



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:13 AM UTC

PDB ID : 6M32 / pdb_00006m32
EMDB ID : EMD-30069
Title : Cryo-EM structure of FMO-RC complex from green sulfur bacteria
Authors : Chen, J.H.; Zhang, X.
Deposited on : 2020-03-02
Resolution : 2.70 Å(reported)

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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

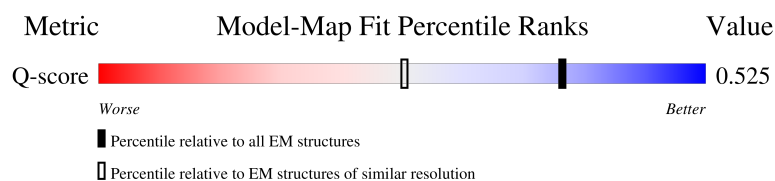
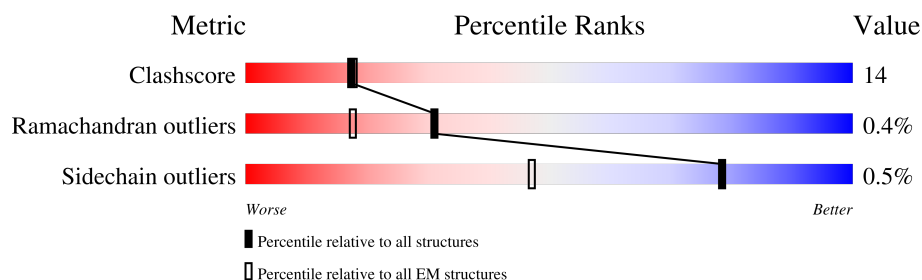
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	E	366	14% 72% 26% .
1	F	366	12% 75% 23% .
1	G	366	9% 73% 24% ..
2	D	143	41% 36% 29% .. 34%

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Mol	Chain	Length	Quality of chain
3	B	231	
4	A	731	
4	a	731	

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
6	SF4	B	301	-	-	X	-
9	F39	A	817	-	X	-	-
9	F39	a	817	-	X	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 23566 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 Bacteriochlorophyll a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	362	Total	C	N	O	S	0	0
			2815	1783	501	524	7		
1	F	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		
1	G	358	Total	C	N	O	S	0	0
			2789	1770	496	516	7		

- Molecule 2 is a protein called P840 reaction center 17 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	94	Total	C	N	O	S	0	0
			766	484	137	141	4		

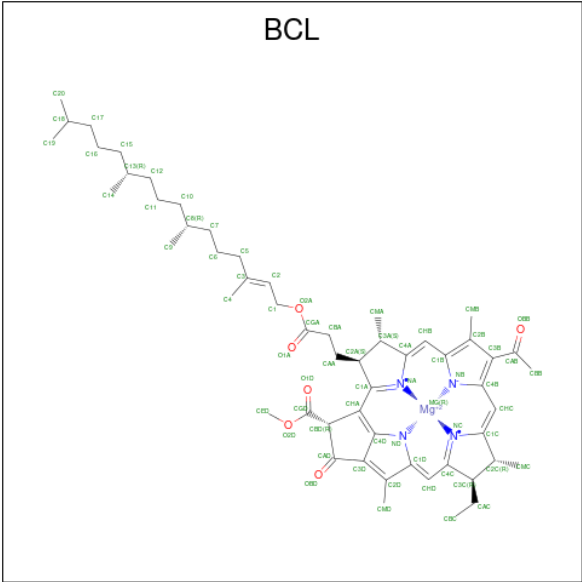
- Molecule 3 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	95	Total	C	N	O	S	0	0
			731	469	115	138	9		

- Molecule 4 is a protein called Photosystem P840 reaction center, large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	628	Total	C	N	O	S	0	0
			5030	3360	798	846	26		
4	a	628	Total	C	N	O	S	0	0
			5030	3360	798	846	26		

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	E	1	Total 46	C 35	Mg 1	N 4	O 6	1
5	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	F	1	Total 66	C 55	Mg 1	N 4	O 6	0

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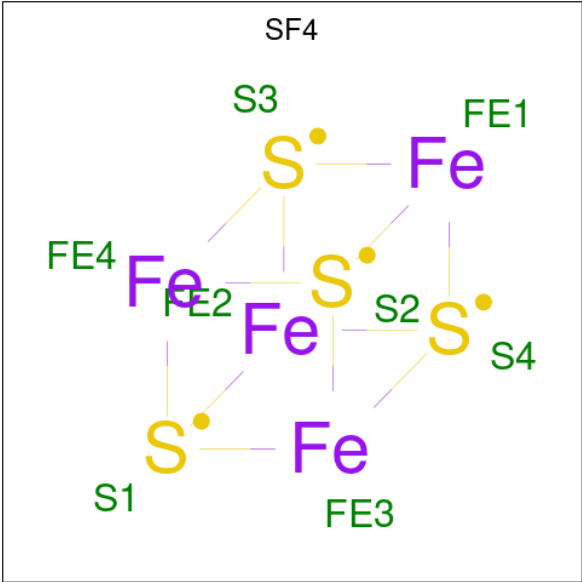
Mol	Chain	Residues	Atoms					AltConf
5	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	F	1	Total 46	C 35	Mg 1	N 4	O 6	1
5	G	1	Total 46	C 35	Mg 1	N 4	O 6	1
5	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	A	1	Total 46	C 35	Mg 1	N 4	O 6	0
5	A	1	Total 56	C 45	Mg 1	N 4	O 6	0
5	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	A	1	Total 46	C 35	Mg 1	N 4	O 6	0
5	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	A	1	Total 46	C 35	Mg 1	N 4	O 6	0
5	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
5	A	1	Total 46	C 35	Mg 1	N 4	O 6	0
5	A	1	Total 46	C 35	Mg 1	N 4	O 6	0

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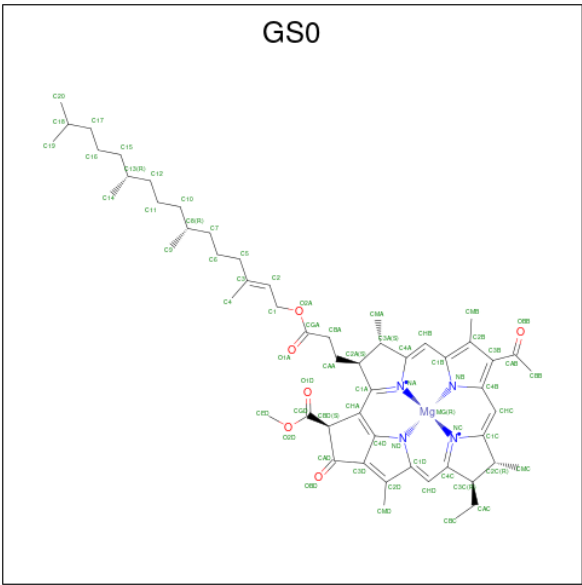
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
5	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 6 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	Fe	S	0
			8	4	4	
6	B	1	Total	Fe	S	0
			8	4	4	
6	A	1	Total	Fe	S	0
			8	4	4	

- Molecule 7 is Bacteriochlorophyll A isomer (CCD ID: GS0) (formula: C₅₅H₇₄MgN₄O₆).



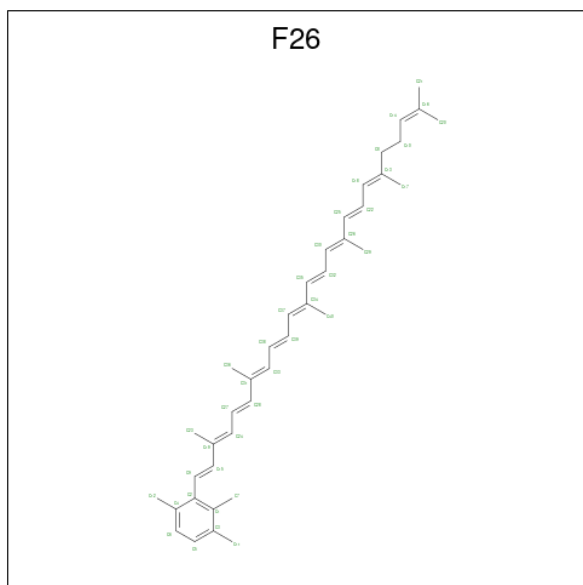
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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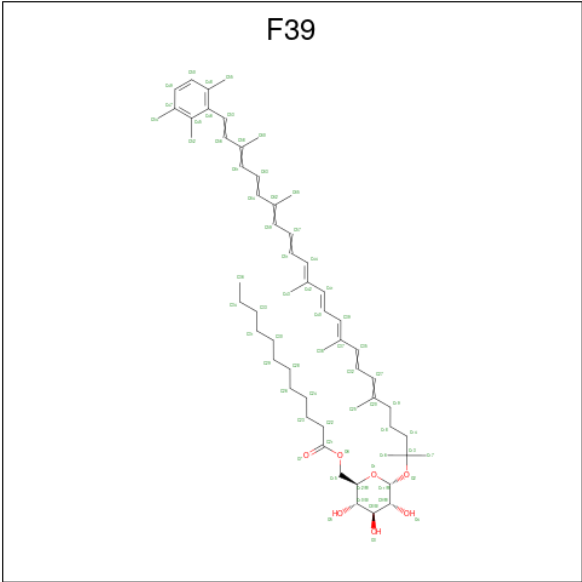
Mol	Chain	Residues	Atoms					AltConf
7	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is 2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E,19E)-3,7,12,16,20,24-hexamethylpentacos-1,3,5,7,9,11,13,15,17,19,23-undecaenyl]-1,3,4-trimethyl-benzene (CCD ID: F26) (formula: $C_{40}H_{52}$).



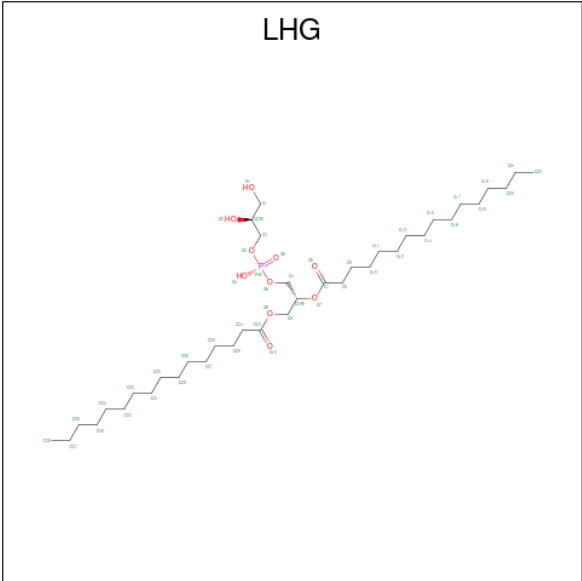
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	C	0
			40	40	
8	a	1	Total	C	0
			40	40	

- Molecule 9 is [(2R,3S,4S,5R,6R)-6-[(10E,12E,14E)-2,6,10,14,19,23-hexamethyl-25-(2,3,6-trimethylphenyl)pentacos-6,8,10,12,14,16,18,20,22,24-decaen-2-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methyl dodecanoate (CCD ID: F39) (formula: $C_{58}H_{86}O_7$).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			65	58	7	
9	a	1	Total	C	O	0
			65	58	7	

- Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



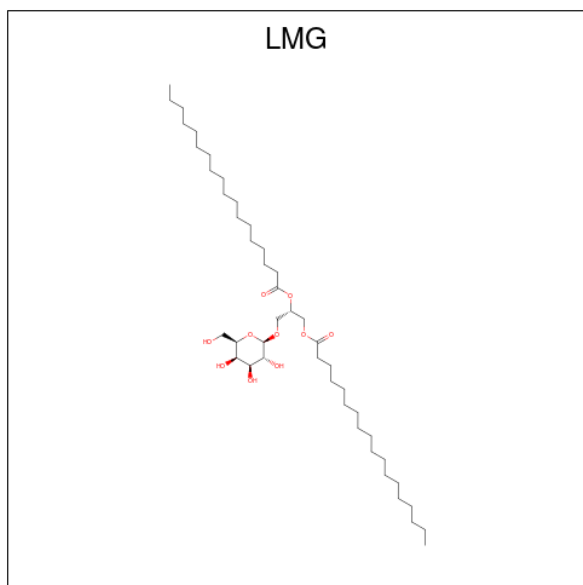
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	O	P	0
			46	35	10	1	

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Mol	Chain	Residues	Atoms				AltConf
10	a	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

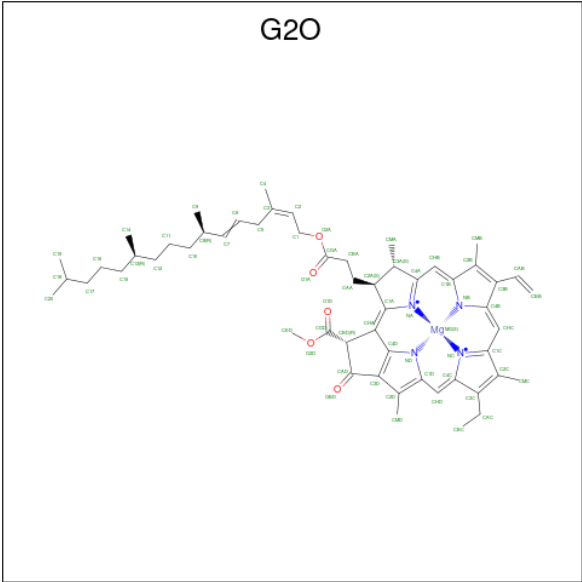


Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O		0
			44	34	10		
11	a	1	Total	C	O		0
			44	34	10		

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Ca	0
			1	1	
12	a	1	Total	Ca	0
			1	1	

- Molecule 13 is Chlorophyll A ester (CCD ID: G2O) (formula: $C_{55}H_{70}MgN_4O_5$).

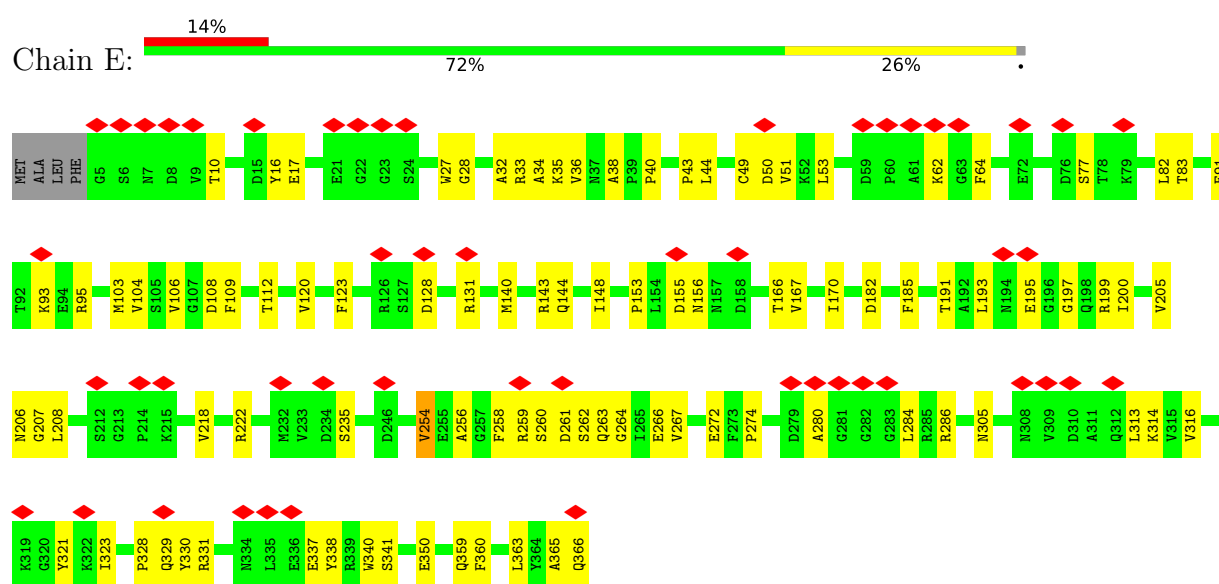


Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

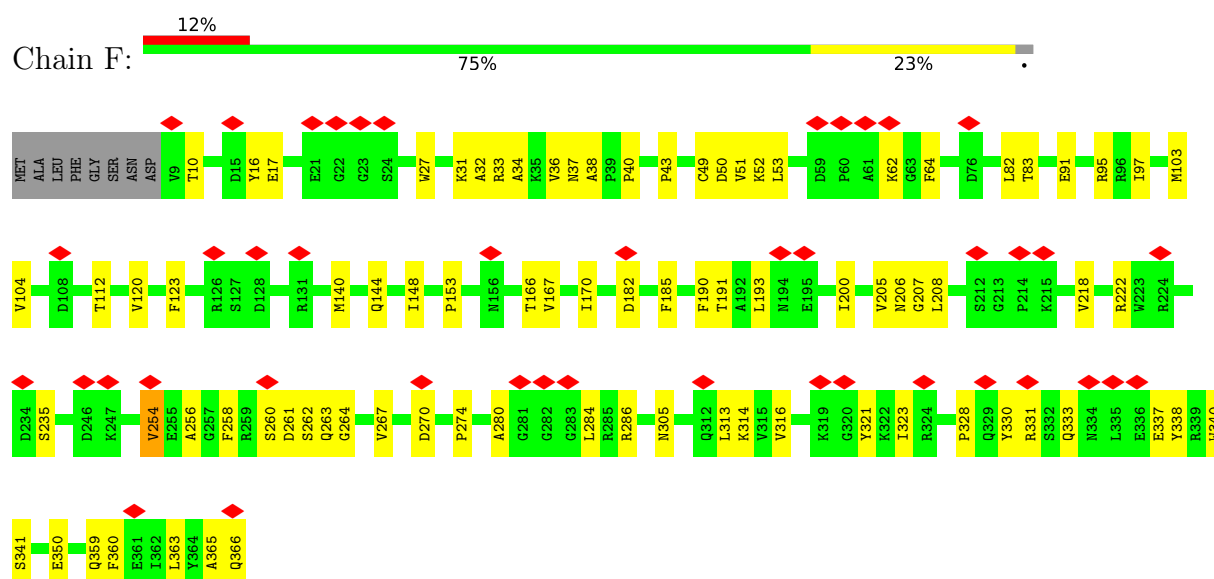
3 Residue-property plots

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.

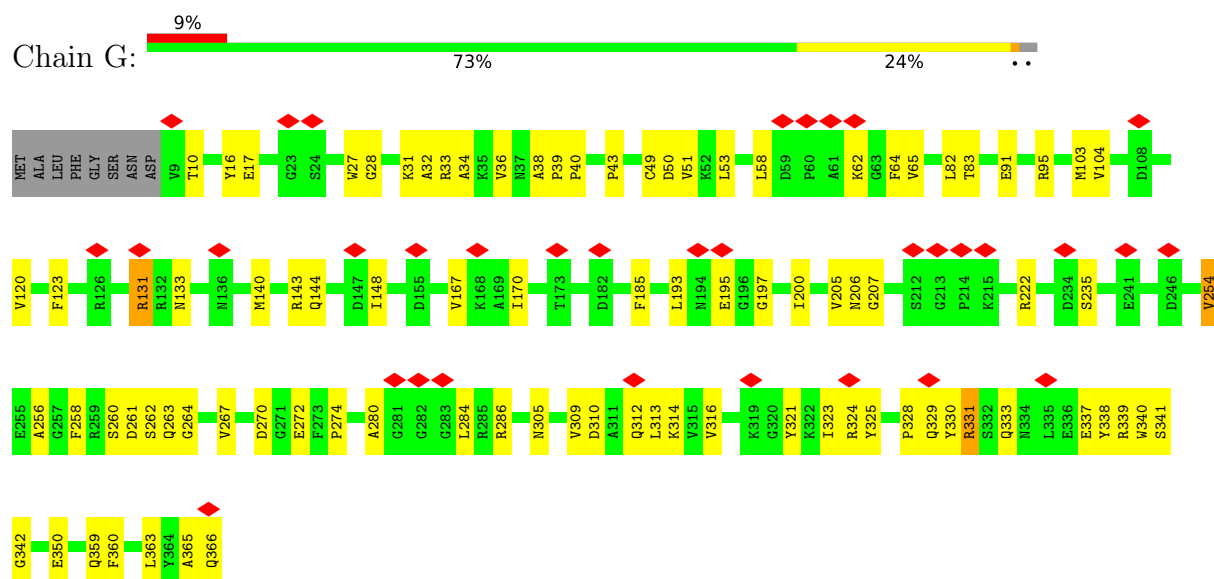
• Molecule 1: Bacteriochlorophyll a protein



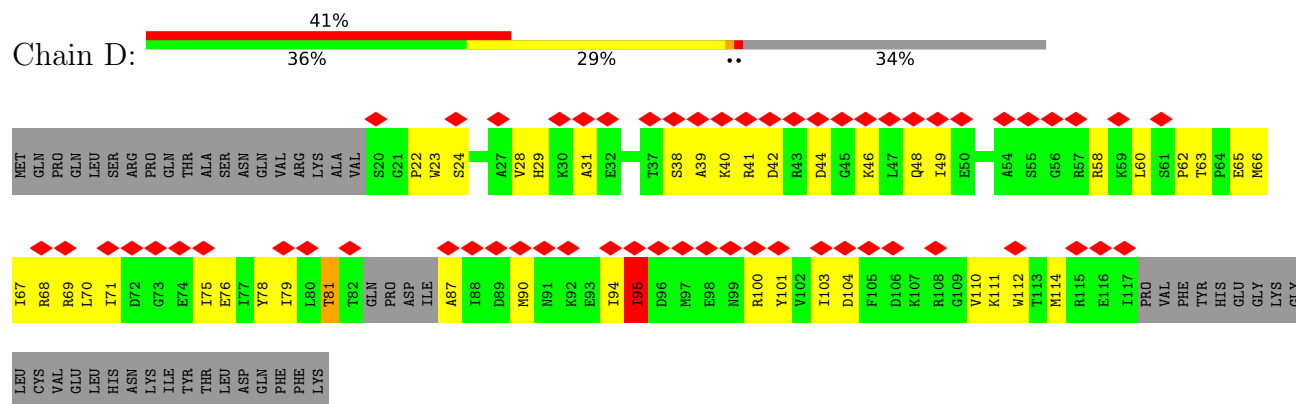
• Molecule 1: Bacteriochlorophyll a protein



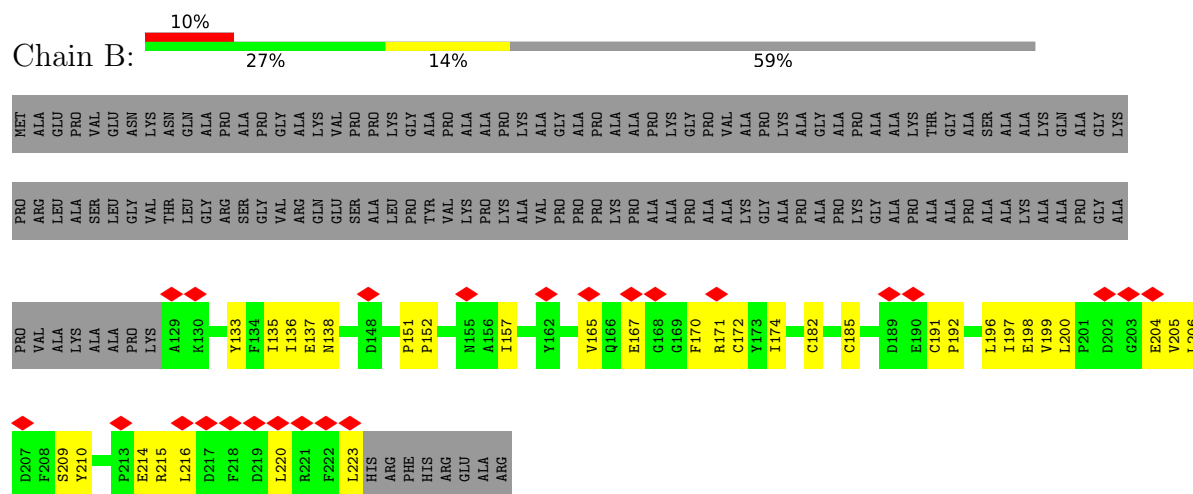
• Molecule 1: Bacteriochlorophyll a protein



- Molecule 2: P840 reaction center 17 kDa protein

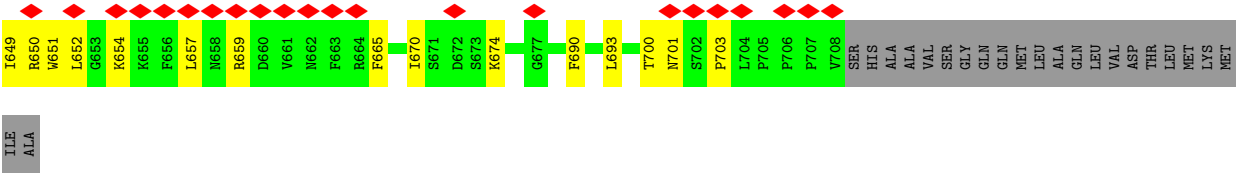


- Molecule 3: Photosystem P840 reaction center iron-sulfur protein



- Molecule 4: Photosystem P840 reaction center, large subunit





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	268430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	38244	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0341	Depositor
Map size ($\text{\AA}$)	209.12001, 209.12001, 209.12001	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, G2O, F26, GS0, LHG, SF4, F39, BCL, CA

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	E	0.24	0/2885	0.52	1/3910 (0.0%)
1	F	0.23	0/2859	0.53	1/3875 (0.0%)
1	G	0.24	0/2859	0.53	1/3875 (0.0%)
2	D	0.22	0/778	0.64	1/1043 (0.1%)
3	B	0.25	0/749	0.55	0/1013
4	A	0.22	0/5207	0.58	9/7097 (0.1%)
4	a	0.22	0/5207	0.55	5/7097 (0.1%)
All	All	0.23	0/20544	0.55	18/27910 (0.1%)

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
3	B	0	1
4	A	0	3
4	a	0	3
All	All	0	7

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	101	PHE	CA-C-N	10.50	132.97	119.84
4	a	101	PHE	C-N-CA	10.50	132.97	119.84
4	A	101	PHE	CA-C-N	9.56	131.79	119.84
4	A	101	PHE	C-N-CA	9.56	131.79	119.84
4	a	266	ASN	N-CA-C	9.27	126.56	107.37

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	311	LYS	Peptide
4	A	344	LYS	Peptide
4	A	519	LYS	Peptide
3	B	216	LEU	Peptide
4	a	311	LYS	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	E	2815	0	2749	83	0
1	F	2789	0	2731	67	0
1	G	2789	0	2731	88	0
2	D	766	0	783	54	0
3	B	731	0	692	35	0
4	A	5030	0	4916	146	0
4	a	5030	0	4916	121	0
5	A	642	0	584	31	0
5	E	508	0	551	25	0
5	F	508	0	551	21	0
5	G	508	0	551	25	0
5	a	642	0	584	27	0
6	A	8	0	0	0	0
6	B	16	0	0	4	0
7	A	66	0	0	0	0
7	a	66	0	0	0	0
8	A	40	0	0	0	0
8	a	40	0	0	0	0
9	A	65	0	0	0	0
9	a	65	0	0	0	0
10	A	46	0	65	0	0
10	a	46	0	65	0	0
11	A	44	0	57	3	0
11	a	44	0	57	3	0
12	A	1	0	0	0	0
12	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	130	0	0	1	0
13	a	130	0	0	2	0
All	All	23566	0	22583	627	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 627 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:583:ASP:OD1	4:a:588:LEU:HB2	1.39	1.18
4:a:202:TYR:CE1	4:a:274:ASP:OD2	2.06	1.09
1:G:331:ARG:NH2	4:A:271:LEU:O	1.87	1.07
1:E:259:ARG:HH11	3:B:215:ARG:HH12	1.05	0.95
1:G:341:SER:OG	4:A:200:LYS:NZ	2.01	0.93

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	E	360/366 (98%)	339 (94%)	21 (6%)	0	100	100
1	F	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
1	G	356/366 (97%)	338 (95%)	18 (5%)	0	100	100
2	D	90/143 (63%)	71 (79%)	17 (19%)	2 (2%)	5	14
3	B	93/231 (40%)	76 (82%)	17 (18%)	0	100	100
4	A	622/731 (85%)	568 (91%)	51 (8%)	3 (0%)	24	48
4	a	622/731 (85%)	571 (92%)	46 (7%)	5 (1%)	16	37
All	All	2499/2934 (85%)	2301 (92%)	188 (8%)	10 (0%)	31	54

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	95	ILE
4	A	102	PRO
4	a	102	PRO
4	A	659	ARG
4	a	659	ARG

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	E	299/302 (99%)	299 (100%)	0	100	100
1	F	296/302 (98%)	296 (100%)	0	100	100
1	G	296/302 (98%)	294 (99%)	2 (1%)	76	90
2	D	83/128 (65%)	83 (100%)	0	100	100
3	B	80/162 (49%)	80 (100%)	0	100	100
4	A	521/599 (87%)	516 (99%)	5 (1%)	68	86
4	a	521/599 (87%)	517 (99%)	4 (1%)	73	88
All	All	2096/2394 (88%)	2085 (100%)	11 (0%)	78	92

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	a	73	GLU
4	a	395	LEU
4	a	502	ARG
4	a	408	LYS
4	A	395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	612	HIS

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Mol	Chain	Res	Type
4	a	303	GLN
4	a	587	HIS
4	a	237	GLN
2	D	48	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, 2 are monoatomic - leaving 65 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
5	BCL	E	378[B]	1	49,54,74	1.94	14 (28%)	55,91,115	2.22	22 (40%)
13	G2O	A	802	-	68,73,73	2.59	22 (32%)	81,113,113	1.34	3 (3%)
5	BCL	F	374	1	69,74,74	1.74	14 (20%)	79,115,115	2.04	28 (35%)
13	G2O	a	803	-	68,73,73	2.63	22 (32%)	81,113,113	1.41	6 (7%)
5	BCL	G	376	1	69,74,74	1.72	15 (21%)	79,115,115	2.10	26 (32%)
5	BCL	a	805	-	59,64,74	1.84	16 (27%)	67,103,115	2.16	23 (34%)
7	GS0	A	801	4	69,74,74	1.74	14 (20%)	79,115,115	1.98	25 (31%)
11	LMG	a	819	-	44,44,55	0.78	2 (4%)	52,52,63	1.33	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	G	378[B]	1	49,54,74	1.95	14 (28%)	55,91,115	2.22	22 (40%)
5	BCL	G	372	-	69,74,74	1.73	14 (20%)	79,115,115	2.06	27 (34%)
5	BCL	a	811	4	69,74,74	1.72	13 (18%)	79,115,115	2.09	25 (31%)
5	BCL	F	372	-	69,74,74	1.73	14 (20%)	79,115,115	2.06	26 (32%)
5	BCL	a	804	4	49,54,74	1.98	15 (30%)	55,91,115	2.25	24 (43%)
9	F39	a	817	-	66,66,66	6.15	59 (89%)	83,85,85	4.32	32 (38%)
5	BCL	E	377	1	69,74,74	1.72	15 (21%)	79,115,115	2.10	27 (34%)
5	BCL	E	372	-	69,74,74	1.73	14 (20%)	79,115,115	2.07	27 (34%)
5	BCL	A	805	-	59,64,74	1.84	16 (27%)	67,103,115	2.15	23 (34%)
5	BCL	E	373	1	69,74,74	1.73	15 (21%)	79,115,115	2.14	27 (34%)
5	BCL	G	375	1	69,74,74	1.71	15 (21%)	79,115,115	2.08	29 (36%)
13	G2O	a	802	-	68,73,73	2.59	22 (32%)	81,113,113	1.33	3 (3%)
10	LHG	A	818	-	45,45,48	0.65	1 (2%)	48,51,54	1.29	6 (12%)
5	BCL	A	814	4	49,54,74	1.96	14 (28%)	55,91,115	2.26	21 (38%)
6	SF4	B	302	3	0,12,12	-	-	-	-	-
5	BCL	F	377	1	69,74,74	1.73	15 (21%)	79,115,115	2.09	26 (32%)
5	BCL	A	806	4	69,74,74	1.71	15 (21%)	79,115,115	2.09	27 (34%)
5	BCL	A	808	4	69,74,74	1.73	14 (20%)	79,115,115	2.04	25 (31%)
5	BCL	a	810	4	49,54,74	1.91	11 (22%)	55,91,115	2.41	20 (36%)
5	BCL	A	804	4	49,54,74	1.98	14 (28%)	55,91,115	2.25	24 (43%)
5	BCL	E	374	1	69,74,74	1.74	14 (20%)	79,115,115	2.03	29 (36%)
5	BCL	E	376	1	69,74,74	1.72	15 (21%)	79,115,115	2.10	26 (32%)
5	BCL	A	809	4	49,54,74	1.97	13 (26%)	55,91,115	2.30	22 (40%)
5	BCL	E	375	1	69,74,74	1.72	16 (23%)	79,115,115	2.08	29 (36%)
5	BCL	A	812	4	69,74,74	1.73	14 (20%)	79,115,115	2.03	25 (31%)
5	BCL	E	371	1	69,74,74	1.74	14 (20%)	79,115,115	2.18	28 (35%)
5	BCL	a	814	4	49,54,74	1.96	12 (24%)	55,91,115	2.26	21 (38%)
10	LHG	a	818	-	45,45,48	0.65	1 (2%)	48,51,54	1.29	6 (12%)
13	G2O	A	803	-	68,73,73	2.62	22 (32%)	81,113,113	1.41	6 (7%)
5	BCL	G	373	1	69,74,74	1.73	16 (23%)	79,115,115	2.14	27 (34%)
5	BCL	F	375	1	69,74,74	1.71	15 (21%)	79,115,115	2.08	29 (36%)
5	BCL	G	374	1	69,74,74	1.74	14 (20%)	79,115,115	2.04	28 (35%)
5	BCL	a	808	4	69,74,74	1.73	14 (20%)	79,115,115	2.03	24 (30%)
5	BCL	a	807	-	49,54,74	1.96	13 (26%)	55,91,115	2.21	21 (38%)
5	BCL	G	371	1	69,74,74	1.74	15 (21%)	79,115,115	2.19	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	A	815	-	49,54,74	1.97	14 (28%)	55,91,115	2.25	22 (40%)
5	BCL	a	809	4	49,54,74	1.97	14 (28%)	55,91,115	2.30	22 (40%)
5	BCL	F	373	1	69,74,74	1.73	15 (21%)	79,115,115	2.14	27 (34%)
5	BCL	a	806	4	69,74,74	1.71	15 (21%)	79,115,115	2.09	27 (34%)
5	BCL	A	810	4	49,54,74	1.91	12 (24%)	55,91,115	2.40	20 (36%)
5	BCL	A	813	-	49,54,74	1.99	15 (30%)	55,91,115	2.24	23 (41%)
8	F26	a	816	-	40,40,40	1.76	12 (30%)	49,50,50	2.09	12 (24%)
5	BCL	a	813	-	49,54,74	1.98	14 (28%)	55,91,115	2.24	22 (40%)
6	SF4	A	821	4	0,12,12	-	-	-	-	-
5	BCL	a	815	-	49,54,74	1.97	14 (28%)	55,91,115	2.26	22 (40%)
5	BCL	G	377	1	69,74,74	1.72	15 (21%)	79,115,115	2.10	26 (32%)
5	BCL	a	812	4	69,74,74	1.72	14 (20%)	79,115,115	2.03	25 (31%)
8	F26	A	816	-	40,40,40	1.75	12 (30%)	49,50,50	2.09	12 (24%)
5	BCL	A	811	4	69,74,74	1.72	15 (21%)	79,115,115	2.09	25 (31%)
5	BCL	F	376	1	69,74,74	1.72	15 (21%)	79,115,115	2.10	26 (32%)
5	BCL	A	807	-	49,54,74	1.95	13 (26%)	55,91,115	2.20	21 (38%)
11	LMG	A	819	-	44,44,55	0.78	2 (4%)	52,52,63	1.33	3 (5%)
6	SF4	B	301	3	0,12,12	-	-	-	-	-
7	GS0	a	801	4	69,74,74	1.75	14 (20%)	79,115,115	1.98	25 (31%)
5	BCL	F	371	1	69,74,74	1.75	15 (21%)	79,115,115	2.19	28 (35%)
5	BCL	F	378[B]	1	49,54,74	1.95	14 (28%)	55,91,115	2.22	22 (40%)
9	F39	A	817	-	66,66,66	6.14	59 (89%)	83,85,85	4.31	32 (38%)

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
5	BCL	E	378[B]	1	-	2/17/113/137	-
13	G2O	A	802	-	-	12/39/115/115	-
5	BCL	F	374	1	-	14/41/137/137	-
13	G2O	a	803	-	-	18/39/115/115	-
5	BCL	G	376	1	-	8/41/137/137	-
5	BCL	a	805	-	-	11/29/125/137	-
7	GS0	A	801	4	-	13/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LMG	a	819	-	-	20/39/59/70	0/1/1/1
5	BCL	G	378[B]	1	-	2/17/113/137	-
5	BCL	G	372	-	-	17/41/137/137	-
5	BCL	a	811	4	-	16/41/137/137	-
5	BCL	F	372	-	-	17/41/137/137	-
5	BCL	a	804	4	-	9/17/113/137	-
9	F39	a	817	-	-	41/58/78/78	0/2/2/2
5	BCL	E	377	1	-	12/41/137/137	-
5	BCL	E	372	-	-	17/41/137/137	-
5	BCL	A	805	-	-	11/29/125/137	-
5	BCL	E	373	1	-	11/41/137/137	-
5	BCL	G	375	1	-	10/41/137/137	-
13	G2O	a	802	-	-	12/39/115/115	-
10	LHG	A	818	-	-	21/50/50/53	-
5	BCL	A	814	4	-	3/17/113/137	-
6	SF4	B	302	3	-	-	0/6/5/5
5	BCL	F	377	1	-	12/41/137/137	-
5	BCL	A	806	4	-	10/41/137/137	-
5	BCL	A	808	4	-	17/41/137/137	-
5	BCL	a	810	4	-	8/17/113/137	-
5	BCL	A	804	4	-	9/17/113/137	-
5	BCL	E	374	1	-	14/41/137/137	-
5	BCL	E	376	1	-	8/41/137/137	-
5	BCL	A	809	4	-	5/17/113/137	-
5	BCL	E	375	1	-	10/41/137/137	-
5	BCL	A	812	4	-	13/41/137/137	-
5	BCL	E	371	1	-	12/41/137/137	-
5	BCL	a	814	4	-	3/17/113/137	-
10	LHG	a	818	-	-	21/50/50/53	-
13	G2O	A	803	-	-	18/39/115/115	-
5	BCL	G	373	1	-	11/41/137/137	-
5	BCL	F	375	1	-	10/41/137/137	-
5	BCL	G	374	1	-	14/41/137/137	-
5	BCL	a	808	4	-	17/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	a	807	-	-	4/17/113/137	-
5	BCL	G	371	1	-	12/41/137/137	-
5	BCL	A	815	-	-	5/17/113/137	-
5	BCL	a	809	4	-	5/17/113/137	-
5	BCL	F	373	1	-	11/41/137/137	-
5	BCL	a	806	4	-	10/41/137/137	-
5	BCL	A	810	4	-	8/17/113/137	-
5	BCL	A	813	-	-	5/17/113/137	-
8	F26	a	816	-	-	15/36/36/36	0/1/1/1
5	BCL	a	813	-	-	5/17/113/137	-
6	SF4	A	821	4	-	-	0/6/5/5
5	BCL	a	815	-	-	5/17/113/137	-
5	BCL	G	377	1	-	12/41/137/137	-
5	BCL	a	812	4	-	14/41/137/137	-
8	F26	A	816	-	-	15/36/36/36	0/1/1/1
5	BCL	A	811	4	-	16/41/137/137	-
5	BCL	F	376	1	-	8/41/137/137	-
5	BCL	A	807	-	-	4/17/113/137	-
11	LMG	A	819	-	-	20/39/59/70	0/1/1/1
6	SF4	B	301	3	-	-	0/6/5/5
7	GS0	a	801	4	-	13/41/137/137	-
5	BCL	F	371	1	-	11/41/137/137	-
5	BCL	F	378[B]	1	-	2/17/113/137	-
9	F39	A	817	-	-	41/58/78/78	0/2/2/2

The worst 5 of 950 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	817	F39	C39-C37	12.63	1.65	1.35
9	A	817	F39	C39-C37	12.61	1.65	1.35
9	A	817	F39	C56-C53	11.83	1.63	1.33
9	a	817	F39	C56-C53	11.81	1.63	1.33
9	A	817	F39	C40-C41	11.71	1.65	1.34

The worst 5 of 1369 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	817	F39	C57-C59-C62	-11.93	110.55	127.28
9	A	817	F39	C57-C59-C62	-11.92	110.56	127.28
9	A	817	F39	C51-C44-C42	-11.38	111.31	127.28
9	a	817	F39	C51-C44-C42	-11.37	111.33	127.28
9	A	817	F39	C40-C39-C37	-11.34	111.37	127.28

There are no chirality outliers.

5 of 750 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	371	BCL	C1A-C2A-CAA-CBA
5	E	371	BCL	C3A-C2A-CAA-CBA
5	E	371	BCL	CBD-CGD-O2D-CED
5	E	371	BCL	O1D-CGD-O2D-CED
5	E	373	BCL	C2C-C3C-CAC-CBC

There are no ring outliers.

49 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	378[B]	BCL	1	0
5	F	374	BCL	3	0
13	a	803	G2O	2	0
5	G	376	BCL	7	0
11	a	819	LMG	3	0
5	G	378[B]	BCL	1	0
5	G	372	BCL	5	0
5	a	811	BCL	4	0
5	F	372	BCL	4	0
5	E	377	BCL	3	0
5	E	372	BCL	3	0
5	E	373	BCL	4	0
5	G	375	BCL	5	0
5	A	814	BCL	2	0
6	B	302	SF4	1	0
5	F	377	BCL	3	0
5	A	806	BCL	4	0
5	A	808	BCL	3	0
5	a	810	BCL	5	0
5	E	374	BCL	2	0
5	E	376	BCL	5	0
5	A	809	BCL	3	0

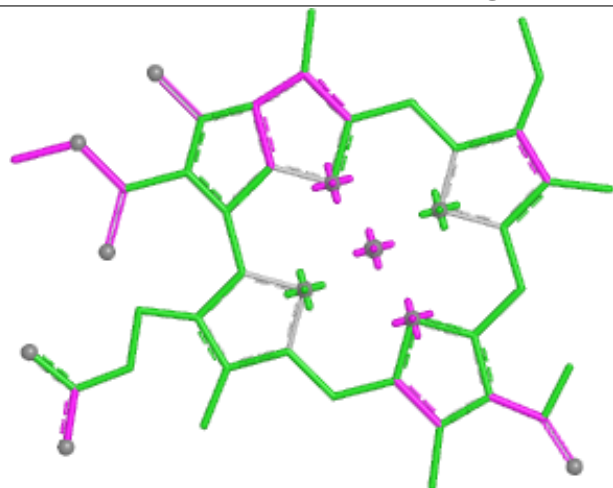
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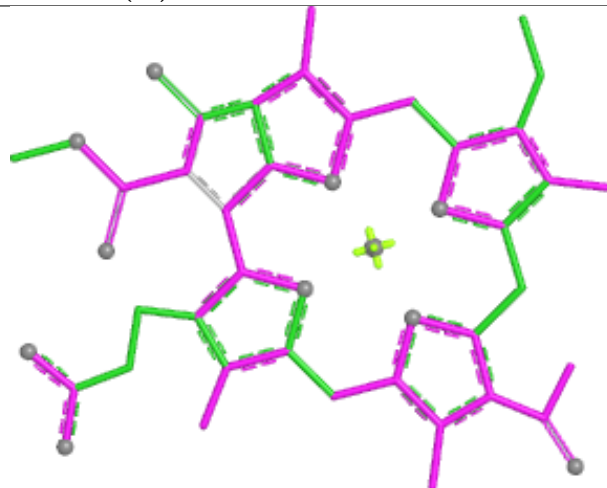
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	375	BCL	6	0
5	A	812	BCL	5	0
5	E	371	BCL	5	0
5	a	814	BCL	2	0
13	A	803	G2O	1	0
5	G	373	BCL	1	0
5	F	375	BCL	6	0
5	G	374	BCL	2	0
5	a	808	BCL	2	0
5	a	807	BCL	3	0
5	G	371	BCL	4	0
5	A	815	BCL	2	0
5	a	809	BCL	3	0
5	F	373	BCL	3	0
5	a	806	BCL	4	0
5	A	810	BCL	6	0
5	A	813	BCL	2	0
5	a	813	BCL	2	0
5	a	815	BCL	2	0
5	G	377	BCL	3	0
5	a	812	BCL	3	0
5	A	811	BCL	4	0
5	F	376	BCL	2	0
5	A	807	BCL	3	0
11	A	819	LMG	3	0
6	B	301	SF4	3	0
5	F	371	BCL	4	0

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

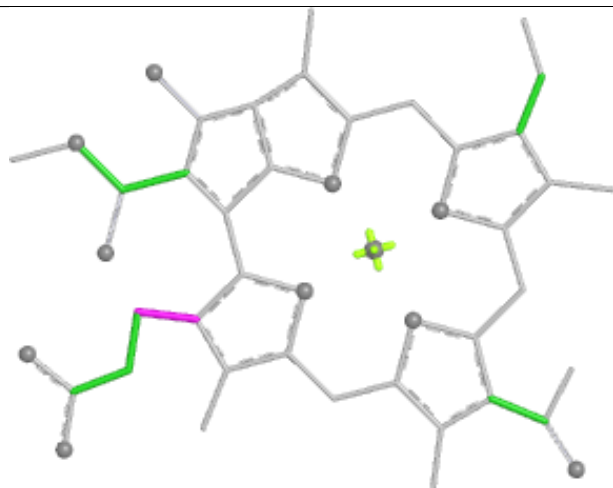
Ligand BCL E 378 (B)



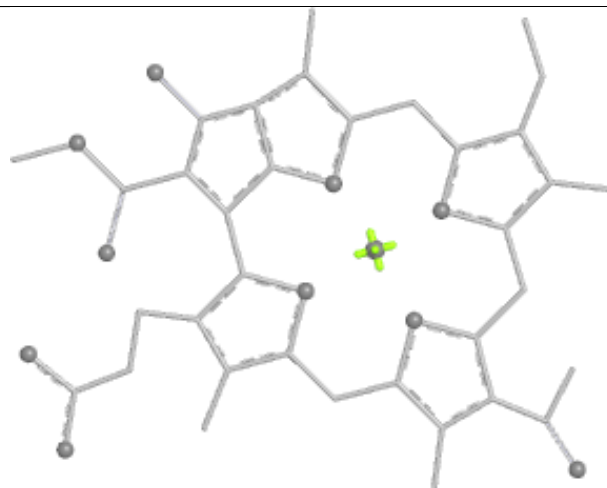
Bond lengths



Bond angles

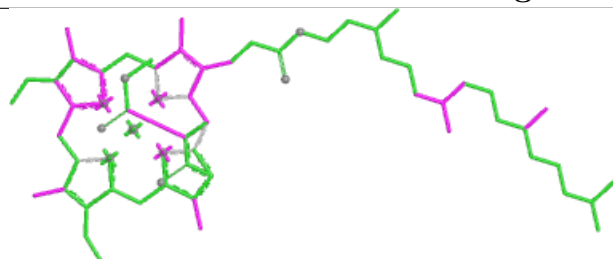


Torsions

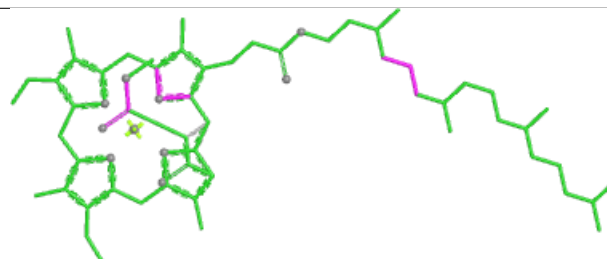


Rings

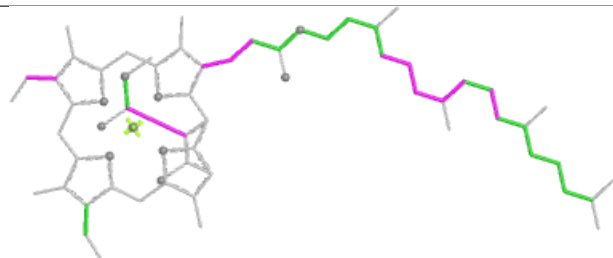
Ligand G2O A 802



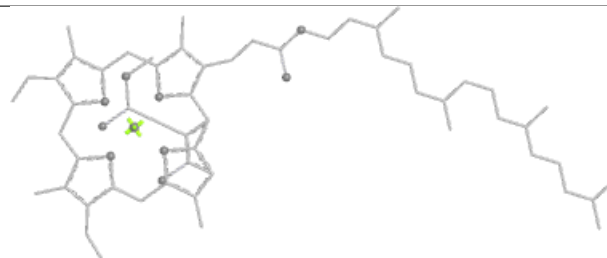
Bond lengths



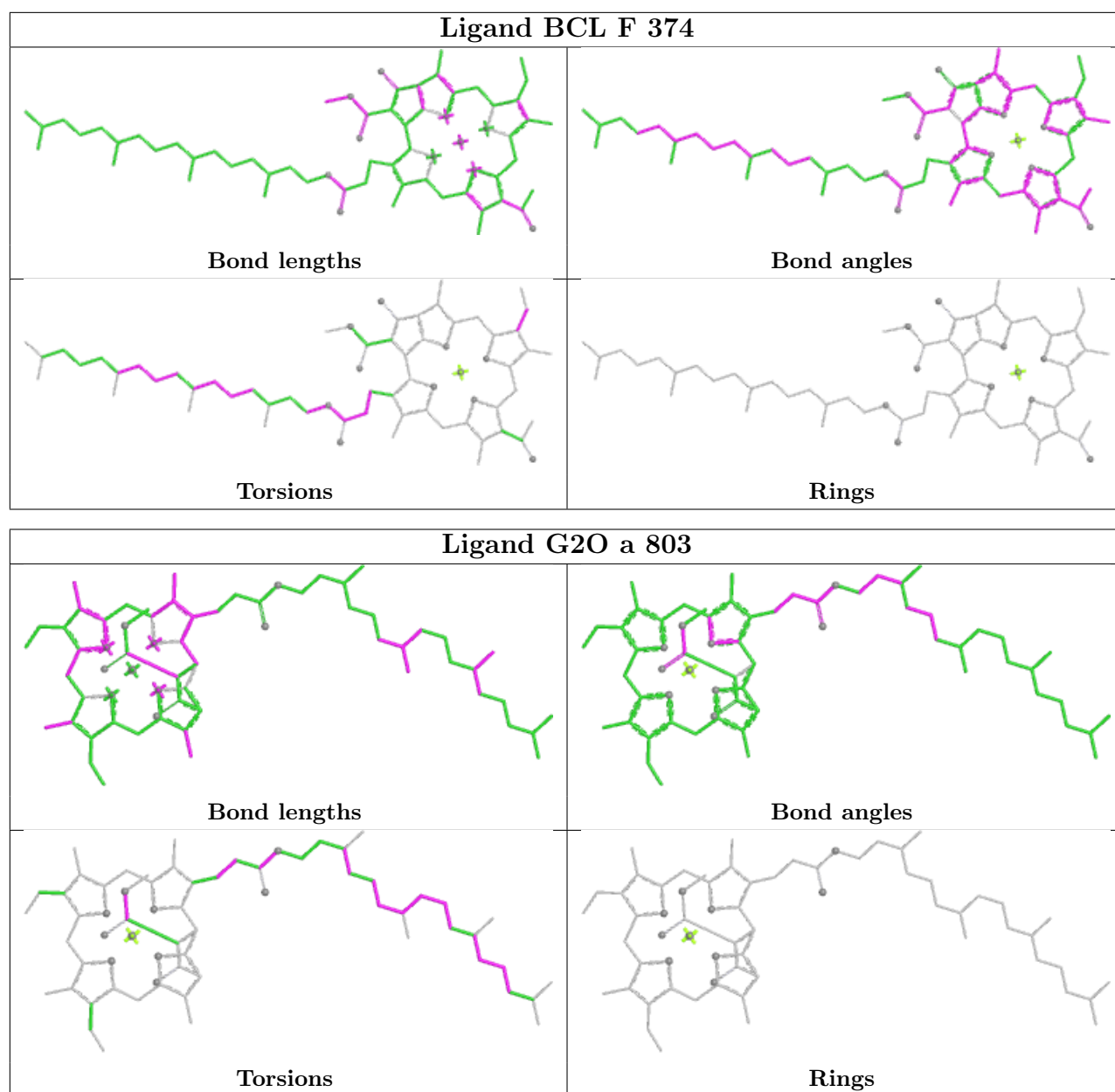
Bond angles

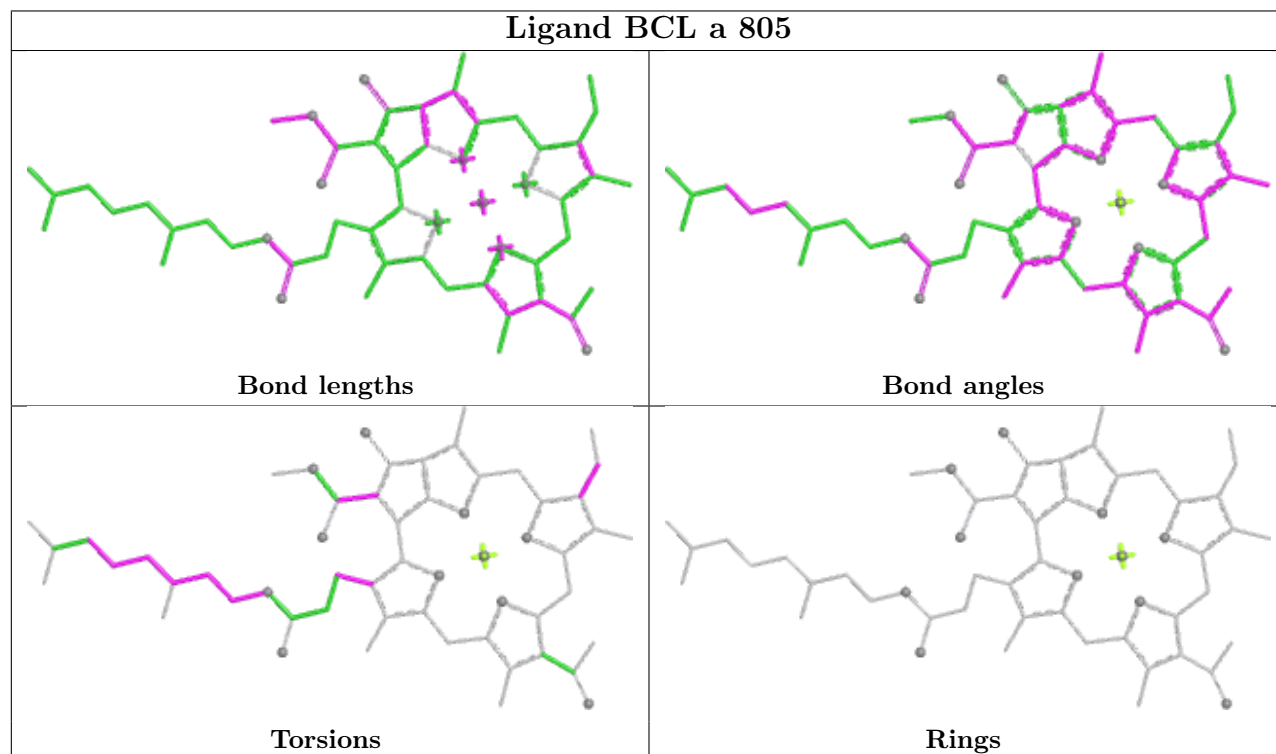
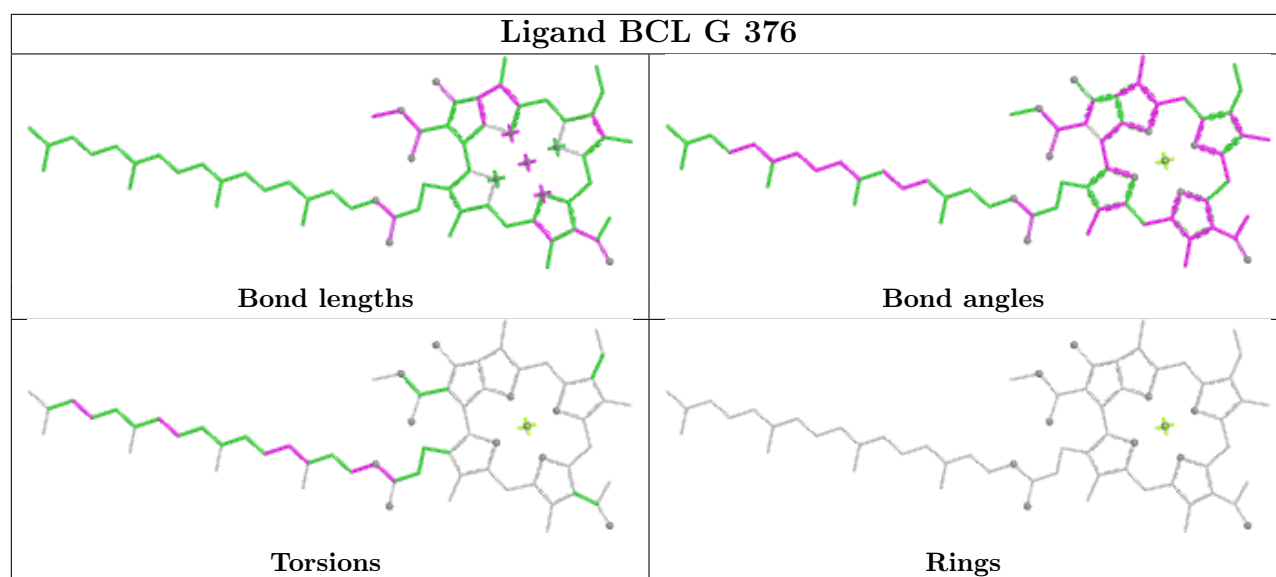


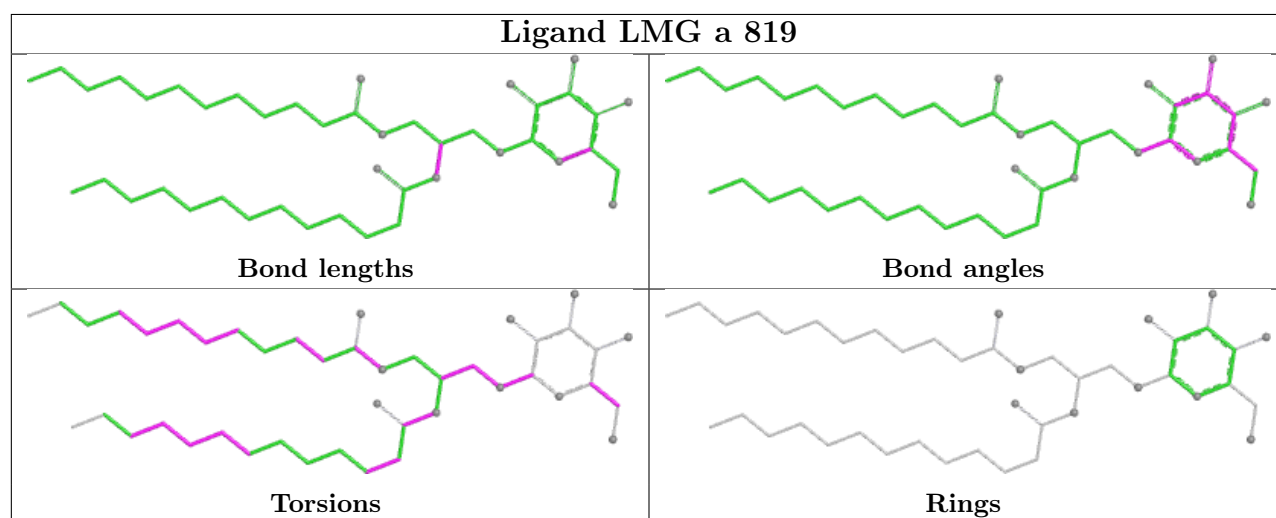
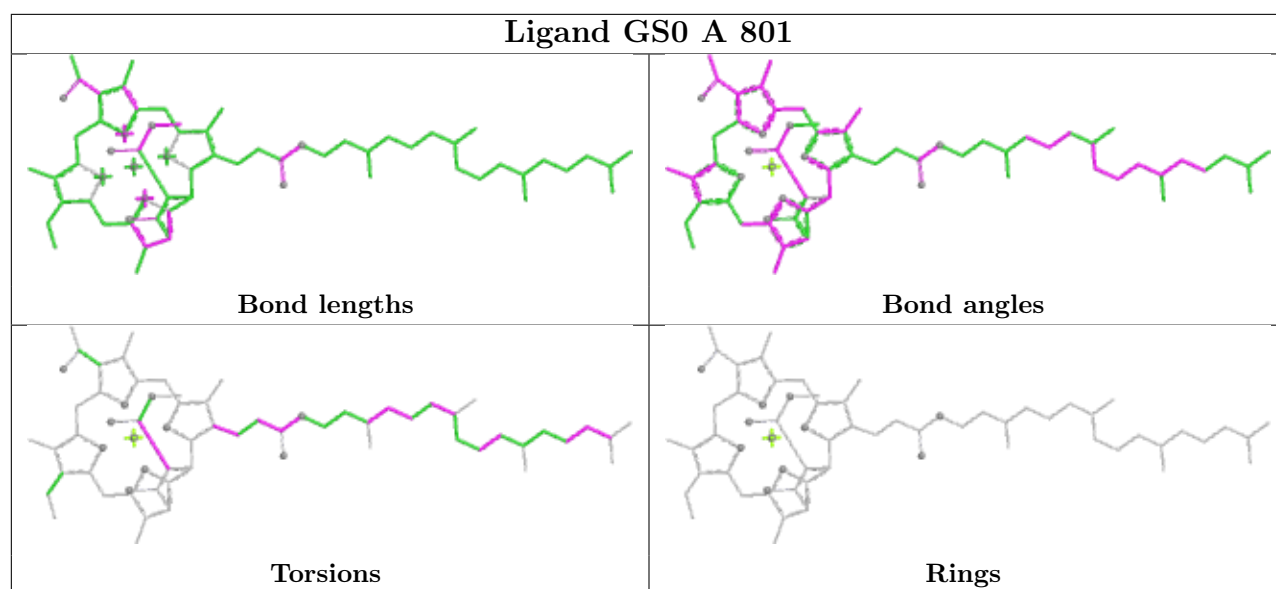
Torsions



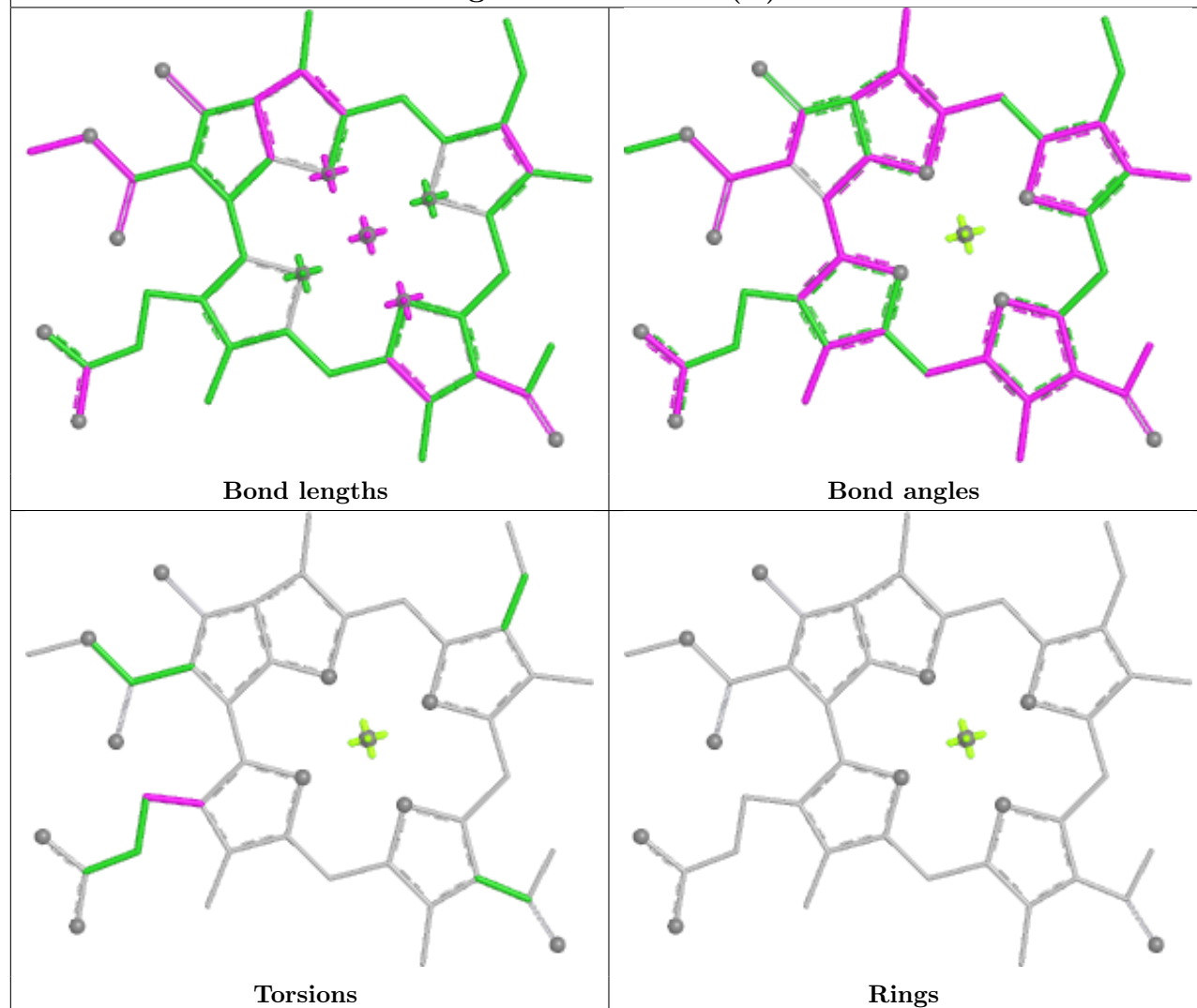
Rings



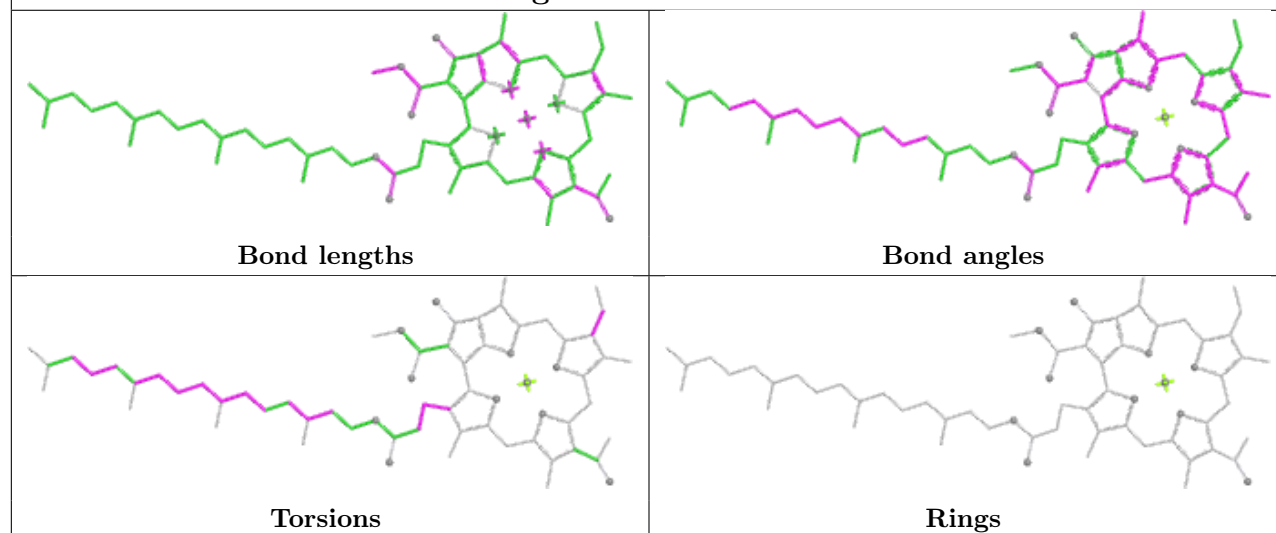


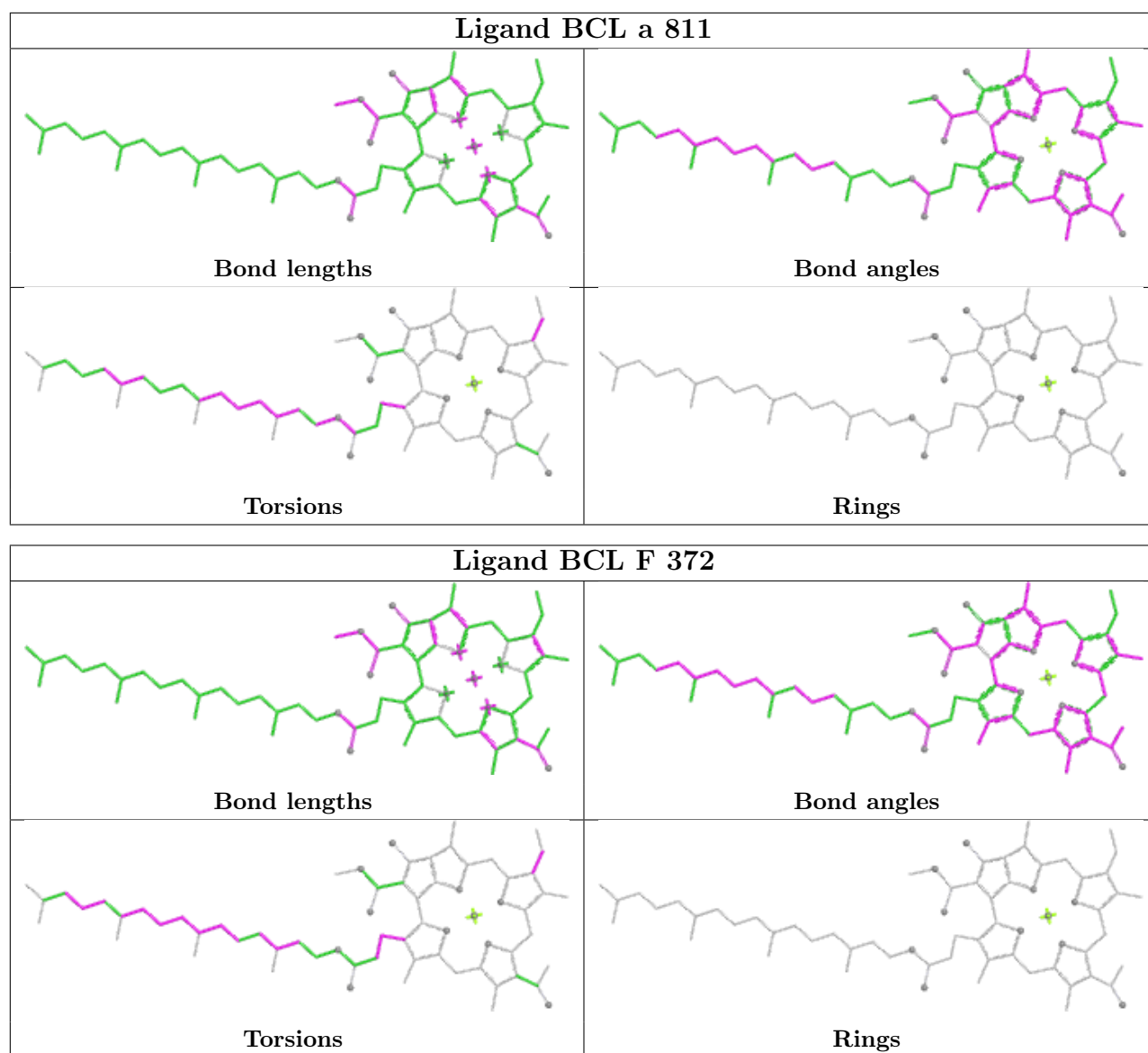


Ligand BCL G 378 (B)

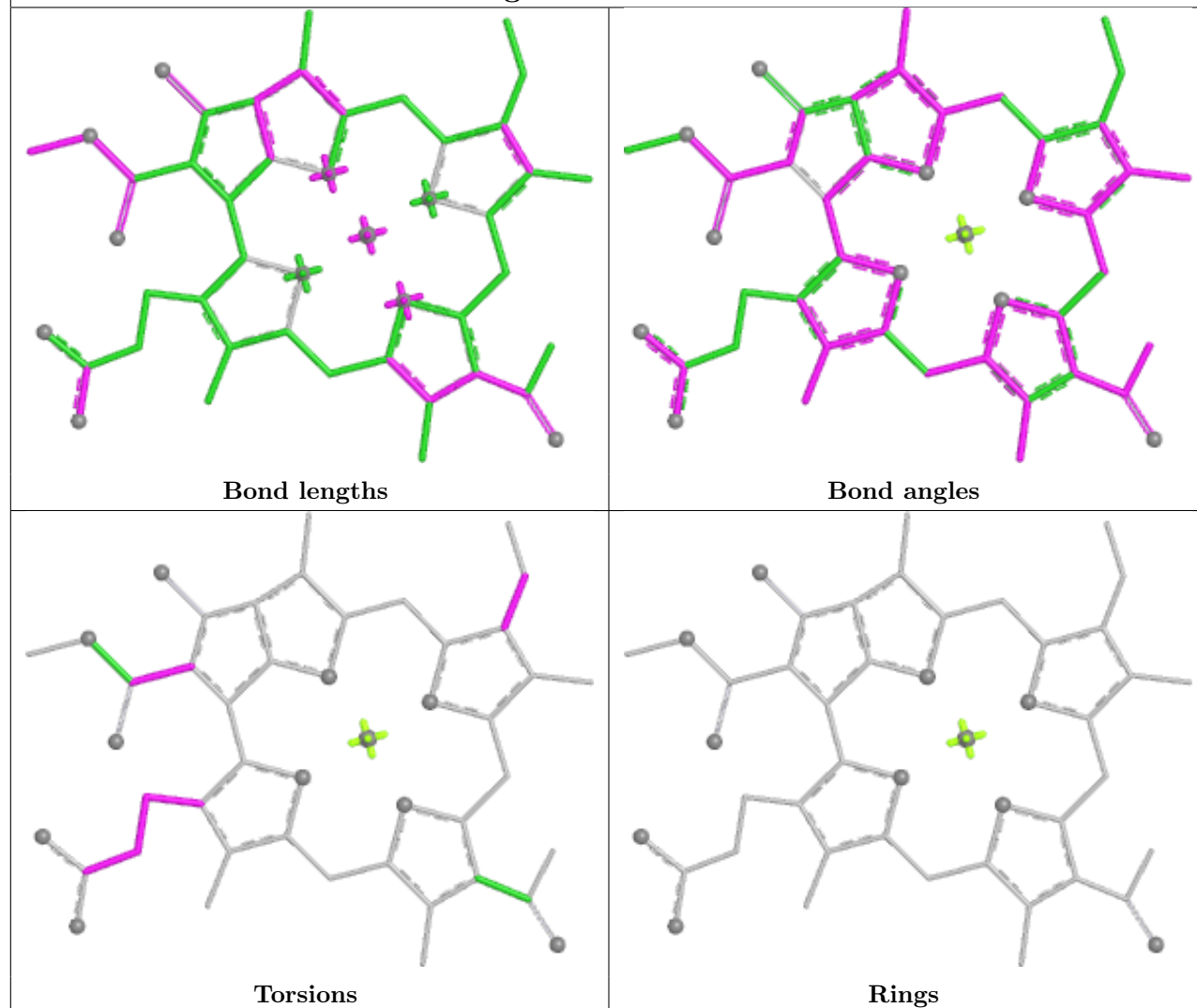


Ligand BCL G 372

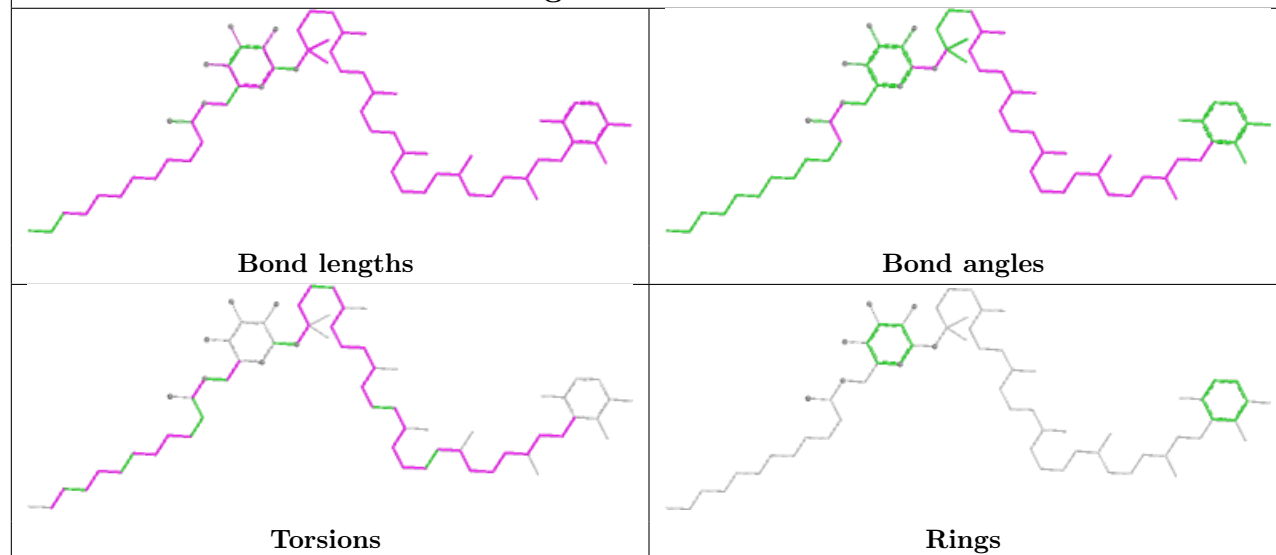


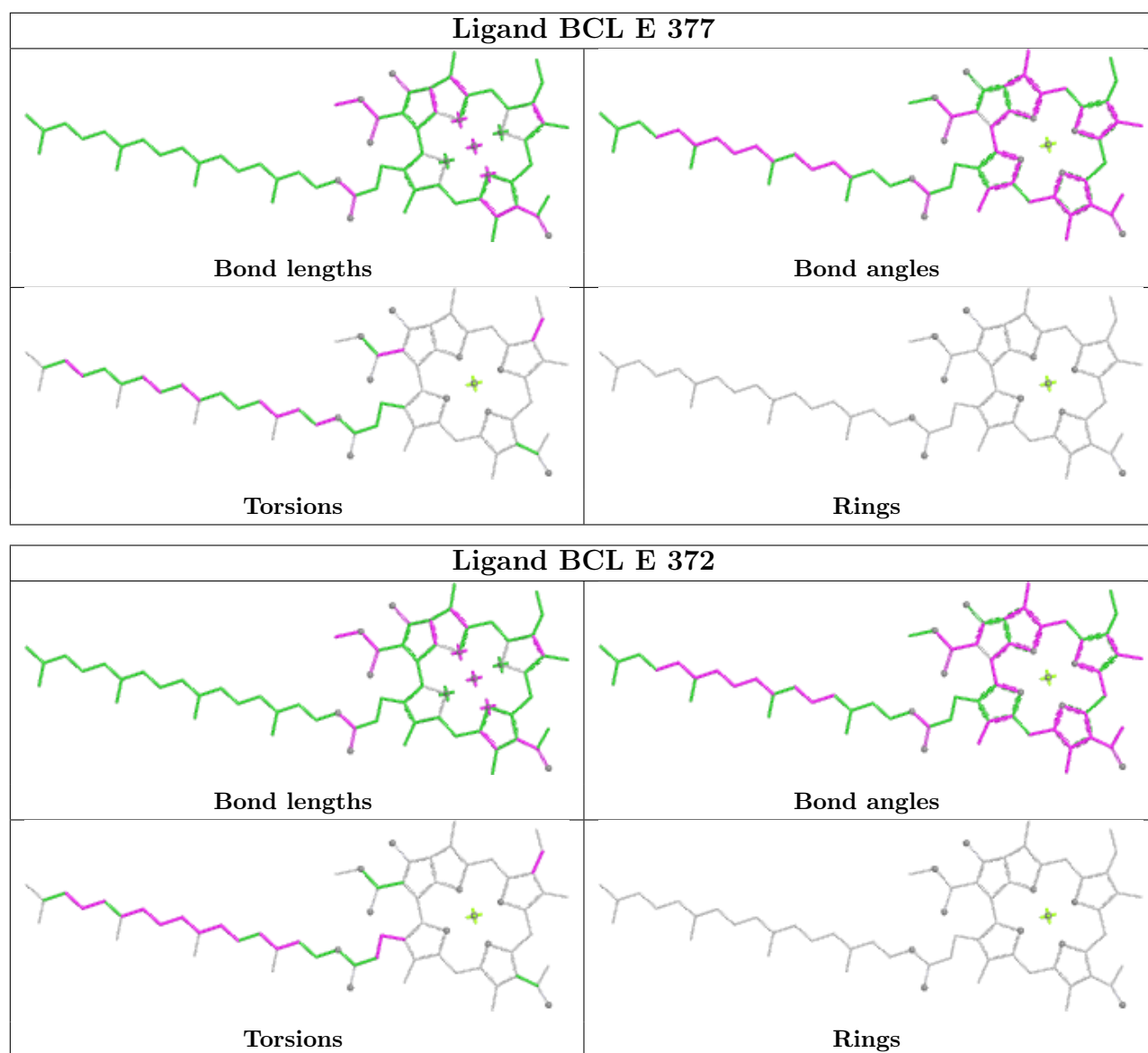


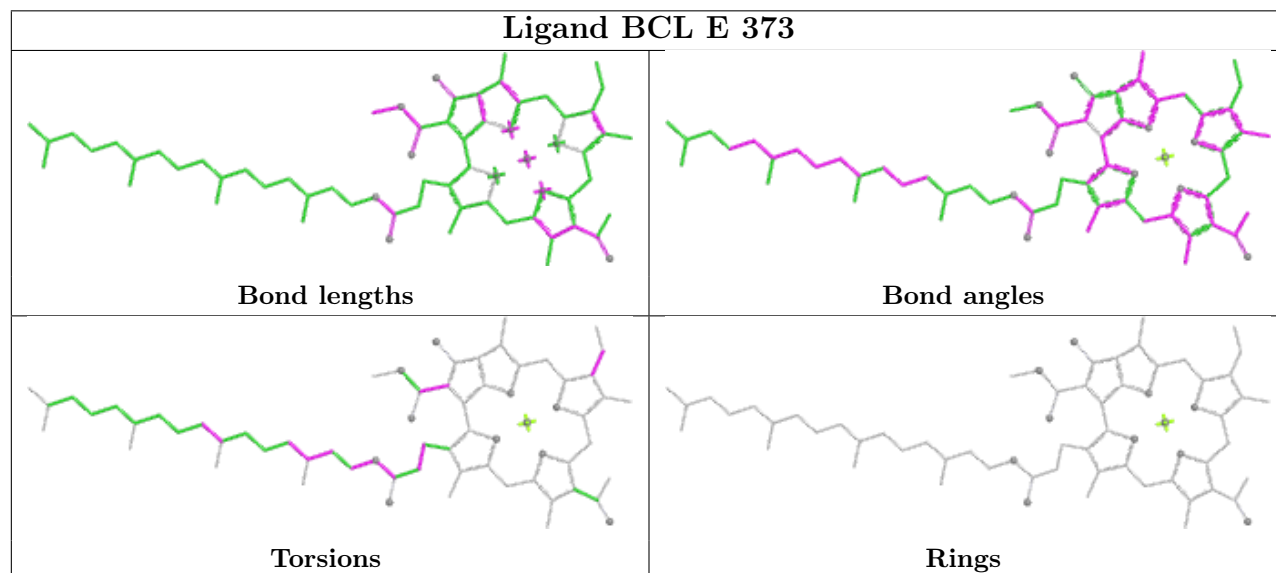
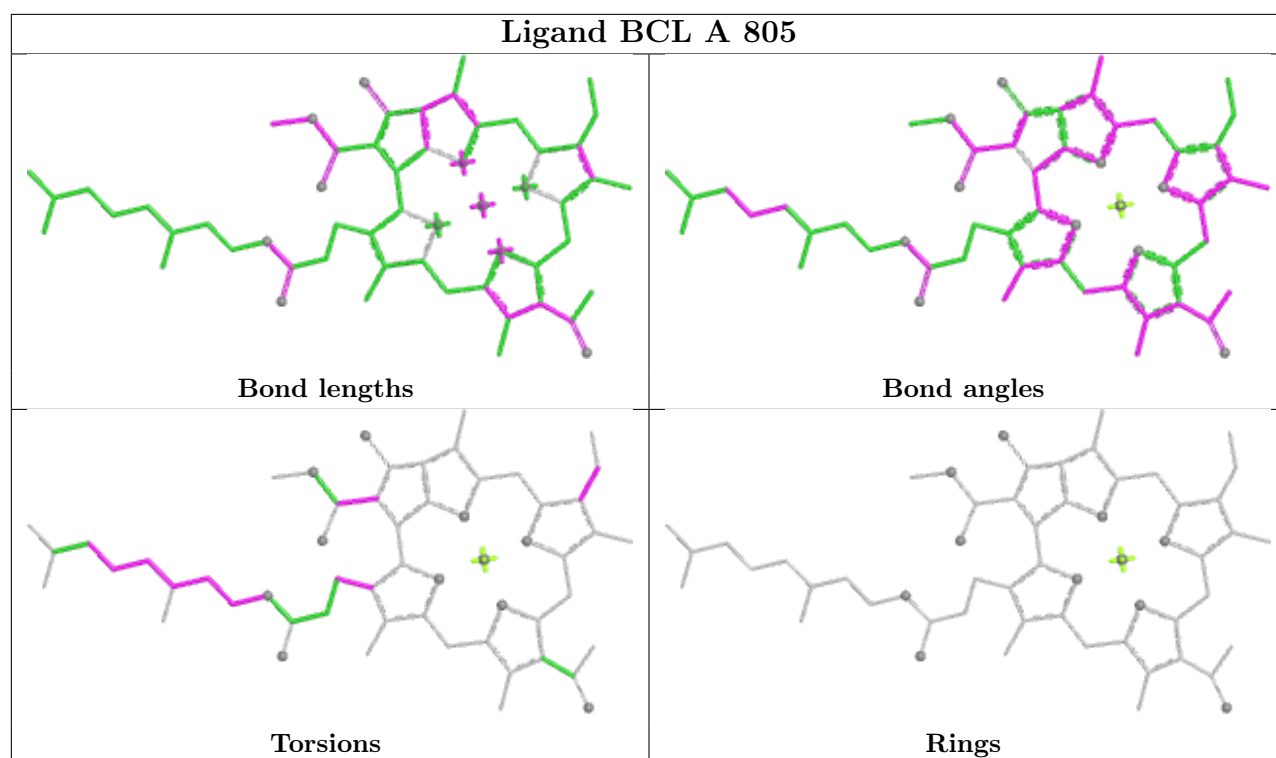
Ligand BCL a 804

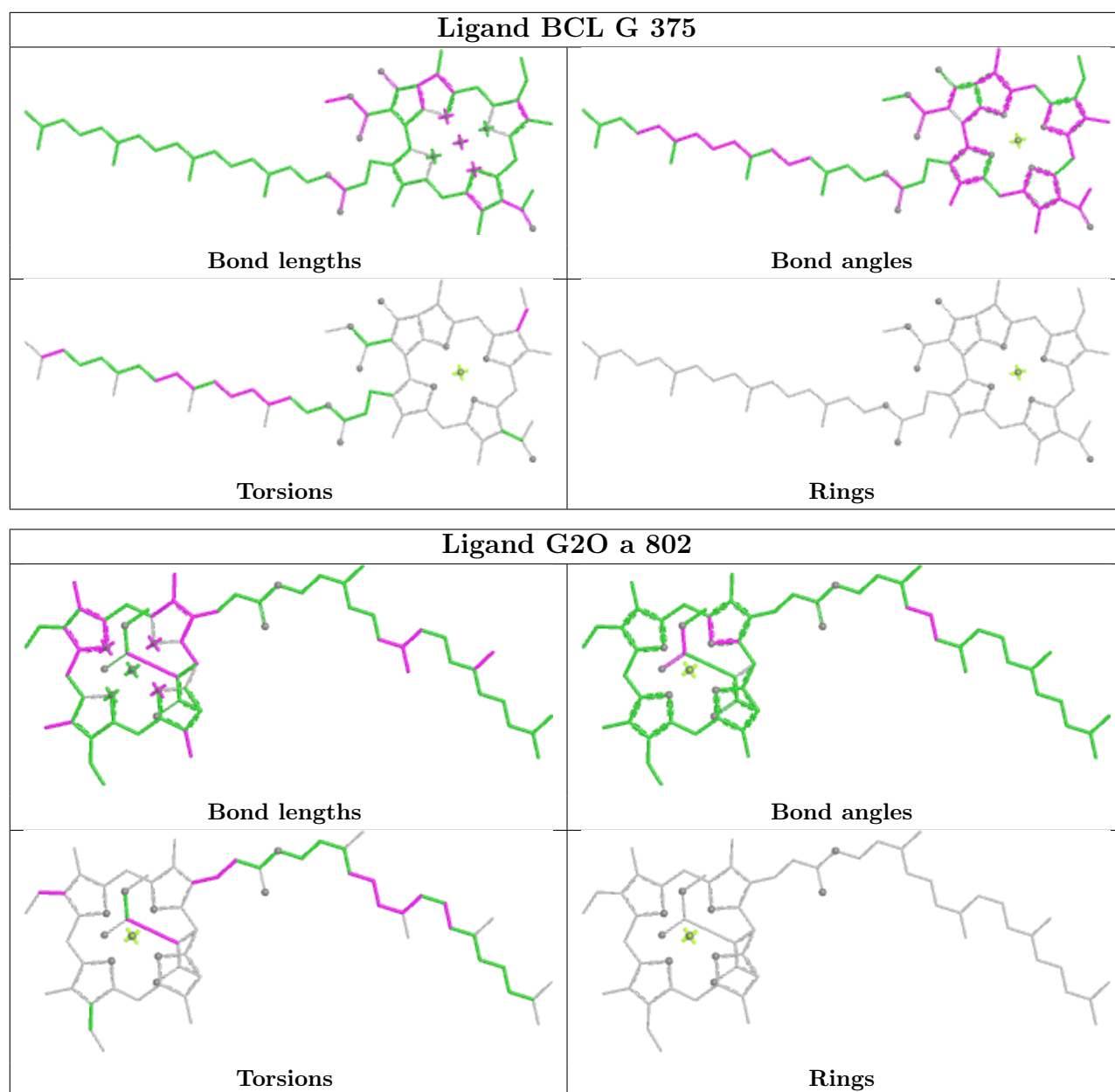


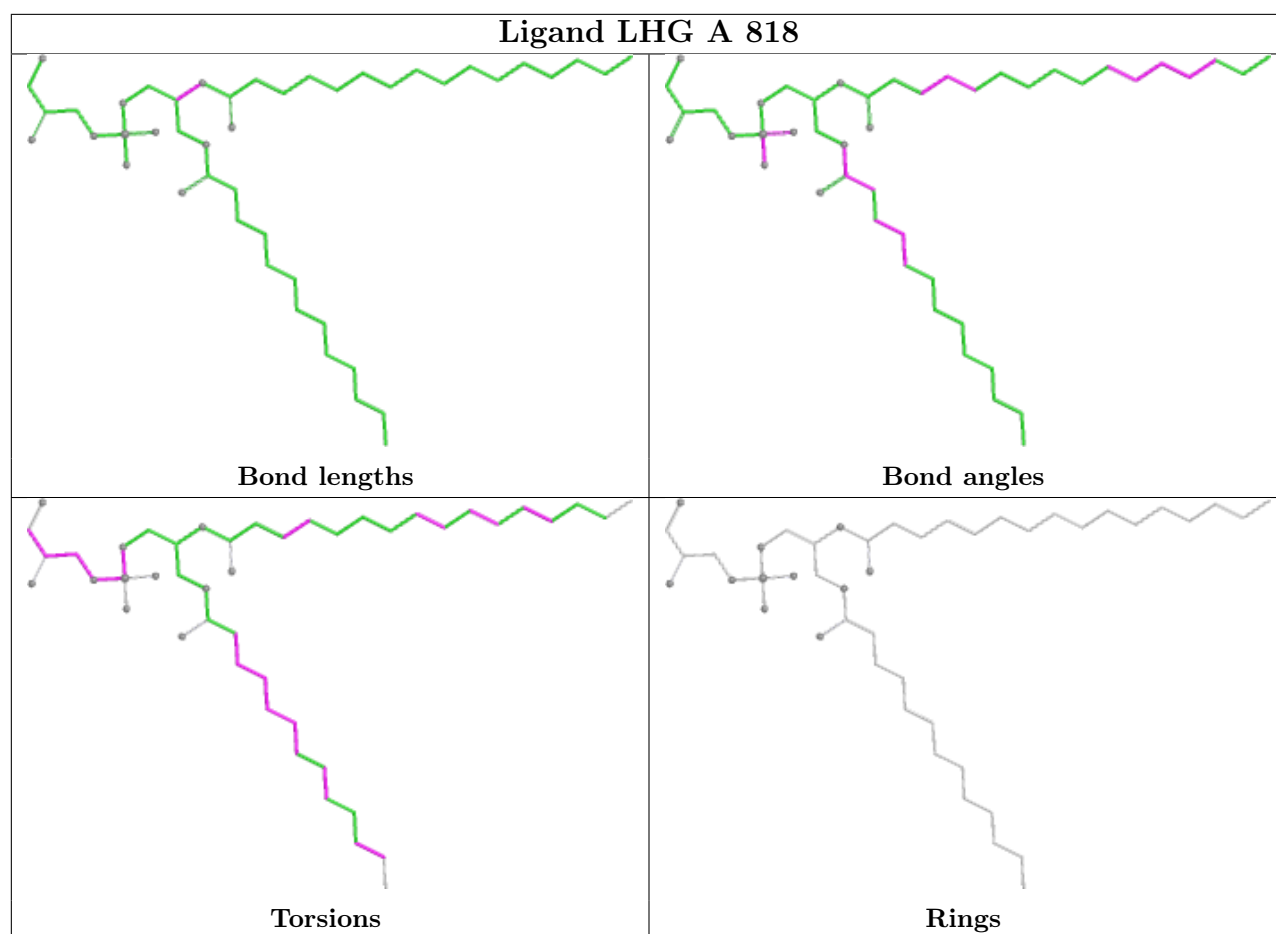
Ligand F39 a 817



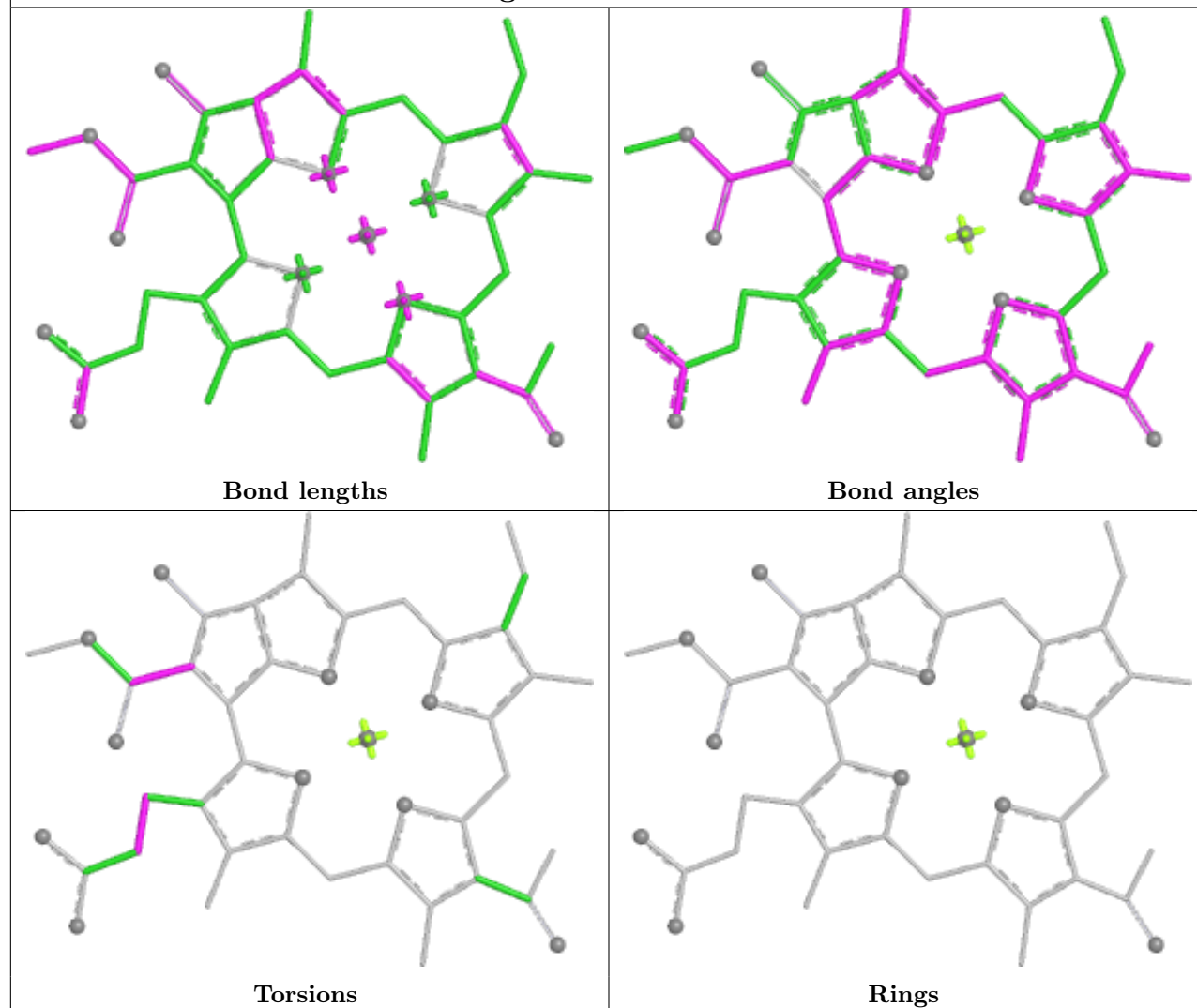




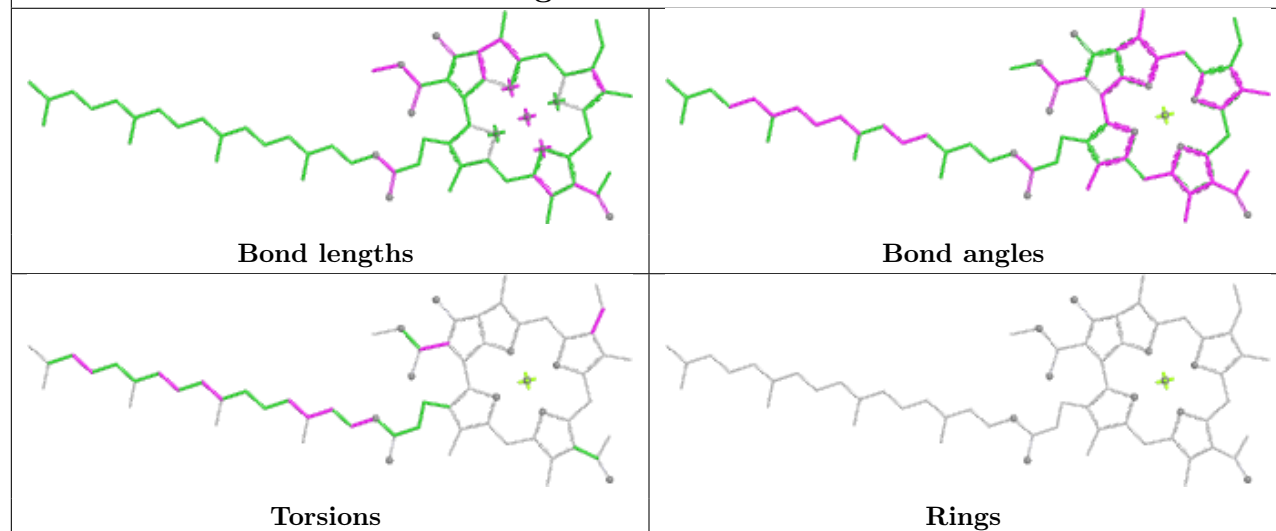


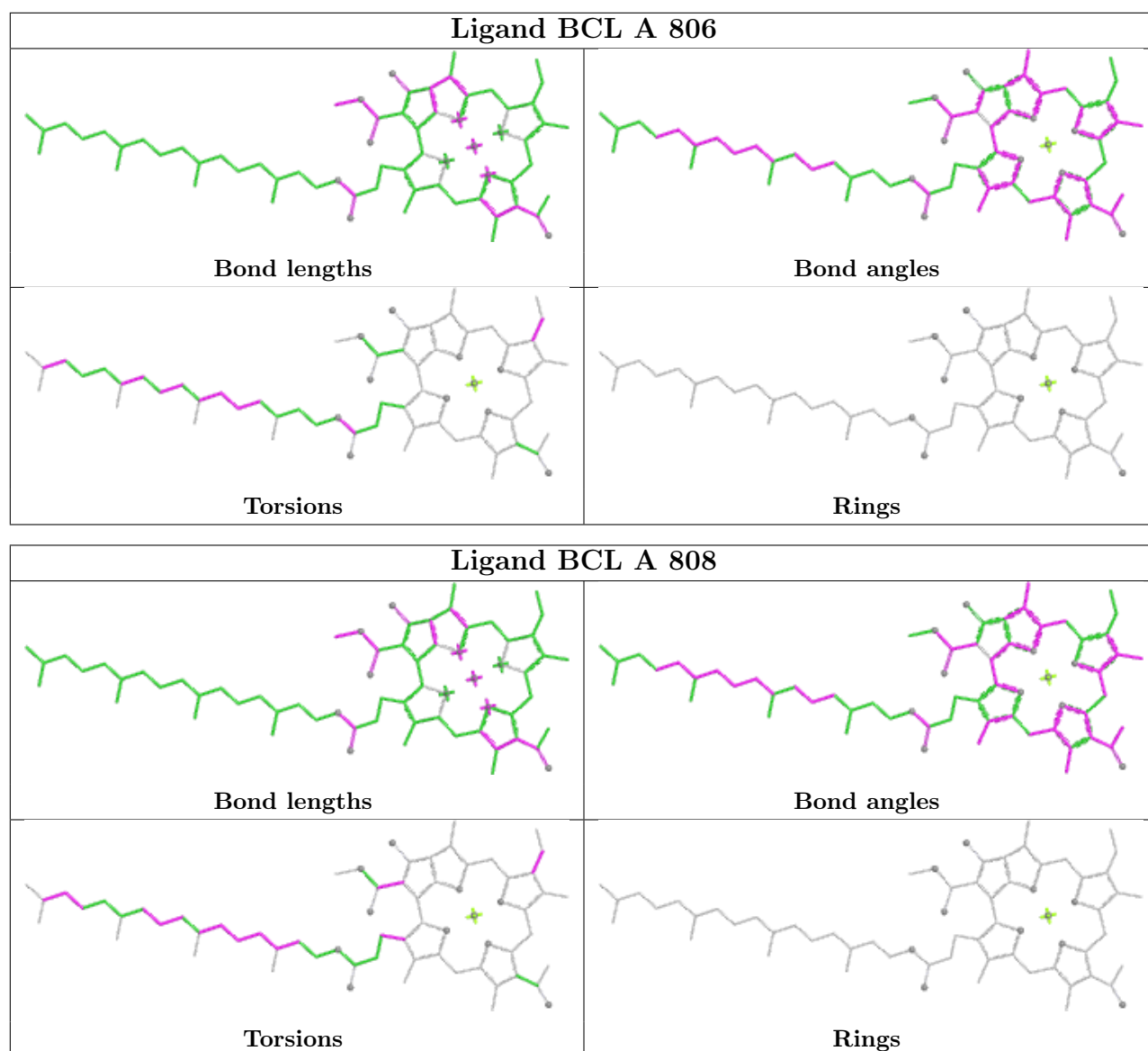


Ligand BCL A 814

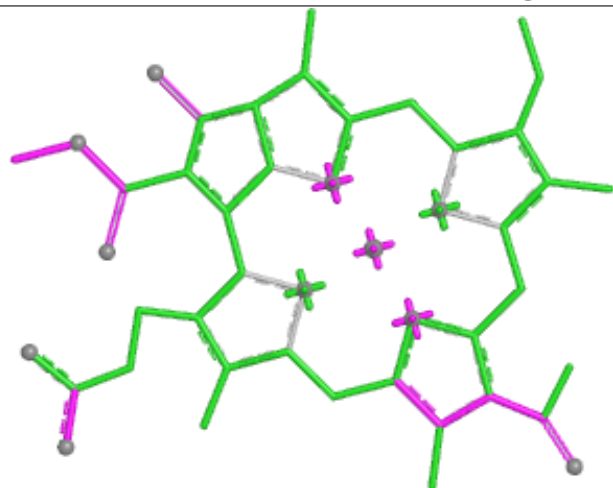


Ligand BCL F 377

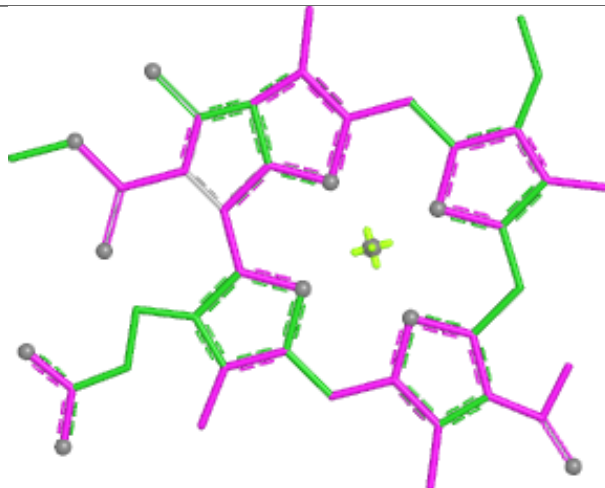




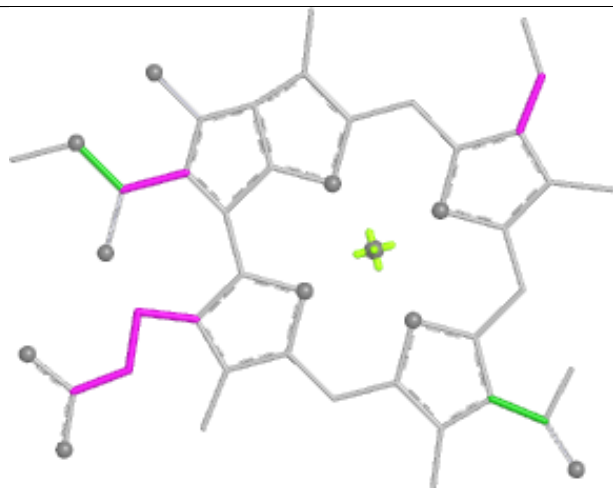
Ligand BCL a 810



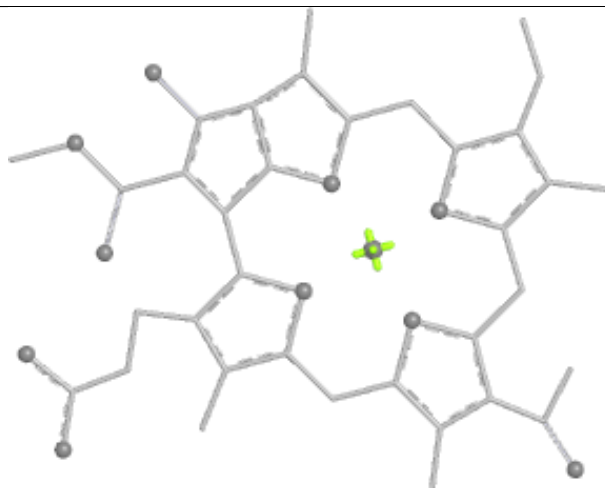
Bond lengths



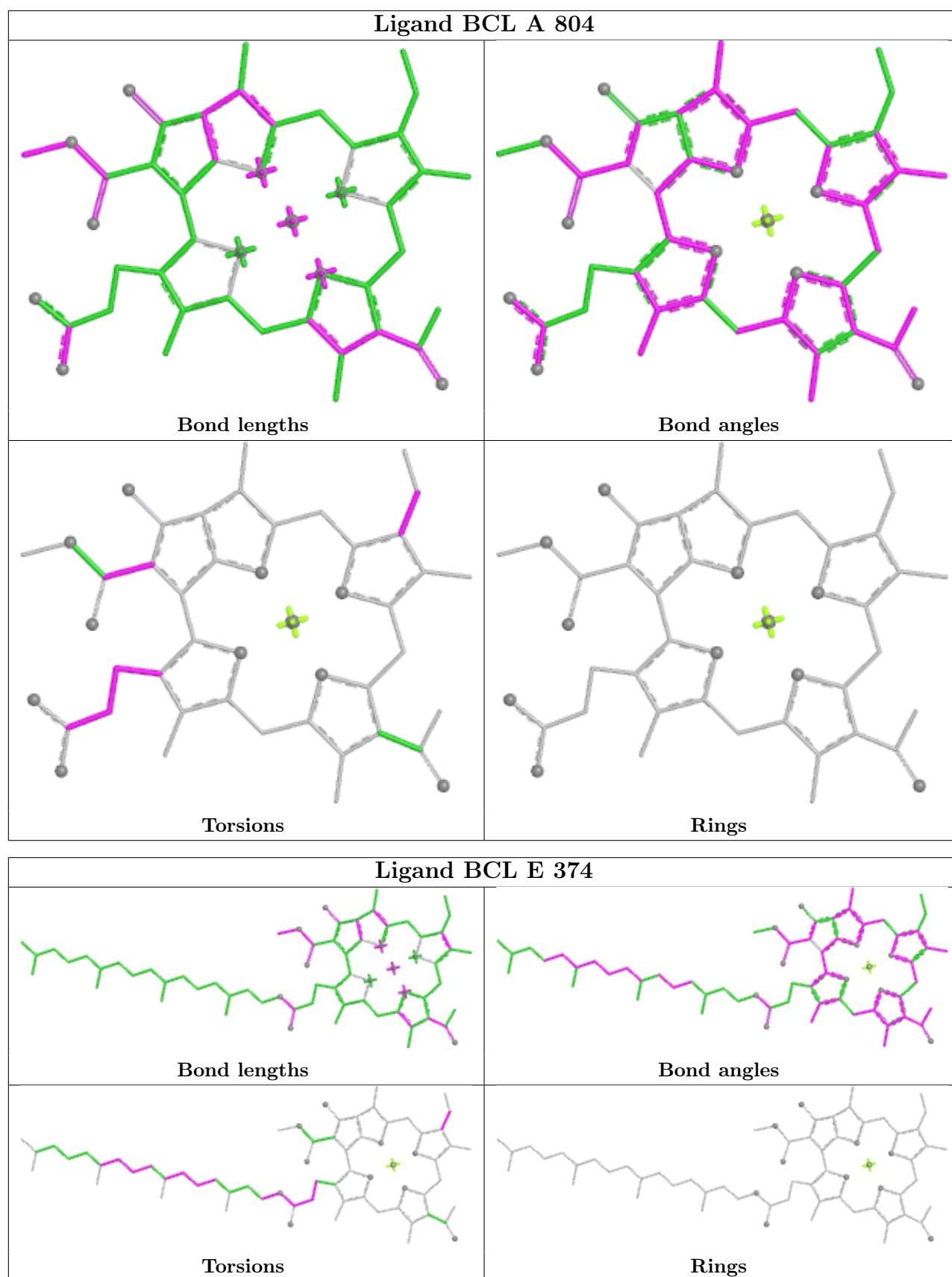
Bond angles

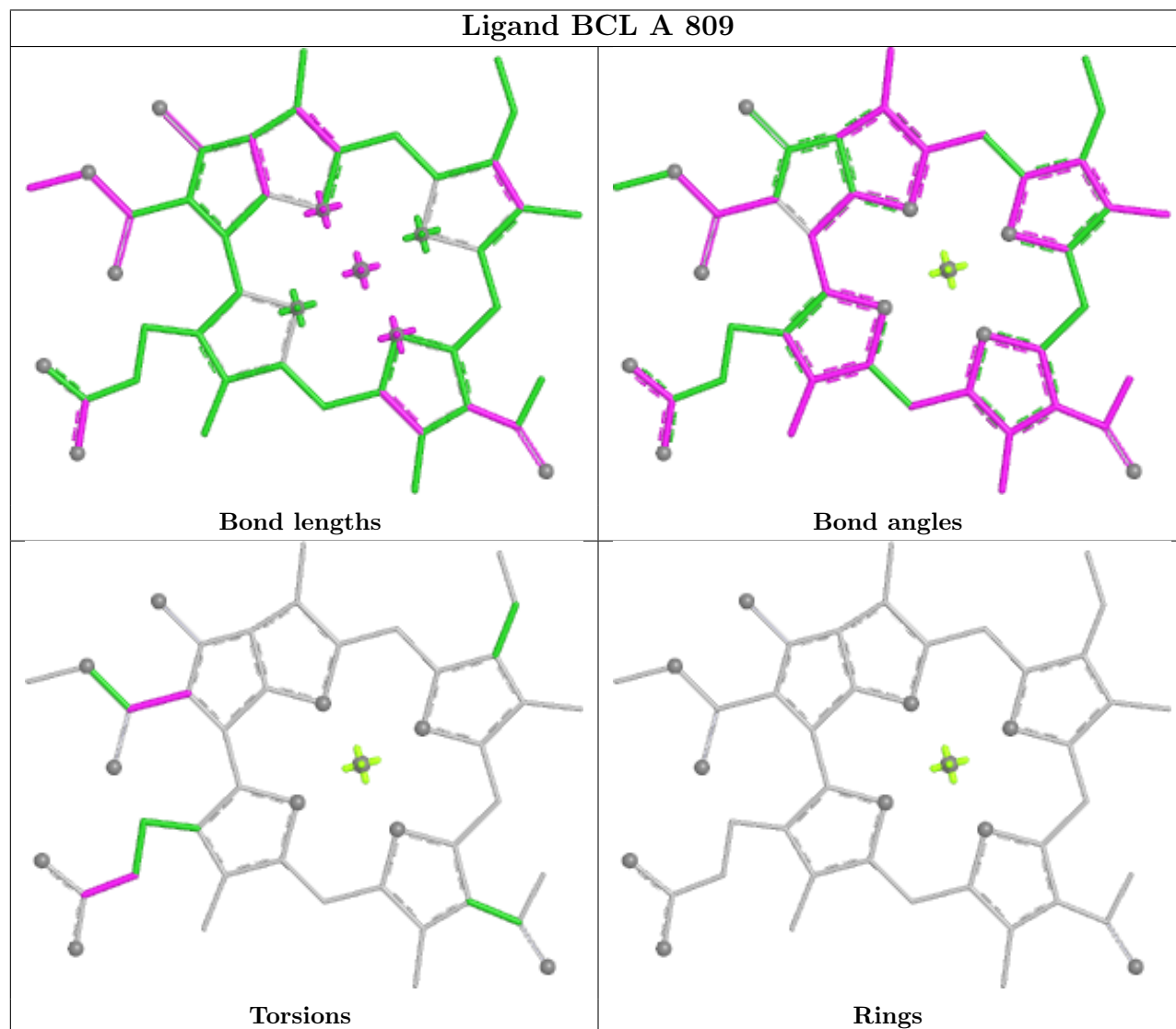
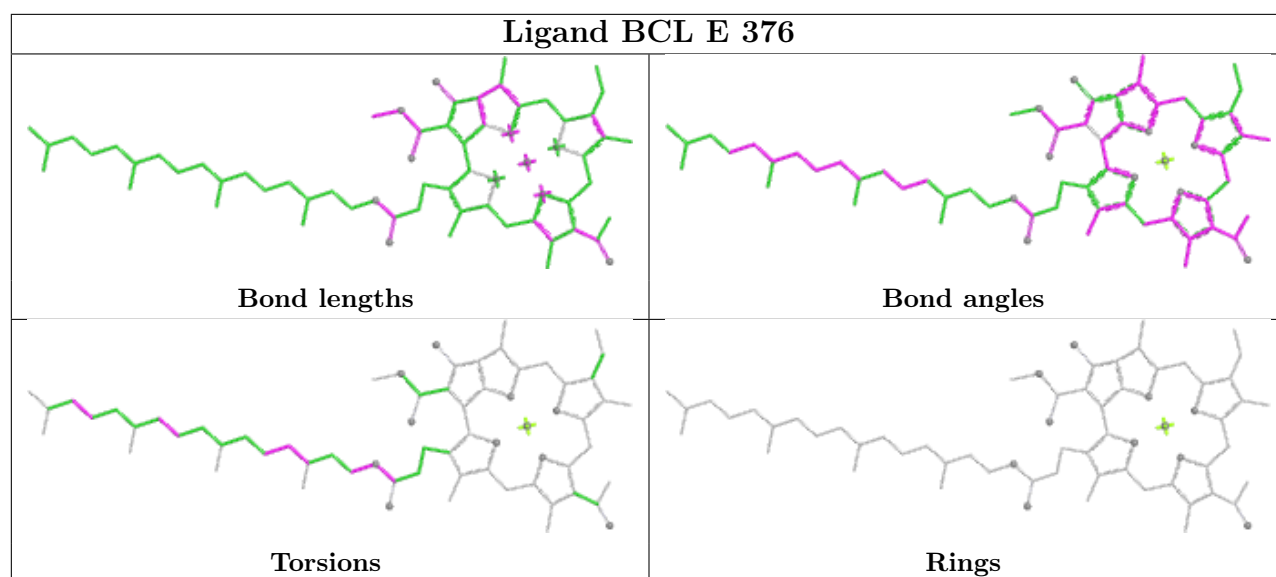


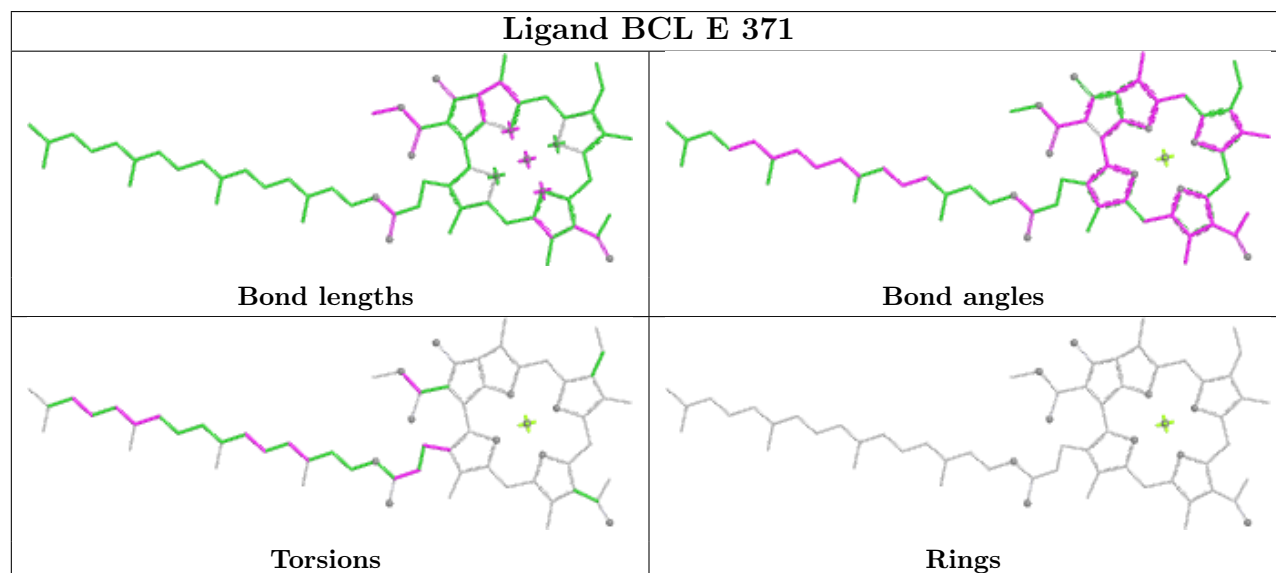
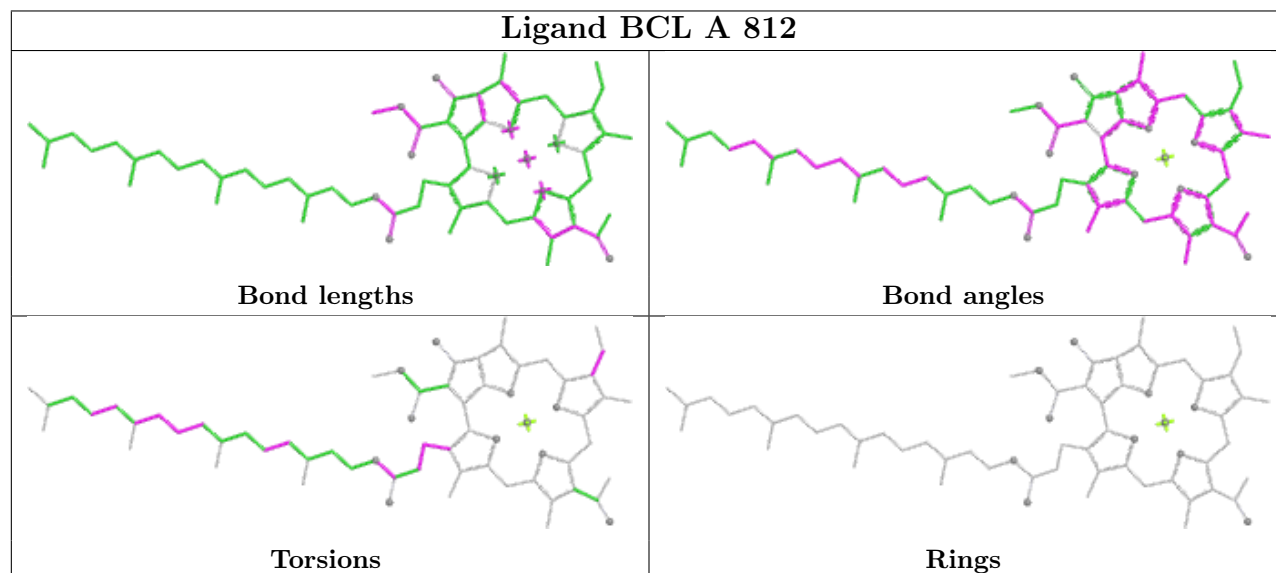
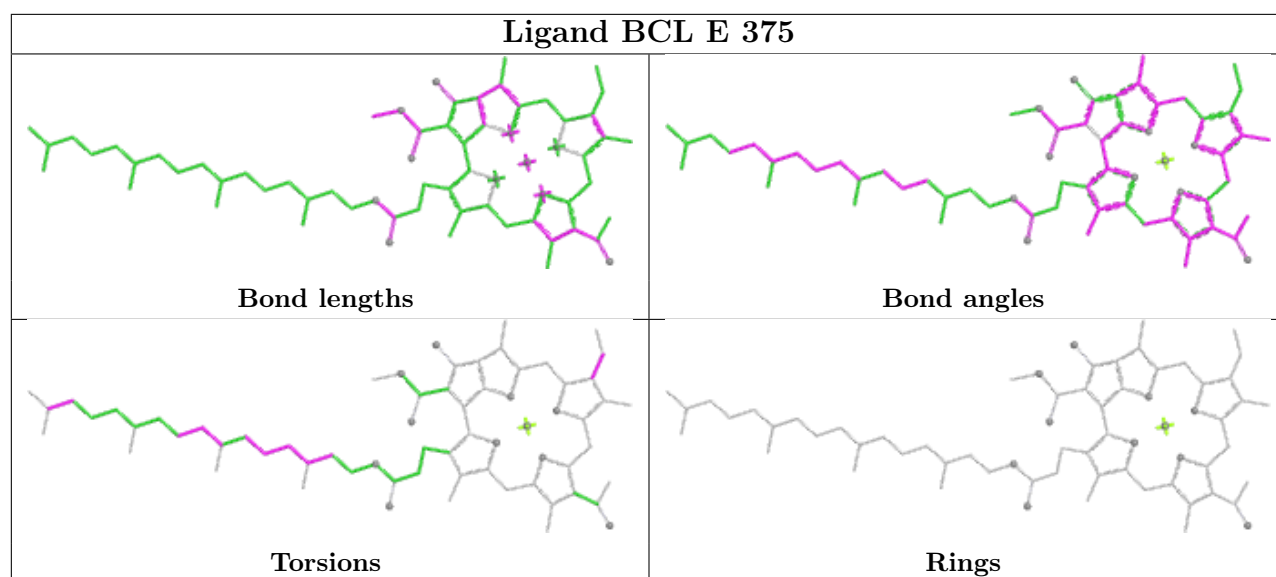
Torsions



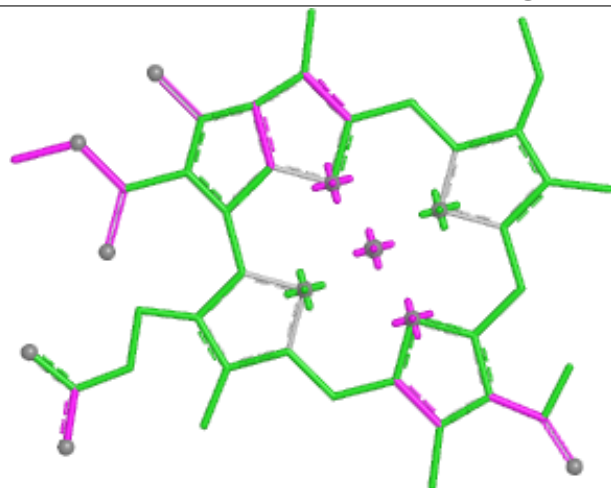
Rings



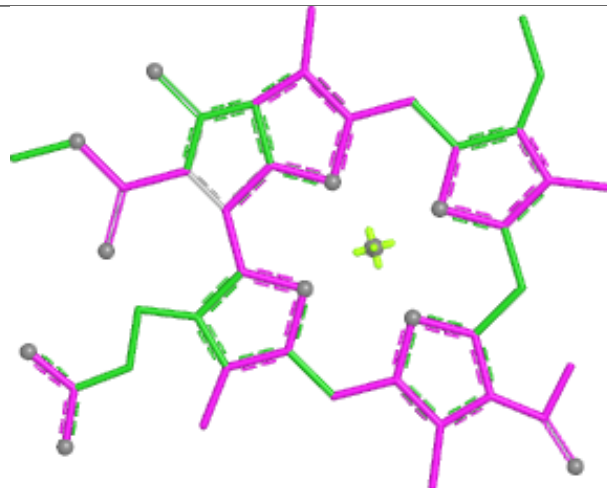




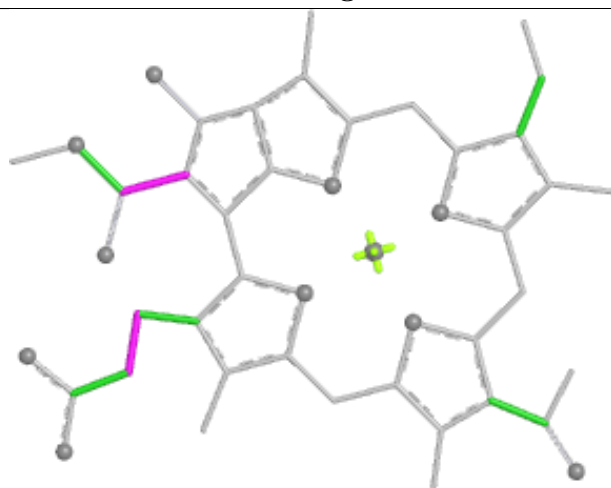
Ligand BCL a 814



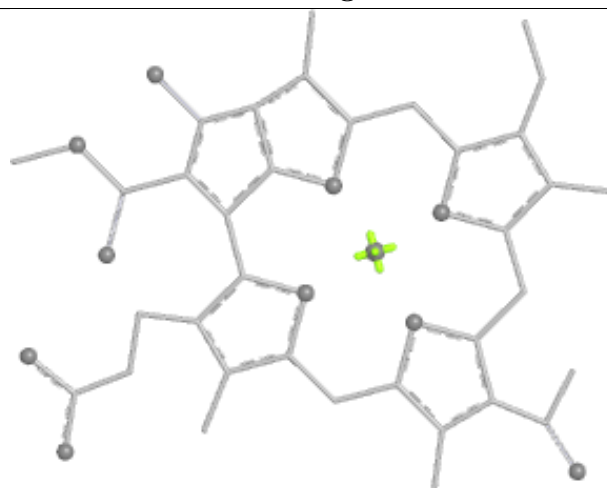
Bond lengths



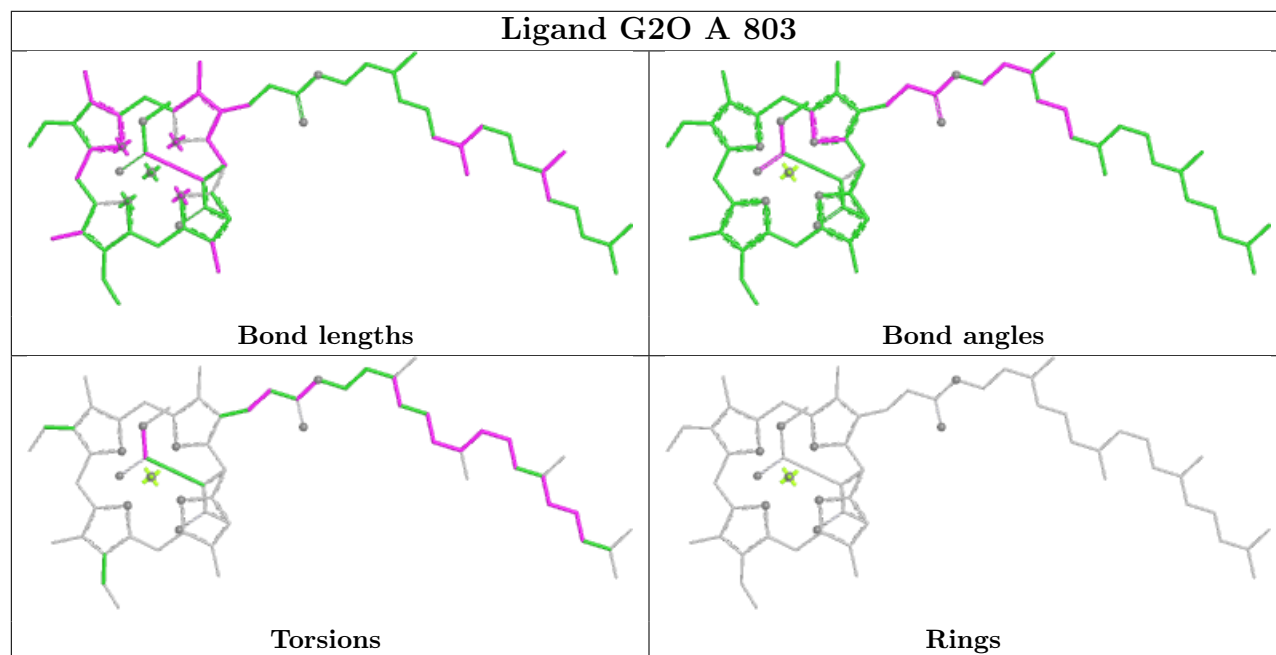
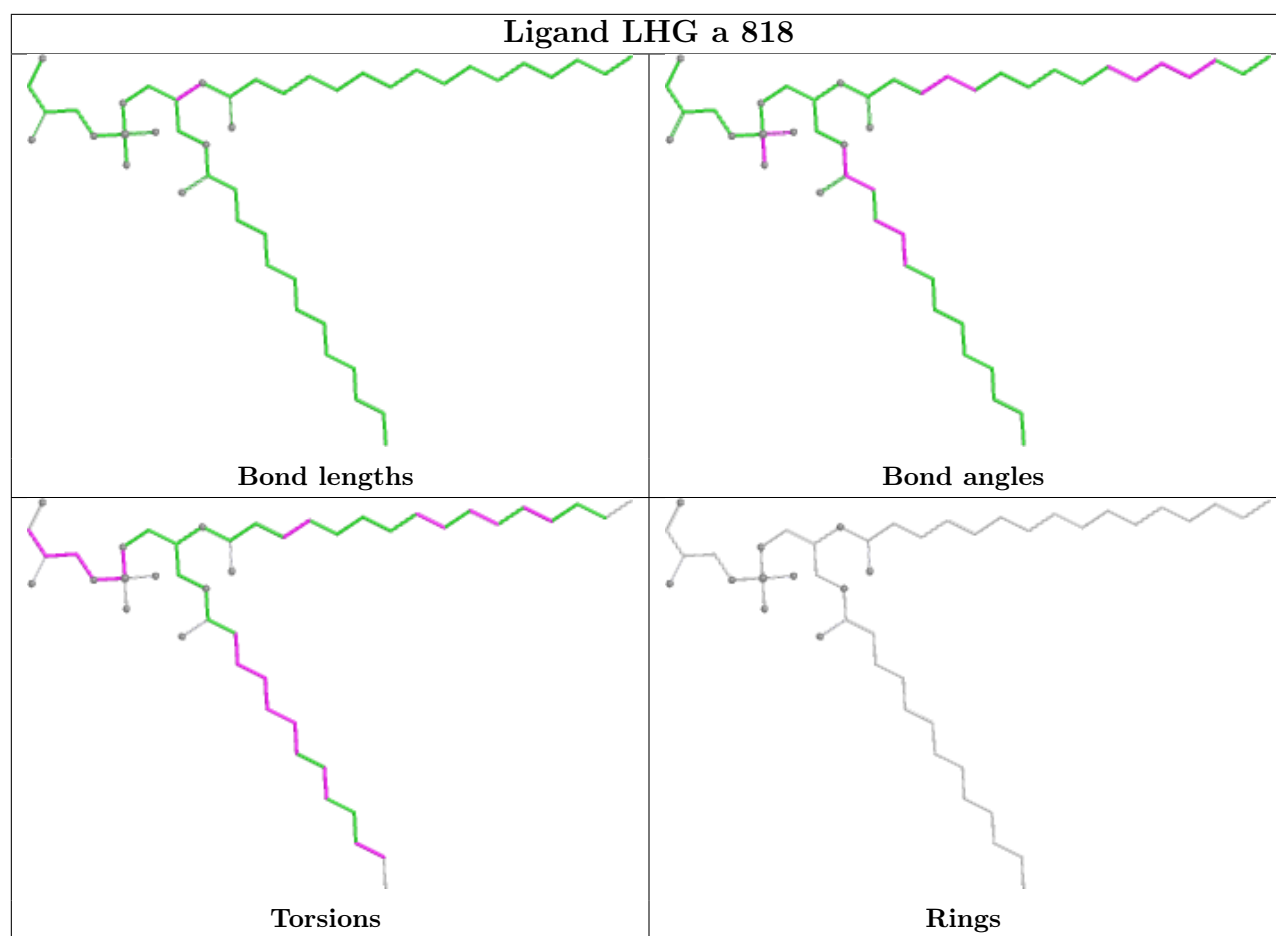
Bond angles

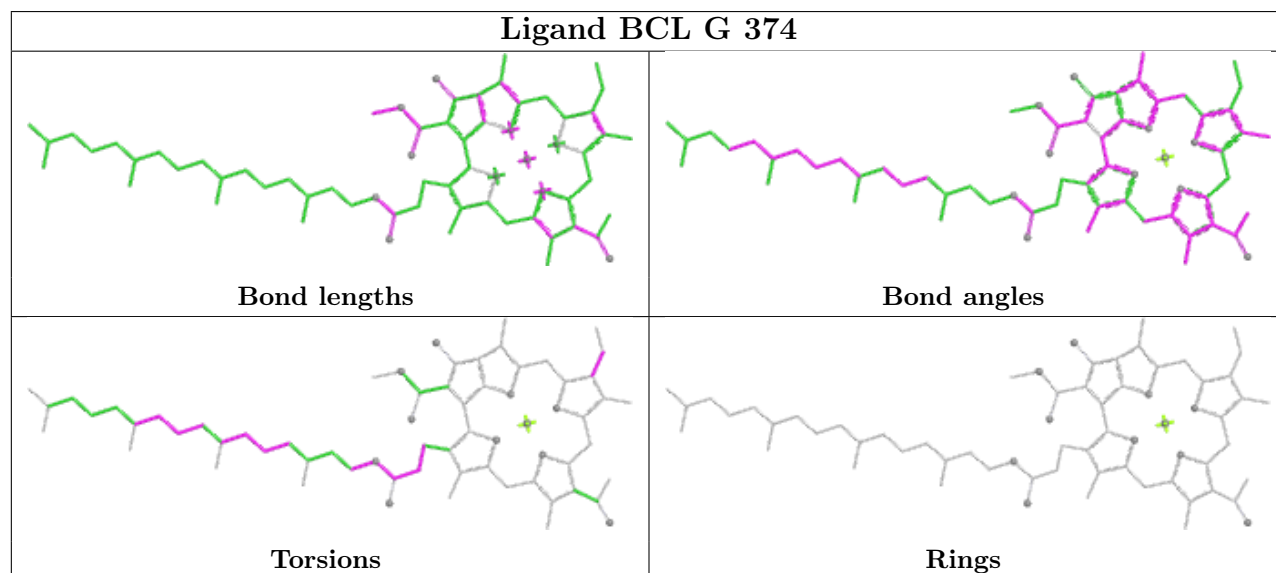
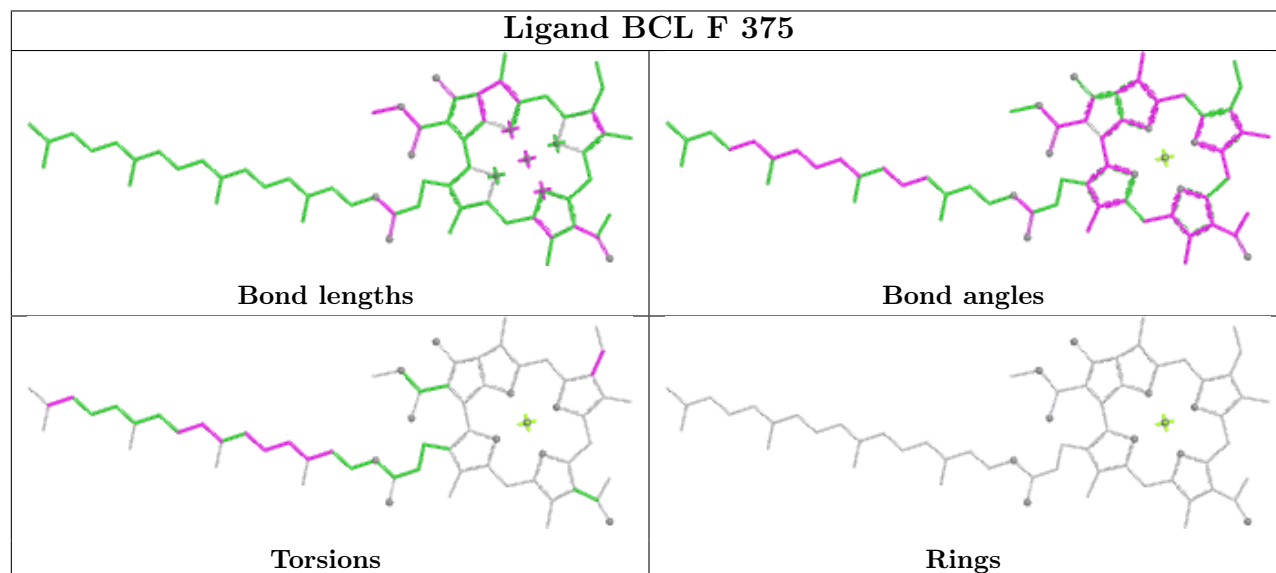
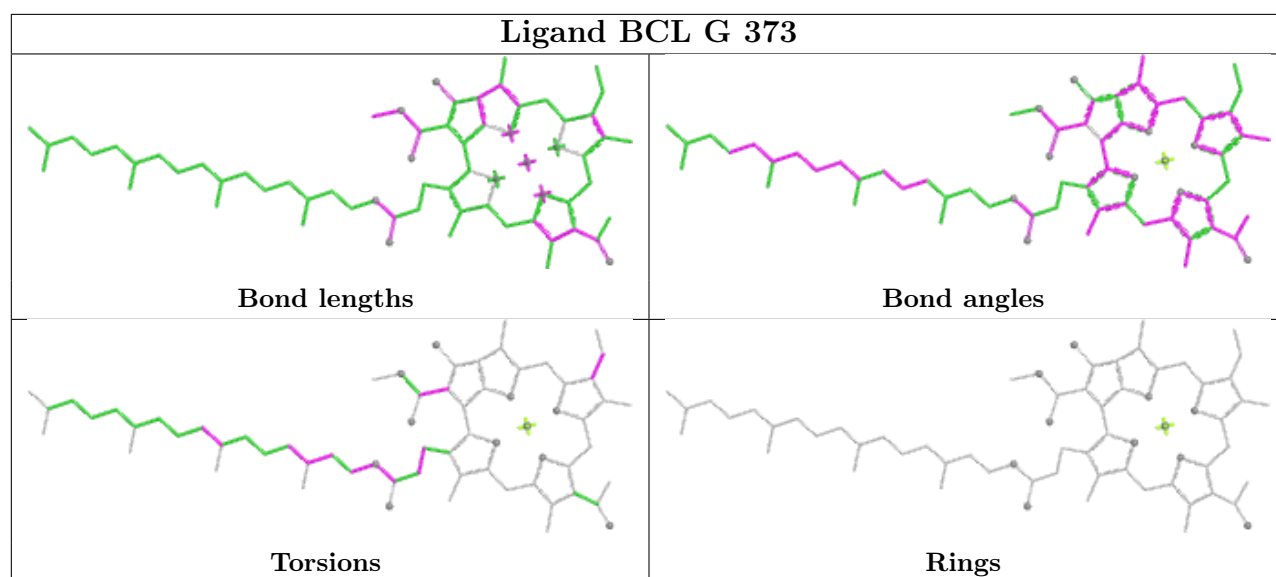


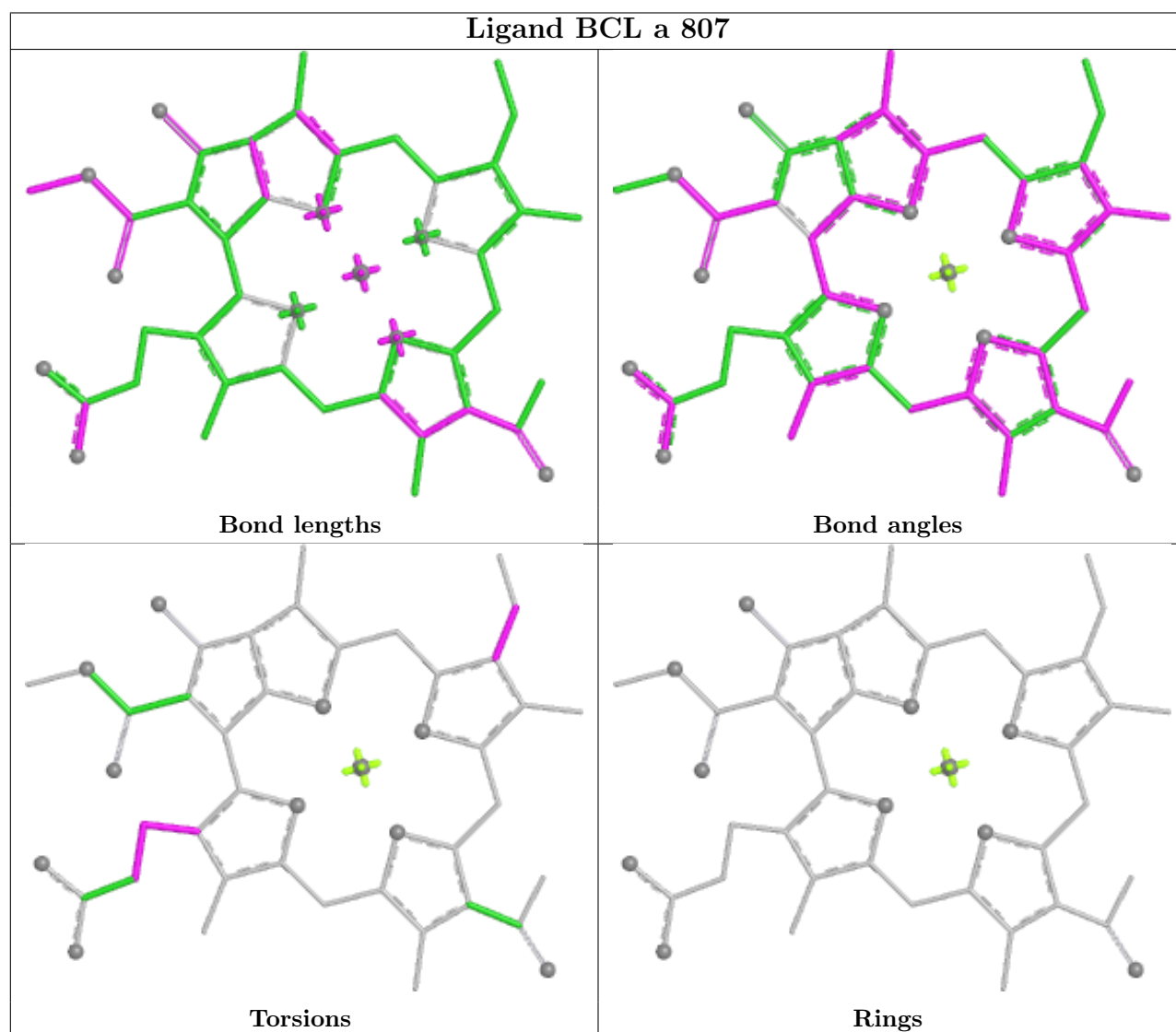
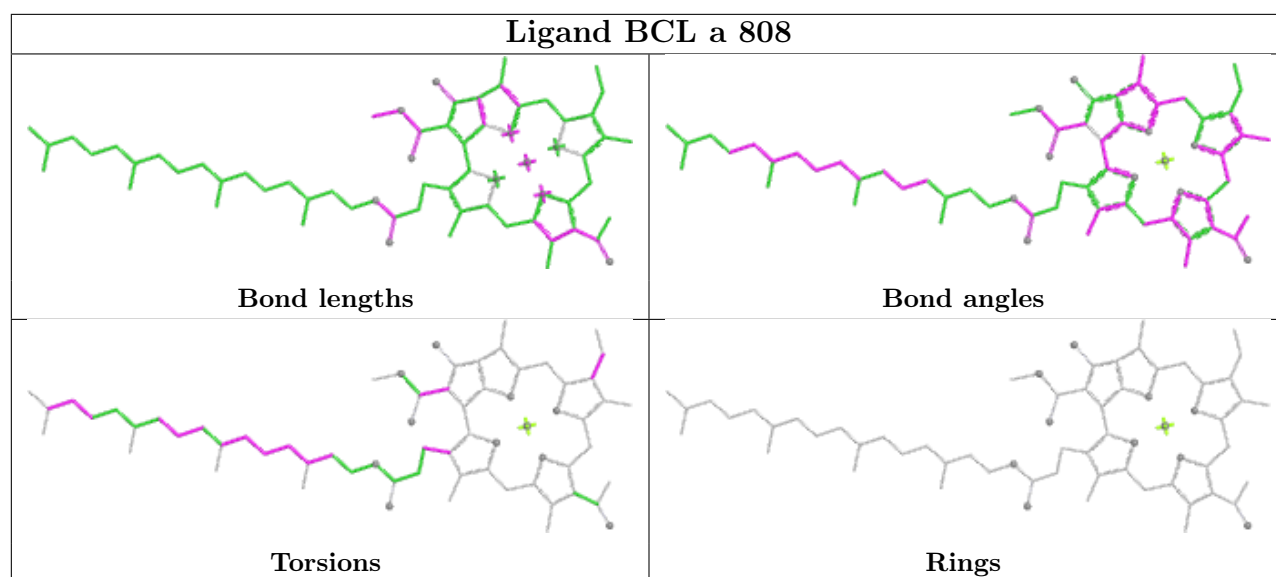
Torsions

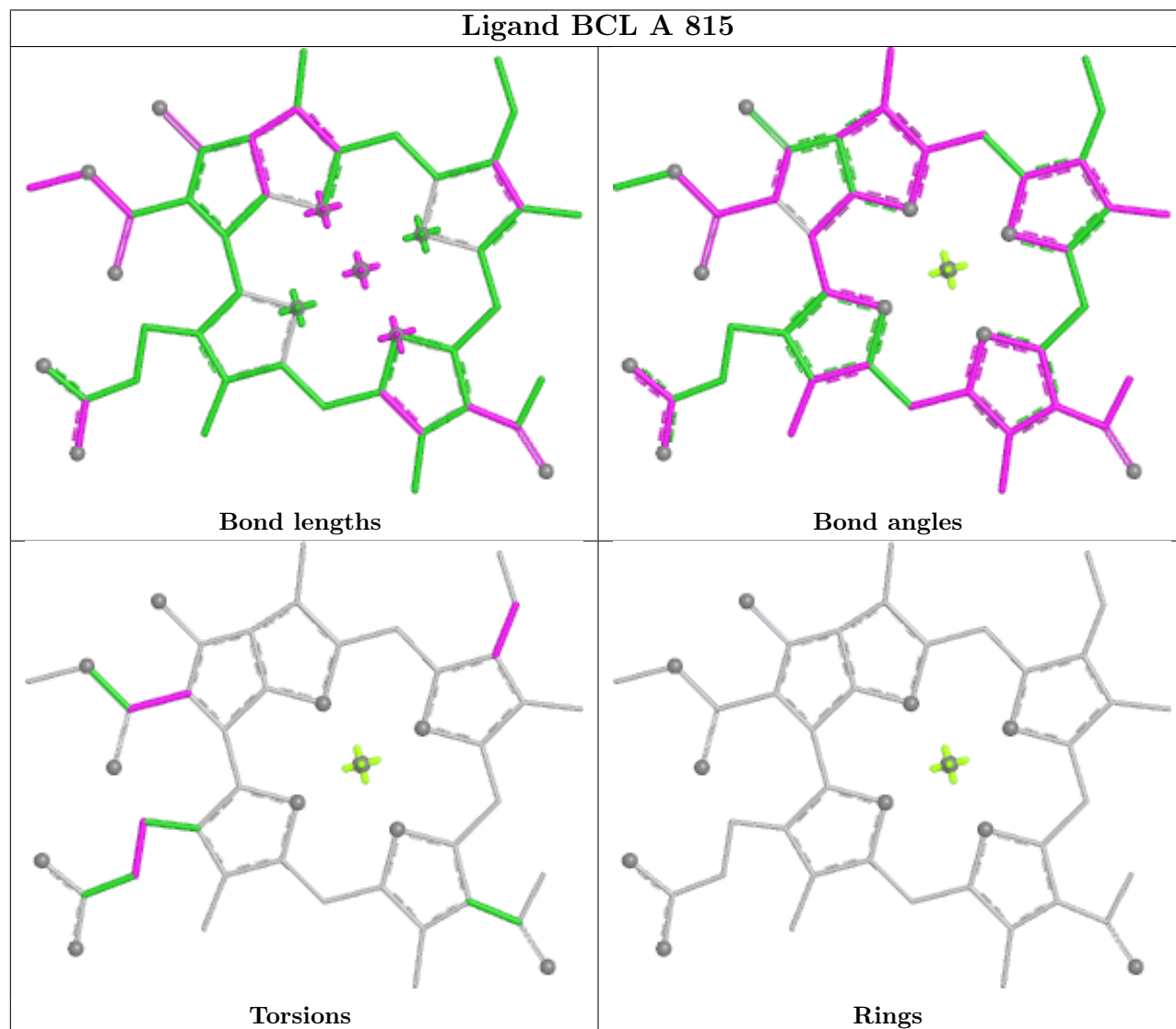
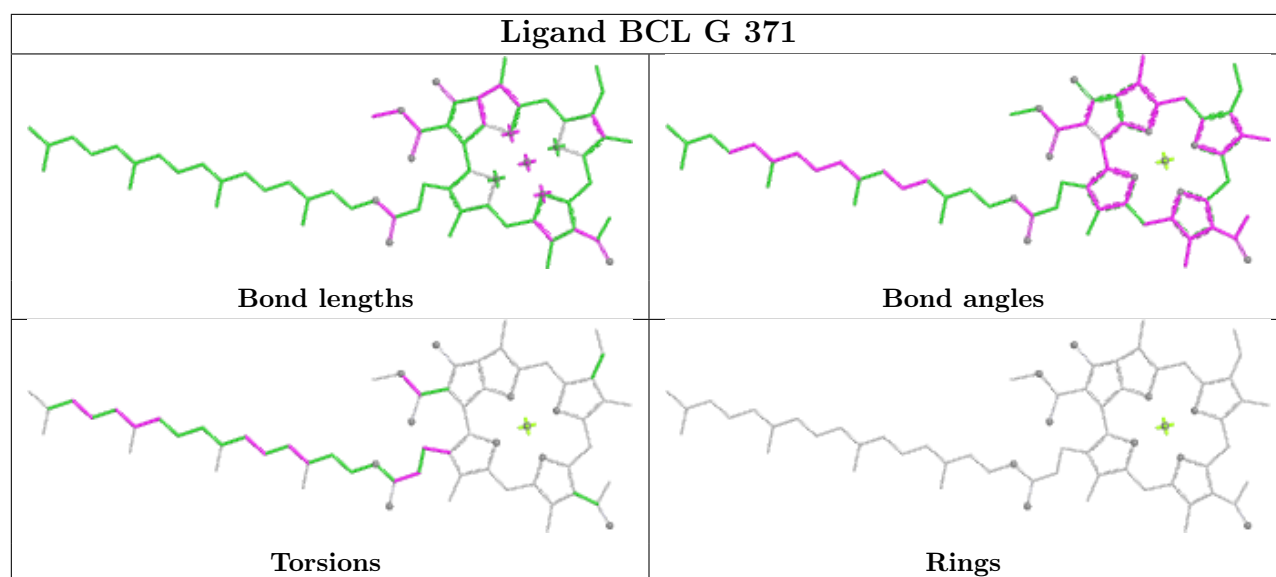


Rings

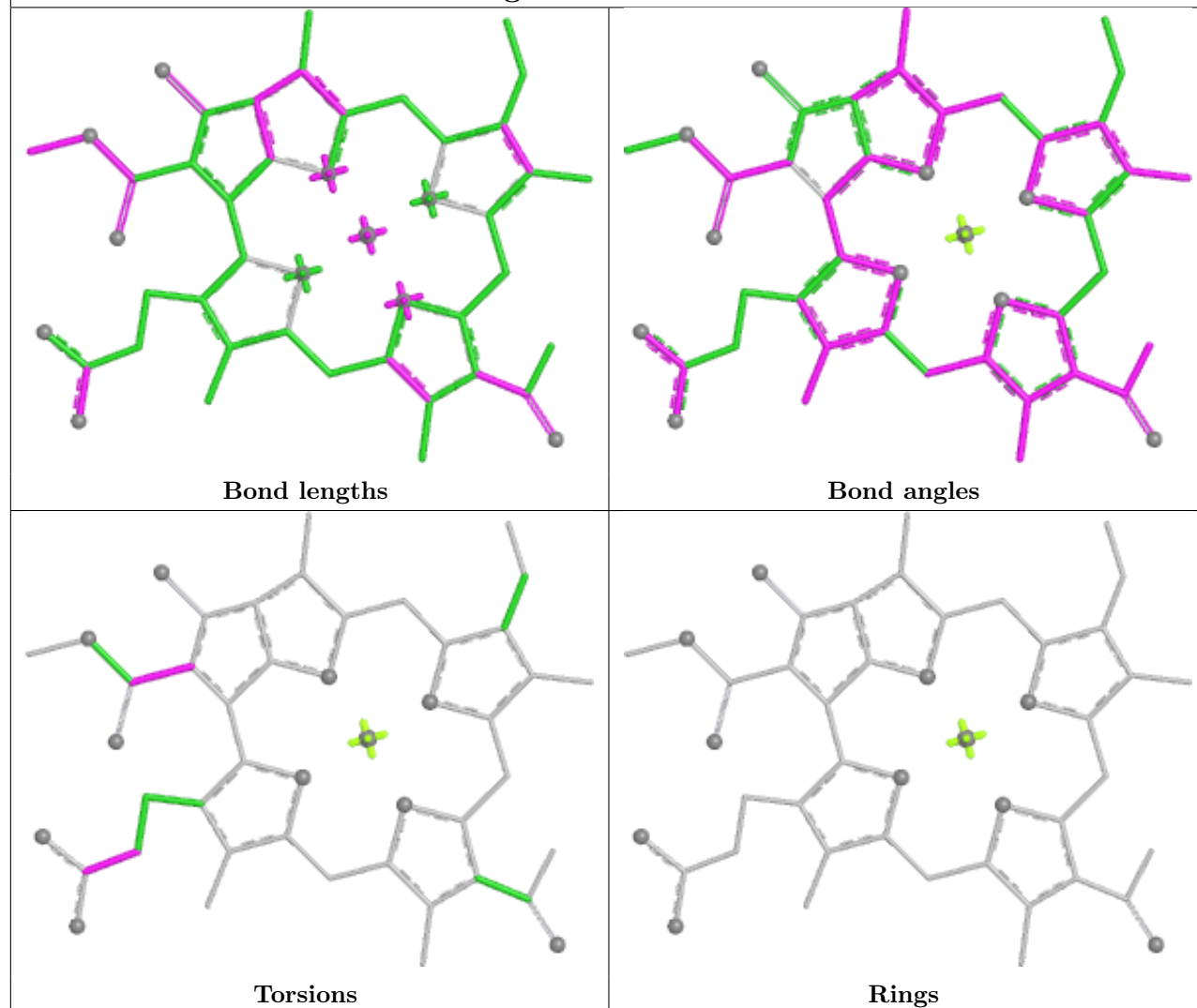




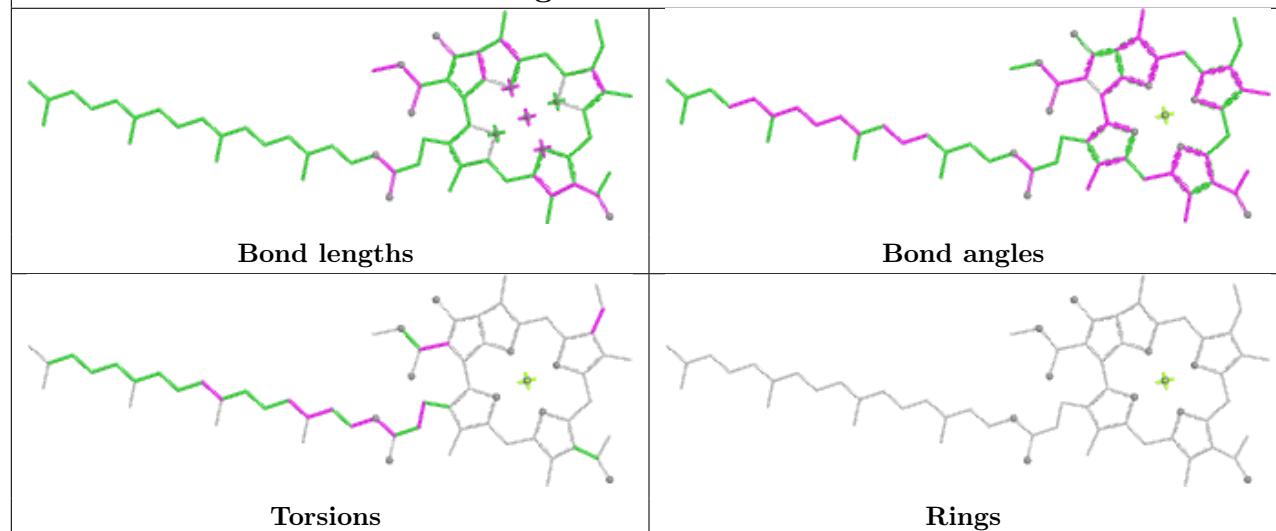


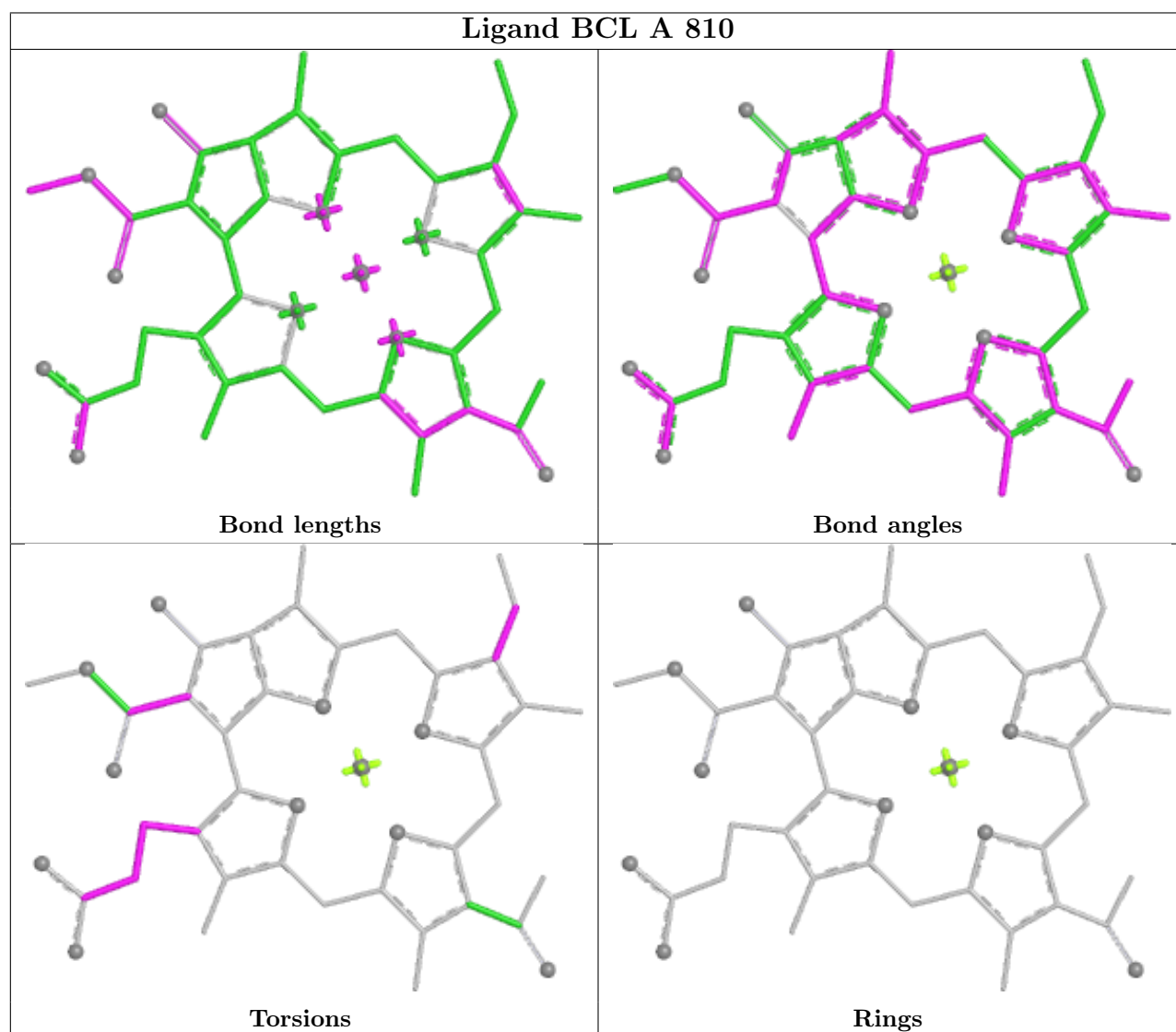
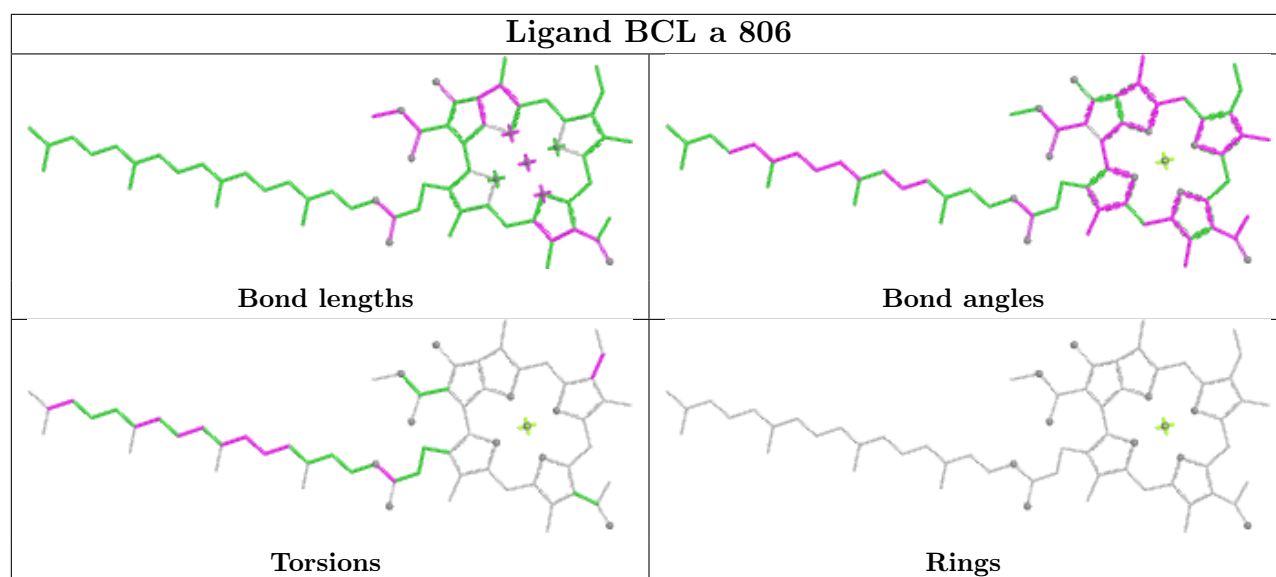


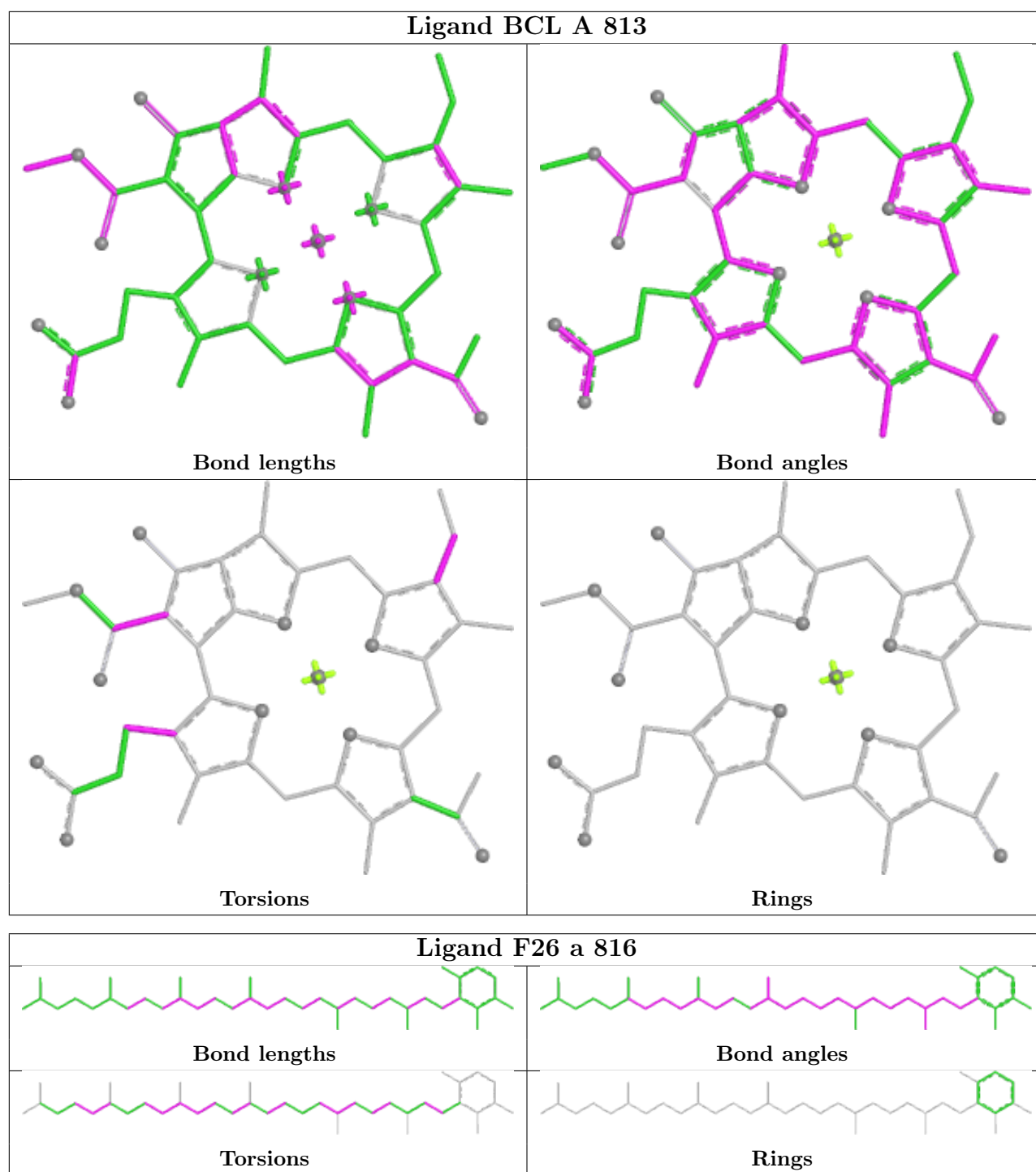
Ligand BCL a 809



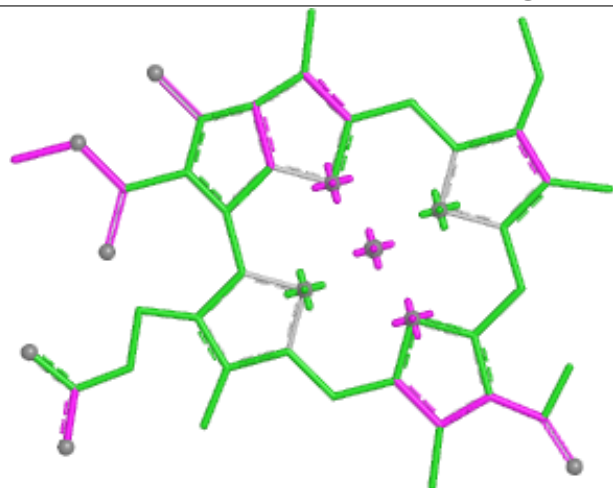
Ligand BCL F 373



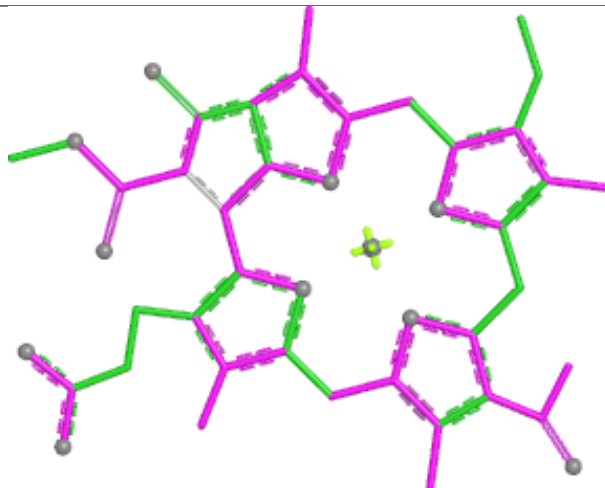




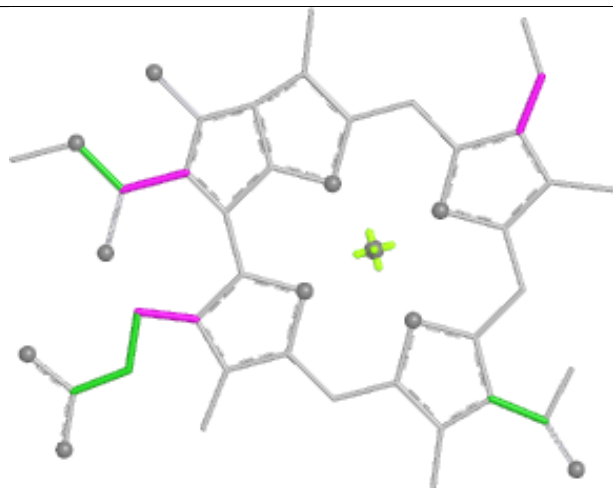
Ligand BCL a 813



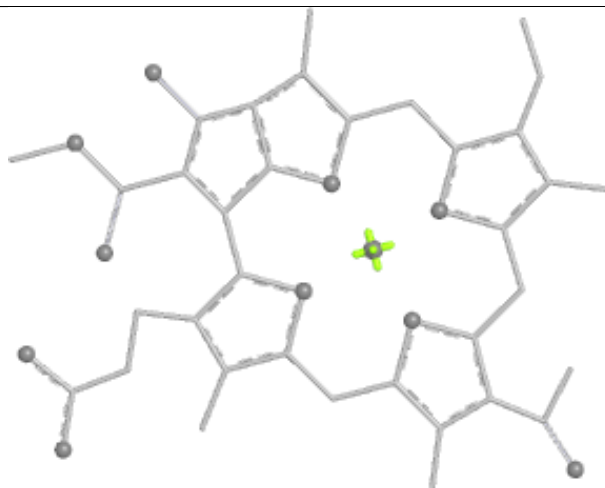
Bond lengths



Bond angles

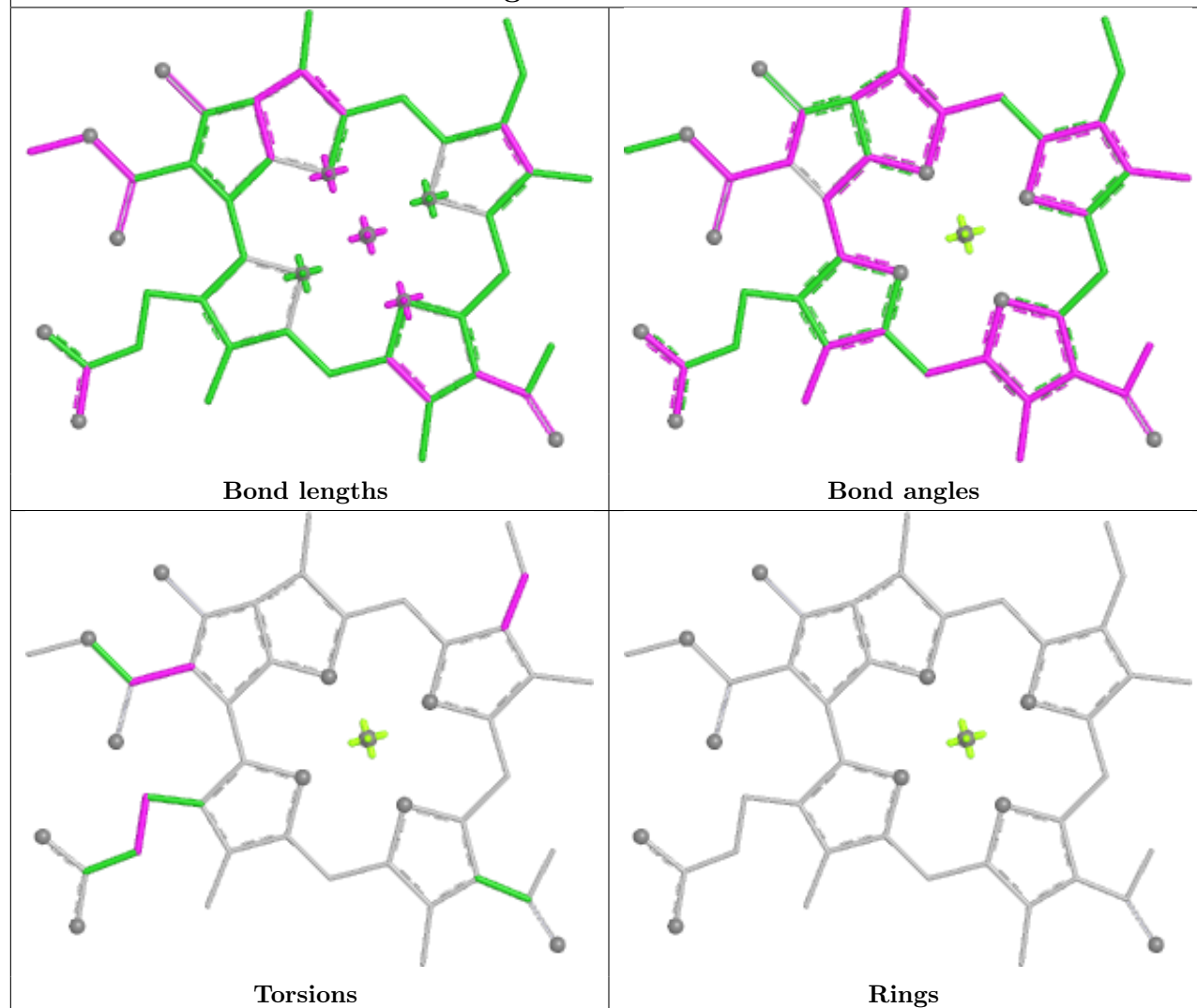


Torsions

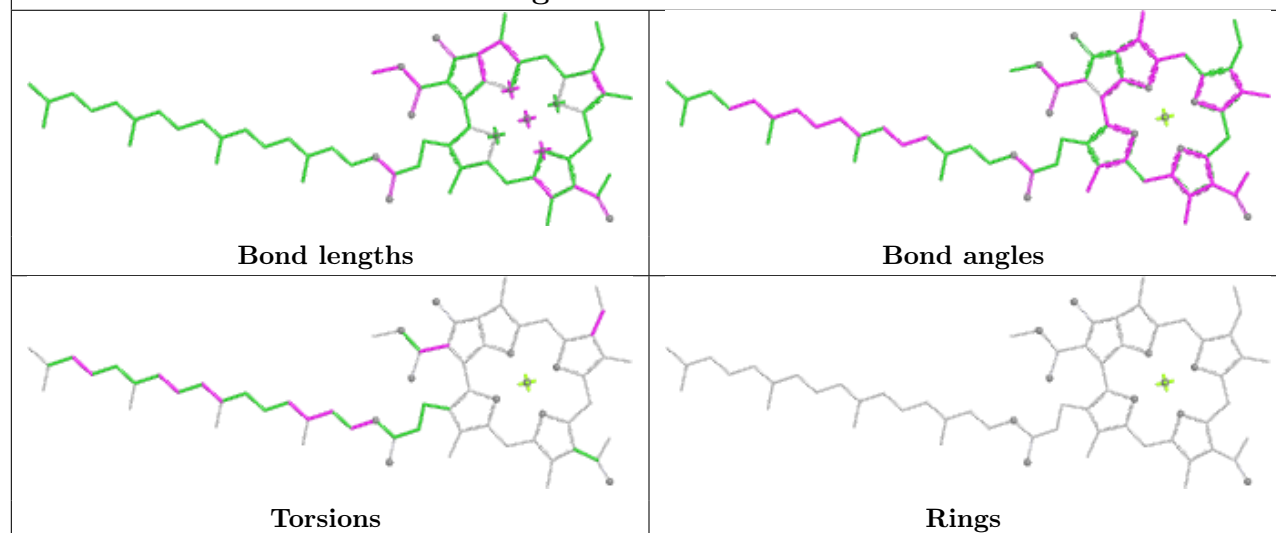


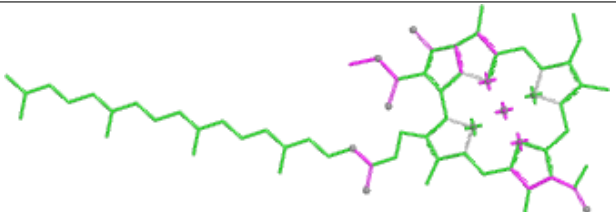
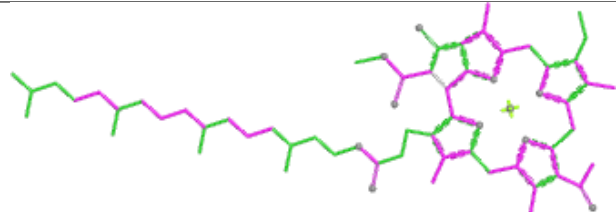
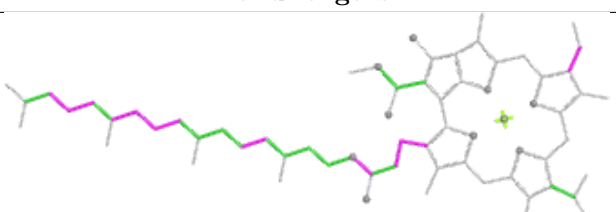
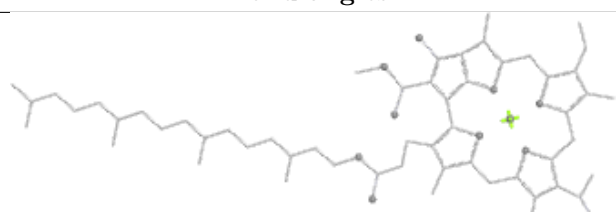
Rings

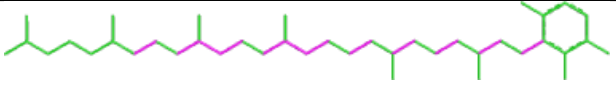
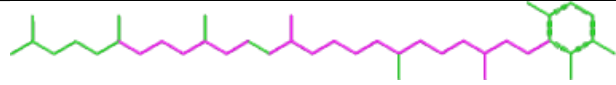
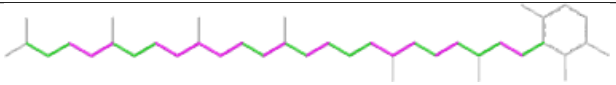
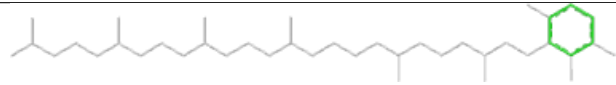
Ligand BCL a 815

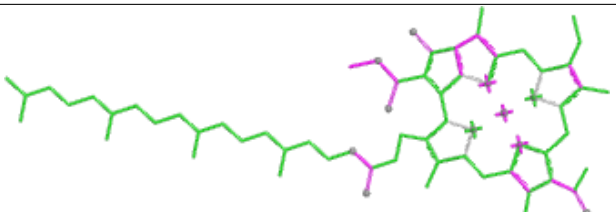
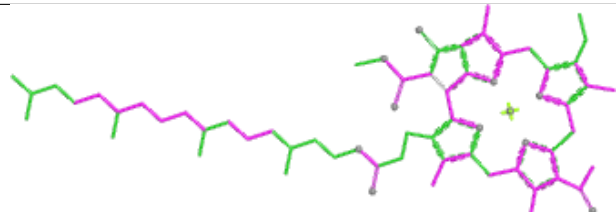
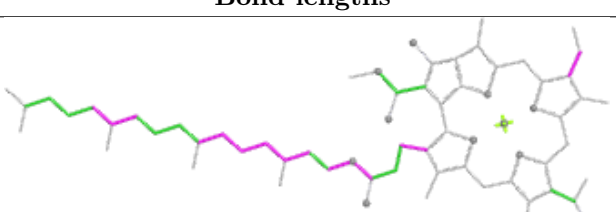
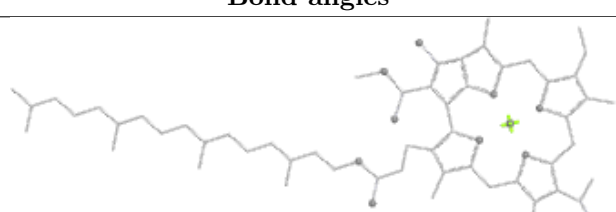


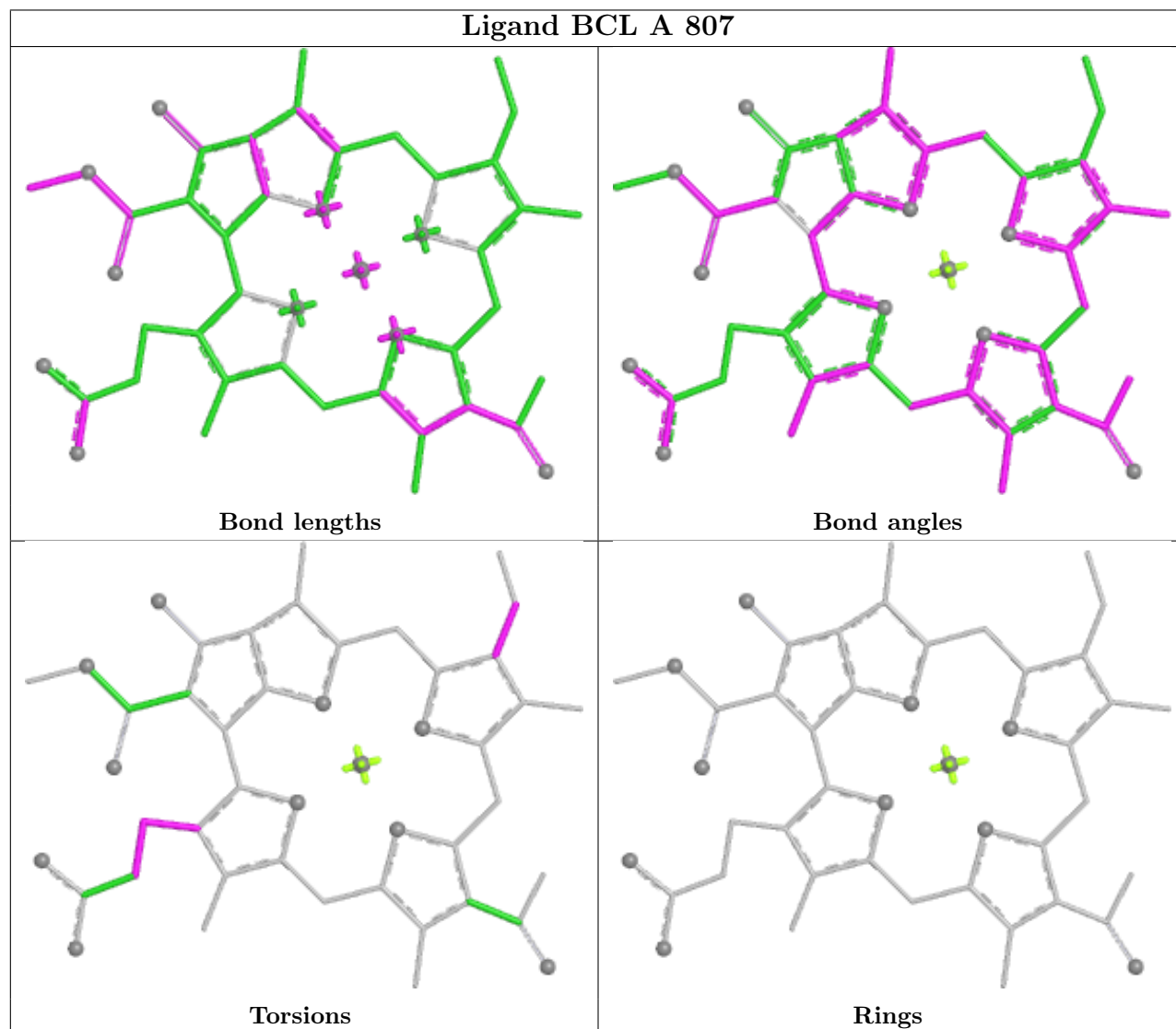
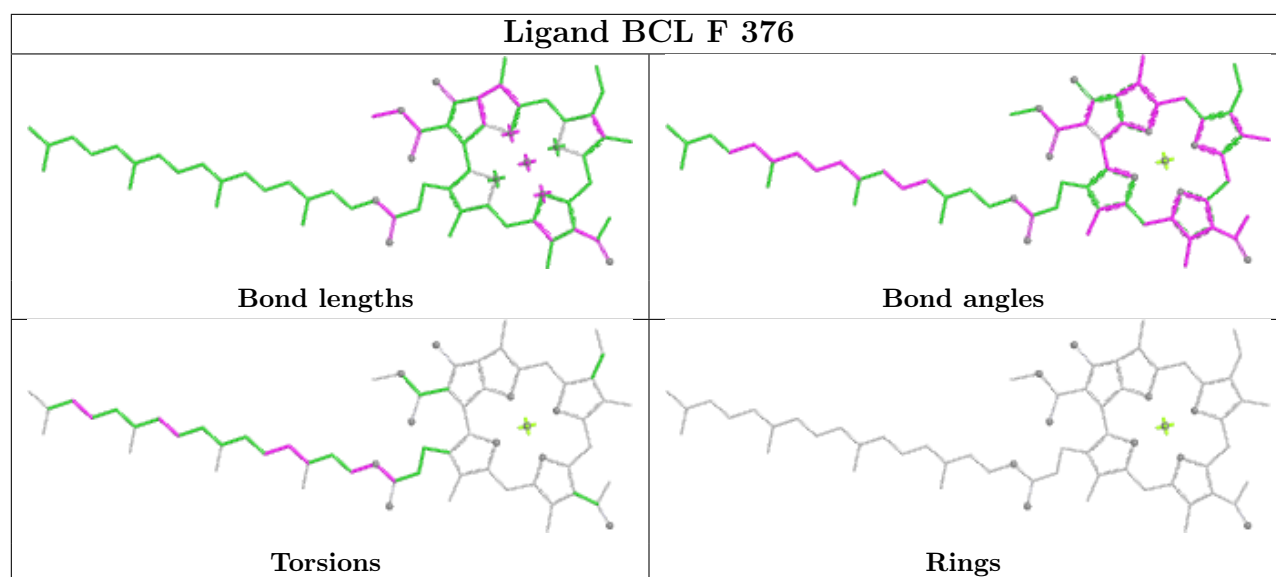
Ligand BCL G 377

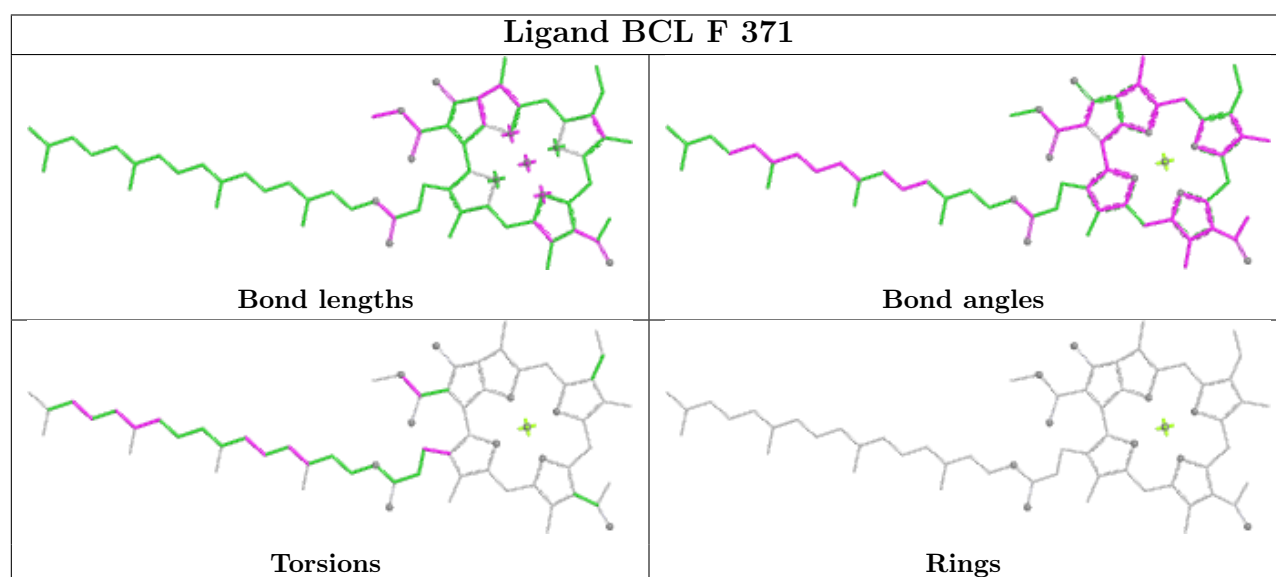
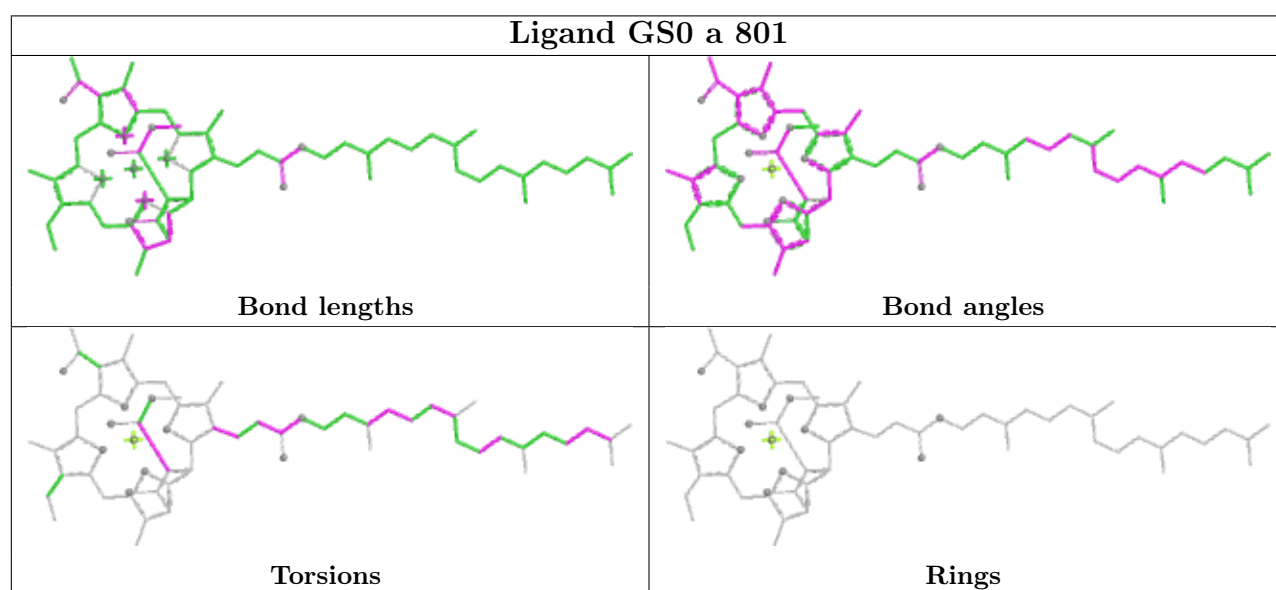
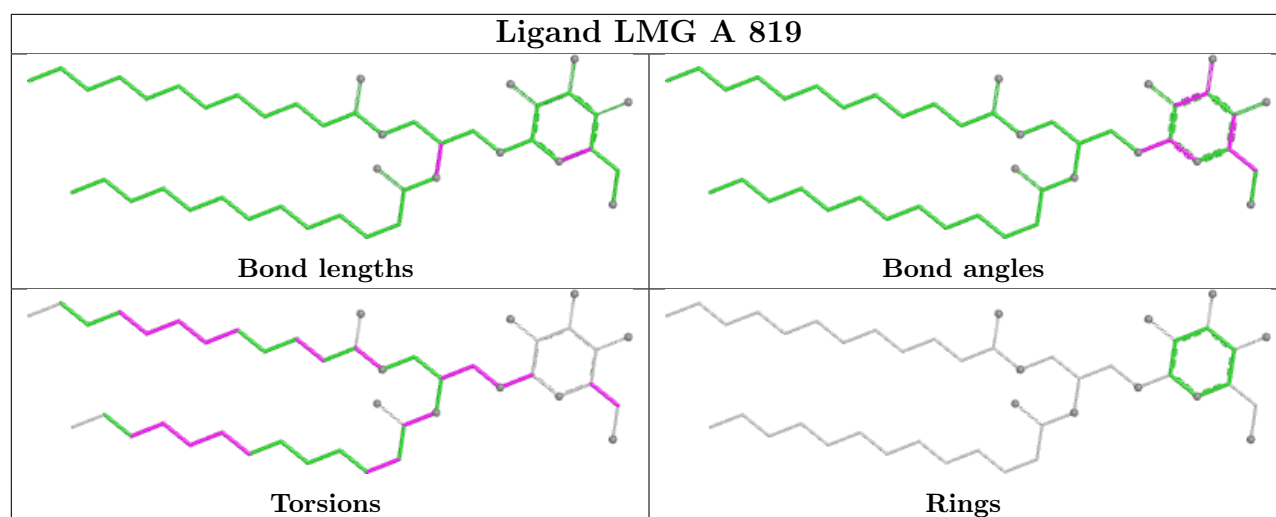


Ligand BCL a 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

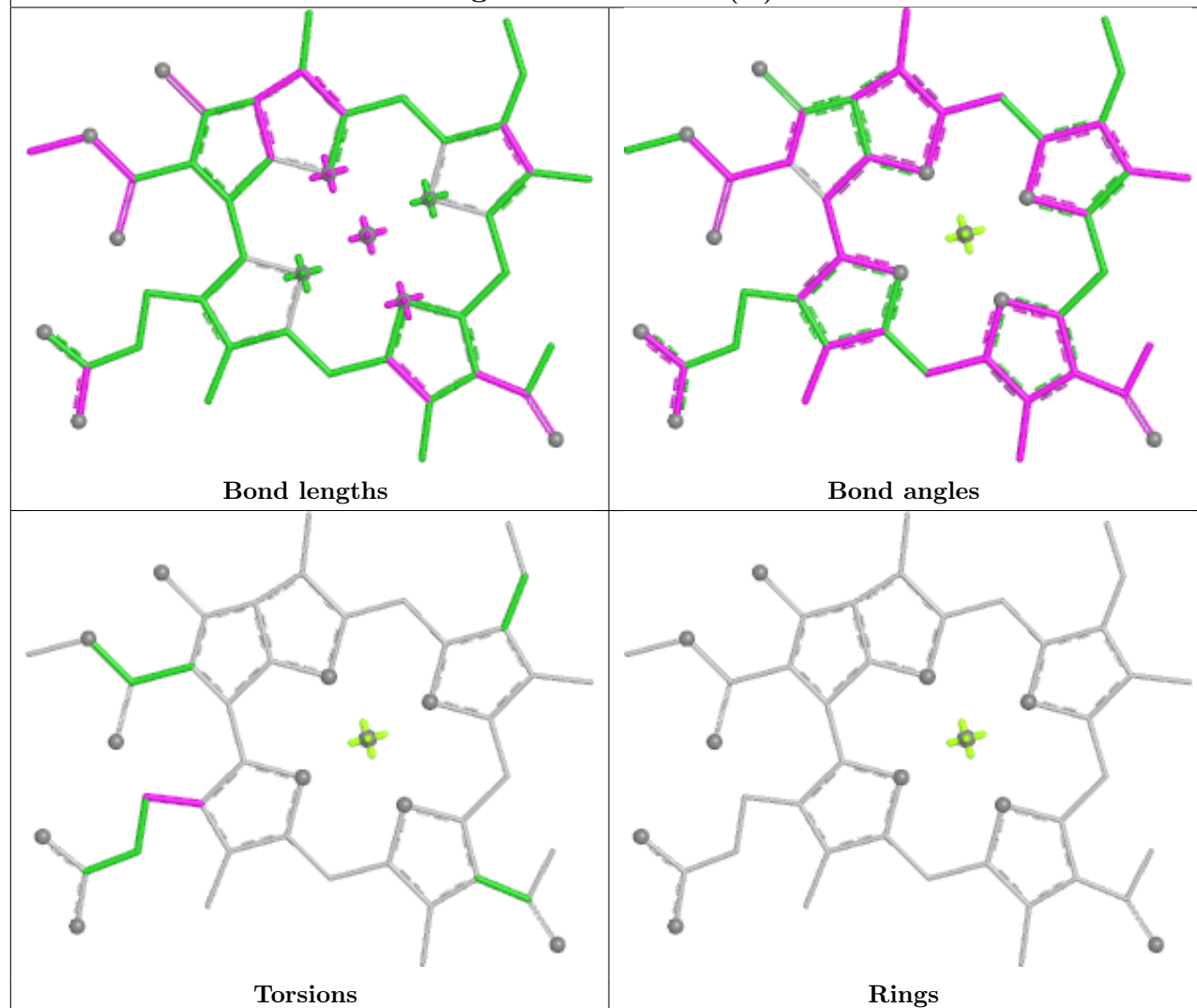
Ligand F26 A 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL A 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

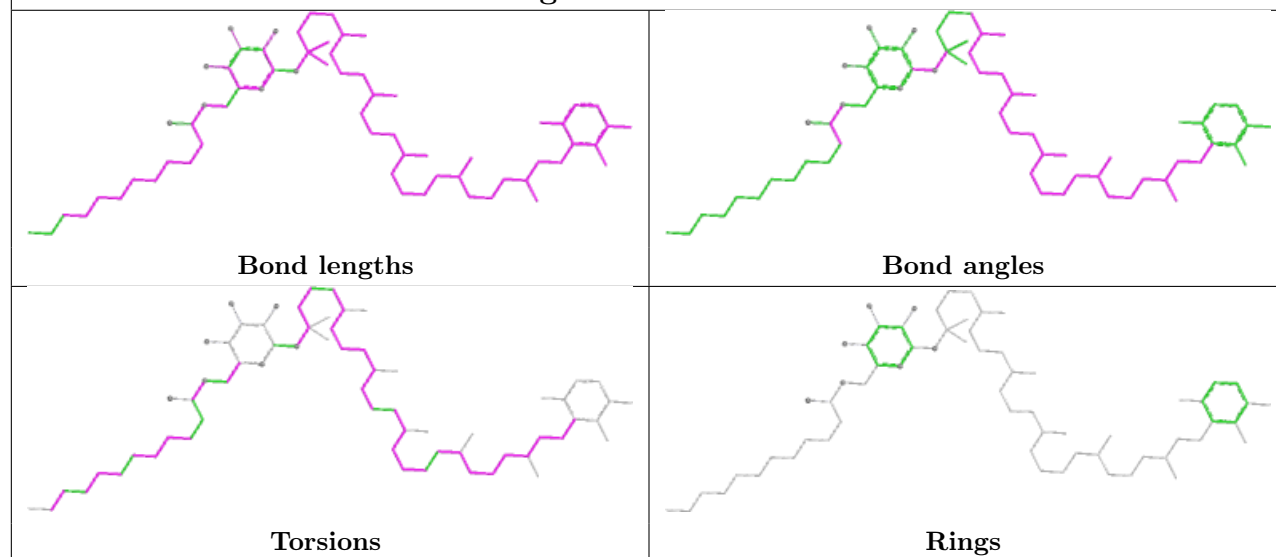




Ligand BCL F 378 (B)



Ligand F39 A 817



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.

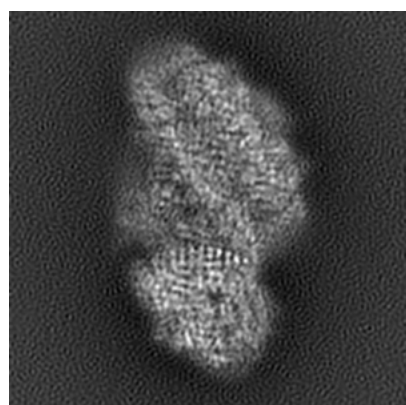
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30069. These allow visual inspection of the internal detail of the map and identification of artifacts.

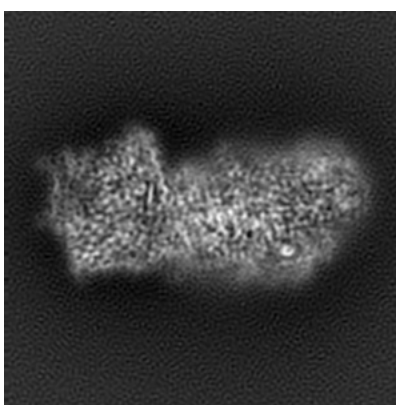
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

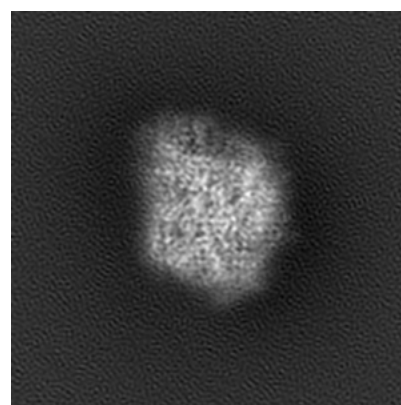
6.1.1 Primary map



X



Y

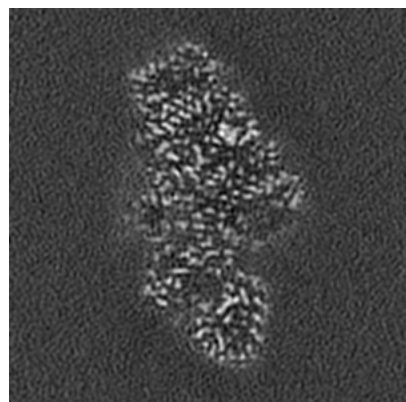


Z

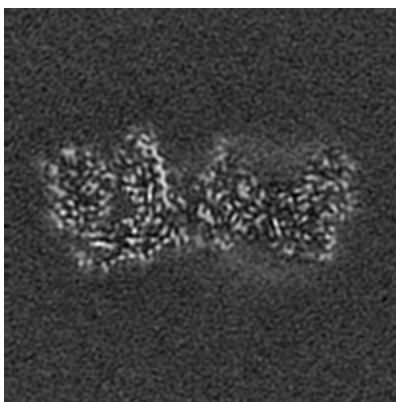
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

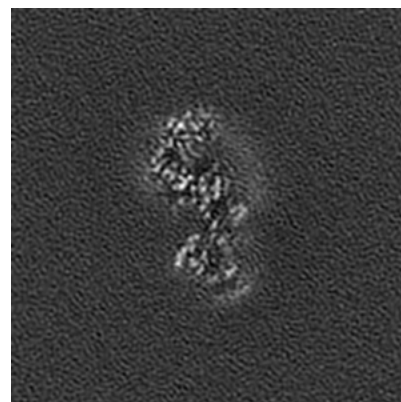
6.2.1 Primary map



X Index: 80



Y Index: 80

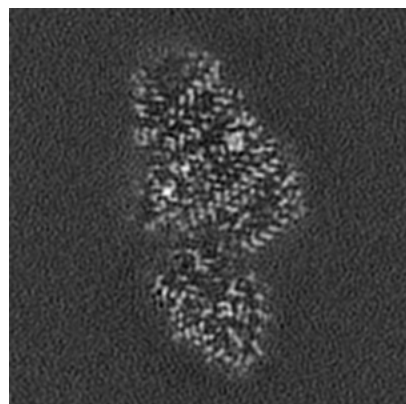


Z Index: 80

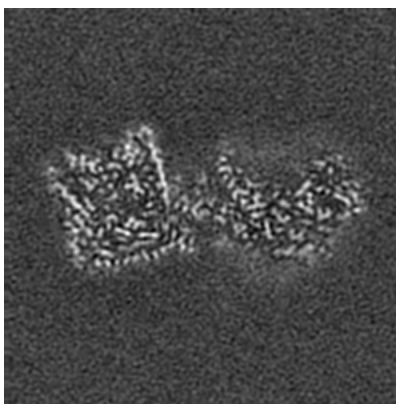
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

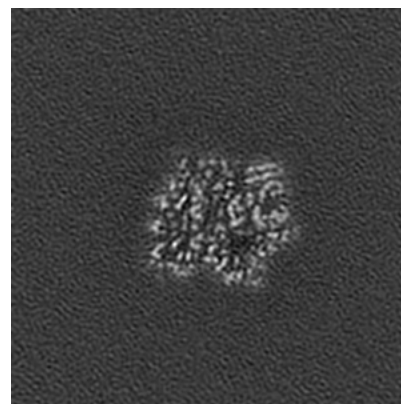
6.3.1 Primary map



X Index: 77



Y Index: 76

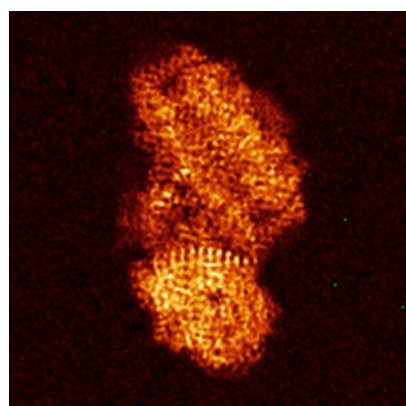


Z Index: 50

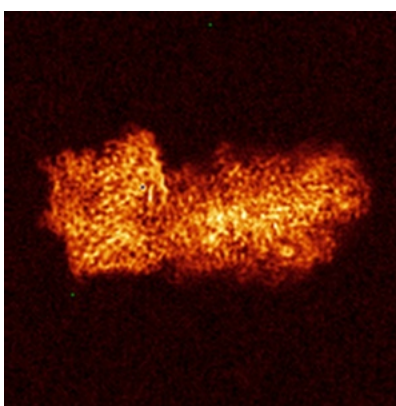
The images above show the largest variance slices of the map in three orthogonal directions.

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

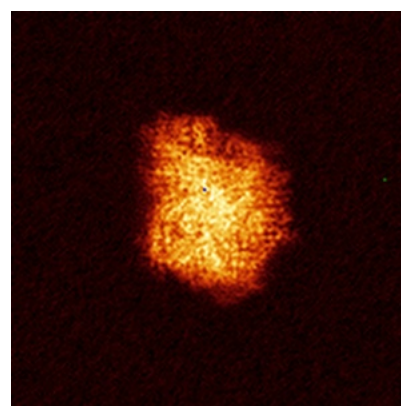
6.4.1 Primary map



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

This section was not generated.

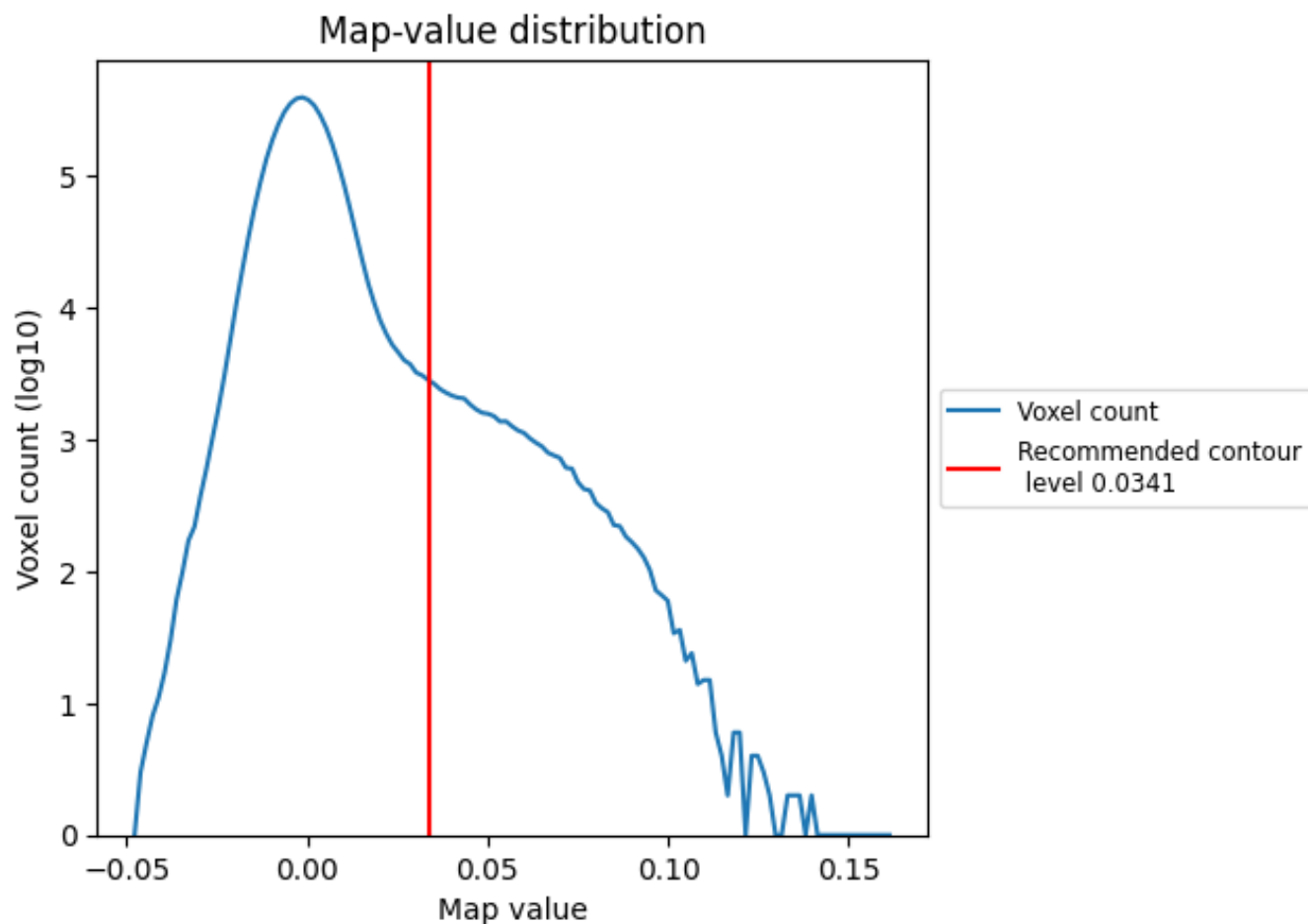
6.6 Mask visualisation

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

7 Map analysis [i](#)

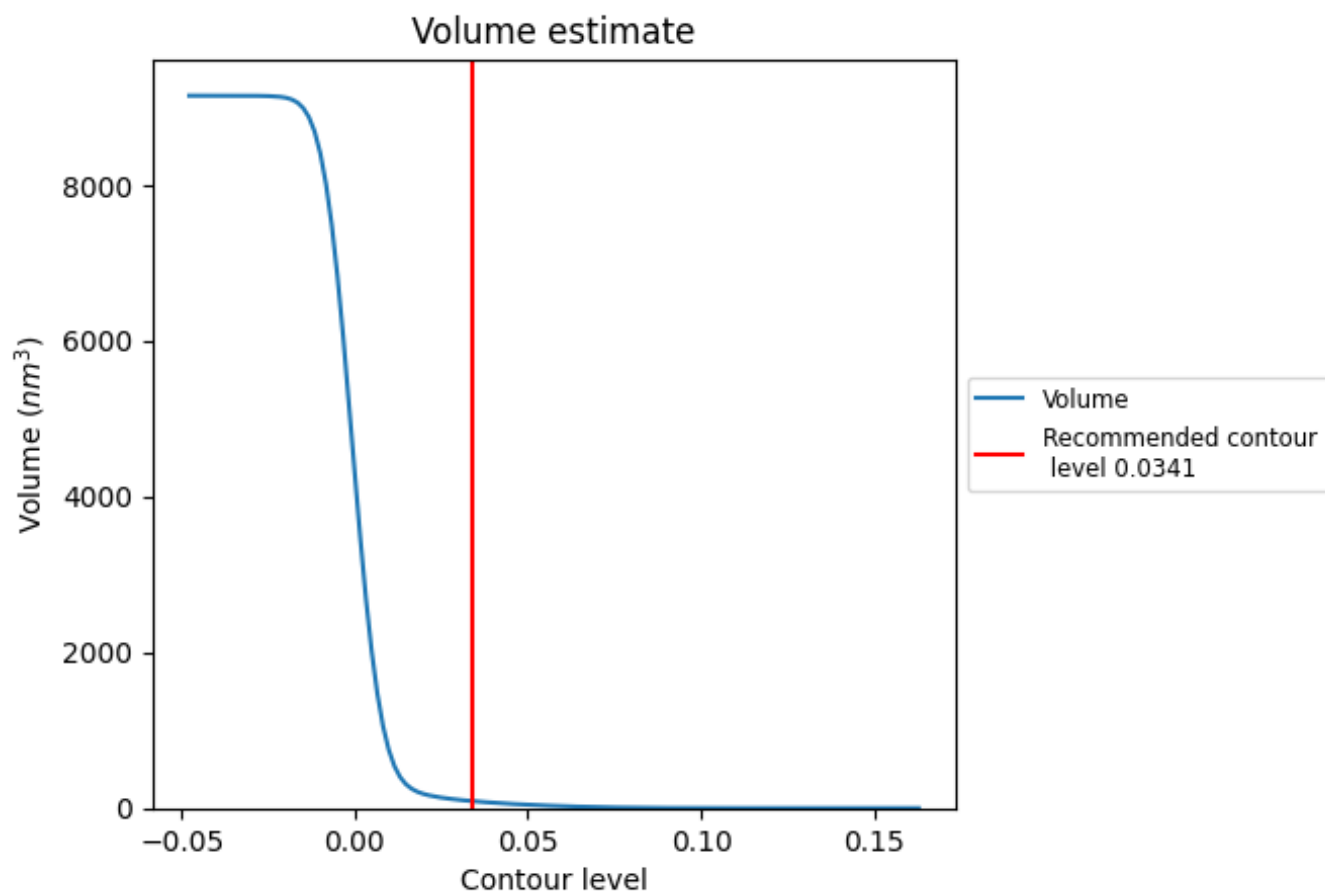
This section contains the results of statistical analysis of the map.

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.

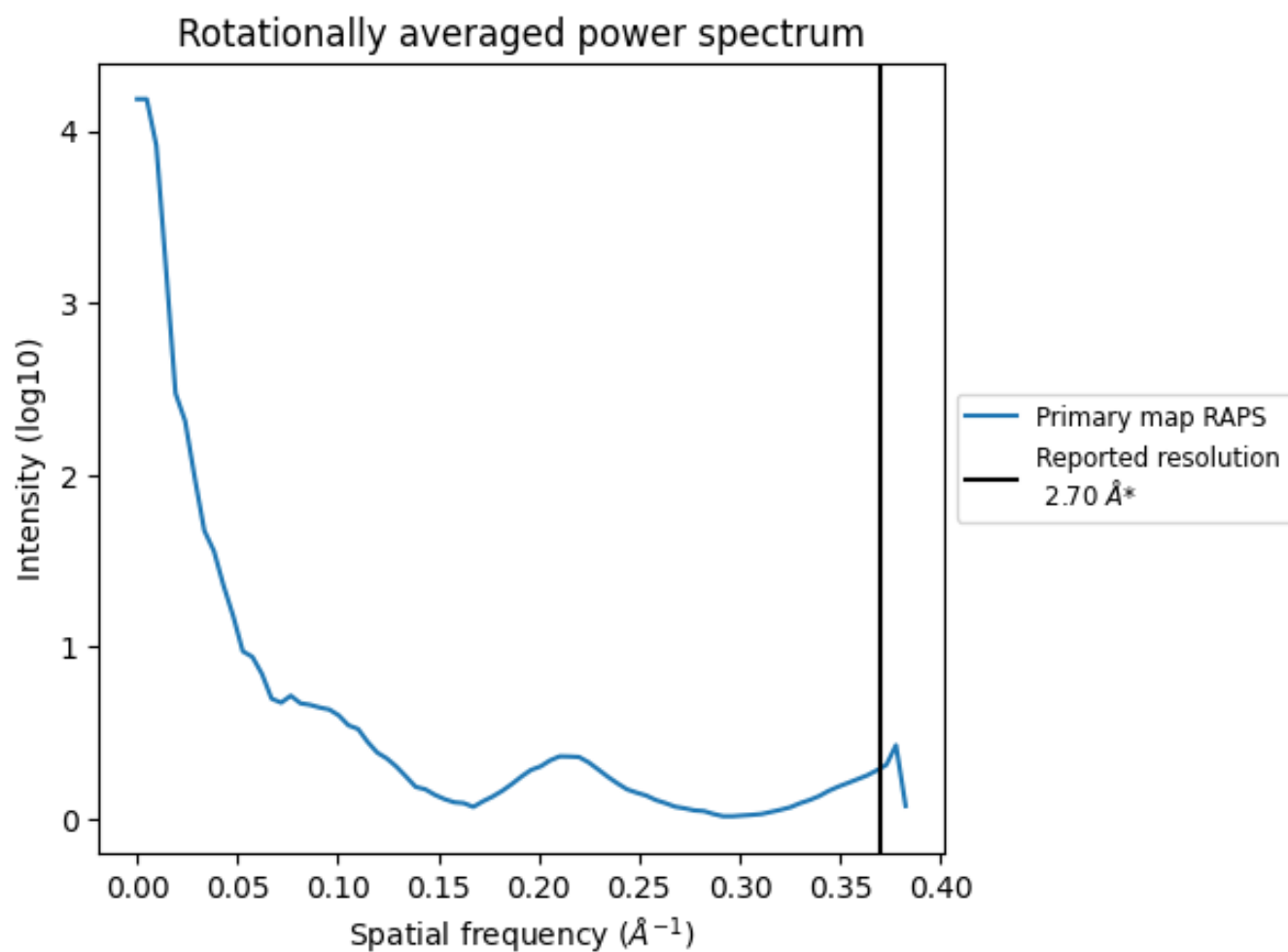
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm³; this corresponds to an approximate mass of 81 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

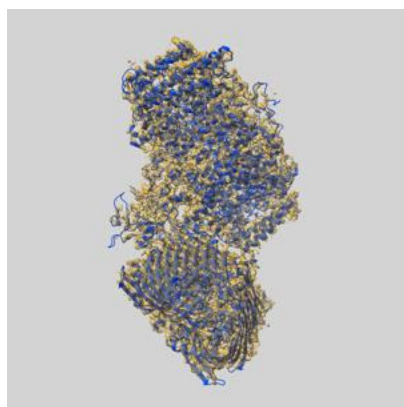
8 Fourier-Shell correlation ⓘ

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

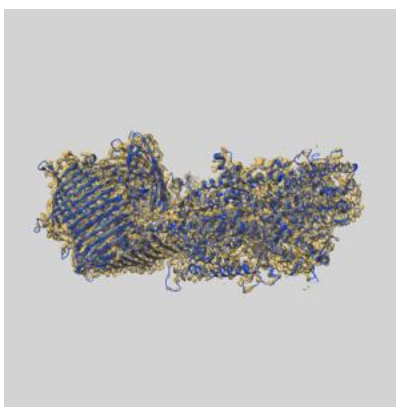
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30069 and PDB model 6M32. Per-residue inclusion information can be found in section [3](#) on page [13](#).

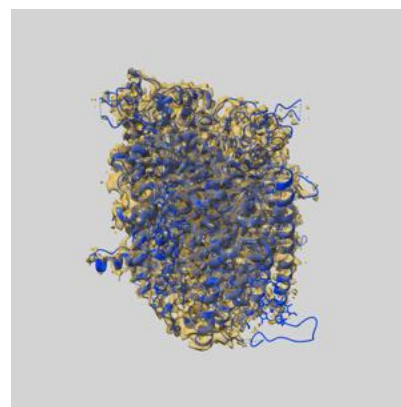
9.1 Map-model overlay [i](#)



X



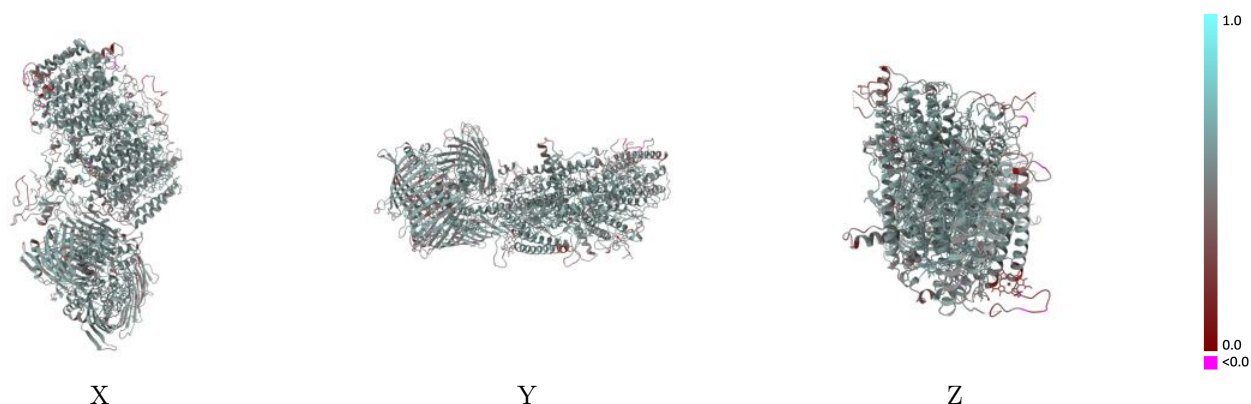
Y



Z

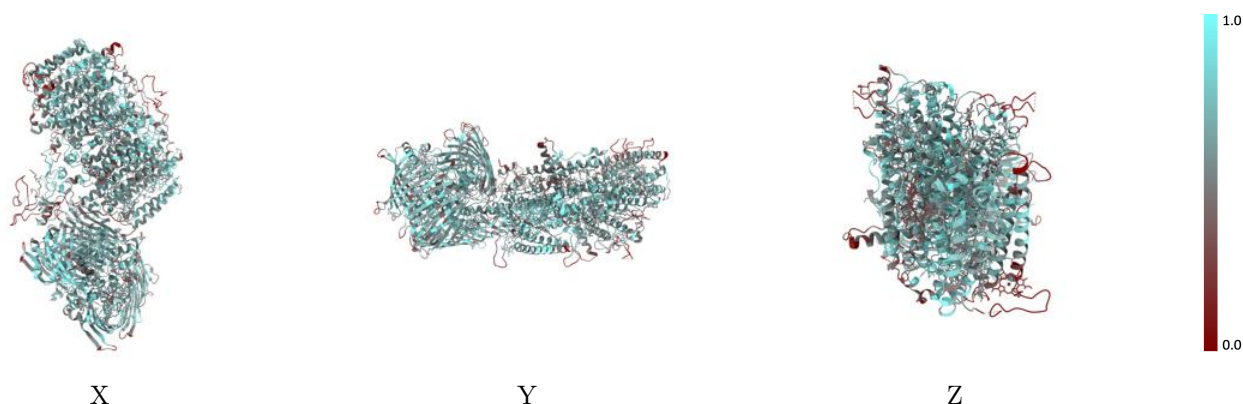
The images above show the 3D surface view of the map at the recommended contour level 0.0341 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



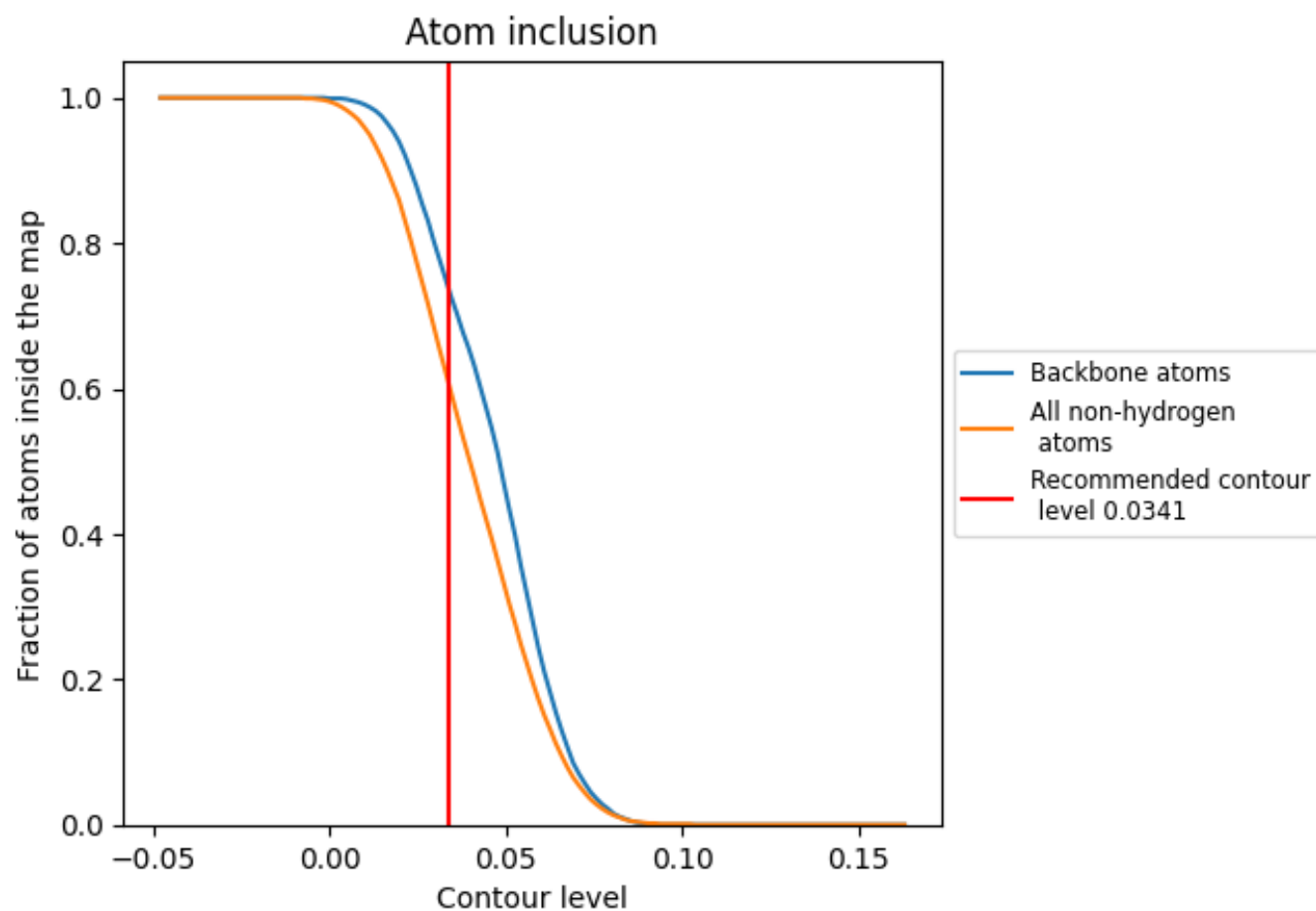
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0341).

9.4 Atom inclusion ⓘ



At the recommended contour level, 73% of all backbone atoms, 60% 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 (0.0341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6030	0.5250
A	0.6030	0.5350
B	0.5750	0.4900
D	0.3100	0.4350
E	0.6450	0.5350
F	0.6390	0.5260
G	0.6610	0.5420
a	0.5710	0.5150

1.0

0.0

<0.0