



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 08:55 AM UTC

PDB ID : 8HFQ / pdb_00008hfq
EMDB ID : EMD-34724
Title : Cryo-EM structure of CpcL-PBS from cyanobacterium Synechocystis sp. PCC 6803
Authors : Zheng, L.; Zhang, Z.; Wang, H.; Zheng, Z.; Gao, N.; Zhao, J.
Deposited on : 2022-11-11
Resolution : 2.64 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:

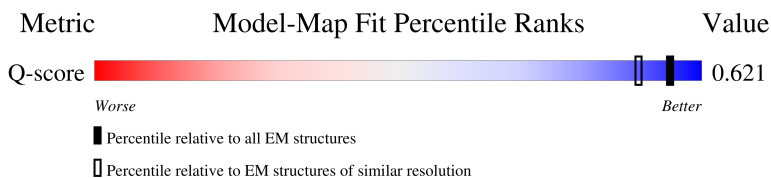
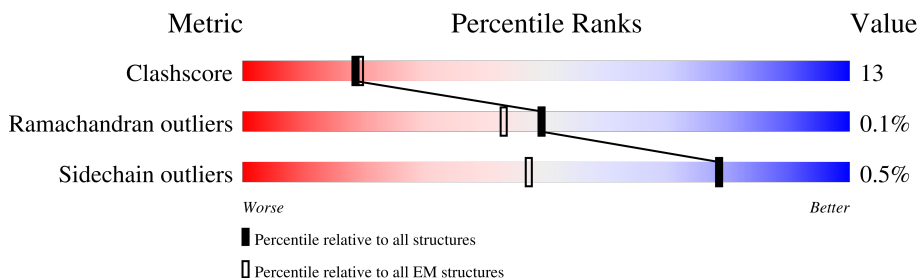
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.64 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	8968 (2.14 - 3.14)

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	A	162	80% 19% .
1	C	162	86% 14%
1	E	162	84% 16%
1	G	162	83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	I	162		82% 18%
1	K	162		83% 17%
1	M	162		78% 22%
1	O	162		82% 18%
1	Q	162		80% 20%
1	S	162		82% 18%
1	U	162		83% 17%
1	W	162		85% 15%
1	Y	162		89% 11%
1	a	162		83% 17%
1	c	162		80% 20%
1	e	162		83% 17%
1	g	162		88% 12%
1	i	162		81% 19%
2	B	172		78% 21% .
2	D	172		81% 19%
2	F	172		88% 12%
2	H	172		83% 17% .
2	J	172		84% 16%
2	L	172		83% 17%
2	N	172		78% 20% .
2	P	172		84% 16%
2	R	172		82% 17% .
2	T	172		78% 21% .
2	V	172		83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	X	172	 80% 20%
2	Z	172	 77% 22% .
2	b	172	 81% 18% .
2	d	172	 84% 16% .
2	f	172	 73% 27%
2	h	172	 78% 21% .
2	j	172	 77% 20% .
3	k	291	 72% 26% ..
4	l	273	 74% 25% .
5	m	413	 12% 7% 80%
6	n	249	 54% 23% . 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CYC	N	201	-	-	X	-
7	CYC	R	201	-	-	X	-
7	CYC	h	201	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 54193 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 C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	C	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	E	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	G	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	I	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	K	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	M	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	O	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	Q	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	S	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	U	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	W	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	Y	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	a	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	c	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	e	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	g	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		

- Molecule 2 is a protein called C-phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	D	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	F	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	H	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	J	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	L	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	N	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	P	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	R	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	T	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	V	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	X	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	Z	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	b	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	d	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	f	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	h	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	j	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		

- Molecule 3 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	k	289	Total	C	N	O	S	0	0
			2282	1438	408	433	3		

- Molecule 4 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	l	272	Total	C	N	O	S	0	0
			2164	1341	404	416	3		

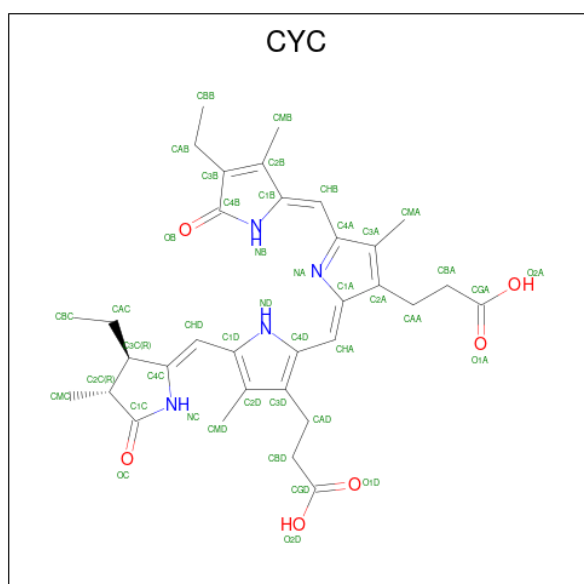
- Molecule 5 is a protein called Ferredoxin–NADP reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	m	81	Total	C	N	O	S	0	0
			626	387	115	120	4		

- Molecule 6 is a protein called Photosystem I-associated linker protein CpcL.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	n	197	Total	C	N	O	S	0	0
			1619	1019	295	300	5		

- Molecule 7 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 43	C 33	N 4	O 6	0
7	B	1	Total 43	C 33	N 4	O 6	0
7	B	1	Total 43	C 33	N 4	O 6	0
7	C	1	Total 43	C 33	N 4	O 6	0
7	D	1	Total 43	C 33	N 4	O 6	0
7	D	1	Total 43	C 33	N 4	O 6	0
7	E	1	Total 43	C 33	N 4	O 6	0
7	F	1	Total 43	C 33	N 4	O 6	0
7	F	1	Total 43	C 33	N 4	O 6	0
7	G	1	Total 43	C 33	N 4	O 6	0
7	H	1	Total 43	C 33	N 4	O 6	0
7	H	1	Total 43	C 33	N 4	O 6	0
7	I	1	Total 43	C 33	N 4	O 6	0
7	J	1	Total 43	C 33	N 4	O 6	0
7	J	1	Total 43	C 33	N 4	O 6	0
7	K	1	Total 43	C 33	N 4	O 6	0
7	L	1	Total 43	C 33	N 4	O 6	0
7	L	1	Total 43	C 33	N 4	O 6	0
7	M	1	Total 43	C 33	N 4	O 6	0
7	N	1	Total 43	C 33	N 4	O 6	0
7	N	1	Total 43	C 33	N 4	O 6	0
7	O	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
7	P	1	Total 43	C 33	N 4	O 6	0
7	P	1	Total 43	C 33	N 4	O 6	0
7	Q	1	Total 43	C 33	N 4	O 6	0
7	R	1	Total 43	C 33	N 4	O 6	0
7	R	1	Total 43	C 33	N 4	O 6	0
7	S	1	Total 43	C 33	N 4	O 6	0
7	T	1	Total 43	C 33	N 4	O 6	0
7	T	1	Total 43	C 33	N 4	O 6	0
7	U	1	Total 43	C 33	N 4	O 6	0
7	V	1	Total 43	C 33	N 4	O 6	0
7	V	1	Total 43	C 33	N 4	O 6	0
7	W	1	Total 43	C 33	N 4	O 6	0
7	X	1	Total 43	C 33	N 4	O 6	0
7	X	1	Total 43	C 33	N 4	O 6	0
7	Y	1	Total 43	C 33	N 4	O 6	0
7	Z	1	Total 43	C 33	N 4	O 6	0
7	Z	1	Total 43	C 33	N 4	O 6	0
7	a	1	Total 43	C 33	N 4	O 6	0
7	b	1	Total 43	C 33	N 4	O 6	0
7	b	1	Total 43	C 33	N 4	O 6	0
7	c	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
7	d	1	Total 43	C 33	N 4	O 6	0
7	d	1	Total 43	C 33	N 4	O 6	0
7	e	1	Total 43	C 33	N 4	O 6	0
7	f	1	Total 43	C 33	N 4	O 6	0
7	f	1	Total 43	C 33	N 4	O 6	0
7	g	1	Total 43	C 33	N 4	O 6	0
7	h	1	Total 43	C 33	N 4	O 6	0
7	h	1	Total 43	C 33	N 4	O 6	0
7	i	1	Total 43	C 33	N 4	O 6	0
7	j	1	Total 43	C 33	N 4	O 6	0
7	j	1	Total 43	C 33	N 4	O 6	0

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: C-phycocyanin alpha subunit

Chain A: 



- Molecule 1: C-phycocyanin alpha subunit

Chain C: 



- Molecule 1: C-phycocyanin alpha subunit

Chain E: 



- Molecule 1: C-phycocyanin alpha subunit

Chain G: 



- Molecule 1: C-phycocyanin alpha subunit

Chain I: 



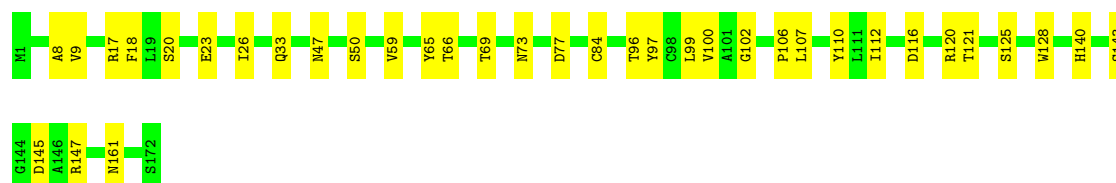
- Molecule 1: C-phycocyanin alpha subunit

Chain K:  83% 17%



- Molecule 1: C-phycocyanin alpha subunit

Chain M:  78% 22%



- Molecule 1: C-phycocyanin alpha subunit

Chain O:  82% 18%



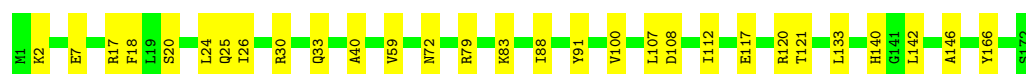
- Molecule 1: C-phycocyanin alpha subunit

Chain Q:  80% 20%



- Molecule 1: C-phycocyanin alpha subunit

Chain S:  82% 18%



- Molecule 1: C-phycocyanin alpha subunit

Chain U:  83% 17%



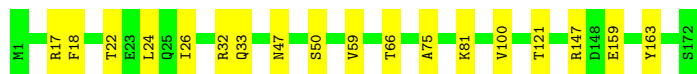
- Molecule 1: C-phycocyanin alpha subunit

Chain W:  85% 15%



- Molecule 1: C-phycoerythrin alpha subunit

Chain Y:  89% 11%



- Molecule 1: C-phycoerythrin alpha subunit

Chain a:  83% 17%



- Molecule 1: C-phycoerythrin alpha subunit

Chain c:  80% 20%



- Molecule 1: C-phycoerythrin alpha subunit

Chain e:  83% 17%



- Molecule 1: C-phycoerythrin alpha subunit

Chain g:  88% 12%



- Molecule 1: C-phycoerythrin alpha subunit

Chain i:  81% 19%



- Molecule 2: C-phycoerythrin beta subunit

Chain B:  78% 21%





• Molecule 2: C-phycoerythrin beta subunit

Chain D: 81% 19%



• Molecule 2: C-phycoerythrin beta subunit

Chain F: 88% 12%



• Molecule 2: C-phycoerythrin beta subunit

Chain H: 83% 17%



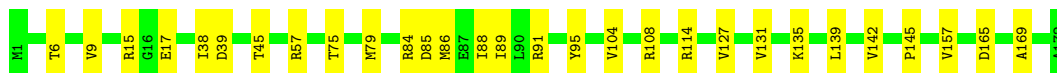
• Molecule 2: C-phycoerythrin beta subunit

Chain J: 84% 16%



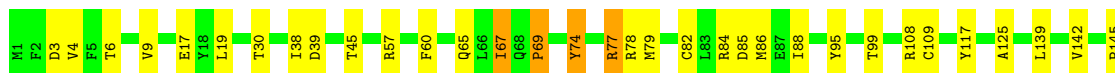
• Molecule 2: C-phycoerythrin beta subunit

Chain L: 83% 17%



• Molecule 2: C-phycoerythrin beta subunit

Chain N: 78% 20%





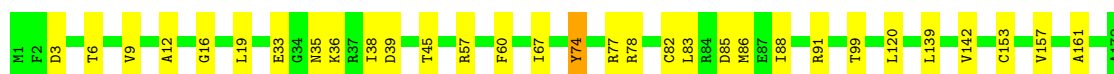
- Molecule 2: C-phycoerythrin beta subunit

Chain P: 84% 16%



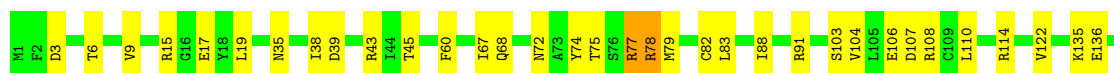
- Molecule 2: C-phycoerythrin beta subunit

Chain R: 82% 17% .



- Molecule 2: C-phycoerythrin beta subunit

Chain T: 78% 21% .



- Molecule 2: C-phycoerythrin beta subunit

Chain V: 83% 17%



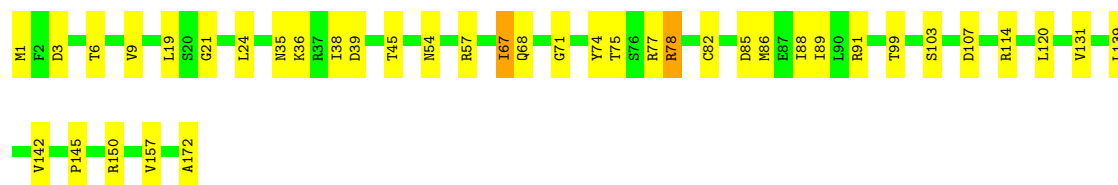
- Molecule 2: C-phycoerythrin beta subunit

Chain X: 80% 20%



- Molecule 2: C-phycoerythrin beta subunit

Chain Z: 77% 22% .



- Molecule 2: C-phycocyanin beta subunit

Chain b: 81% 18% .



- Molecule 2: C-phycocyanin beta subunit

Chain d: 84% 16% .



- Molecule 2: C-phycocyanin beta subunit

Chain f: 73% 27% .



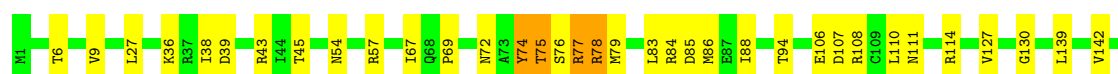
- Molecule 2: C-phycocyanin beta subunit

Chain h: 78% 21% .

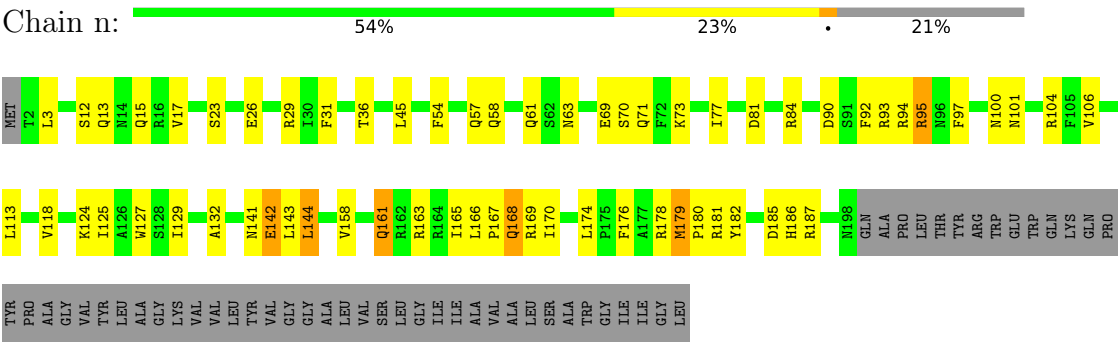


- Molecule 2: C-phycocyanin beta subunit

Chain j: 77% 20% .







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124441	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0164	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CYC

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	A	0.31	0/1261	0.57	0/1709
1	C	0.20	0/1261	0.45	0/1709
1	E	0.20	0/1261	0.48	0/1709
1	G	0.21	0/1261	0.46	0/1709
1	I	0.22	0/1261	0.49	0/1709
1	K	0.22	0/1261	0.45	0/1709
1	M	0.22	0/1261	0.49	0/1709
1	O	0.20	0/1261	0.49	0/1709
1	Q	0.23	0/1261	0.50	0/1709
1	S	0.22	0/1261	0.47	0/1709
1	U	0.26	0/1261	0.53	0/1709
1	W	0.21	0/1261	0.45	0/1709
1	Y	0.20	0/1261	0.42	0/1709
1	a	0.20	0/1261	0.45	0/1709
1	c	0.23	0/1261	0.51	0/1709
1	e	0.24	0/1261	0.52	0/1709
1	g	0.21	0/1261	0.49	0/1709
1	i	0.22	0/1261	0.50	0/1709
2	B	0.30	0/1284	0.64	3/1739 (0.2%)
2	D	0.27	0/1284	0.54	0/1739
2	F	0.26	0/1284	0.51	1/1739 (0.1%)
2	H	0.26	0/1284	0.53	1/1739 (0.1%)
2	J	0.27	0/1284	0.52	2/1739 (0.1%)
2	L	0.28	0/1284	0.56	1/1739 (0.1%)
2	N	0.32	0/1284	0.56	1/1739 (0.1%)
2	P	0.31	0/1284	0.55	0/1739
2	R	0.32	0/1284	0.56	1/1739 (0.1%)
2	T	0.36	0/1284	0.60	2/1739 (0.1%)
2	V	0.29	0/1284	0.58	2/1739 (0.1%)
2	X	0.31	0/1284	0.52	0/1739
2	Z	0.36	0/1284	0.56	1/1739 (0.1%)
2	b	0.30	0/1284	0.58	1/1739 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	d	0.34	0/1284	0.65	1/1739 (0.1%)
2	f	0.33	0/1284	0.59	2/1739 (0.1%)
2	h	0.31	0/1284	0.54	1/1739 (0.1%)
2	j	0.33	0/1284	0.57	1/1739 (0.1%)
3	k	0.30	0/2327	0.63	2/3149 (0.1%)
4	l	0.25	0/2201	0.54	3/2972 (0.1%)
5	m	0.34	0/635	0.64	0/854
6	n	0.35	0/1651	0.72	4/2230 (0.2%)
All	All	0.27	0/52624	0.54	30/71269 (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
1	U	0	1
2	N	0	1
2	T	0	2
2	Z	0	2
2	j	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	k	183	GLU	N-CA-C	-8.41	95.64	108.67
6	n	179	MET	CA-C-N	7.64	127.80	120.31
6	n	179	MET	C-N-CA	7.64	127.80	120.31
4	l	160	GLN	N-CA-C	7.08	120.48	110.50
2	B	74	TYR	N-CA-CB	6.89	118.07	110.35

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	77	ARG	Sidechain
2	T	77	ARG	Sidechain
2	T	78	ARG	Sidechain
1	U	32	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	Z	77	ARG	Sidechain

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	A	1240	0	1206	27	0
1	C	1240	0	1206	23	0
1	E	1240	0	1206	23	0
1	G	1240	0	1206	36	0
1	I	1240	0	1206	23	0
1	K	1240	0	1207	32	0
1	M	1240	0	1207	34	0
1	O	1240	0	1206	23	0
1	Q	1240	0	1206	36	0
1	S	1240	0	1206	23	0
1	U	1240	0	1206	33	0
1	W	1240	0	1206	20	0
1	Y	1240	0	1206	15	0
1	a	1240	0	1207	24	0
1	c	1240	0	1206	30	0
1	e	1240	0	1206	29	0
1	g	1240	0	1206	21	0
1	i	1240	0	1207	29	0
2	B	1270	0	1262	36	0
2	D	1270	0	1262	36	0
2	F	1270	0	1263	30	0
2	H	1270	0	1261	35	0
2	J	1270	0	1262	33	0
2	L	1270	0	1262	33	0
2	N	1270	0	1262	45	0
2	P	1270	0	1263	34	0
2	R	1270	0	1262	32	0
2	T	1270	0	1263	30	0
2	V	1270	0	1262	31	0
2	X	1270	0	1263	40	0
2	Z	1270	0	1262	32	0
2	b	1270	0	1262	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	1270	0	1262	22	0
2	f	1270	0	1263	47	0
2	h	1270	0	1262	34	0
2	j	1270	0	1262	43	0
3	k	2282	0	2261	93	0
4	l	2164	0	2118	75	0
5	m	626	0	639	58	0
6	n	1619	0	1590	65	0
7	A	43	0	37	7	0
7	B	86	0	74	33	0
7	C	43	0	37	7	0
7	D	86	0	75	35	0
7	E	43	0	37	9	0
7	F	86	0	76	35	0
7	G	43	0	37	14	0
7	H	86	0	75	31	0
7	I	43	0	37	4	0
7	J	86	0	75	30	0
7	K	43	0	38	14	0
7	L	86	0	74	30	0
7	M	43	0	38	12	0
7	N	86	0	75	41	0
7	O	43	0	37	8	0
7	P	86	0	76	30	0
7	Q	43	0	37	10	0
7	R	86	0	75	32	0
7	S	43	0	37	7	0
7	T	86	0	76	24	0
7	U	43	0	37	5	0
7	V	86	0	75	27	0
7	W	43	0	37	14	0
7	X	86	0	76	31	0
7	Y	43	0	37	4	0
7	Z	86	0	75	35	0
7	a	43	0	38	12	0
7	b	86	0	75	22	0
7	c	43	0	37	11	0
7	d	86	0	75	16	0
7	e	43	0	37	7	0
7	f	86	0	76	26	0
7	g	43	0	37	9	0
7	h	86	0	75	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	i	43	0	38	13	0
7	j	86	0	75	32	0
All	All	54193	0	53063	1391	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1391 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:M:84:CYS:SG	7:M:201:CYC:HAC2	1.21	1.70
2:F:82:CYS:SG	7:F:201:CYC:HAC2	1.27	1.68
1:i:84:CYS:SG	7:i:201:CYC:HAC2	1.13	1.67
1:K:84:CYS:SG	7:K:201:CYC:HAC2	1.14	1.65
2:f:82:CYS:SG	7:f:201:CYC:HAC2	1.35	1.62

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	A	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	C	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	E	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	G	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	I	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	K	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	M	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	O	160/162 (99%)	159 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	S	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	U	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	W	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	Y	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	a	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	c	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	e	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	g	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	i	160/162 (99%)	160 (100%)	0	0	100	100
2	B	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	D	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	F	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	H	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	J	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	L	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	N	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	31
2	P	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	R	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	T	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	31
2	V	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
2	X	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	Z	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	31
2	b	170/172 (99%)	166 (98%)	3 (2%)	1 (1%)	21	31
2	d	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	f	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
2	h	170/172 (99%)	167 (98%)	2 (1%)	1 (1%)	21	31
2	j	170/172 (99%)	163 (96%)	5 (3%)	2 (1%)	10	15
3	k	287/291 (99%)	279 (97%)	8 (3%)	0	100	100
4	l	270/273 (99%)	264 (98%)	6 (2%)	0	100	100
5	m	79/413 (19%)	76 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	n	195/249 (78%)	187 (96%)	8 (4%)	0	100	100
All	All	6771/7238 (94%)	6652 (98%)	112 (2%)	7 (0%)	49	64

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	j	75	THR
2	N	69	PRO
2	Z	75	THR
2	b	75	THR
2	h	75	THR

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	A	126/126 (100%)	124 (98%)	2 (2%)	55	73
1	C	126/126 (100%)	126 (100%)	0	100	100
1	E	126/126 (100%)	126 (100%)	0	100	100
1	G	126/126 (100%)	126 (100%)	0	100	100
1	I	126/126 (100%)	126 (100%)	0	100	100
1	K	126/126 (100%)	126 (100%)	0	100	100
1	M	126/126 (100%)	126 (100%)	0	100	100
1	O	126/126 (100%)	126 (100%)	0	100	100
1	Q	126/126 (100%)	126 (100%)	0	100	100
1	S	126/126 (100%)	126 (100%)	0	100	100
1	U	126/126 (100%)	126 (100%)	0	100	100
1	W	126/126 (100%)	126 (100%)	0	100	100
1	Y	126/126 (100%)	126 (100%)	0	100	100
1	a	126/126 (100%)	126 (100%)	0	100	100
1	c	126/126 (100%)	126 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	126/126 (100%)	126 (100%)	0	100	100
1	g	126/126 (100%)	126 (100%)	0	100	100
1	i	126/126 (100%)	126 (100%)	0	100	100
2	B	128/128 (100%)	128 (100%)	0	100	100
2	D	128/128 (100%)	128 (100%)	0	100	100
2	F	128/128 (100%)	128 (100%)	0	100	100
2	H	128/128 (100%)	128 (100%)	0	100	100
2	J	128/128 (100%)	128 (100%)	0	100	100
2	L	128/128 (100%)	128 (100%)	0	100	100
2	N	128/128 (100%)	126 (98%)	2 (2%)	55	73
2	P	128/128 (100%)	128 (100%)	0	100	100
2	R	128/128 (100%)	128 (100%)	0	100	100
2	T	128/128 (100%)	126 (98%)	2 (2%)	55	73
2	V	128/128 (100%)	128 (100%)	0	100	100
2	X	128/128 (100%)	127 (99%)	1 (1%)	73	84
2	Z	128/128 (100%)	126 (98%)	2 (2%)	55	73
2	b	128/128 (100%)	127 (99%)	1 (1%)	73	84
2	d	128/128 (100%)	127 (99%)	1 (1%)	73	84
2	f	128/128 (100%)	128 (100%)	0	100	100
2	h	128/128 (100%)	126 (98%)	2 (2%)	55	73
2	j	128/128 (100%)	126 (98%)	2 (2%)	55	73
3	k	244/246 (99%)	242 (99%)	2 (1%)	73	84
4	l	229/230 (100%)	229 (100%)	0	100	100
5	m	71/351 (20%)	70 (99%)	1 (1%)	59	75
6	n	173/211 (82%)	167 (96%)	6 (4%)	32	51
All	All	5289/5610 (94%)	5265 (100%)	24 (0%)	78	89

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	j	72	ASN
5	m	38	ASP
3	k	277	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	n	93	ARG
2	X	67	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	70	GLN
3	k	276	ASN
1	e	161	ASN
1	i	33	GLN
6	n	71	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](#)

54 ligands are modelled in this entry.

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	$\# Z > 2$
7	CYC	A	201	1	46,46,46	2.28	17 (36%)	63,67,67	3.28	28 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CYC	B	202	-	46,46,46	2.84	19 (41%)	63,67,67	2.57	20 (31%)
7	CYC	T	201	-	46,46,46	2.53	14 (30%)	63,67,67	2.32	25 (39%)
7	CYC	d	201	-	46,46,46	2.24	13 (28%)	63,67,67	3.31	26 (41%)
7	CYC	d	202	-	46,46,46	2.85	19 (41%)	63,67,67	2.57	21 (33%)
7	CYC	N	201	2	46,46,46	2.62	14 (30%)	63,67,67	2.60	20 (31%)
7	CYC	a	201	-	46,46,46	2.27	18 (39%)	63,67,67	3.27	28 (44%)
7	CYC	j	202	-	46,46,46	2.85	18 (39%)	63,67,67	2.57	21 (33%)
7	CYC	R	202	-	46,46,46	2.85	19 (41%)	63,67,67	2.57	20 (31%)
7	CYC	O	201	1	46,46,46	2.28	18 (39%)	63,67,67	3.28	26 (41%)
7	CYC	Y	201	1	46,46,46	2.27	17 (36%)	63,67,67	3.28	28 (44%)
7	CYC	L	201	2	46,46,46	2.61	14 (30%)	63,67,67	2.27	22 (34%)
7	CYC	J	202	-	46,46,46	2.84	18 (39%)	63,67,67	2.57	21 (33%)
7	CYC	h	201	-	46,46,46	2.60	14 (30%)	63,67,67	2.29	20 (31%)
7	CYC	H	201	2	46,46,46	2.58	13 (28%)	63,67,67	2.30	23 (36%)
7	CYC	D	201	2	46,46,46	3.17	19 (41%)	63,67,67	2.14	16 (25%)
7	CYC	c	201	1	46,46,46	2.27	18 (39%)	63,67,67	3.28	26 (41%)
7	CYC	h	202	-	46,46,46	2.83	19 (41%)	63,67,67	2.57	20 (31%)
7	CYC	C	201	1	46,46,46	2.26	17 (36%)	63,67,67	3.29	28 (44%)
7	CYC	F	201	-	46,46,46	3.10	18 (39%)	63,67,67	2.21	16 (25%)
7	CYC	E	201	1	46,46,46	2.27	18 (39%)	63,67,67	3.30	28 (44%)
7	CYC	H	202	-	46,46,46	2.84	19 (41%)	63,67,67	2.57	21 (33%)
7	CYC	F	202	-	46,46,46	2.84	19 (41%)	63,67,67	2.57	21 (33%)
7	CYC	S	201	1	46,46,46	2.27	17 (36%)	63,67,67	3.29	27 (42%)
7	CYC	J	201	-	46,46,46	2.55	14 (30%)	63,67,67	2.28	24 (38%)
7	CYC	G	201	1	46,46,46	2.27	17 (36%)	63,67,67	3.28	28 (44%)
7	CYC	R	201	-	46,46,46	2.22	13 (28%)	63,67,67	3.34	27 (42%)
7	CYC	b	201	2	46,46,46	2.59	14 (30%)	63,67,67	2.31	23 (36%)
7	CYC	b	202	-	46,46,46	2.84	19 (41%)	63,67,67	2.57	20 (31%)
7	CYC	U	201	1	46,46,46	2.28	17 (36%)	63,67,67	3.29	28 (44%)
7	CYC	P	201	-	46,46,46	2.81	18 (39%)	63,67,67	2.30	18 (28%)
7	CYC	P	202	-	46,46,46	2.84	18 (39%)	63,67,67	2.57	21 (33%)
7	CYC	Z	201	2	46,46,46	2.23	13 (28%)	63,67,67	3.32	27 (42%)
7	CYC	W	201	1	46,46,46	2.28	18 (39%)	63,67,67	3.28	28 (44%)
7	CYC	Z	202	-	46,46,46	2.84	18 (39%)	63,67,67	2.57	21 (33%)
7	CYC	g	201	-	46,46,46	2.26	17 (36%)	63,67,67	3.27	28 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CYC	f	201	-	46,46,46	2.24	14 (30%)	63,67,67	3.33	27 (42%)
7	CYC	N	202	-	46,46,46	2.84	19 (41%)	63,67,67	2.56	20 (31%)
7	CYC	L	202	-	46,46,46	2.84	18 (39%)	63,67,67	2.56	20 (31%)
7	CYC	I	201	1	46,46,46	2.27	17 (36%)	63,67,67	3.27	27 (42%)
7	CYC	f	202	-	46,46,46	2.85	18 (39%)	63,67,67	2.57	20 (31%)
7	CYC	V	201	2	46,46,46	2.25	14 (30%)	63,67,67	3.34	27 (42%)
7	CYC	D	202	-	46,46,46	2.84	19 (41%)	63,67,67	2.57	21 (33%)
7	CYC	e	201	1	46,46,46	2.27	18 (39%)	63,67,67	3.28	28 (44%)
7	CYC	i	201	-	46,46,46	2.26	17 (36%)	63,67,67	3.27	29 (46%)
7	CYC	T	202	-	46,46,46	2.83	19 (41%)	63,67,67	2.57	20 (31%)
7	CYC	M	201	-	46,46,46	2.28	18 (39%)	63,67,67	3.26	27 (42%)
7	CYC	B	201	-	46,46,46	3.64	20 (43%)	63,67,67	2.31	16 (25%)
7	CYC	X	201	-	46,46,46	2.61	14 (30%)	63,67,67	2.62	22 (34%)
7	CYC	j	201	-	46,46,46	3.13	17 (36%)	63,67,67	2.35	18 (28%)
7	CYC	K	201	-	46,46,46	2.27	18 (39%)	63,67,67	3.29	28 (44%)
7	CYC	V	202	-	46,46,46	2.84	18 (39%)	63,67,67	2.57	20 (31%)
7	CYC	Q	201	1	46,46,46	2.27	17 (36%)	63,67,67	3.29	28 (44%)
7	CYC	X	202	-	46,46,46	2.84	19 (41%)	63,67,67	2.57	20 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CYC	A	201	1	-	9/26/74/74	0/4/4/4
7	CYC	B	202	-	-	9/26/74/74	0/4/4/4
7	CYC	T	201	-	-	11/26/74/74	0/4/4/4
7	CYC	d	201	-	-	9/26/74/74	0/4/4/4
7	CYC	d	202	-	-	9/26/74/74	0/4/4/4
7	CYC	N	201	2	-	11/26/74/74	0/4/4/4
7	CYC	a	201	-	-	9/26/74/74	0/4/4/4
7	CYC	j	202	-	-	9/26/74/74	0/4/4/4
7	CYC	R	202	-	-	9/26/74/74	0/4/4/4
7	CYC	O	201	1	-	9/26/74/74	0/4/4/4
7	CYC	Y	201	1	-	9/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CYC	L	201	2	-	11/26/74/74	0/4/4/4
7	CYC	J	202	-	-	9/26/74/74	0/4/4/4
7	CYC	h	201	-	-	10/26/74/74	0/4/4/4
7	CYC	H	201	2	-	10/26/74/74	0/4/4/4
7	CYC	D	201	2	-	9/26/74/74	0/4/4/4
7	CYC	c	201	1	-	9/26/74/74	0/4/4/4
7	CYC	h	202	-	-	9/26/74/74	0/4/4/4
7	CYC	C	201	1	-	9/26/74/74	0/4/4/4
7	CYC	F	201	-	-	10/26/74/74	0/4/4/4
7	CYC	E	201	1	-	9/26/74/74	0/4/4/4
7	CYC	H	202	-	-	9/26/74/74	0/4/4/4
7	CYC	F	202	-	-	9/26/74/74	0/4/4/4
7	CYC	S	201	1	-	9/26/74/74	0/4/4/4
7	CYC	J	201	-	-	8/26/74/74	0/4/4/4
7	CYC	G	201	1	-	9/26/74/74	0/4/4/4
7	CYC	R	201	-	-	9/26/74/74	0/4/4/4
7	CYC	b	201	2	-	10/26/74/74	0/4/4/4
7	CYC	b	202	-	-	9/26/74/74	0/4/4/4
7	CYC	U	201	1	-	9/26/74/74	0/4/4/4
7	CYC	P	201	-	-	9/26/74/74	0/4/4/4
7	CYC	P	202	-	-	9/26/74/74	0/4/4/4
7	CYC	Z	201	2	-	9/26/74/74	0/4/4/4
7	CYC	W	201	1	-	9/26/74/74	0/4/4/4
7	CYC	Z	202	-	-	9/26/74/74	0/4/4/4
7	CYC	g	201	-	-	9/26/74/74	0/4/4/4
7	CYC	f	201	-	-	9/26/74/74	0/4/4/4
7	CYC	N	202	-	-	9/26/74/74	0/4/4/4
7	CYC	L	202	-	-	9/26/74/74	0/4/4/4
7	CYC	I	201	1	-	9/26/74/74	0/4/4/4
7	CYC	f	202	-	-	9/26/74/74	0/4/4/4
7	CYC	V	201	2	-	9/26/74/74	0/4/4/4
7	CYC	D	202	-	-	9/26/74/74	0/4/4/4
7	CYC	e	201	1	-	9/26/74/74	0/4/4/4
7	CYC	i	201	-	-	9/26/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CYC	T	202	-	-	9/26/74/74	0/4/4/4
7	CYC	M	201	-	-	9/26/74/74	0/4/4/4
7	CYC	B	201	-	-	11/26/74/74	0/4/4/4
7	CYC	X	201	-	-	10/26/74/74	0/4/4/4
7	CYC	j	201	-	-	9/26/74/74	0/4/4/4
7	CYC	K	201	-	-	9/26/74/74	0/4/4/4
7	CYC	V	202	-	-	9/26/74/74	0/4/4/4
7	CYC	Q	201	1	-	9/26/74/74	0/4/4/4
7	CYC	X	202	-	-	9/26/74/74	0/4/4/4

The worst 5 of 919 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	201	CYC	C1C-NC	10.51	1.51	1.37
7	j	201	CYC	C3C-C4C	10.23	1.72	1.50
7	X	201	CYC	C1B-NB	9.33	1.53	1.37
7	B	201	CYC	C1B-NB	9.30	1.53	1.37
7	b	201	CYC	C1B-NB	9.27	1.53	1.37

The worst 5 of 1263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	201	CYC	C3B-C4B-NB	12.71	116.90	106.77
7	f	201	CYC	C3B-C4B-NB	12.67	116.87	106.77
7	V	201	CYC	C3B-C4B-NB	12.63	116.84	106.77
7	O	201	CYC	C3B-C4B-NB	12.62	116.83	106.77
7	U	201	CYC	C3B-C4B-NB	12.59	116.81	106.77

There are no chirality outliers.

5 of 498 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	201	CYC	NA-C4A-CHB-C1B
7	A	201	CYC	C3A-C4A-CHB-C1B
7	A	201	CYC	C4C-C3C-CAC-CBC
7	B	201	CYC	C2C-C3C-CAC-CBC
7	B	201	CYC	C4C-C3C-CAC-CBC

There are no ring outliers.

54 monomers are involved in 714 short contacts:

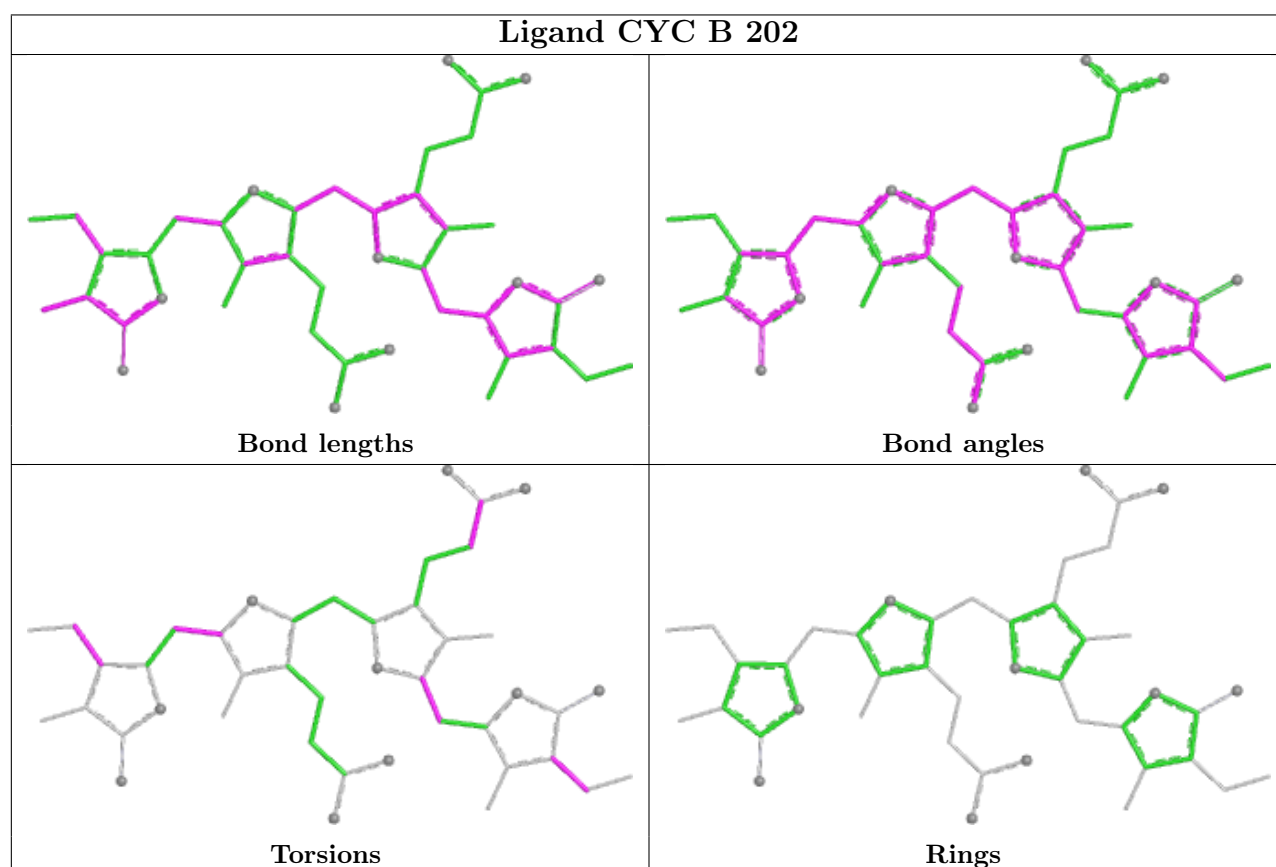
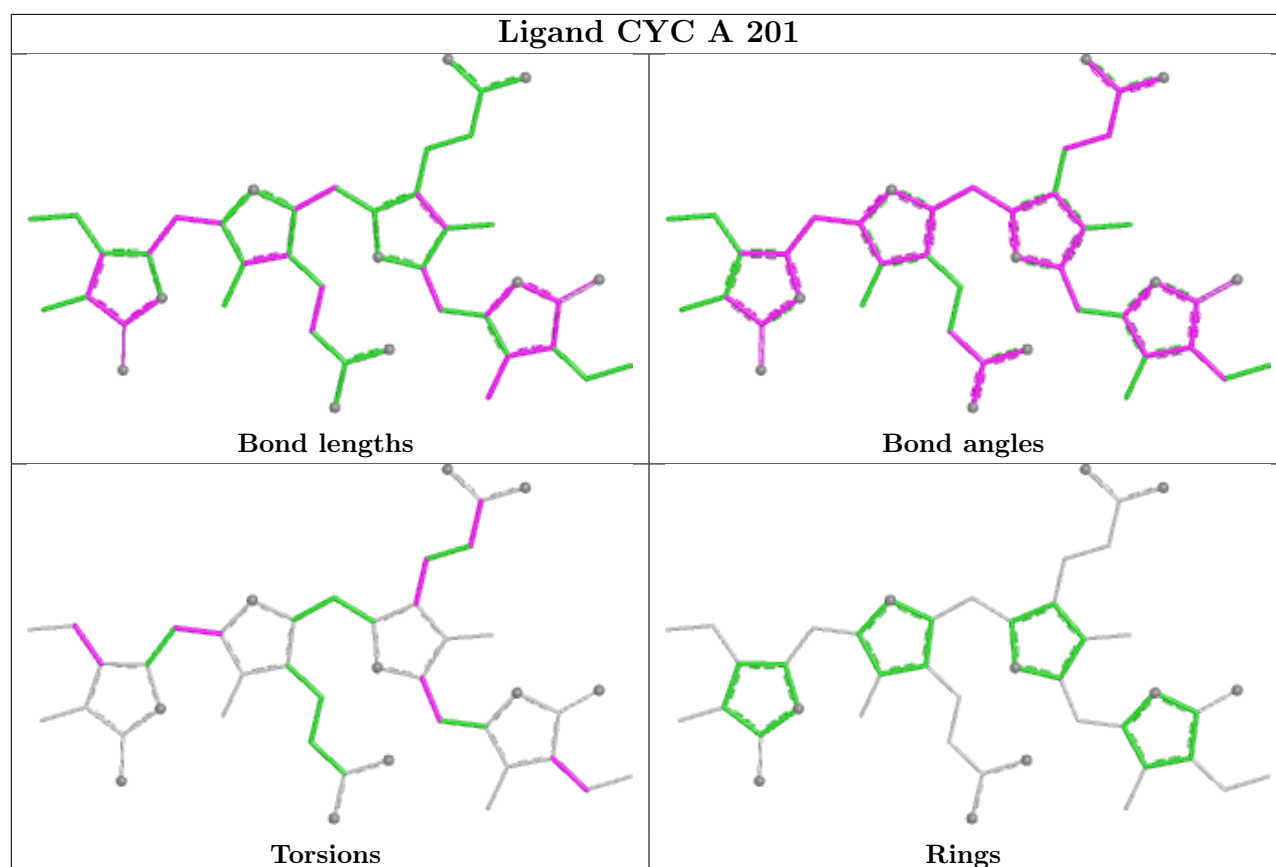
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	201	CYC	7	0
7	B	202	CYC	19	0
7	T	201	CYC	9	0
7	d	201	CYC	6	0
7	d	202	CYC	10	0
7	N	201	CYC	24	0
7	a	201	CYC	12	0
7	j	202	CYC	19	0
7	R	202	CYC	11	0
7	O	201	CYC	8	0
7	Y	201	CYC	4	0
7	L	201	CYC	12	0
7	J	202	CYC	13	0
7	h	201	CYC	24	0
7	H	201	CYC	11	0
7	D	201	CYC	18	0
7	c	201	CYC	11	0
7	h	202	CYC	13	0
7	C	201	CYC	7	0
7	F	201	CYC	19	0
7	E	201	CYC	9	0
7	H	202	CYC	20	0
7	F	202	CYC	16	0
7	S	201	CYC	7	0
7	J	201	CYC	17	0
7	G	201	CYC	14	0
7	R	201	CYC	21	0
7	b	201	CYC	11	0
7	b	202	CYC	11	0
7	U	201	CYC	5	0
7	P	201	CYC	19	0
7	P	202	CYC	11	0
7	Z	201	CYC	16	0
7	W	201	CYC	14	0
7	Z	202	CYC	19	0
7	g	201	CYC	9	0
7	f	201	CYC	13	0
7	N	202	CYC	17	0
7	L	202	CYC	18	0
7	I	201	CYC	4	0
7	f	202	CYC	13	0
7	V	201	CYC	9	0

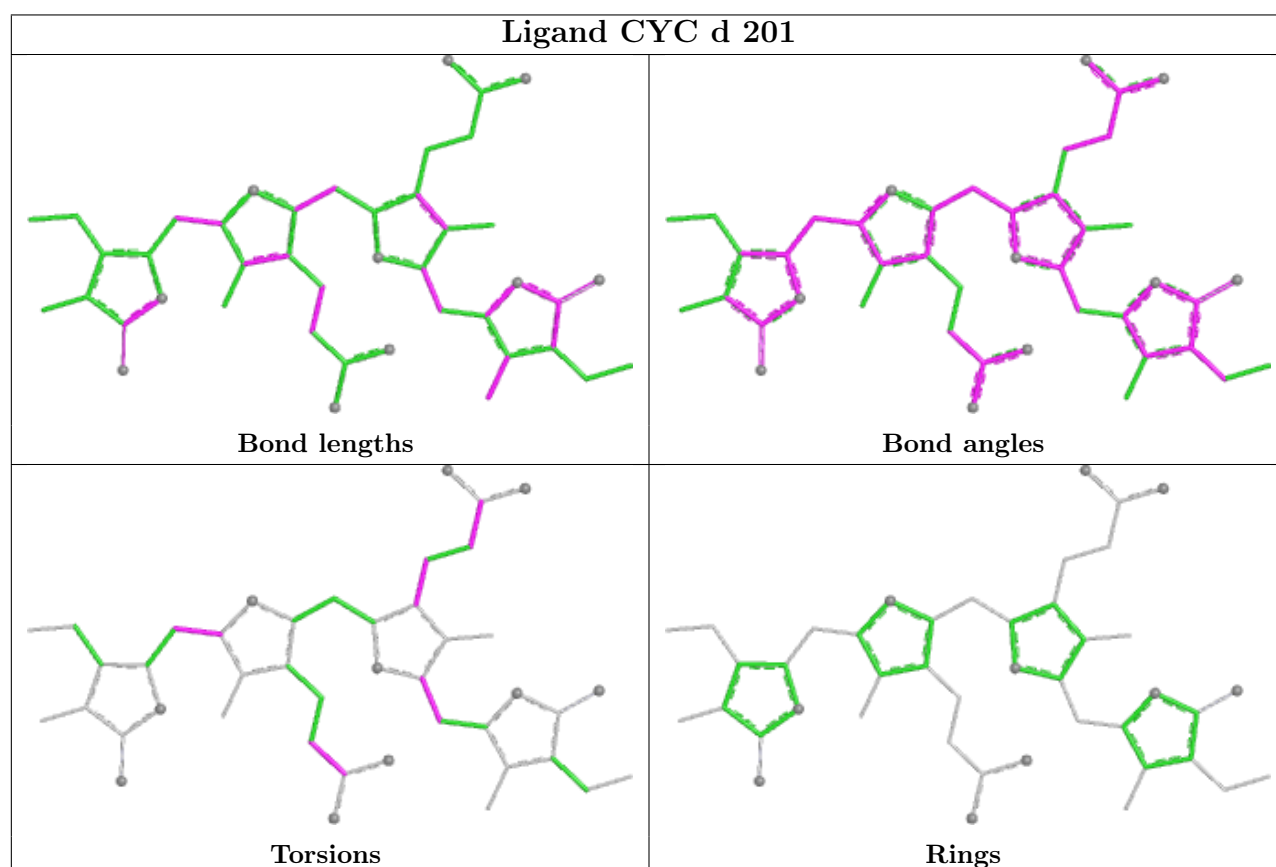
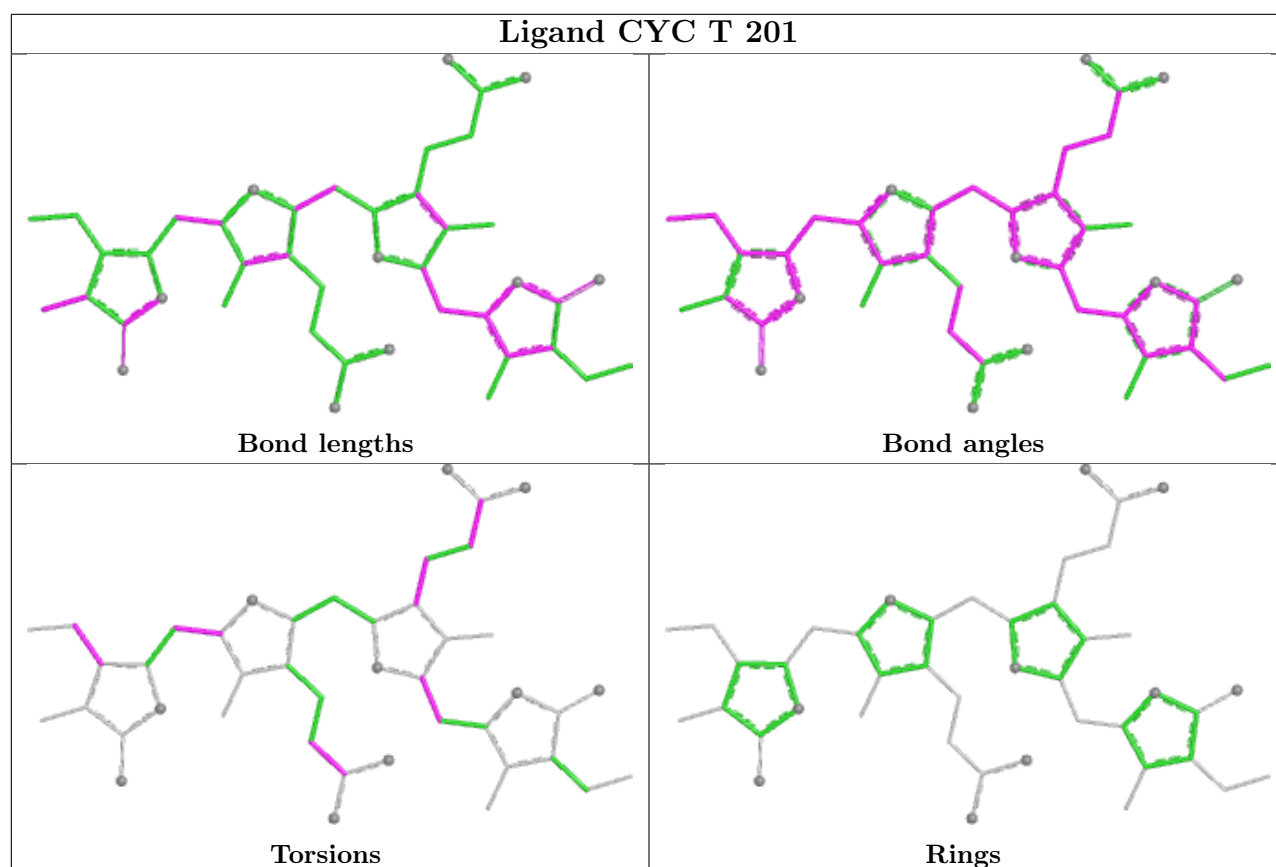
Continued on next page...

Continued from previous page...

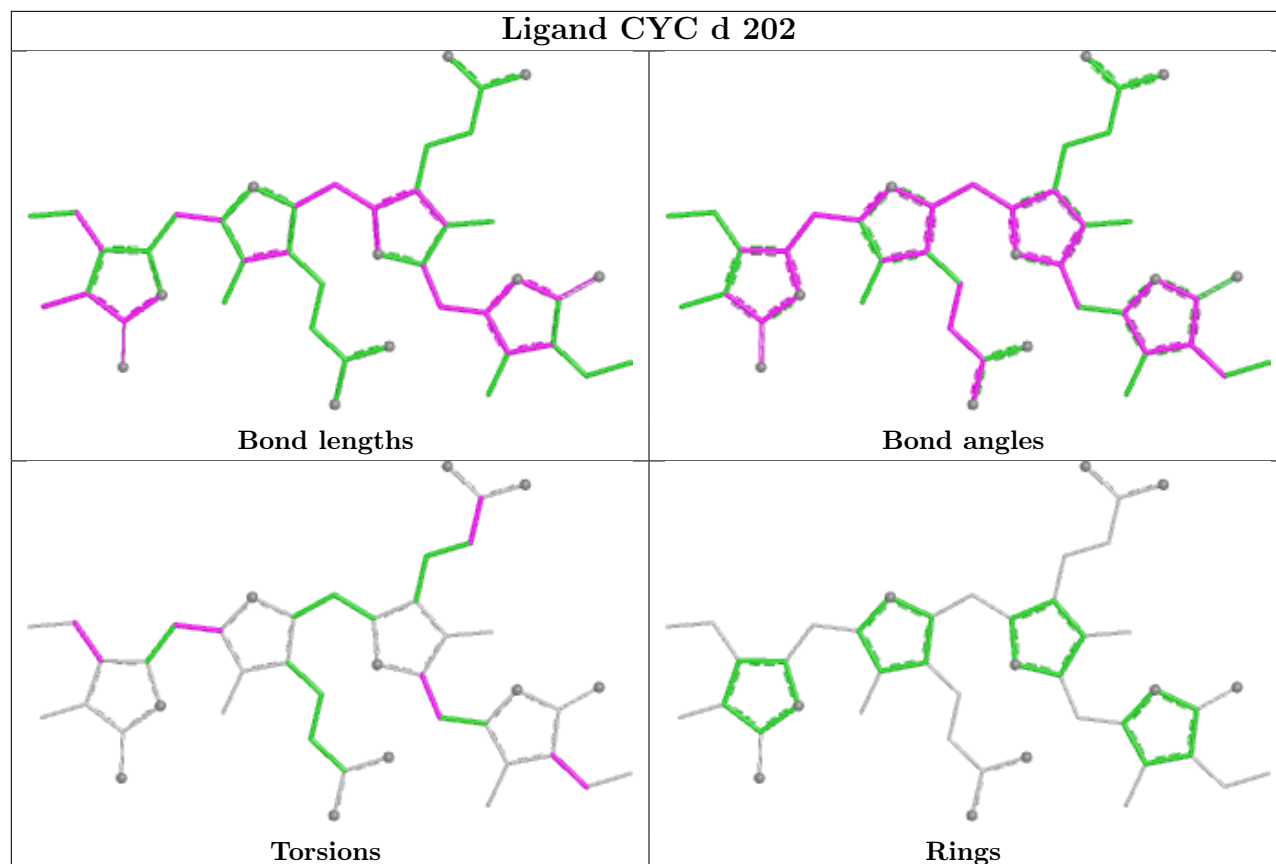
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	202	CYC	17	0
7	e	201	CYC	7	0
7	i	201	CYC	13	0
7	T	202	CYC	15	0
7	M	201	CYC	12	0
7	B	201	CYC	14	0
7	X	201	CYC	14	0
7	j	201	CYC	13	0
7	K	201	CYC	14	0
7	V	202	CYC	18	0
7	Q	201	CYC	10	0
7	X	202	CYC	17	0

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.

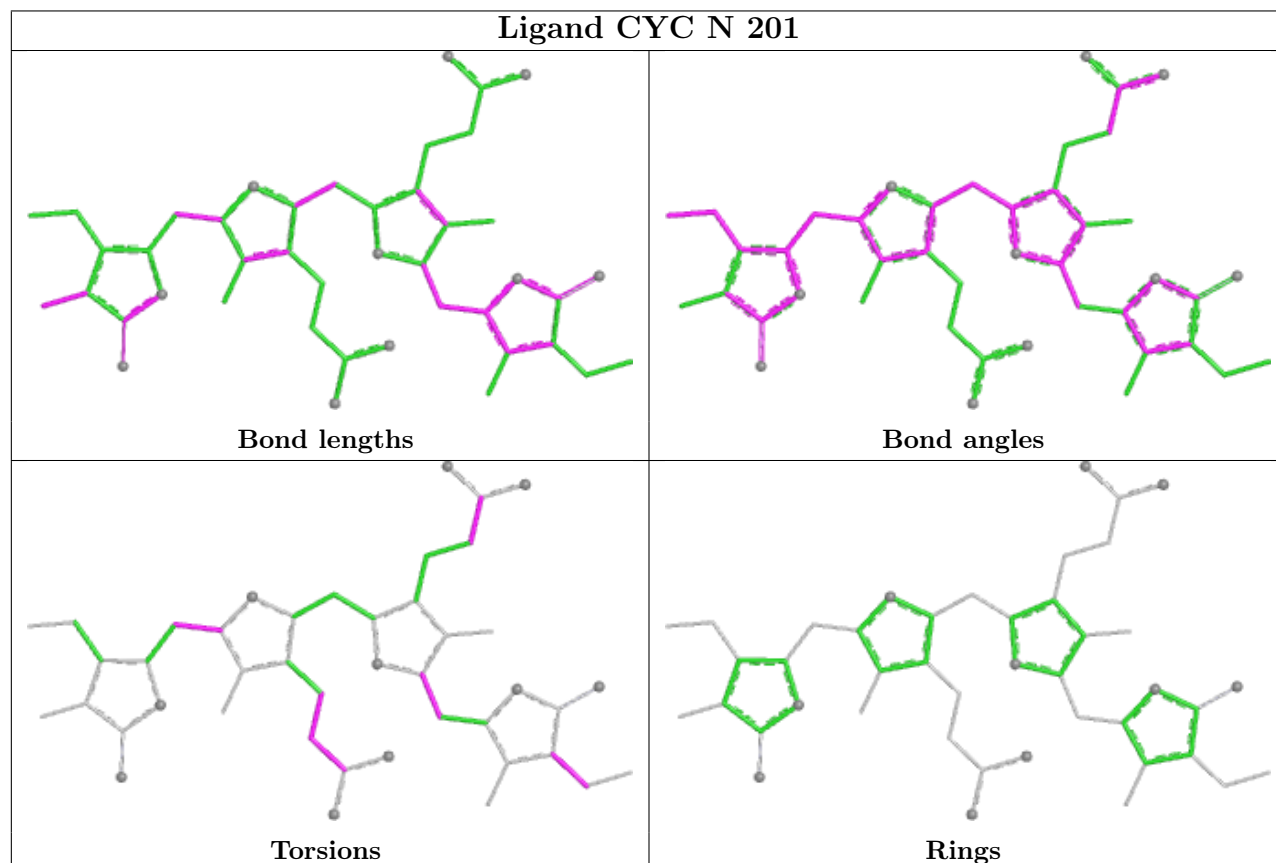




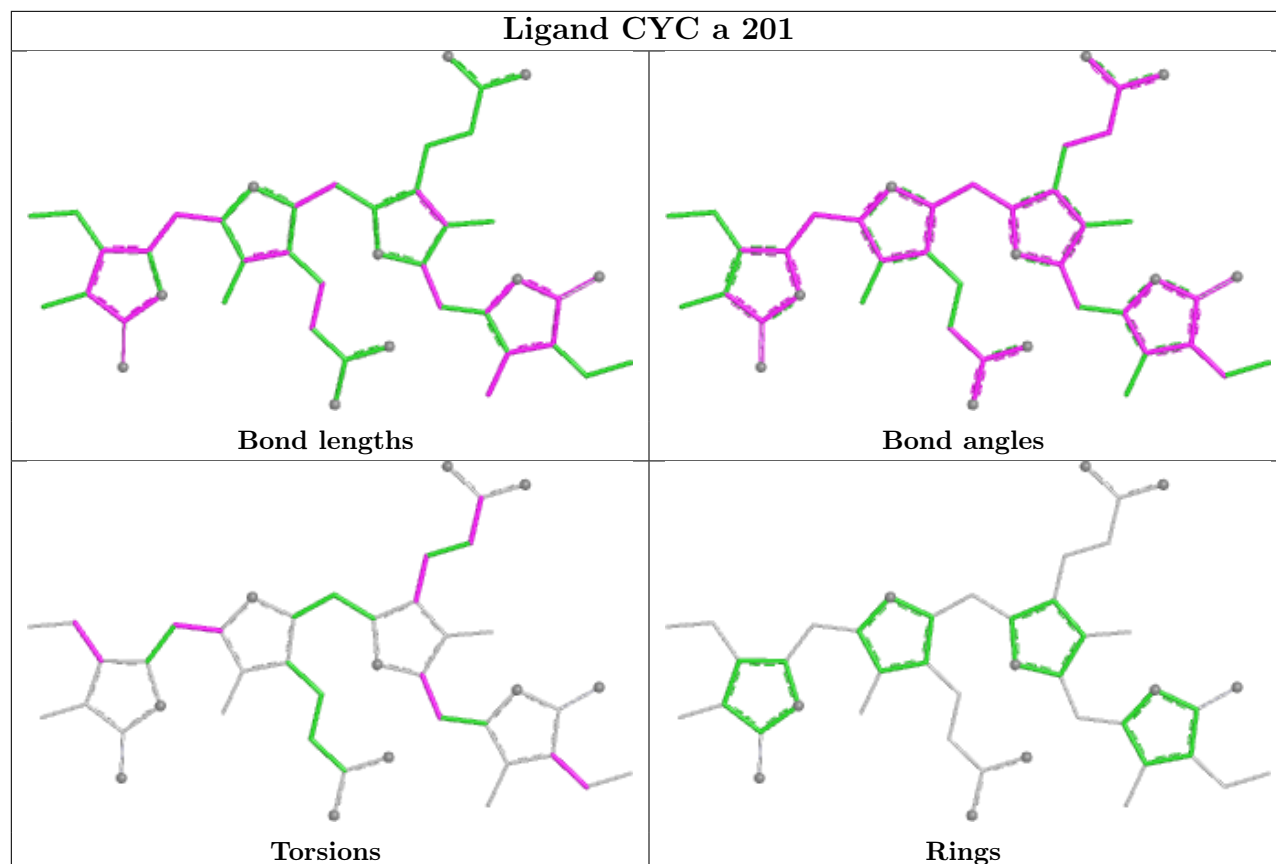
Ligand CYC d 202



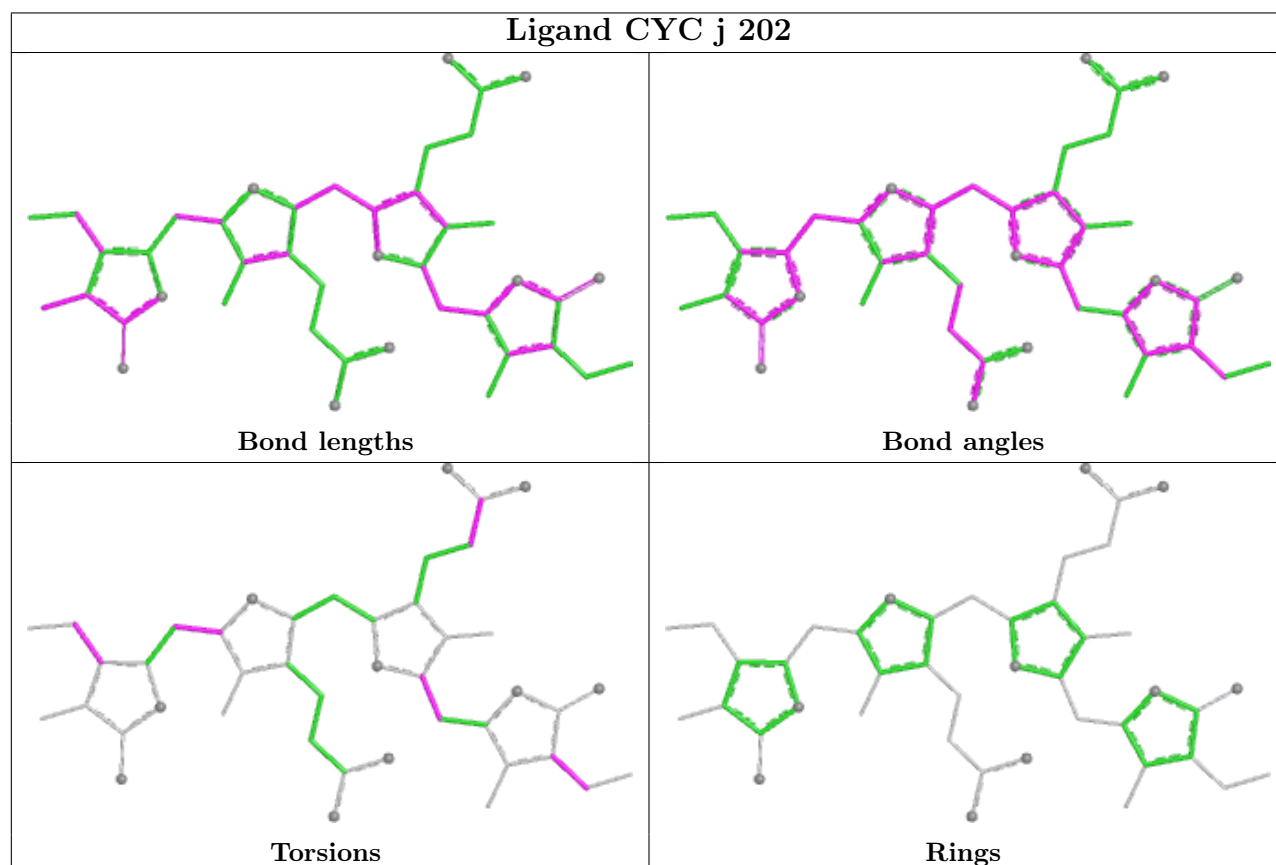
Ligand CYC N 201

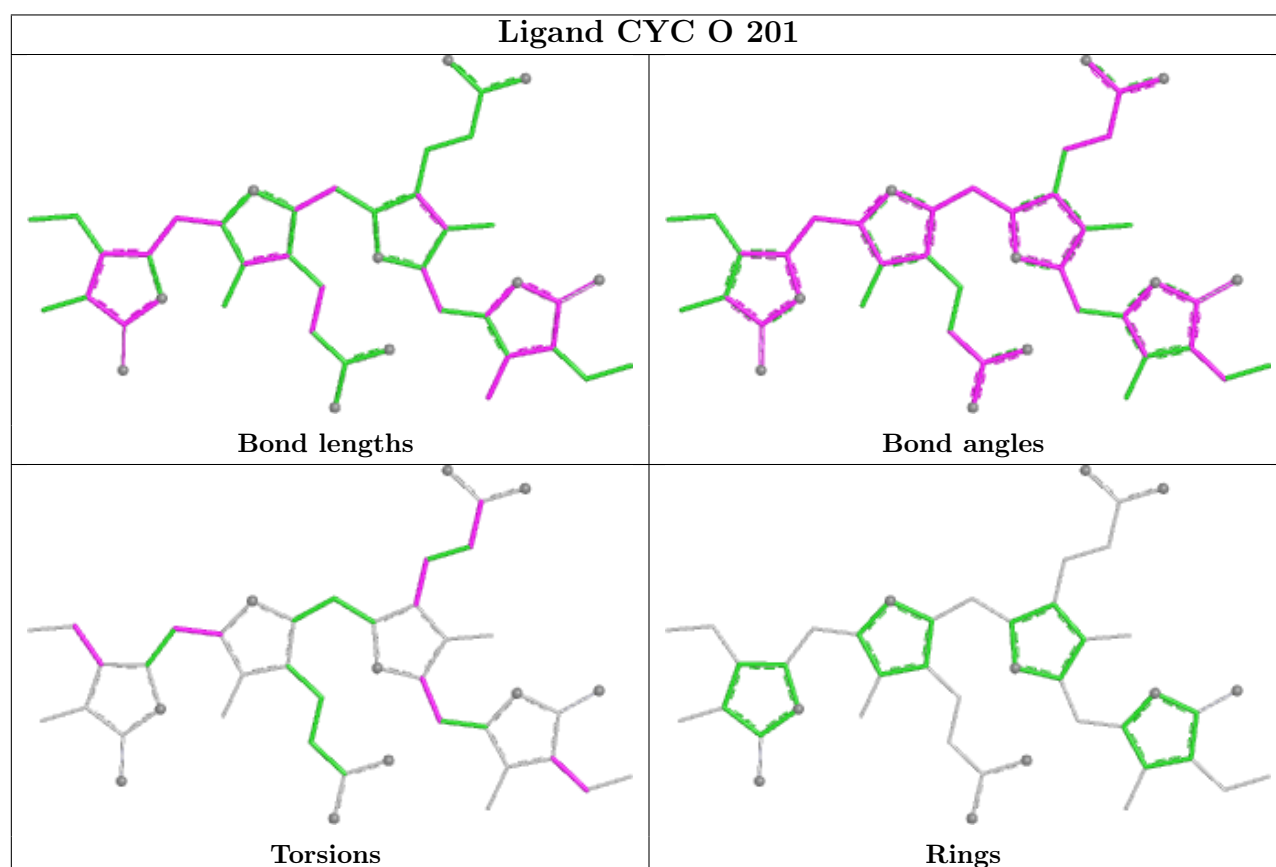
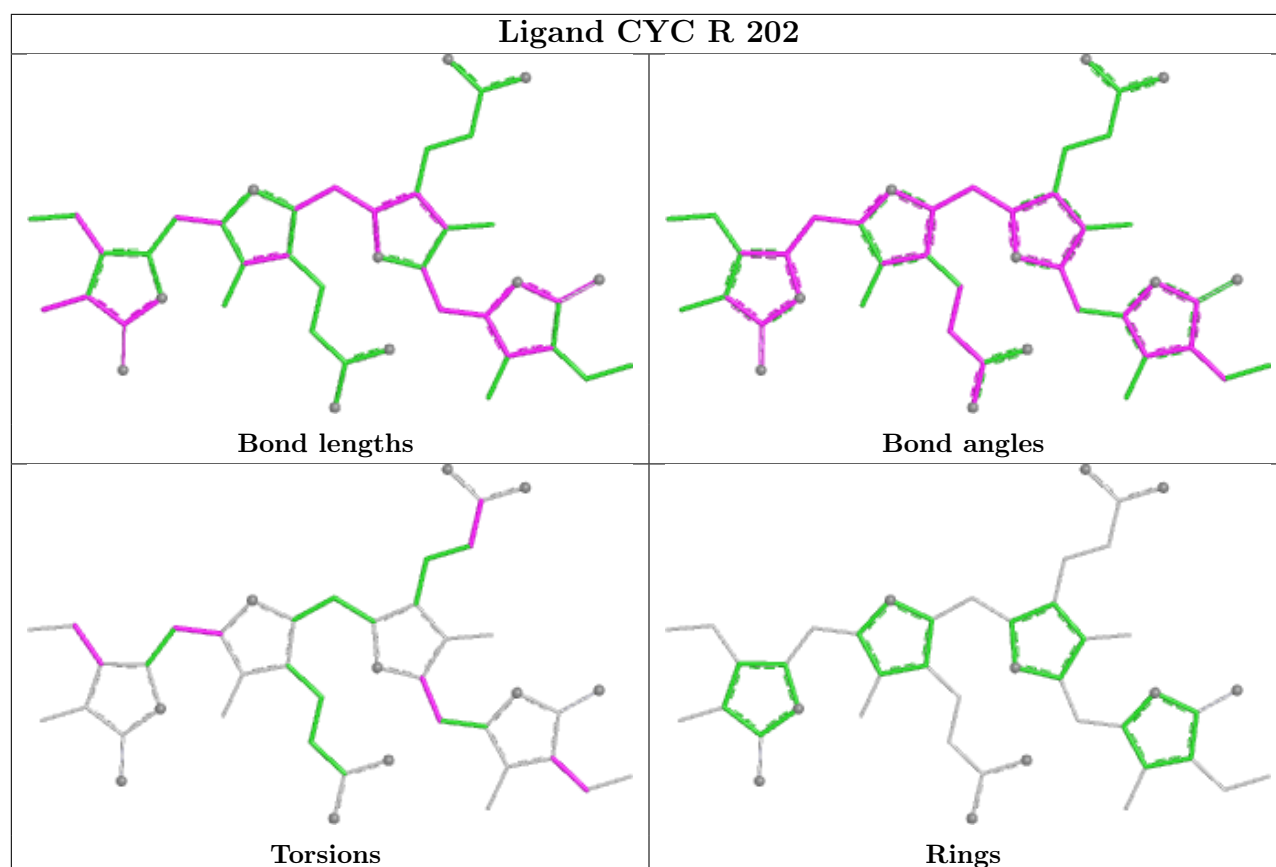


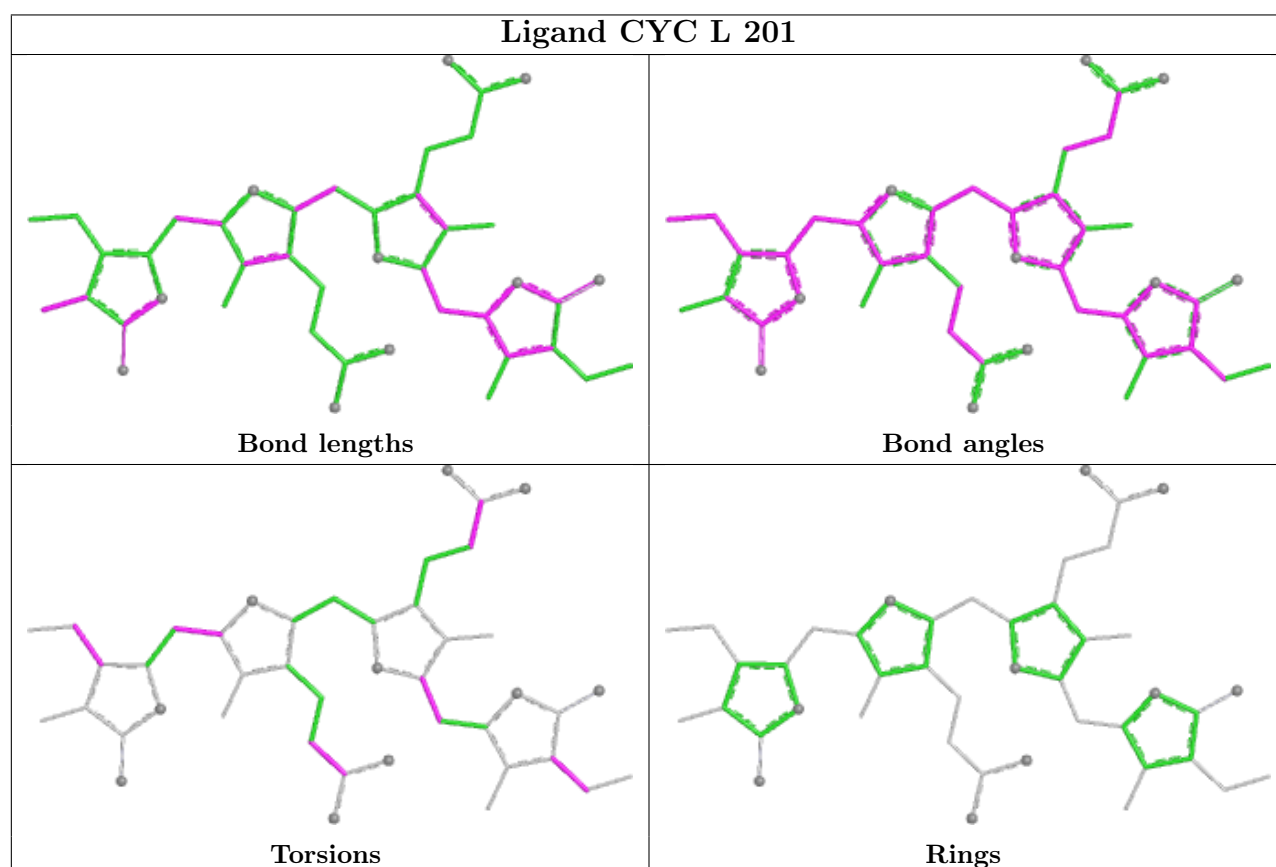
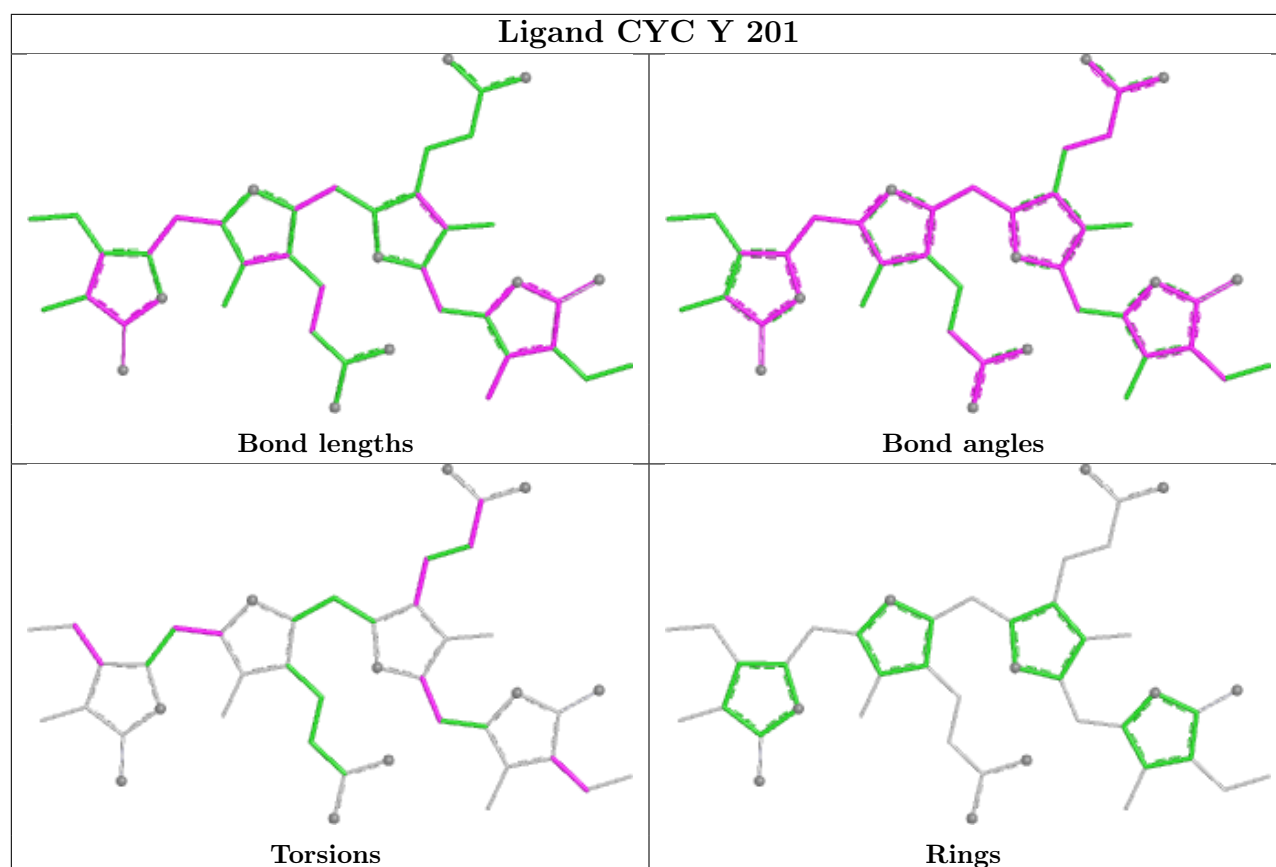
Ligand CYC a 201



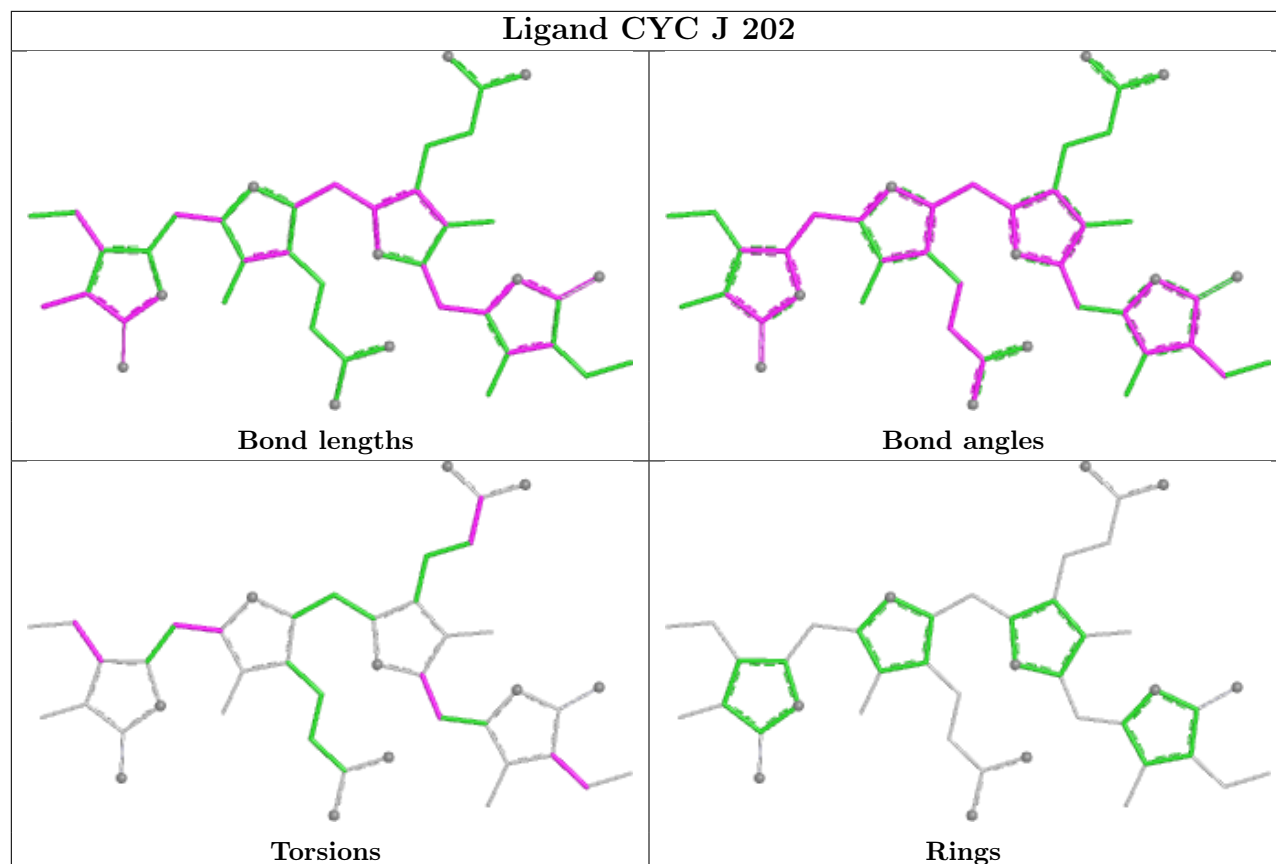
Ligand CYC j 202



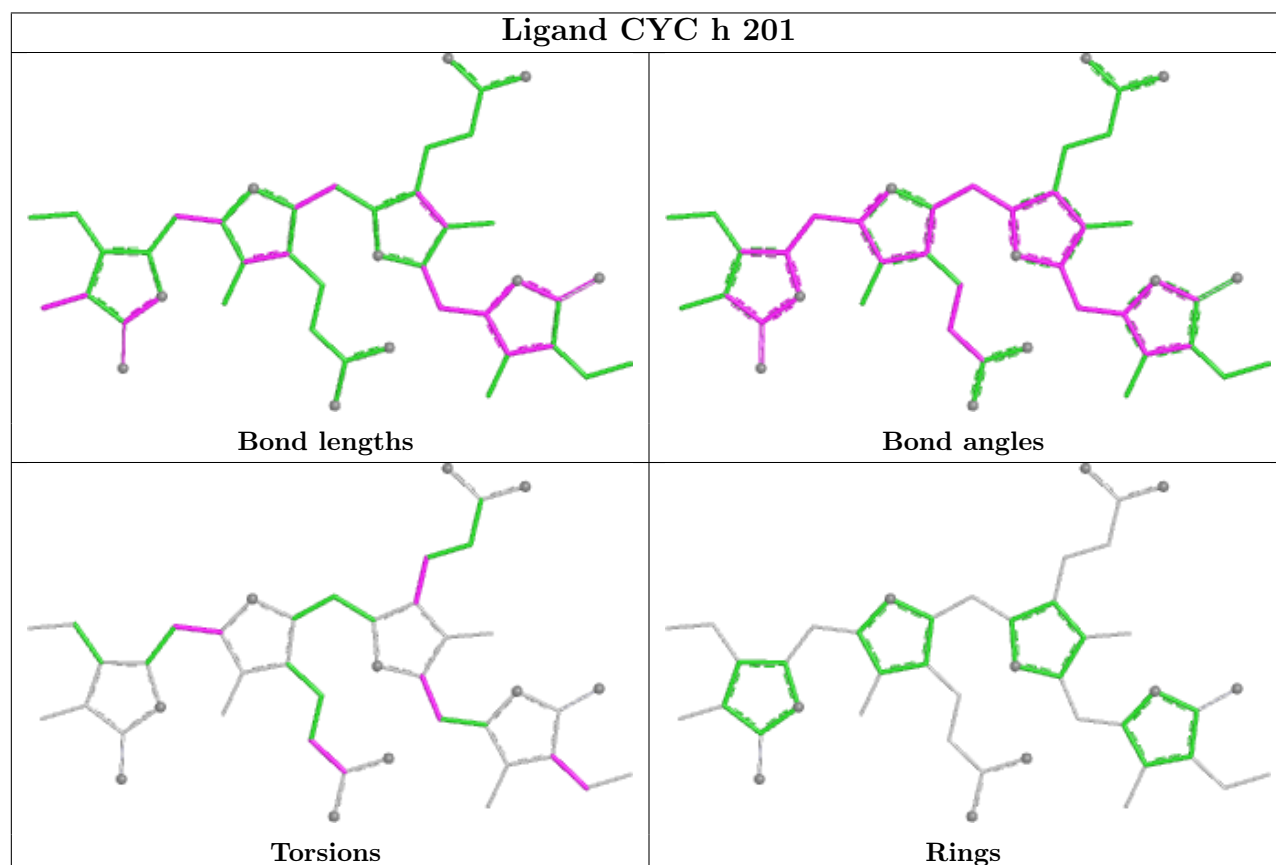


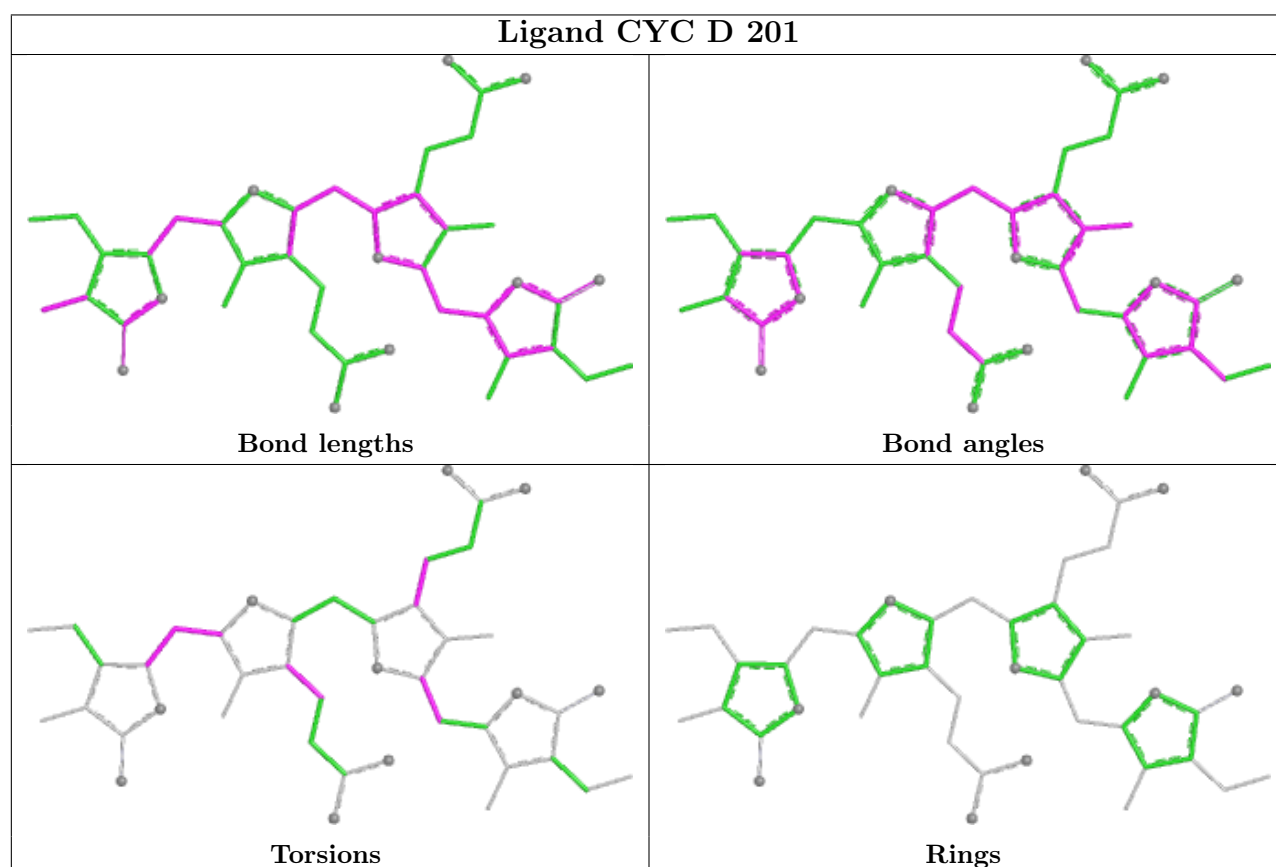
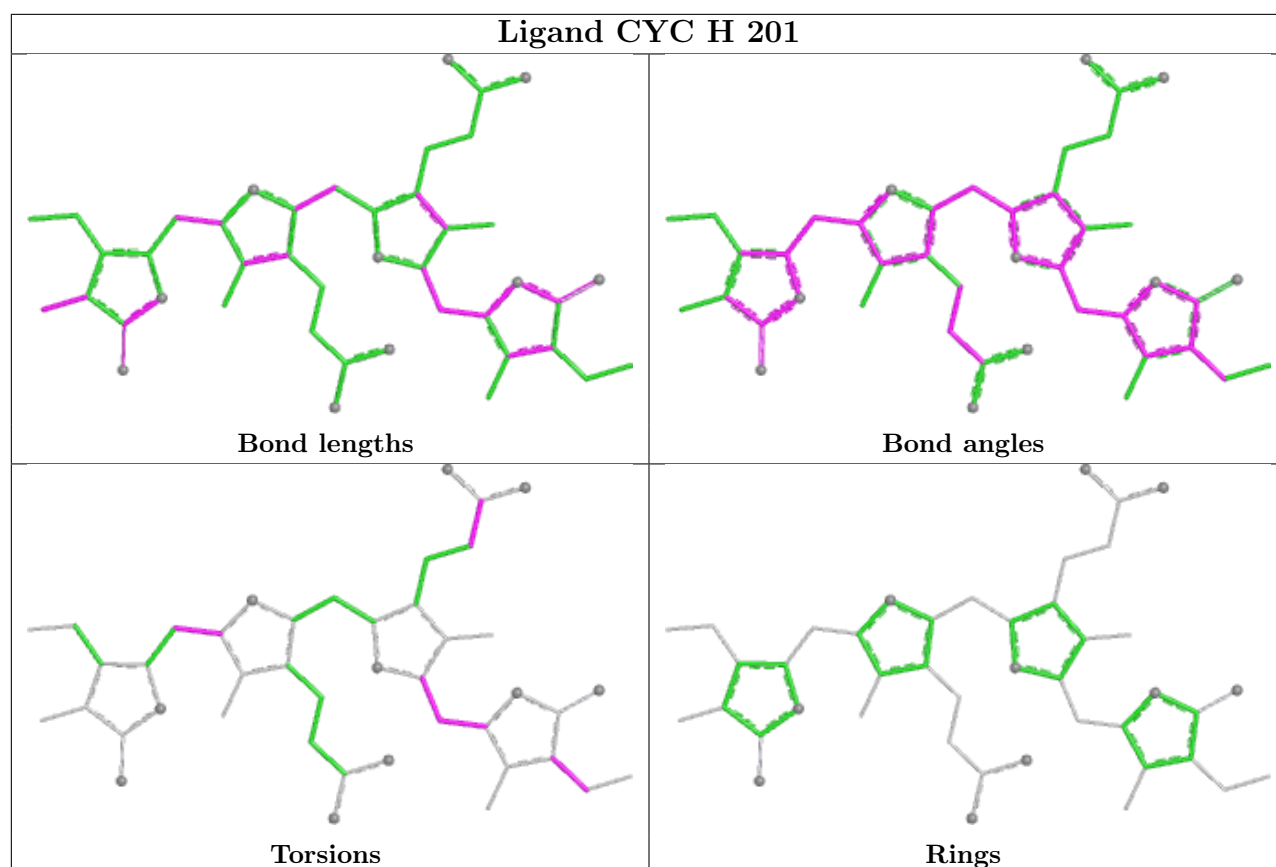


Ligand CYC J 202

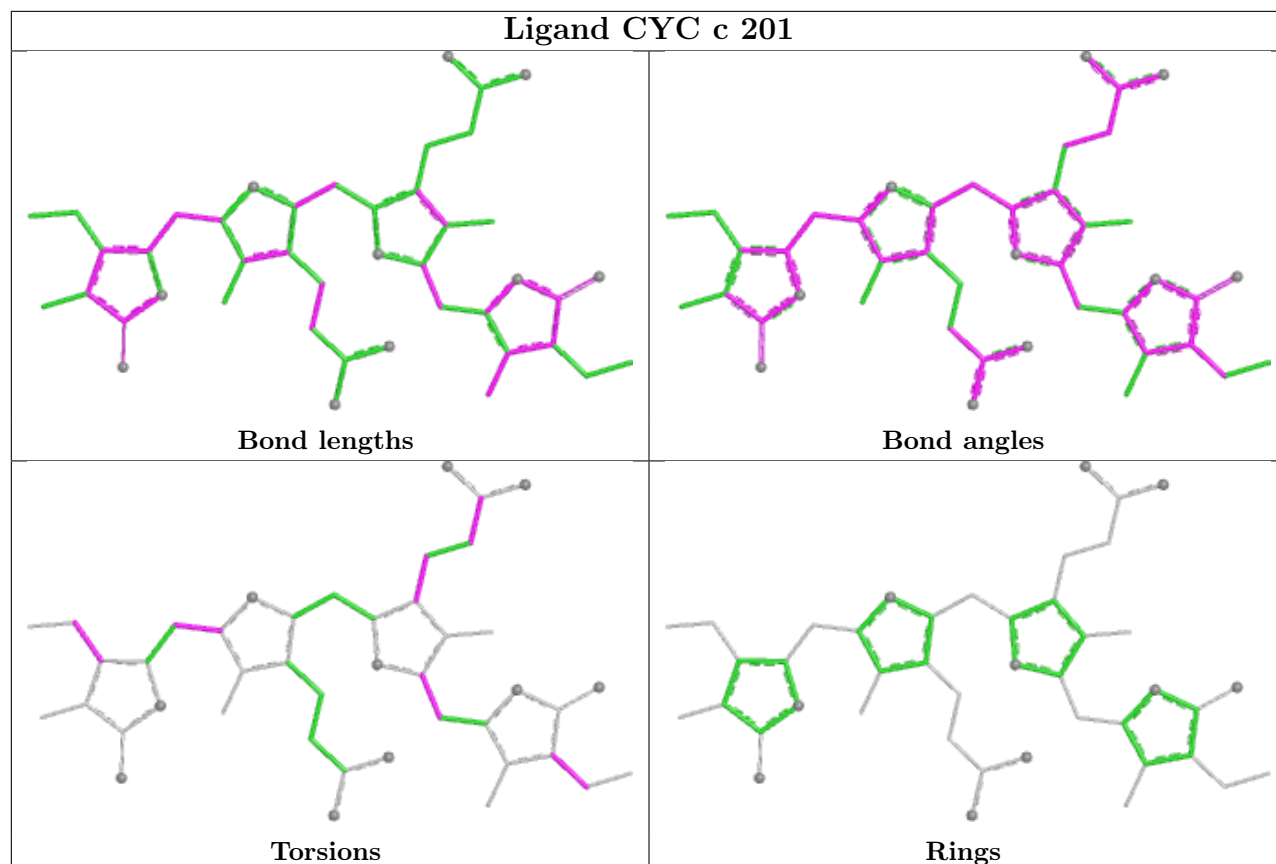


Ligand CYC h 201

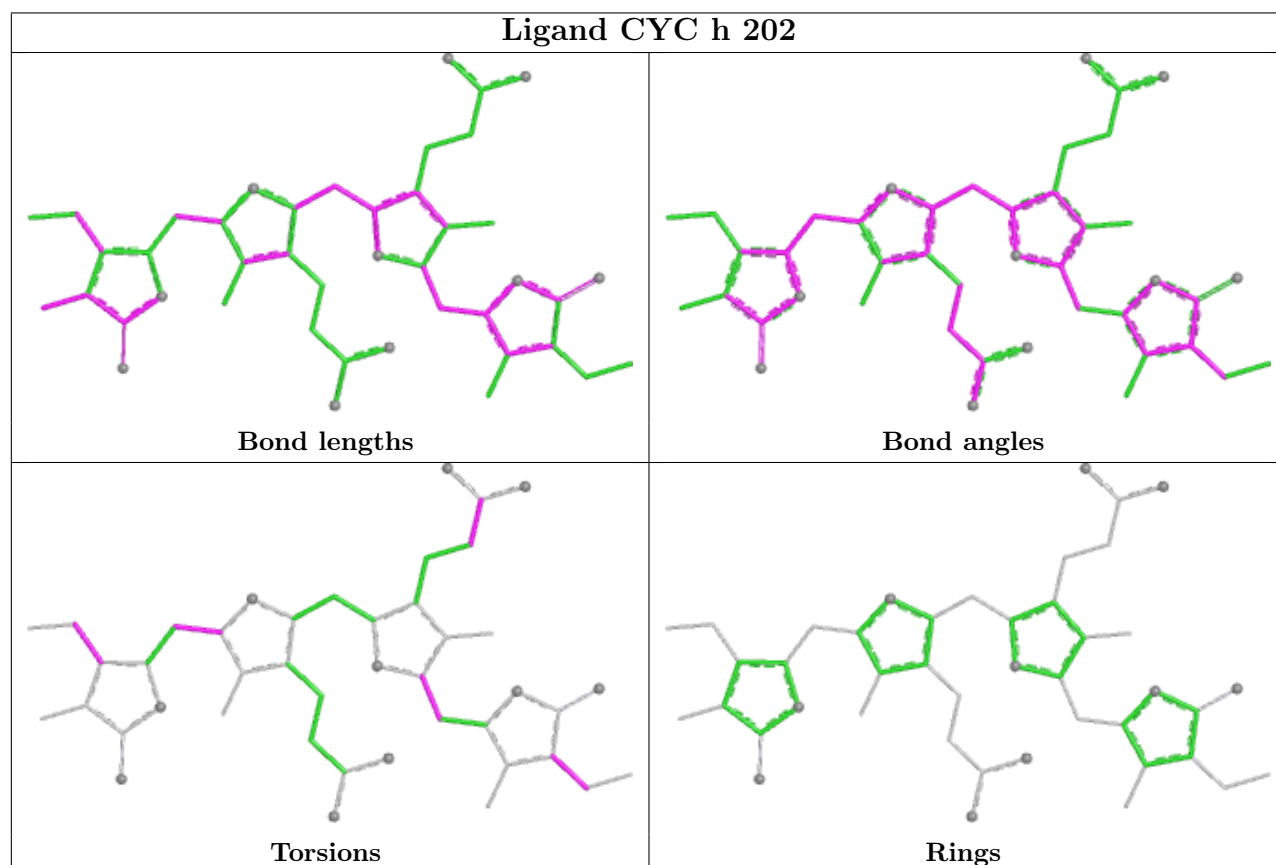


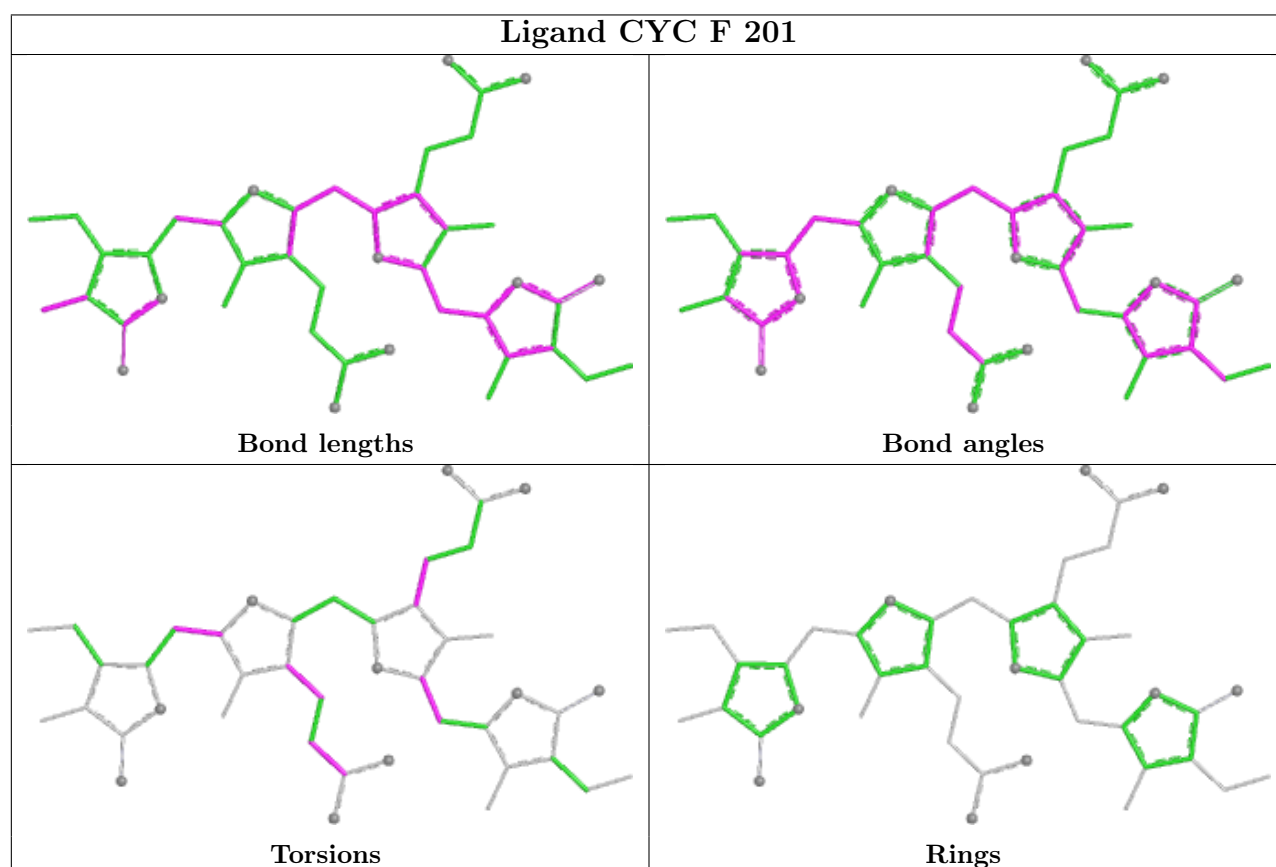
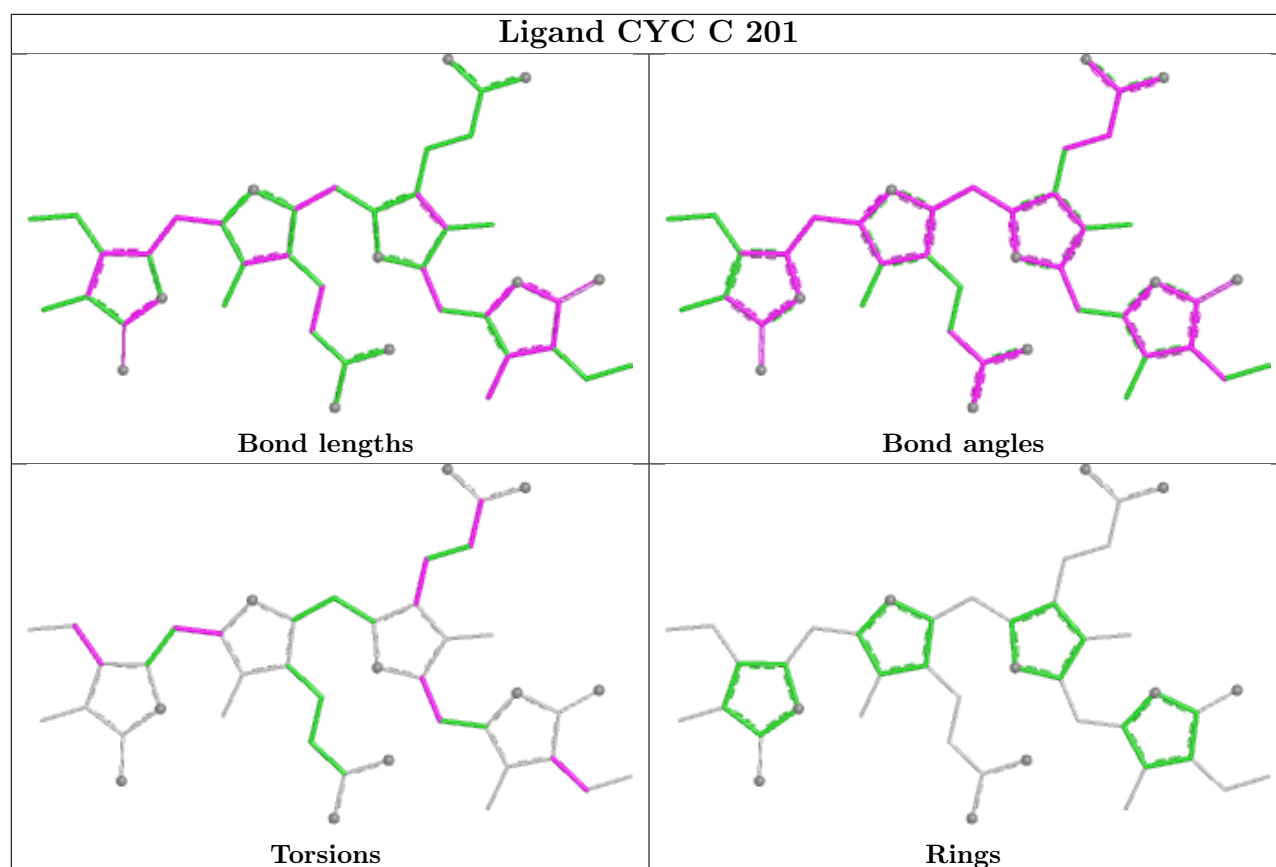


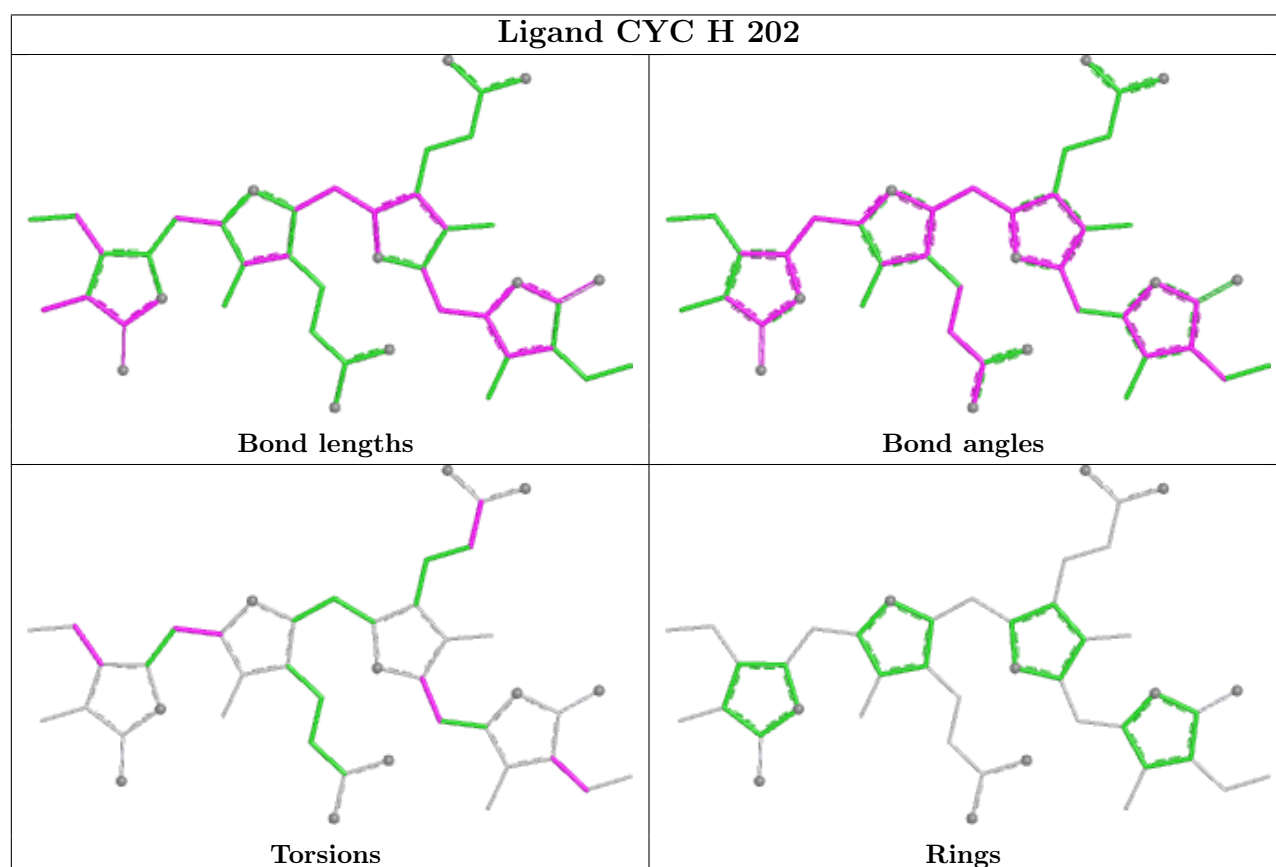
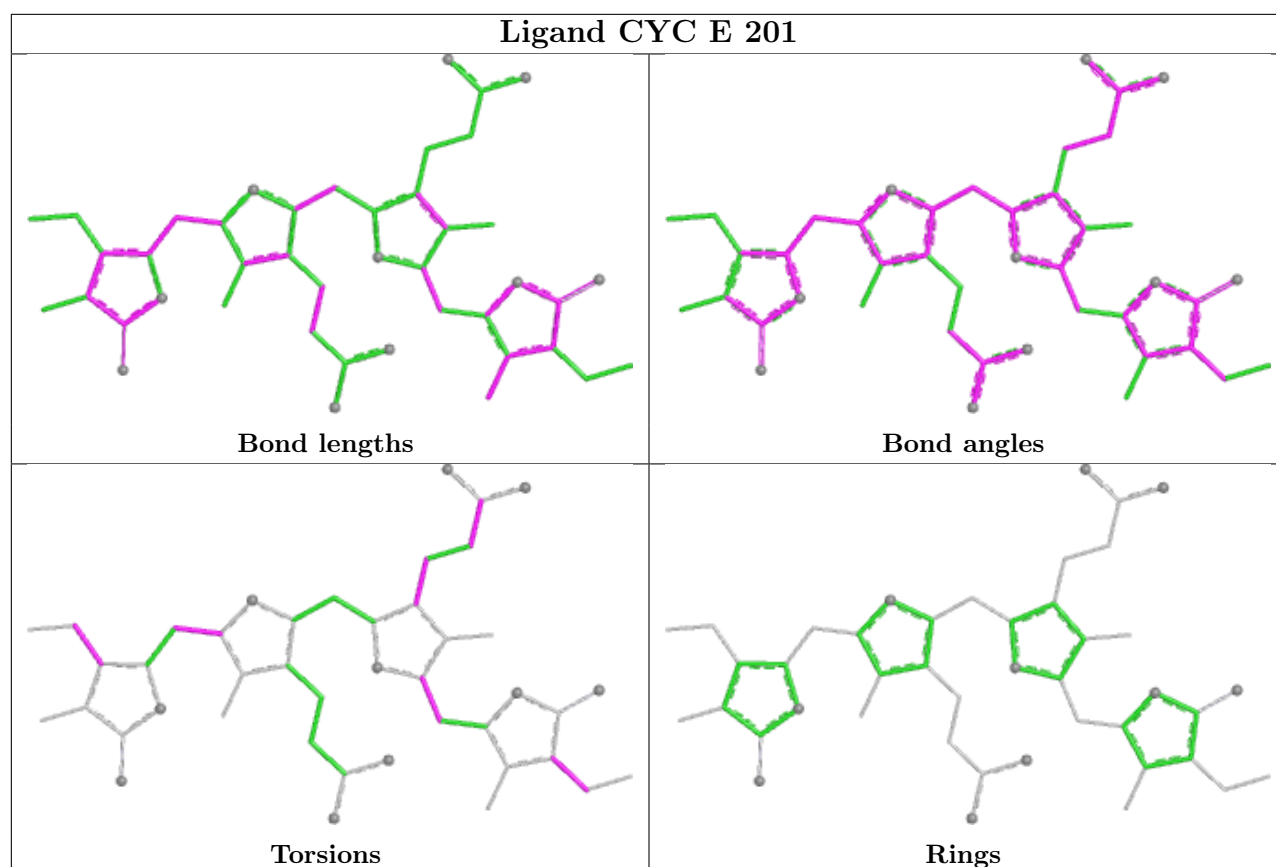
Ligand CYC c 201



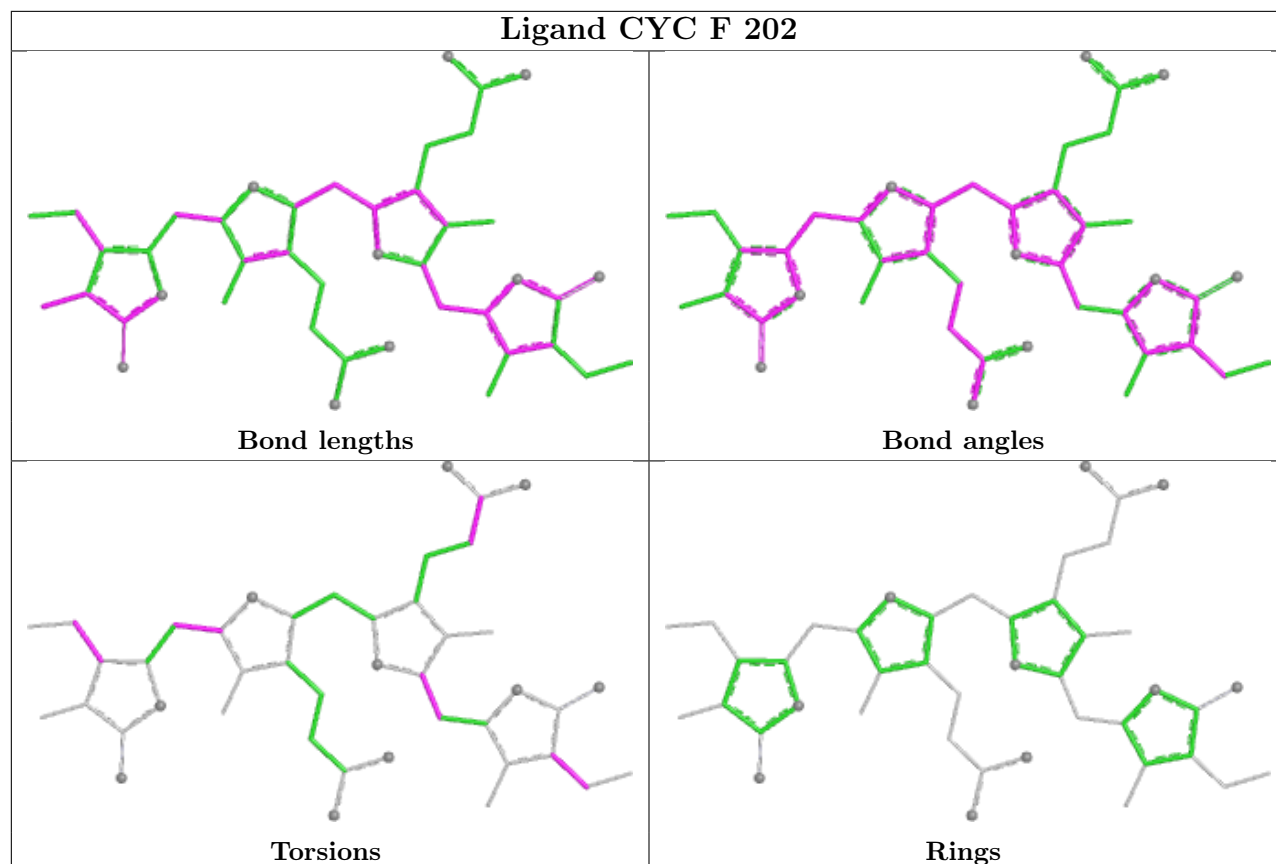
Ligand CYC h 202



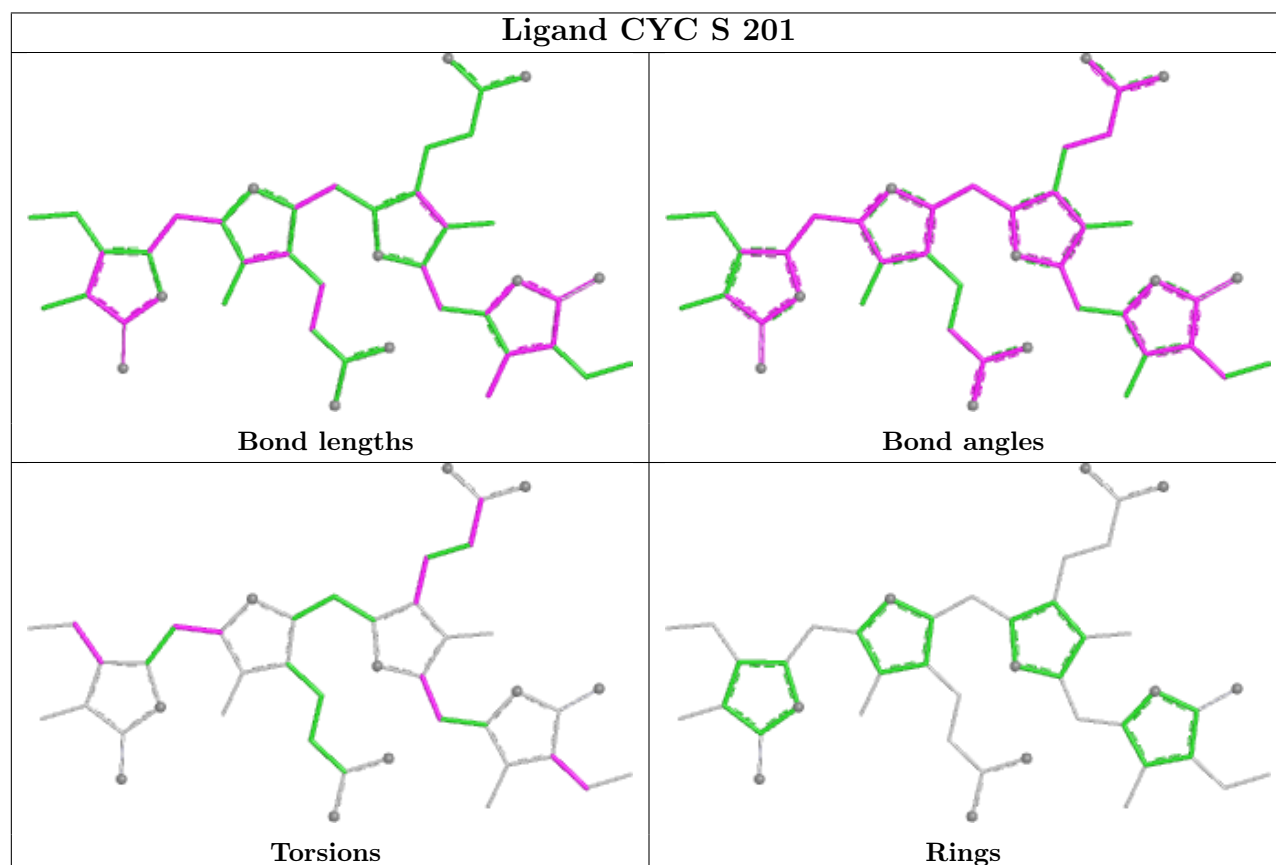




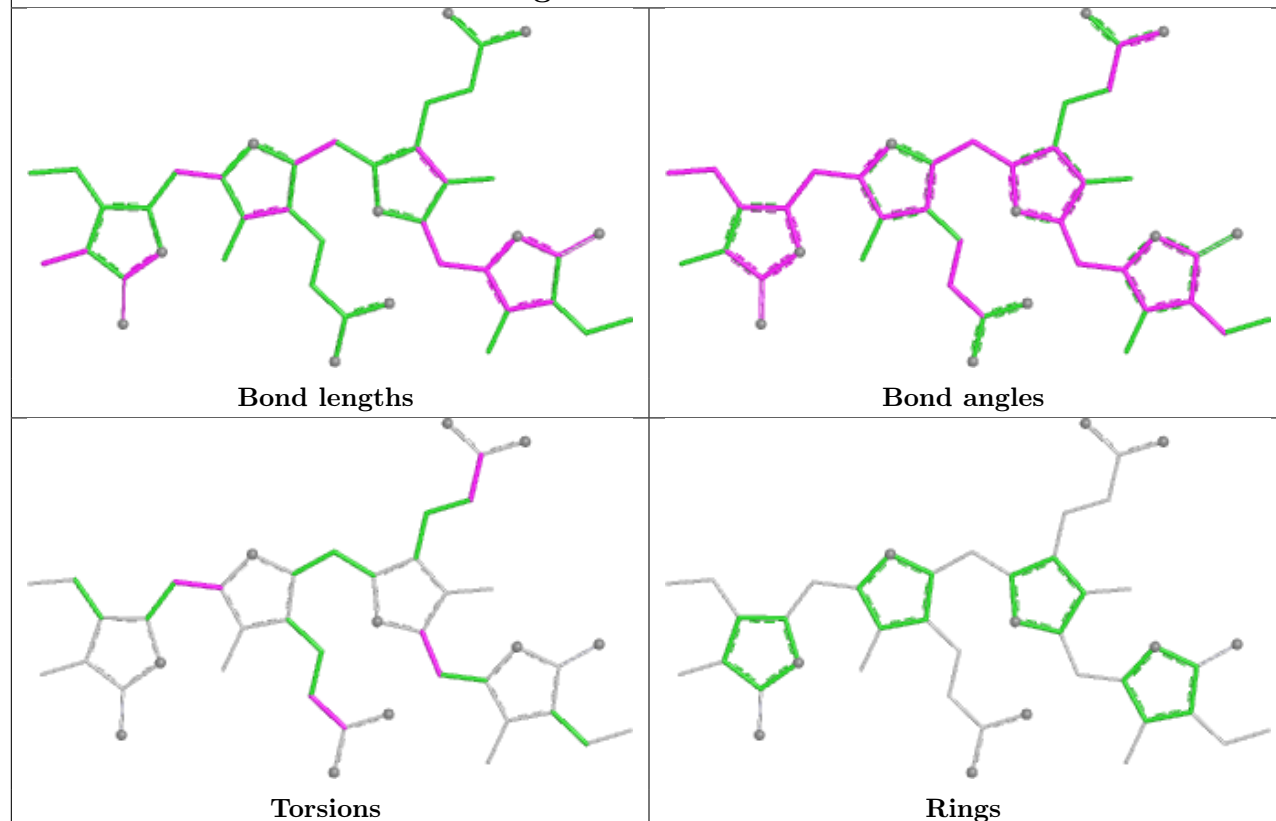
Ligand CYC F 202



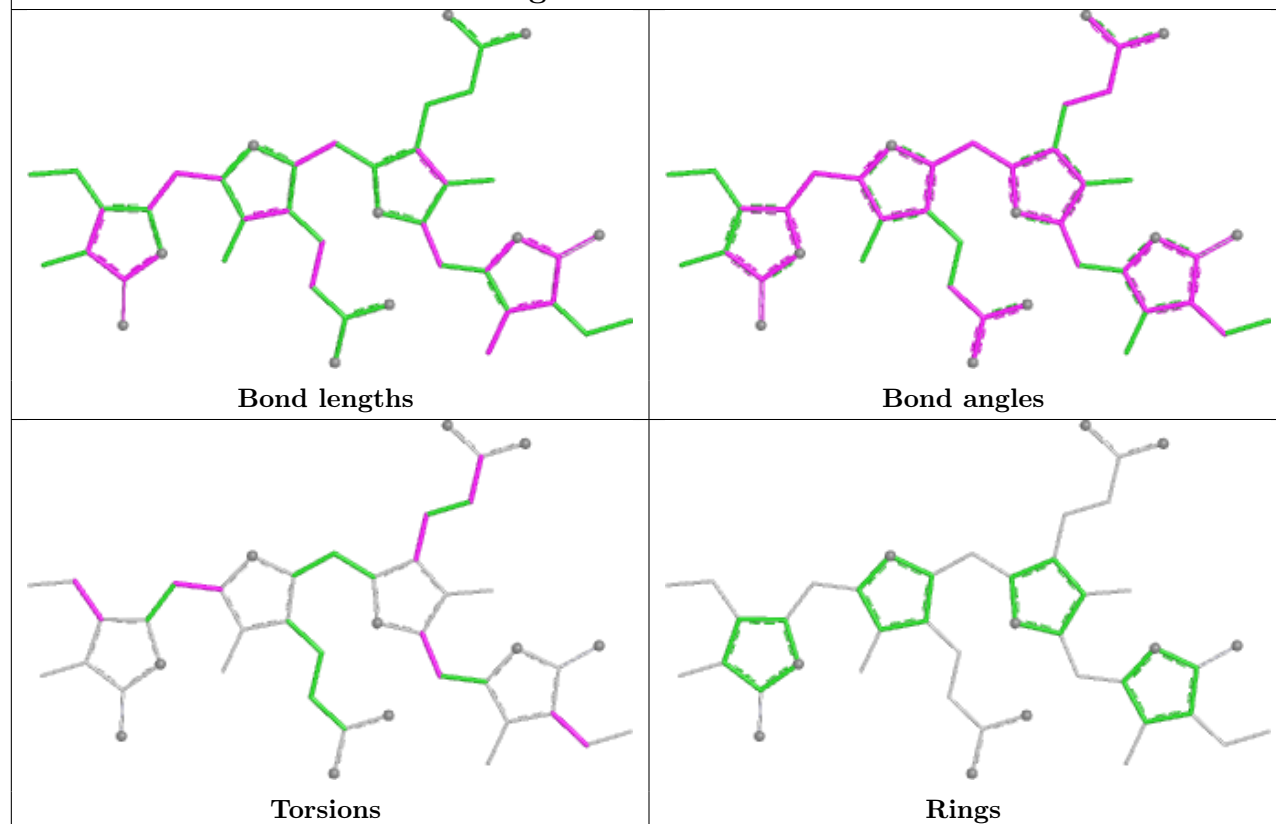
Ligand CYC S 201

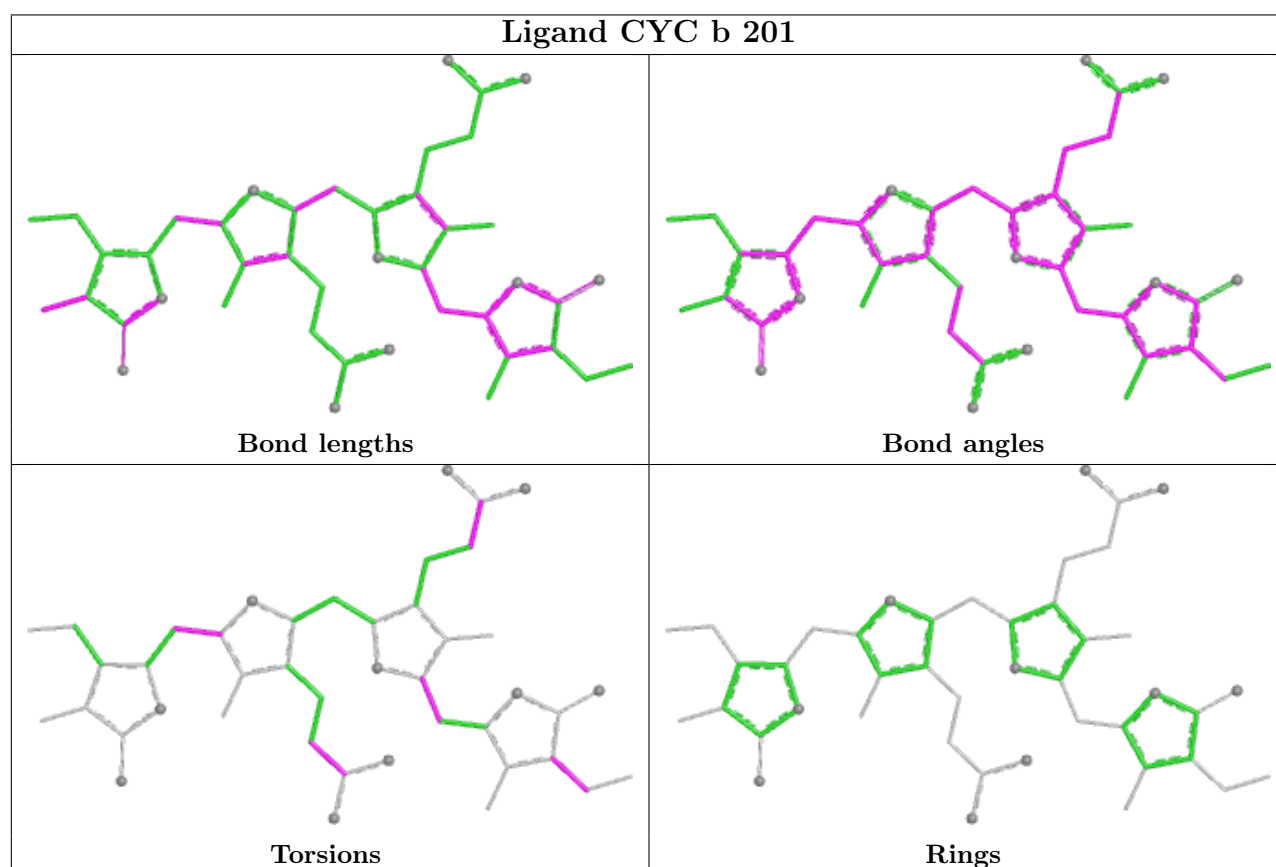
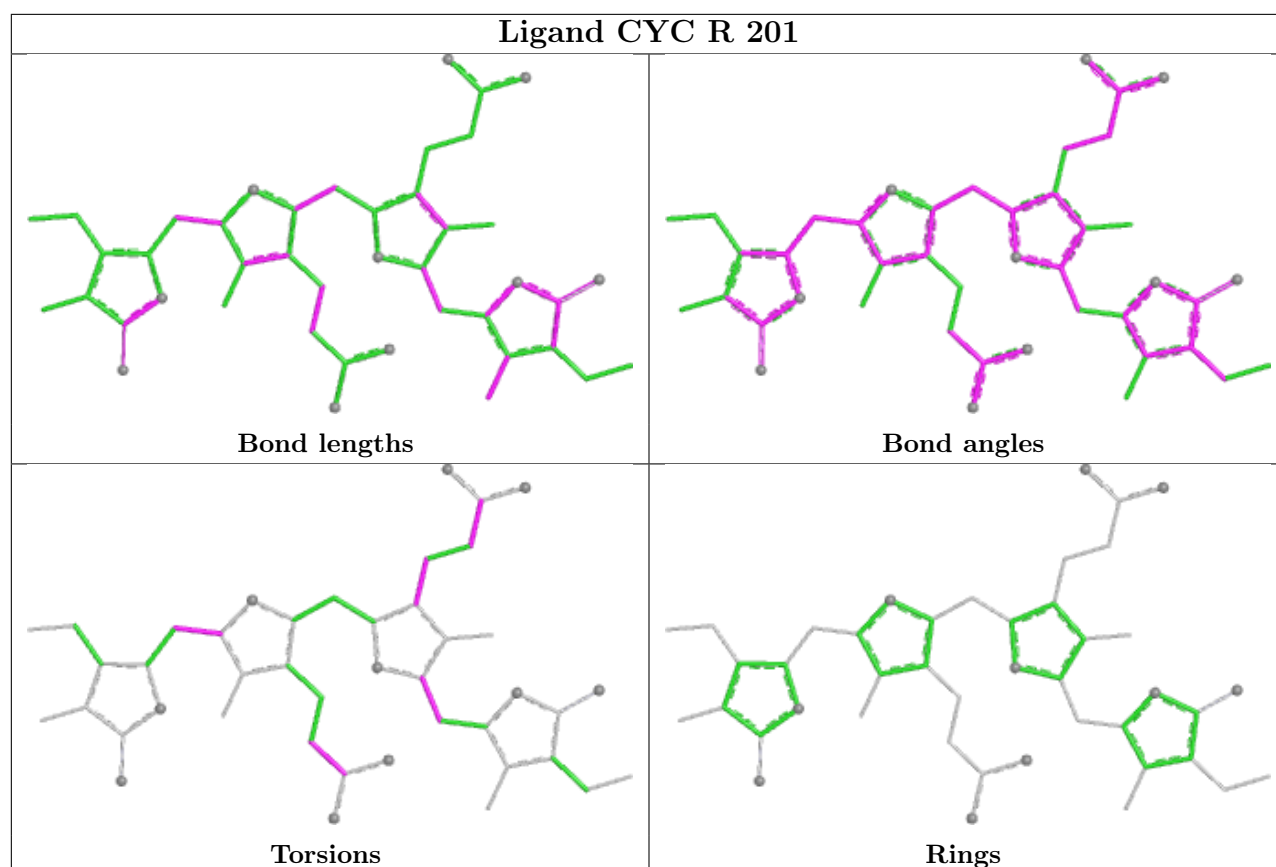


Ligand CYC J 201

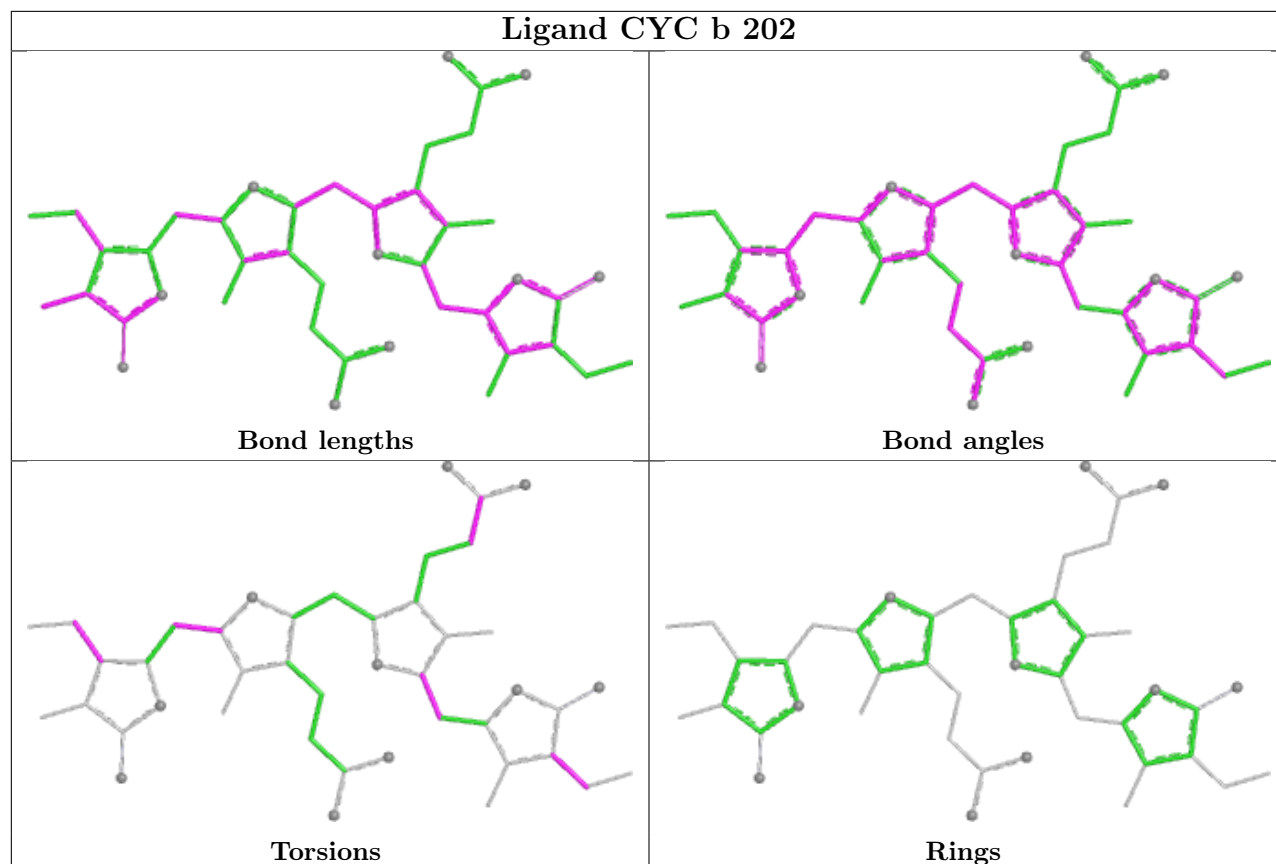


Ligand CYC G 201

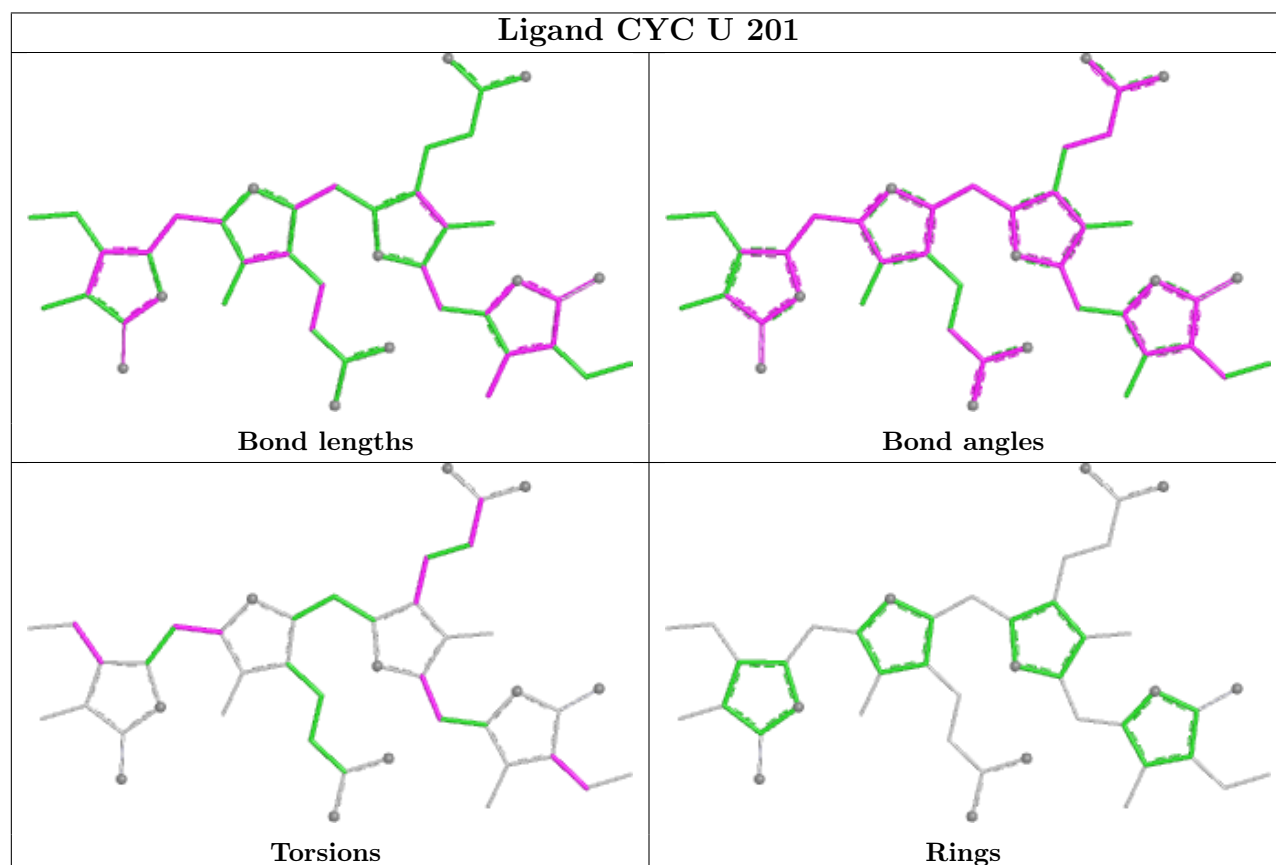


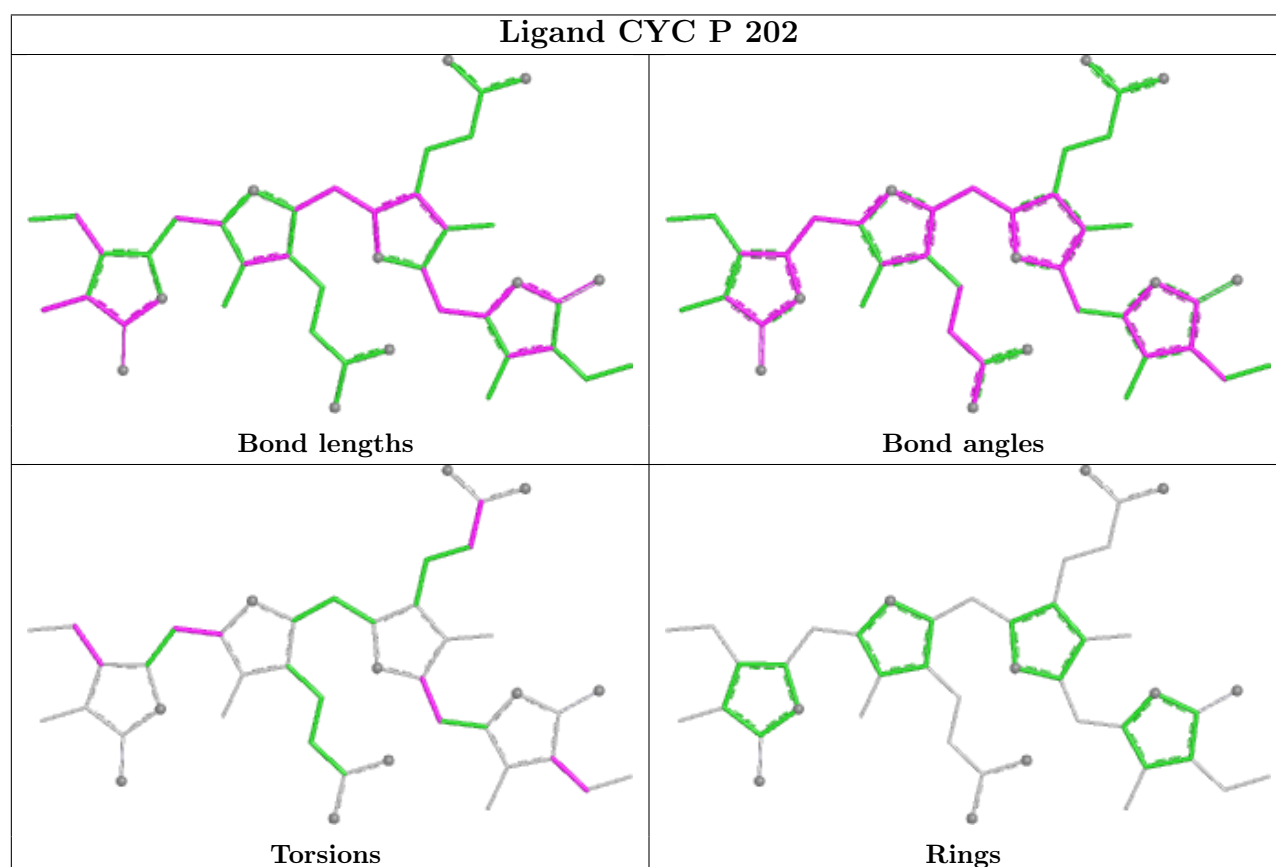
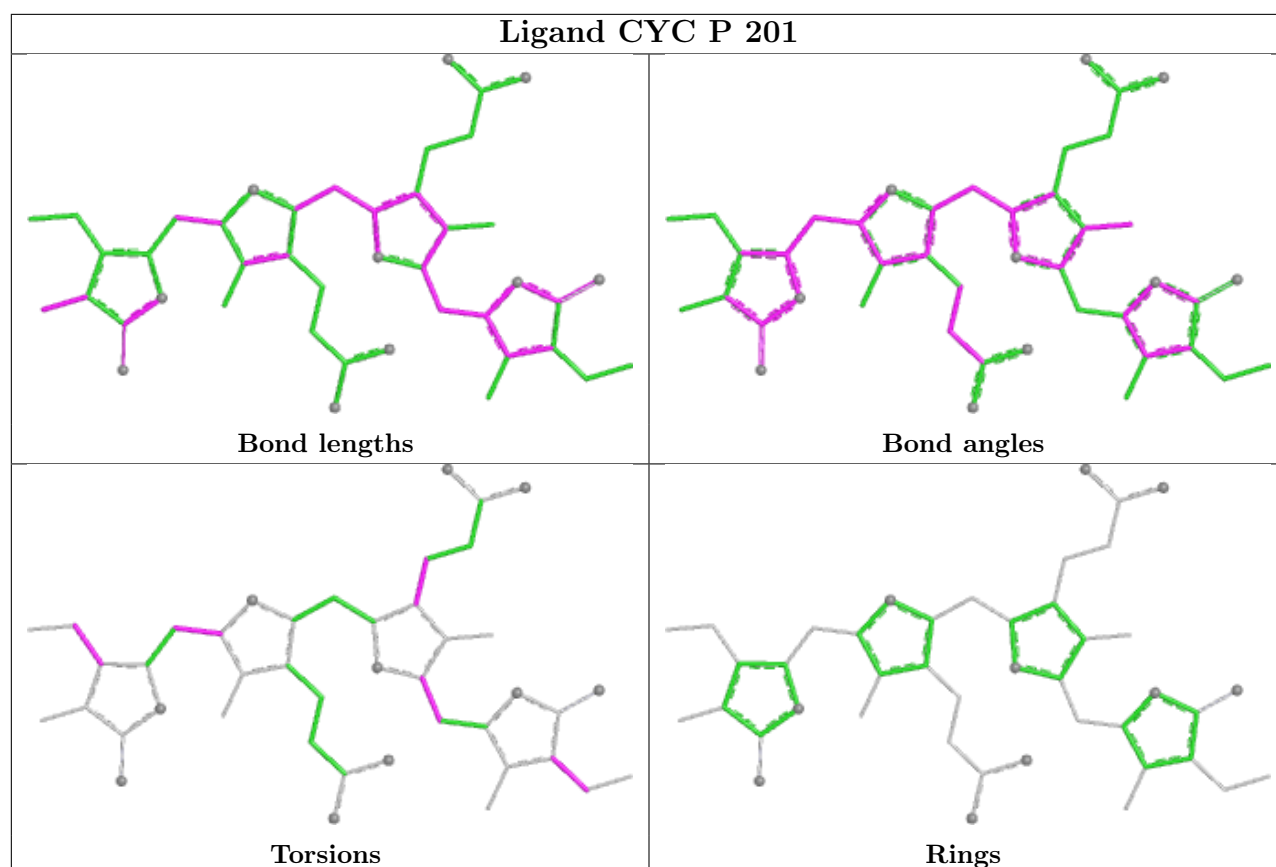


Ligand CYC b 202

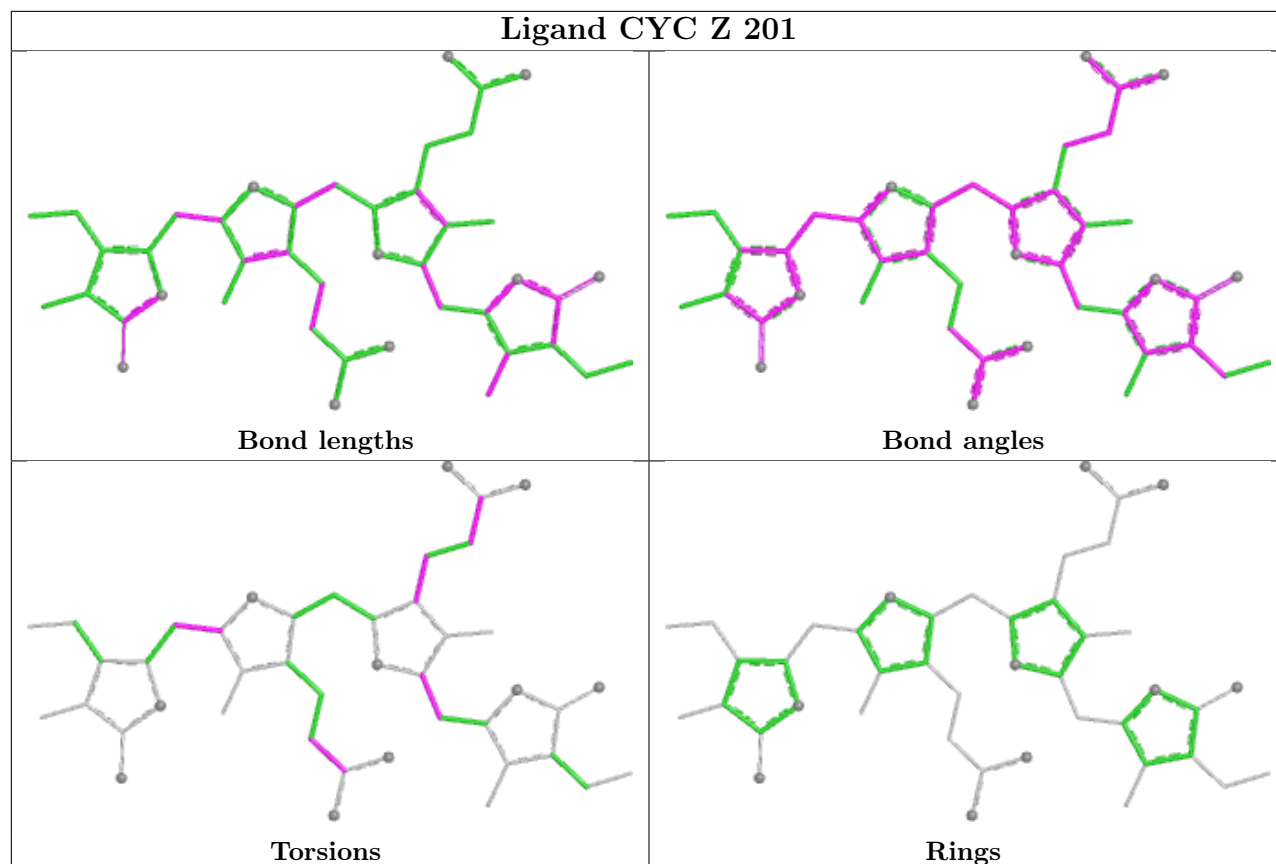


Ligand CYC U 201

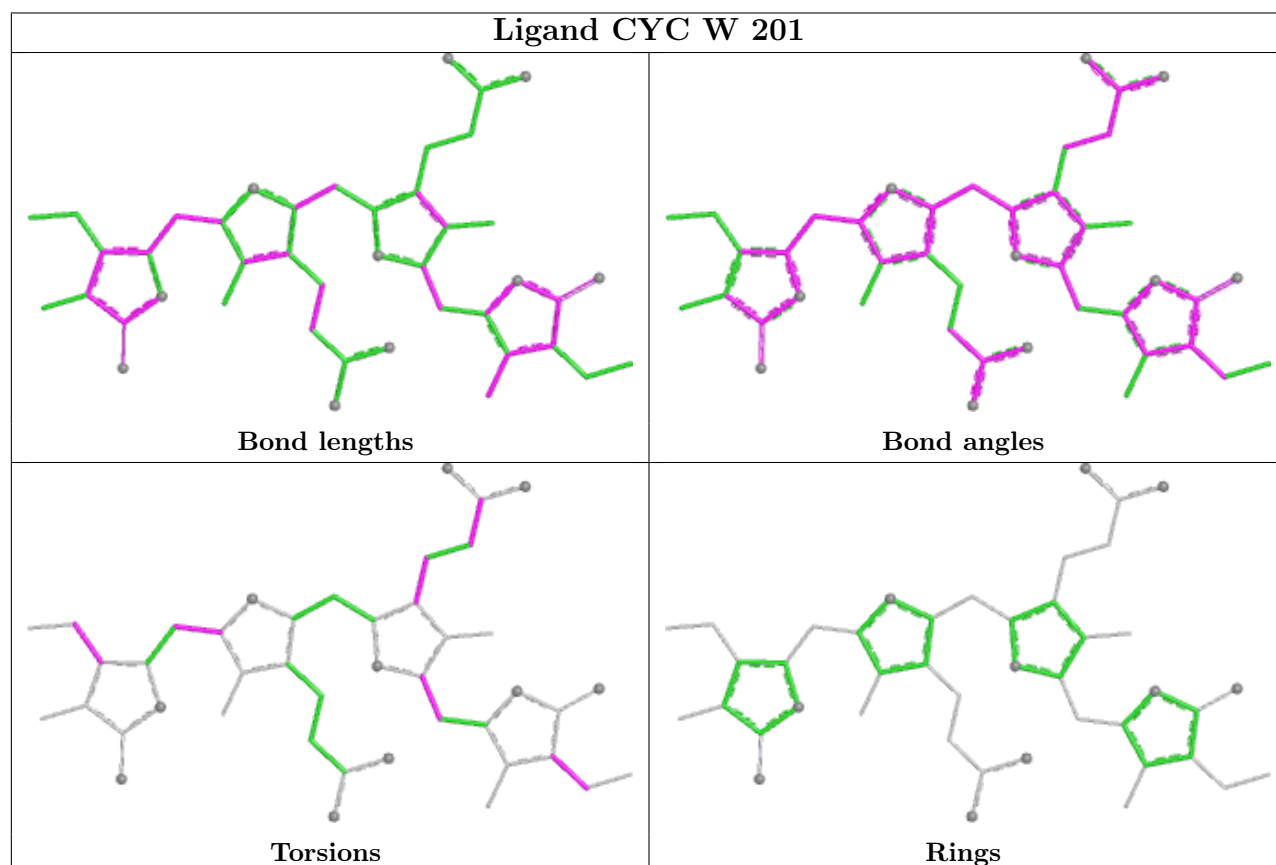




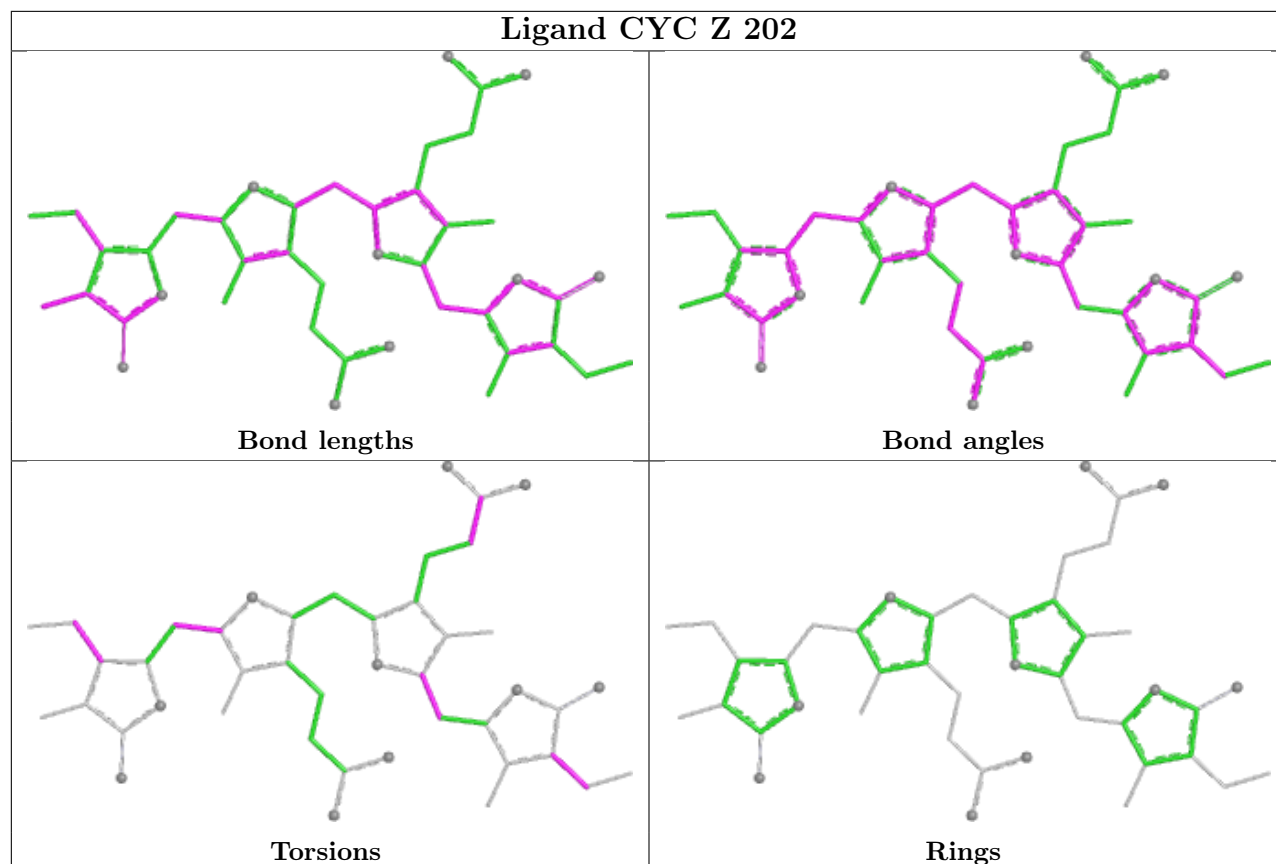
Ligand CYC Z 201



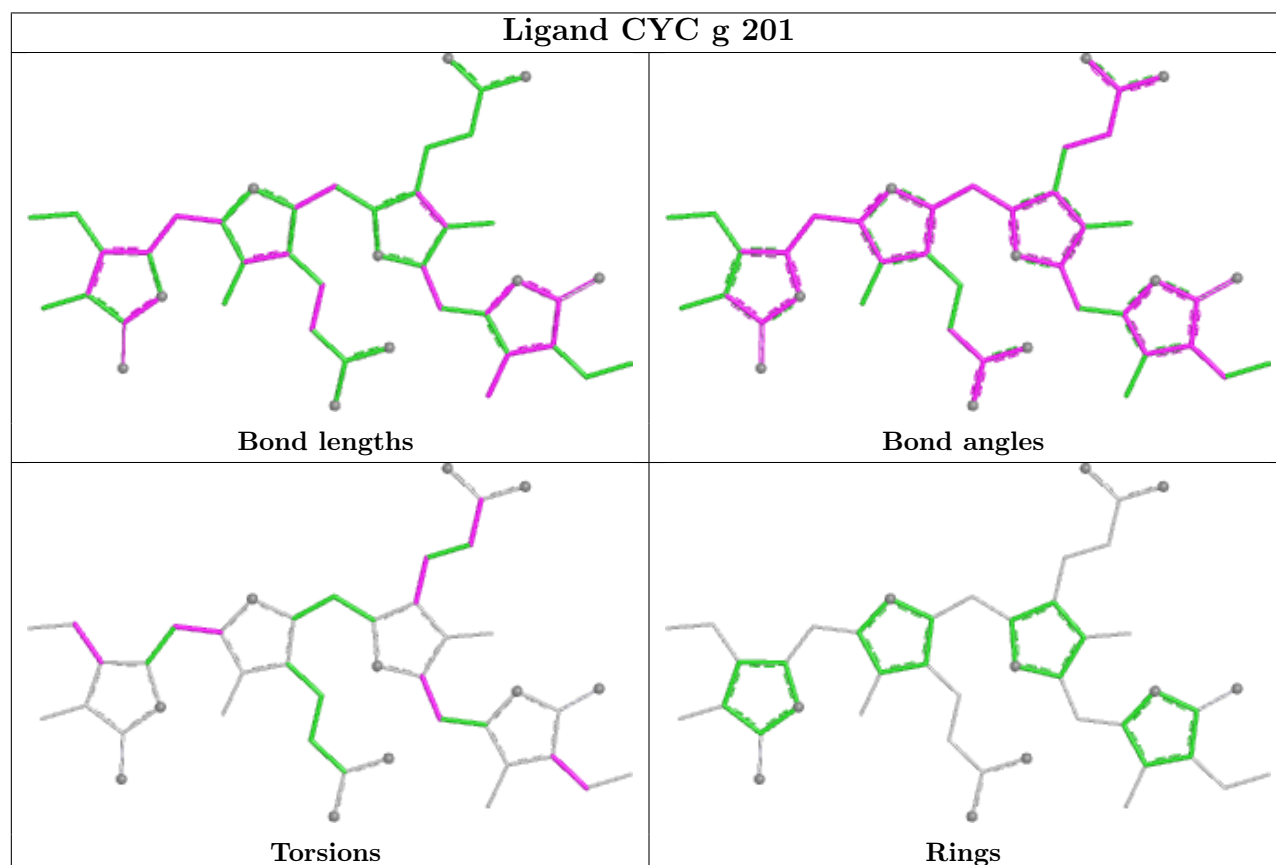
Ligand CYC W 201

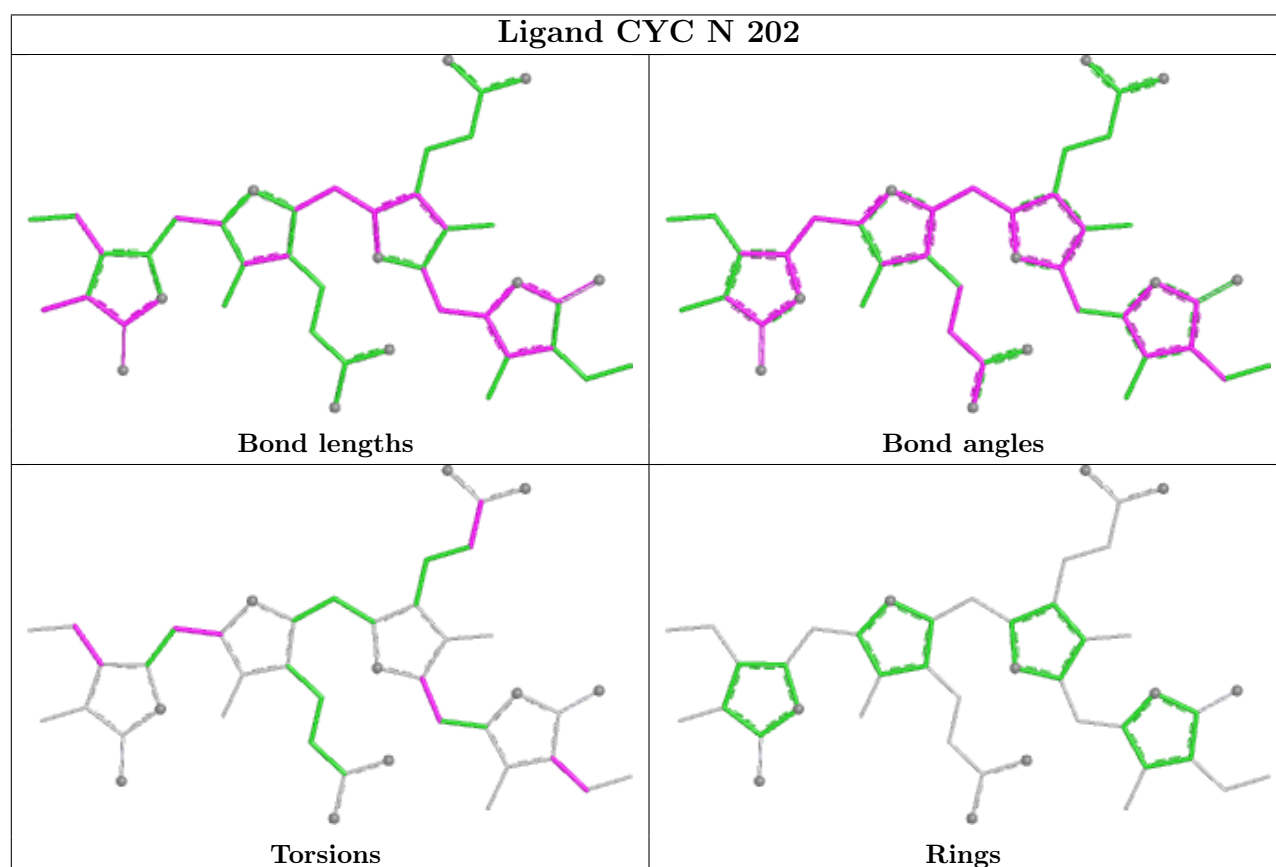
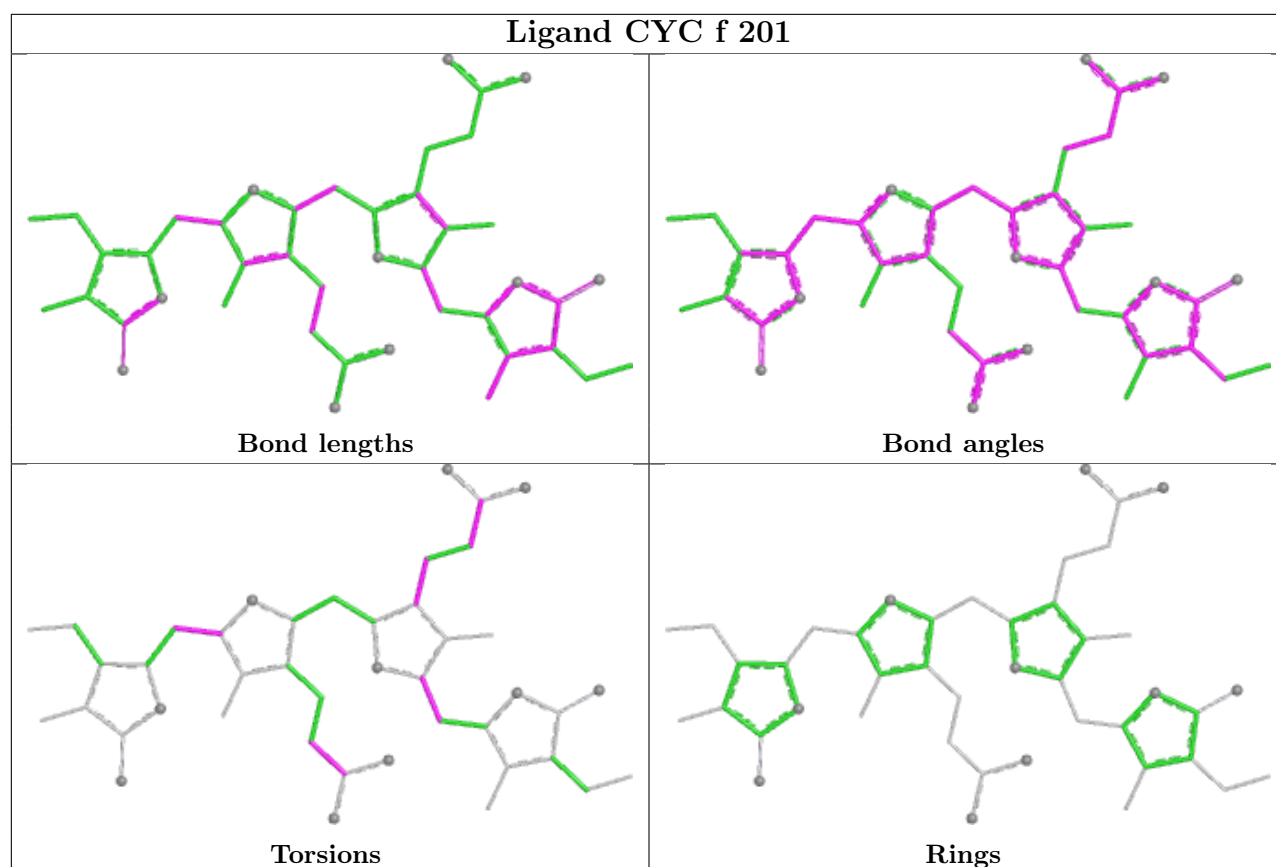


Ligand CYC Z 202

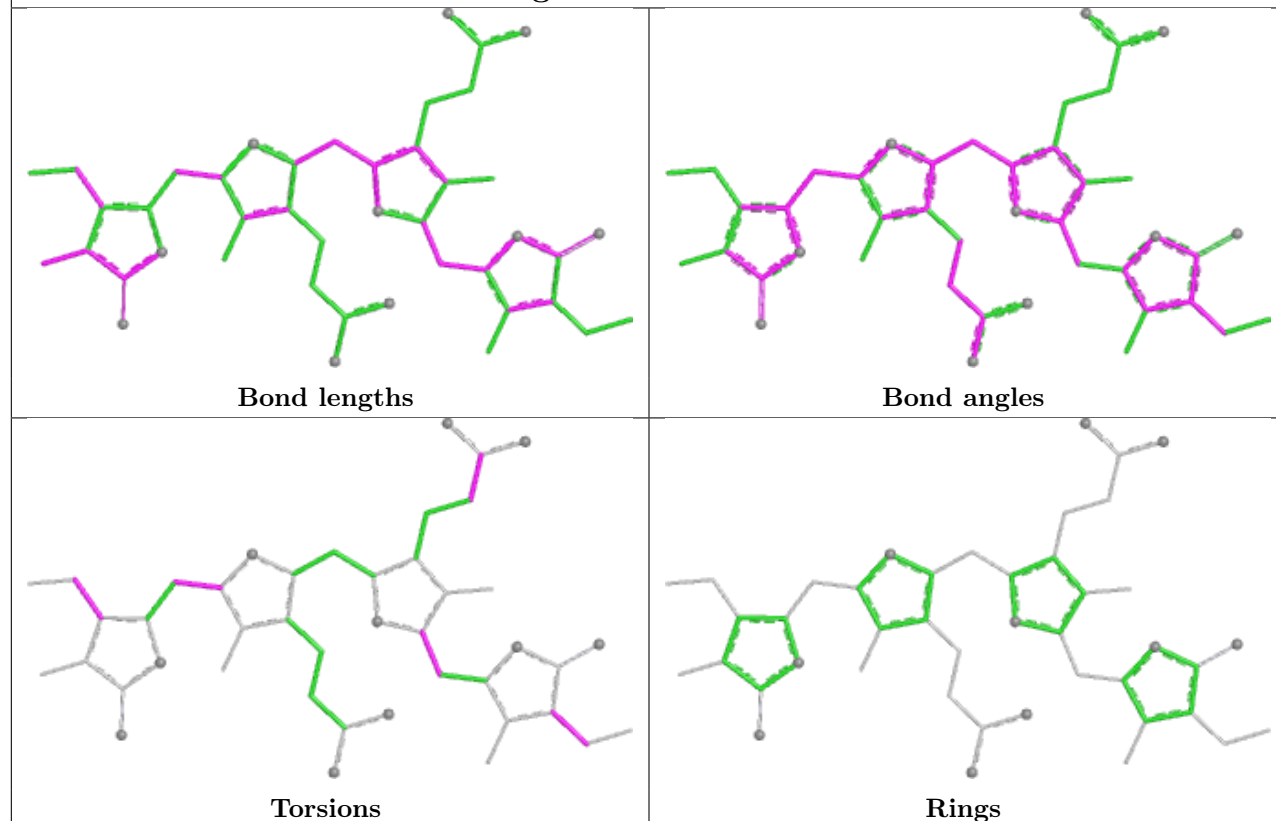


Ligand CYC g 201

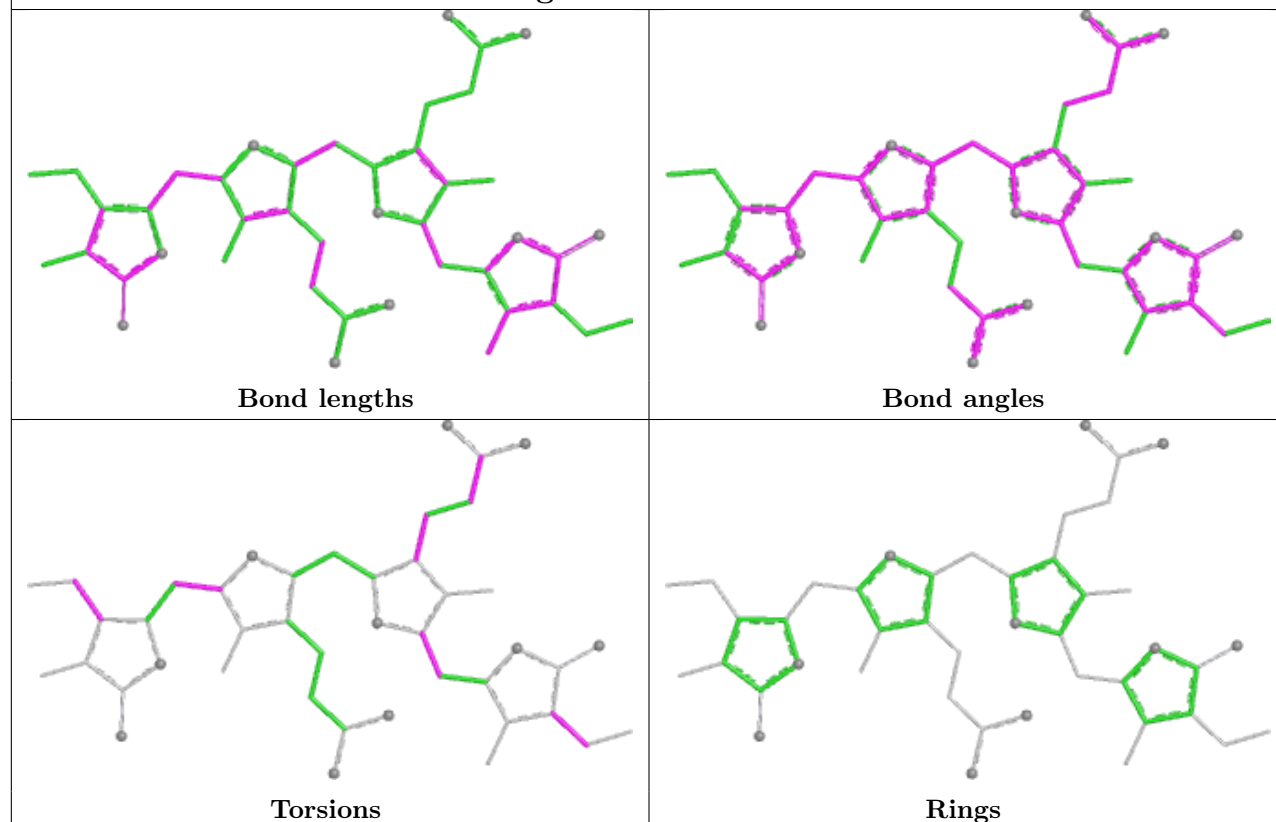




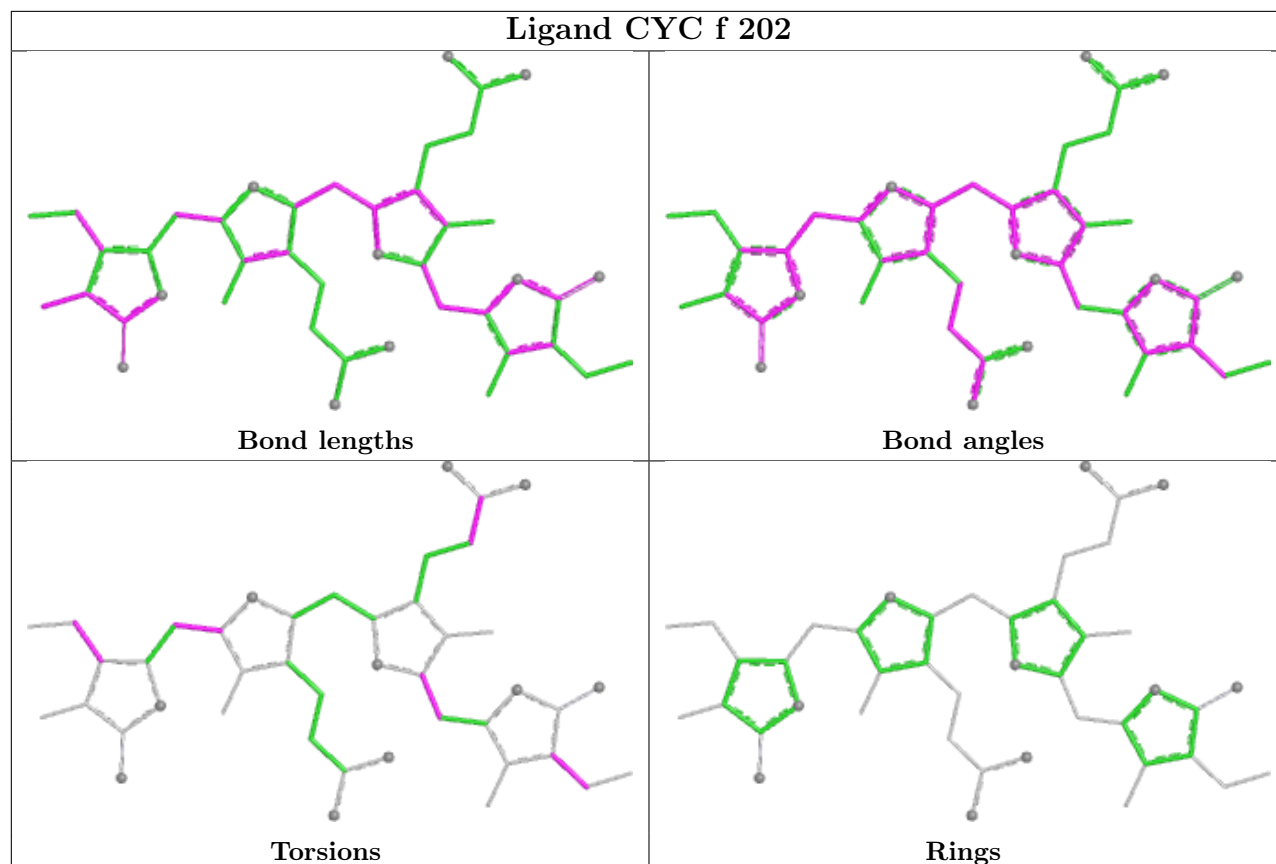
Ligand CYC L 202



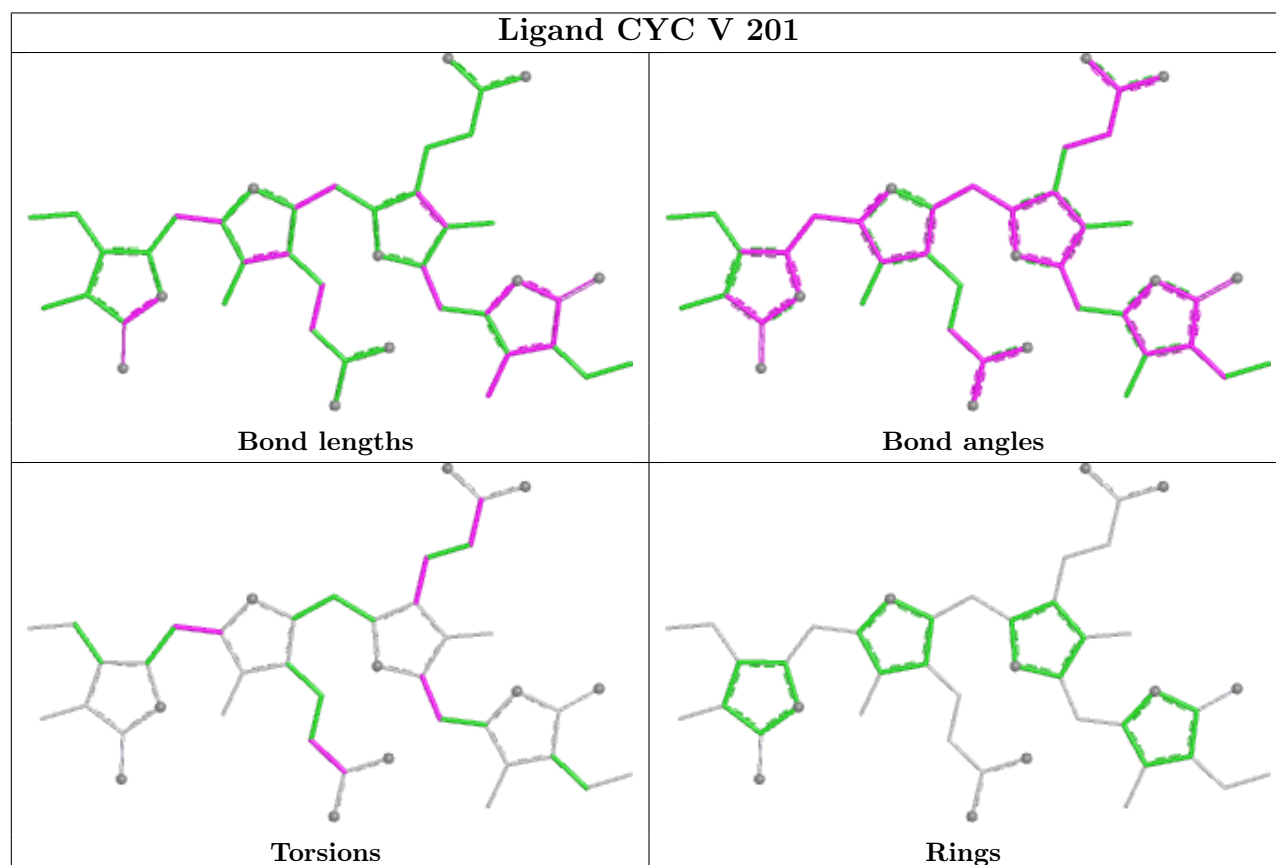
Ligand CYC I 201

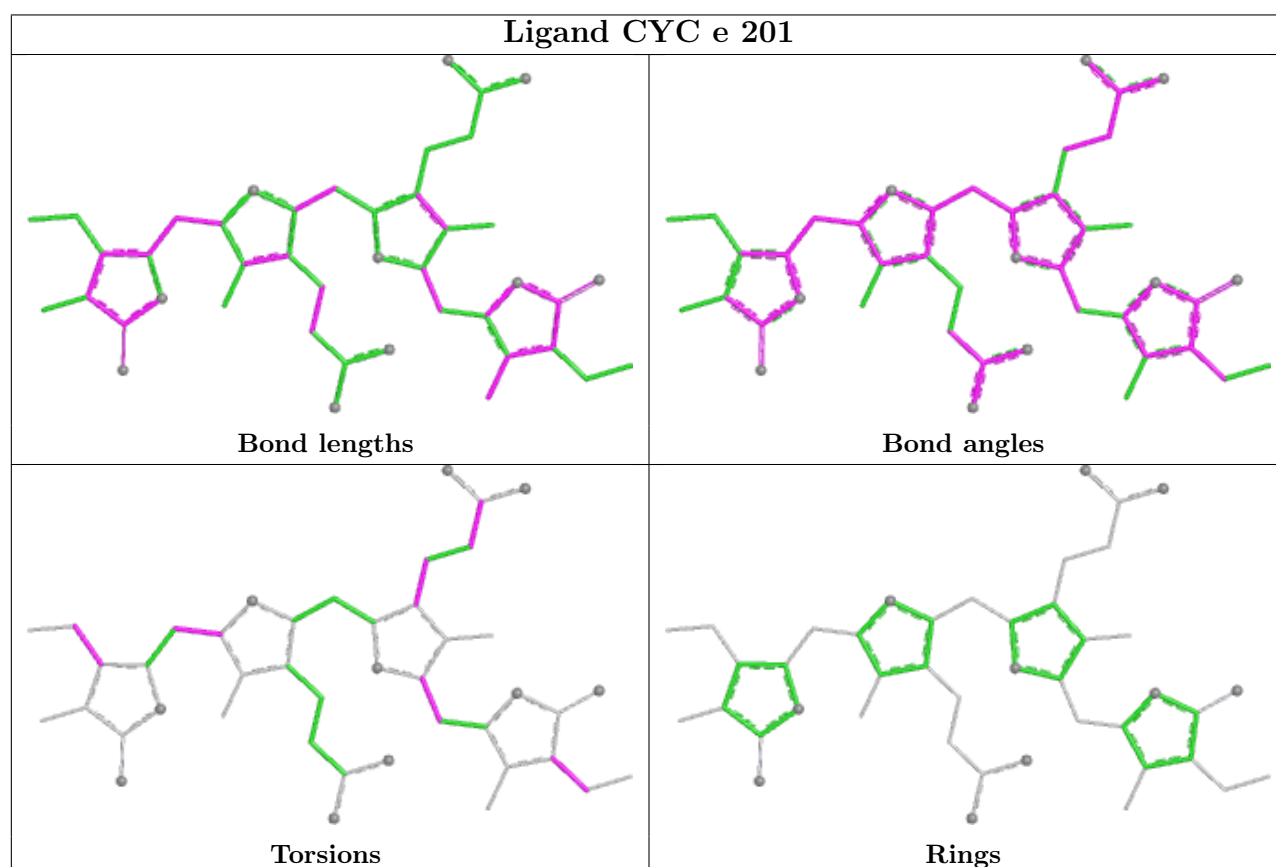
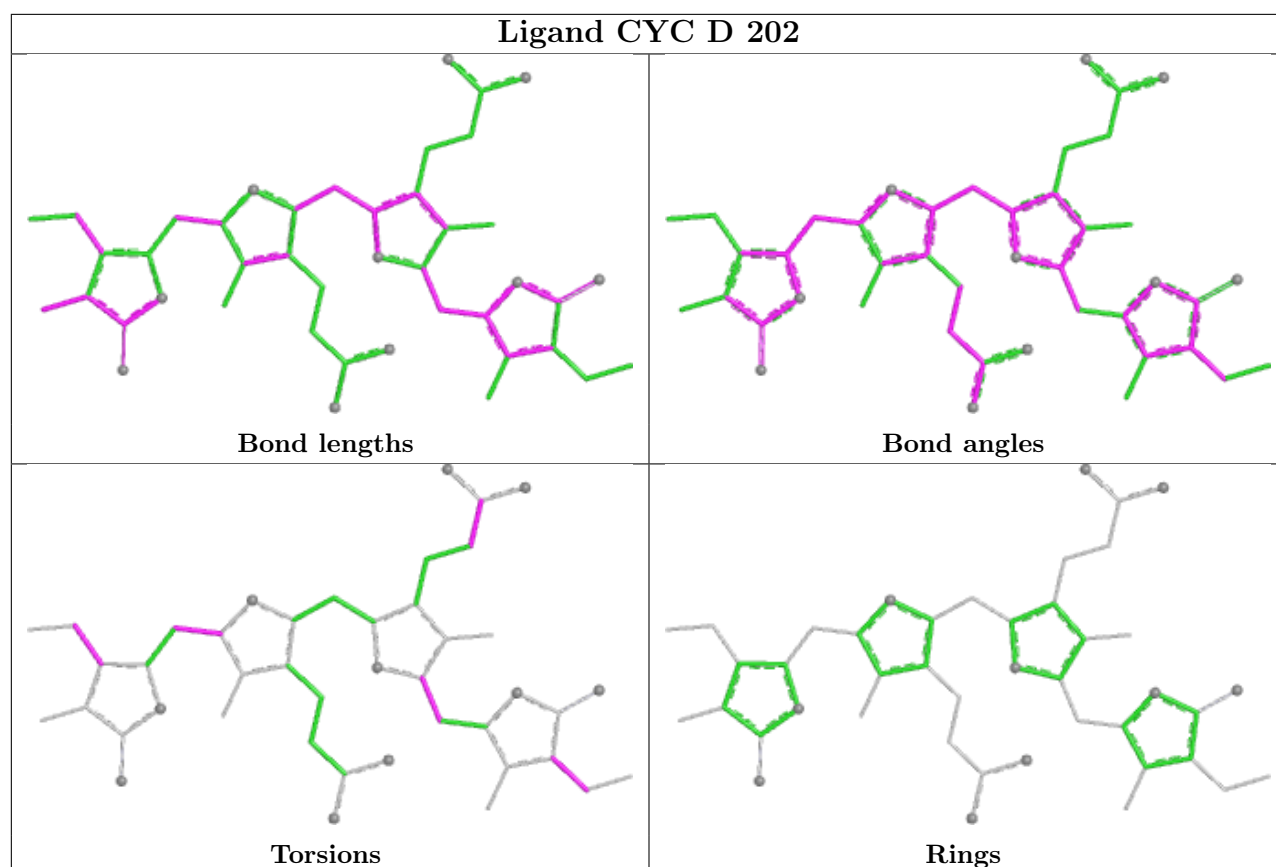


Ligand CYC f 202

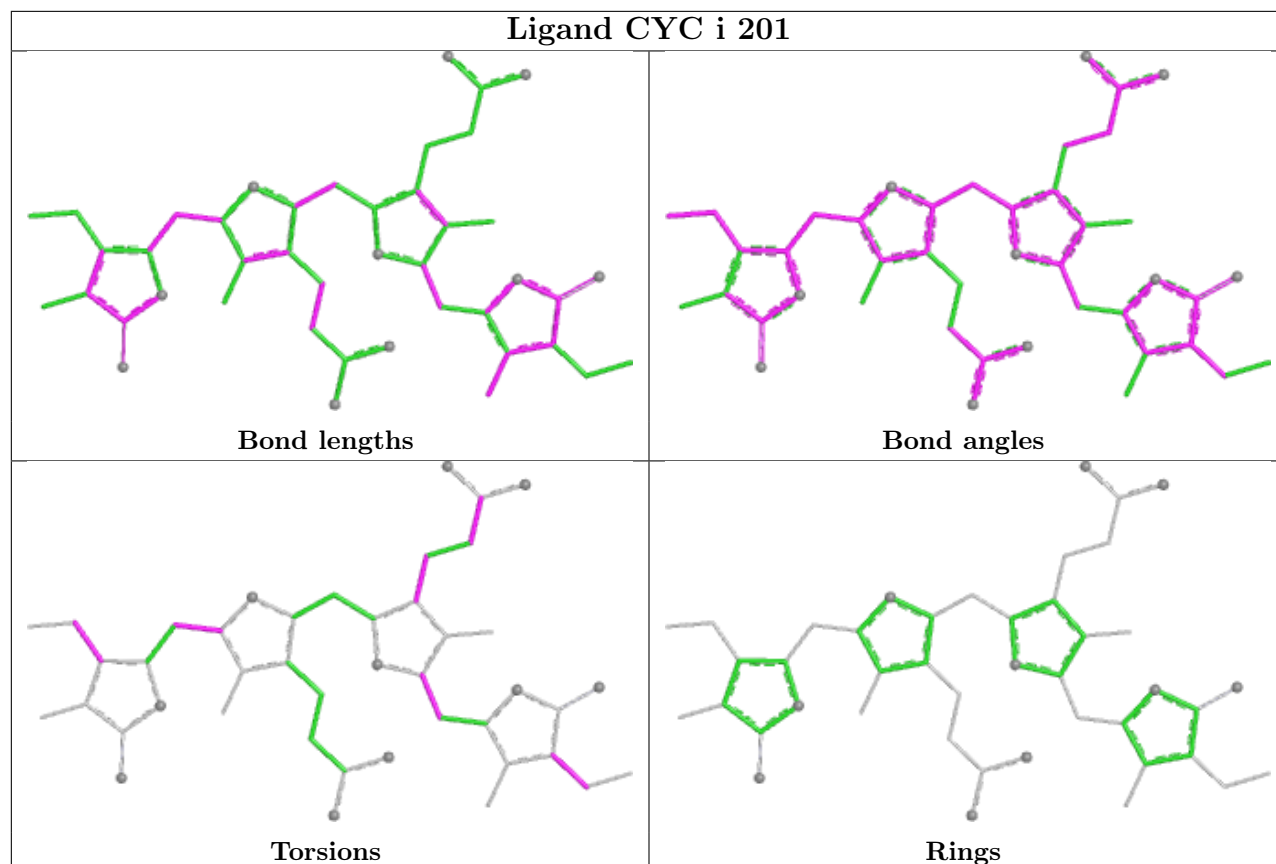


Ligand CYC V 201

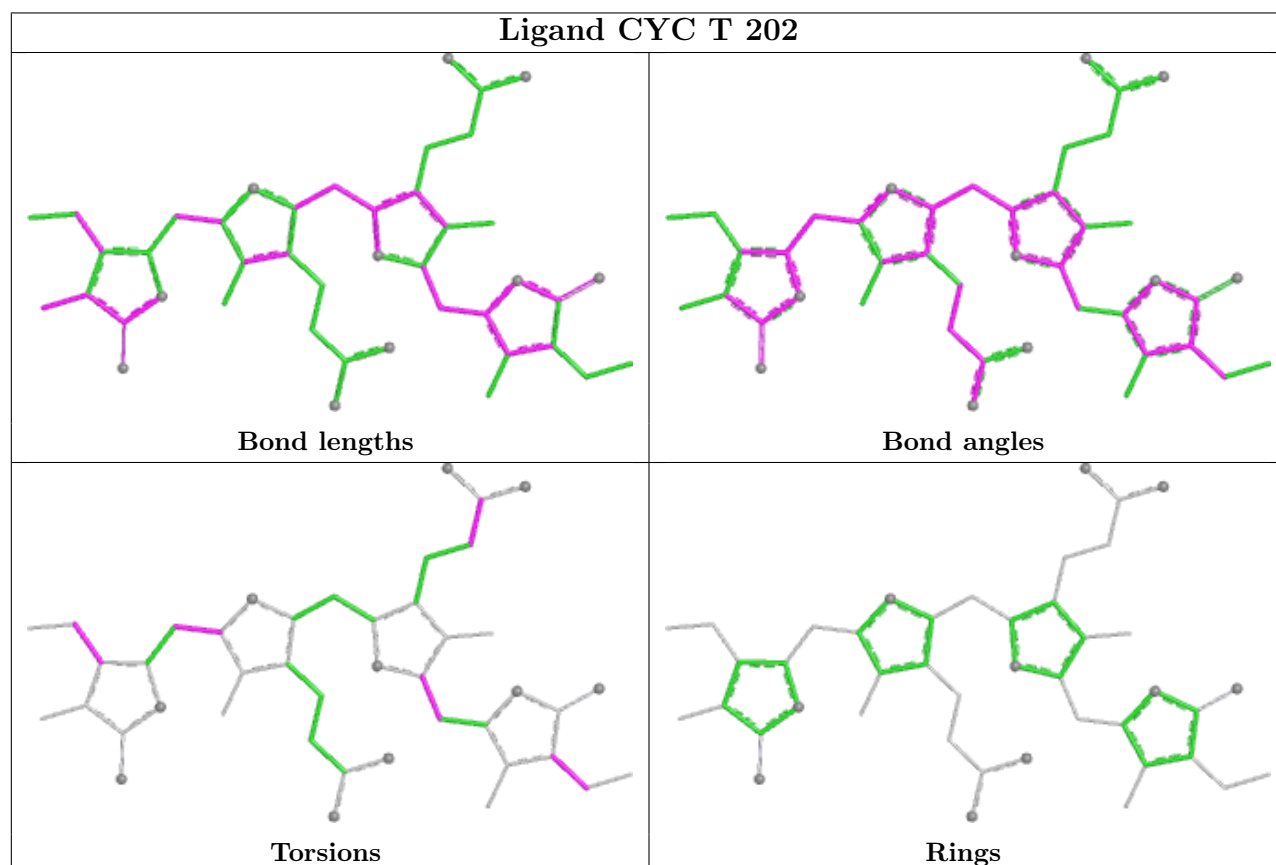


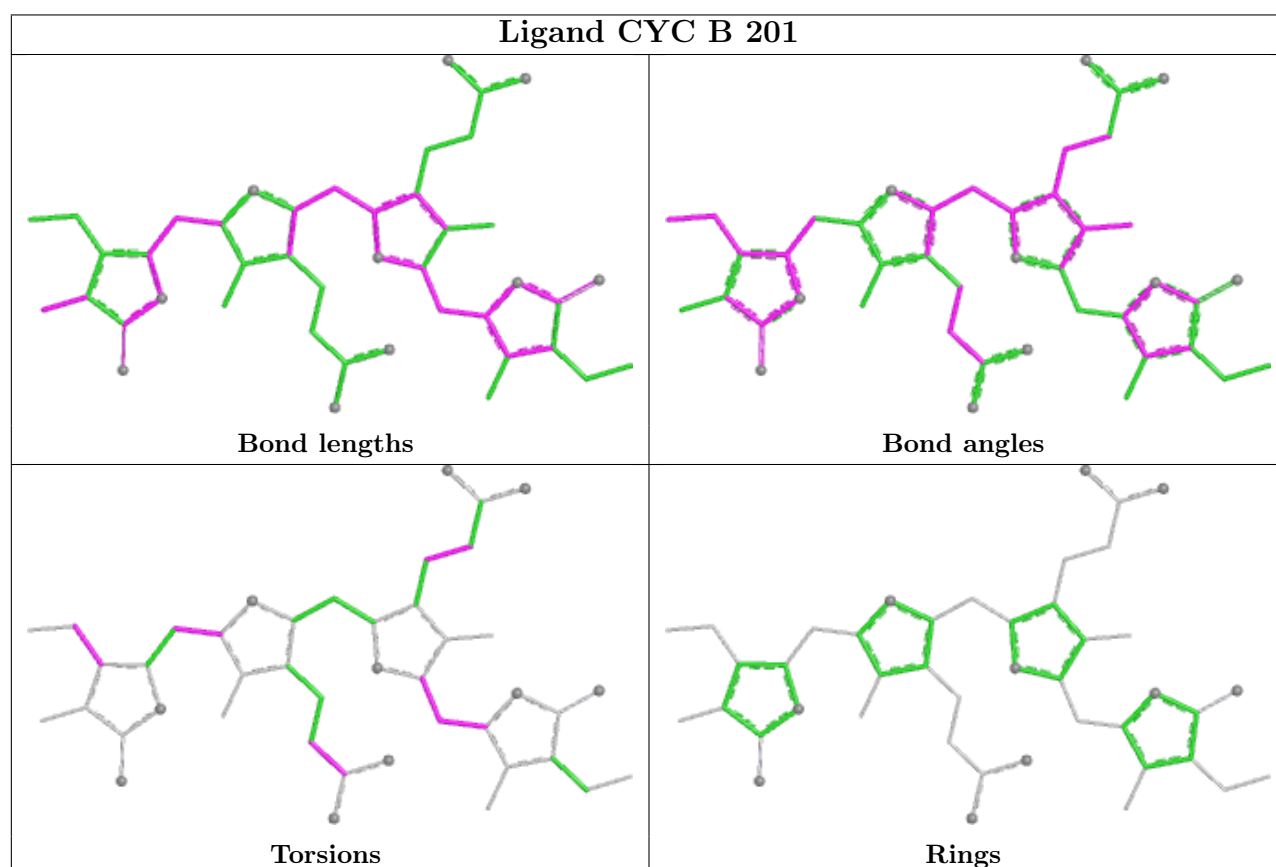
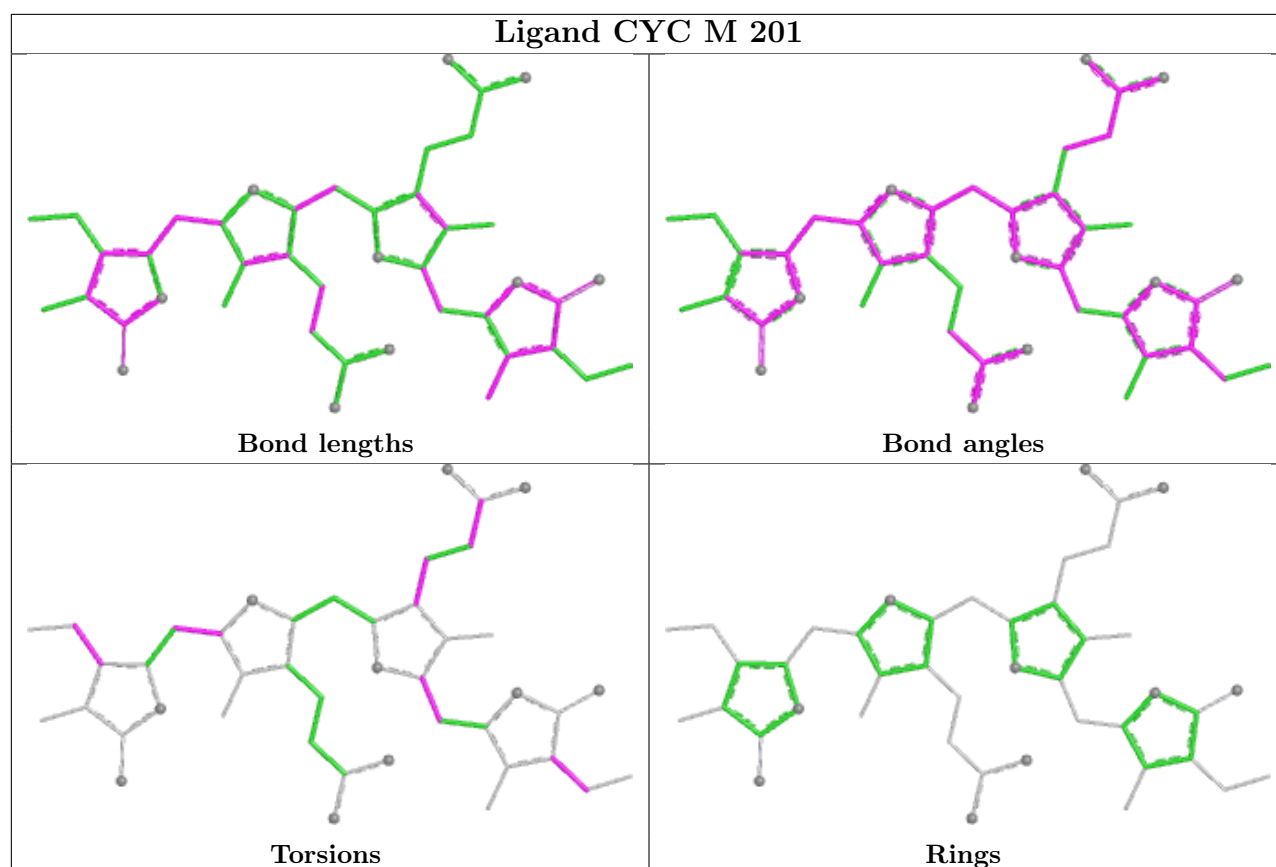


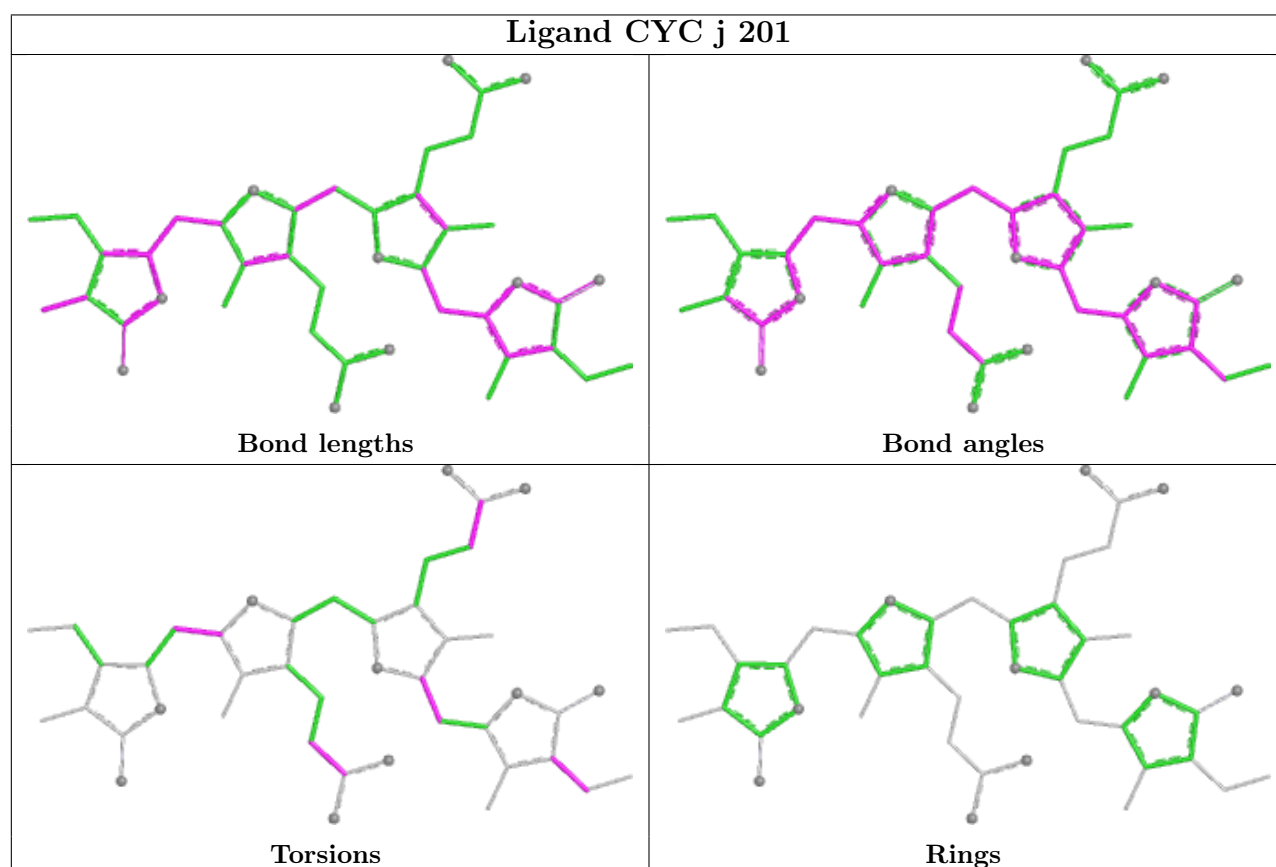
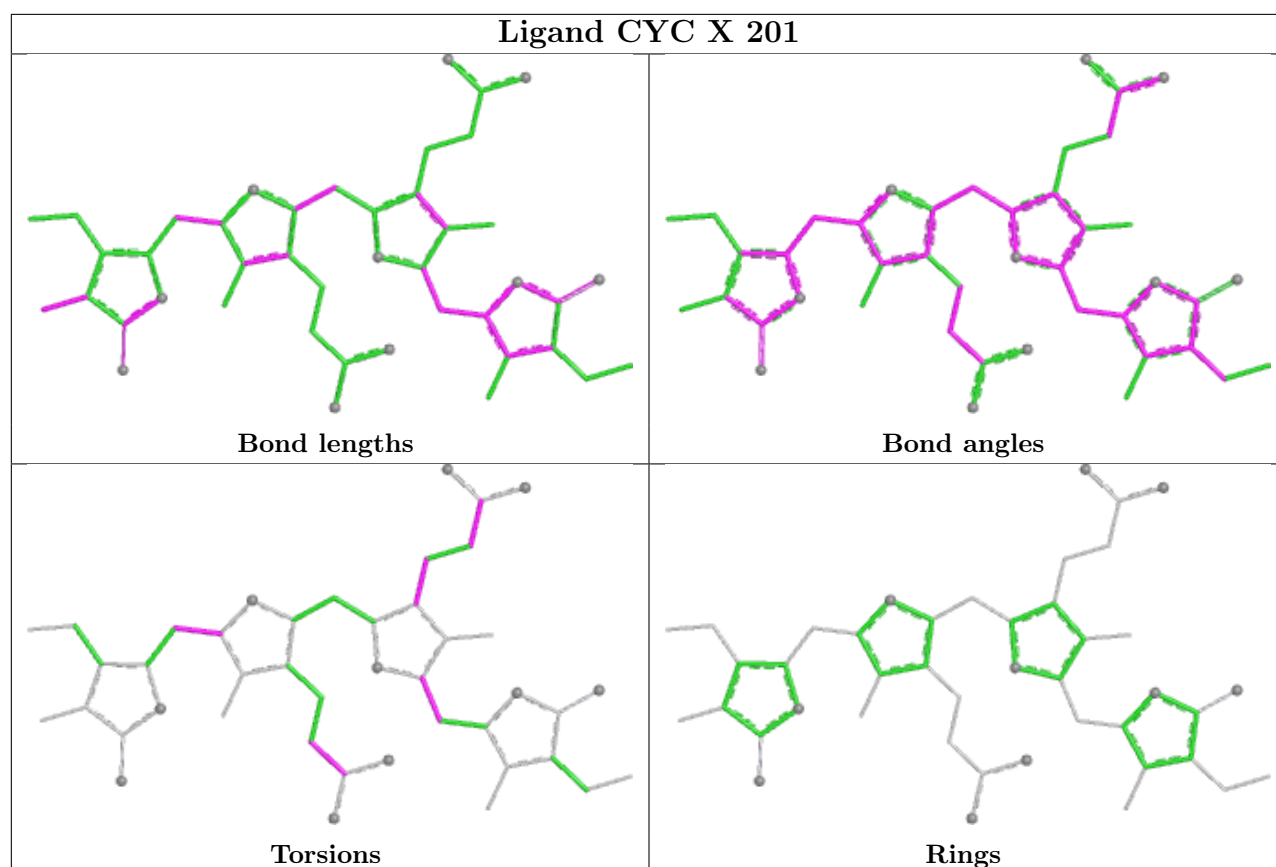
Ligand CYC i 201

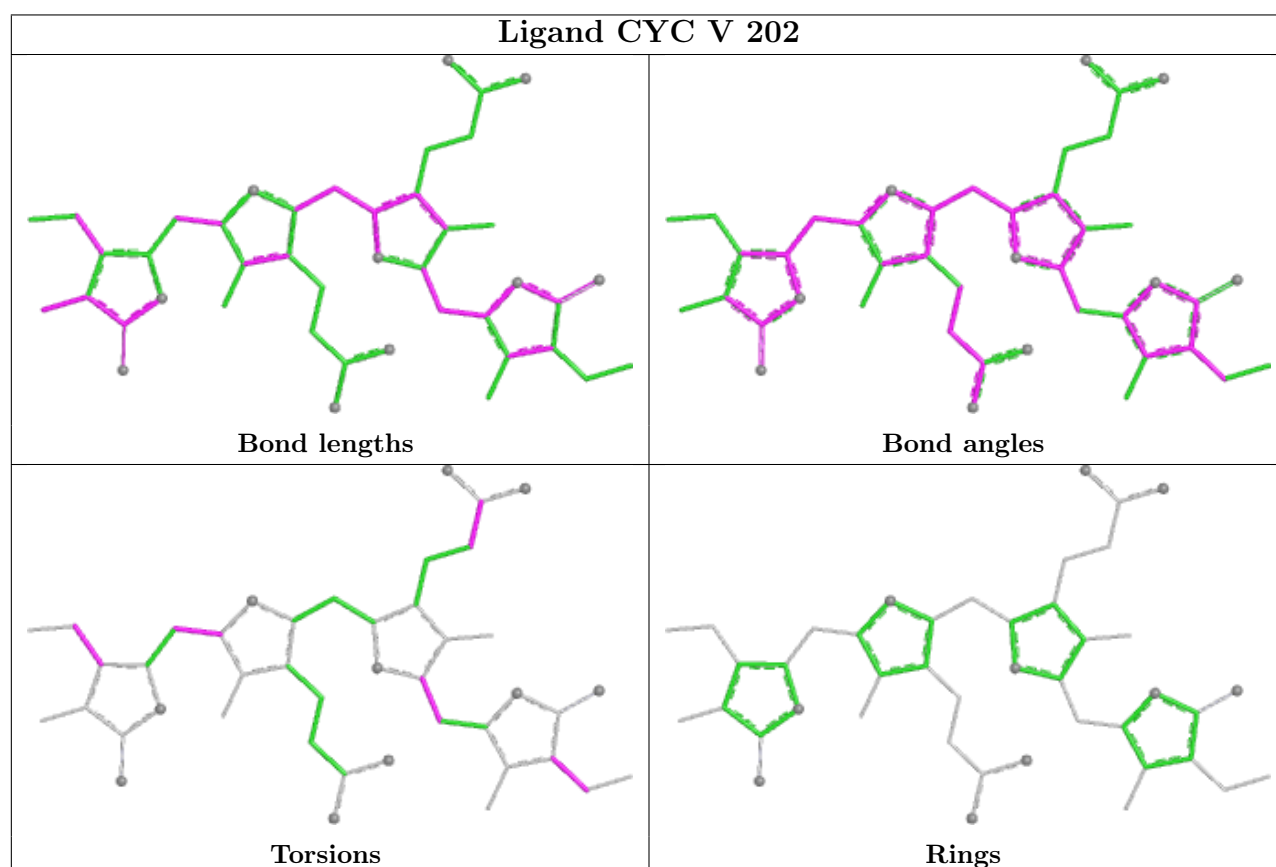
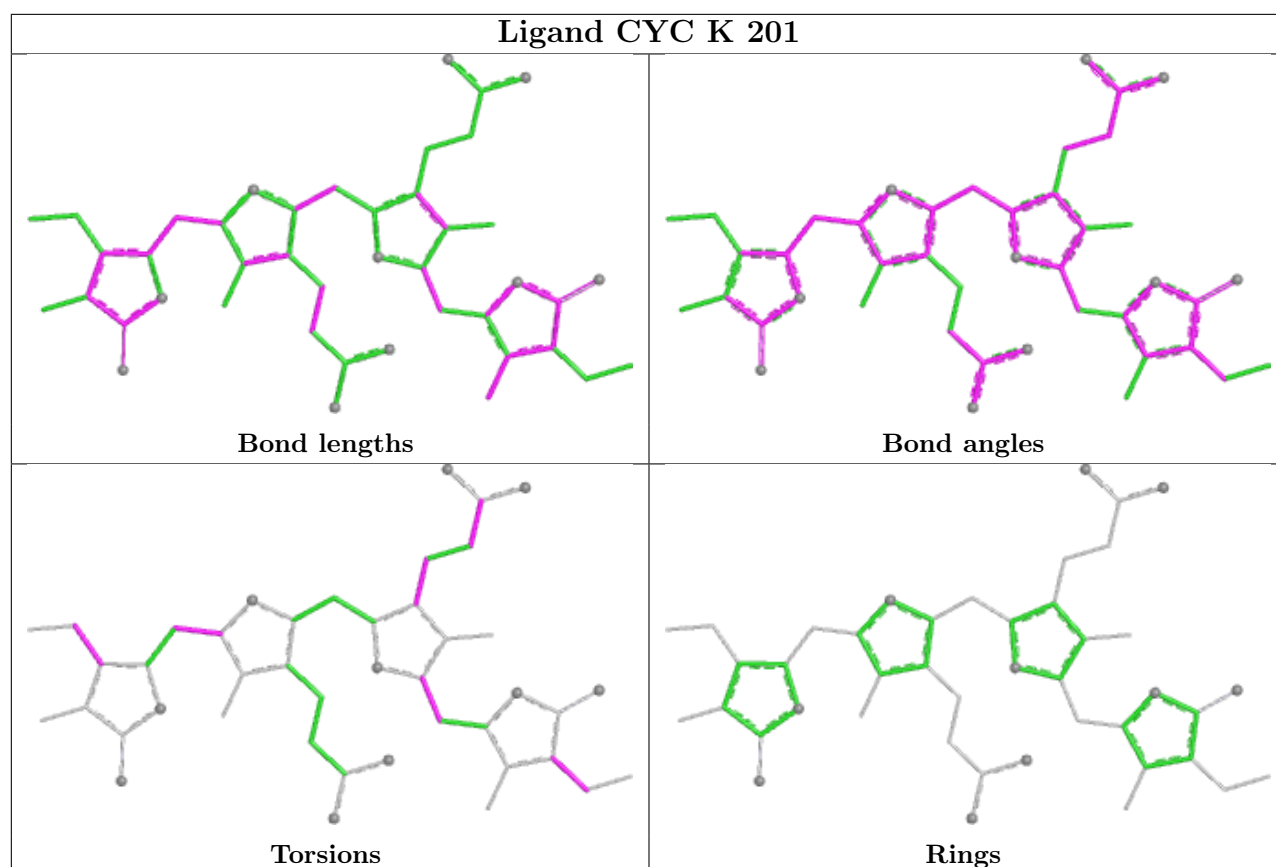


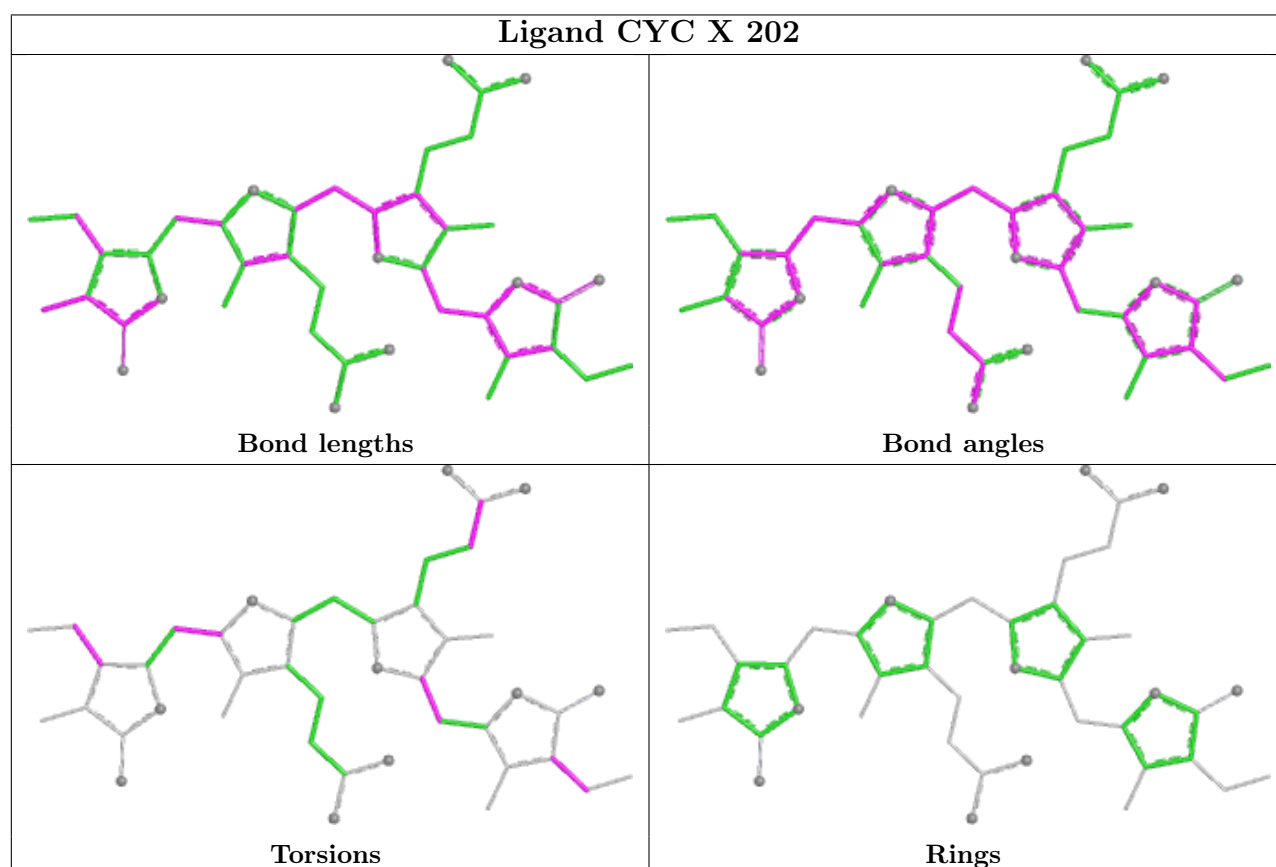
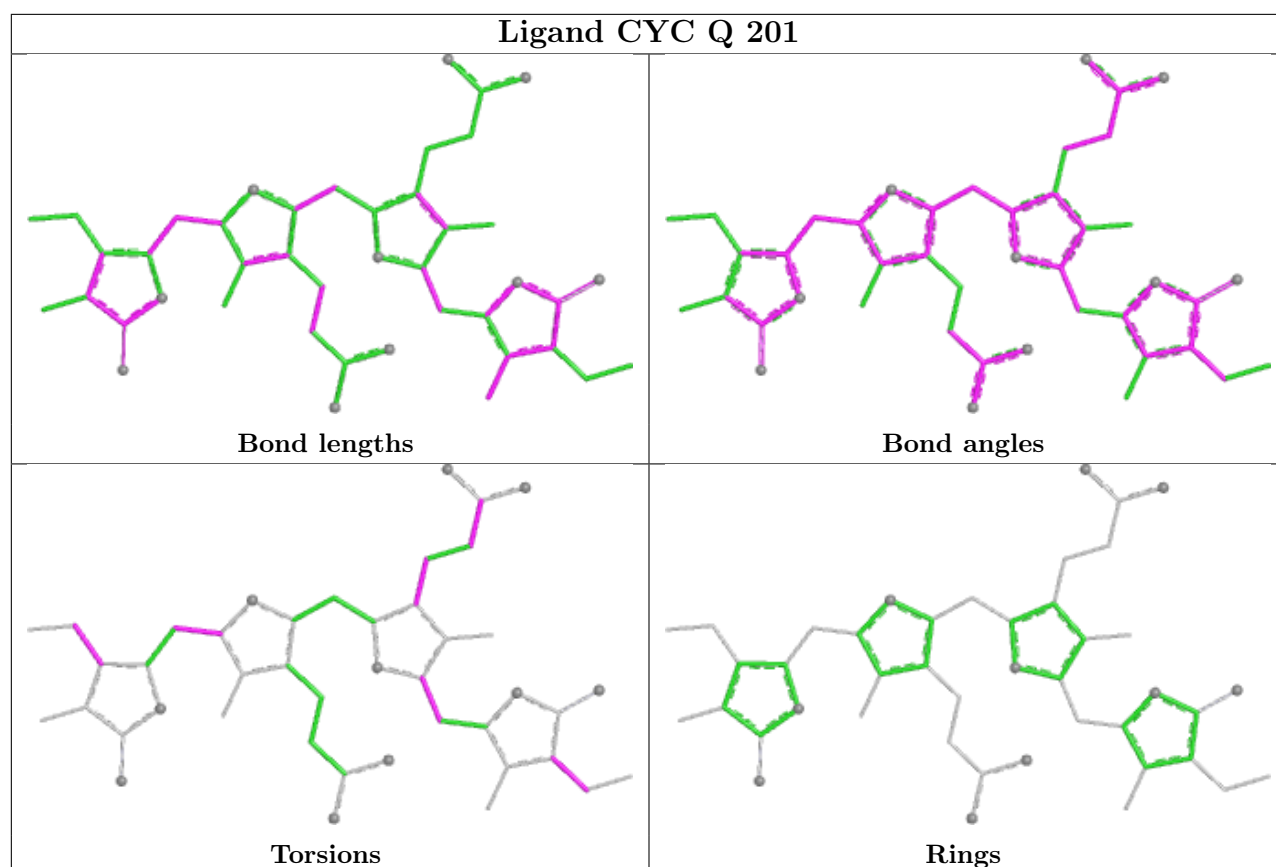
Ligand CYC T 202











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.

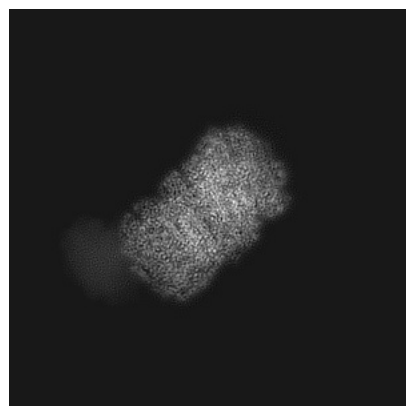
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34724. These allow visual inspection of the internal detail of the map and identification of artifacts.

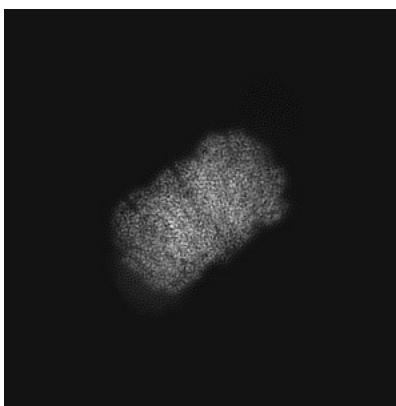
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

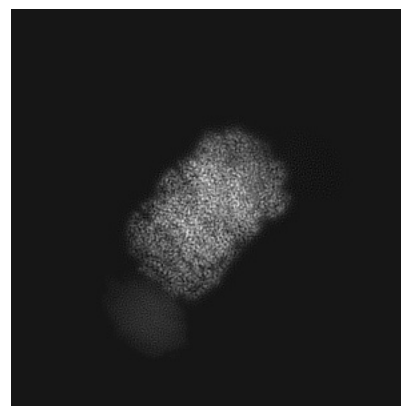
6.1.1 Primary map



X

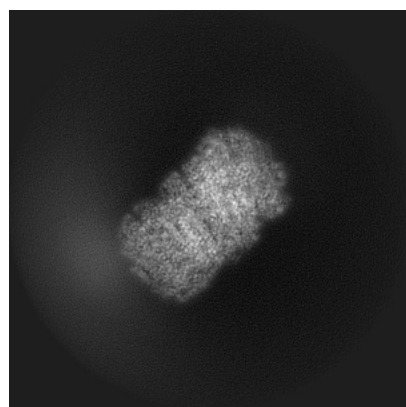


Y

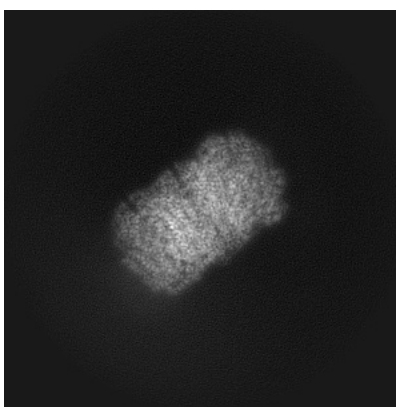


Z

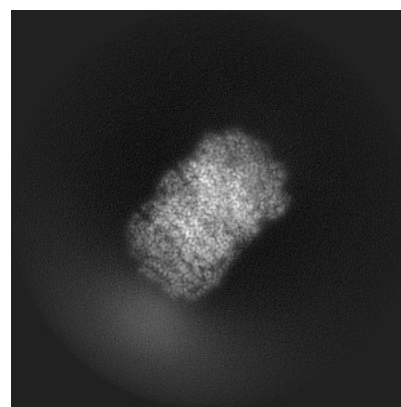
6.1.2 Raw map



X



Y

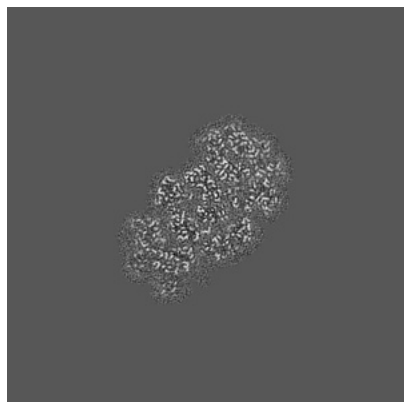


Z

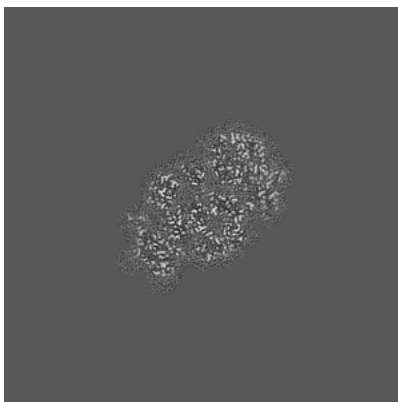
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

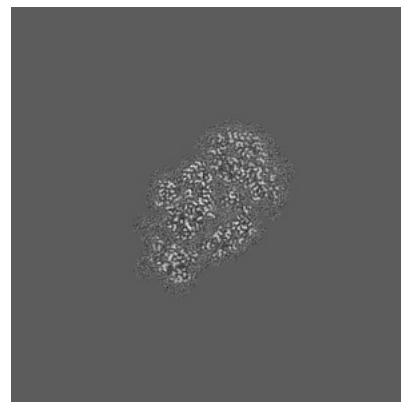
6.2.1 Primary map



X Index: 180

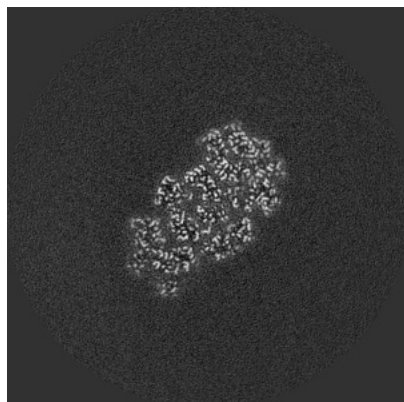


Y Index: 180

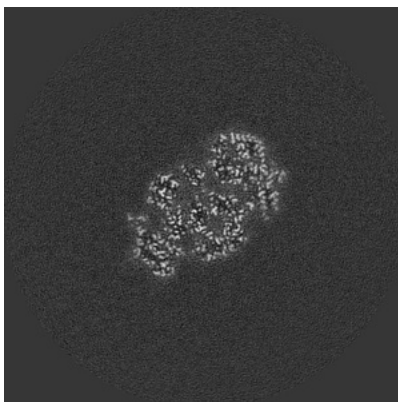


Z Index: 180

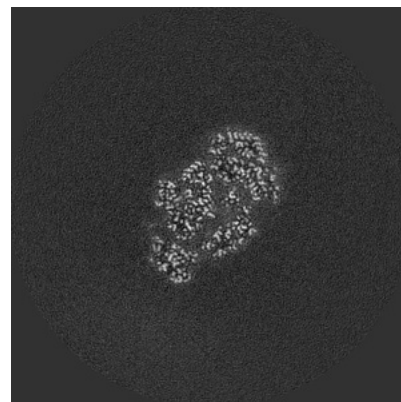
6.2.2 Raw map



X Index: 180



Y Index: 180

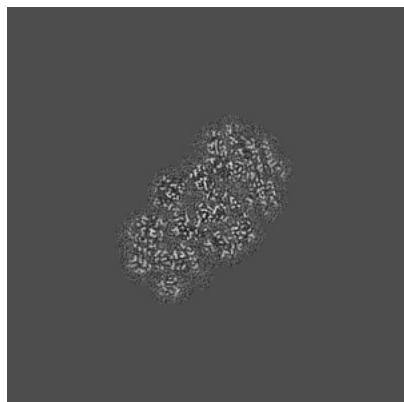


Z Index: 180

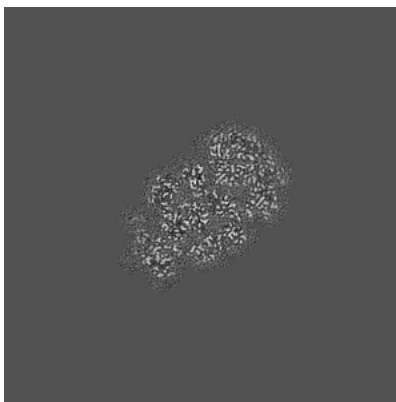
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

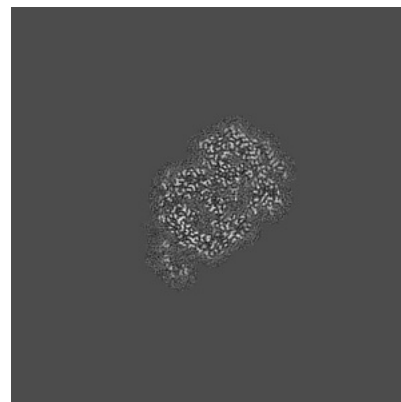
6.3.1 Primary map



X Index: 178

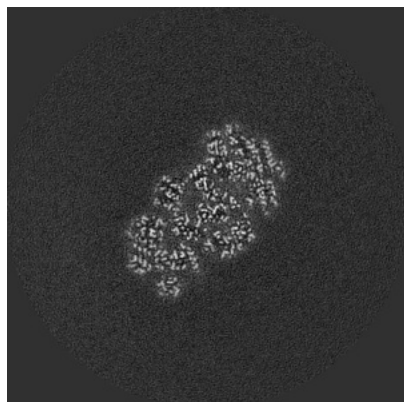


Y Index: 182

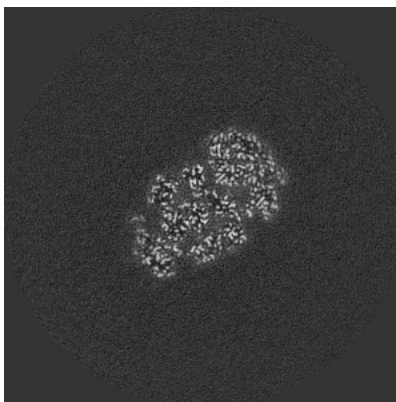


Z Index: 187

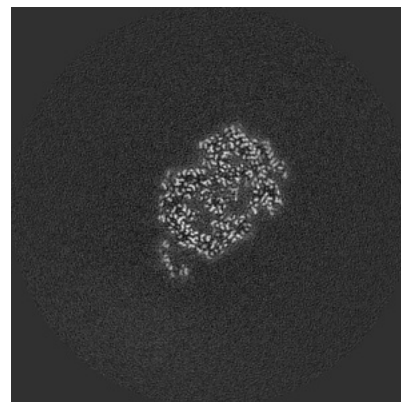
6.3.2 Raw map



X Index: 178



Y Index: 182

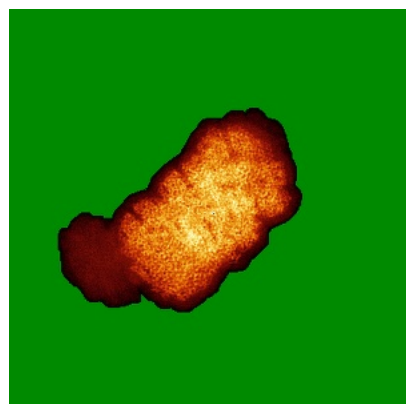


Z Index: 187

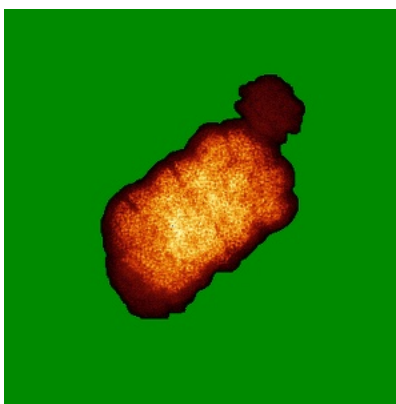
The images above show the largest variance slices of the map in three orthogonal directions.

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

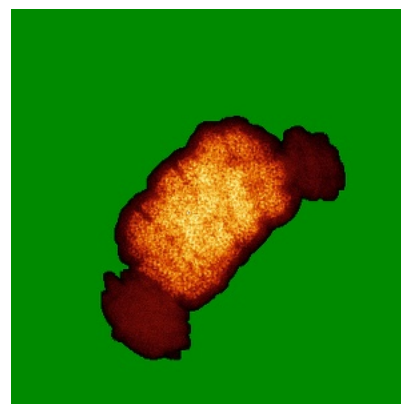
6.4.1 Primary map



X

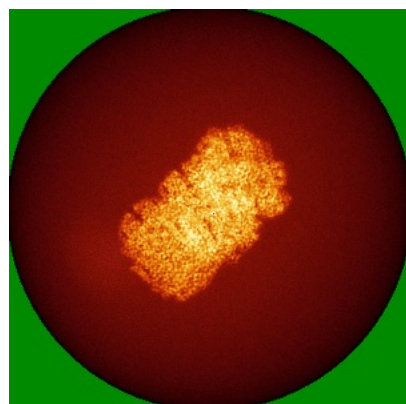


Y

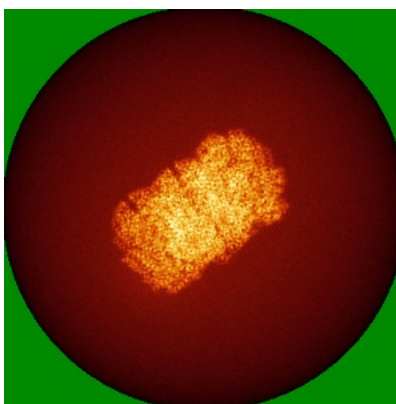


Z

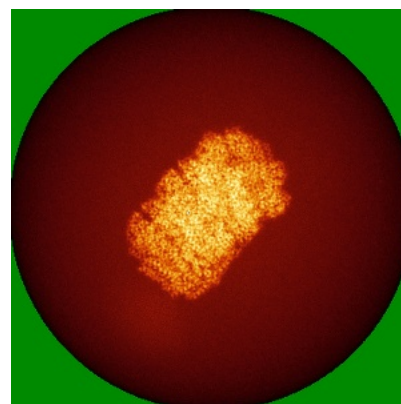
6.4.2 Raw map



X



Y

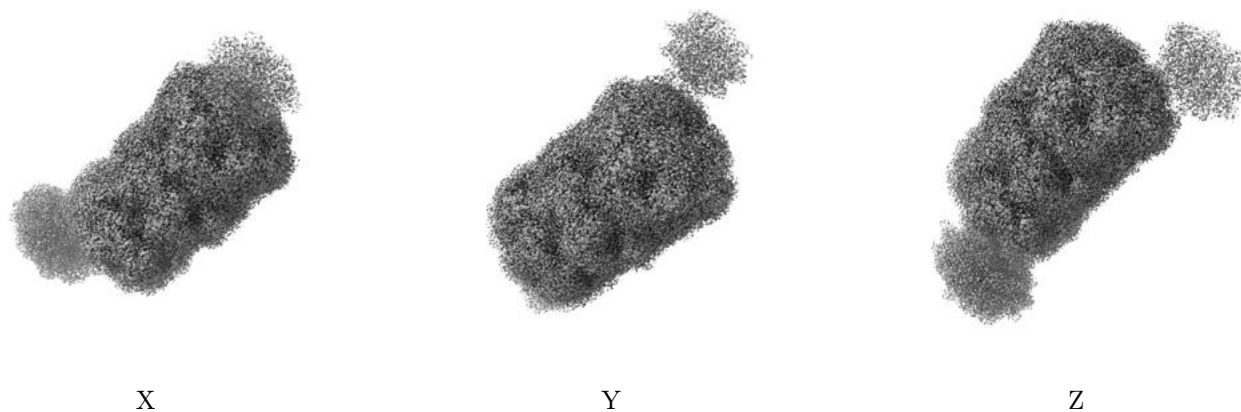


Z

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

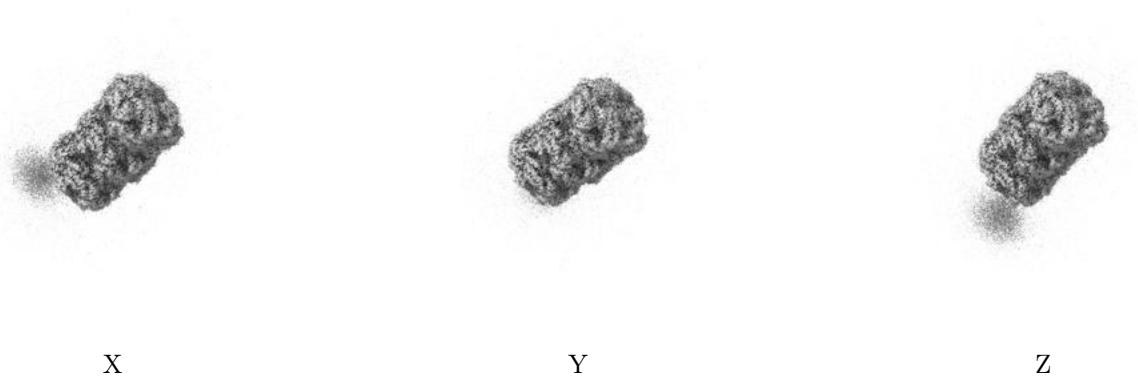
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0164. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

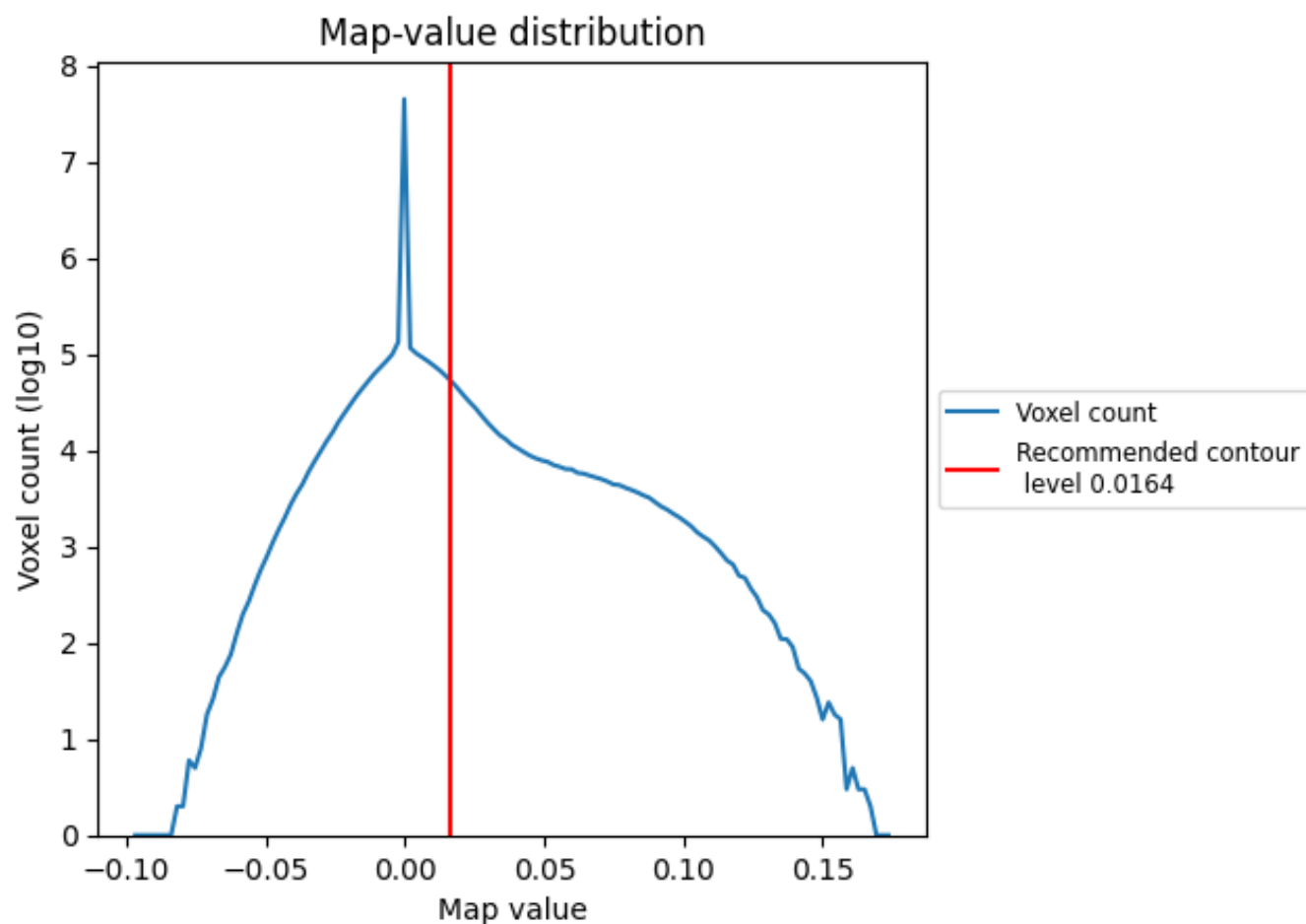
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

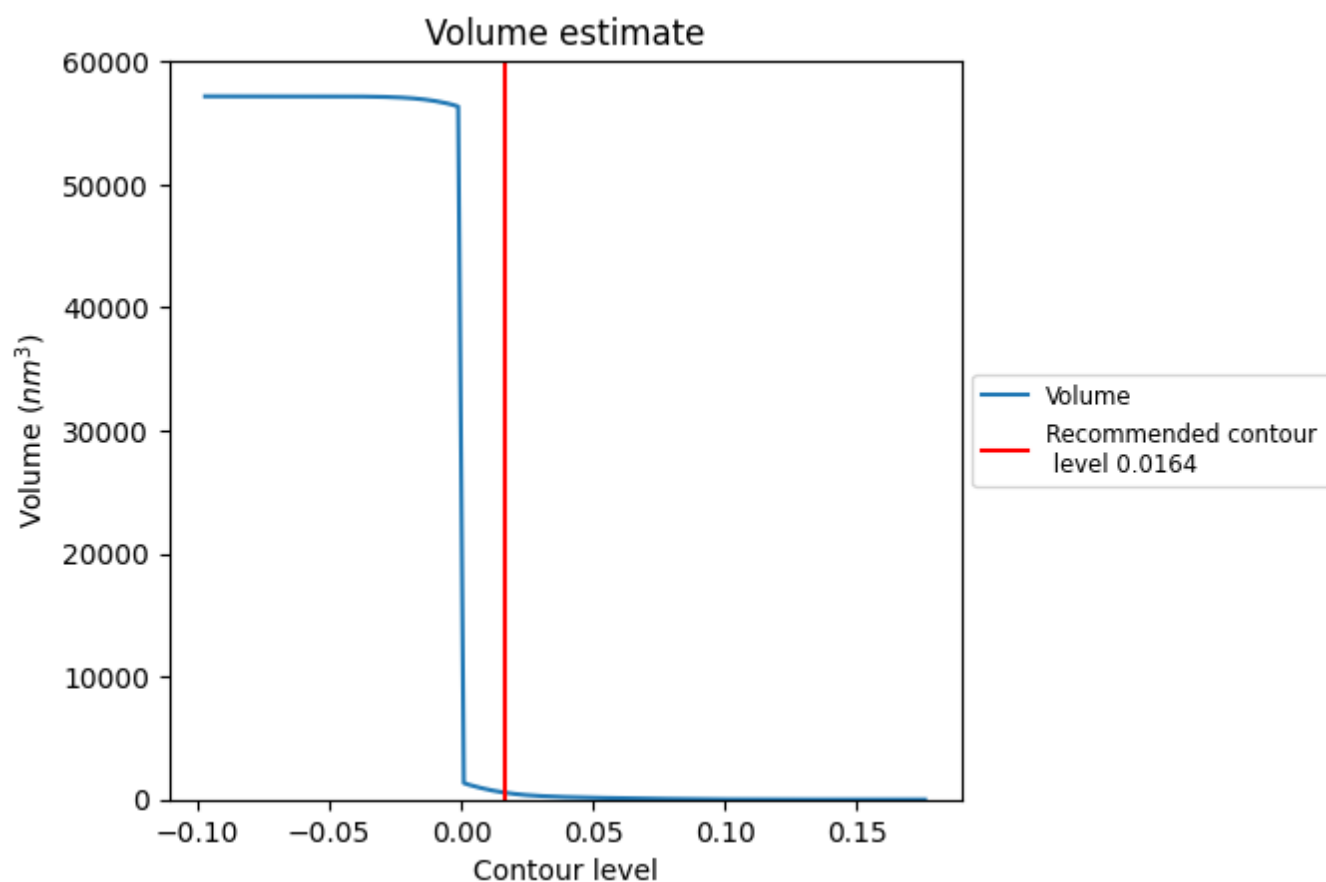
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

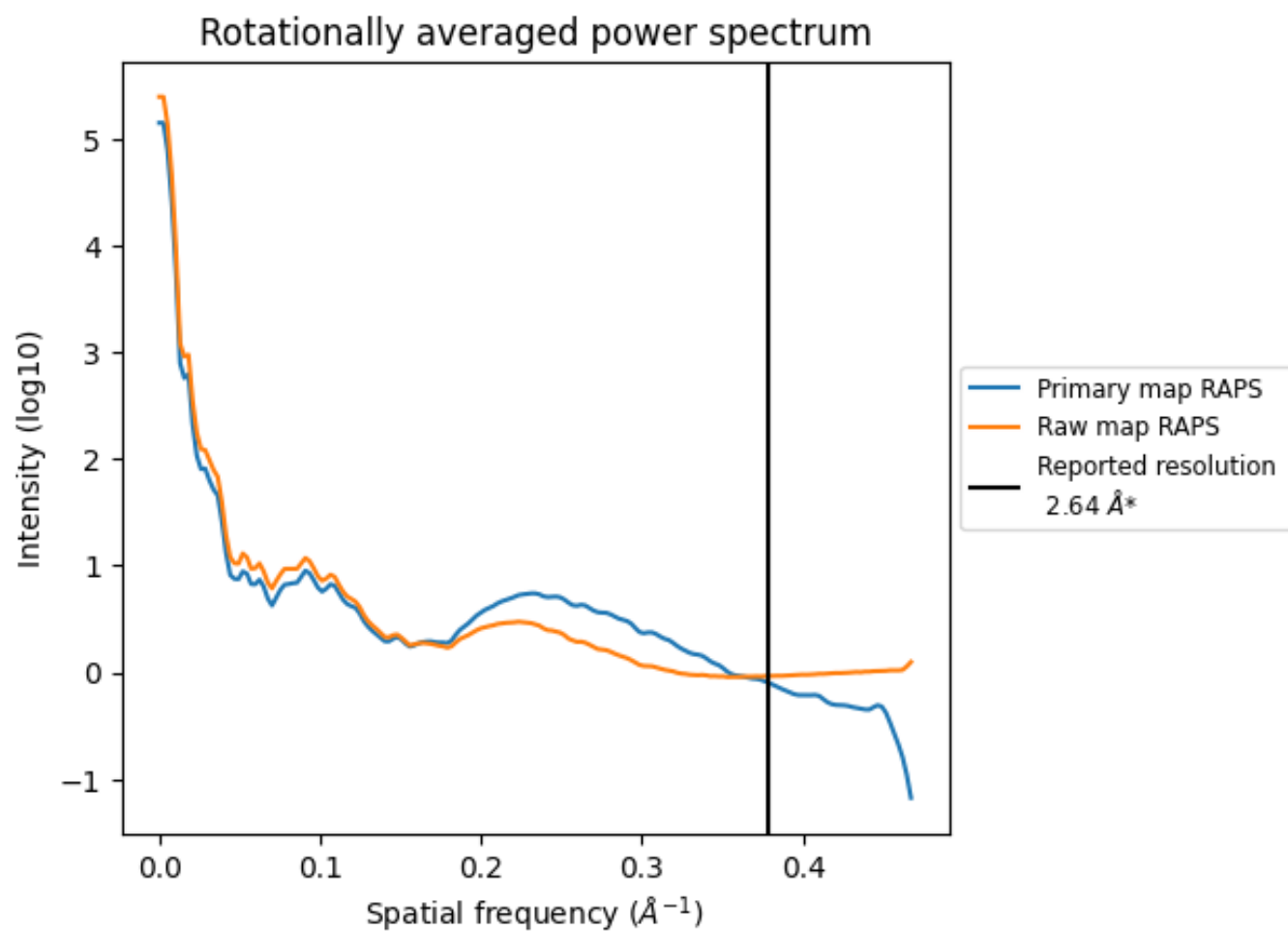
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 571 nm³; this corresponds to an approximate mass of 516 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 ⓘ

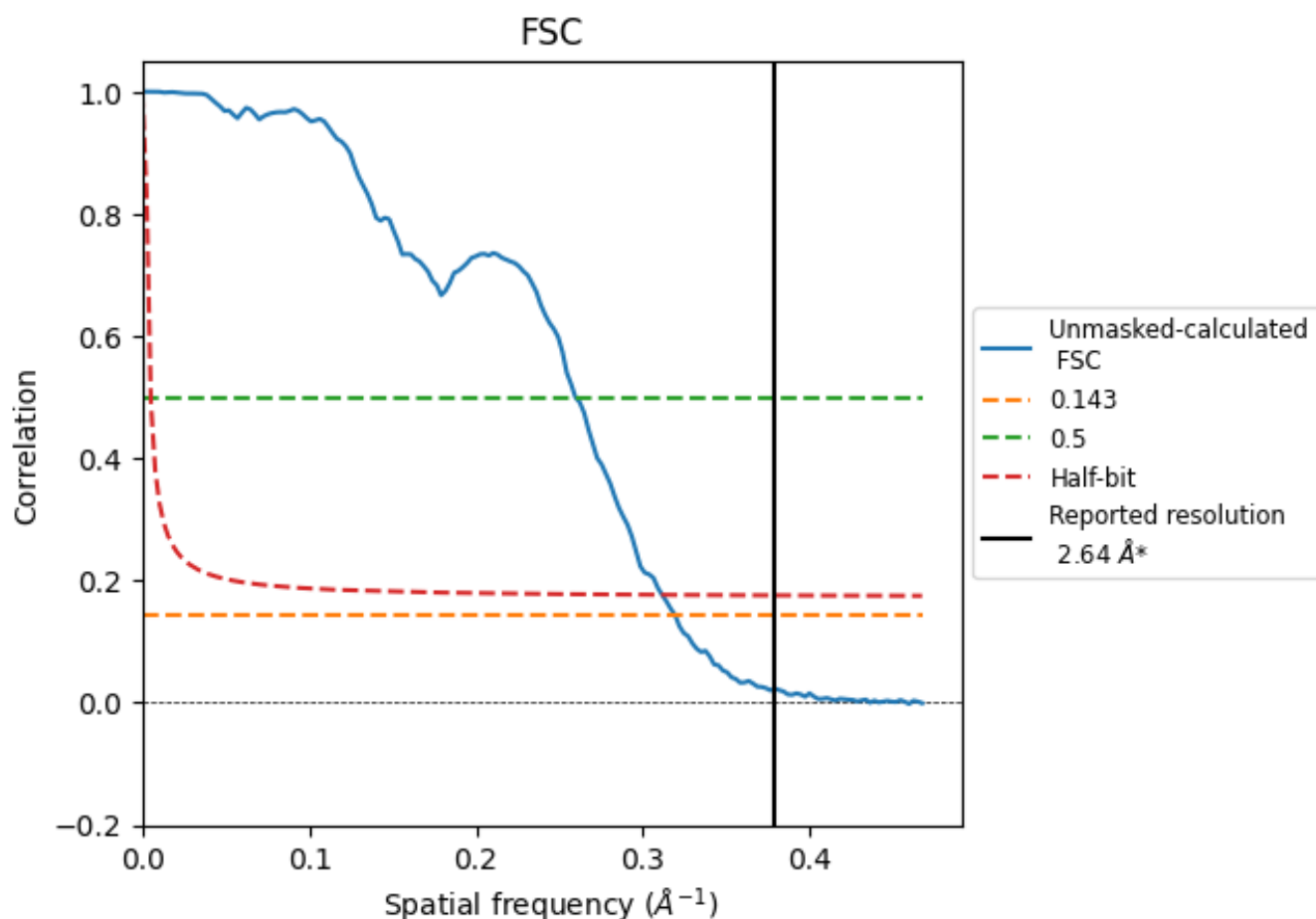


*Reported resolution corresponds to spatial frequency of 0.379 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.379 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

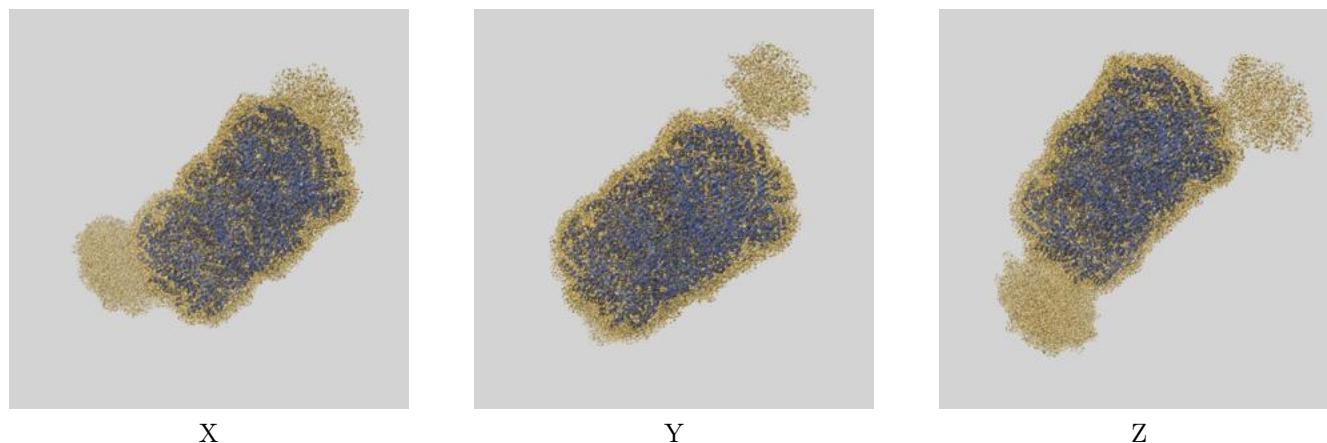
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.13	3.85	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.64 by more than 10 %

9 Map-model fit [i](#)

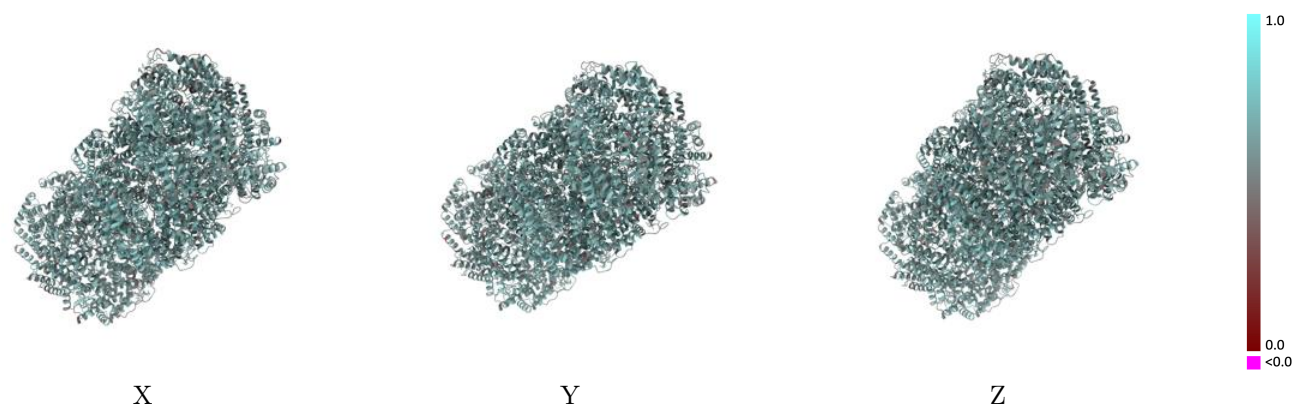
This section contains information regarding the fit between EMDB map EMD-34724 and PDB model 8HFQ. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



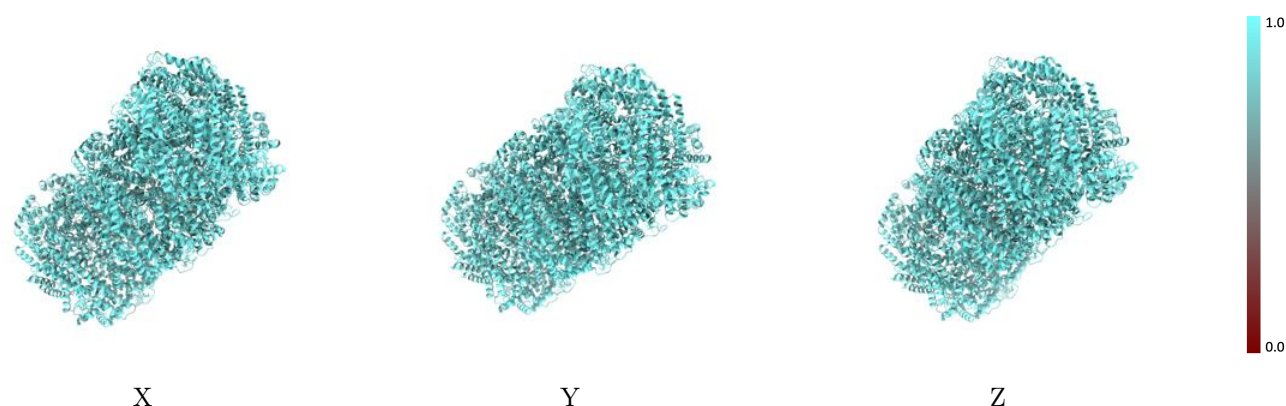
The images above show the 3D surface view of the map at the recommended contour level 0.0164 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



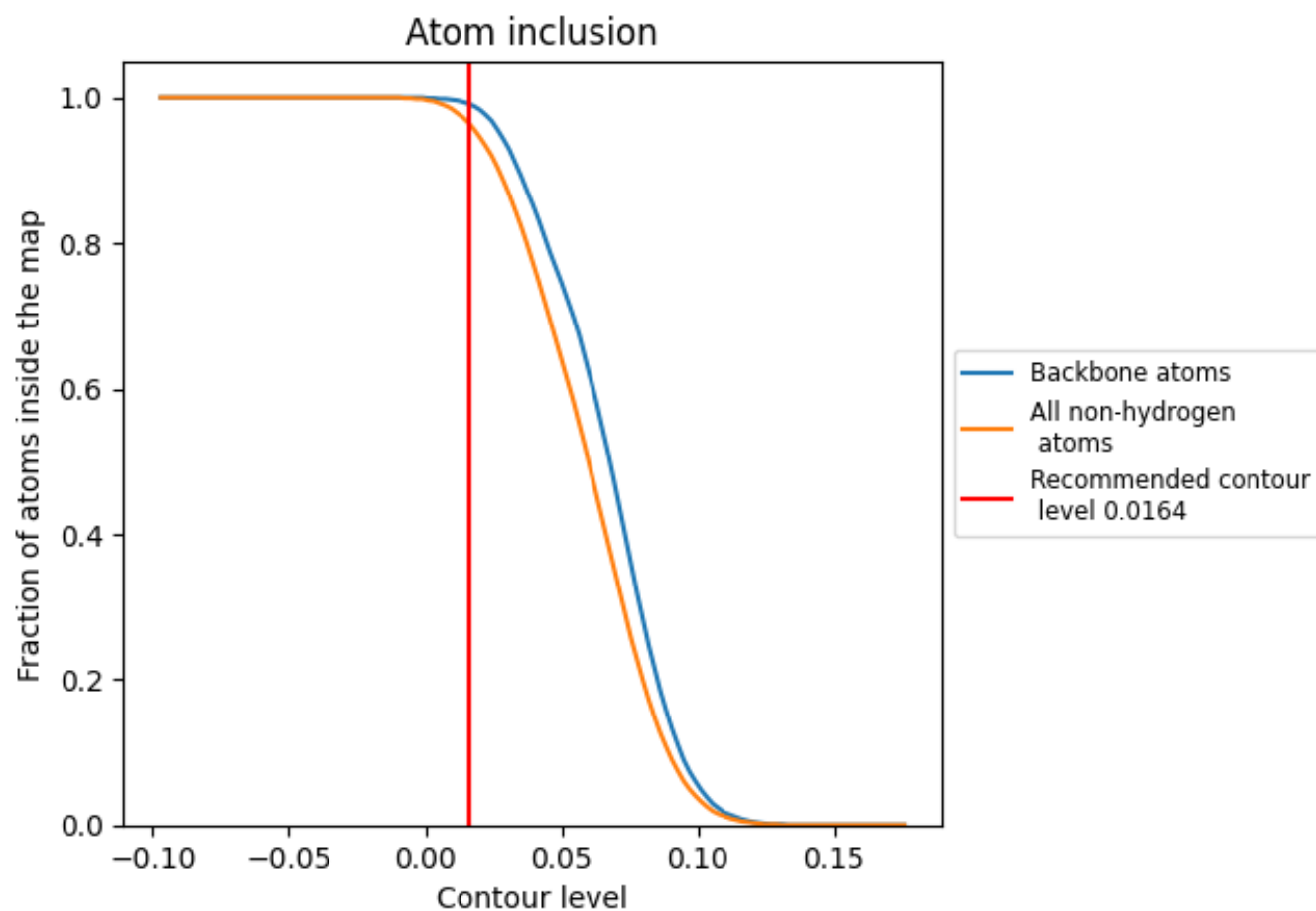
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0164).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.0164) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.6210
A	 0.9620	 0.6180
B	 0.9530	 0.6170
C	 0.9580	 0.6230
D	 0.9370	 0.5910
E	 0.9540	 0.5990
F	 0.9450	 0.6010
G	 0.9710	 0.6330
H	 0.9570	 0.6290
I	 0.9520	 0.6120
J	 0.9590	 0.6100
K	 0.9560	 0.6120
L	 0.9530	 0.6220
M	 0.9700	 0.6370
N	 0.9690	 0.6360
O	 0.9710	 0.6440
P	 0.9770	 0.6500
Q	 0.9750	 0.6390
R	 0.9700	 0.6390
S	 0.9710	 0.6370
T	 0.9720	 0.6420
U	 0.9720	 0.6340
V	 0.9670	 0.6350
W	 0.9780	 0.6430
X	 0.9680	 0.6410
Y	 0.9740	 0.6120
Z	 0.9550	 0.5990
a	 0.9680	 0.6020
b	 0.9700	 0.6210
c	 0.9740	 0.6250
d	 0.9670	 0.6240
e	 0.9580	 0.5850
f	 0.9560	 0.5970
g	 0.9580	 0.6020
h	 0.9650	 0.6080



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9670	 0.6140
j	 0.9540	 0.5860
k	 0.9770	 0.6450
l	 0.9670	 0.6240
m	 0.9420	 0.5800
n	 0.9570	 0.6200