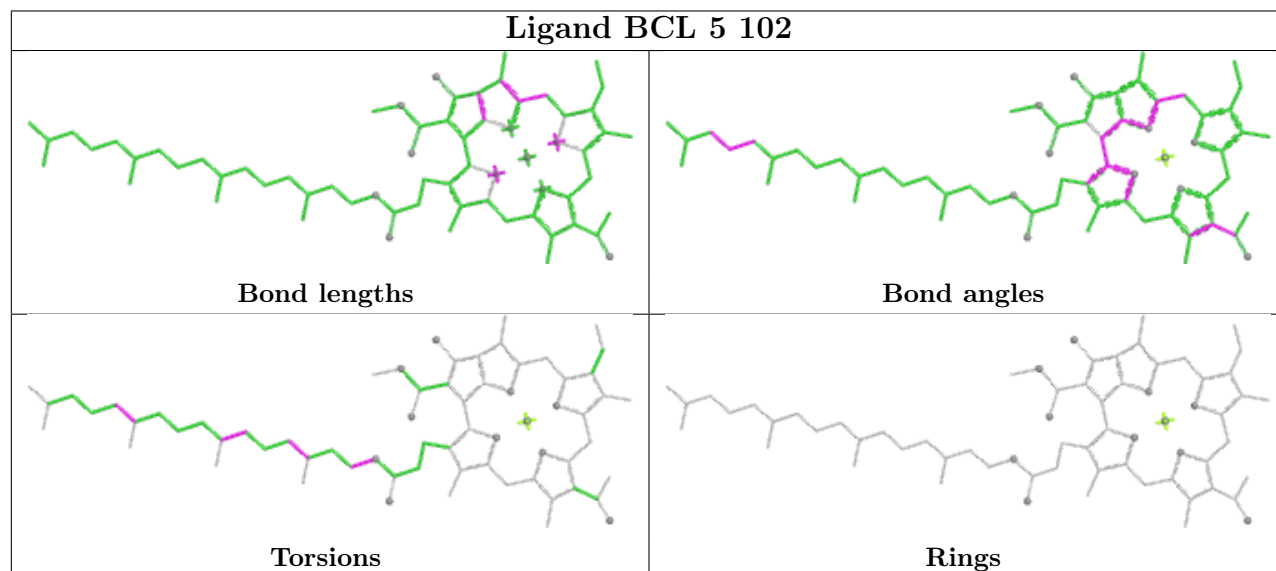
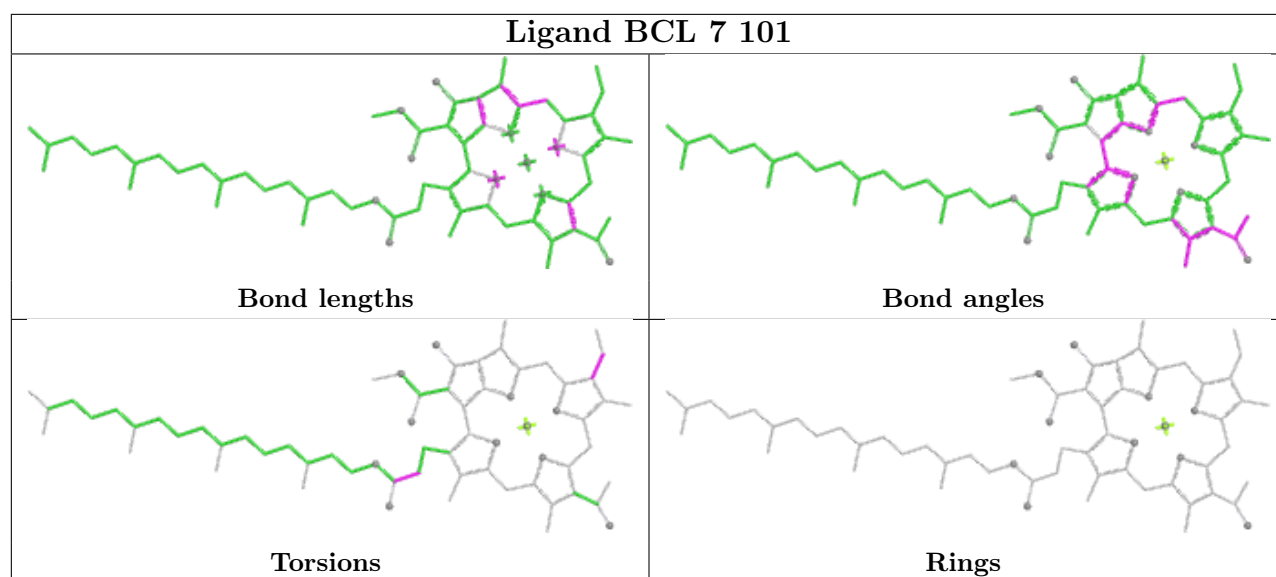


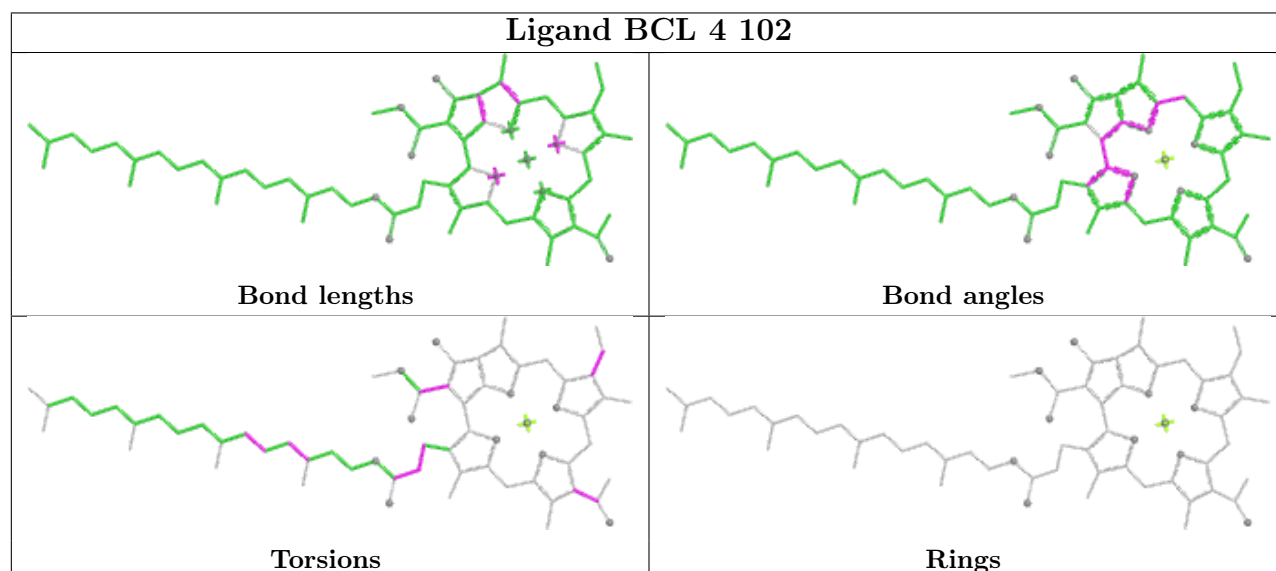
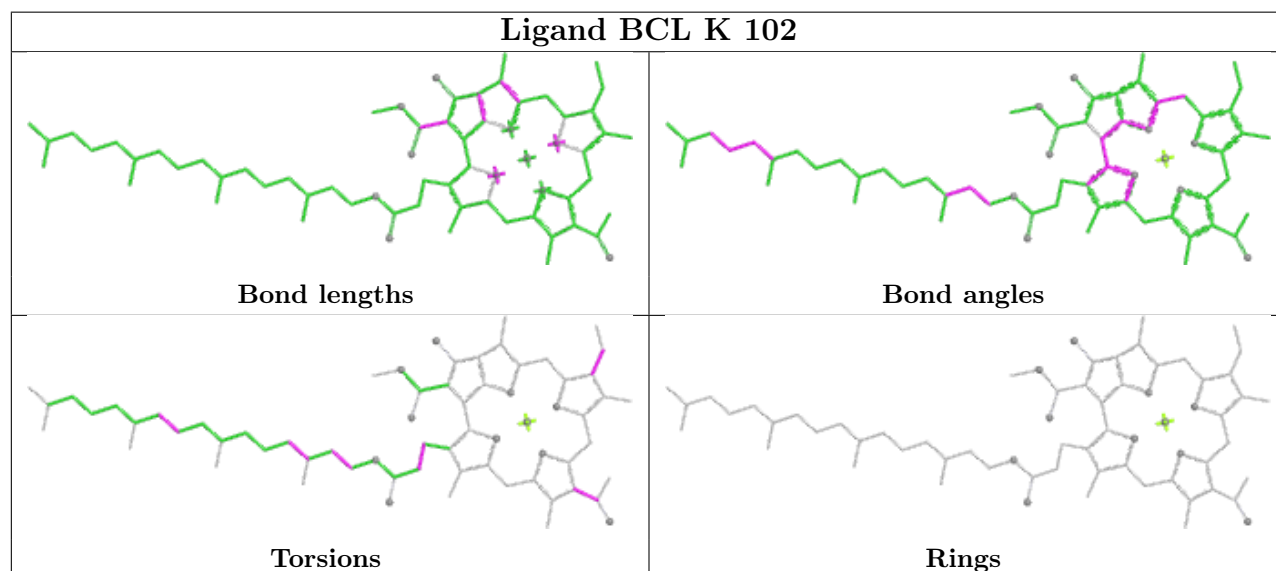
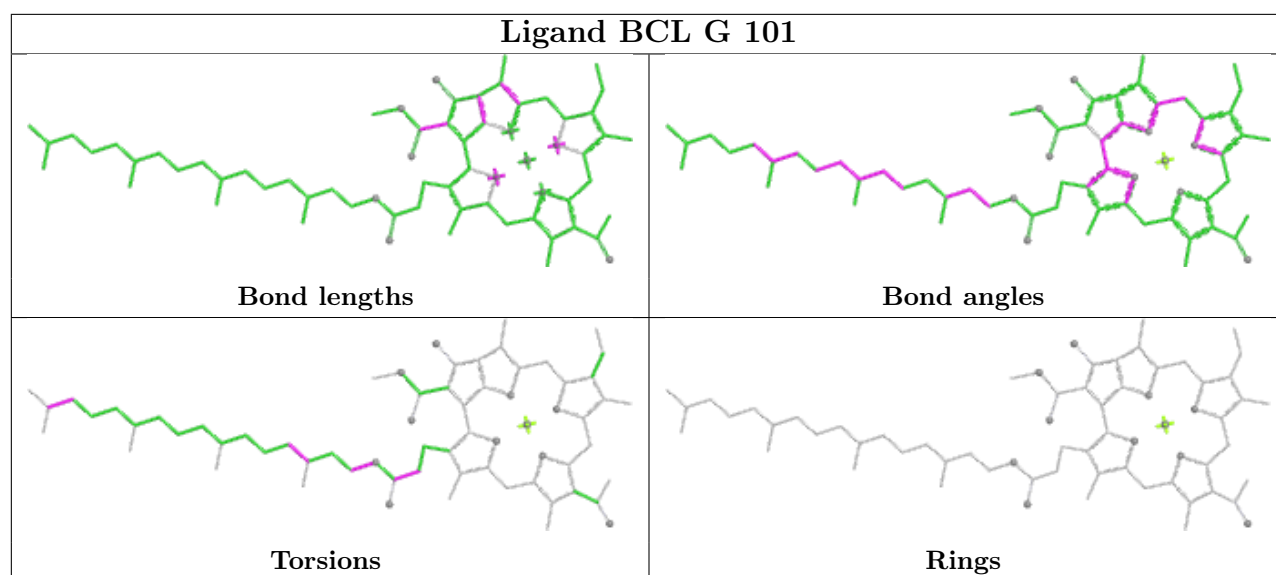
Ligand BCL T 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

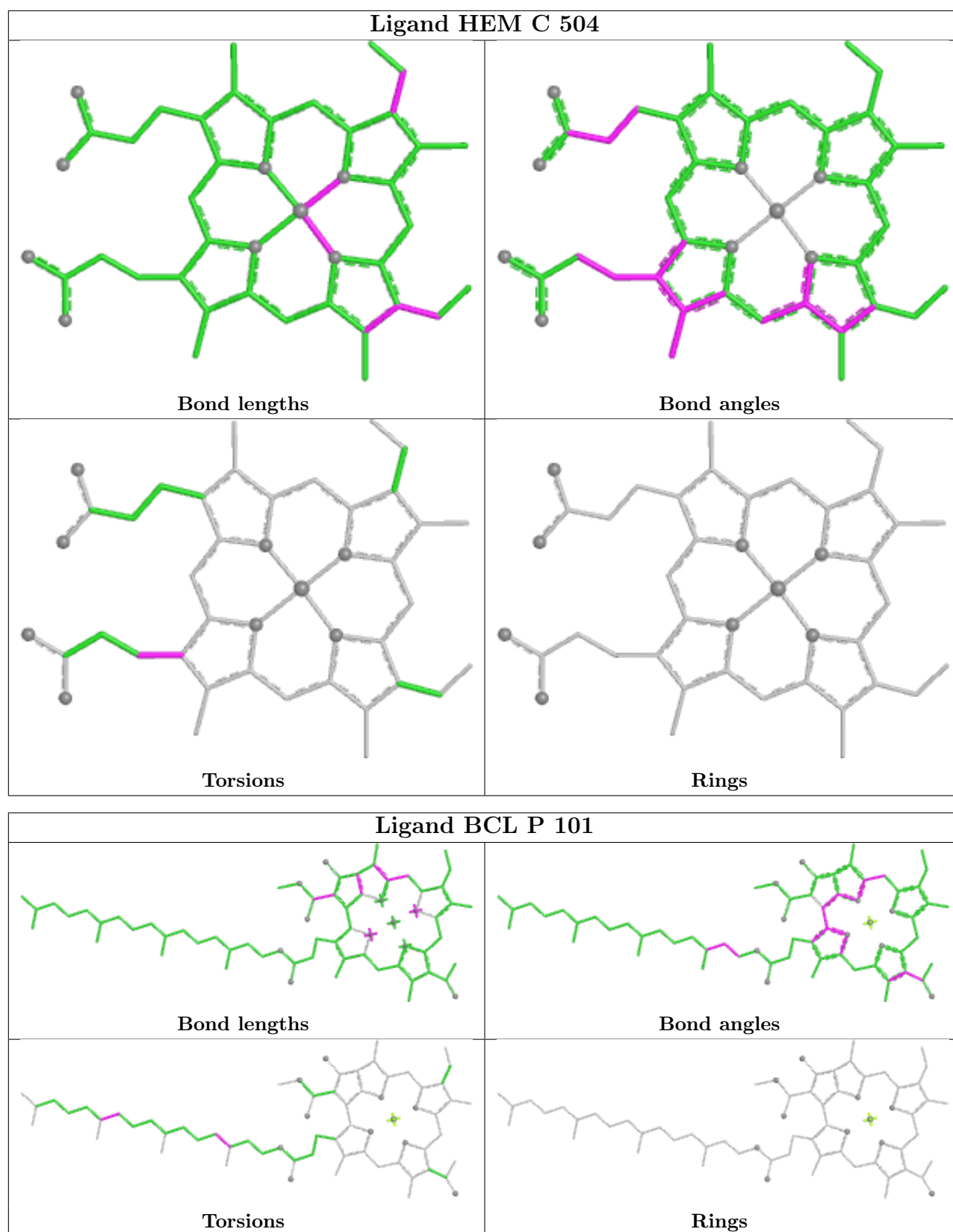
Ligand BCL W 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

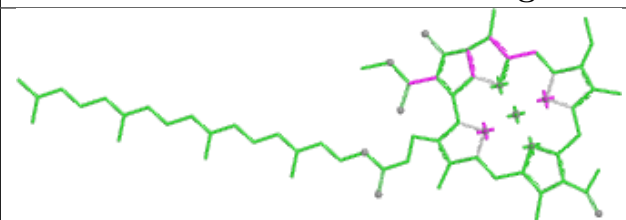
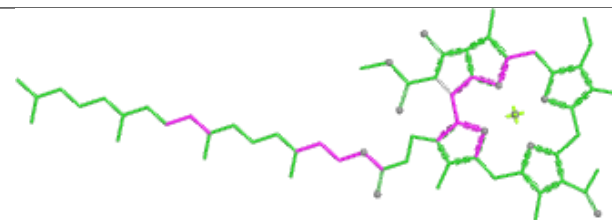
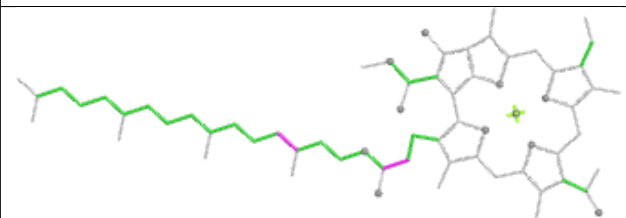
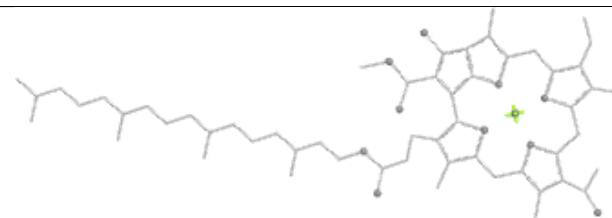
Ligand BCL F 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

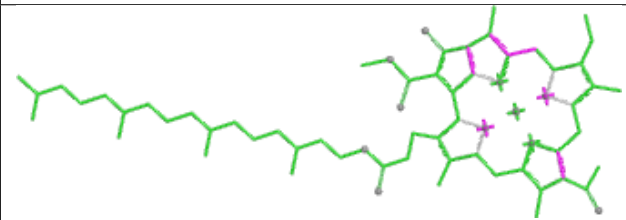
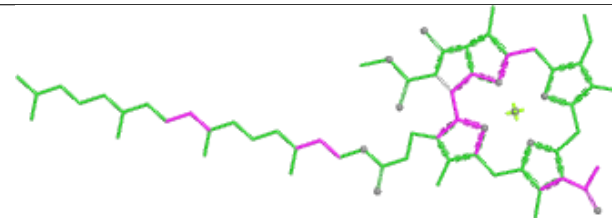
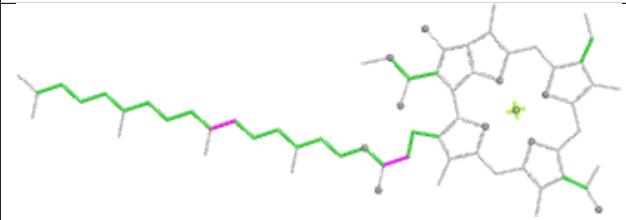
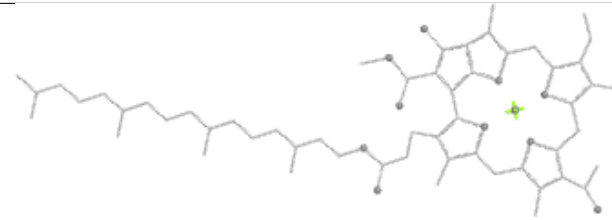


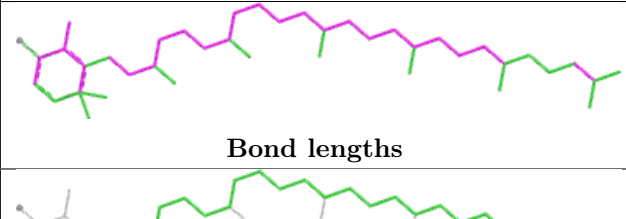
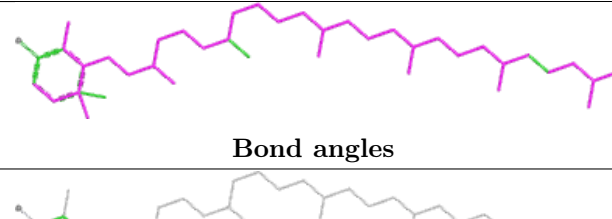


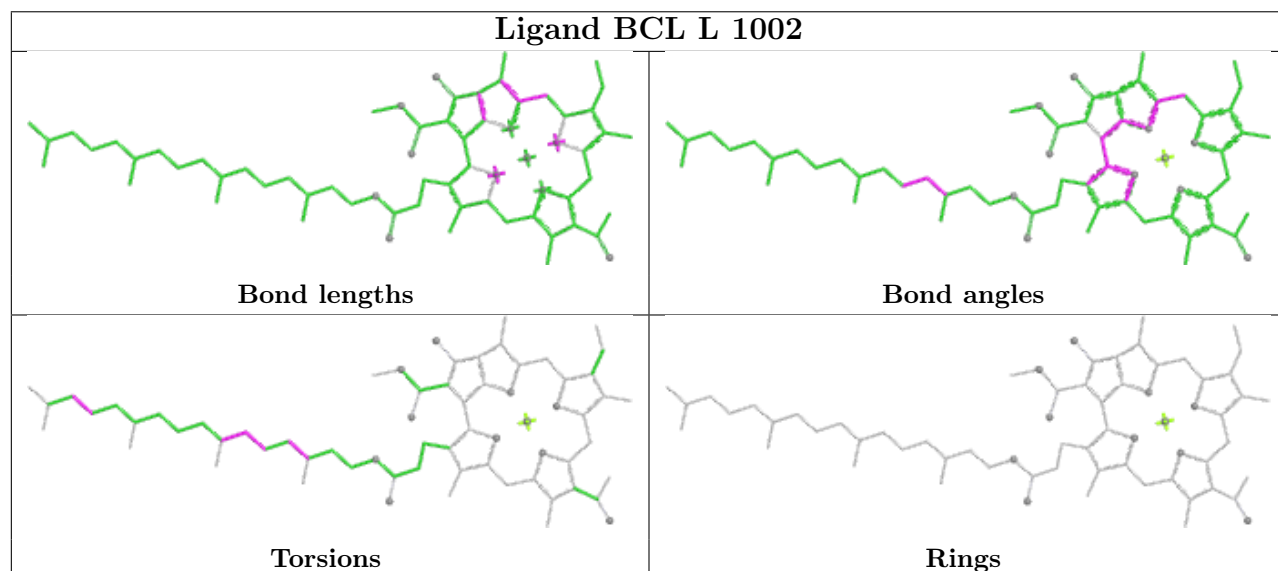
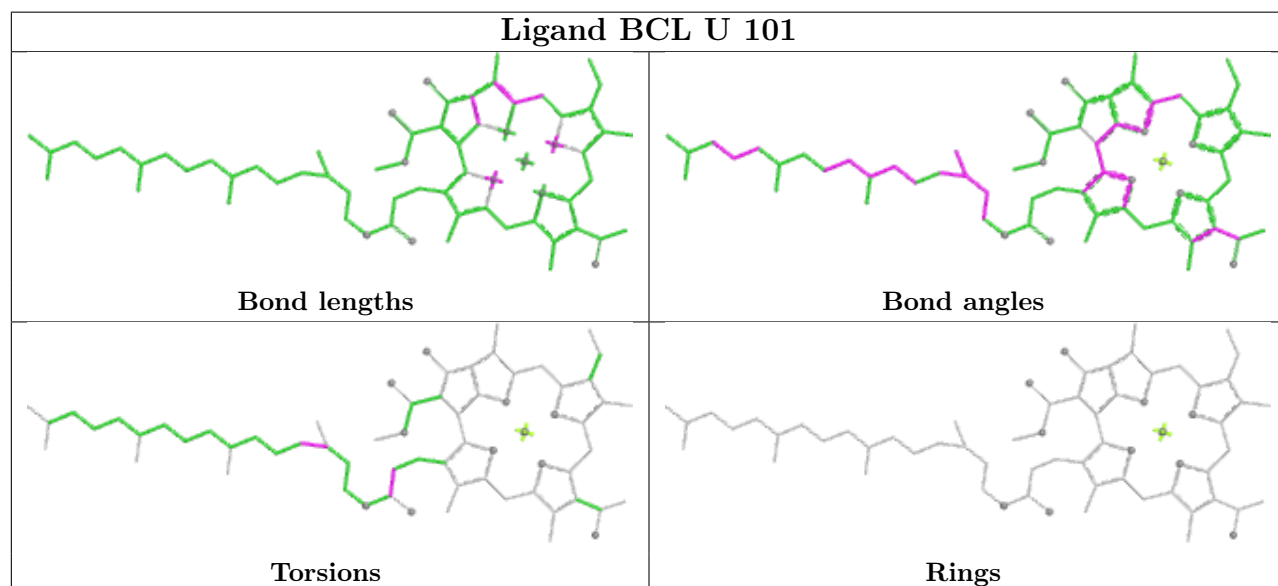
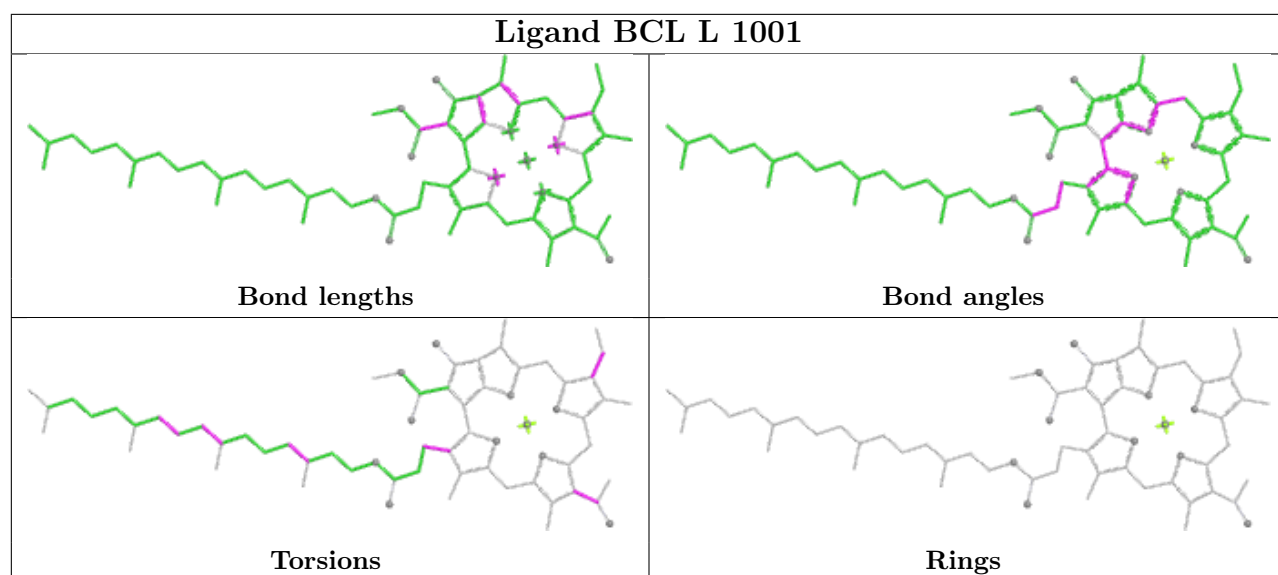


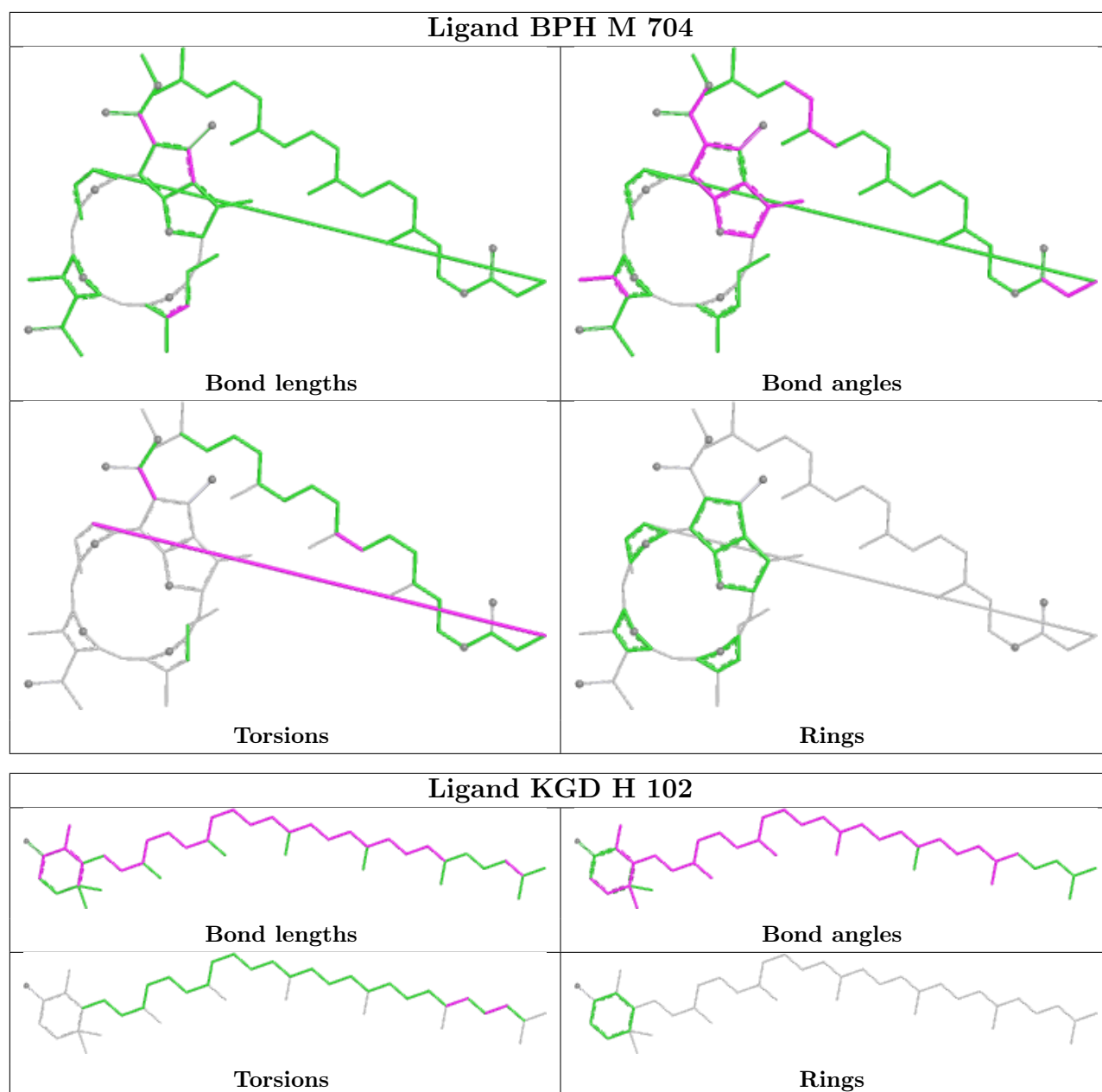


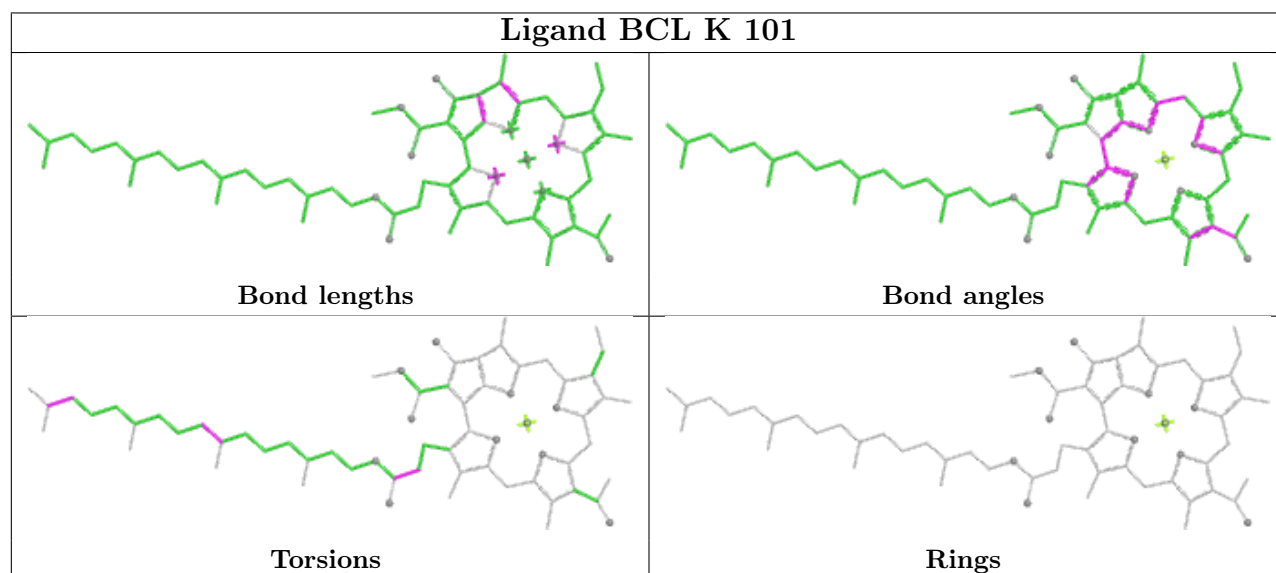
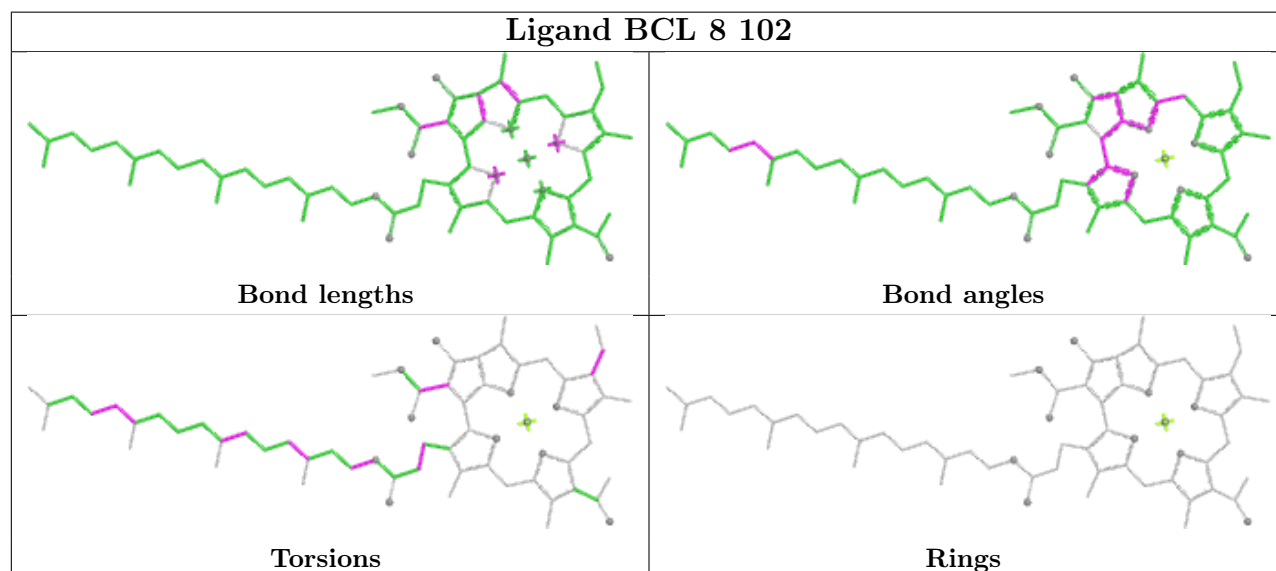
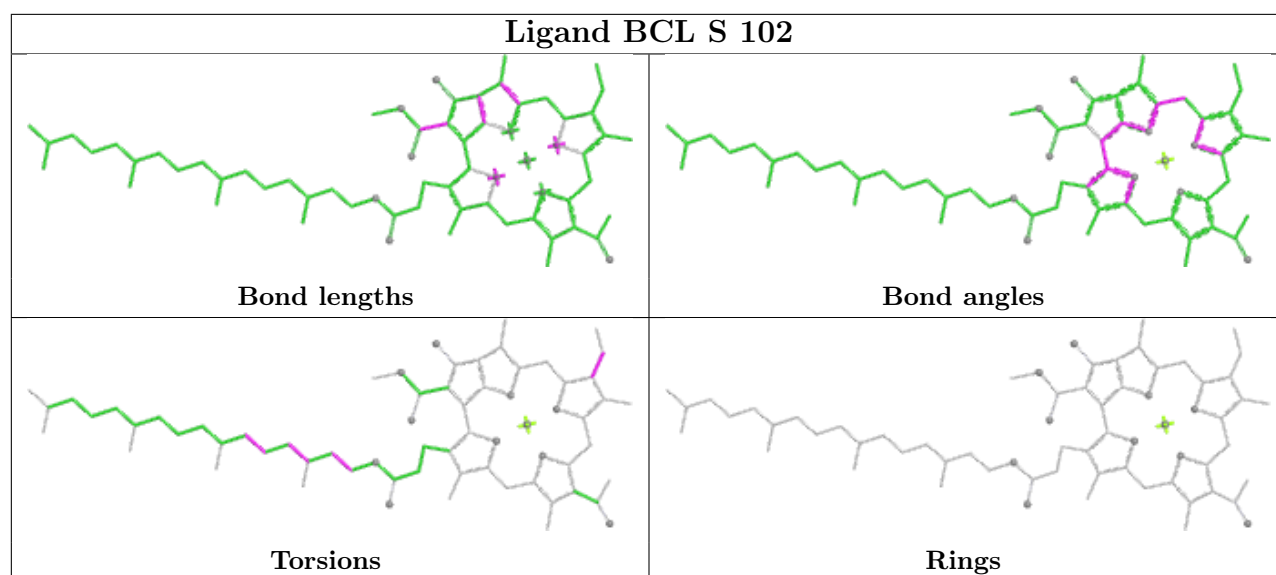
Ligand BCL M 703	
	
Bond lengths	Bond angles
	
Torsions	Rings

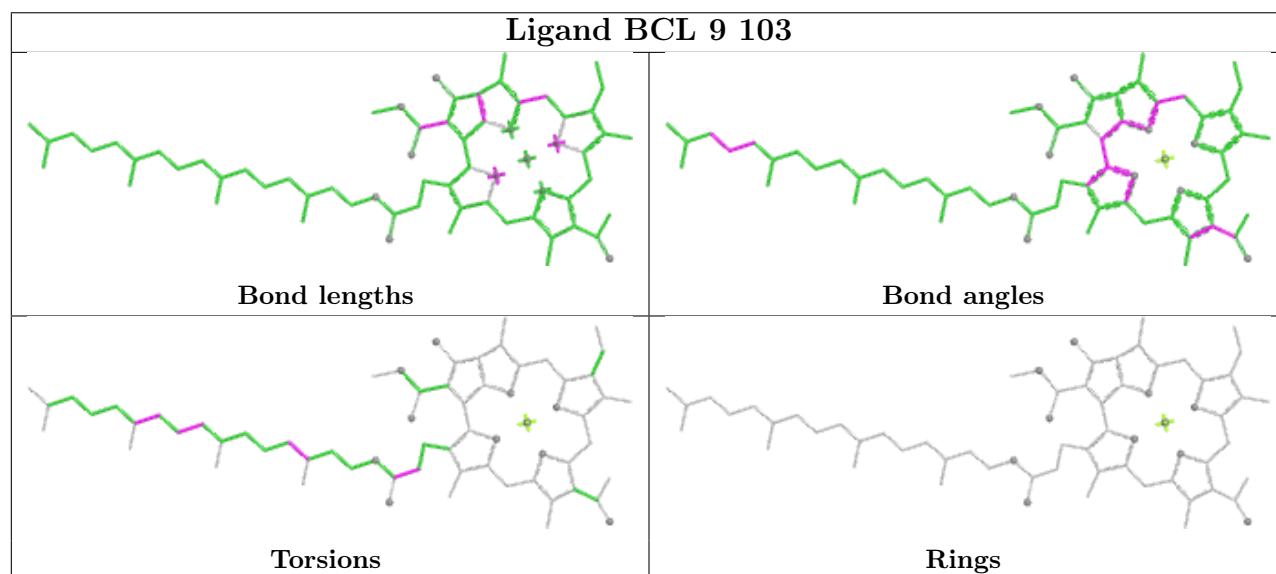
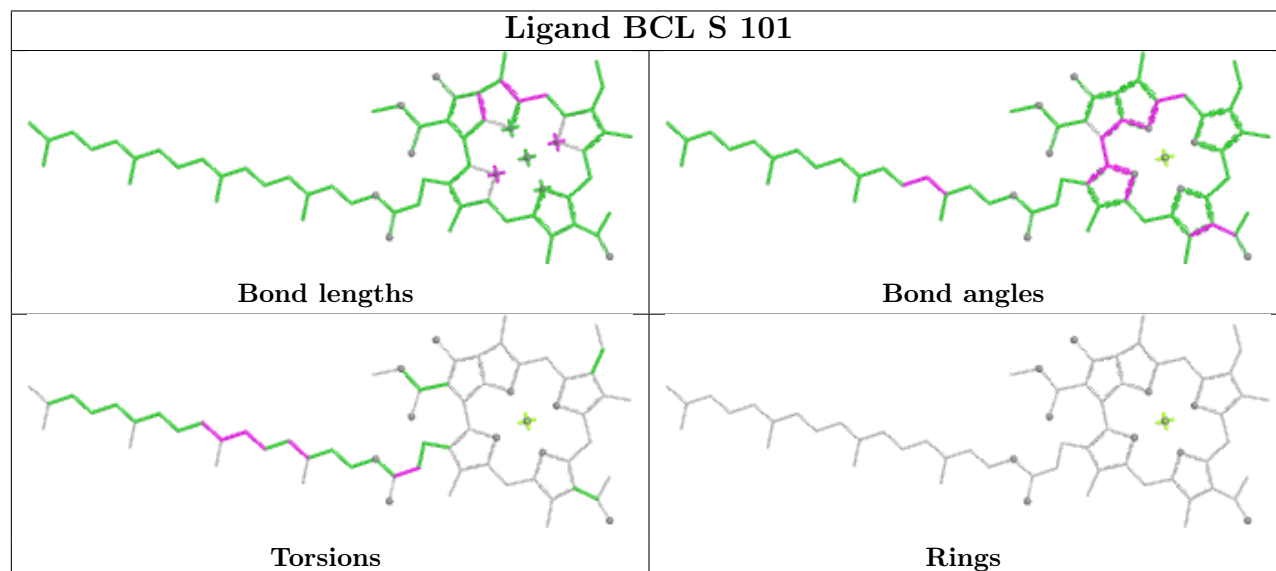
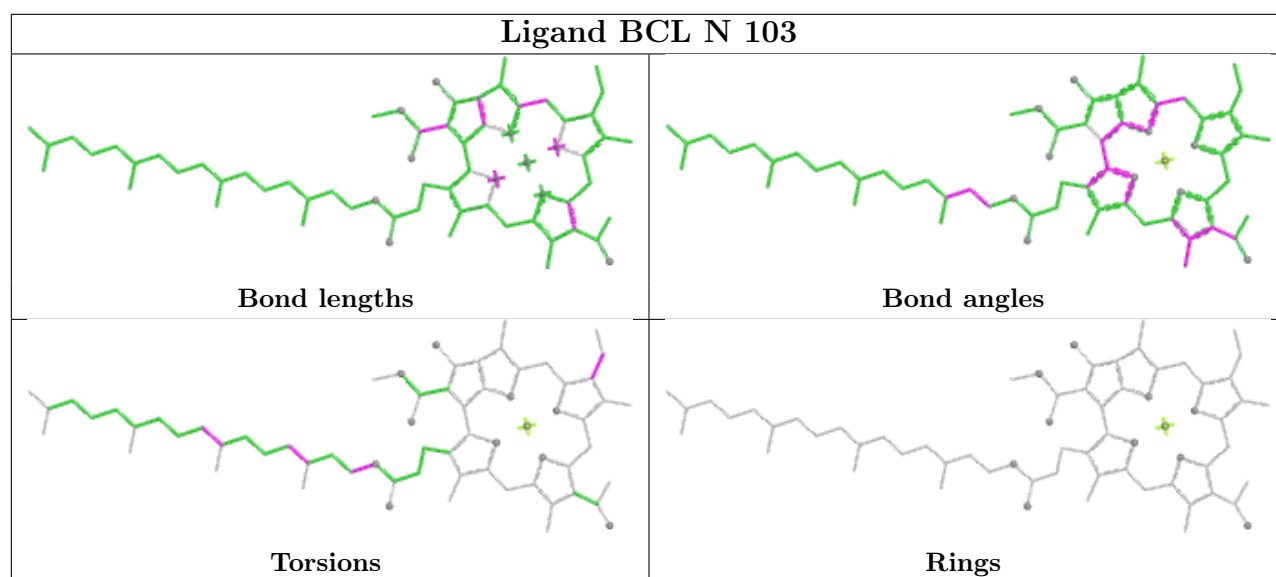
Ligand BCL V 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

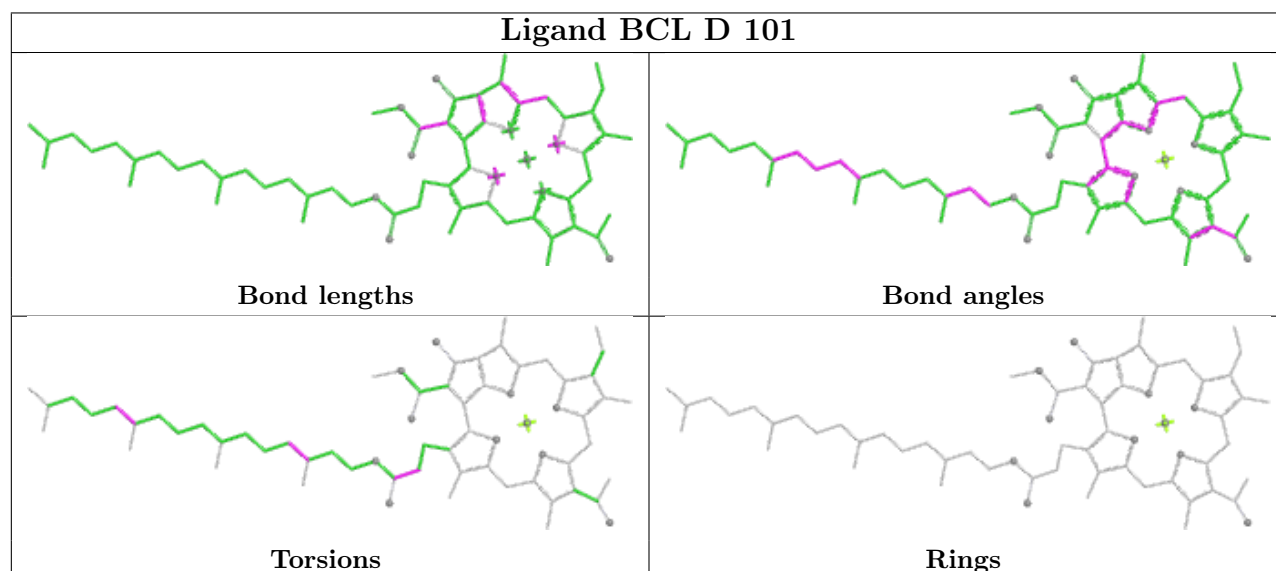
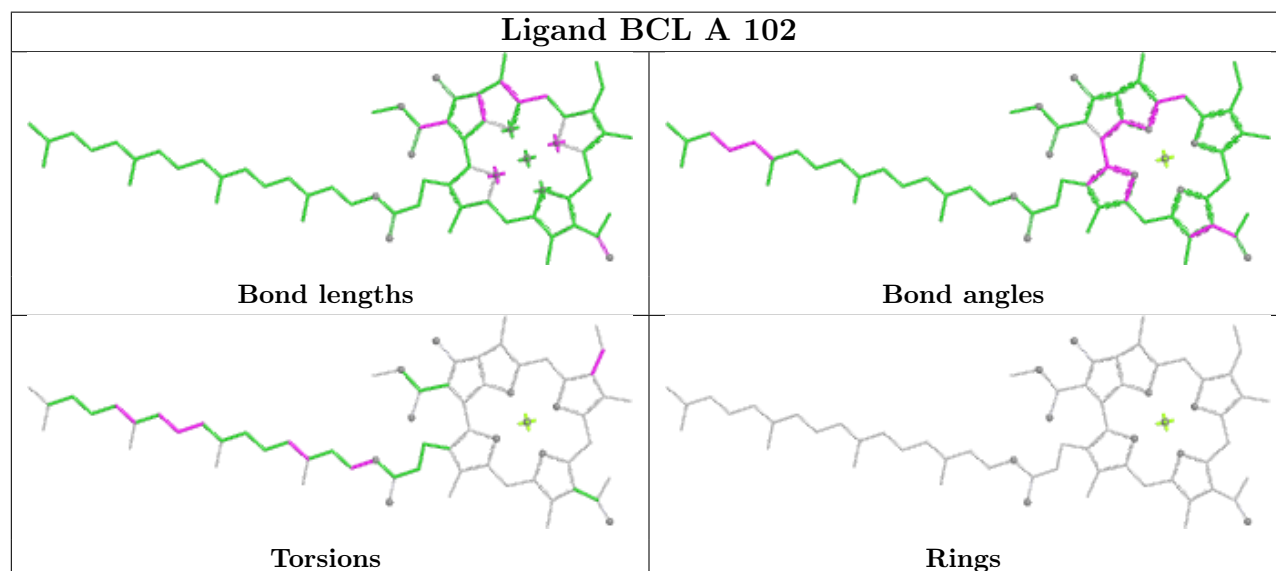
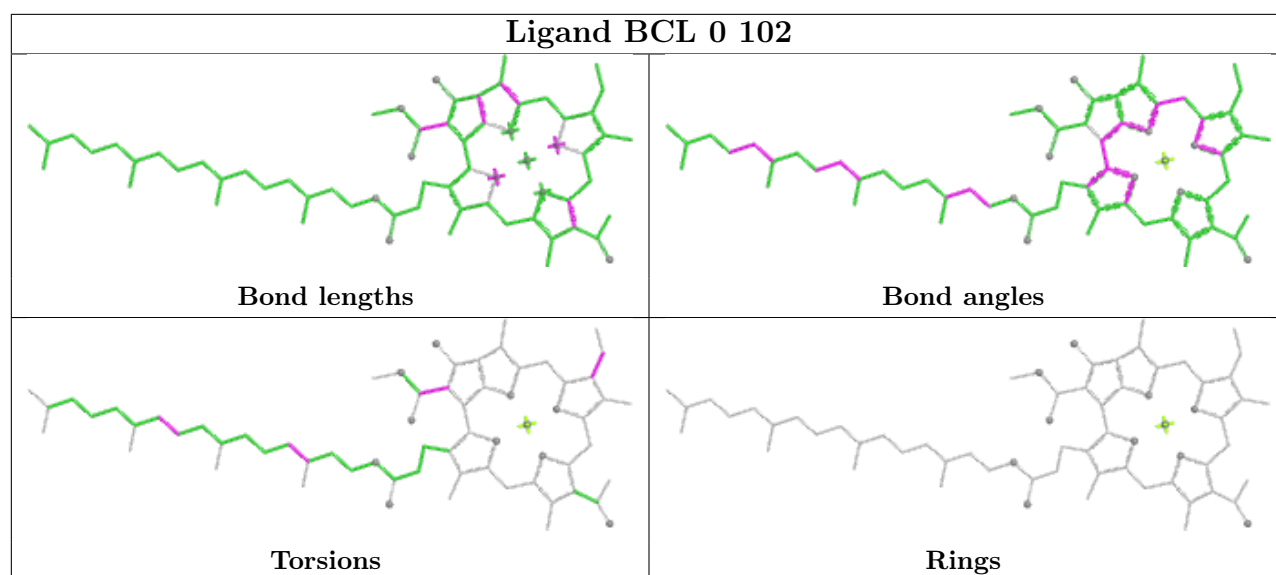
Ligand KGD 5 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

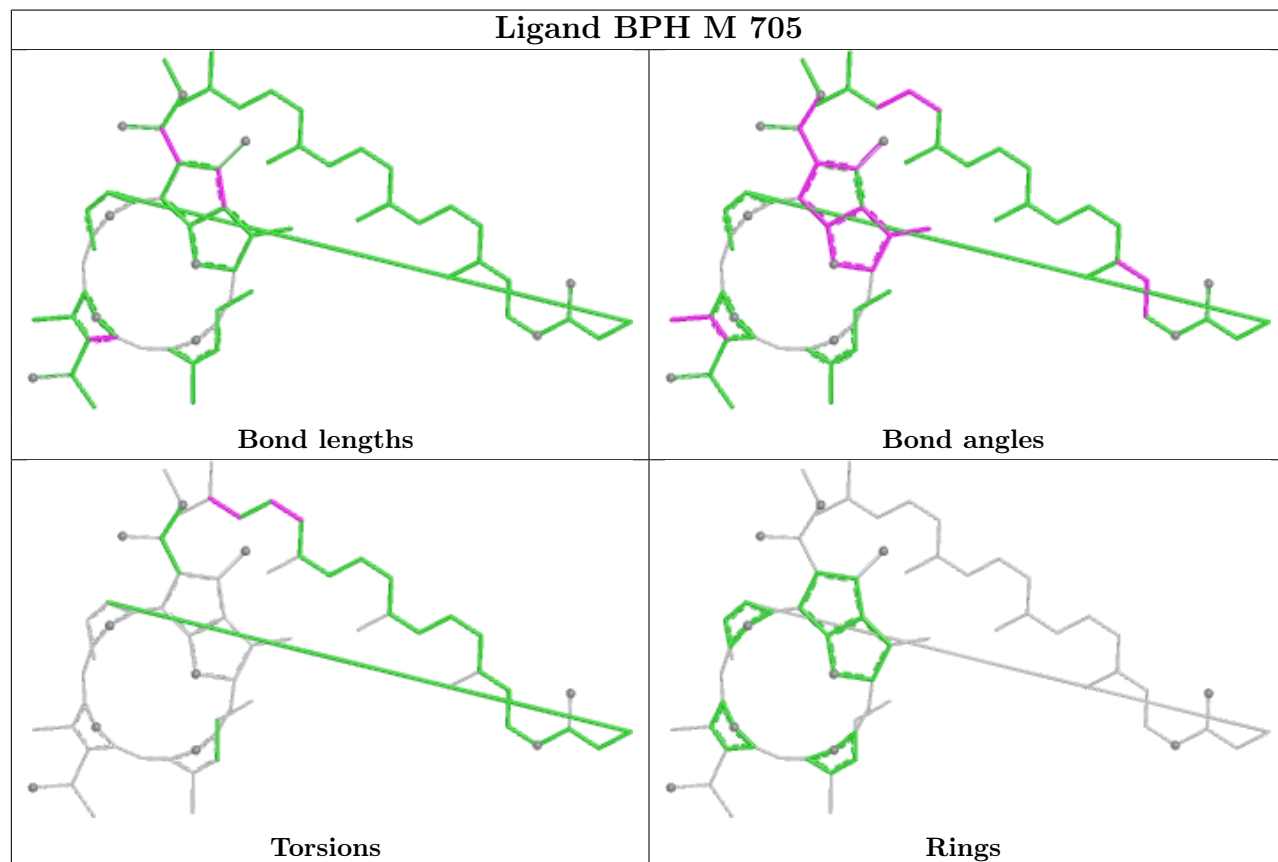
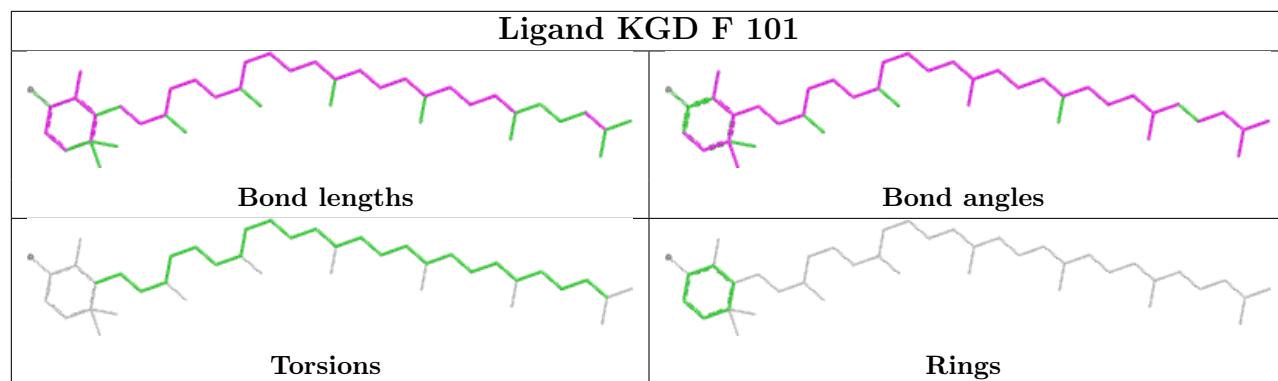


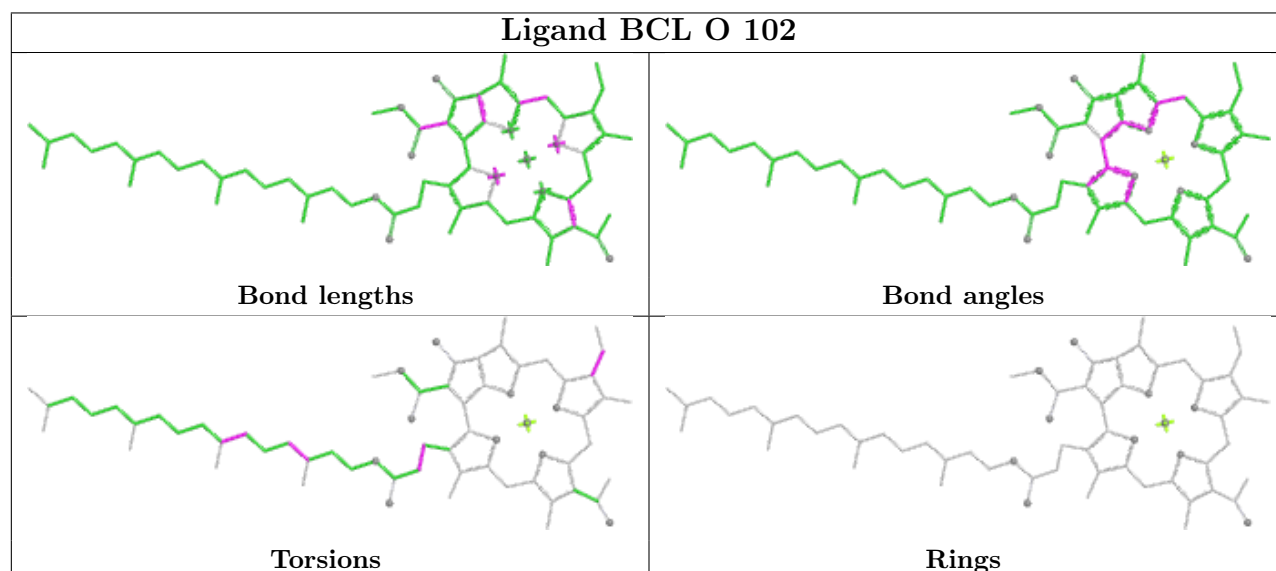
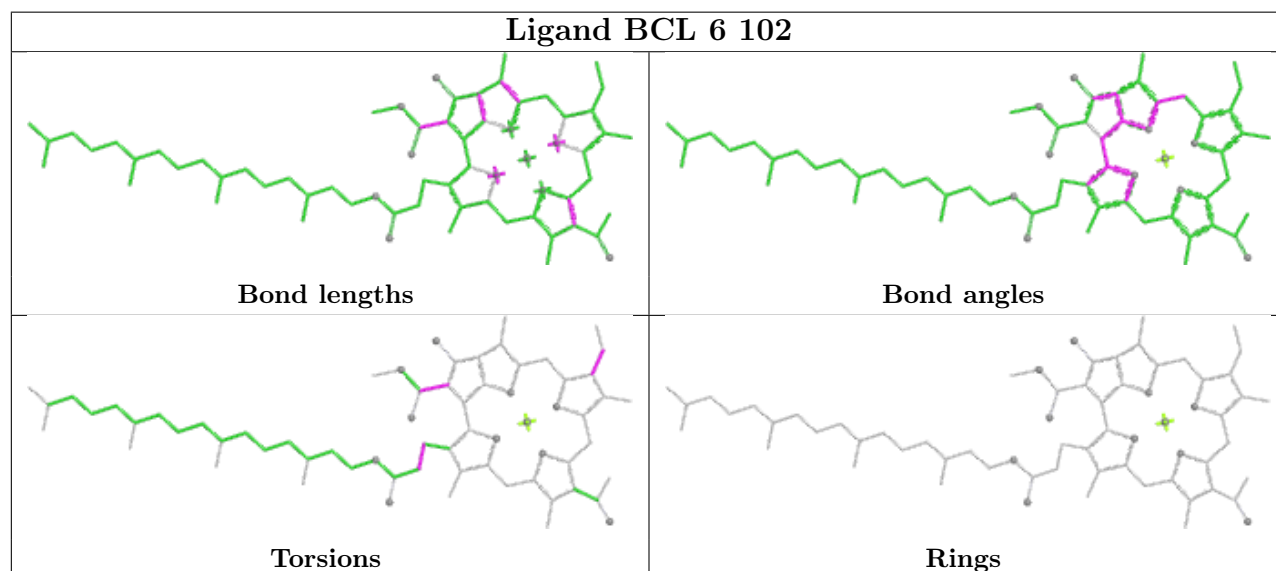
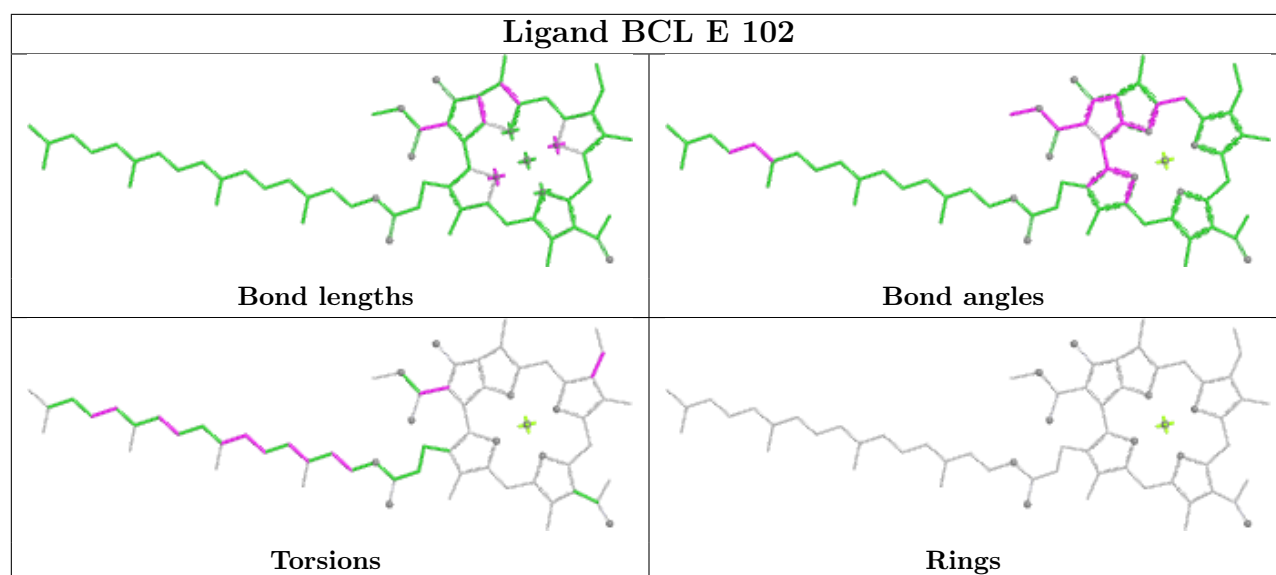


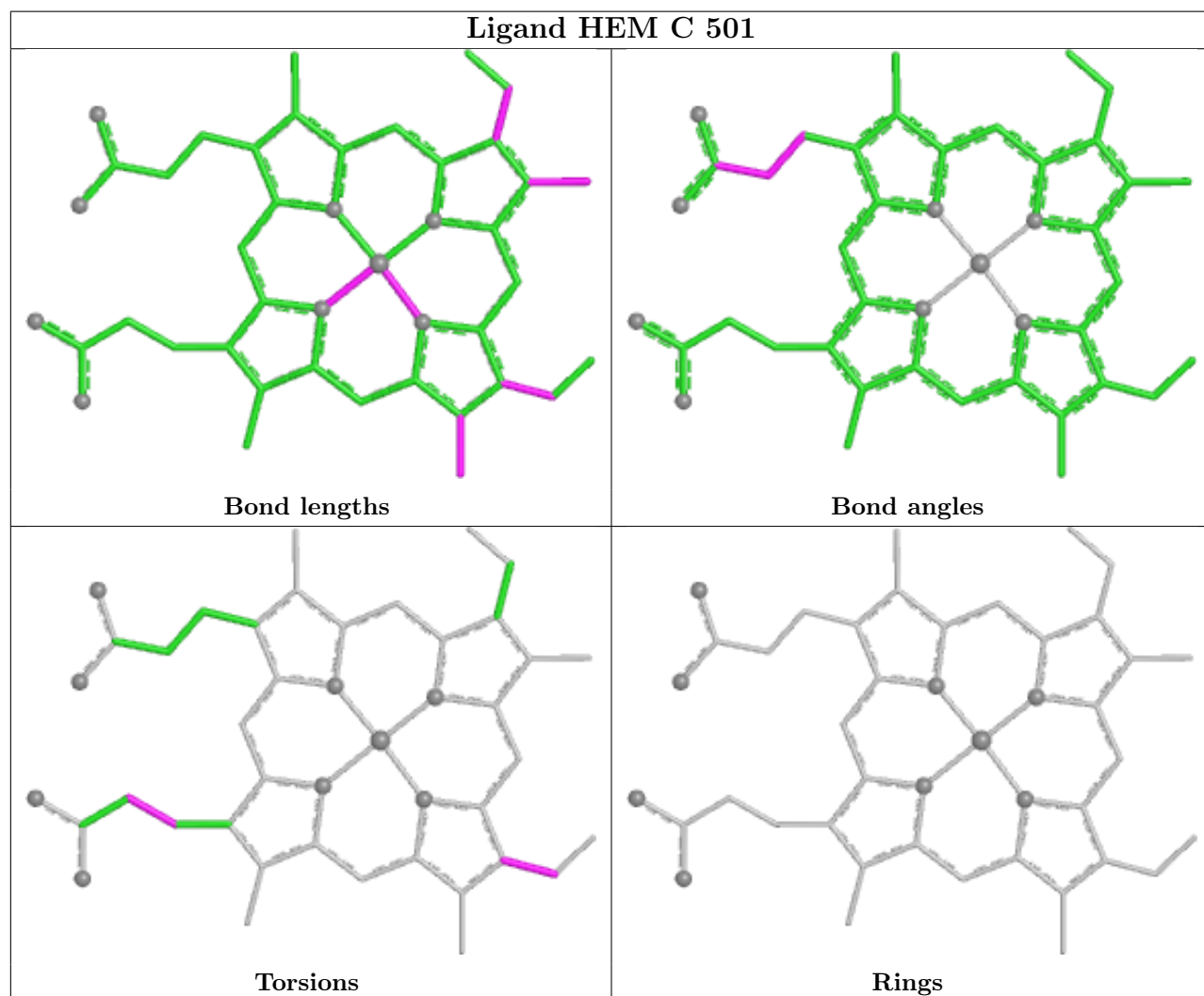
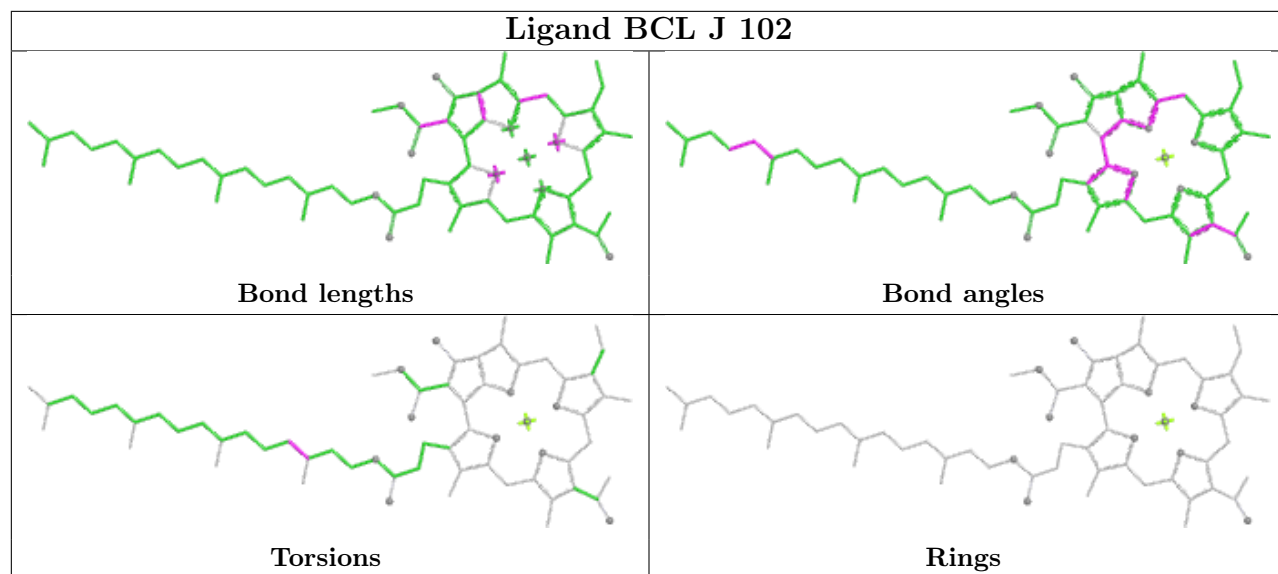


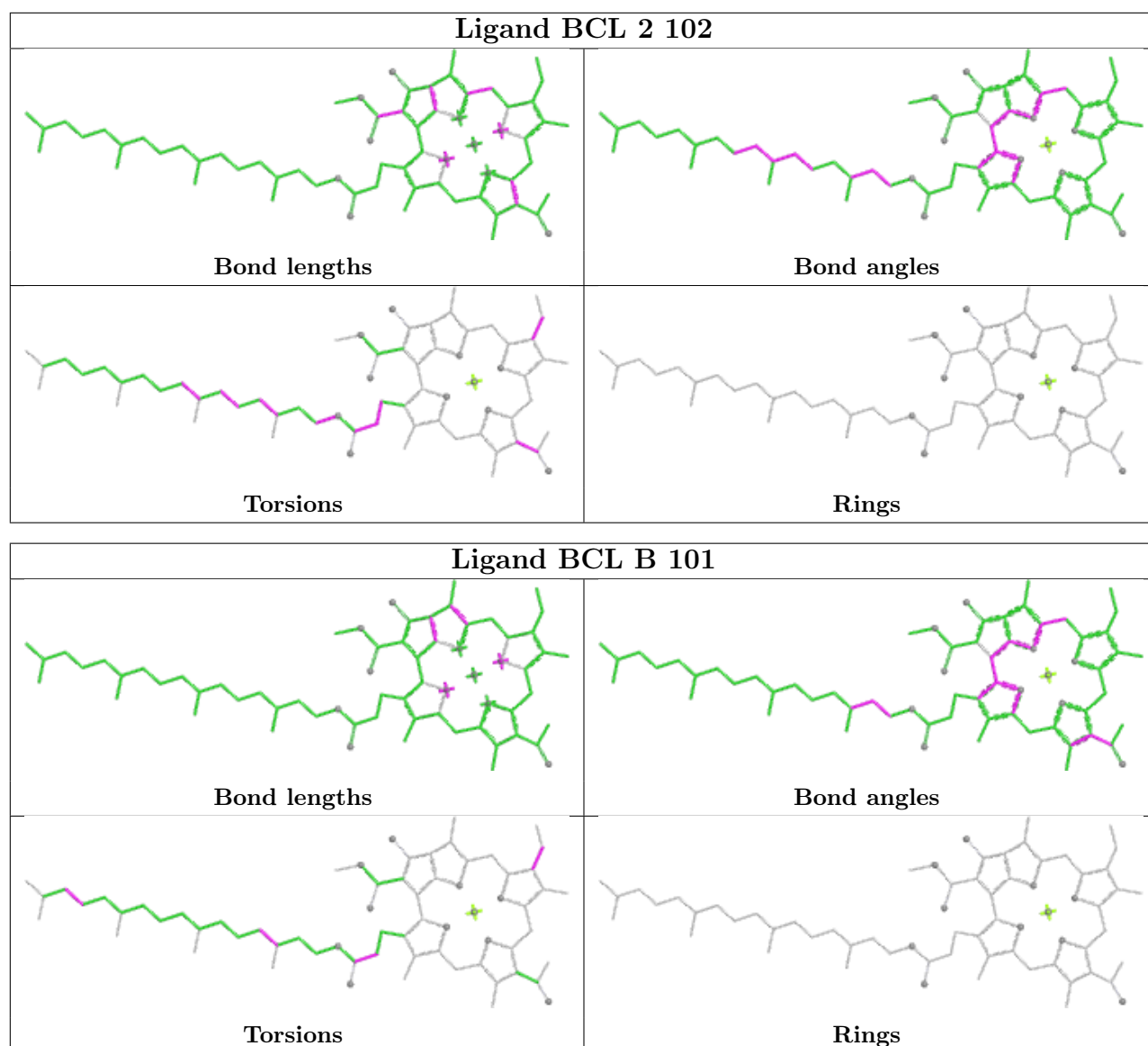


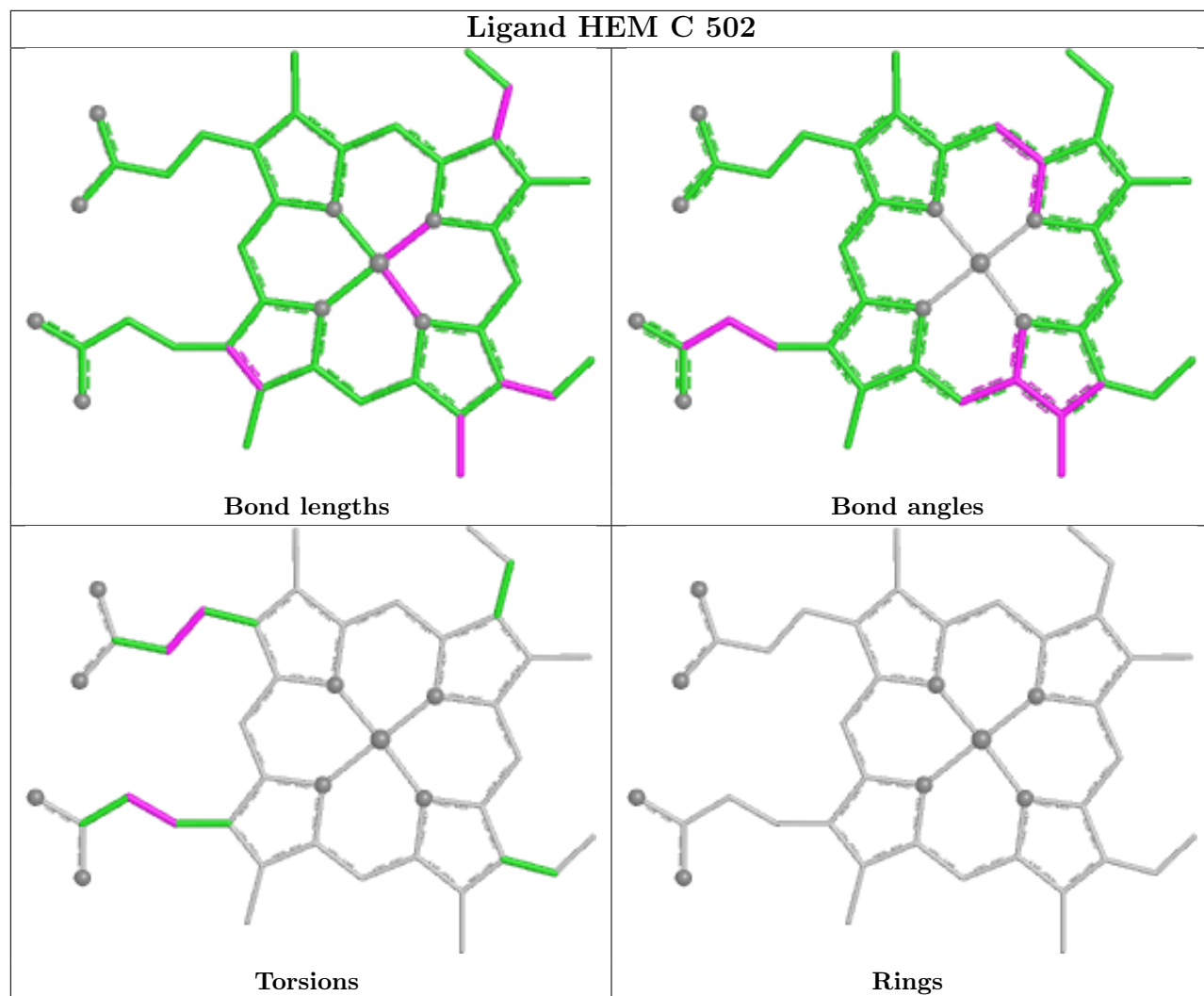


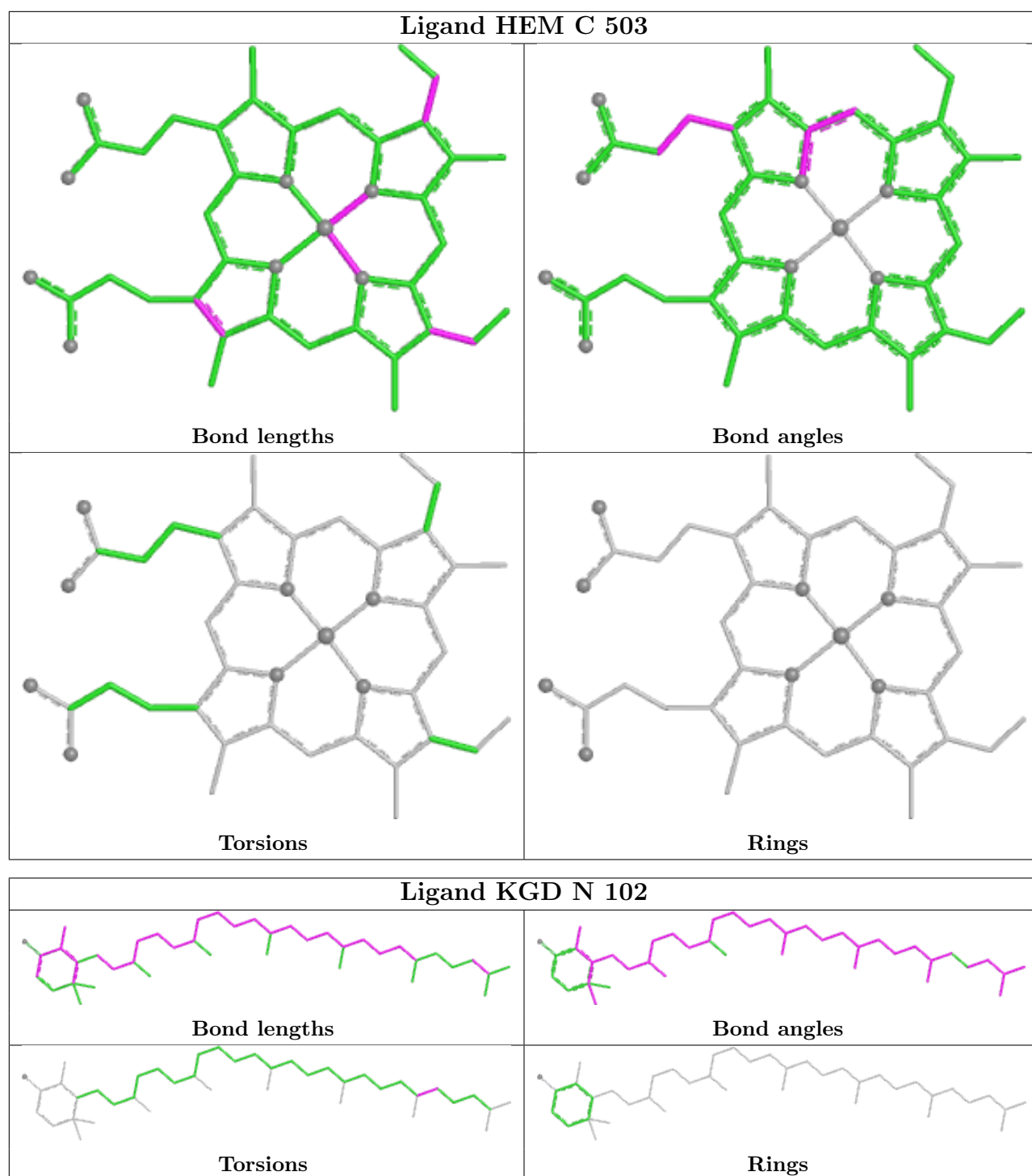


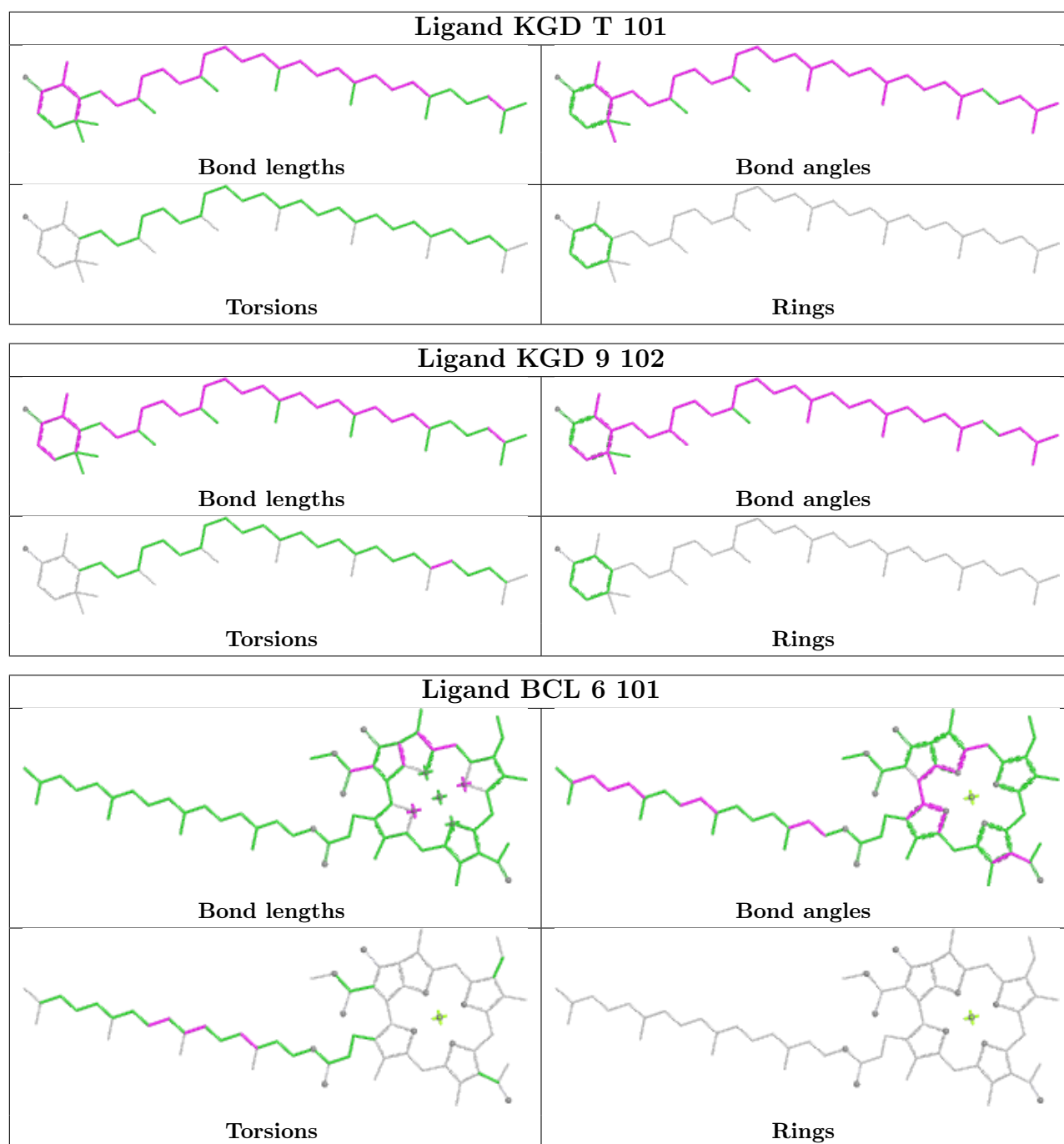


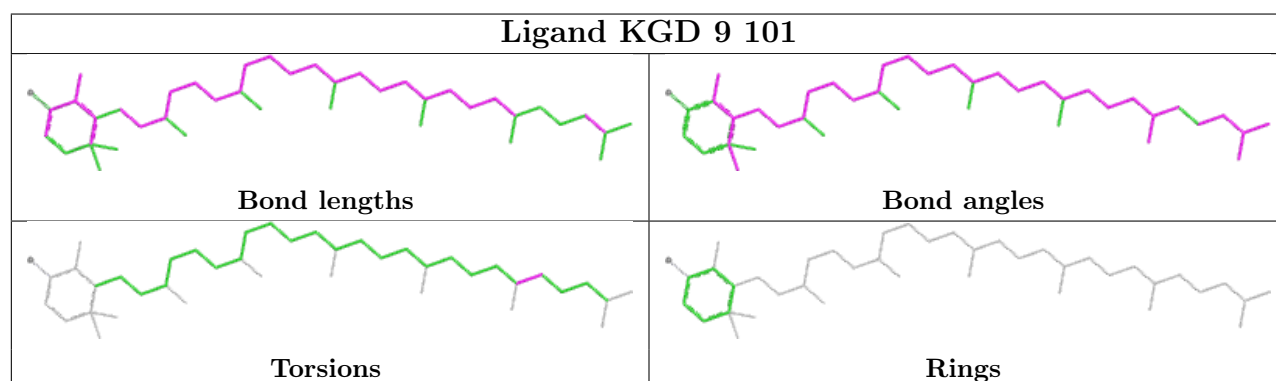
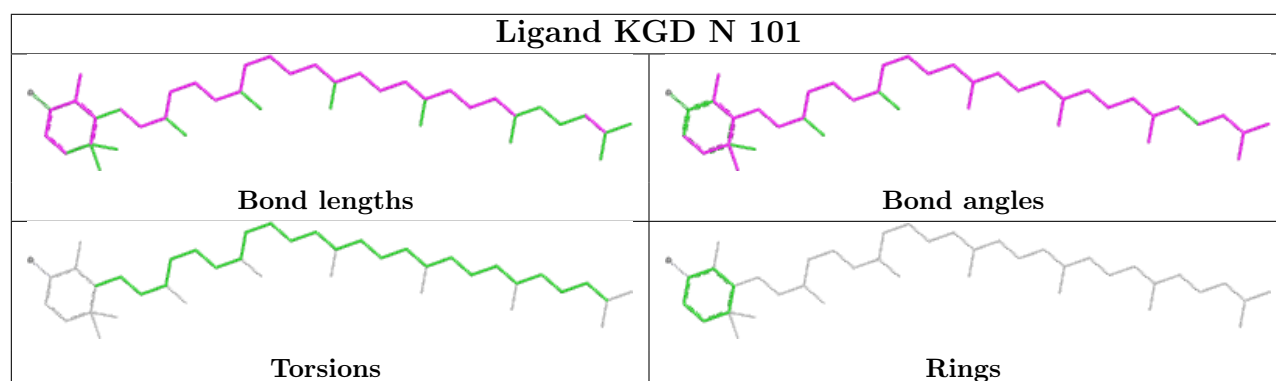
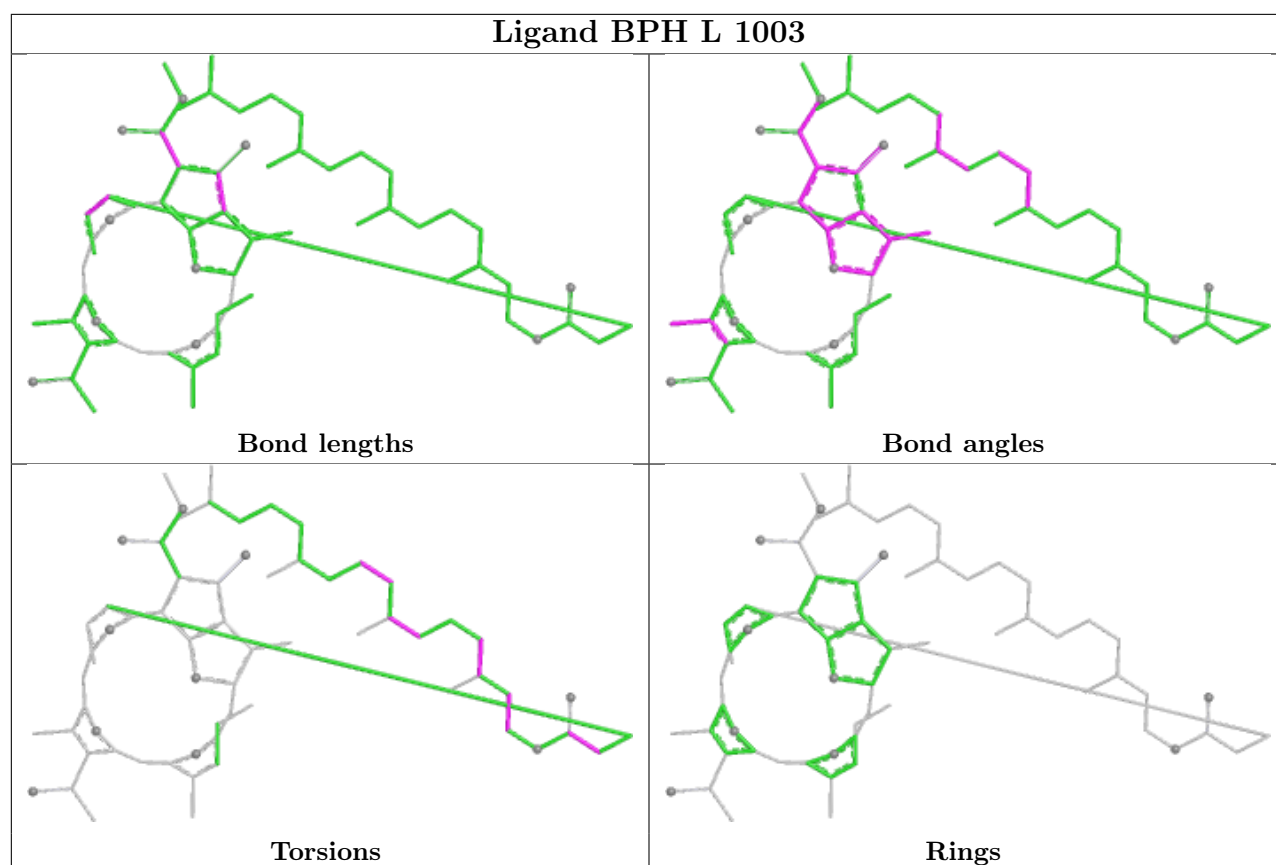


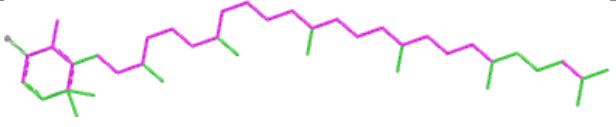
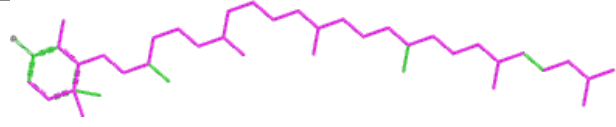
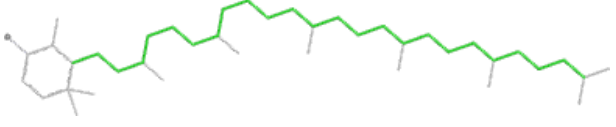
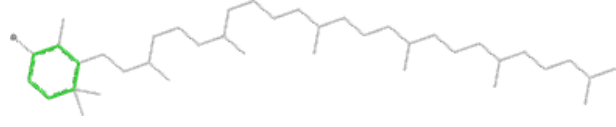


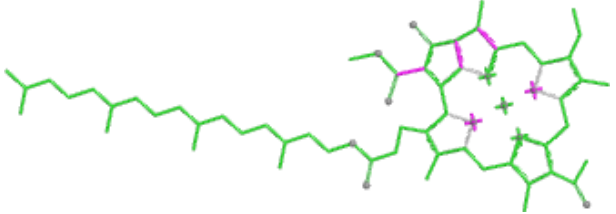
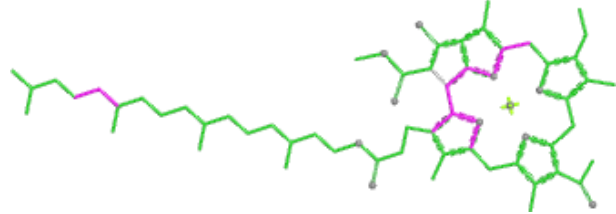
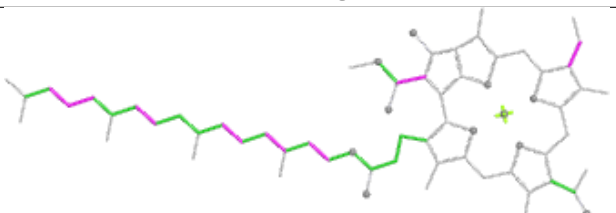
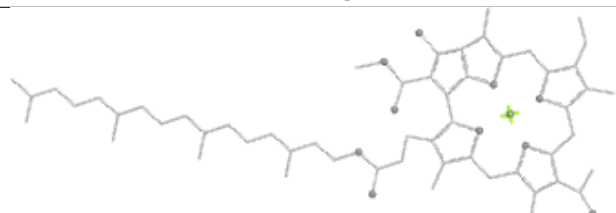


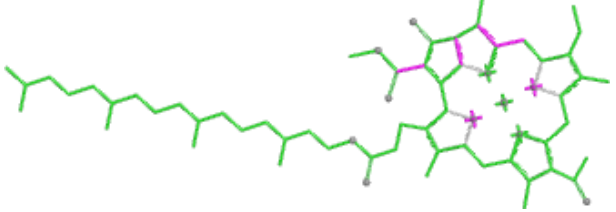
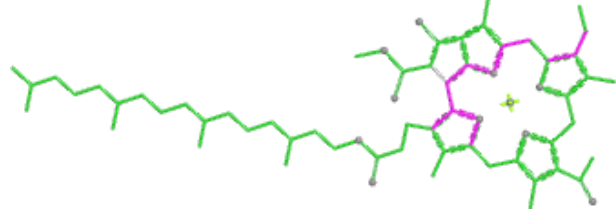
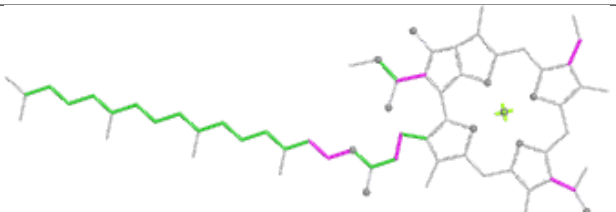
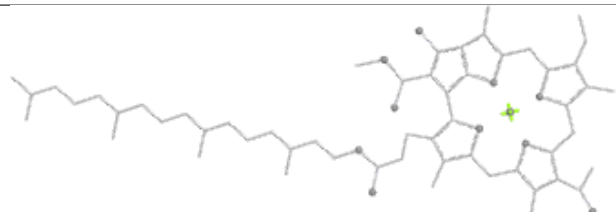


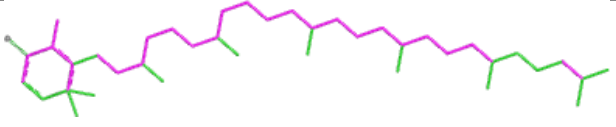
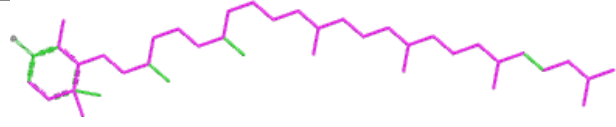
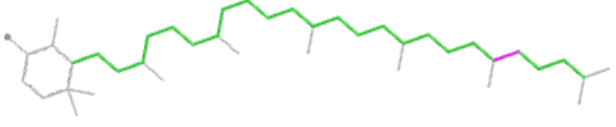
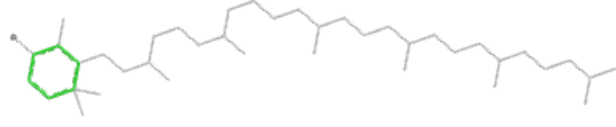


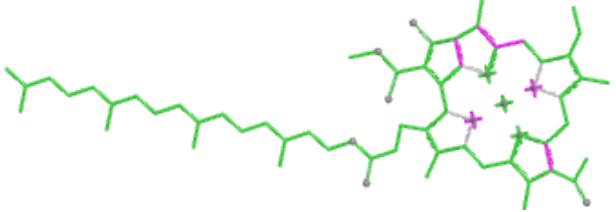
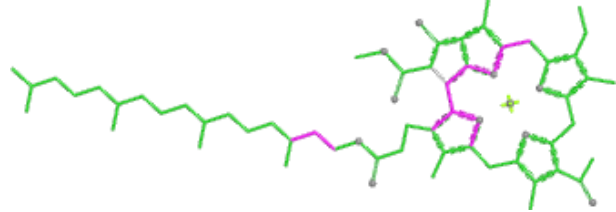
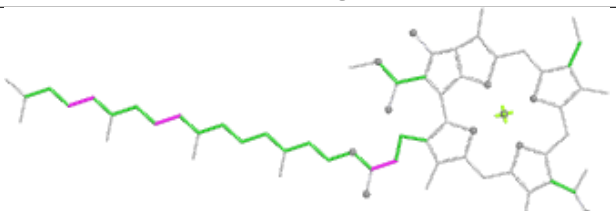
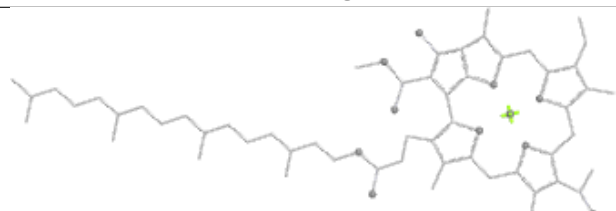


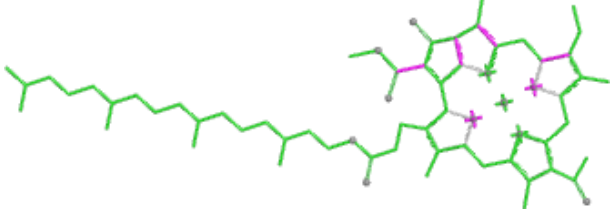
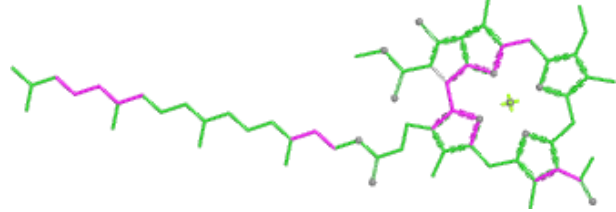
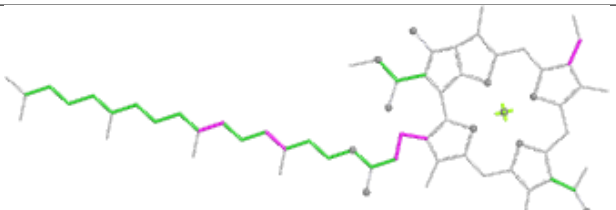
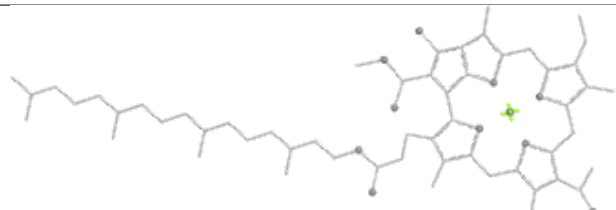
Ligand KGD J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

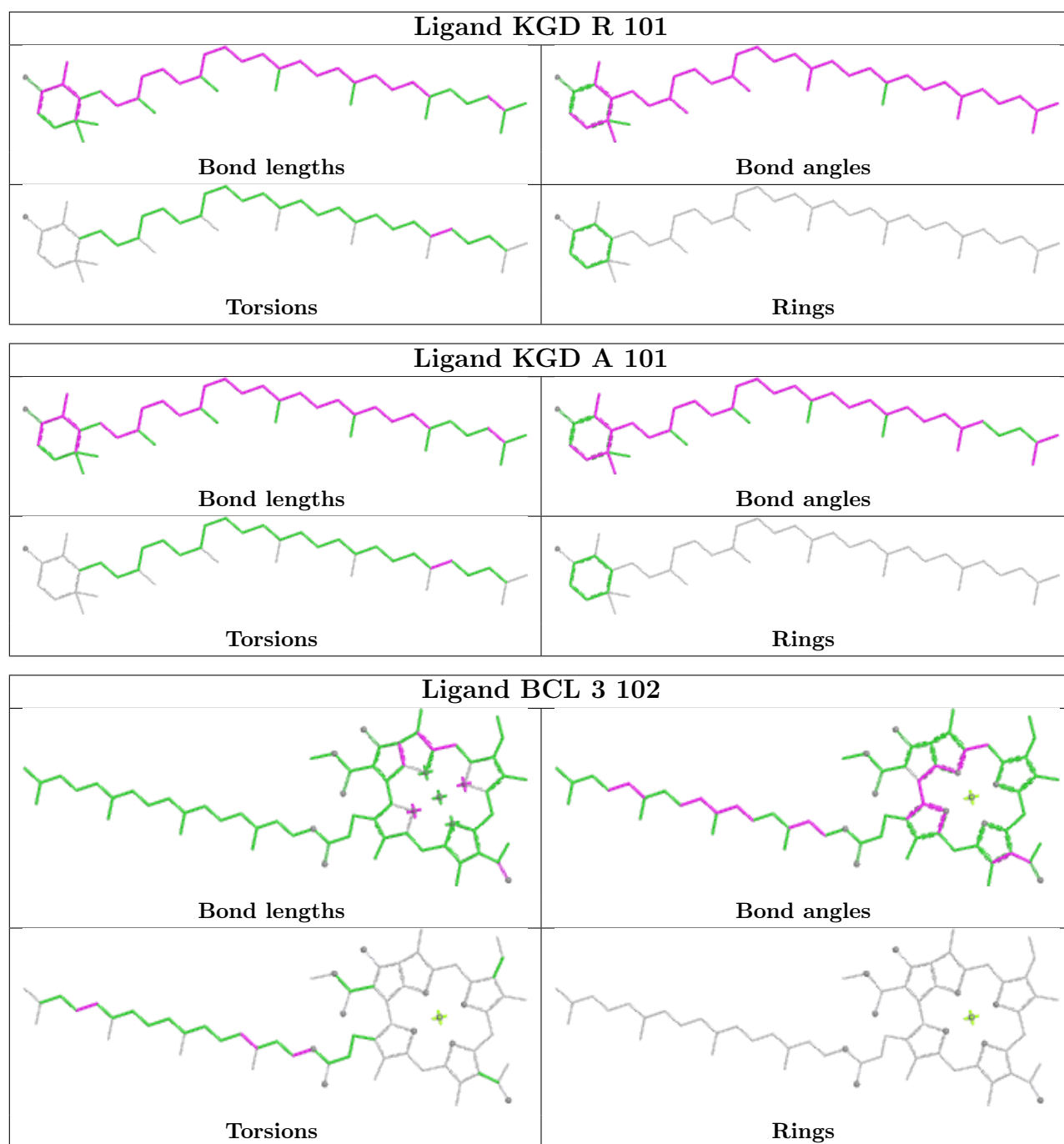
Ligand BCL G 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

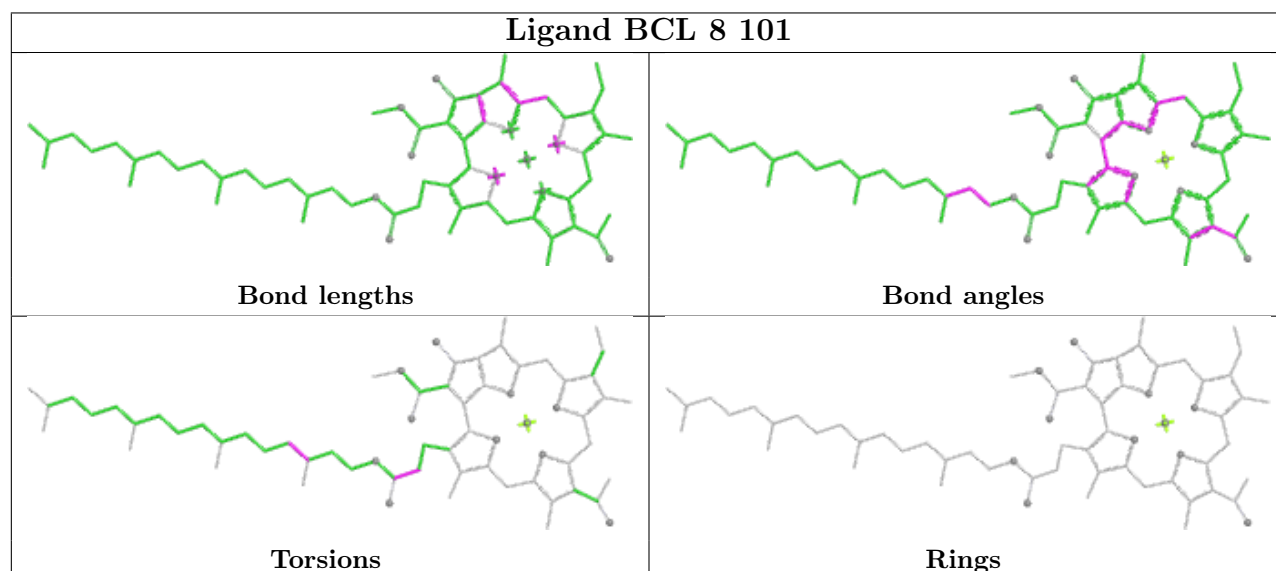
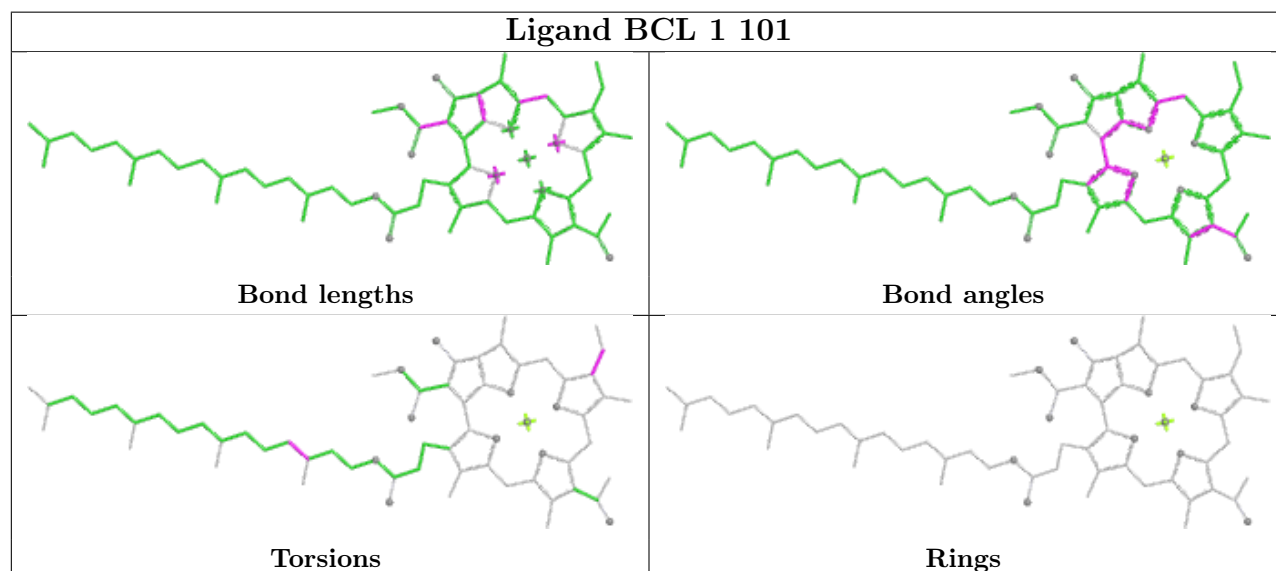
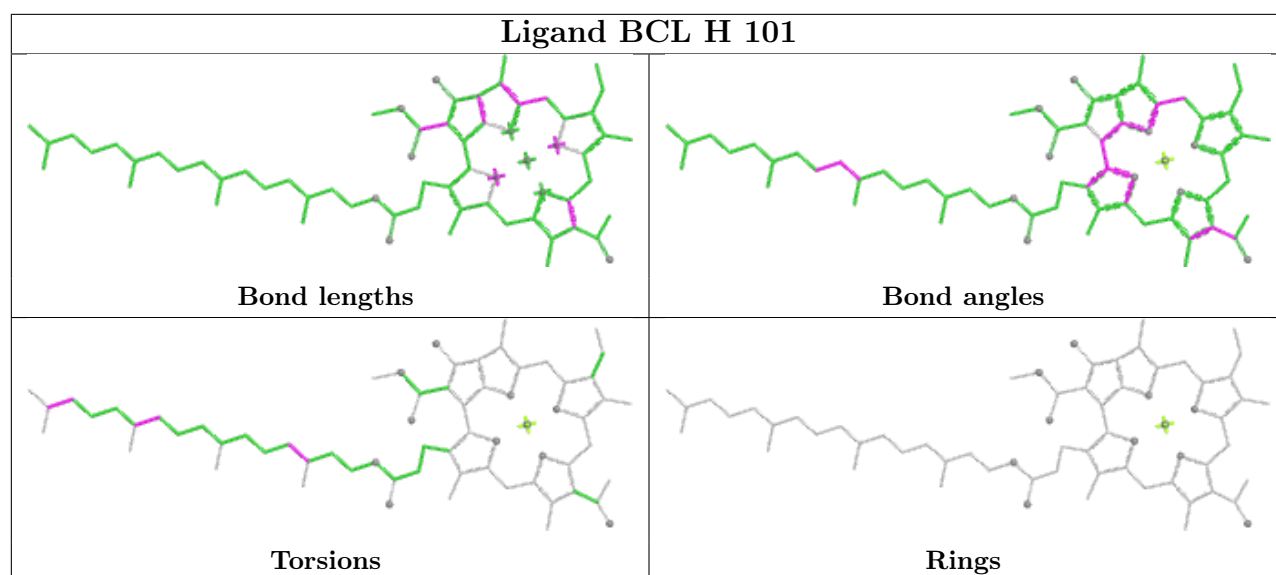
Ligand BCL U 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

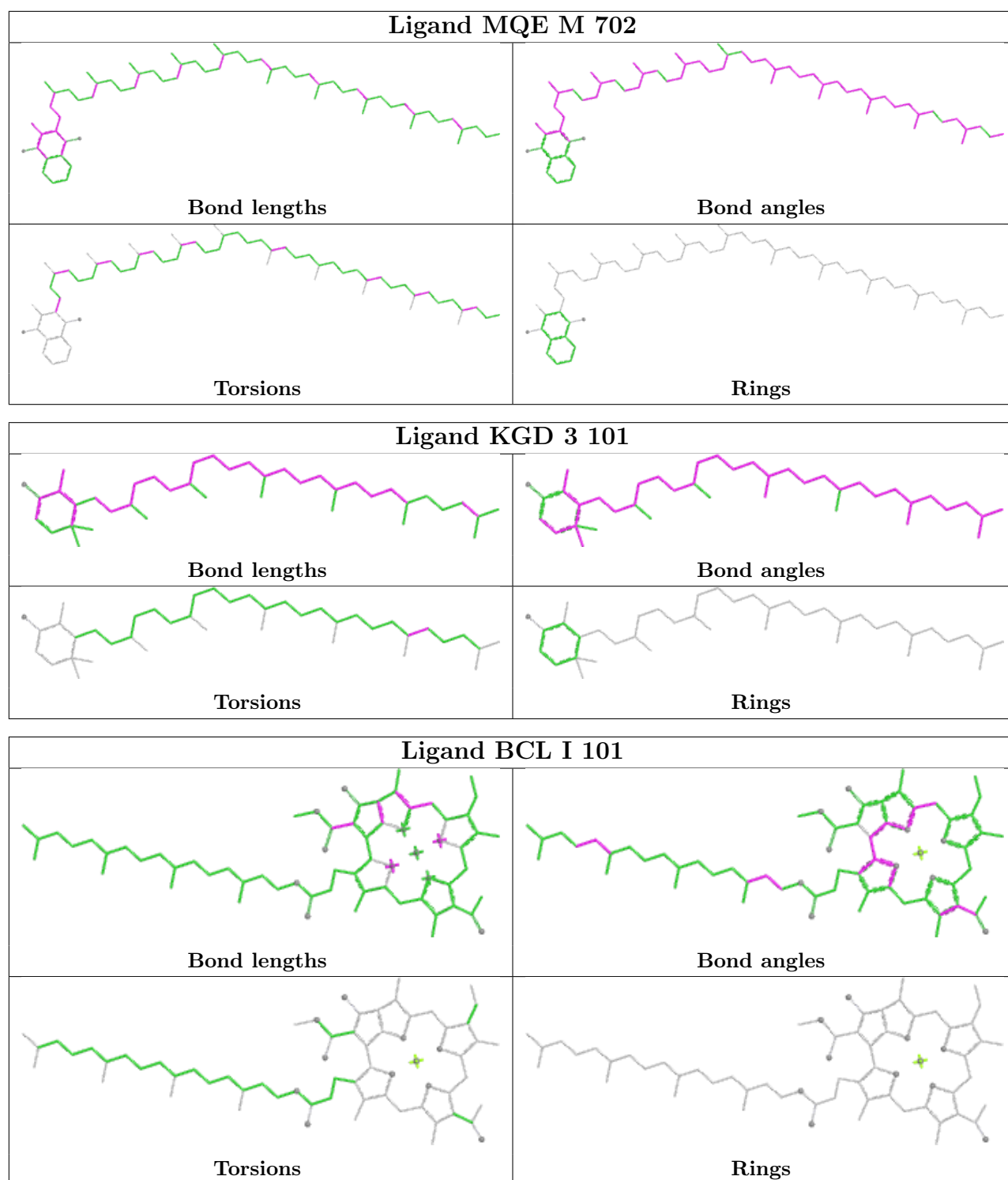
Ligand KGD T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

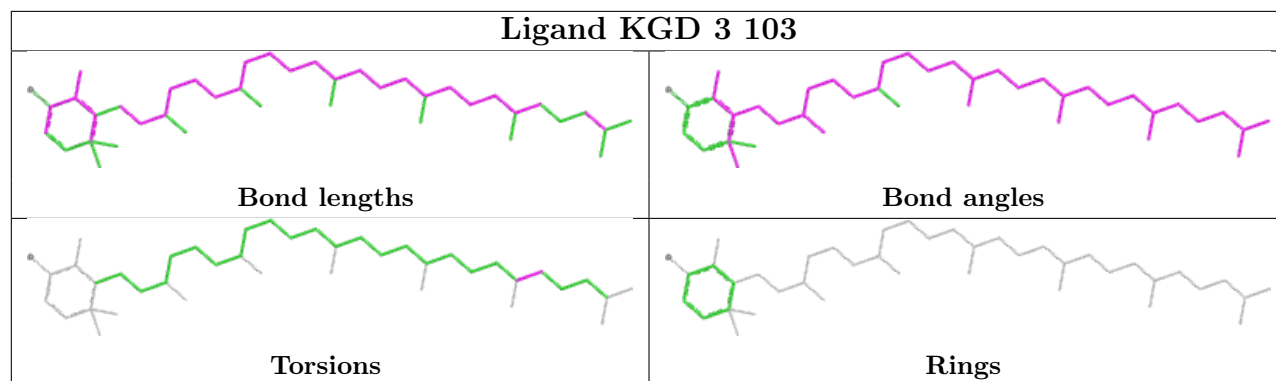
Ligand BCL 2 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL 4 101	
	
Bond lengths	Bond angles
	
Torsions	Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

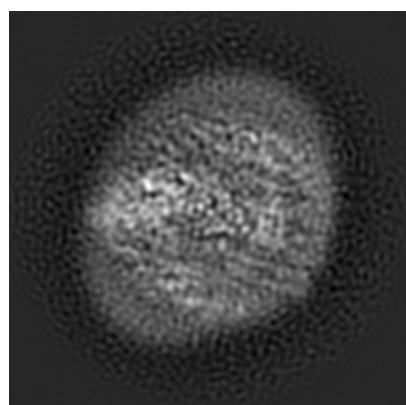
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6828. These allow visual inspection of the internal detail of the map and identification of artifacts.

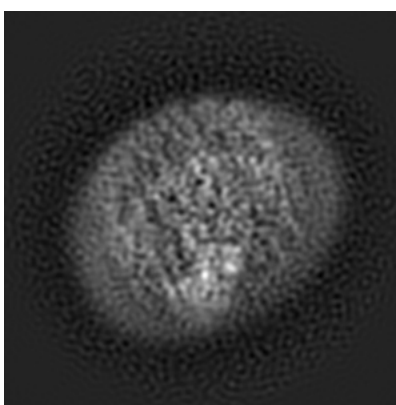
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

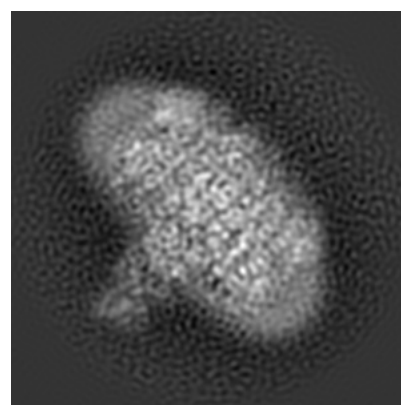
6.1.1 Primary map



X



Y

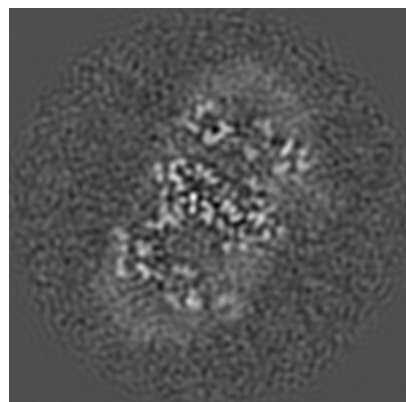


Z

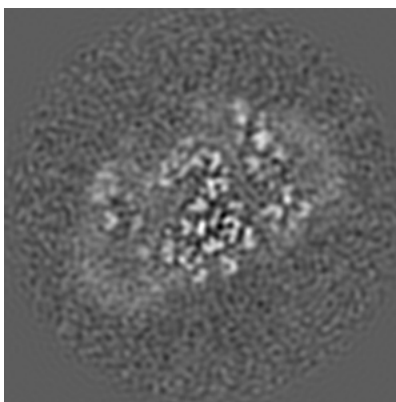
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

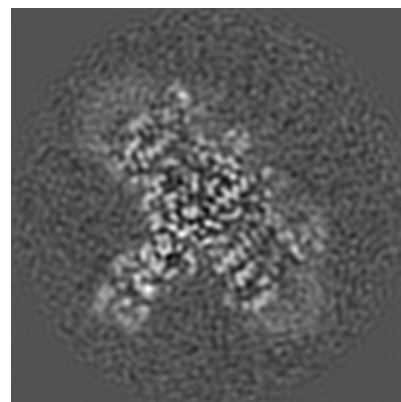
6.2.1 Primary map



X Index: 96



Y Index: 96

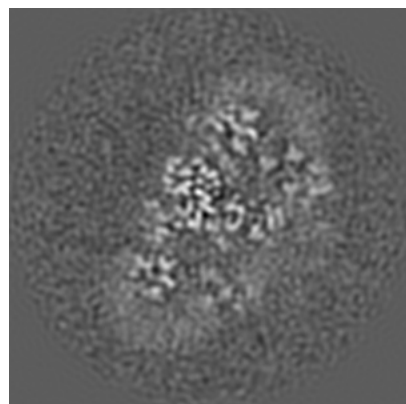


Z Index: 96

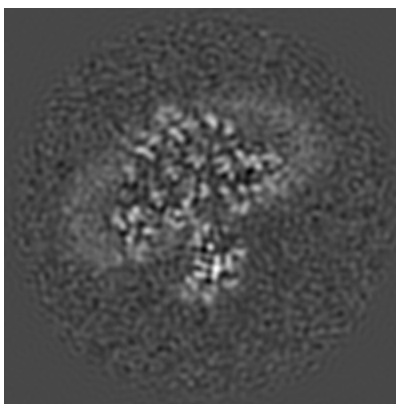
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

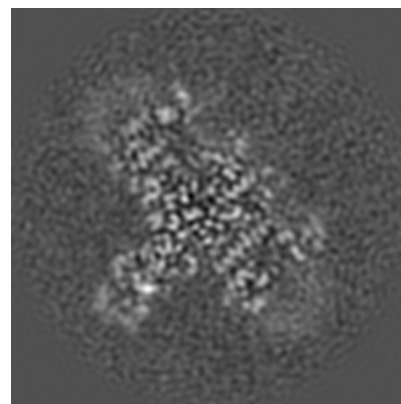
6.3.1 Primary map



X Index: 88



Y Index: 71

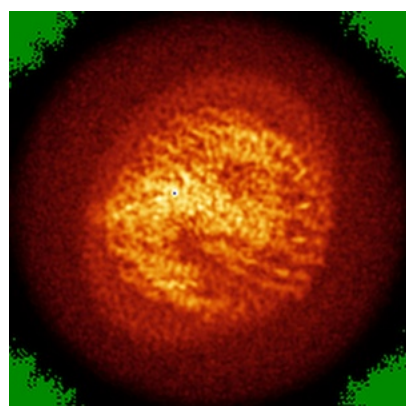


Z Index: 97

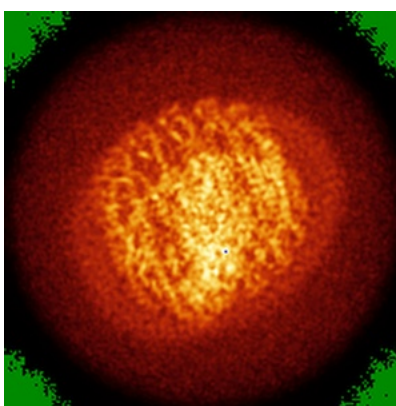
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

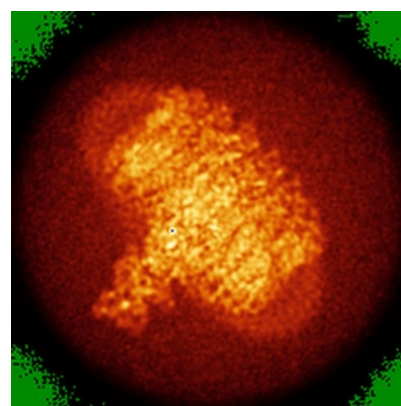
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

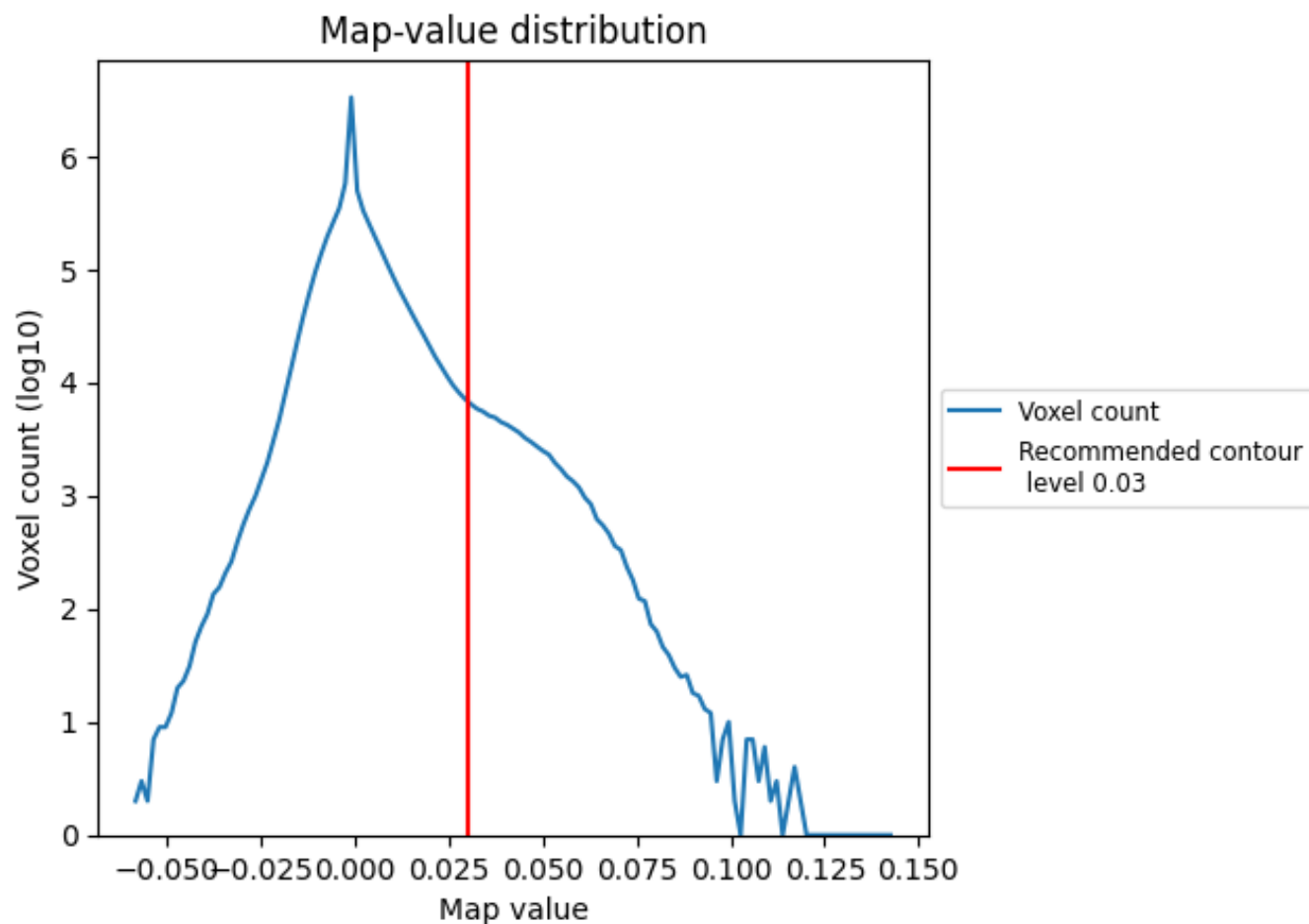
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

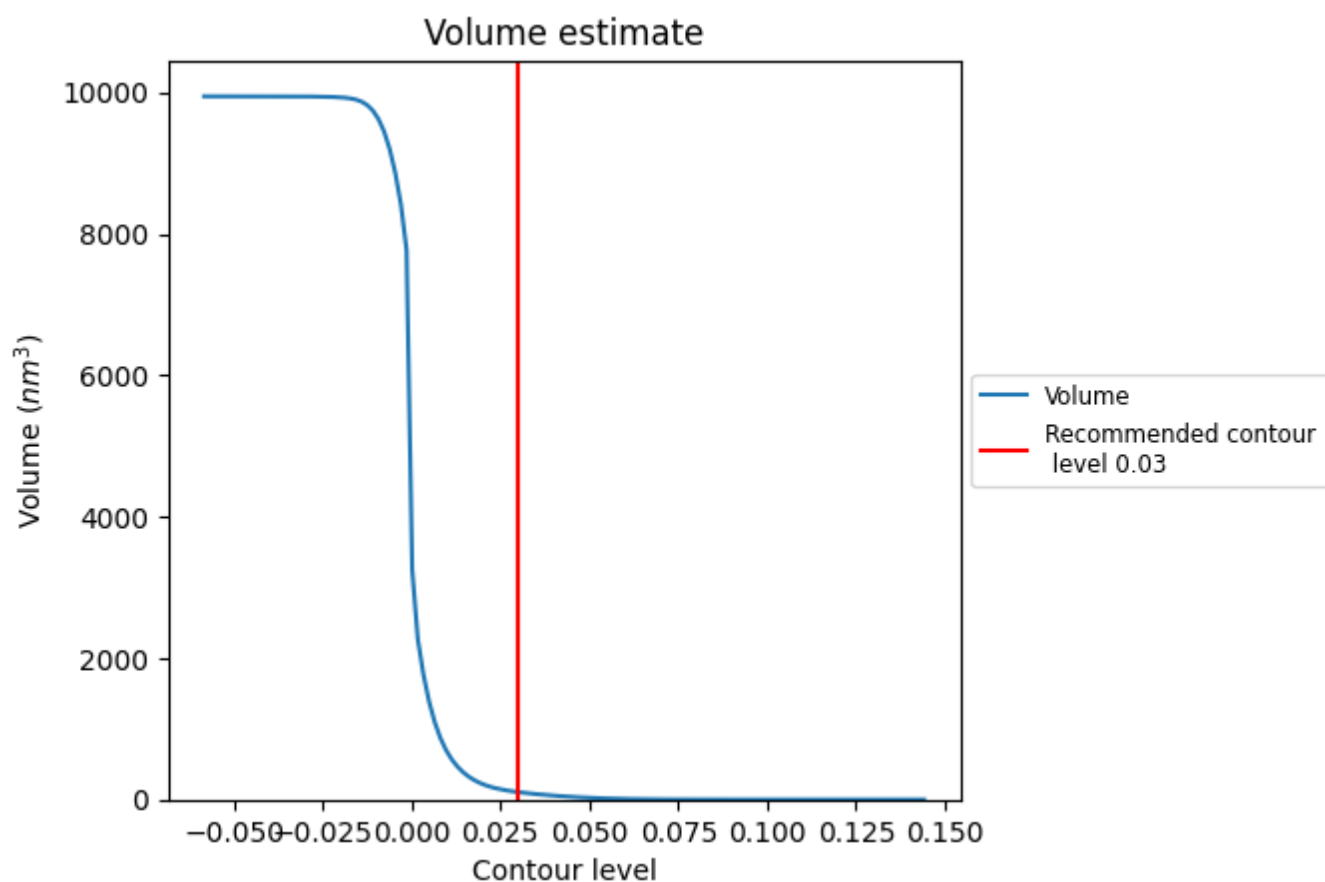
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

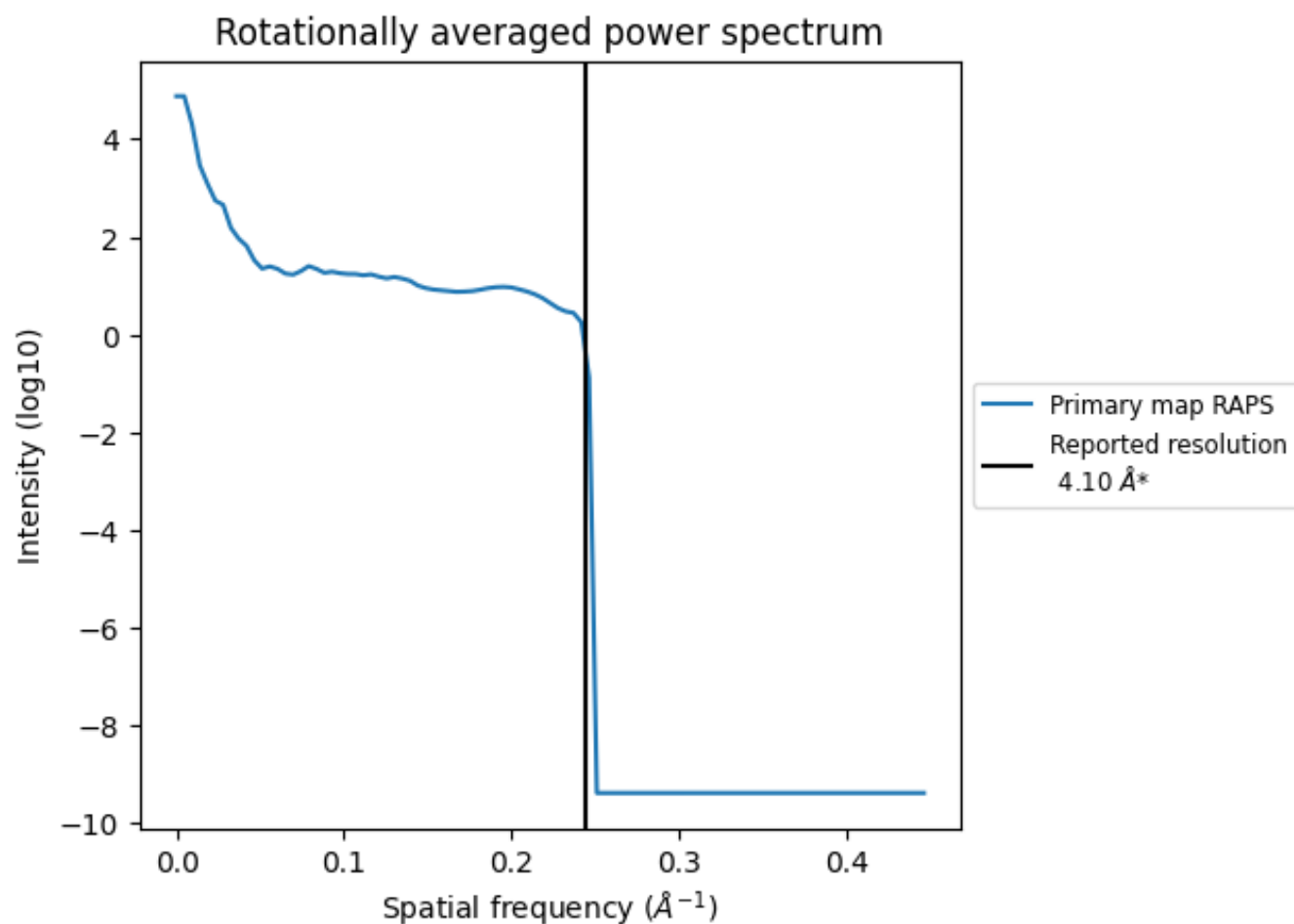
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm^3 ; this corresponds to an approximate mass of 95 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

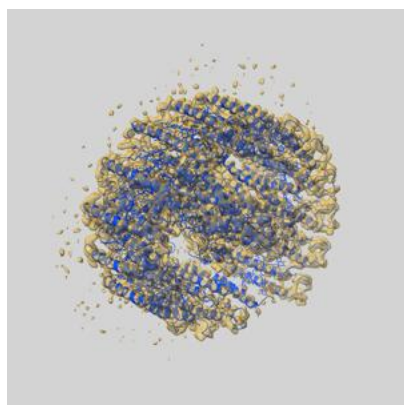
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

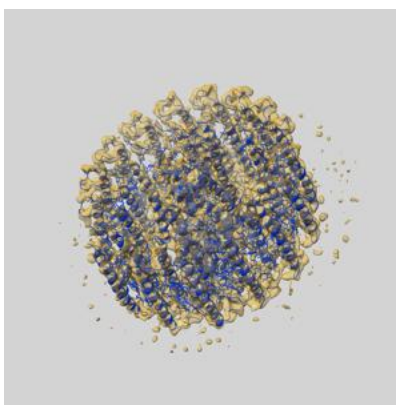
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6828 and PDB model 5YQ7. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

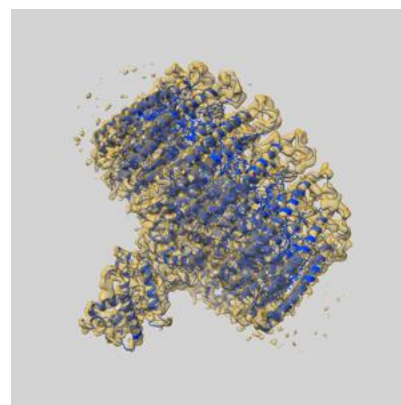
9.1 Map-model overlay [i](#)



X



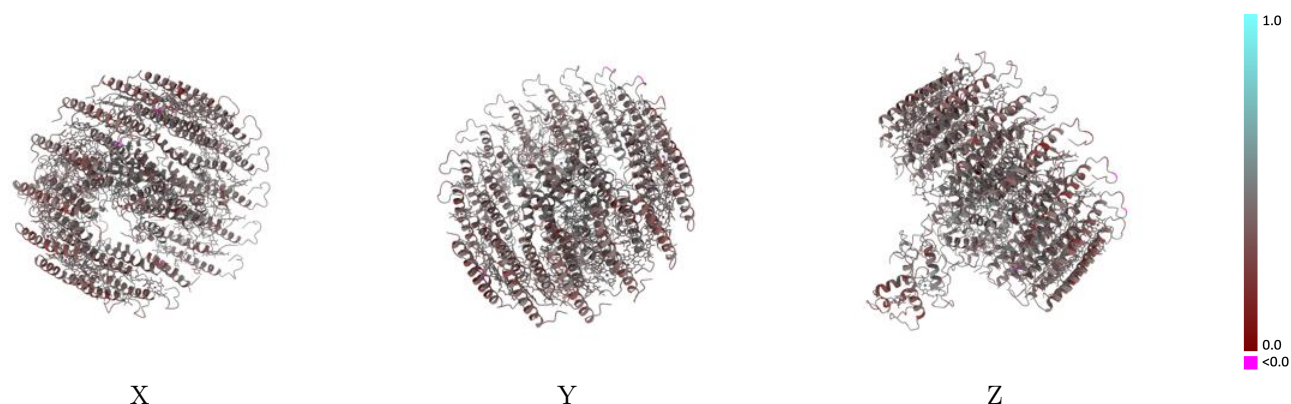
Y



Z

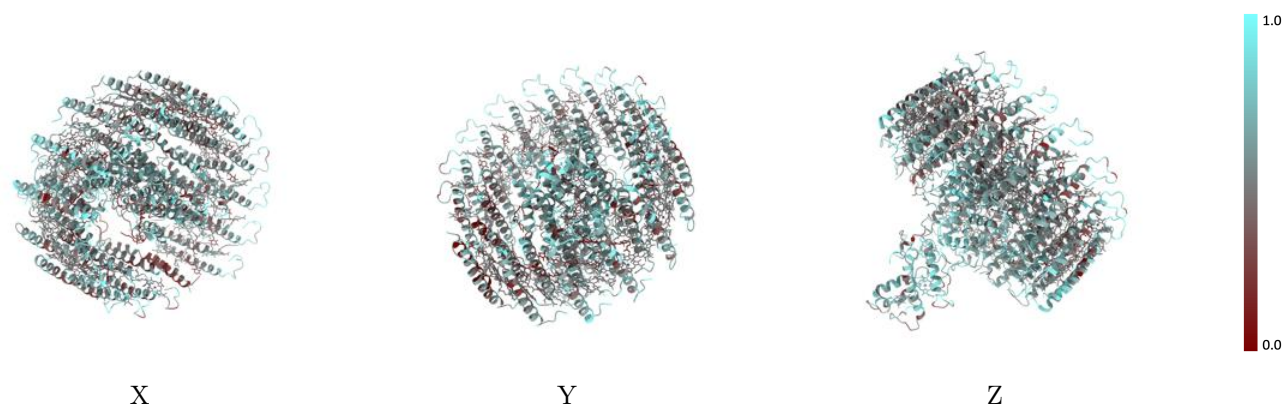
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



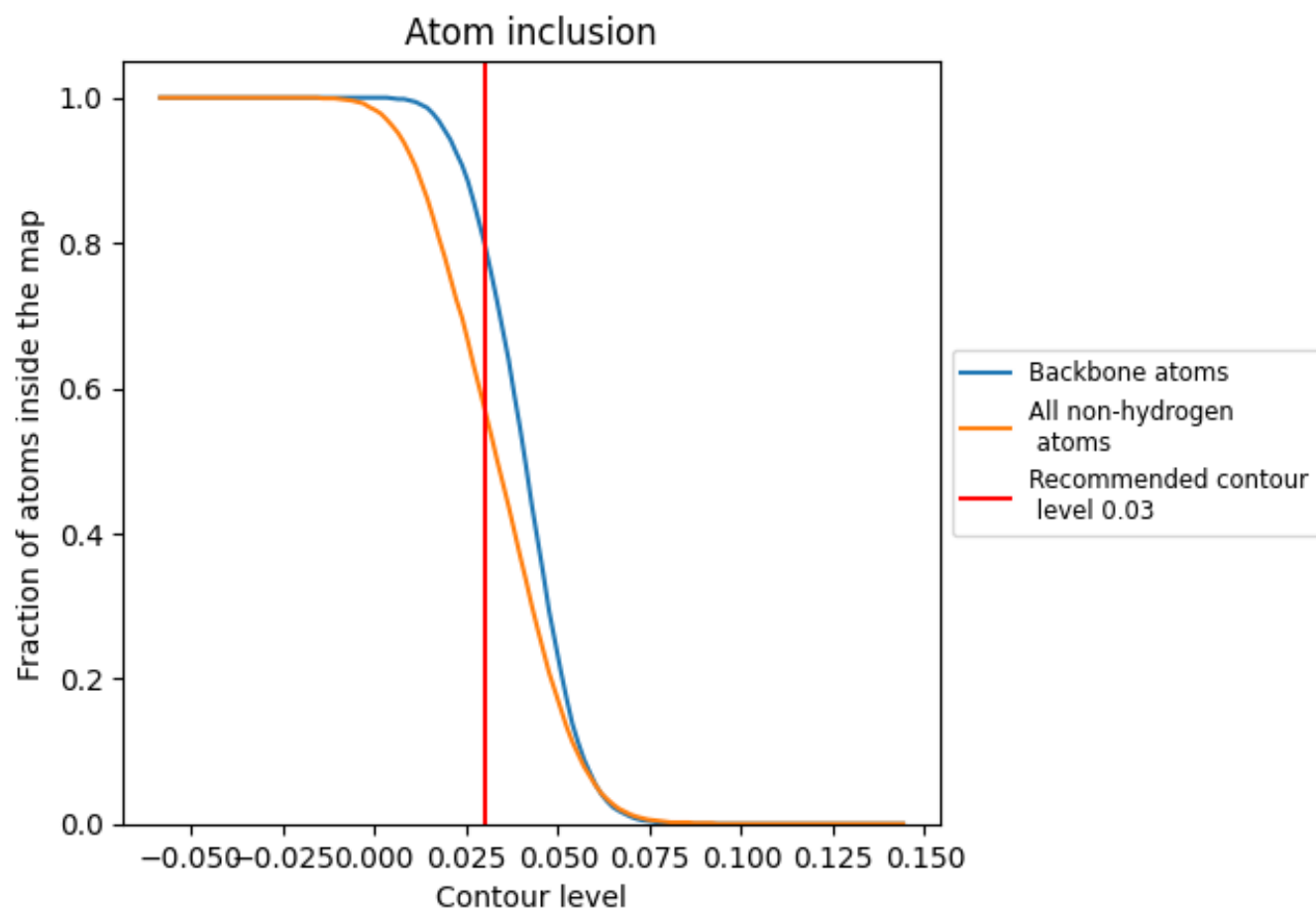
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 57% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5730	 0.4020
0	 0.6020	 0.3920
1	 0.5000	 0.4110
2	 0.5200	 0.3830
3	 0.4660	 0.3850
4	 0.5610	 0.3770
5	 0.5080	 0.3910
6	 0.5770	 0.3830
7	 0.5750	 0.4120
8	 0.5910	 0.3740
9	 0.5060	 0.4030
A	 0.5460	 0.4000
B	 0.6300	 0.3980
C	 0.6340	 0.3950
D	 0.5870	 0.4120
E	 0.6120	 0.3990
F	 0.5160	 0.4020
G	 0.5790	 0.3880
H	 0.5470	 0.4010
I	 0.5860	 0.3860
J	 0.5320	 0.3990
K	 0.5940	 0.4020
L	 0.5970	 0.4220
M	 0.6170	 0.4280
N	 0.4690	 0.3990
O	 0.5910	 0.3910
P	 0.5960	 0.4190
Q	 0.5810	 0.3960
R	 0.5180	 0.3920
S	 0.5990	 0.4020
T	 0.4440	 0.3910
U	 0.5590	 0.3950
V	 0.4480	 0.3660
W	 0.5290	 0.3790
X	 0.0430	 0.2960
Y	 0.7280	 0.4360

