



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:23 AM UTC

PDB ID : 8IMN / pdb_00008imn
EMDB ID : EMD-35570
Title : Rt1I-Rt1II, Rt2'I-Rt2'II, Rt3I-Rt3II cylinder in cyanobacterial phycobilisome from *Anthocerotibacter panamensis* (Cluster F)
Authors : Wang, C.H.; Yang, C.H.; Wu, H.Y.; Jiang, H.W.; Ho, M.C.; Ho, M.Y.
Deposited on : 2023-03-07
Resolution : 3.07 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

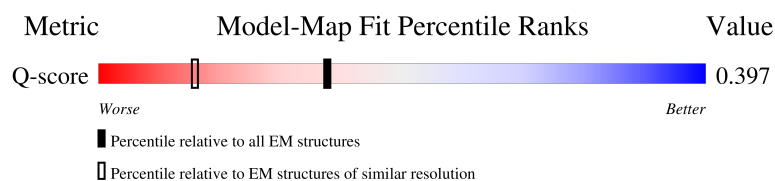
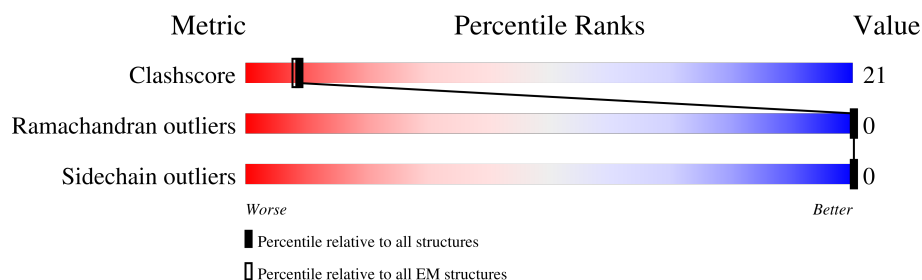
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 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.



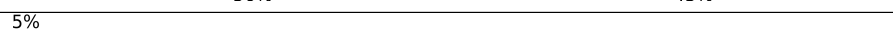
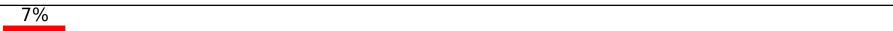
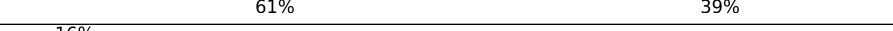
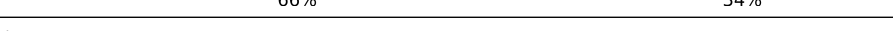
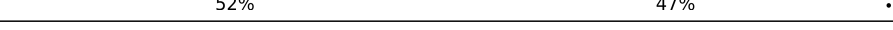
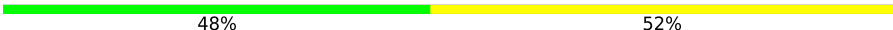
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13977 (2.57 - 3.57)

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	5	1182	
2	A	163	
2	B	163	
2	C	163	

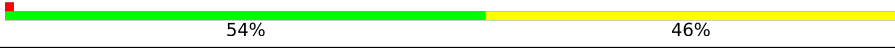
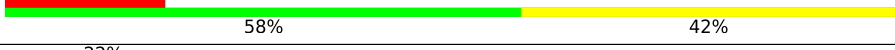
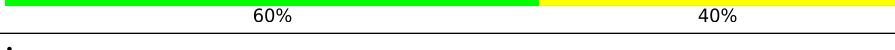
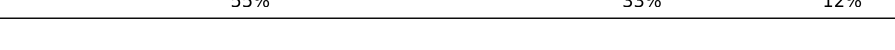
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Mol	Chain	Length	Quality of chain
2	D	163	 65% 34%
2	E	163	 63% 37%
2	F	163	 68% 31%
2	N	163	 7% 56% 43%
2	O	163	 5% 63% 37%
2	P	163	 70% 53% 47%
2	Q	163	 7% 61% 39%
2	R	163	 16% 60% 40%
2	S	163	 1% 66% 34%
2	a	163	 1% 44% 55%
2	b	163	 6% 55% 45%
2	c	163	 25% 55% 45%
2	d	163	 1% 64% 35%
2	e	163	 1% 52% 47%
2	f	163	 48% 52%
3	G	172	 65% 35%
3	H	172	 1% 55% 45%
3	I	172	 1% 66% 34%
3	J	172	 70% 30%
3	K	172	 70% 30%
3	L	172	 1% 67% 33%
3	T	172	 1% 57% 43%
3	U	172	 51% 65% 35%
3	V	172	 41% 55% 45%
3	W	172	 69% 31%

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Mol	Chain	Length	Quality of chain
3	X	172	
3	Y	172	
3	g	172	
3	h	172	
3	i	172	
3	j	172	
3	k	172	
3	l	172	
4	M	78	
4	Z	78	
4	m	78	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 55489 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 CpcN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	702	Total	C	N	O	S	0	0
			5659	3562	995	1093	9		

- Molecule 2 is a protein called CpcA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	B	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		
2	C	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	D	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	E	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	F	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	N	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	O	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		
2	P	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	Q	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	R	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	S	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	a	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	b	163	Total	C	N	O	S	0	0
			1262	804	217	239	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	d	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	e	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		
2	f	162	Total	C	N	O	S	0	0
			1254	799	216	238	1		

- Molecule 3 is a protein called CpcB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	H	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	I	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	J	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	K	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	L	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	T	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	U	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	V	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	W	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	X	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	Y	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	g	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	h	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	i	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		

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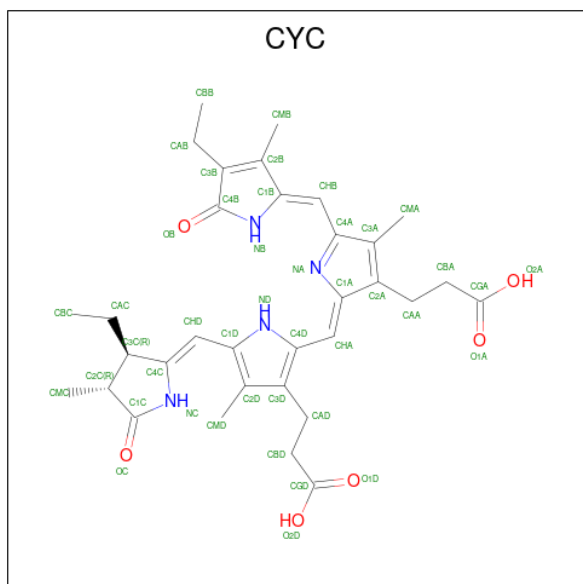
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	j	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	k	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		
3	l	172	Total	C	N	O	S	0	0
			1293	807	226	252	8		

- Molecule 4 is a protein called CpcD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	69	Total	C	N	O	S	0	0
			546	345	101	99	1		
4	Z	69	Total	C	N	O	S	0	0
			546	345	101	99	1		
4	m	69	Total	C	N	O	S	0	0
			546	345	101	99	1		

- Molecule 5 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
5	5	1	Total	C	N	O	0
			43	33	4	6	
5	5	1	Total	C	N	O	0
			43	33	4	6	
5	A	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total 43	C 33	N 4	O 6	0
5	C	1	Total 43	C 33	N 4	O 6	0
5	D	1	Total 43	C 33	N 4	O 6	0
5	E	1	Total 43	C 33	N 4	O 6	0
5	F	1	Total 43	C 33	N 4	O 6	0
5	G	1	Total 43	C 33	N 4	O 6	0
5	G	1	Total 43	C 33	N 4	O 6	0
5	H	1	Total 43	C 33	N 4	O 6	0
5	H	1	Total 43	C 33	N 4	O 6	0
5	I	1	Total 43	C 33	N 4	O 6	0
5	I	1	Total 43	C 33	N 4	O 6	0
5	J	1	Total 43	C 33	N 4	O 6	0
5	J	1	Total 43	C 33	N 4	O 6	0
5	K	1	Total 43	C 33	N 4	O 6	0
5	K	1	Total 43	C 33	N 4	O 6	0
5	L	1	Total 43	C 33	N 4	O 6	0
5	N	1	Total 43	C 33	N 4	O 6	0
5	O	1	Total 43	C 33	N 4	O 6	0
5	P	1	Total 43	C 33	N 4	O 6	0
5	Q	1	Total 43	C 33	N 4	O 6	0
5	R	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
5	S	1	Total 43	C 33	N 4	O 6	0
5	T	1	Total 43	C 33	N 4	O 6	0
5	T	1	Total 43	C 33	N 4	O 6	0
5	U	1	Total 43	C 33	N 4	O 6	0
5	U	1	Total 43	C 33	N 4	O 6	0
5	V	1	Total 43	C 33	N 4	O 6	0
5	V	1	Total 43	C 33	N 4	O 6	0
5	W	1	Total 43	C 33	N 4	O 6	0
5	W	1	Total 43	C 33	N 4	O 6	0
5	X	1	Total 43	C 33	N 4	O 6	0
5	X	1	Total 43	C 33	N 4	O 6	0
5	Y	1	Total 43	C 33	N 4	O 6	0
5	Y	1	Total 43	C 33	N 4	O 6	0
5	a	1	Total 43	C 33	N 4	O 6	0
5	b	1	Total 43	C 33	N 4	O 6	0
5	c	1	Total 43	C 33	N 4	O 6	0
5	d	1	Total 43	C 33	N 4	O 6	0
5	e	1	Total 43	C 33	N 4	O 6	0
5	f	1	Total 43	C 33	N 4	O 6	0
5	g	1	Total 43	C 33	N 4	O 6	0
5	g	1	Total 43	C 33	N 4	O 6	0

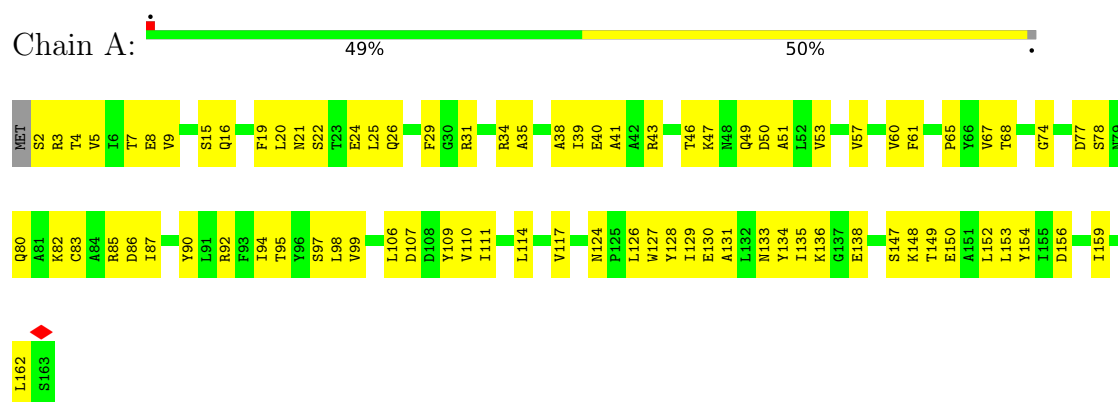
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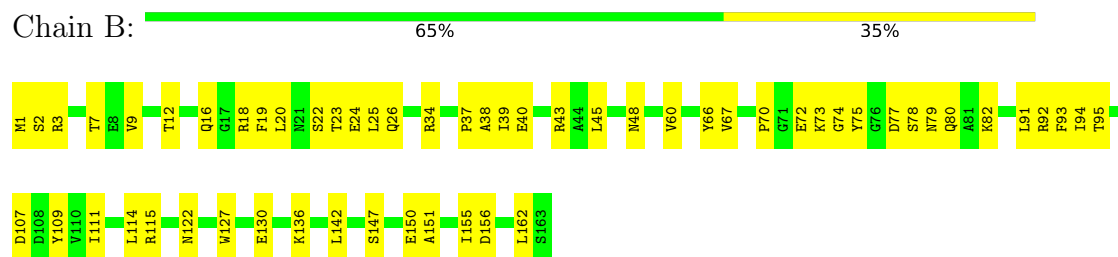
Mol	Chain	Residues	Atoms				AltConf
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5	h	1	Total	C	N	O	0
			43	33	4	6	
5	i	1	Total	C	N	O	0
			43	33	4	6	
5	i	1	Total	C	N	O	0
			43	33	4	6	
5	j	1	Total	C	N	O	0
			43	33	4	6	
5	j	1	Total	C	N	O	0
			43	33	4	6	
5	k	1	Total	C	N	O	0
			43	33	4	6	
5	k	1	Total	C	N	O	0
			43	33	4	6	
5	l	1	Total	C	N	O	0
			43	33	4	6	

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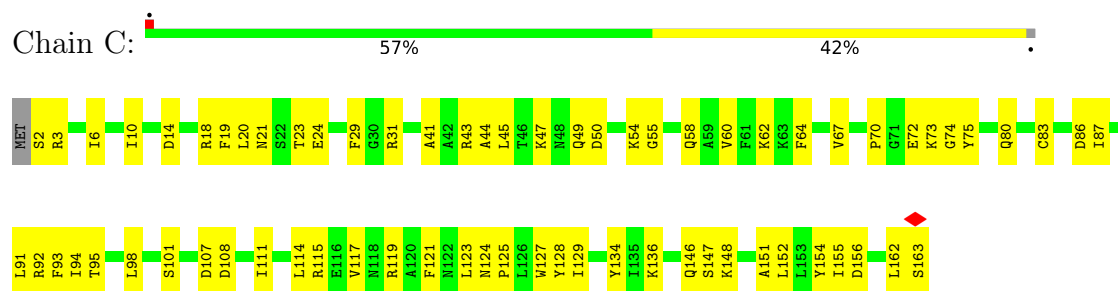
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- Molecule 2: CpcA

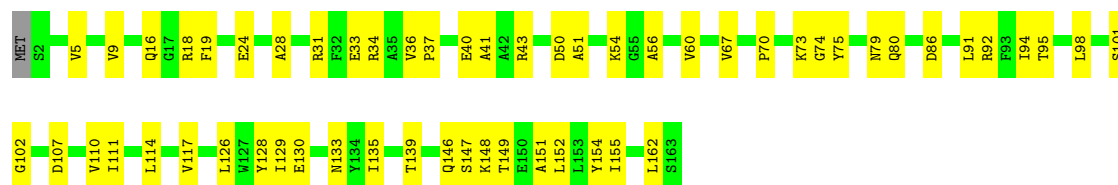


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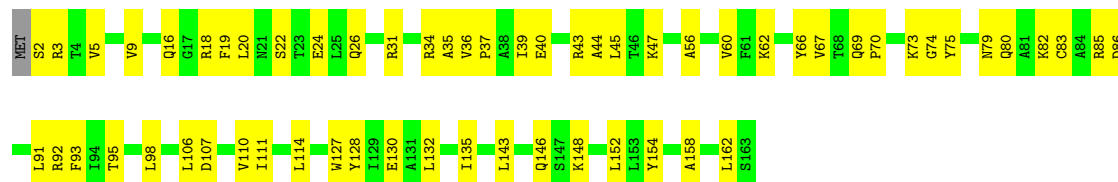
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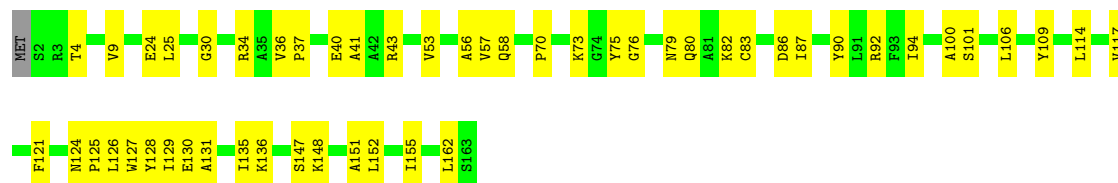
- Molecule 2: CpcA

Chain E: 63% 37%



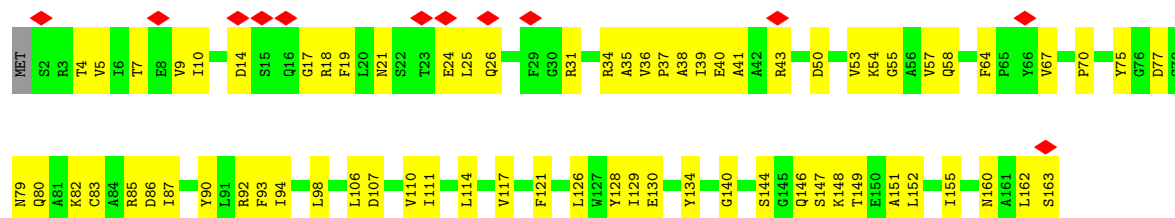
- Molecule 2: CpcA

Chain F: 68% 31%



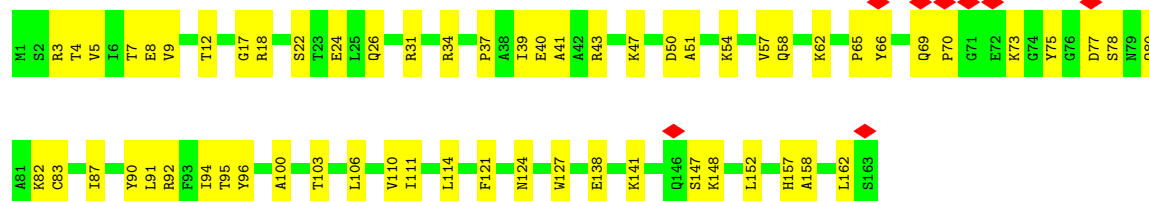
- Molecule 2: CpcA

Chain N: 7% 56% 43%

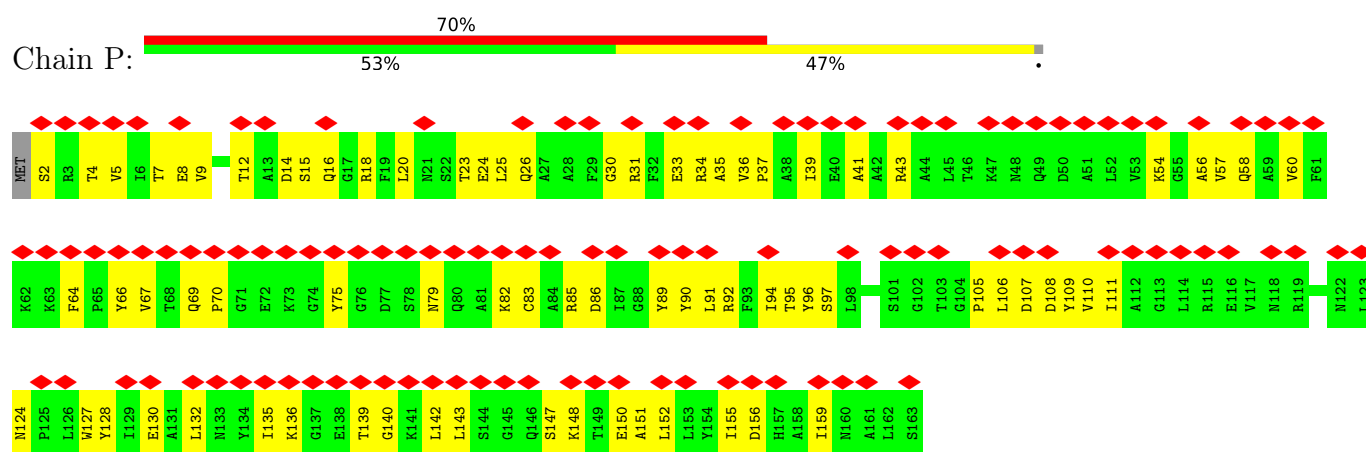


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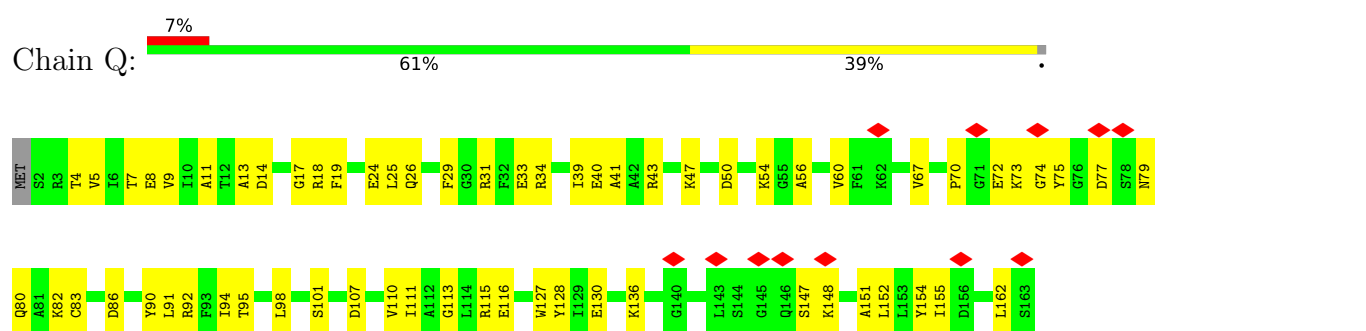
Chain O: 5% 63% 37%



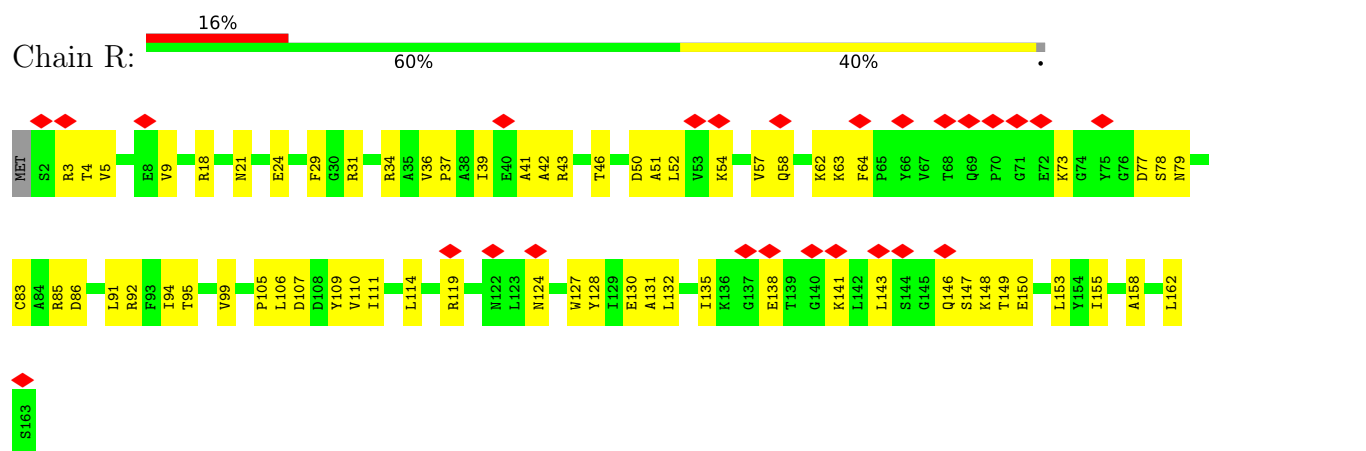
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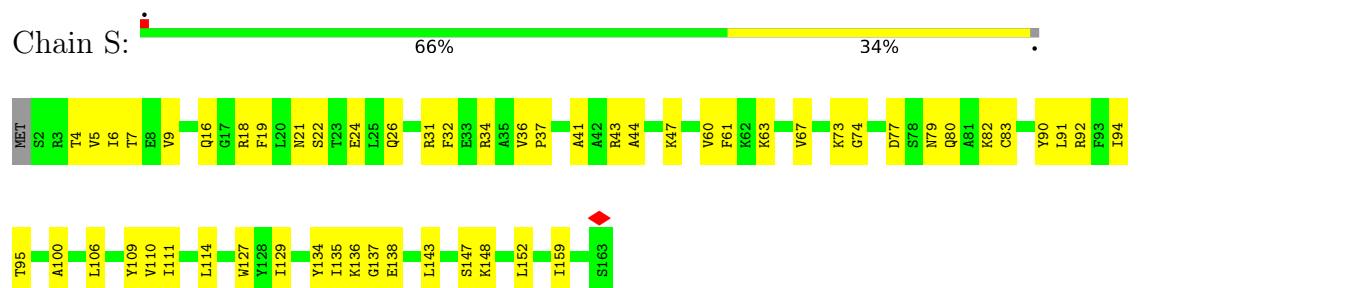
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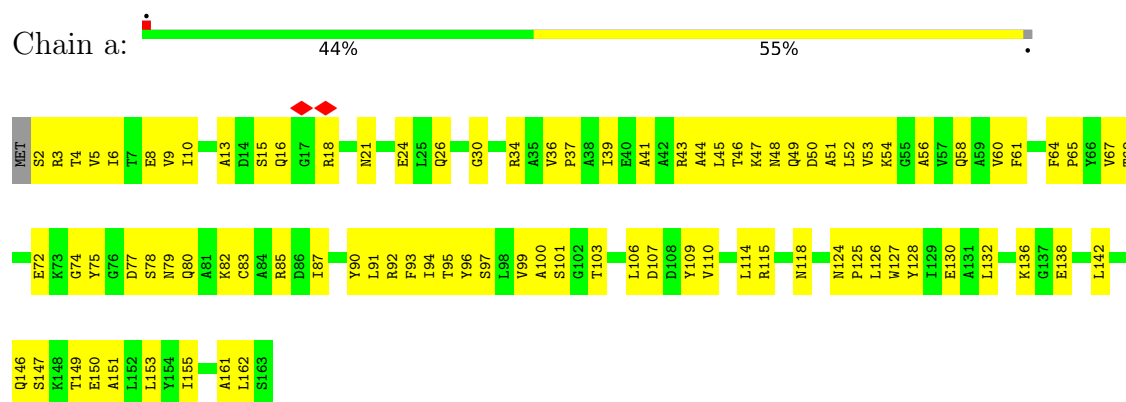
• Molecule 2: CpcA



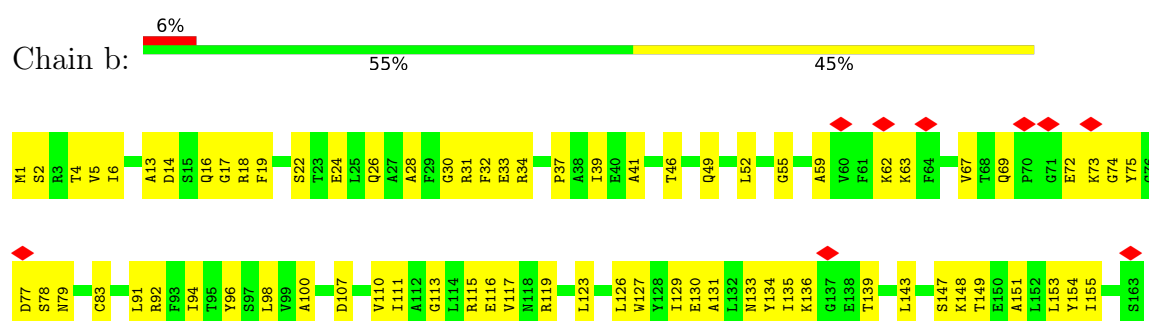
• Molecule 2: CpcA



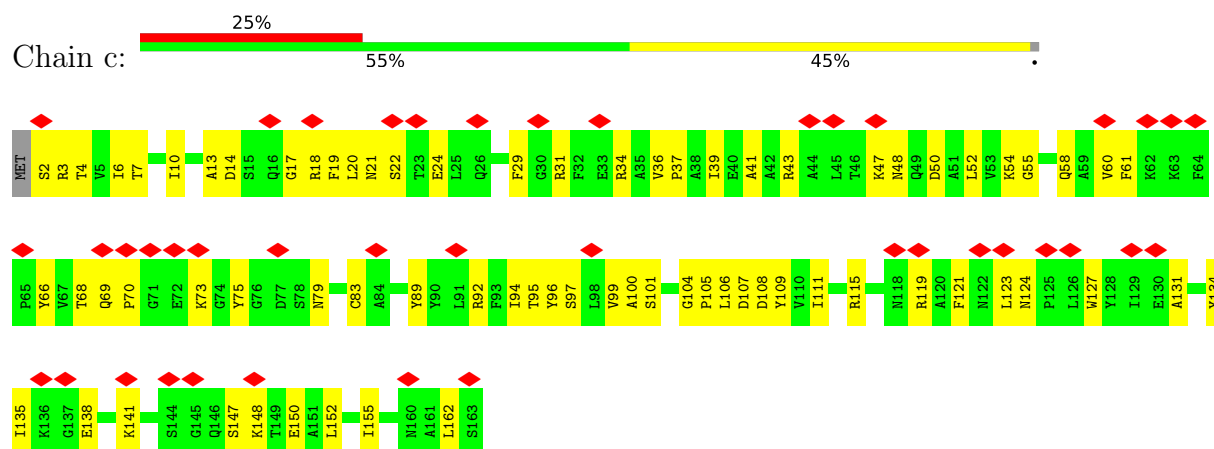
- Molecule 2: CpcA



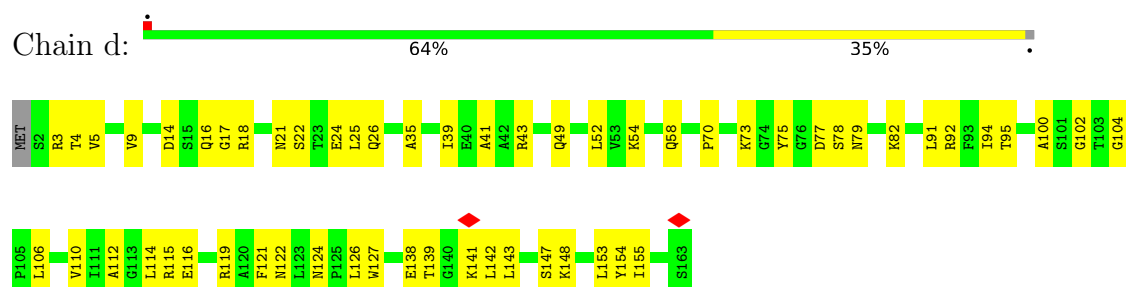
- Molecule 2: CpcA



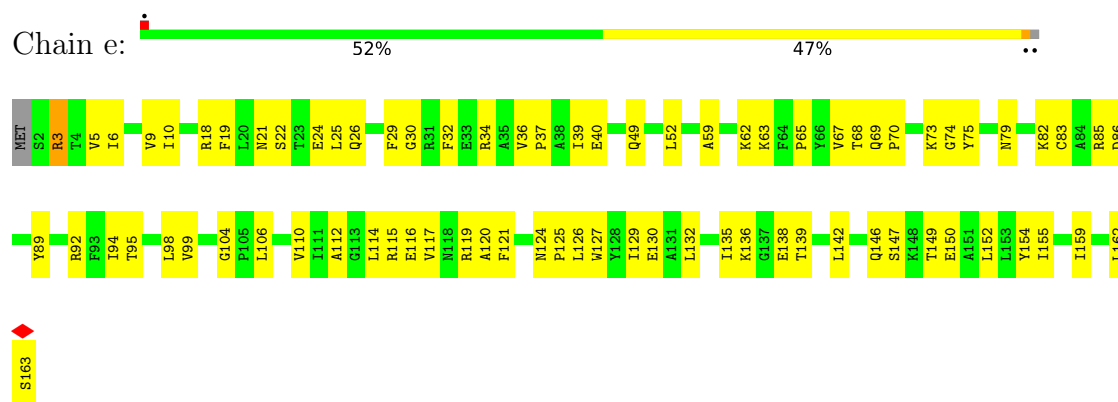
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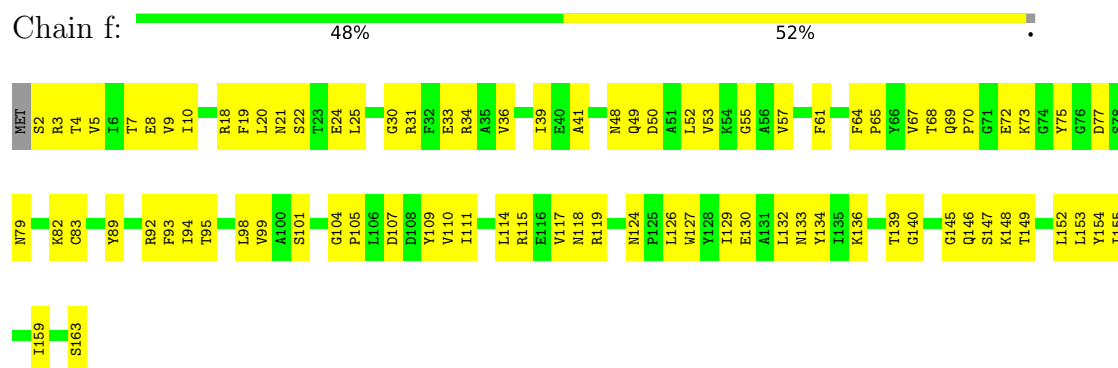
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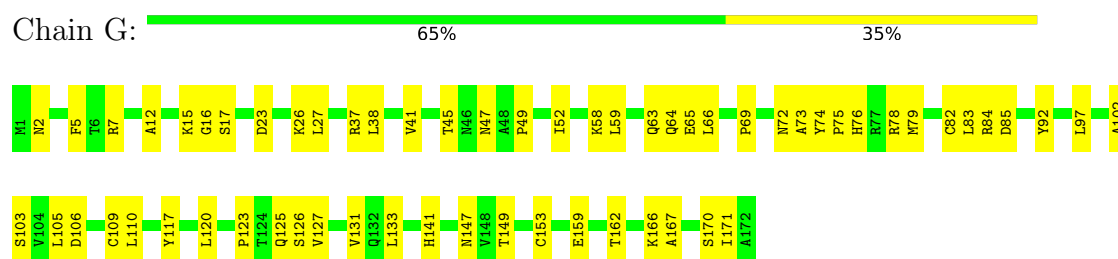
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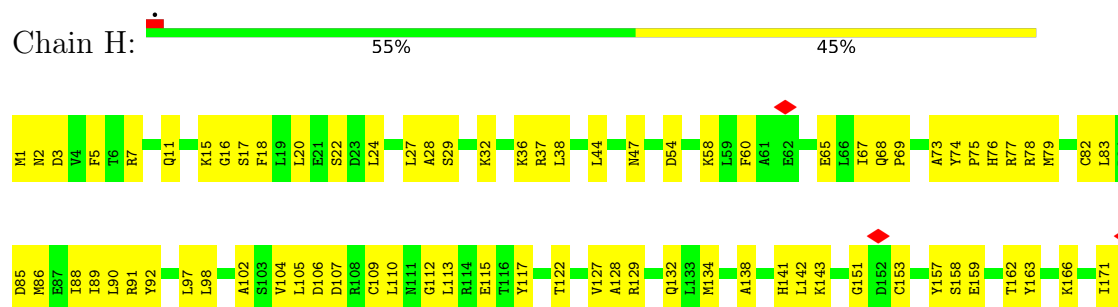
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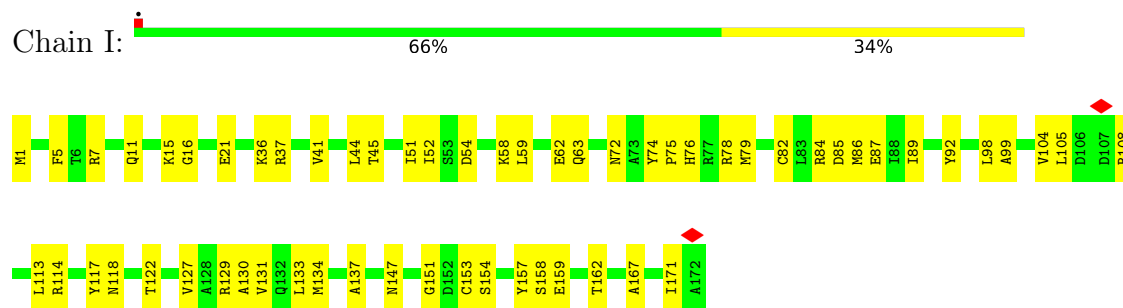
- Molecule 3: CpcB



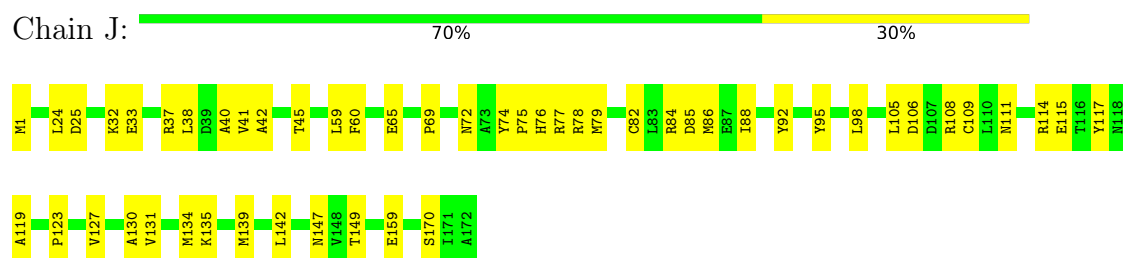
- Molecule 3: CpcB



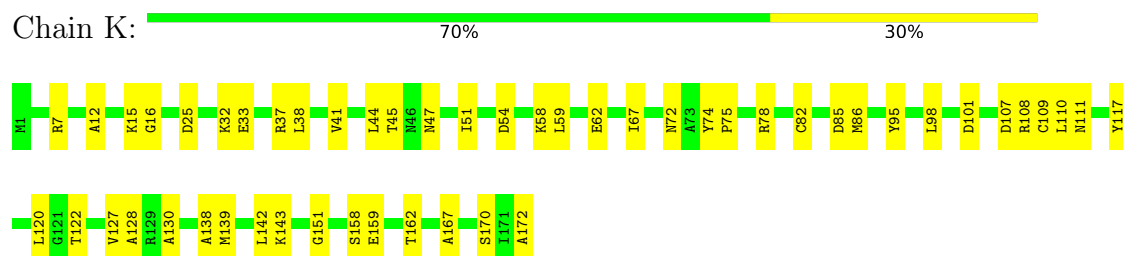
- Molecule 3: CpcB



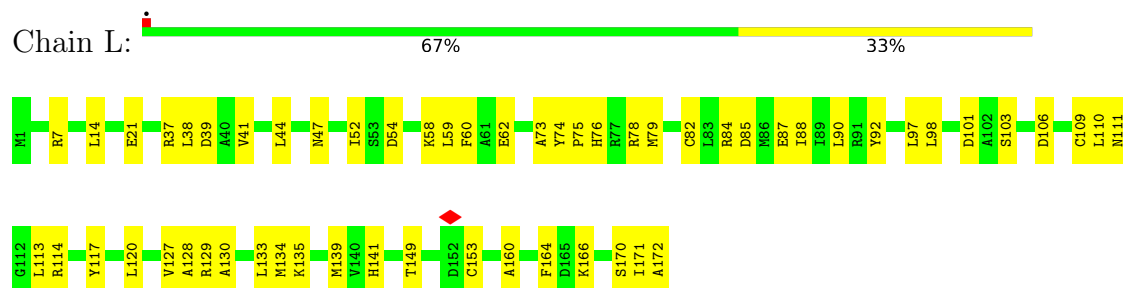
- Molecule 3: CpcB



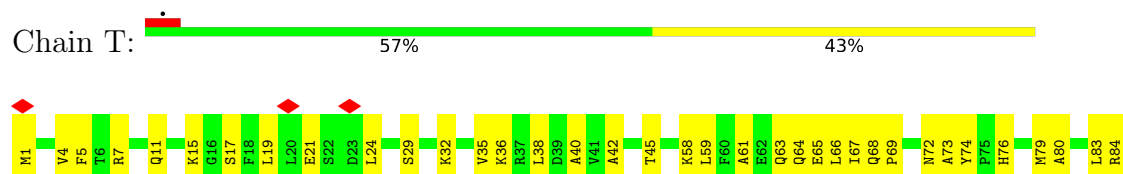
- Molecule 3: CpcB

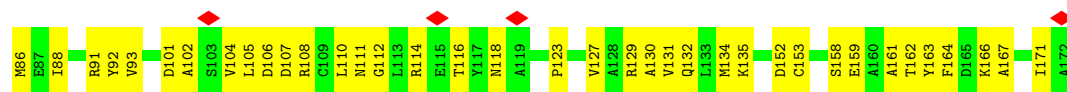


- Molecule 3: CpcB

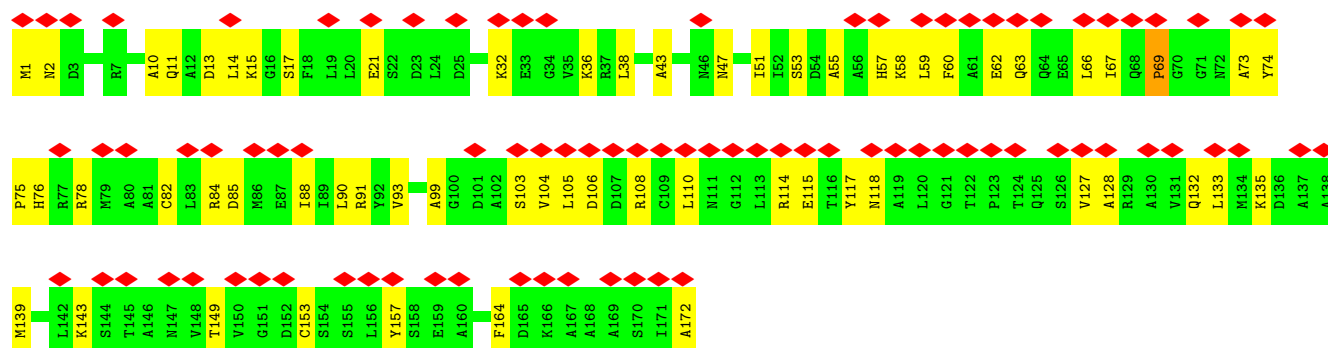


- Molecule 3: CpcB

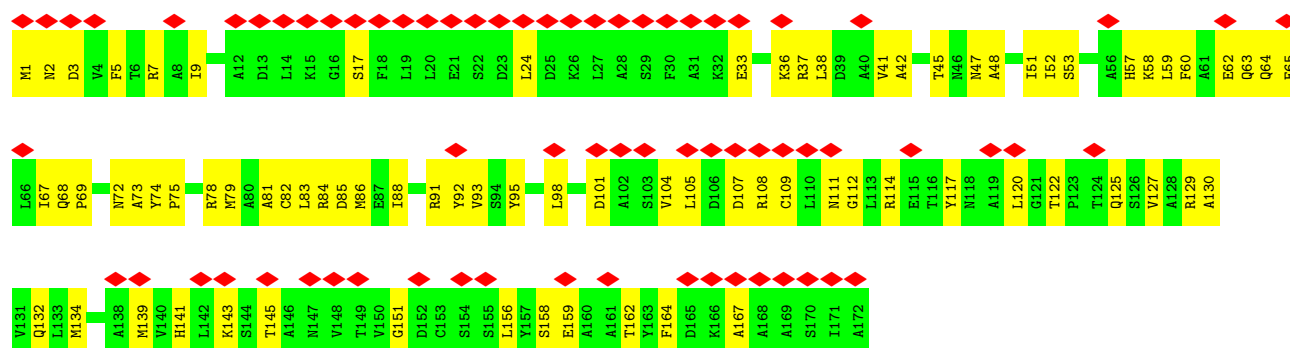
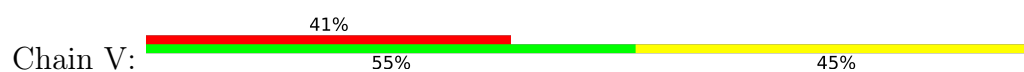




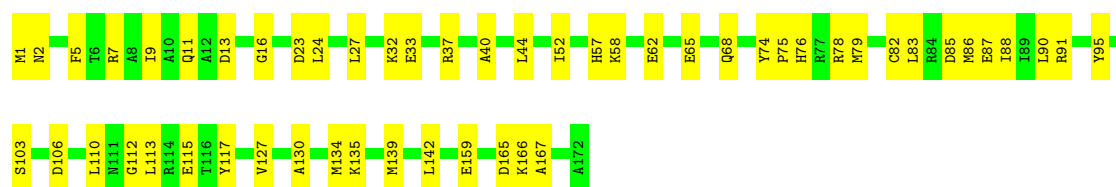
• Molecule 3: CpcB



• Molecule 3: CpcB

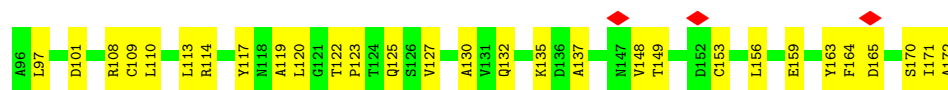


• Molecule 3: CpcB

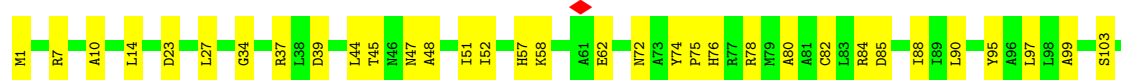


• Molecule 3: CpcB





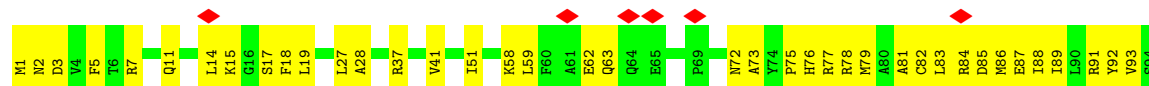
- Molecule 3: CpcB



- Molecule 3: CpcB

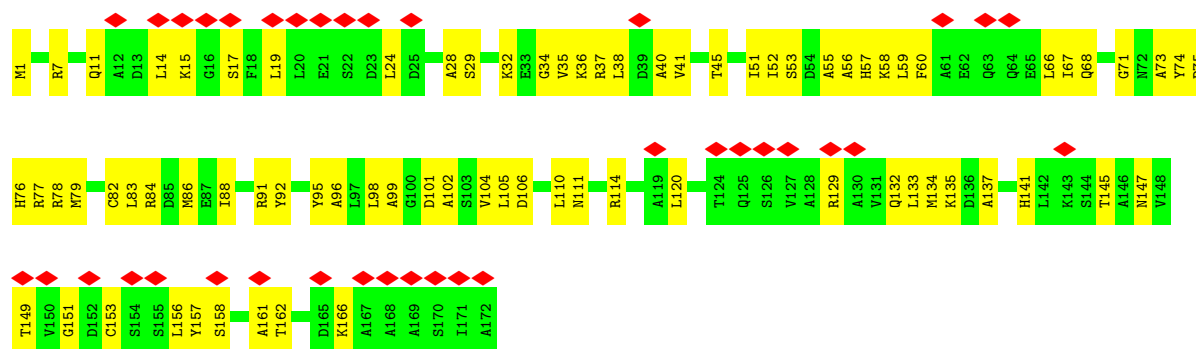


- Molecule 3: CpcB

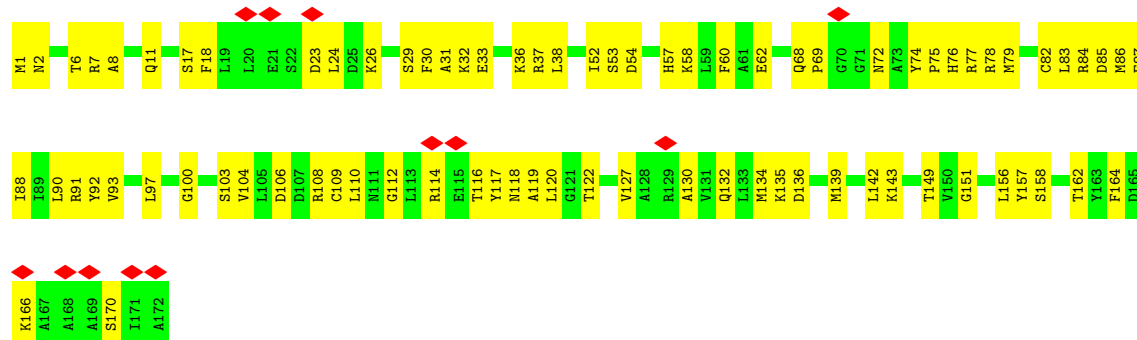


- Molecule 3: CpcB

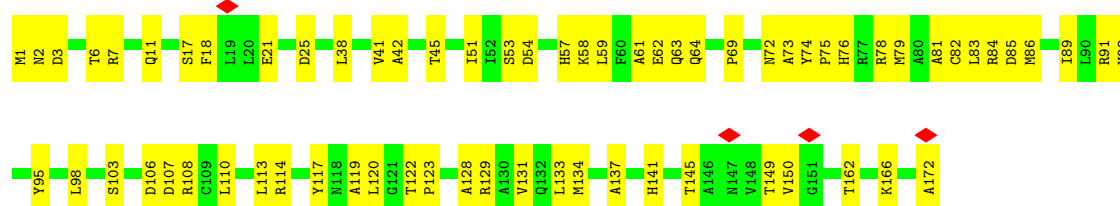




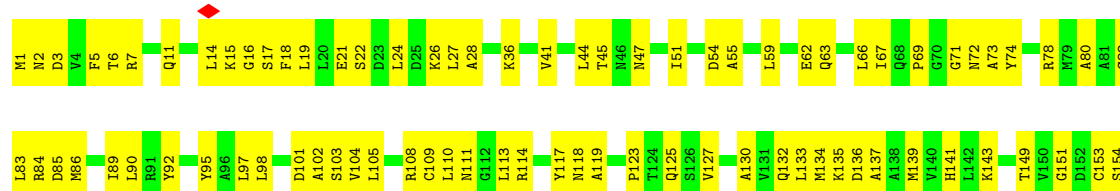
• Molecule 3: CpcB



• Molecule 3: CpcB



• Molecule 3: CpcB

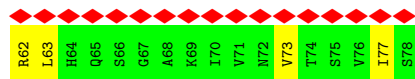
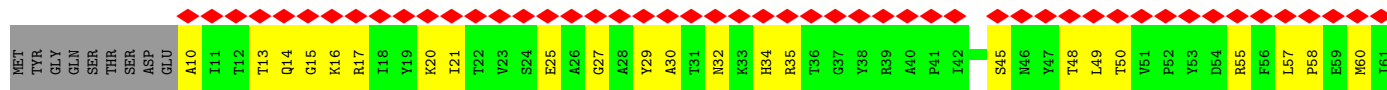
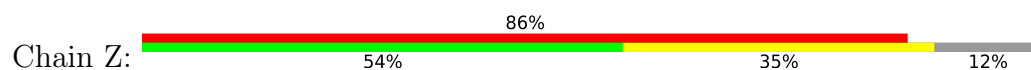




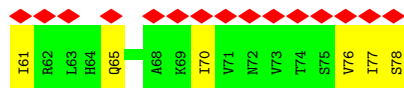
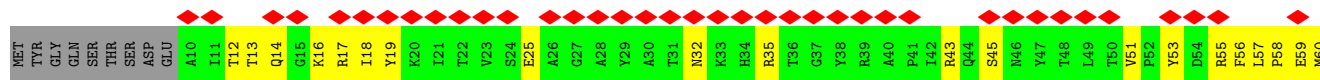
• Molecule 4: CpcD



• Molecule 4: CpcD



• Molecule 4: CpcD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1109579	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.163	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.038	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	721.48, 721.48, 721.48	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.061, 1.061, 1.061	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	5	0.23	0/5786	0.45	2/7836 (0.0%)
2	A	0.23	0/1277	0.45	0/1729
2	B	0.28	0/1285	0.45	0/1739
2	C	0.21	0/1277	0.45	0/1729
2	D	0.29	0/1277	0.43	0/1729
2	E	0.26	0/1277	0.51	0/1729
2	F	0.30	0/1277	0.45	0/1729
2	N	0.23	0/1277	0.47	0/1729
2	O	0.23	0/1285	0.45	0/1739
2	P	0.17	0/1277	0.42	0/1729
2	Q	0.21	0/1277	0.45	0/1729
2	R	0.20	0/1277	0.45	0/1729
2	S	0.35	0/1277	0.49	2/1729 (0.1%)
2	a	0.19	0/1277	0.48	0/1729
2	b	0.15	0/1285	0.37	0/1739
2	c	0.16	0/1277	0.42	0/1729
2	d	0.15	0/1277	0.36	0/1729
2	e	0.20	0/1277	0.51	0/1729
2	f	0.27	0/1277	0.51	0/1729
3	G	0.20	0/1310	0.46	0/1772
3	H	0.19	0/1310	0.45	0/1772
3	I	0.19	0/1310	0.37	0/1772
3	J	0.29	0/1310	0.44	0/1772
3	K	0.28	0/1310	0.37	0/1772
3	L	0.28	0/1310	0.40	0/1772
3	T	0.20	0/1310	0.46	0/1772
3	U	0.28	1/1310 (0.1%)	0.61	3/1772 (0.2%)
3	V	0.17	0/1310	0.42	0/1772
3	W	0.30	0/1310	0.45	0/1772
3	X	0.22	0/1310	0.40	0/1772
3	Y	0.25	0/1310	0.41	0/1772
3	g	0.17	0/1310	0.43	0/1772

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	h	0.14	0/1310	0.36	0/1772
3	i	0.15	0/1310	0.41	0/1772
3	j	0.19	0/1310	0.45	0/1772
3	k	0.15	0/1310	0.37	0/1772
3	l	0.21	0/1310	0.43	0/1772
4	M	0.13	0/556	0.38	0/753
4	Z	0.15	0/556	0.42	0/753
4	m	0.15	0/556	0.46	0/753
All	All	0.22	1/54044 (0.0%)	0.44	7/73143 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	e	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	69	PRO	CG-CD	-6.27	1.29	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	69	PRO	CA-N-CD	-12.99	93.82	112.00
3	U	69	PRO	N-CD-CG	-9.11	89.53	103.20
2	S	137	GLY	CA-C-N	-5.72	112.02	122.38
2	S	137	GLY	C-N-CA	-5.72	112.02	122.38
3	U	69	PRO	CA-CB-CG	-5.60	93.85	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	e	3	ARG	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	5	5659	0	5457	216	0
2	A	1254	0	1254	74	0
2	B	1262	0	1267	48	0
2	C	1254	0	1255	63	0
2	D	1254	0	1255	46	0
2	E	1254	0	1255	63	0
2	F	1254	0	1255	47	0
2	N	1254	0	1253	69	0
2	O	1262	0	1267	48	0
2	P	1254	0	1255	62	0
2	Q	1254	0	1255	68	0
2	R	1254	0	1255	60	0
2	S	1254	0	1255	50	0
2	a	1254	0	1255	87	0
2	b	1262	0	1267	70	0
2	c	1254	0	1255	72	0
2	d	1254	0	1255	54	0
2	e	1254	0	1255	74	0
2	f	1254	0	1255	90	0
3	G	1293	0	1297	51	0
3	H	1293	0	1297	73	0
3	I	1293	0	1297	53	0
3	J	1293	0	1297	54	0
3	K	1293	0	1297	42	0
3	L	1293	0	1297	45	0
3	T	1293	0	1297	60	0
3	U	1293	0	1297	55	0
3	V	1293	0	1297	63	0
3	W	1293	0	1297	54	0
3	X	1293	0	1297	70	0
3	Y	1293	0	1297	47	0
3	g	1293	0	1297	70	0
3	h	1293	0	1297	68	0
3	i	1293	0	1297	75	0
3	j	1293	0	1297	83	0
3	k	1293	0	1297	69	0
3	l	1293	0	1297	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	546	0	563	29	0
4	Z	546	0	563	25	0
4	m	546	0	563	30	0
5	5	86	0	73	19	0
5	A	43	0	38	3	0
5	B	43	0	38	9	0
5	C	43	0	38	7	0
5	D	43	0	38	1	0
5	E	43	0	38	8	0
5	F	43	0	37	6	0
5	G	86	0	76	11	0
5	H	86	0	76	20	0
5	I	86	0	74	12	0
5	J	86	0	76	16	0
5	K	86	0	76	9	0
5	L	43	0	38	5	0
5	N	43	0	38	7	0
5	O	43	0	38	13	0
5	P	43	0	38	4	0
5	Q	43	0	38	10	0
5	R	43	0	38	4	0
5	S	43	0	37	5	0
5	T	86	0	76	9	0
5	U	86	0	76	7	0
5	V	86	0	76	7	0
5	W	86	0	76	11	0
5	X	86	0	76	10	0
5	Y	86	0	76	13	0
5	a	43	0	38	4	0
5	b	43	0	38	2	0
5	c	43	0	38	8	0
5	d	43	0	38	7	0
5	e	43	0	38	4	0
5	f	43	0	38	6	0
5	g	86	0	76	15	0
5	h	86	0	76	13	0
5	i	86	0	76	9	0
5	j	86	0	76	9	0
5	k	86	0	76	13	0
5	l	43	0	38	7	0
All	All	55489	0	55160	2309	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 21.

The worst 5 of 2309 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)
3:X:72:ASN:ND2	3:X:122:THR:HA	1.78	0.98
2:a:72:GLU:HB3	2:a:75:TYR:HB2	1.42	0.97
5:O:200:CYC:HMA3	5:O:200:CYC:HB	1.27	0.96
3:h:75:PRO:O	3:h:77:ARG:NH1	2.05	0.90
5:W:200:CYC:HMD1	5:W:200:CYC:HC	1.37	0.88

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	5	700/1182 (59%)	665 (95%)	35 (5%)	0	100	100
2	A	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	B	161/163 (99%)	154 (96%)	7 (4%)	0	100	100
2	C	160/163 (98%)	155 (97%)	5 (3%)	0	100	100
2	D	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	E	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
2	F	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	N	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	O	161/163 (99%)	158 (98%)	3 (2%)	0	100	100
2	P	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	Q	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	R	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
2	S	160/163 (98%)	155 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	a	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	b	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
2	c	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
2	d	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
2	e	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
2	f	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
3	G	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	H	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
3	I	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
3	K	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	L	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
3	T	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	U	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
3	V	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
3	W	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
3	X	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	Y	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	g	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
3	h	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	i	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	j	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
3	k	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	l	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
4	M	67/78 (86%)	62 (92%)	5 (8%)	0	100	100
4	Z	67/78 (86%)	62 (92%)	5 (8%)	0	100	100
4	m	67/78 (86%)	65 (97%)	2 (3%)	0	100	100
All	All	6844/7446 (92%)	6630 (97%)	214 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	5	594/1003 (59%)	594 (100%)	0	100	100
2	A	128/129 (99%)	128 (100%)	0	100	100
2	B	129/129 (100%)	129 (100%)	0	100	100
2	C	128/129 (99%)	128 (100%)	0	100	100
2	D	128/129 (99%)	128 (100%)	0	100	100
2	E	128/129 (99%)	128 (100%)	0	100	100
2	F	128/129 (99%)	128 (100%)	0	100	100
2	N	128/129 (99%)	128 (100%)	0	100	100
2	O	129/129 (100%)	129 (100%)	0	100	100
2	P	128/129 (99%)	128 (100%)	0	100	100
2	Q	128/129 (99%)	128 (100%)	0	100	100
2	R	128/129 (99%)	128 (100%)	0	100	100
2	S	128/129 (99%)	128 (100%)	0	100	100
2	a	128/129 (99%)	128 (100%)	0	100	100
2	b	129/129 (100%)	129 (100%)	0	100	100
2	c	128/129 (99%)	128 (100%)	0	100	100
2	d	128/129 (99%)	128 (100%)	0	100	100
2	e	128/129 (99%)	128 (100%)	0	100	100
2	f	128/129 (99%)	128 (100%)	0	100	100
3	G	133/133 (100%)	133 (100%)	0	100	100
3	H	133/133 (100%)	133 (100%)	0	100	100
3	I	133/133 (100%)	133 (100%)	0	100	100
3	J	133/133 (100%)	133 (100%)	0	100	100
3	K	133/133 (100%)	133 (100%)	0	100	100
3	L	133/133 (100%)	133 (100%)	0	100	100
3	T	133/133 (100%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	U	133/133 (100%)	133 (100%)	0	100	100
3	V	133/133 (100%)	133 (100%)	0	100	100
3	W	133/133 (100%)	133 (100%)	0	100	100
3	X	133/133 (100%)	133 (100%)	0	100	100
3	Y	133/133 (100%)	133 (100%)	0	100	100
3	g	133/133 (100%)	133 (100%)	0	100	100
3	h	133/133 (100%)	133 (100%)	0	100	100
3	i	133/133 (100%)	133 (100%)	0	100	100
3	j	133/133 (100%)	133 (100%)	0	100	100
3	k	133/133 (100%)	133 (100%)	0	100	100
3	l	133/133 (100%)	133 (100%)	0	100	100
4	M	59/67 (88%)	59 (100%)	0	100	100
4	Z	59/67 (88%)	59 (100%)	0	100	100
4	m	59/67 (88%)	59 (100%)	0	100	100
All	All	5472/5920 (92%)	5472 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
3	Y	47	ASN
2	c	58	GLN
3	k	72	ASN
3	Y	72	ASN
2	a	146	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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$
5	CYC	k	200	-	46,46,46	5.29	26 (56%)	63,67,67	4.02	16 (25%)
5	CYC	U	200	-	46,46,46	5.33	25 (54%)	63,67,67	3.97	17 (26%)
5	CYC	I	200	-	46,46,46	5.26	26 (56%)	63,67,67	3.92	13 (20%)
5	CYC	T	201	-	46,46,46	5.27	26 (56%)	63,67,67	4.06	15 (23%)
5	CYC	D	200	-	46,46,46	5.20	27 (58%)	63,67,67	4.27	18 (28%)
5	CYC	c	200	-	46,46,46	5.35	26 (56%)	63,67,67	4.02	16 (25%)
5	CYC	j	200	-	46,46,46	5.27	26 (56%)	63,67,67	4.06	17 (26%)
5	CYC	W	200	-	46,46,46	5.22	25 (54%)	63,67,67	3.99	18 (28%)
5	CYC	V	201	-	46,46,46	5.29	25 (54%)	63,67,67	4.20	11 (17%)
5	CYC	k	201	-	46,46,46	5.34	25 (54%)	63,67,67	3.98	15 (23%)
5	CYC	Y	201	-	46,46,46	5.29	26 (56%)	63,67,67	4.07	15 (23%)
5	CYC	A	200	-	46,46,46	5.25	26 (56%)	63,67,67	4.25	15 (23%)
5	CYC	I	201	-	46,46,46	5.23	25 (54%)	63,67,67	4.28	16 (25%)
5	CYC	l	201	-	46,46,46	5.33	26 (56%)	63,67,67	4.07	15 (23%)
5	CYC	Q	200	-	46,46,46	5.31	27 (58%)	63,67,67	4.15	15 (23%)
5	CYC	R	200	-	46,46,46	5.36	25 (54%)	63,67,67	4.03	14 (22%)
5	CYC	V	200	-	46,46,46	5.30	26 (56%)	63,67,67	4.09	13 (20%)
5	CYC	E	200	-	46,46,46	5.27	26 (56%)	63,67,67	3.95	18 (28%)
5	CYC	i	200	-	46,46,46	5.34	25 (54%)	63,67,67	3.99	14 (22%)
5	CYC	5	1202	-	46,46,46	5.29	26 (56%)	63,67,67	4.02	13 (20%)
5	CYC	i	201	-	46,46,46	5.33	25 (54%)	63,67,67	4.13	12 (19%)
5	CYC	f	200	-	46,46,46	5.28	26 (56%)	63,67,67	4.28	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CYC	5	1201	-	46,46,46	5.23	26 (56%)	63,67,67	3.92	16 (25%)
5	CYC	W	201	-	46,46,46	5.24	26 (56%)	63,67,67	4.07	13 (20%)
5	CYC	j	201	-	46,46,46	5.27	26 (56%)	63,67,67	4.20	13 (20%)
5	CYC	O	200	-	46,46,46	5.29	26 (56%)	63,67,67	4.26	17 (26%)
5	CYC	G	201	-	46,46,46	5.32	26 (56%)	63,67,67	3.98	14 (22%)
5	CYC	g	200	-	46,46,46	5.35	25 (54%)	63,67,67	3.89	15 (23%)
5	CYC	d	200	-	46,46,46	5.34	25 (54%)	63,67,67	3.81	13 (20%)
5	CYC	S	200	-	46,46,46	5.22	26 (56%)	63,67,67	4.29	14 (22%)
5	CYC	B	200	-	46,46,46	5.31	26 (56%)	63,67,67	4.15	16 (25%)
5	CYC	X	201	-	46,46,46	5.30	26 (56%)	63,67,67	4.03	14 (22%)
5	CYC	L	201	-	46,46,46	5.26	26 (56%)	63,67,67	4.01	18 (28%)
5	CYC	K	201	-	46,46,46	5.22	26 (56%)	63,67,67	4.17	17 (26%)
5	CYC	J	200	-	46,46,46	5.27	26 (56%)	63,67,67	4.08	16 (25%)
5	CYC	H	201	-	46,46,46	5.31	26 (56%)	63,67,67	4.16	13 (20%)
5	CYC	F	200	-	46,46,46	5.21	27 (58%)	63,67,67	3.94	14 (22%)
5	CYC	K	200	-	46,46,46	5.25	25 (54%)	63,67,67	4.07	16 (25%)
5	CYC	b	200	-	46,46,46	5.33	26 (56%)	63,67,67	4.13	14 (22%)
5	CYC	G	200	-	46,46,46	5.30	26 (56%)	63,67,67	3.88	14 (22%)
5	CYC	e	200	-	46,46,46	5.32	26 (56%)	63,67,67	4.06	13 (20%)
5	CYC	U	201	-	46,46,46	5.30	26 (56%)	63,67,67	4.12	14 (22%)
5	CYC	T	200	-	46,46,46	5.33	26 (56%)	63,67,67	3.88	14 (22%)
5	CYC	X	200	-	46,46,46	5.29	25 (54%)	63,67,67	4.10	15 (23%)
5	CYC	a	200	-	46,46,46	5.34	26 (56%)	63,67,67	4.19	17 (26%)
5	CYC	g	201	-	46,46,46	5.28	26 (56%)	63,67,67	3.99	13 (20%)
5	CYC	Y	200	-	46,46,46	5.22	26 (56%)	63,67,67	4.03	16 (25%)
5	CYC	C	200	-	46,46,46	5.28	25 (54%)	63,67,67	3.92	14 (22%)
5	CYC	H	200	-	46,46,46	5.30	26 (56%)	63,67,67	4.11	19 (30%)
5	CYC	N	200	-	46,46,46	5.26	26 (56%)	63,67,67	4.16	19 (30%)
5	CYC	P	200	-	46,46,46	5.35	24 (52%)	63,67,67	3.86	15 (23%)
5	CYC	h	201	-	46,46,46	5.32	26 (56%)	63,67,67	4.09	14 (22%)
5	CYC	h	200	-	46,46,46	5.32	26 (56%)	63,67,67	3.97	17 (26%)
5	CYC	J	201	-	46,46,46	5.25	26 (56%)	63,67,67	4.18	14 (22%)

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	CYC	k	200	-	-	14/26/74/74	0/4/4/4
5	CYC	U	200	-	-	6/26/74/74	0/4/4/4
5	CYC	I	200	-	-	11/26/74/74	0/4/4/4
5	CYC	T	201	-	-	12/26/74/74	0/4/4/4
5	CYC	D	200	-	-	14/26/74/74	0/4/4/4
5	CYC	c	200	-	-	16/26/74/74	0/4/4/4
5	CYC	j	200	-	-	10/26/74/74	0/4/4/4
5	CYC	W	200	-	-	13/26/74/74	0/4/4/4
5	CYC	V	201	-	-	12/26/74/74	0/4/4/4
5	CYC	k	201	-	-	7/26/74/74	0/4/4/4
5	CYC	Y	201	-	-	19/26/74/74	0/4/4/4
5	CYC	A	200	-	-	18/26/74/74	0/4/4/4
5	CYC	I	201	-	-	10/26/74/74	0/4/4/4
5	CYC	l	201	-	-	15/26/74/74	0/4/4/4
5	CYC	Q	200	-	-	13/26/74/74	0/4/4/4
5	CYC	R	200	-	-	14/26/74/74	0/4/4/4
5	CYC	V	200	-	-	11/26/74/74	0/4/4/4
5	CYC	E	200	-	-	14/26/74/74	0/4/4/4
5	CYC	i	200	-	-	14/26/74/74	0/4/4/4
5	CYC	5	1202	-	-	11/26/74/74	0/4/4/4
5	CYC	i	201	-	-	16/26/74/74	0/4/4/4
5	CYC	f	200	-	-	16/26/74/74	0/4/4/4
5	CYC	5	1201	-	-	8/26/74/74	0/4/4/4
5	CYC	W	201	-	-	10/26/74/74	0/4/4/4
5	CYC	j	201	-	-	9/26/74/74	0/4/4/4
5	CYC	O	200	-	-	16/26/74/74	0/4/4/4
5	CYC	G	201	-	-	15/26/74/74	0/4/4/4
5	CYC	g	200	-	-	7/26/74/74	0/4/4/4
5	CYC	d	200	-	-	16/26/74/74	0/4/4/4
5	CYC	S	200	-	-	16/26/74/74	0/4/4/4
5	CYC	B	200	-	-	18/26/74/74	0/4/4/4
5	CYC	X	201	-	-	13/26/74/74	0/4/4/4
5	CYC	L	201	-	-	14/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYC	K	201	-	-	14/26/74/74	0/4/4/4
5	CYC	J	200	-	-	8/26/74/74	0/4/4/4
5	CYC	H	201	-	-	16/26/74/74	0/4/4/4
5	CYC	F	200	-	-	14/26/74/74	0/4/4/4
5	CYC	K	200	-	-	11/26/74/74	0/4/4/4
5	CYC	b	200	-	-	11/26/74/74	0/4/4/4
5	CYC	G	200	-	-	11/26/74/74	0/4/4/4
5	CYC	e	200	-	-	17/26/74/74	0/4/4/4
5	CYC	U	201	-	-	17/26/74/74	0/4/4/4
5	CYC	T	200	-	-	8/26/74/74	0/4/4/4
5	CYC	X	200	-	-	13/26/74/74	0/4/4/4
5	CYC	a	200	-	-	21/26/74/74	0/4/4/4
5	CYC	g	201	-	-	15/26/74/74	0/4/4/4
5	CYC	Y	200	-	-	10/26/74/74	0/4/4/4
5	CYC	C	200	-	-	16/26/74/74	0/4/4/4
5	CYC	H	200	-	-	13/26/74/74	0/4/4/4
5	CYC	N	200	-	-	12/26/74/74	0/4/4/4
5	CYC	P	200	-	-	12/26/74/74	0/4/4/4
5	CYC	h	201	-	-	13/26/74/74	0/4/4/4
5	CYC	h	200	-	-	12/26/74/74	0/4/4/4
5	CYC	J	201	-	-	18/26/74/74	0/4/4/4

The worst 5 of 1392 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	200	CYC	C2C-C1C	13.78	1.64	1.52
5	a	200	CYC	C2C-C1C	13.68	1.64	1.52
5	f	200	CYC	C2C-C1C	13.62	1.64	1.52
5	R	200	CYC	C2C-C1C	13.61	1.64	1.52
5	b	200	CYC	C2C-C1C	13.55	1.64	1.52

The worst 5 of 810 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	200	CYC	OC-C1C-C2C	-22.17	108.55	126.17
5	J	200	CYC	OC-C1C-C2C	-22.07	108.62	126.17
5	K	200	CYC	OC-C1C-C2C	-21.85	108.80	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	201	CYC	OC-C1C-C2C	-21.84	108.81	126.17
5	e	200	CYC	OC-C1C-C2C	-21.31	109.23	126.17

There are no chirality outliers.

5 of 710 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	5	1201	CYC	NA-C4A-CHB-C1B
5	5	1201	CYC	C3A-C4A-CHB-C1B
5	5	1201	CYC	C4C-C3C-CAC-CBC
5	5	1201	CYC	NC-C4C-CHD-C1D
5	5	1201	CYC	C3C-C4C-CHD-C1D

There are no ring outliers.

54 monomers are involved in 323 short contacts:

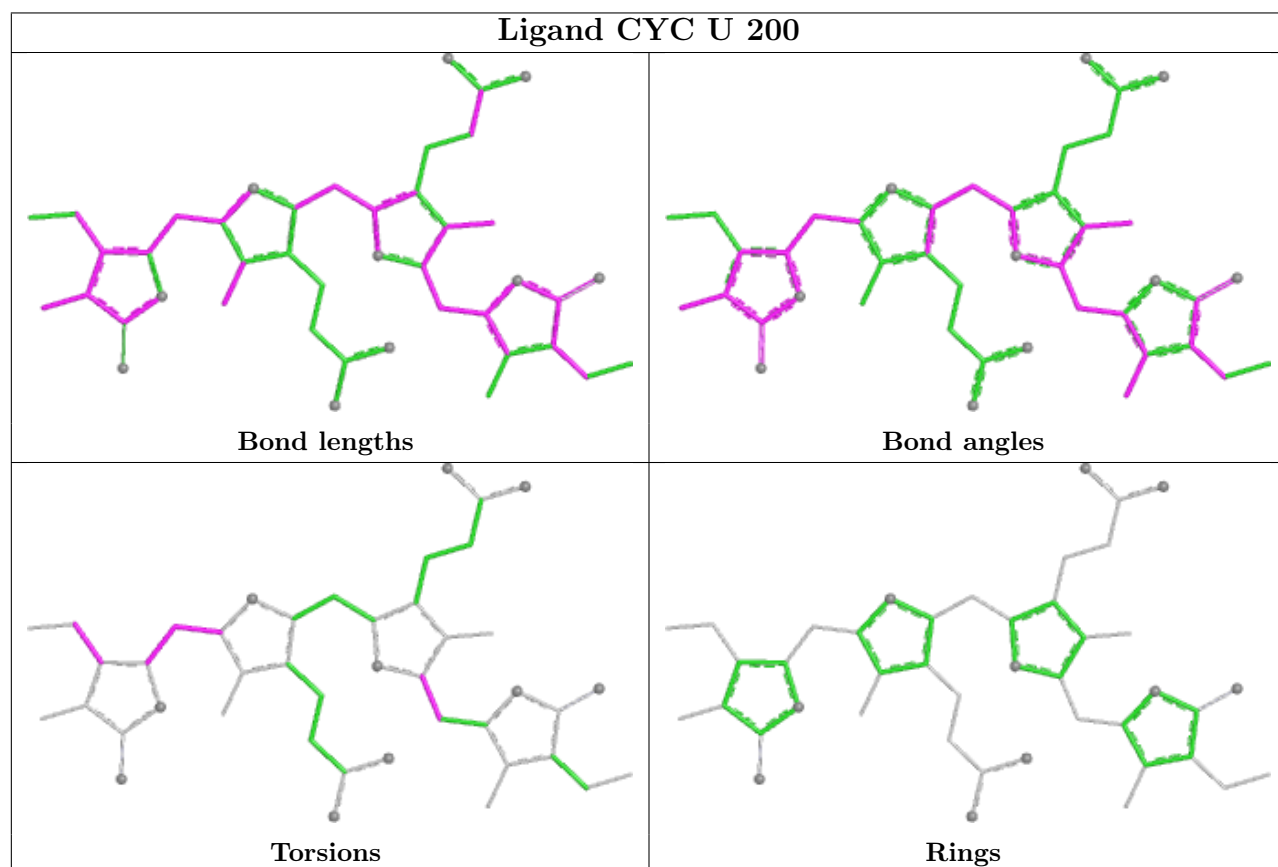
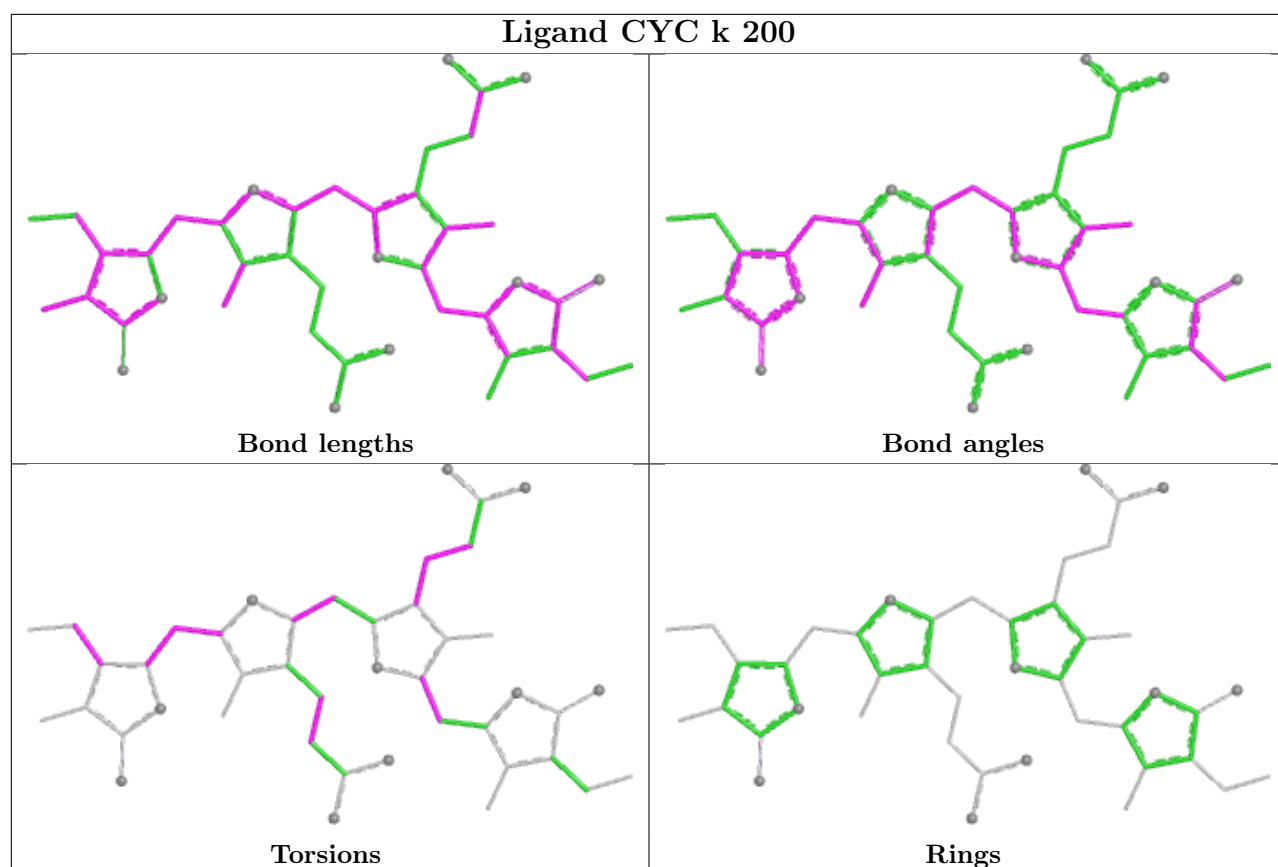
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	k	200	CYC	9	0
5	U	200	CYC	3	0
5	I	200	CYC	8	0
5	T	201	CYC	7	0
5	D	200	CYC	1	0
5	c	200	CYC	8	0
5	j	200	CYC	6	0
5	W	200	CYC	10	0
5	V	201	CYC	3	0
5	k	201	CYC	4	0
5	Y	201	CYC	5	0
5	A	200	CYC	3	0
5	I	201	CYC	4	0
5	l	201	CYC	7	0
5	Q	200	CYC	10	0
5	R	200	CYC	4	0
5	V	200	CYC	4	0
5	E	200	CYC	8	0
5	i	200	CYC	5	0
5	5	1202	CYC	12	0
5	i	201	CYC	4	0
5	f	200	CYC	6	0
5	5	1201	CYC	7	0
5	W	201	CYC	1	0

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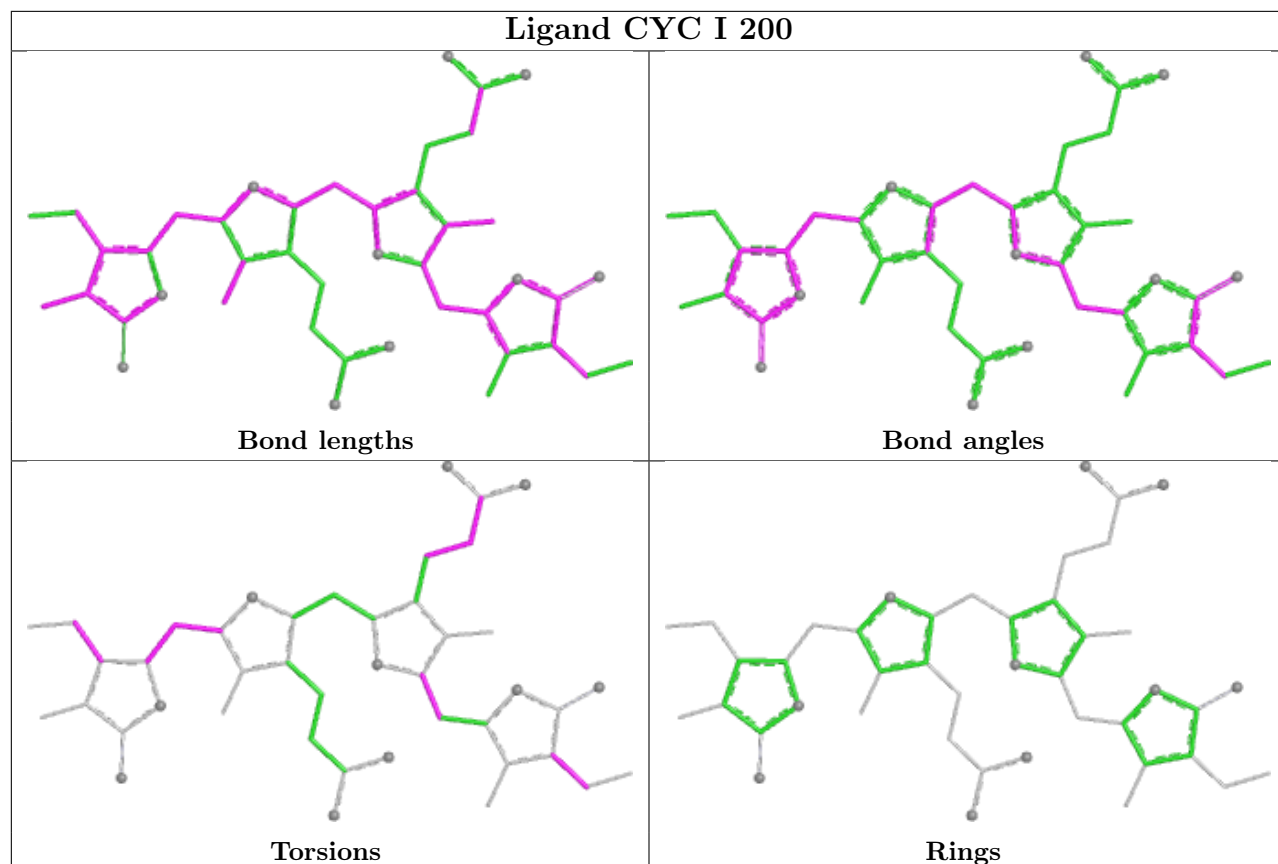
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	j	201	CYC	3	0
5	O	200	CYC	13	0
5	G	201	CYC	6	0
5	g	200	CYC	6	0
5	d	200	CYC	7	0
5	S	200	CYC	5	0
5	B	200	CYC	9	0
5	X	201	CYC	4	0
5	L	201	CYC	5	0
5	K	201	CYC	4	0
5	J	200	CYC	12	0
5	H	201	CYC	5	0
5	F	200	CYC	6	0
5	K	200	CYC	5	0
5	b	200	CYC	2	0
5	G	200	CYC	5	0
5	e	200	CYC	4	0
5	U	201	CYC	4	0
5	T	200	CYC	2	0
5	X	200	CYC	6	0
5	a	200	CYC	4	0
5	g	201	CYC	9	0
5	Y	200	CYC	8	0
5	C	200	CYC	7	0
5	H	200	CYC	15	0
5	N	200	CYC	7	0
5	P	200	CYC	4	0
5	h	201	CYC	2	0
5	h	200	CYC	11	0
5	J	201	CYC	4	0

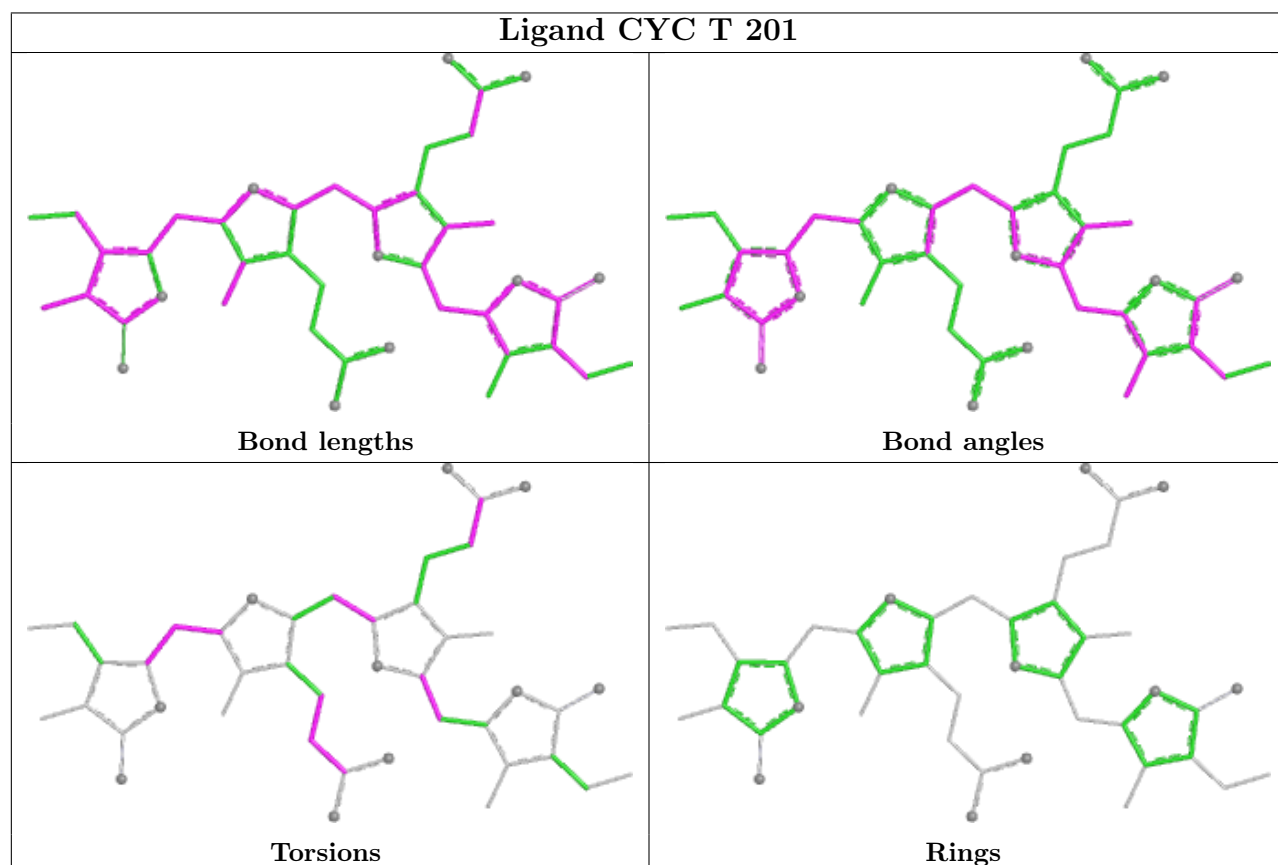
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

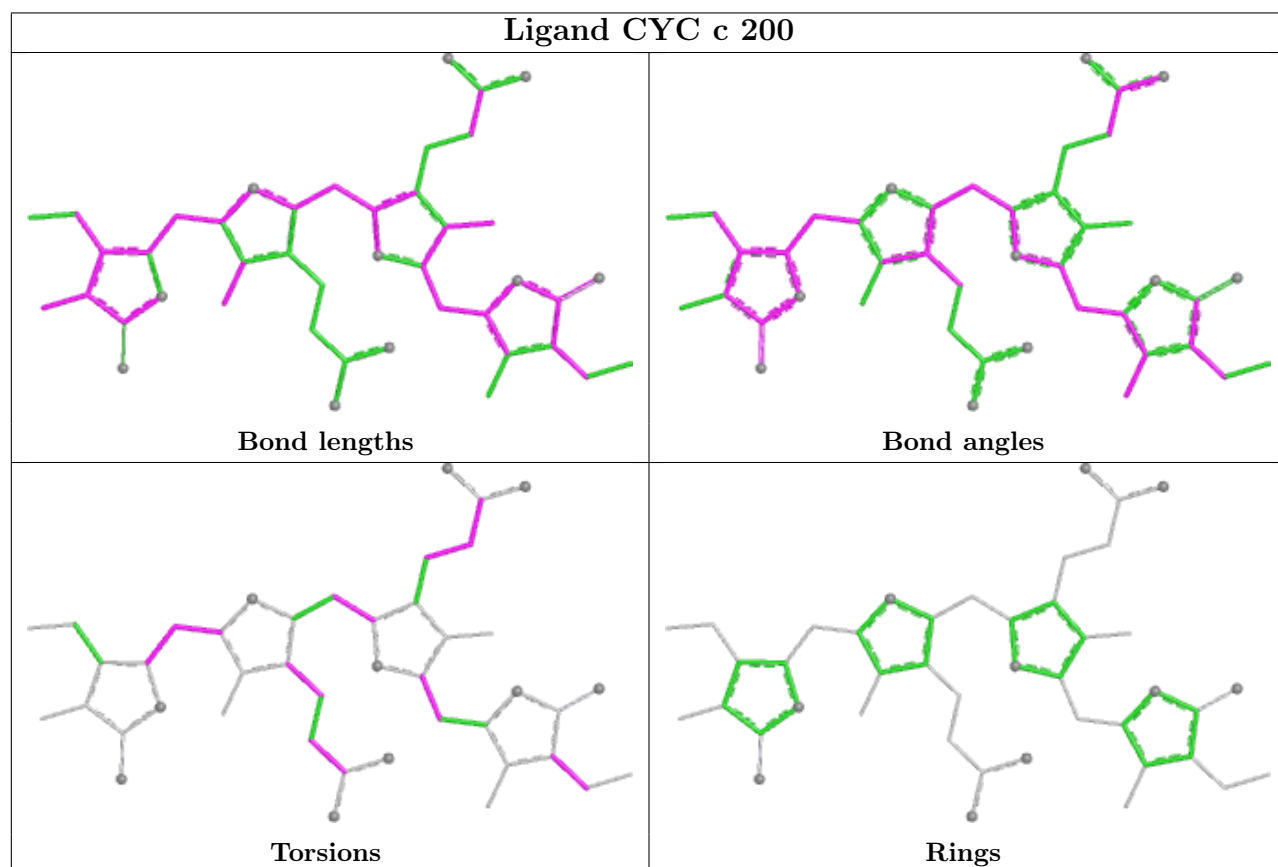
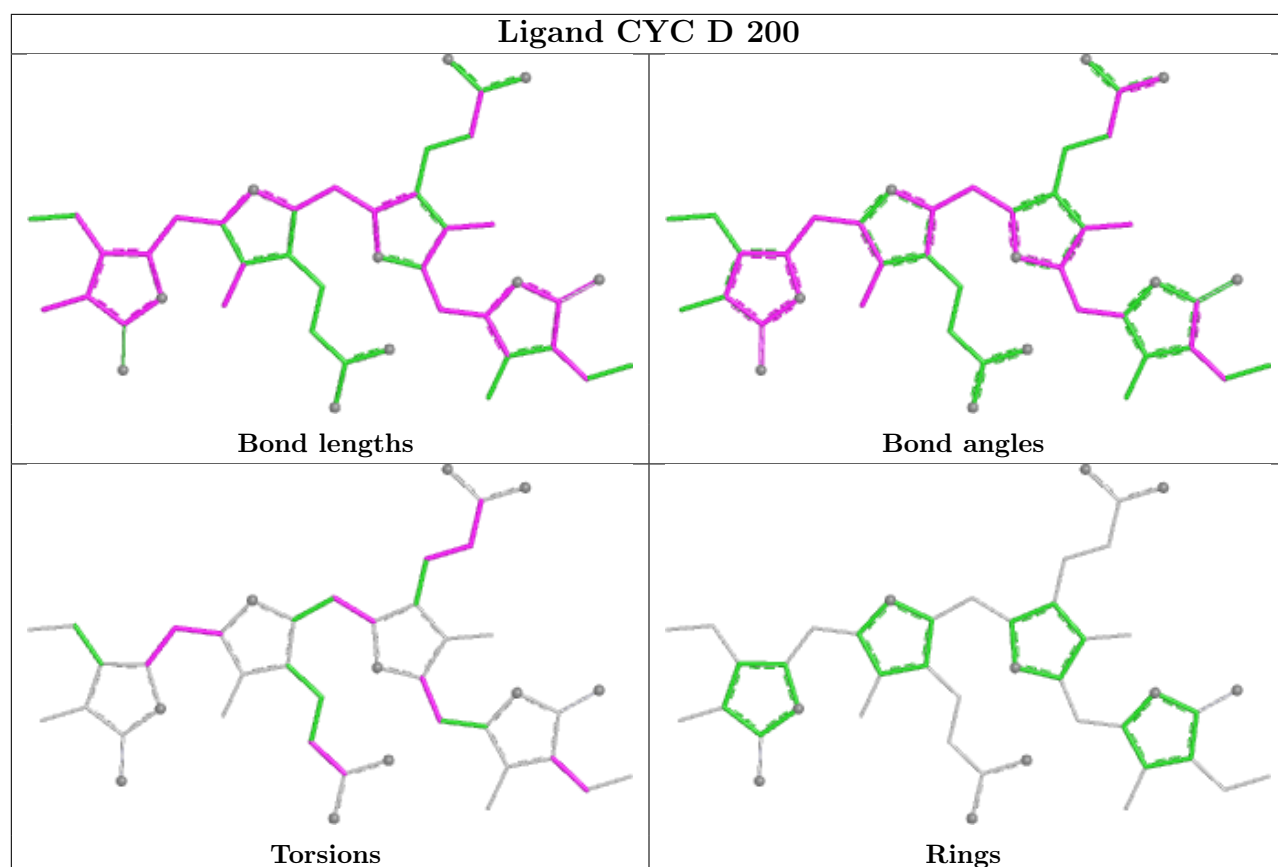


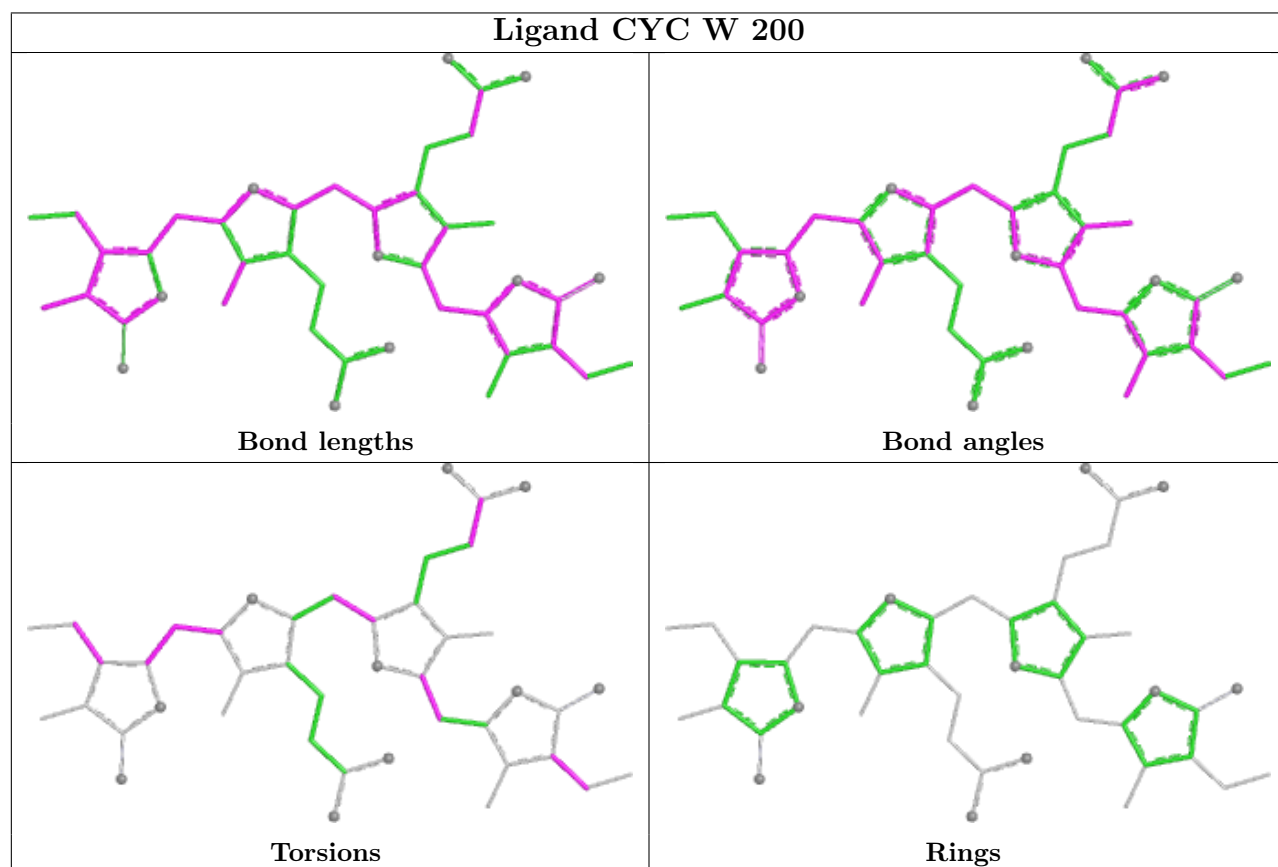
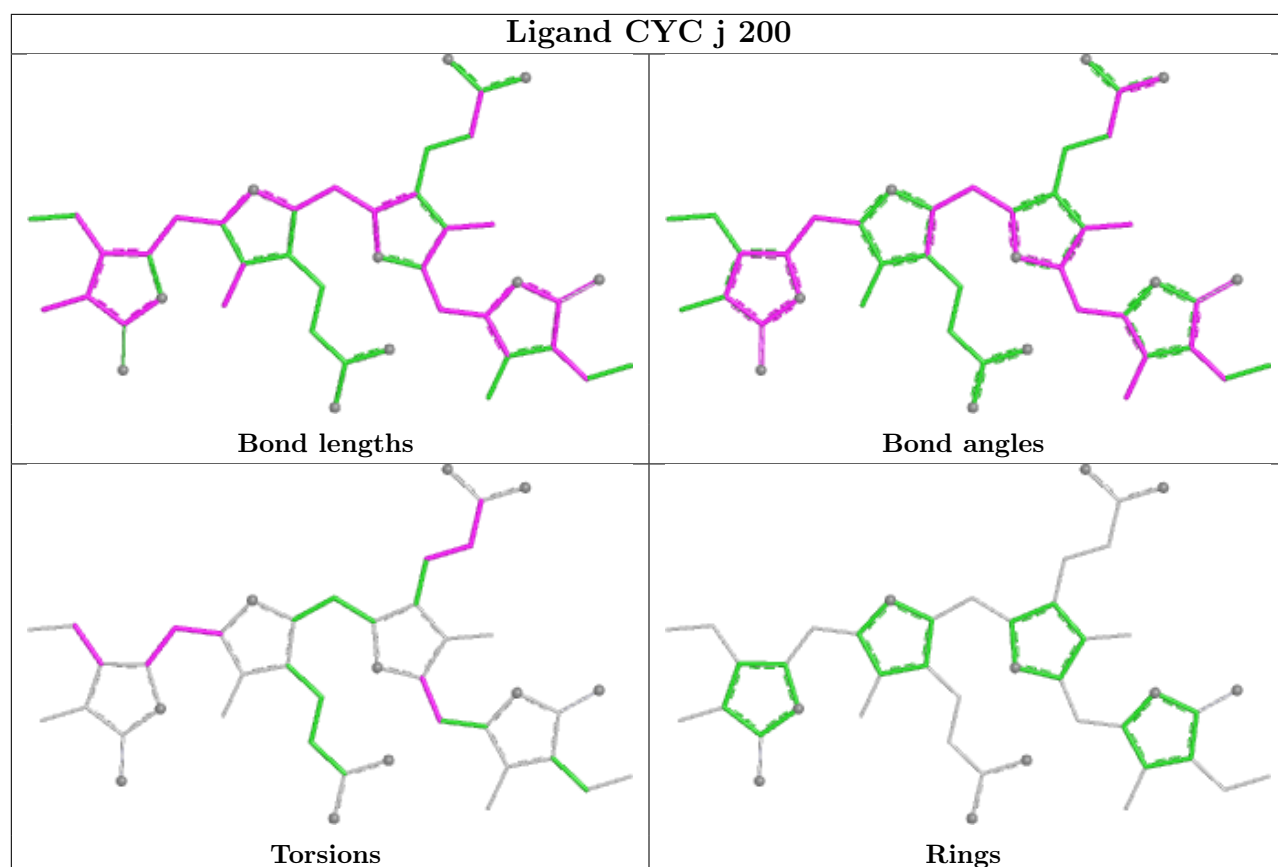
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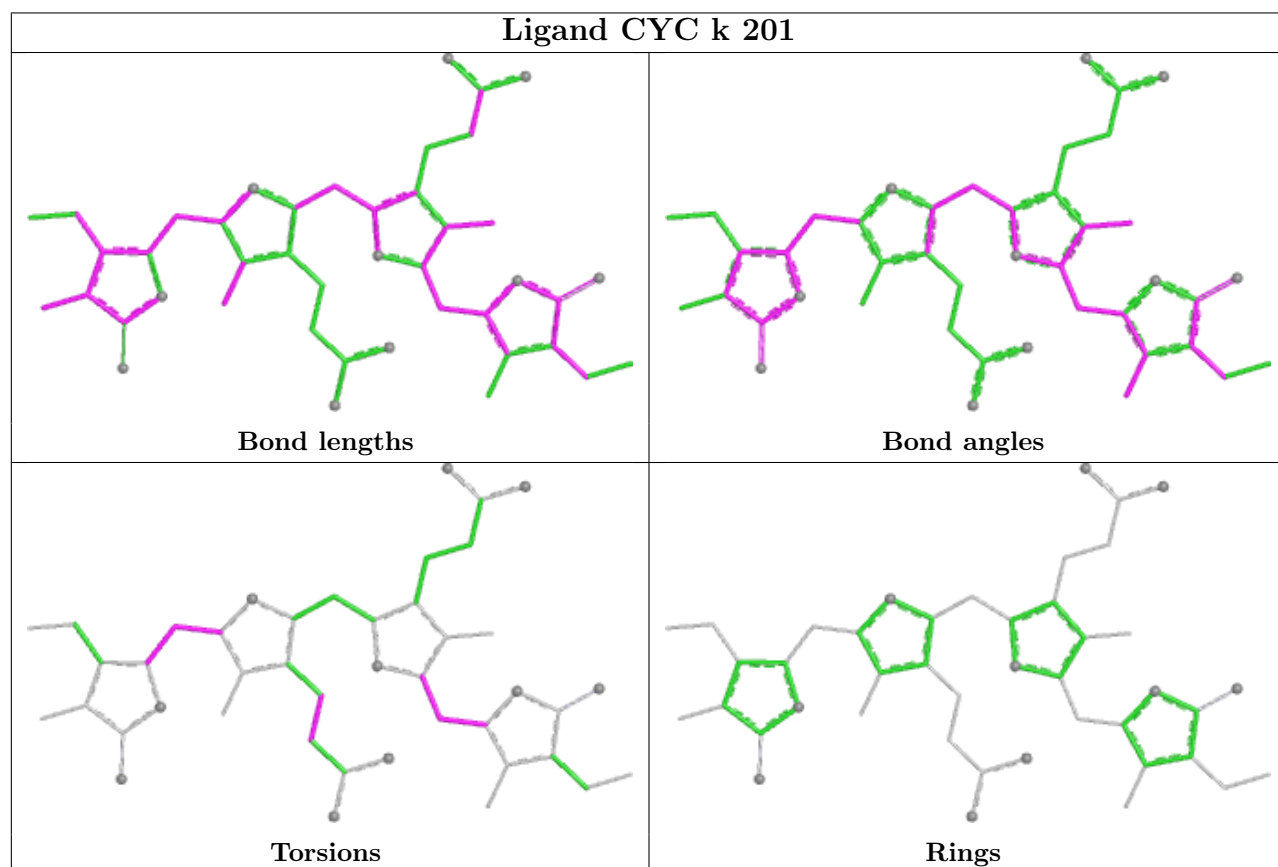
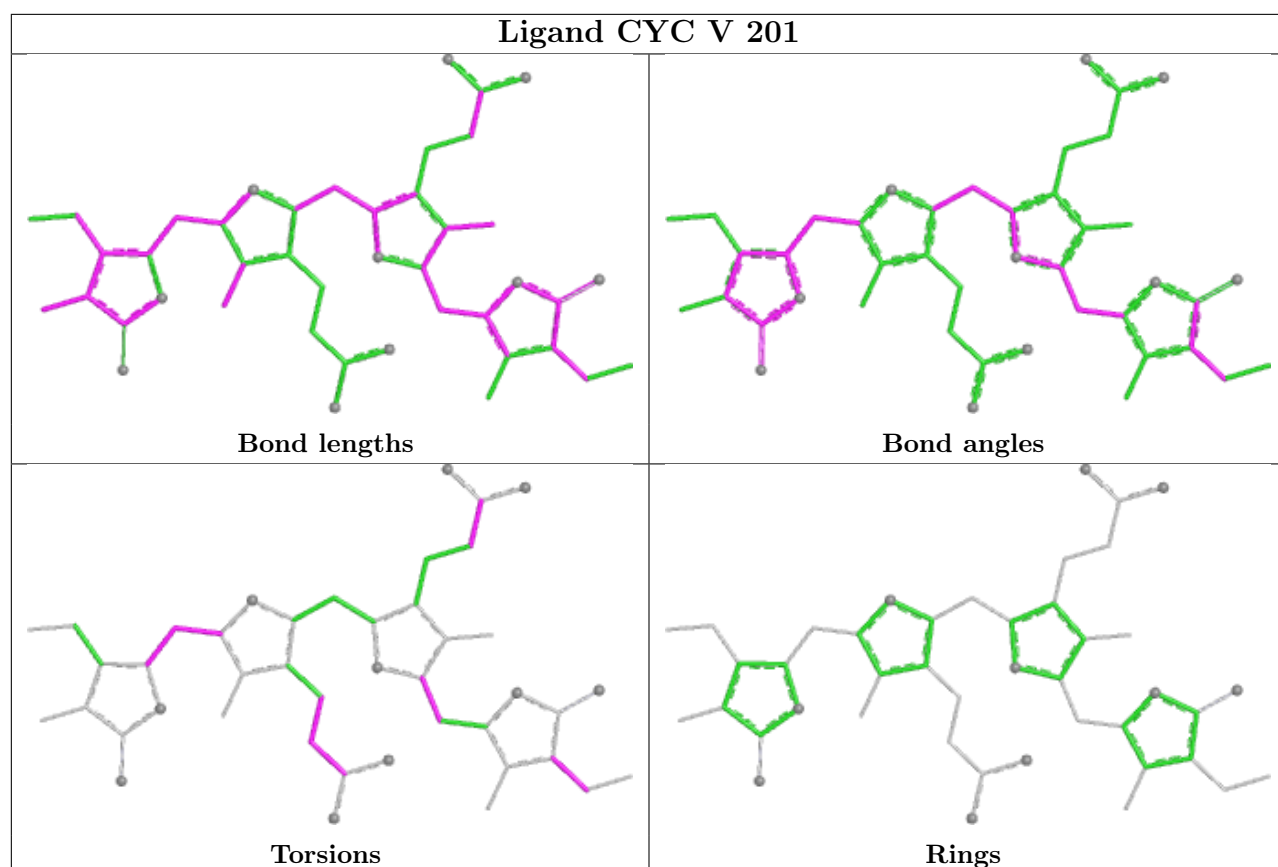


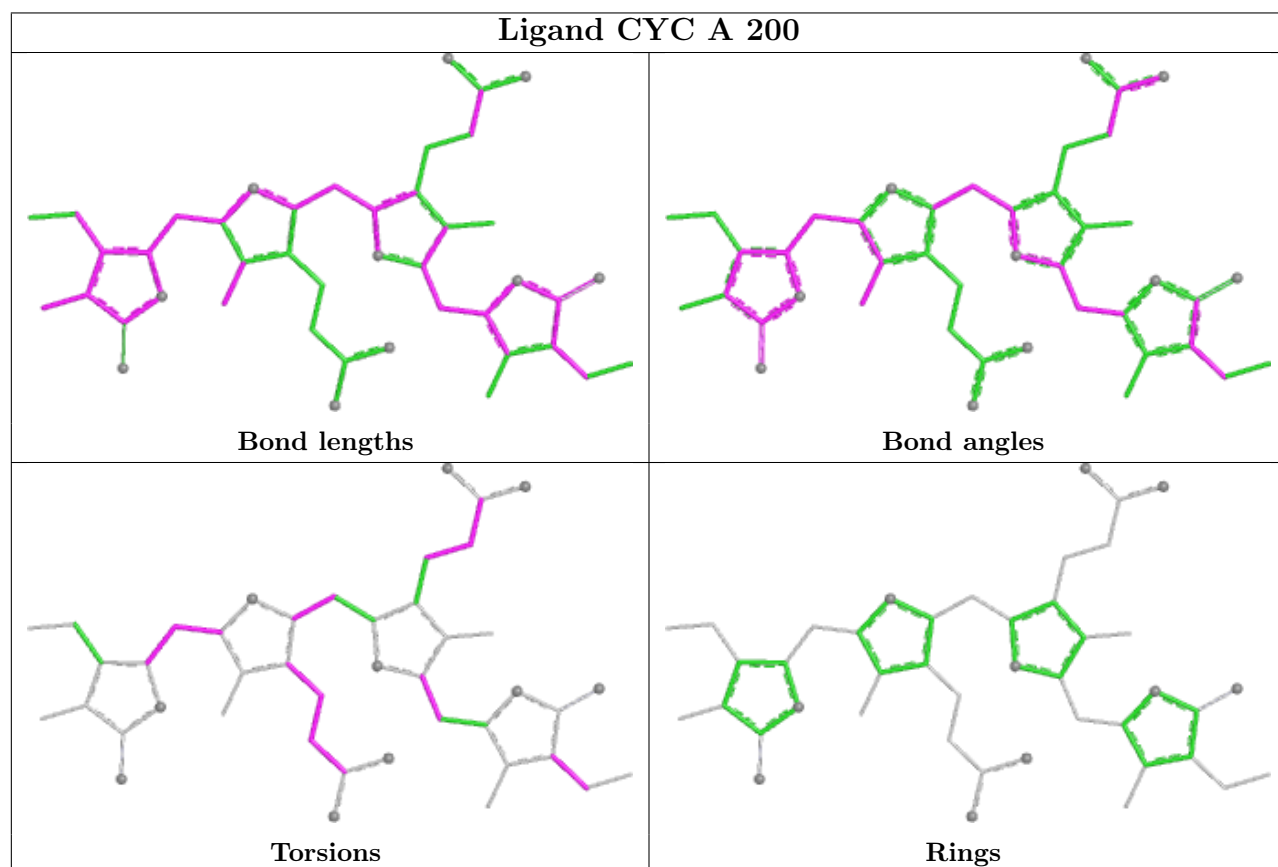
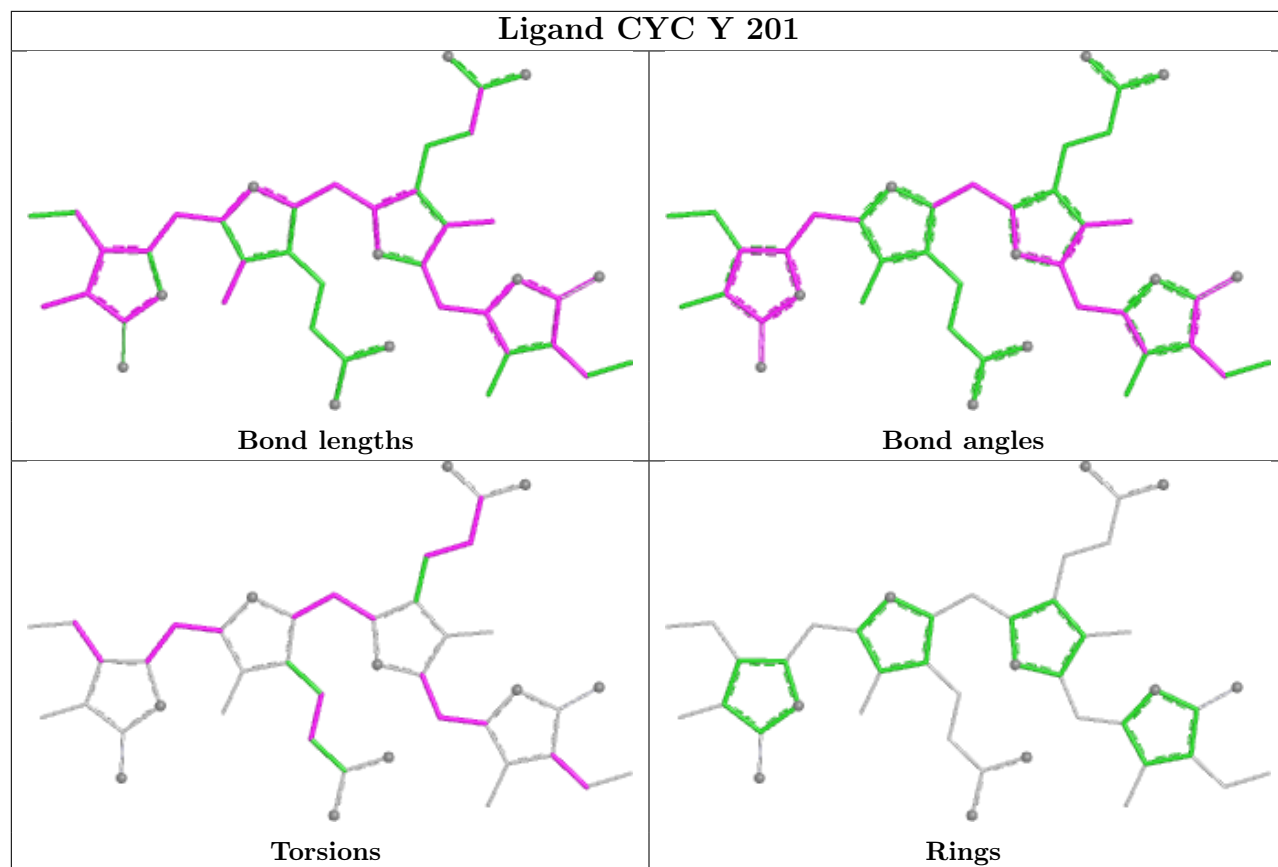
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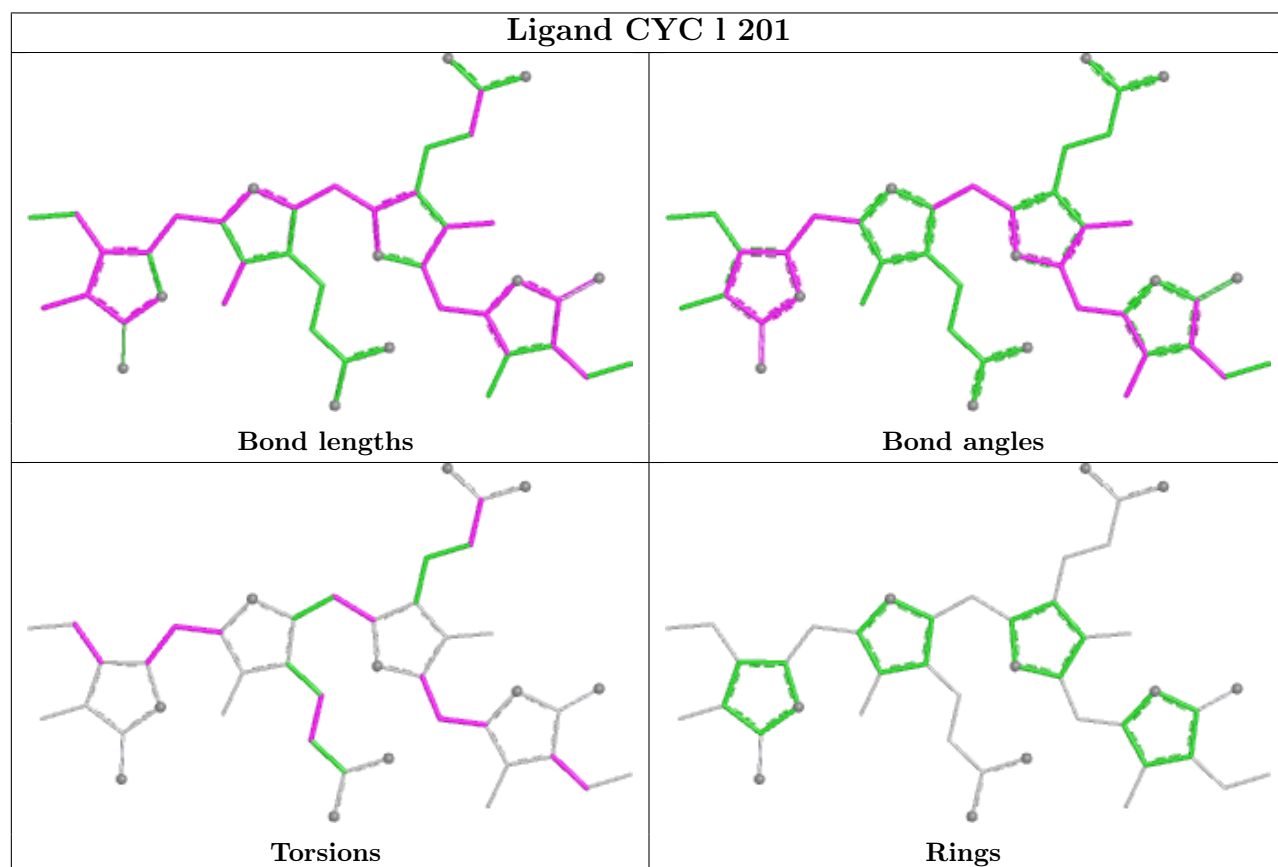
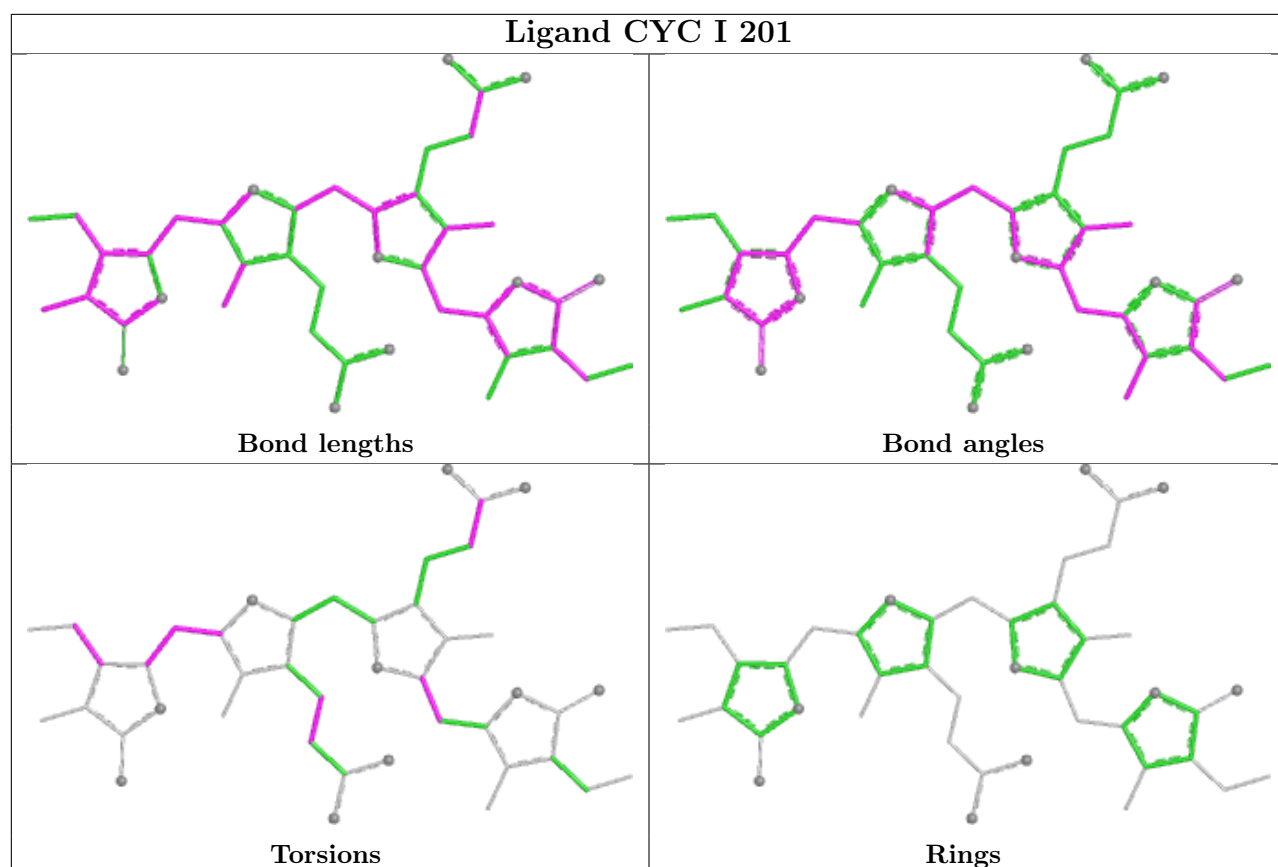


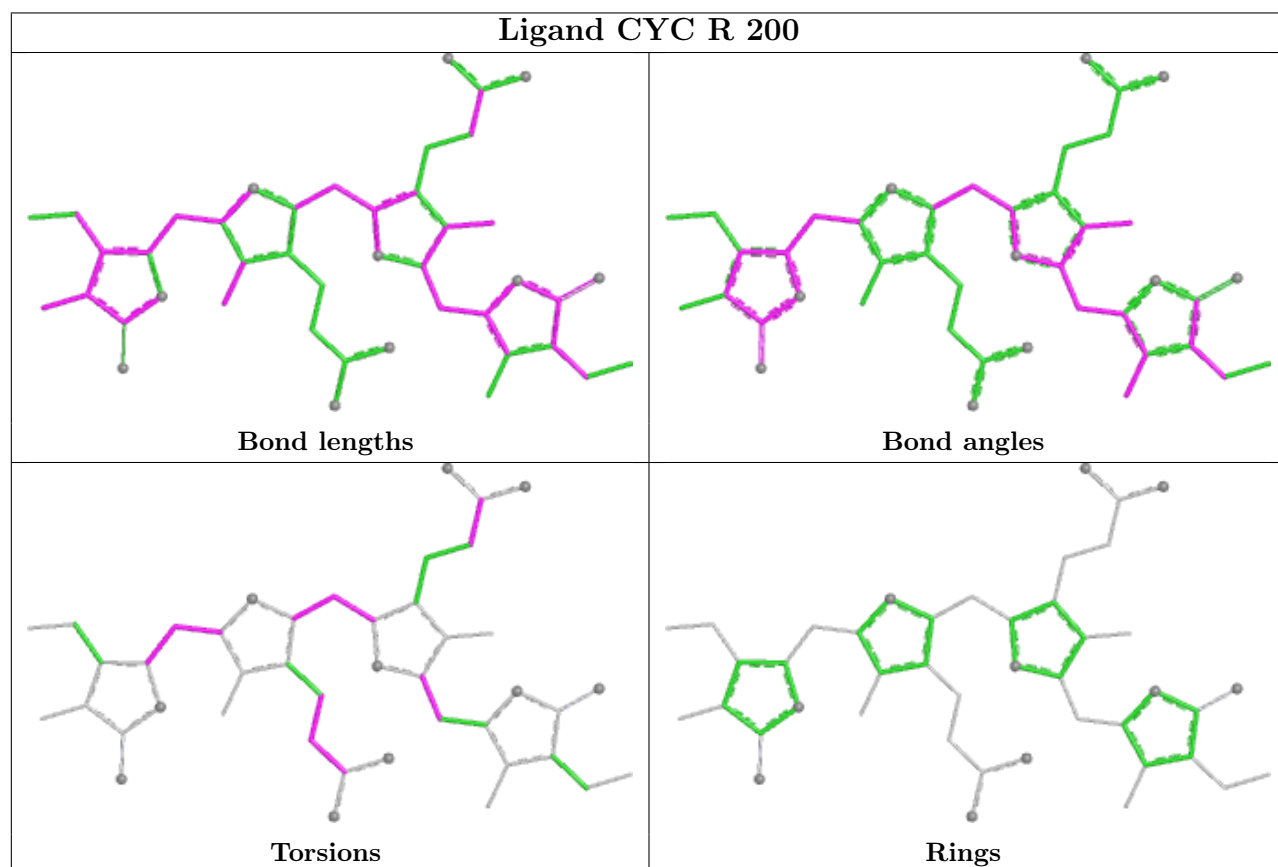
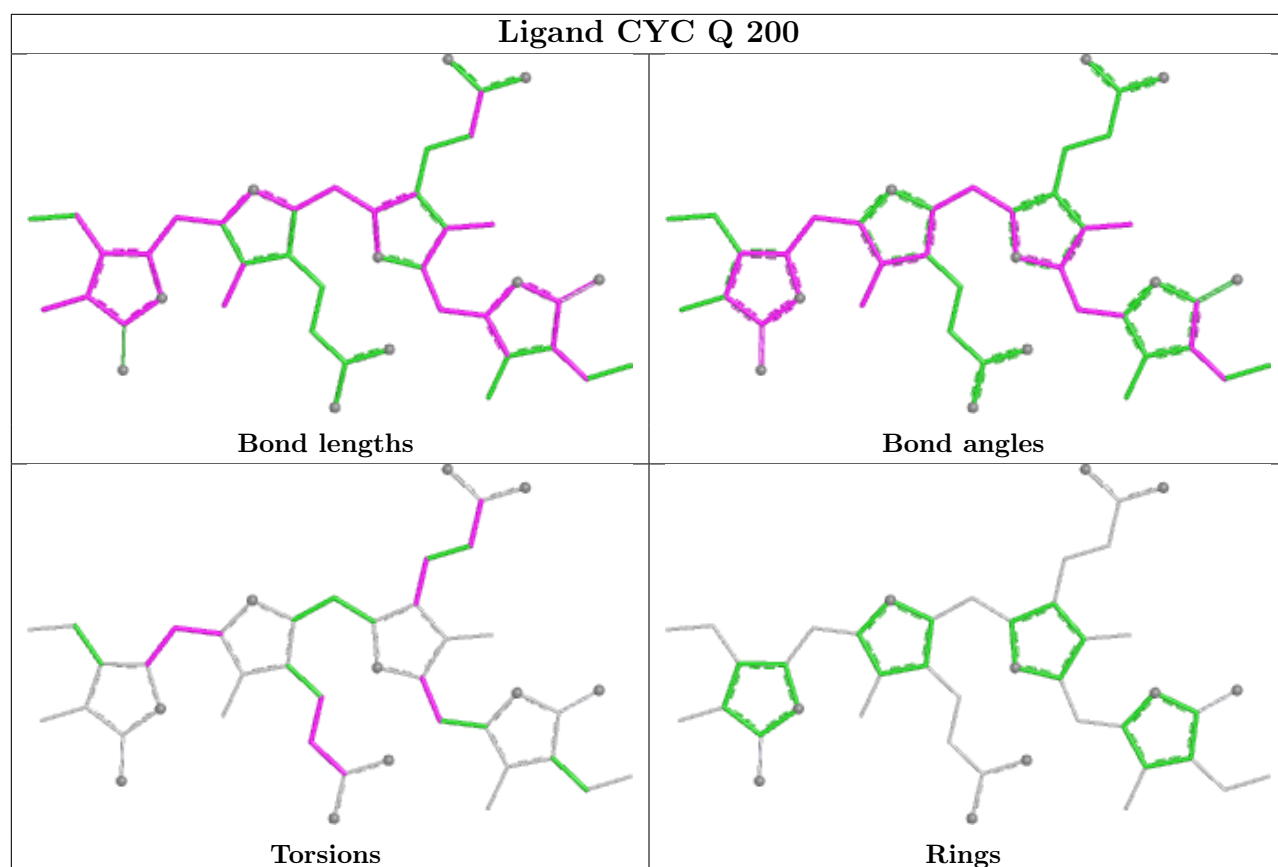


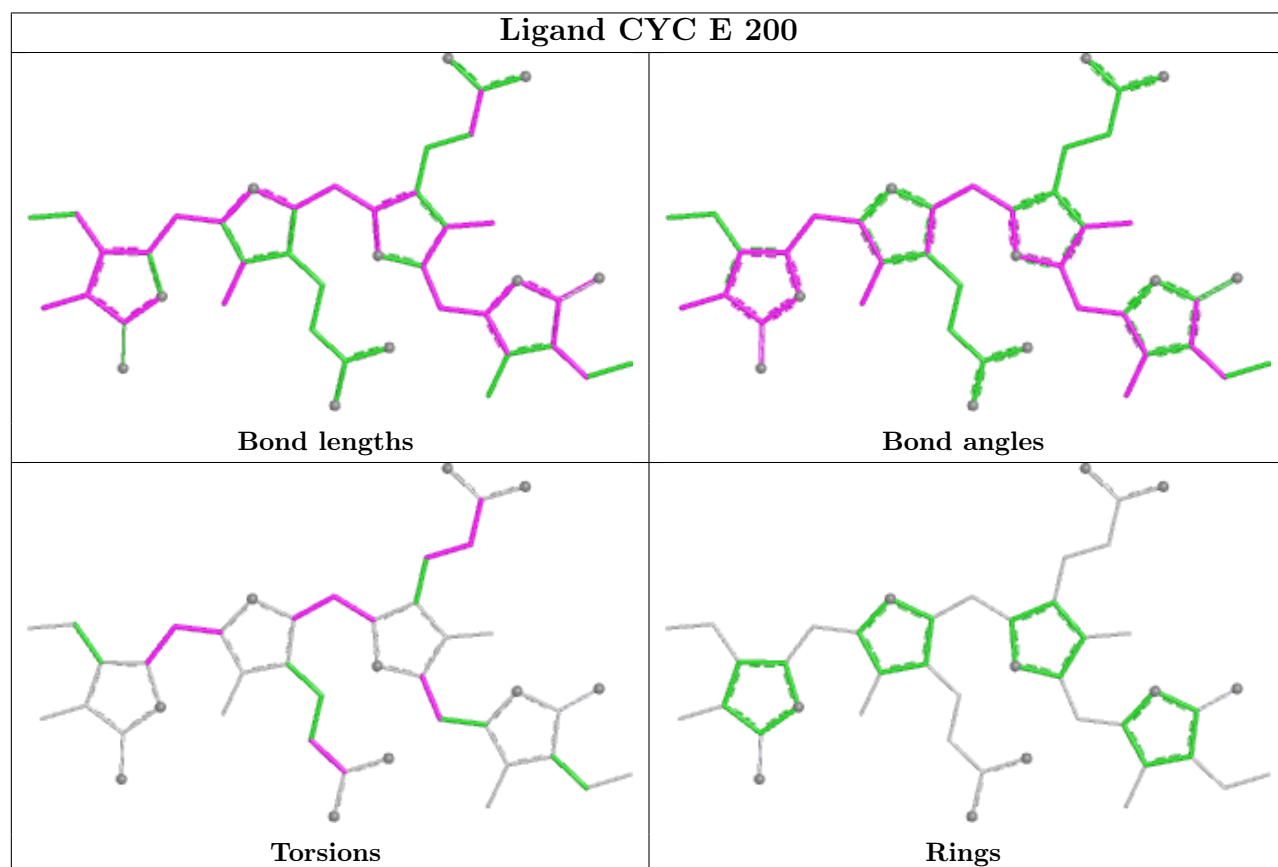
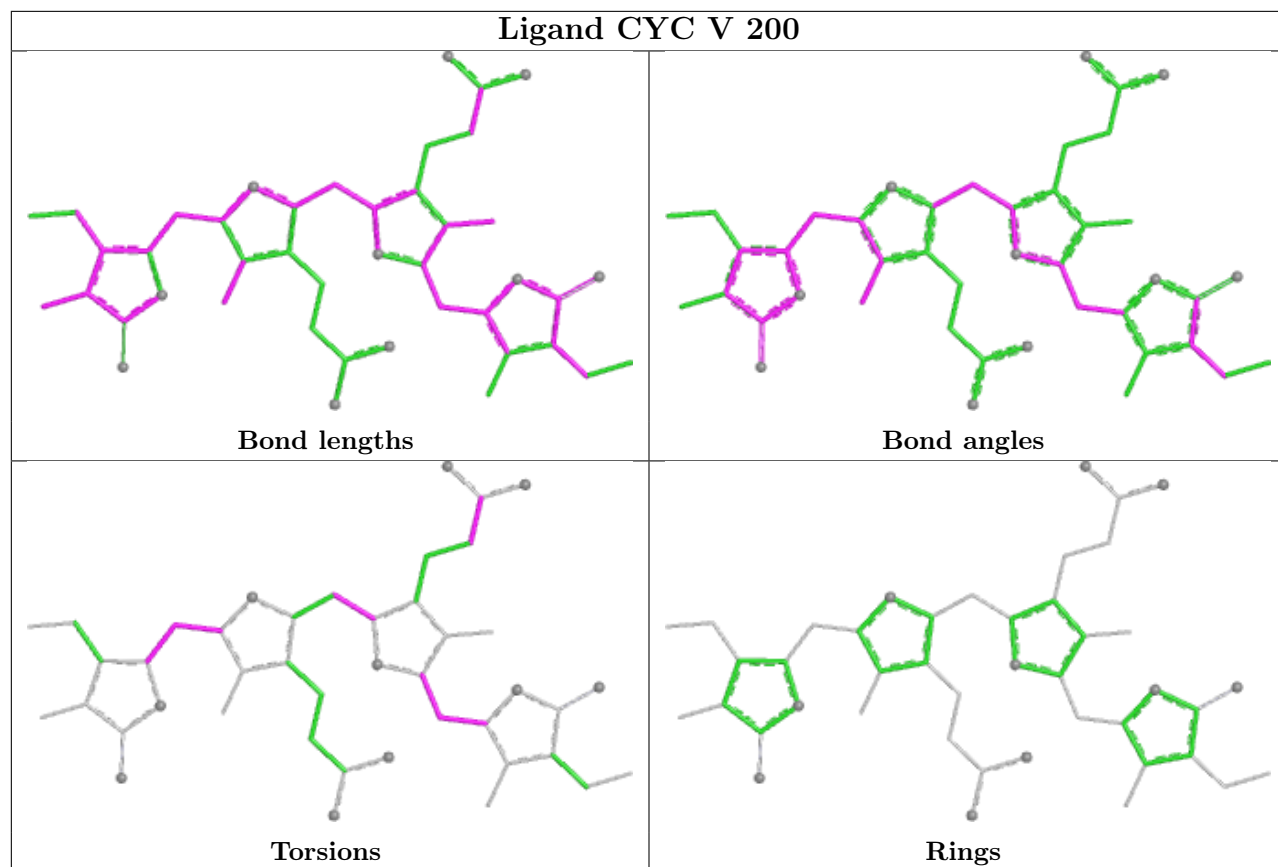


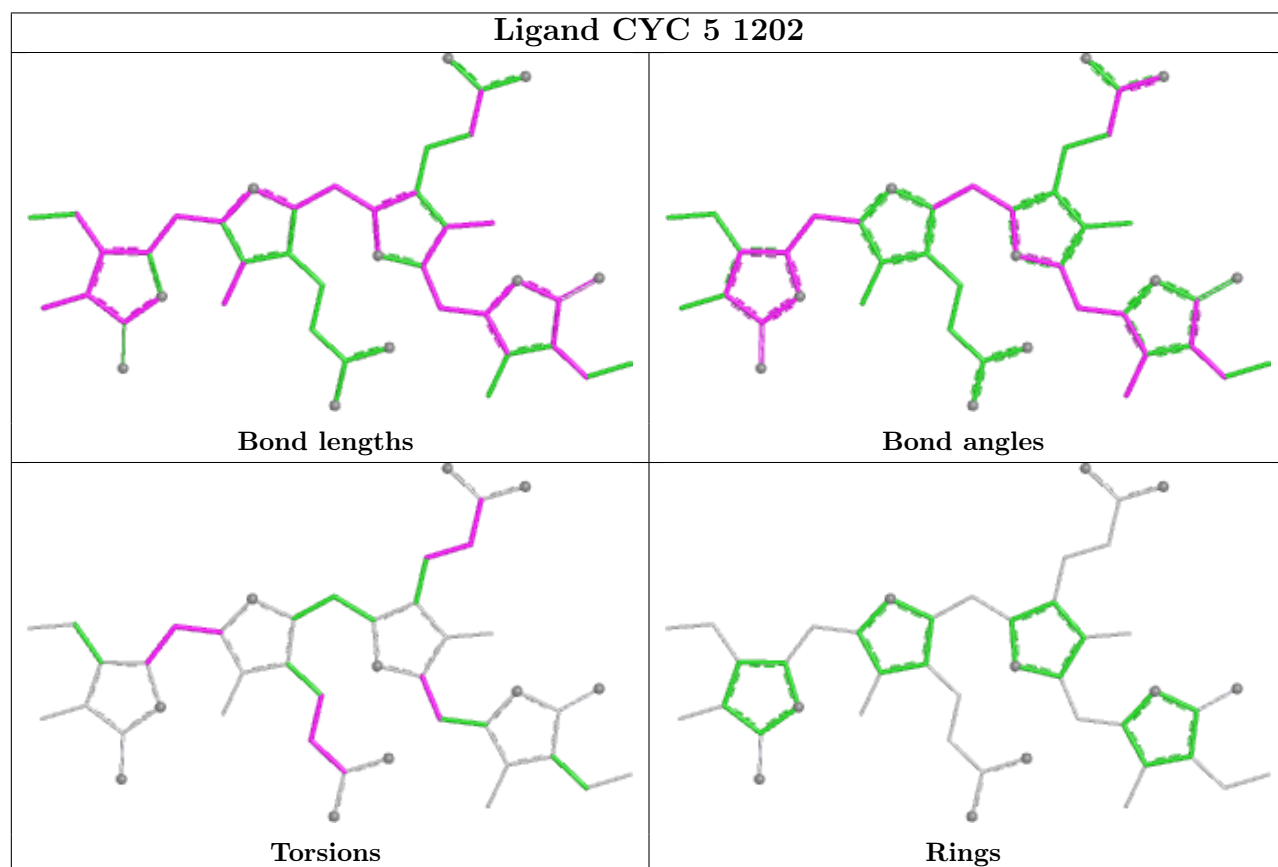
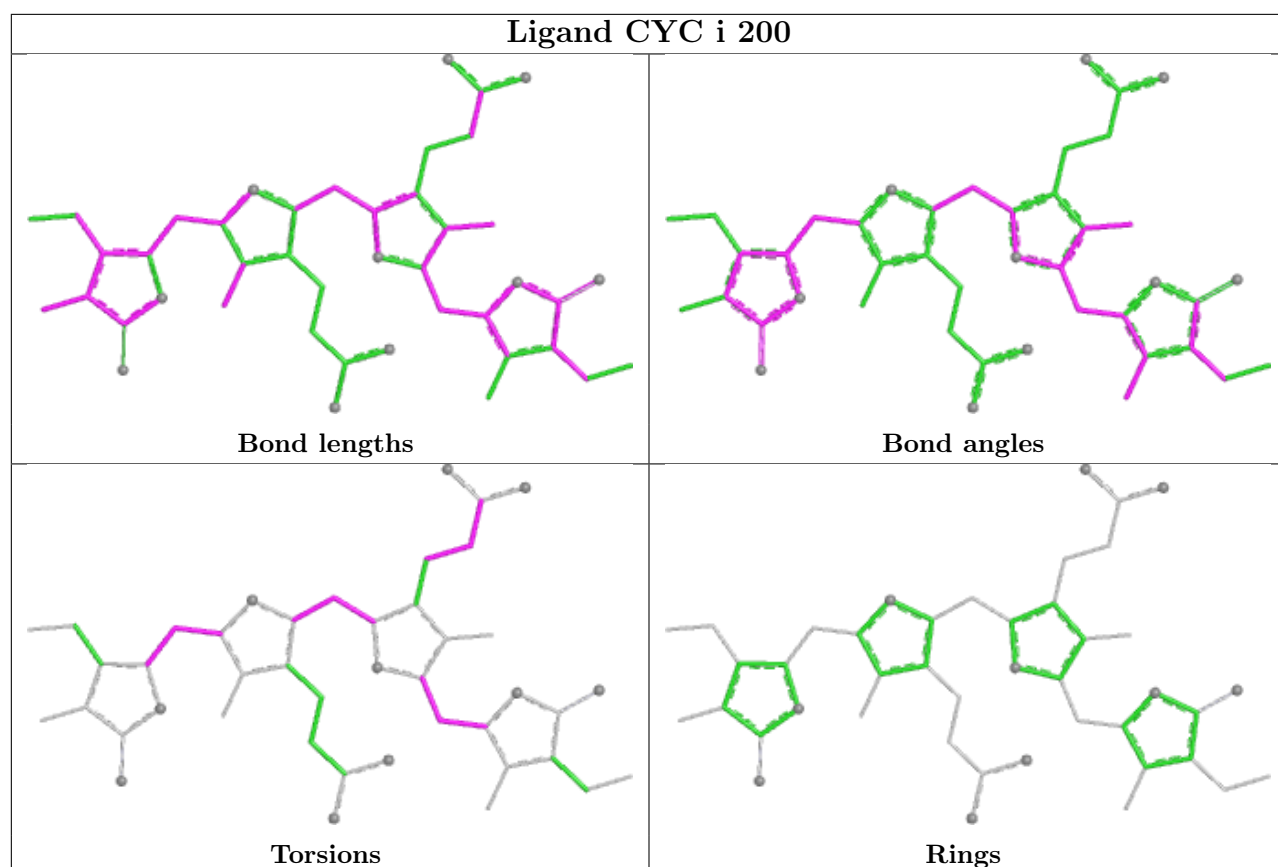




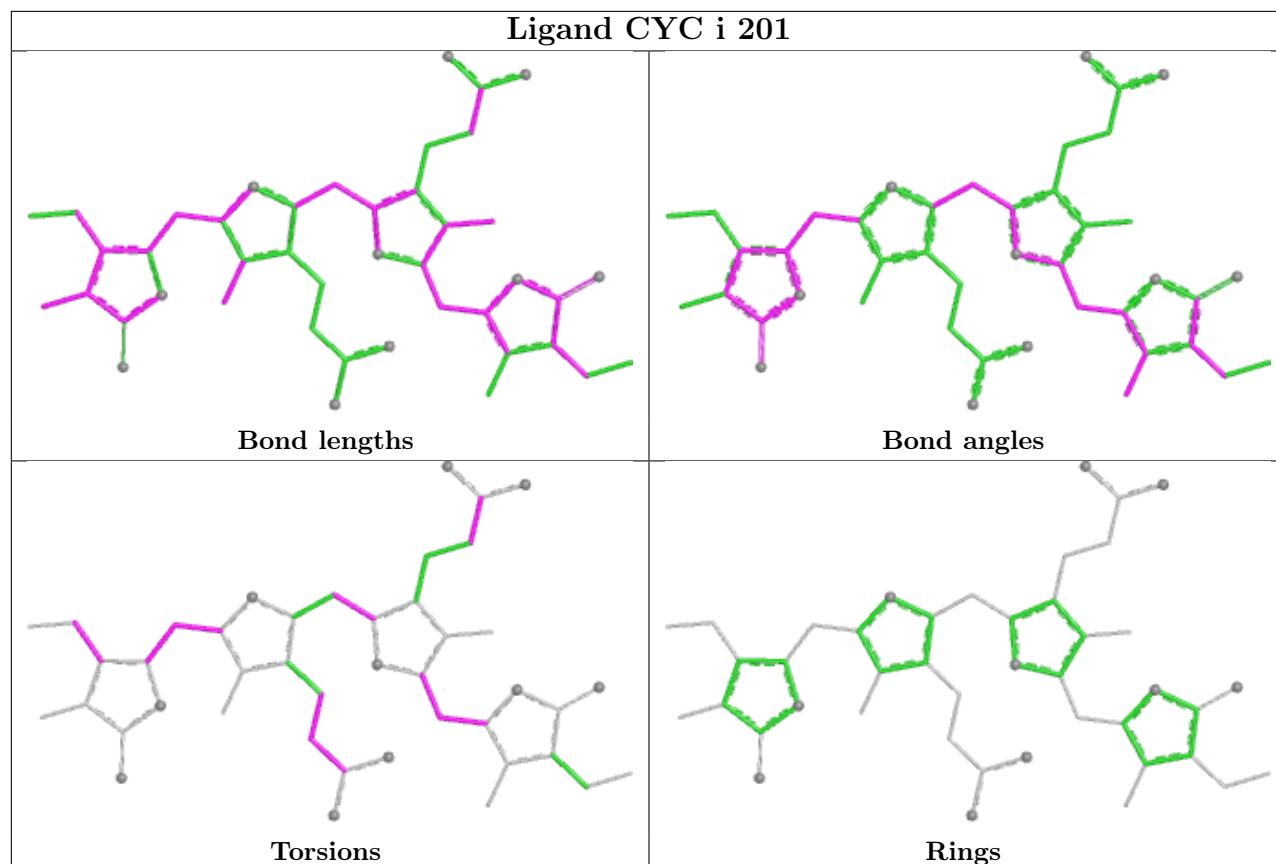




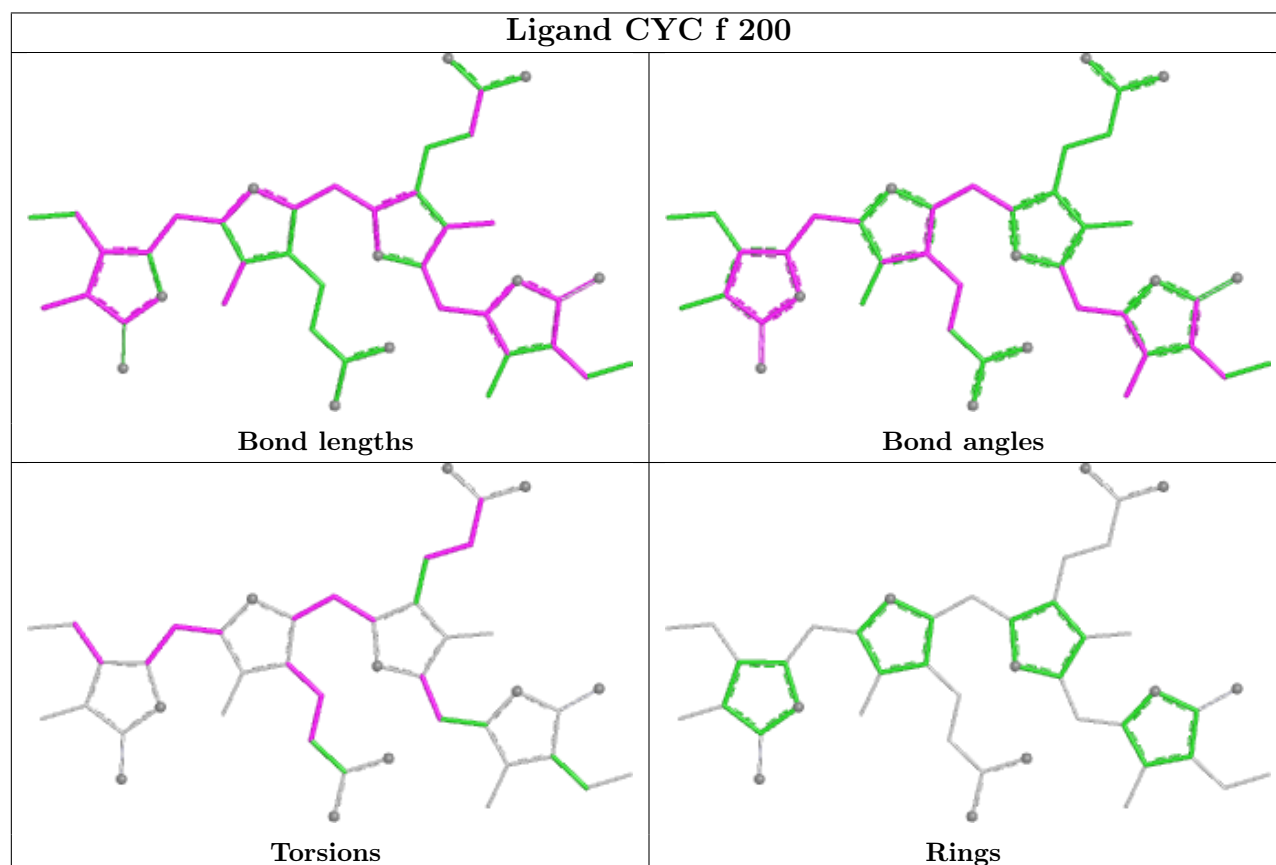


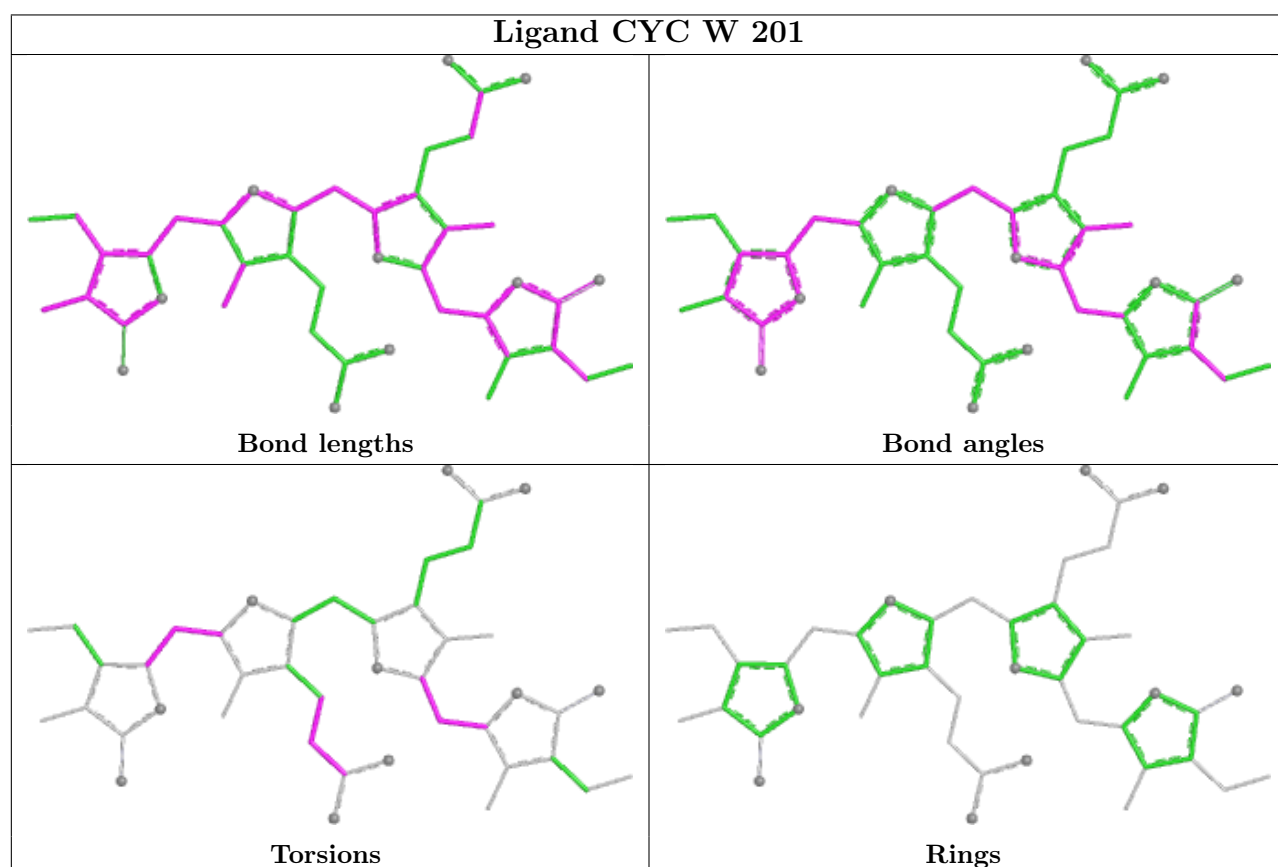
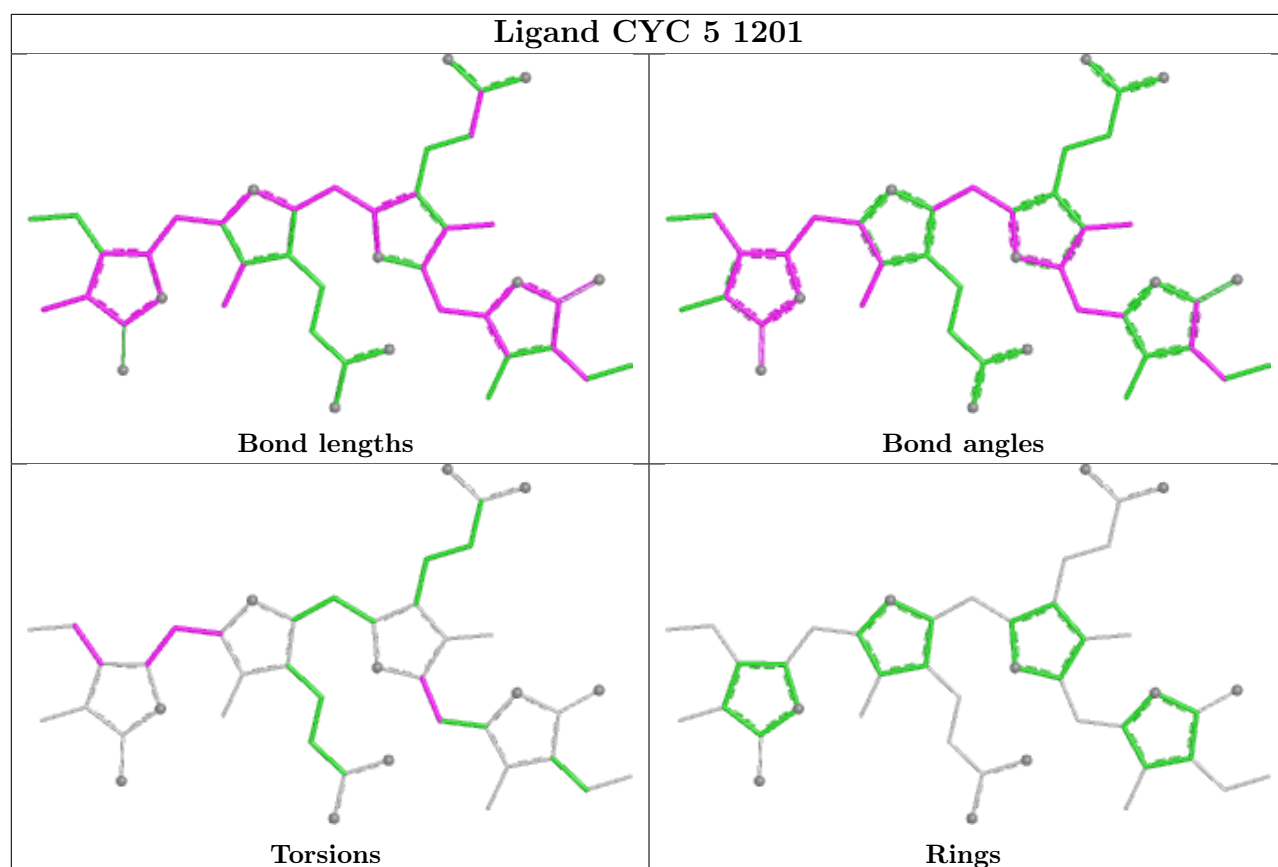


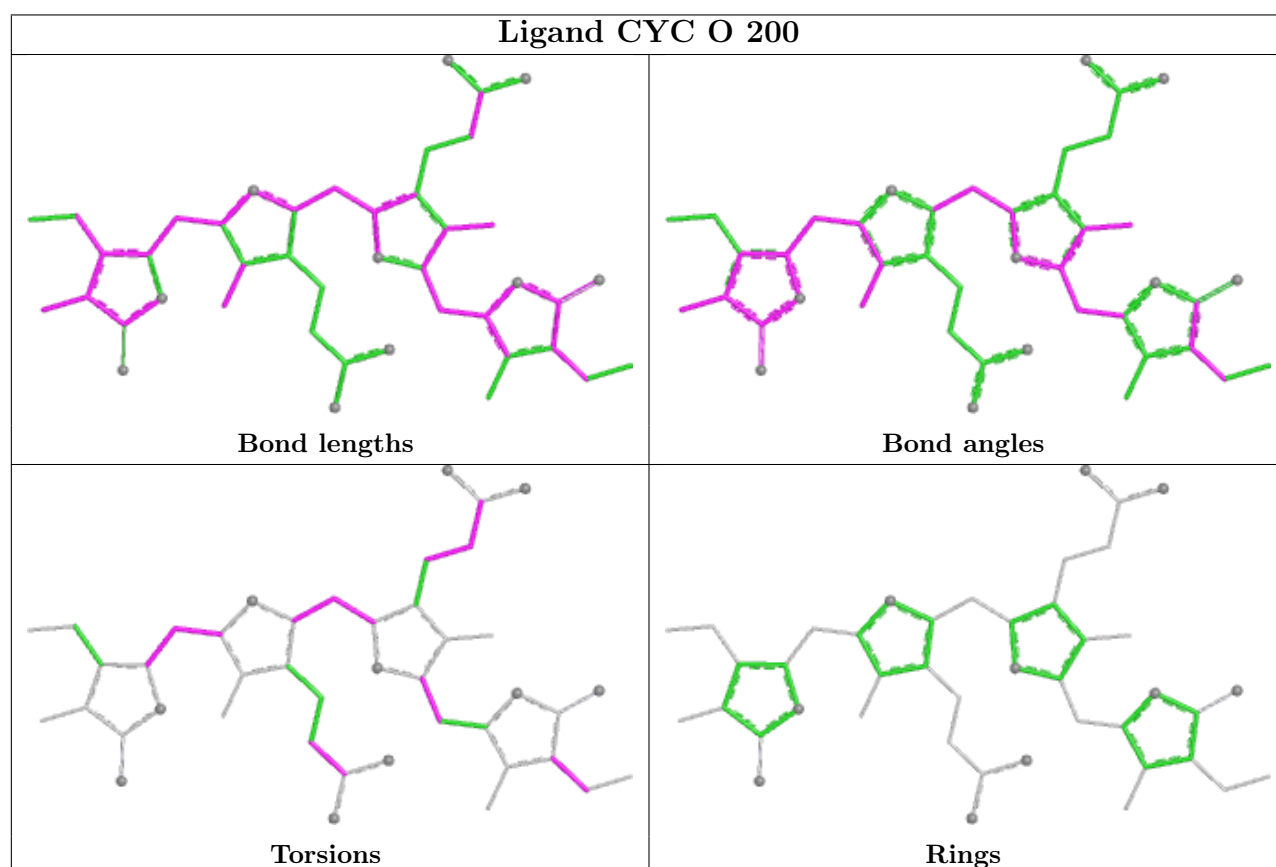
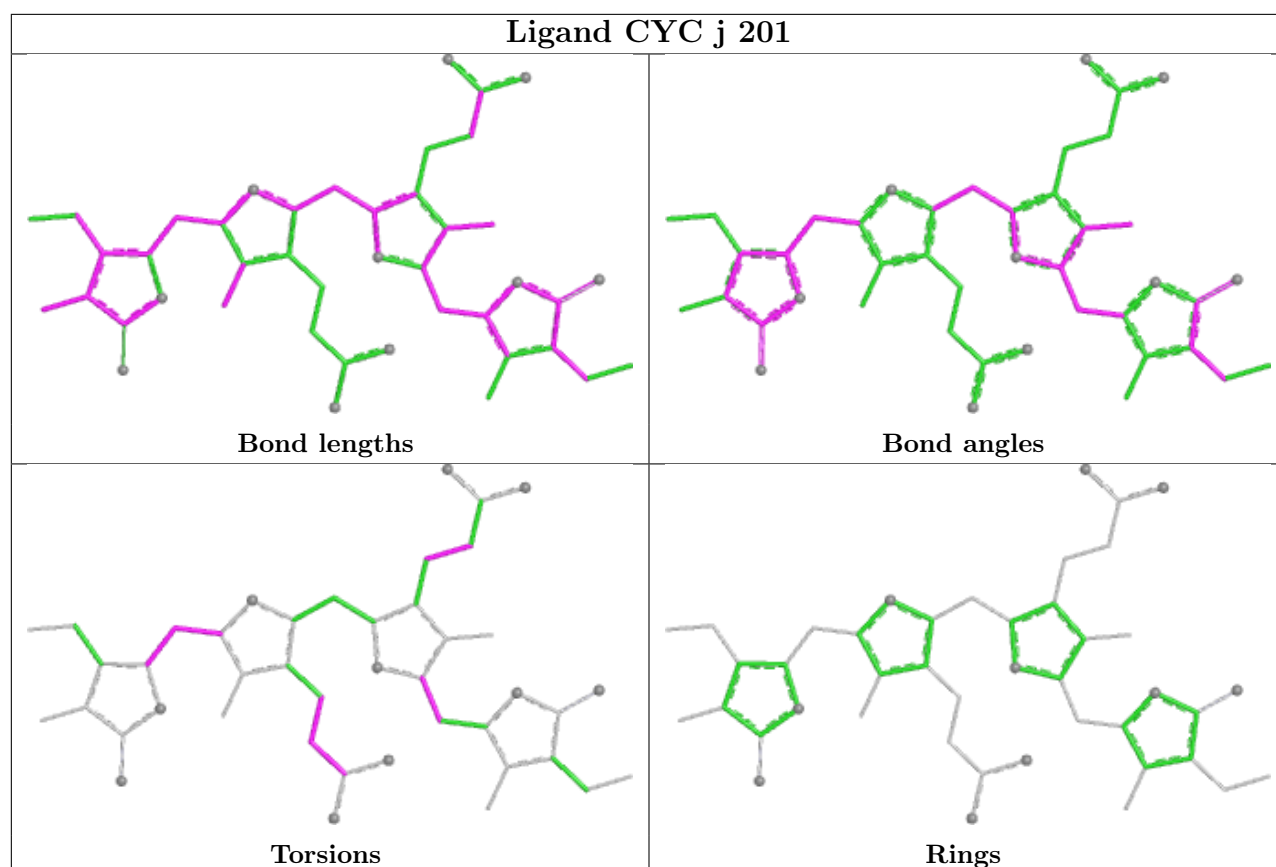
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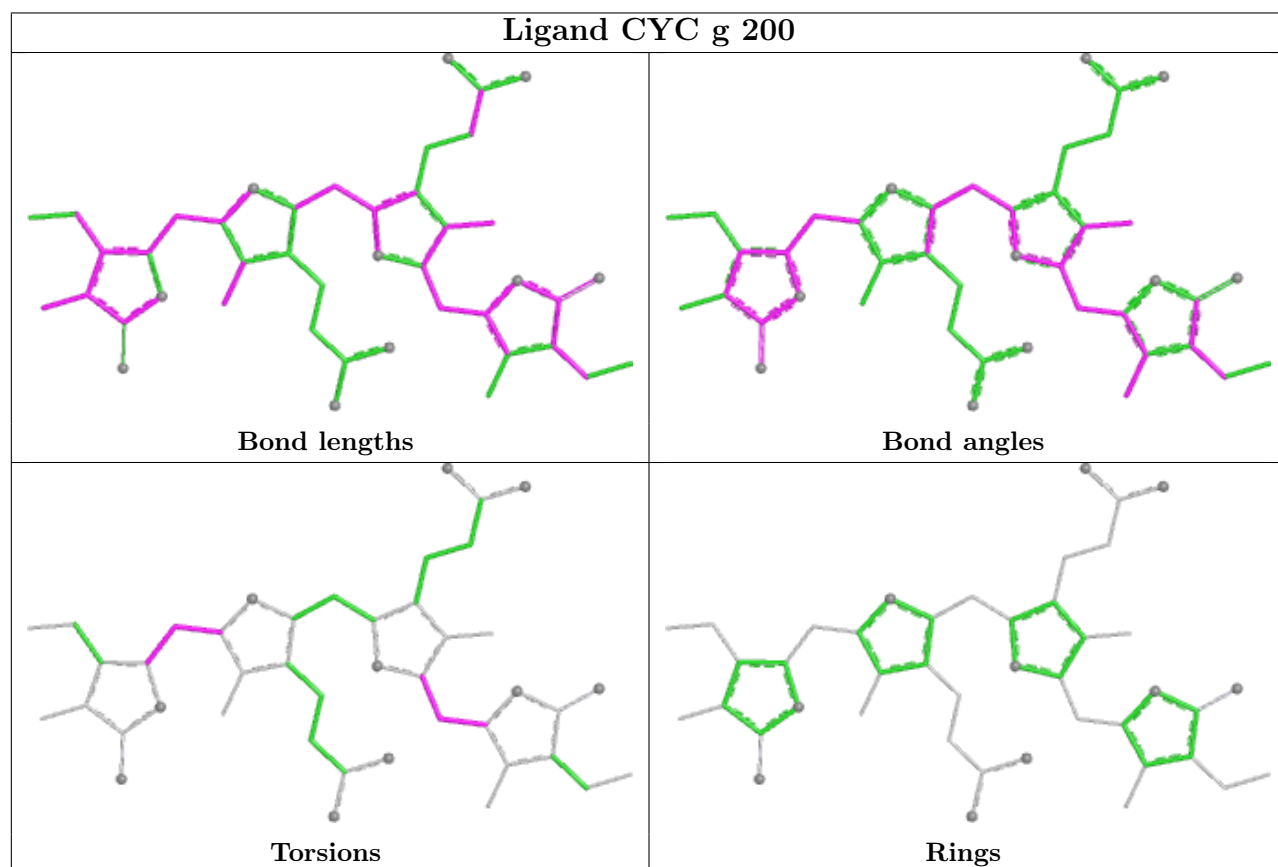
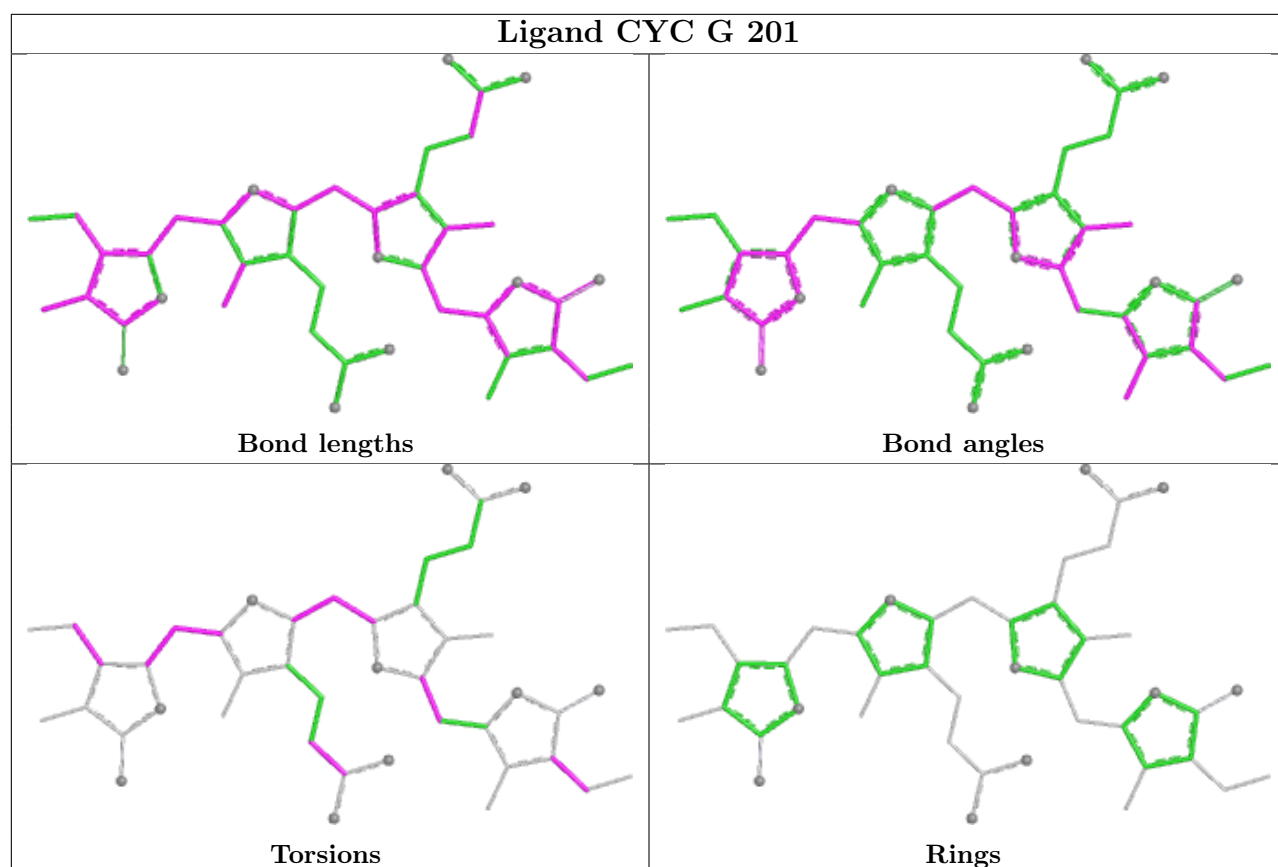


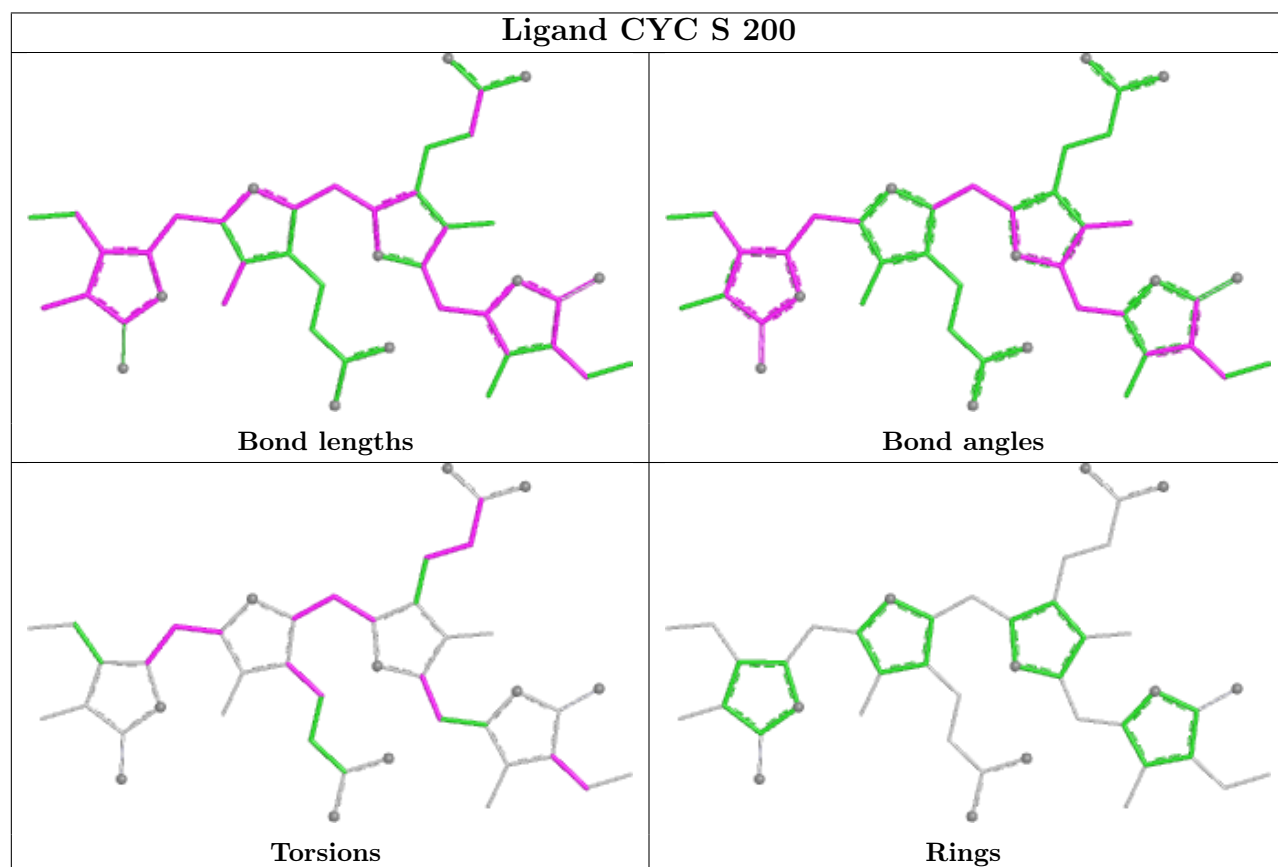
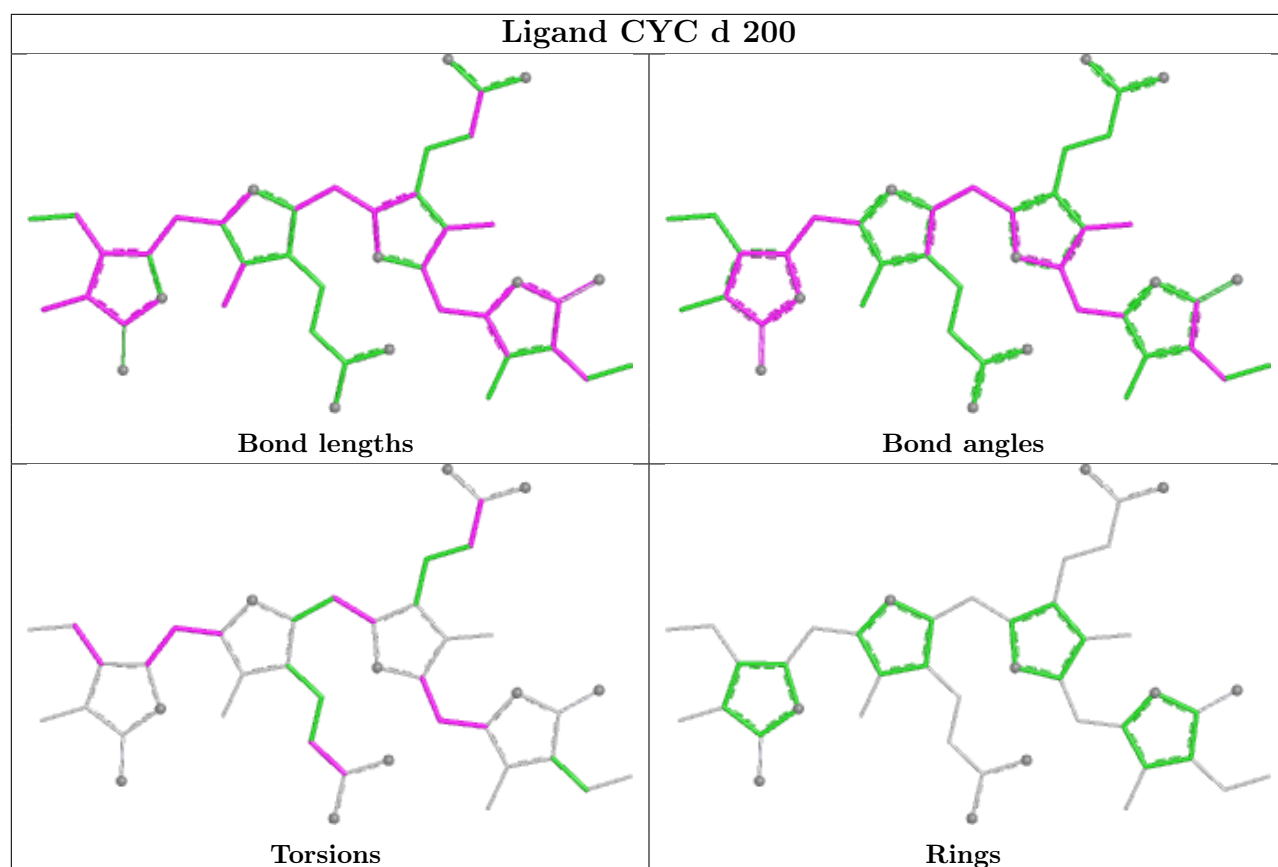
Ligand CYC f 200

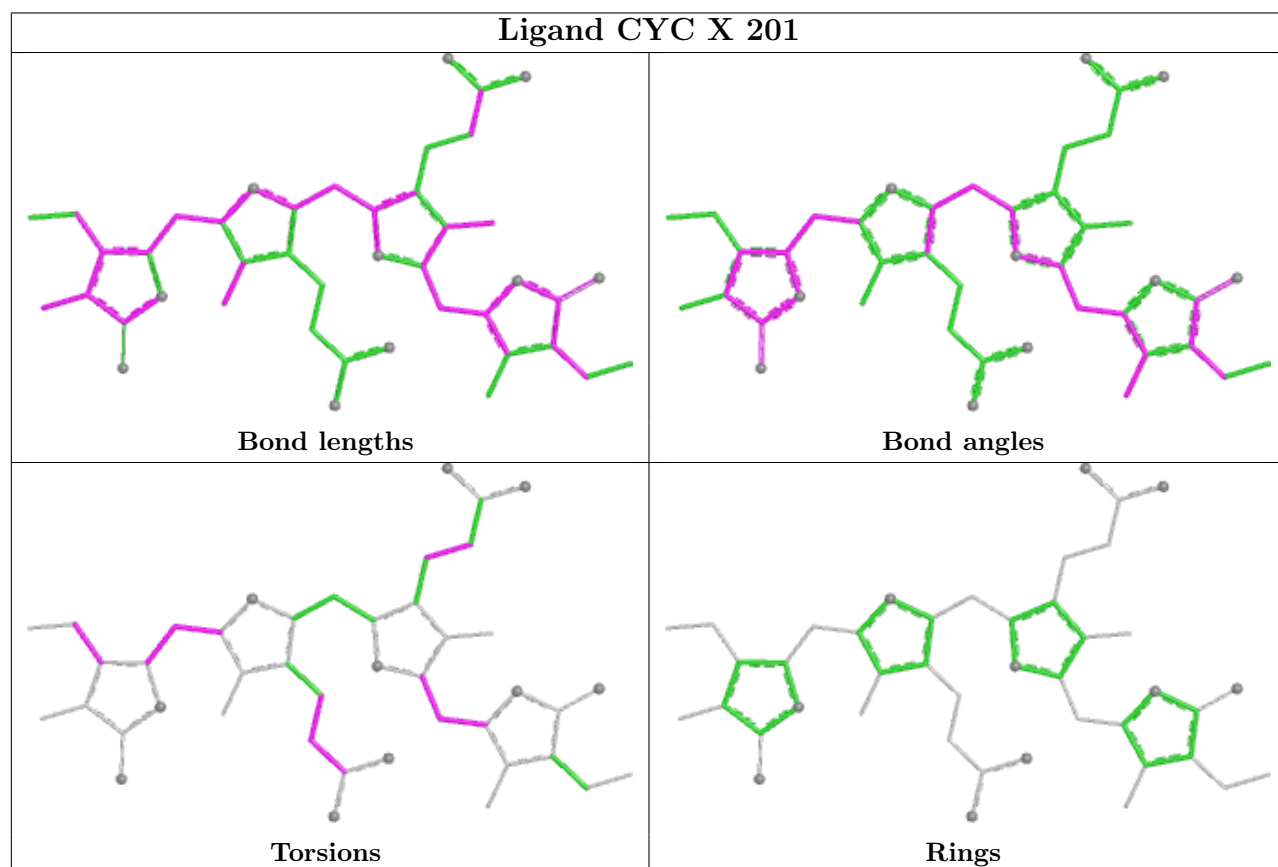
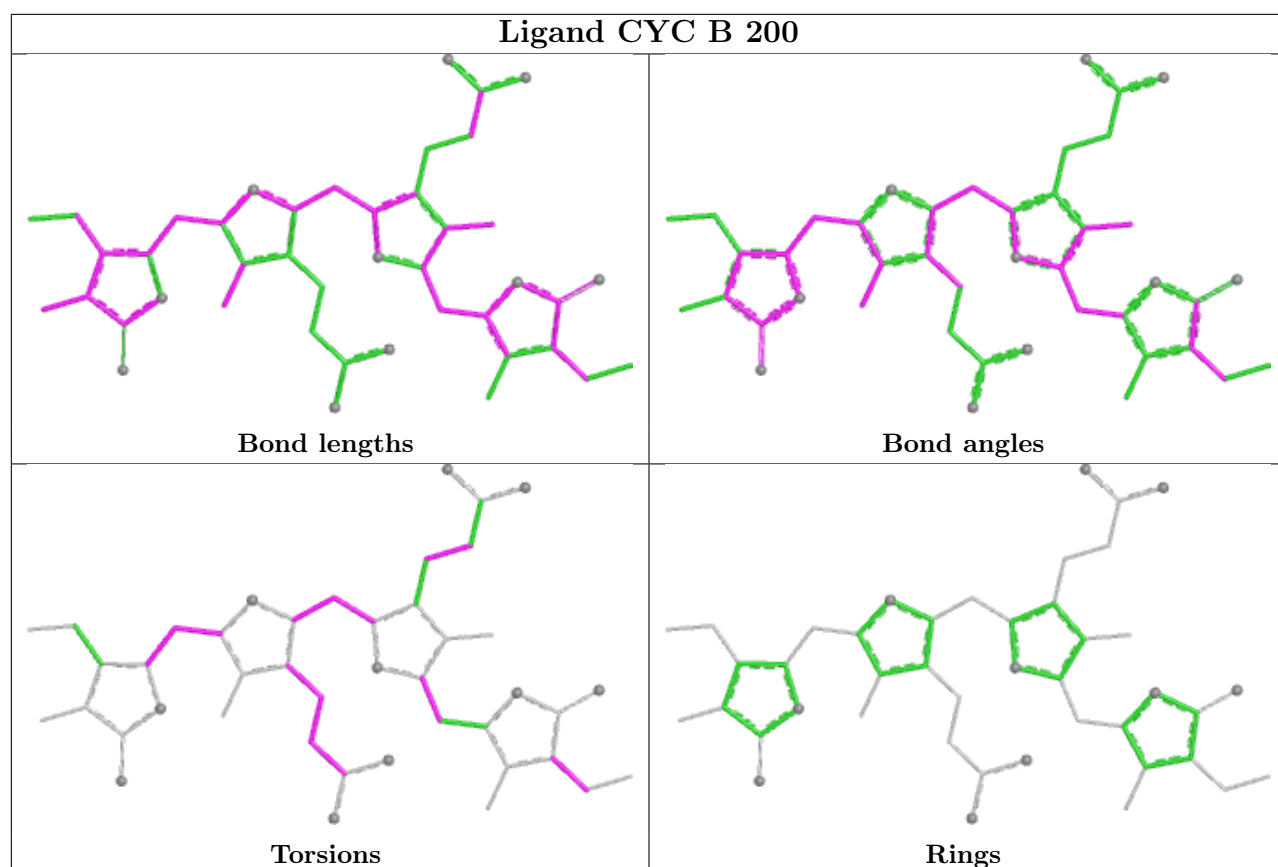


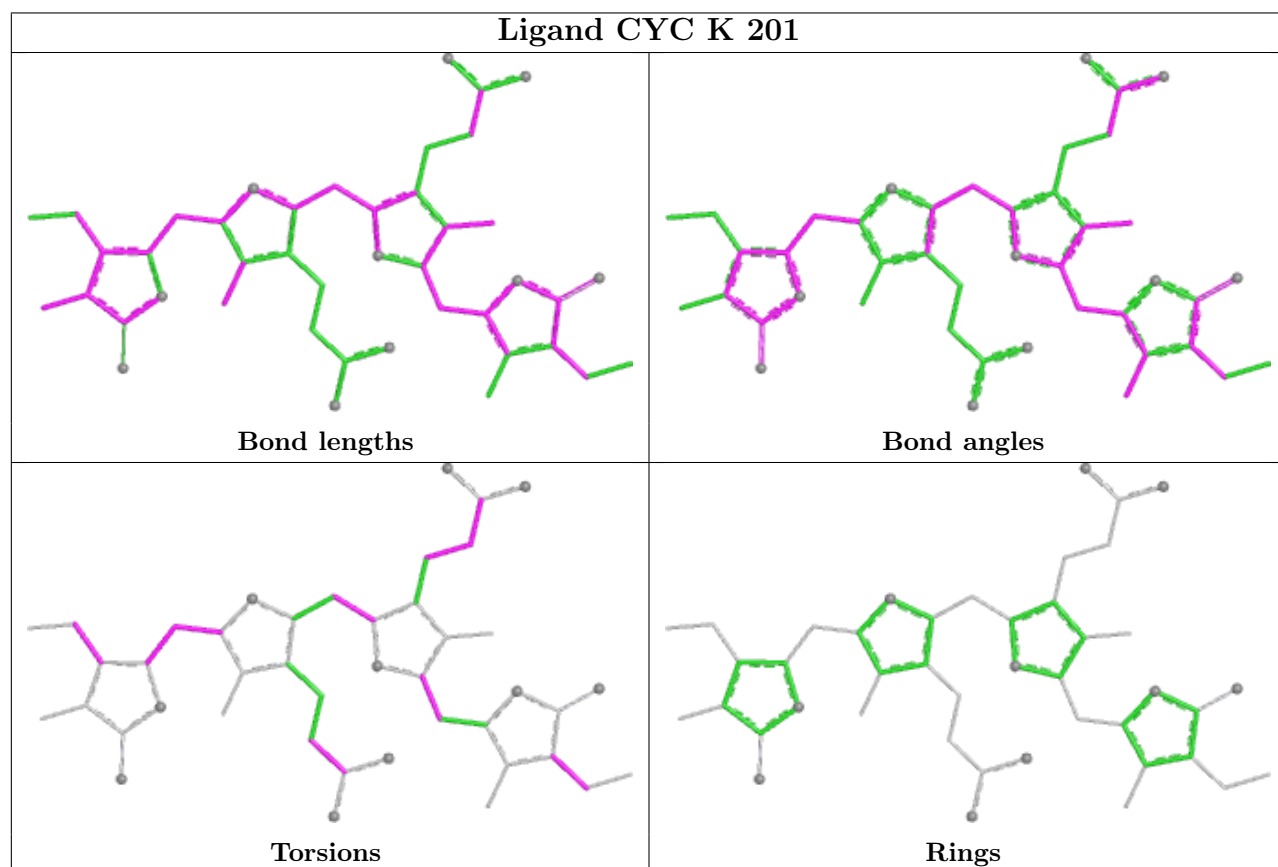
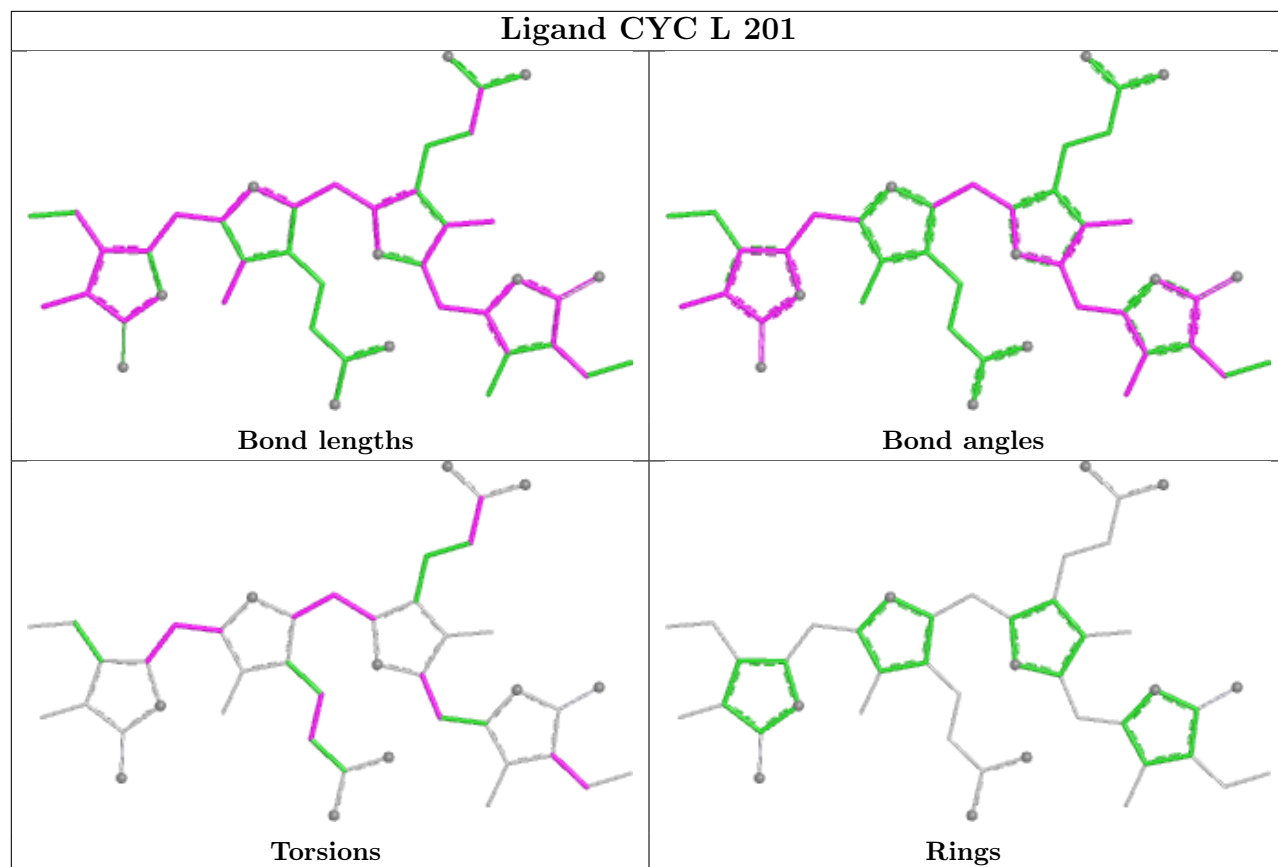


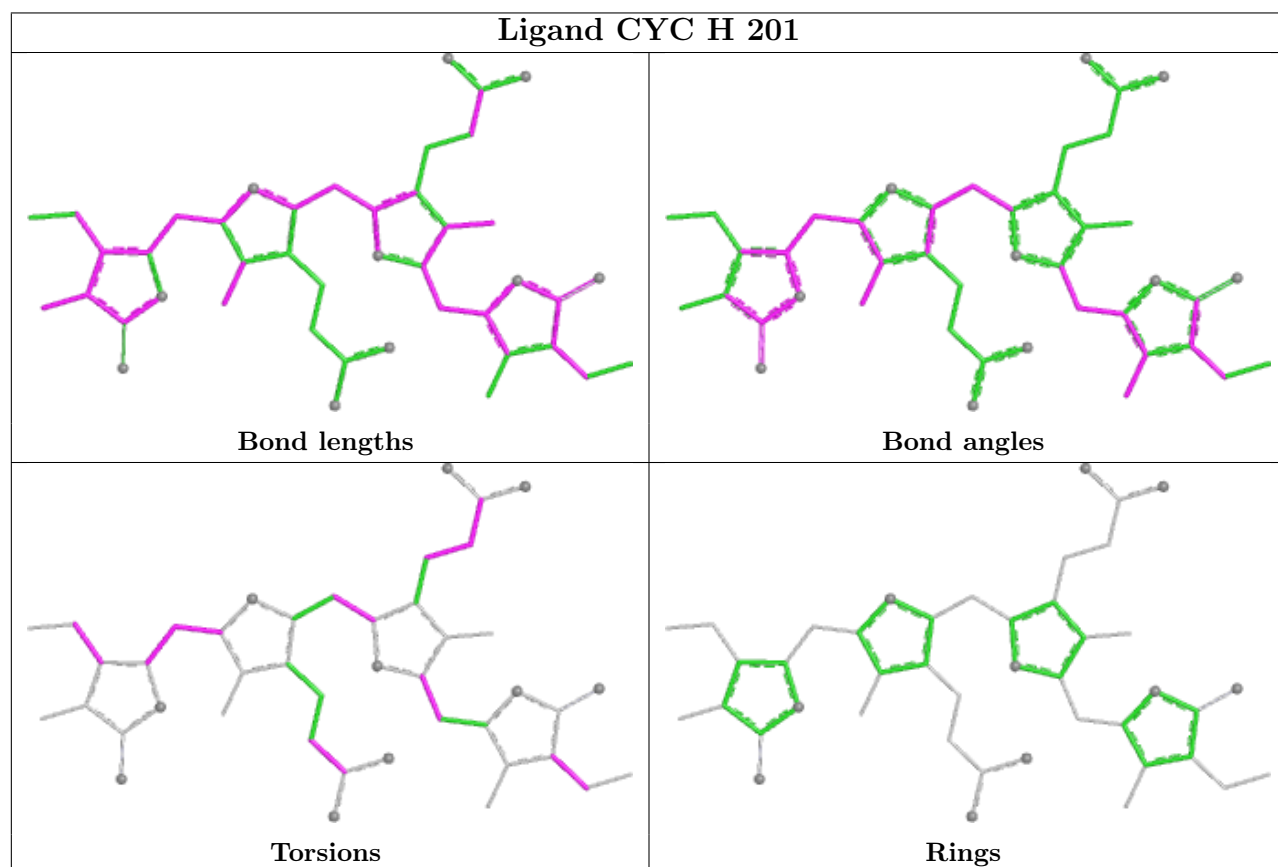
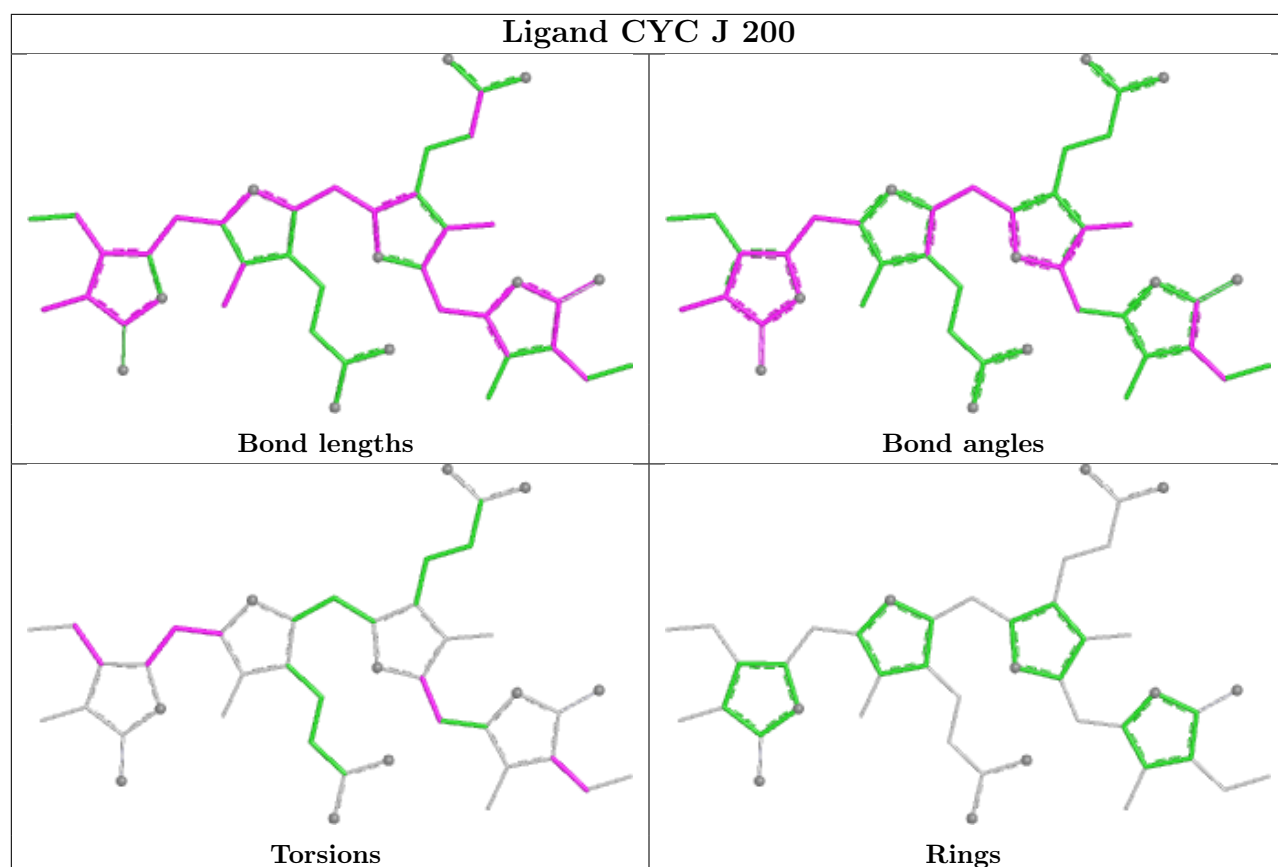


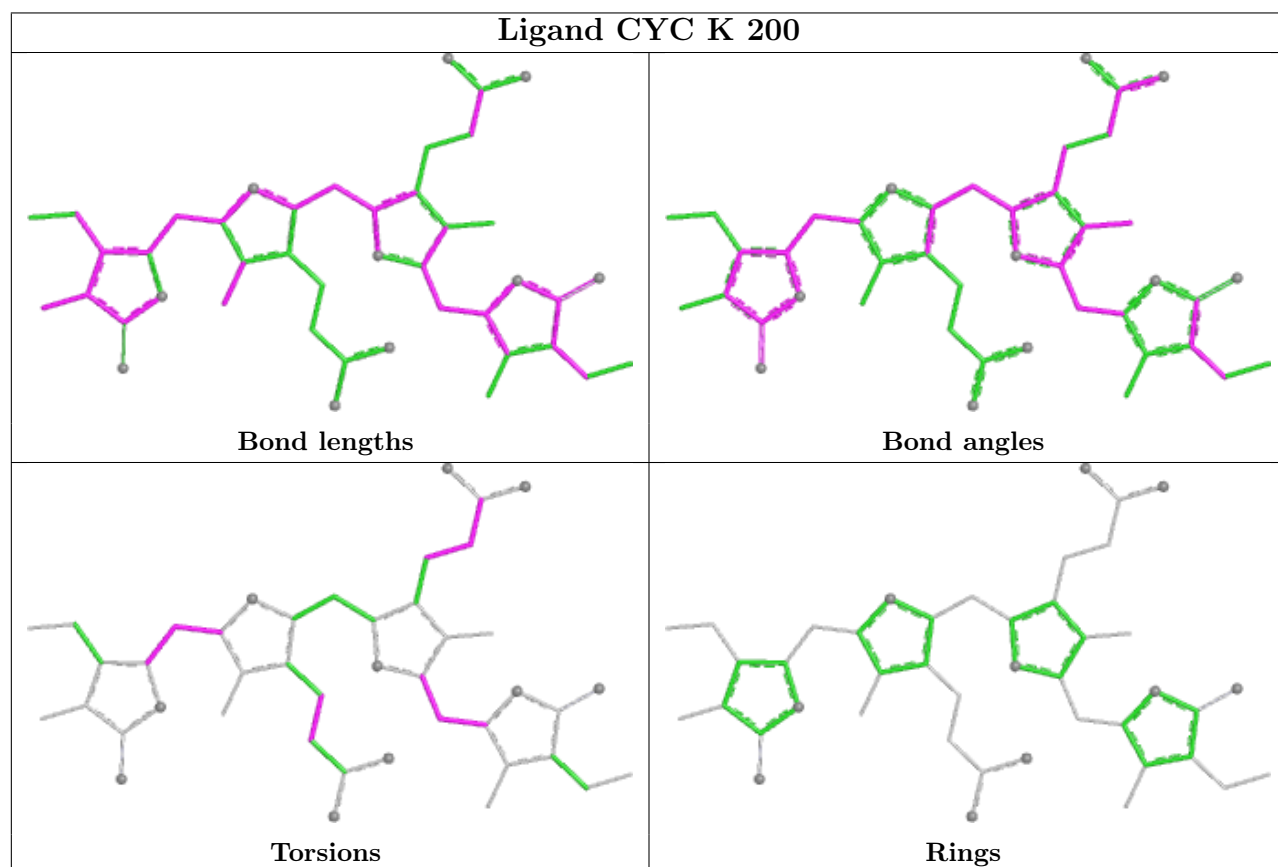
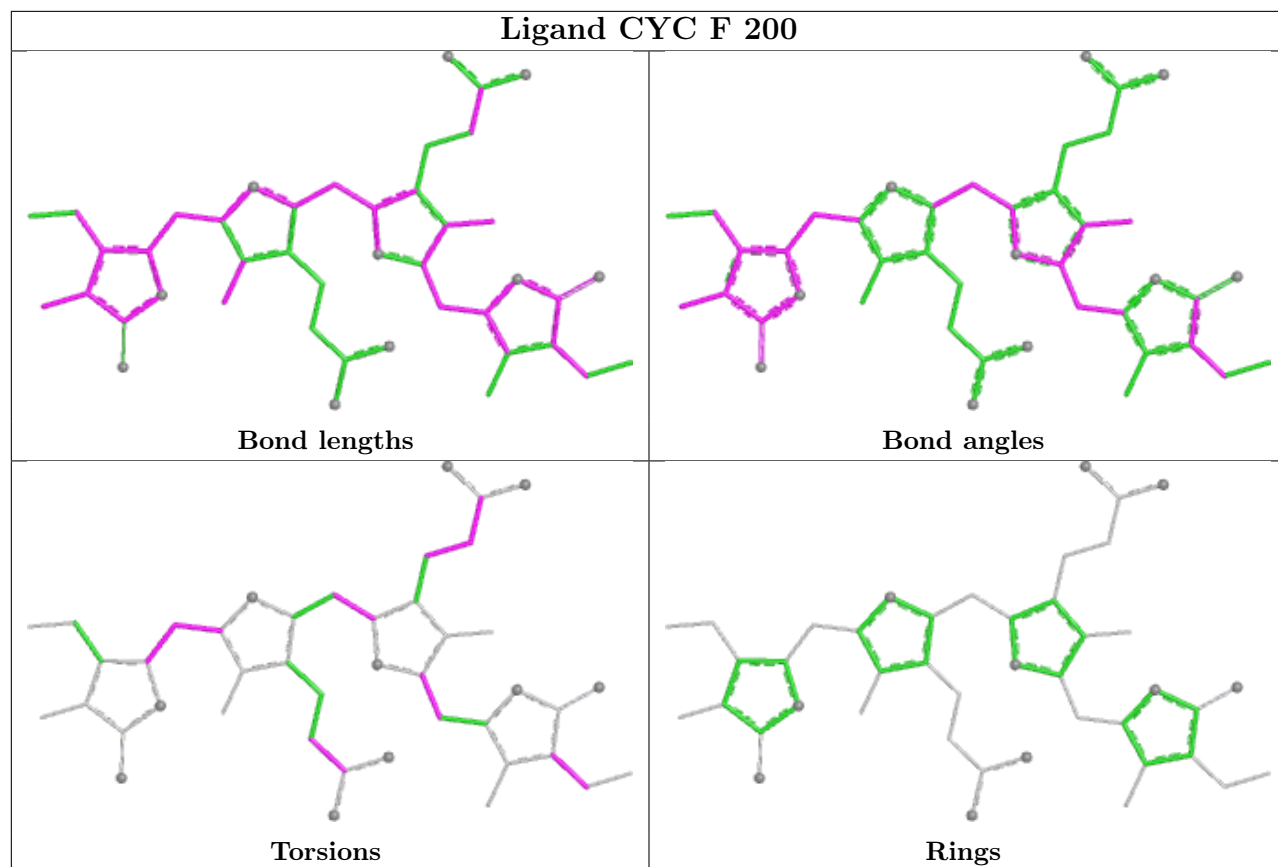


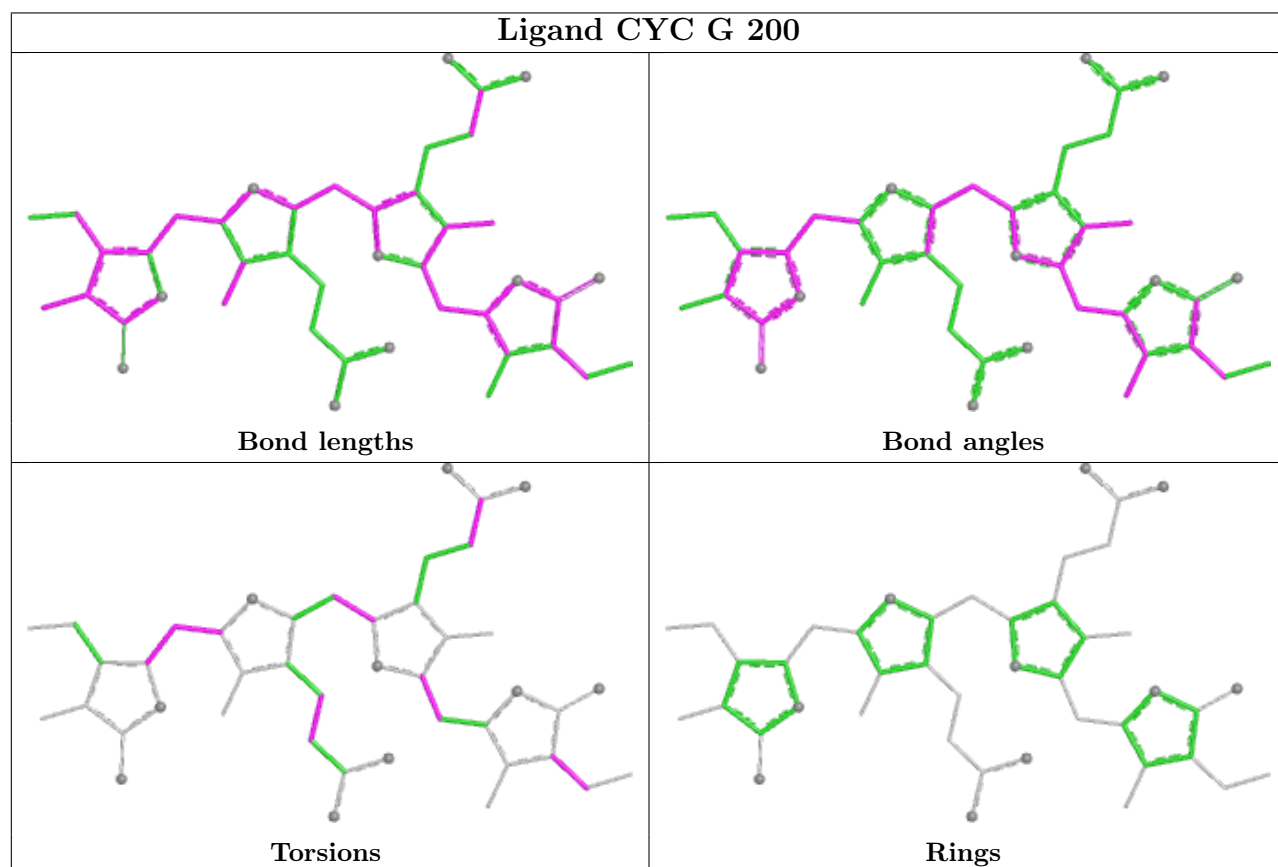
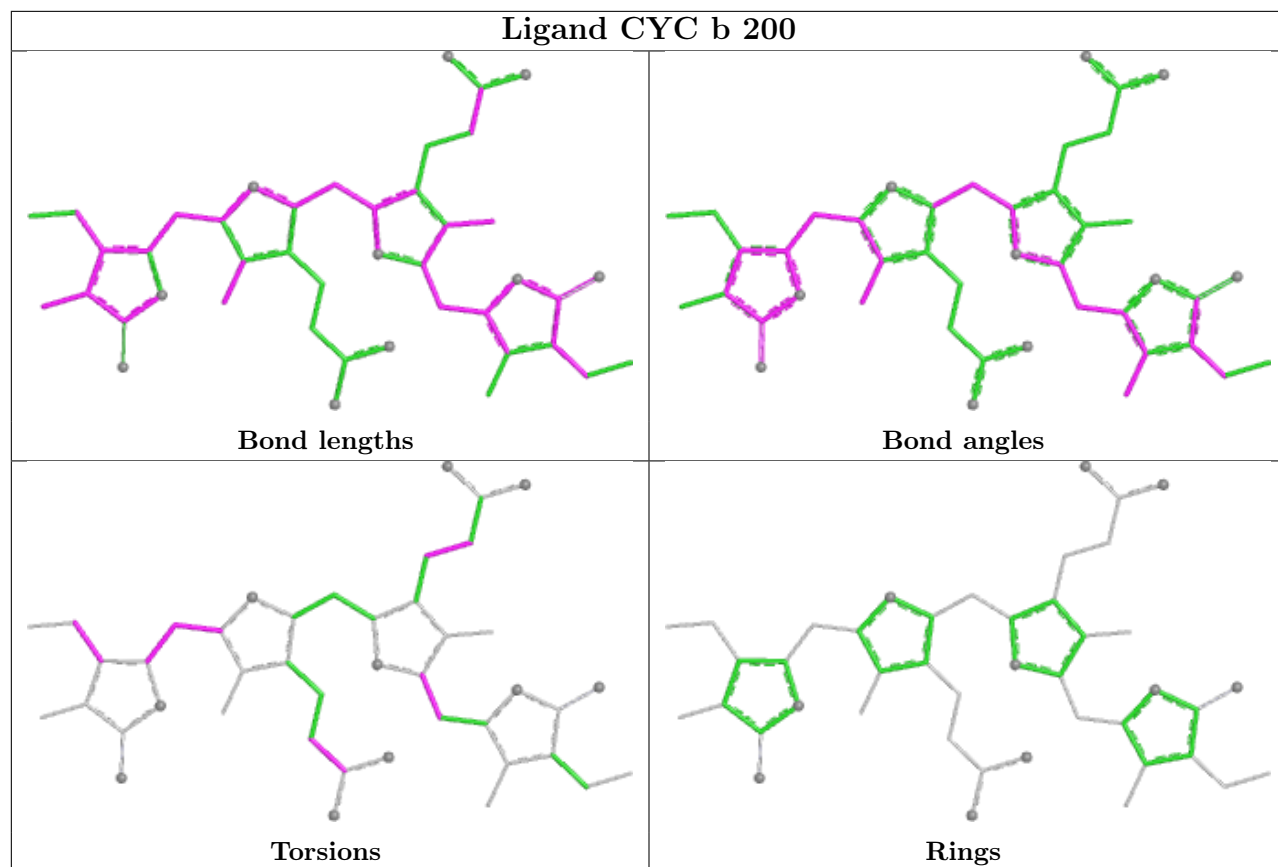




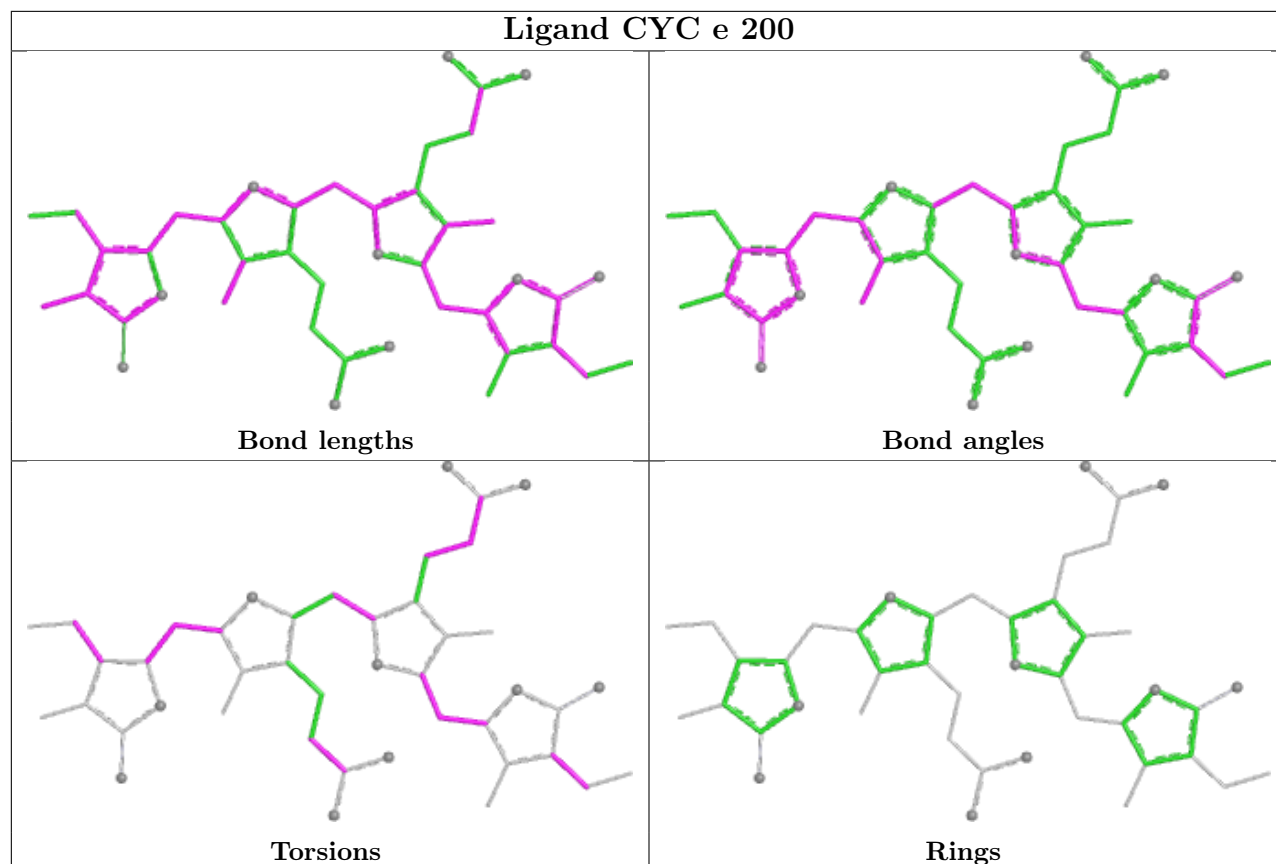




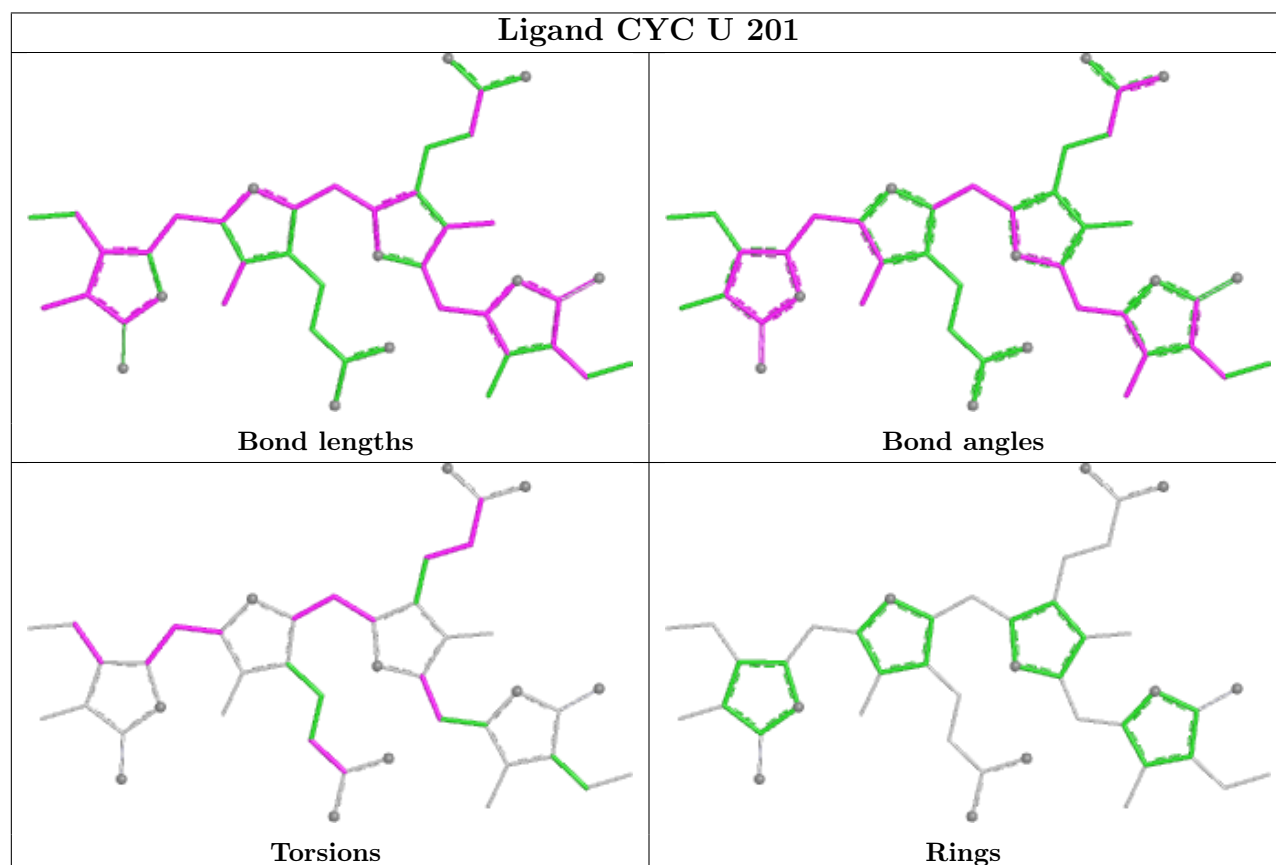


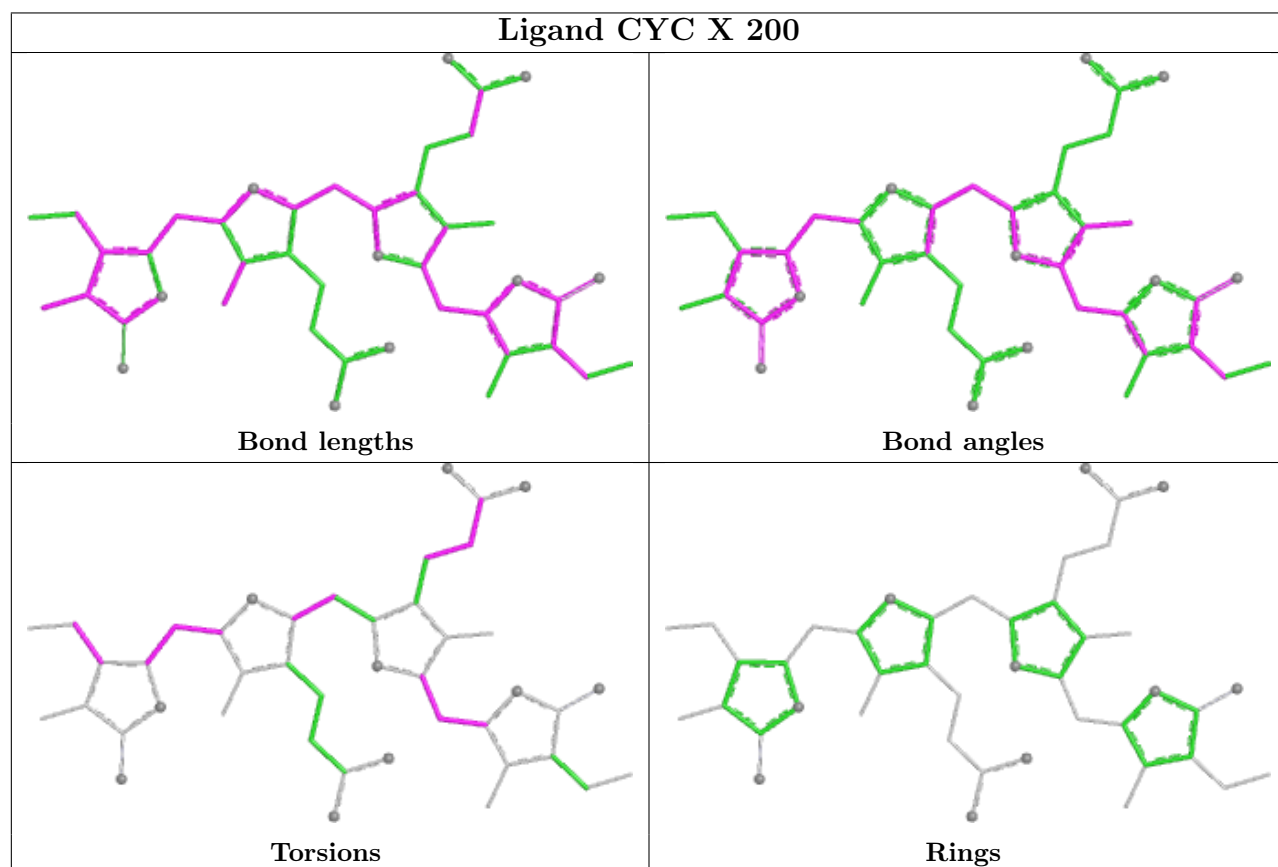
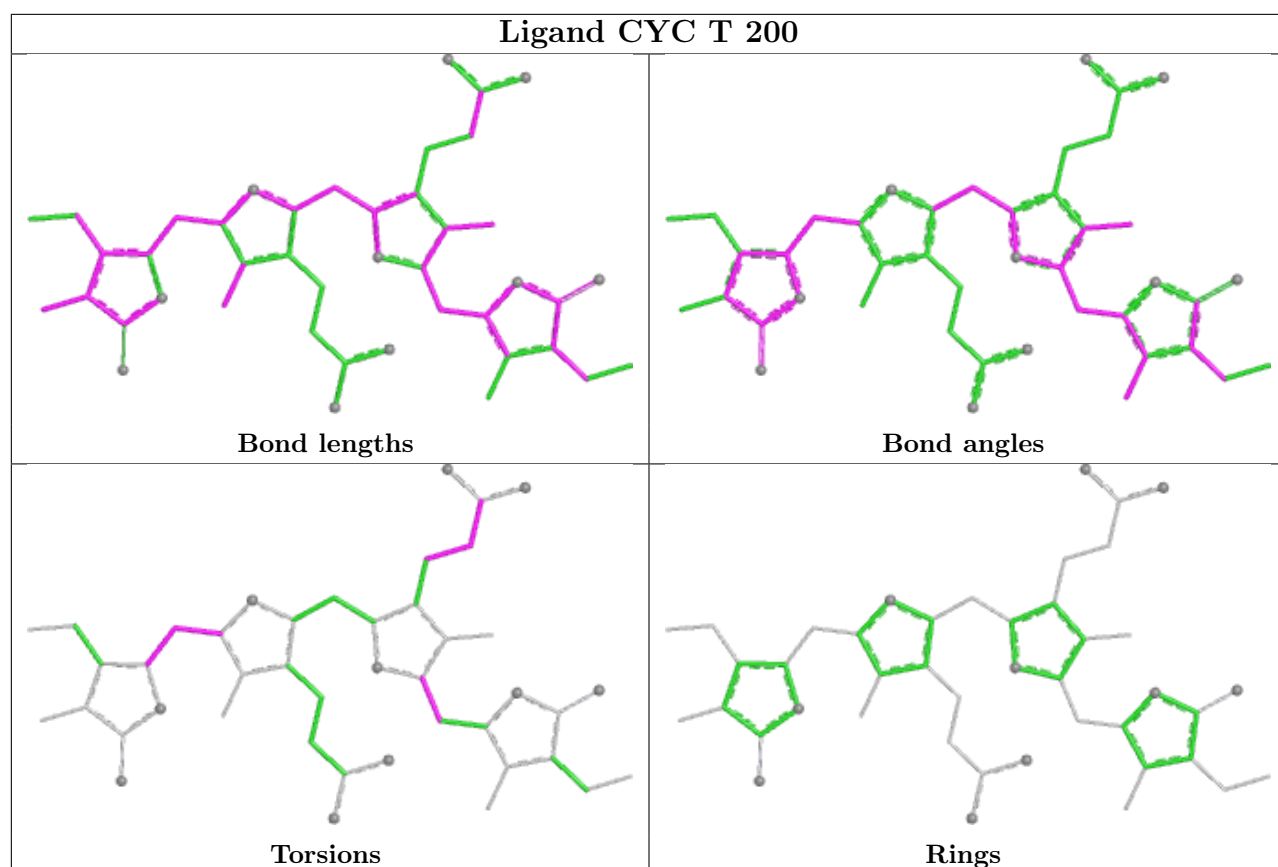


Ligand CYC e 200

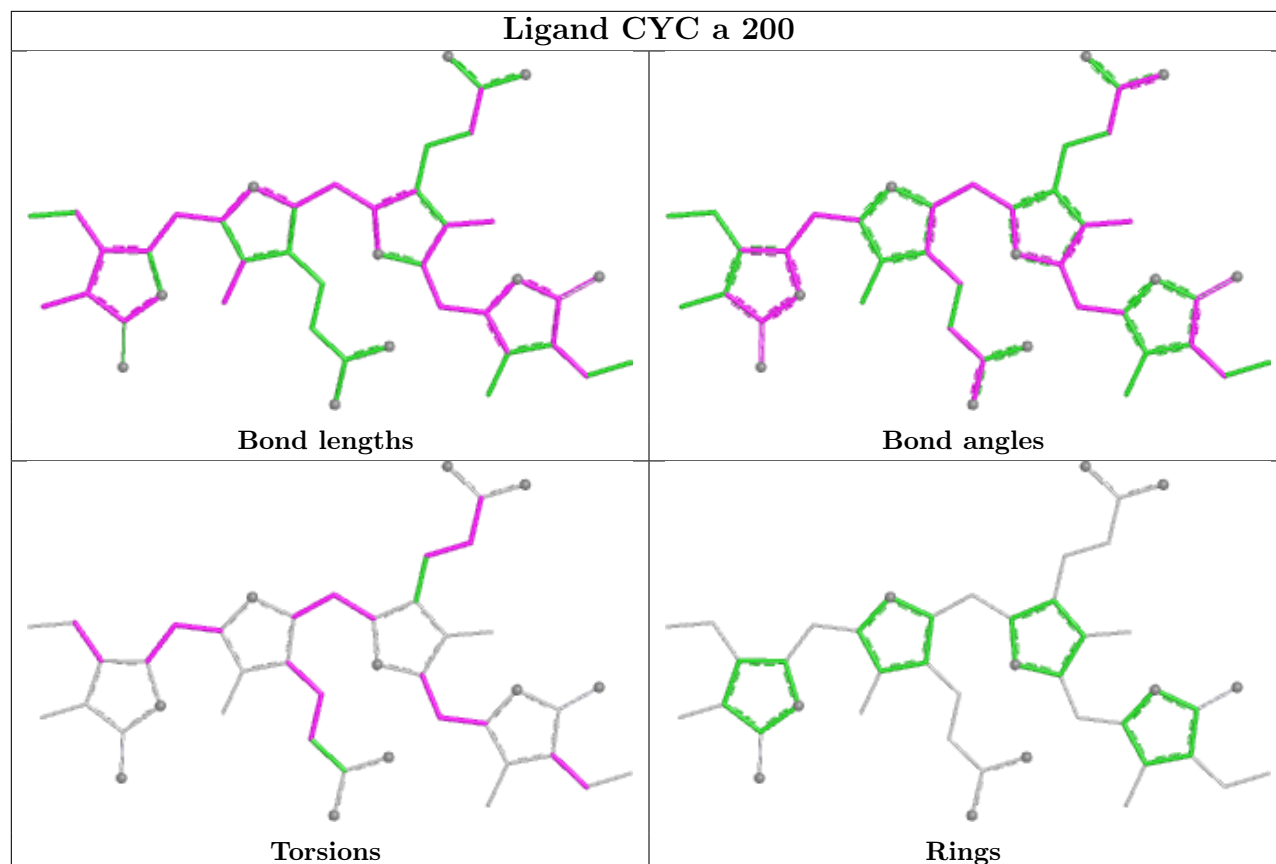


Ligand CYC U 201

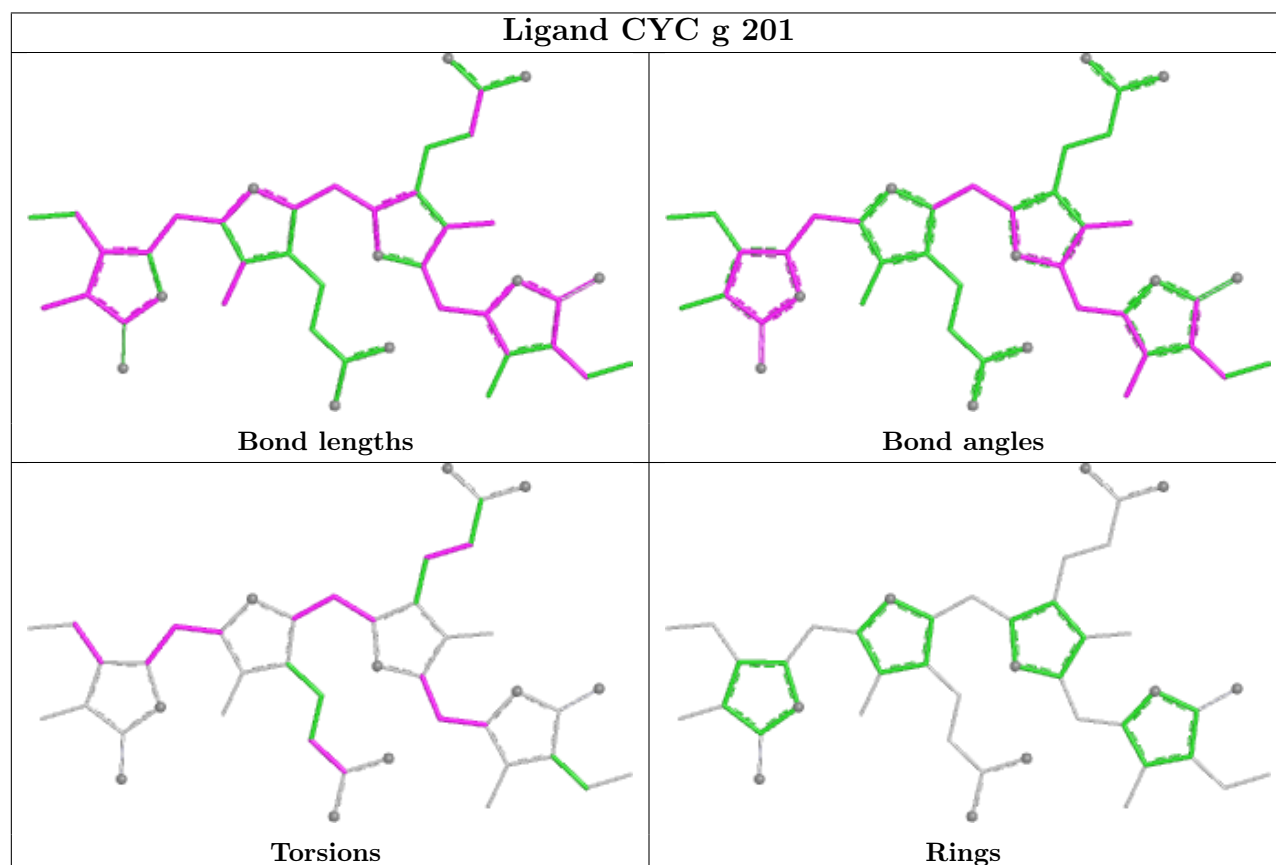


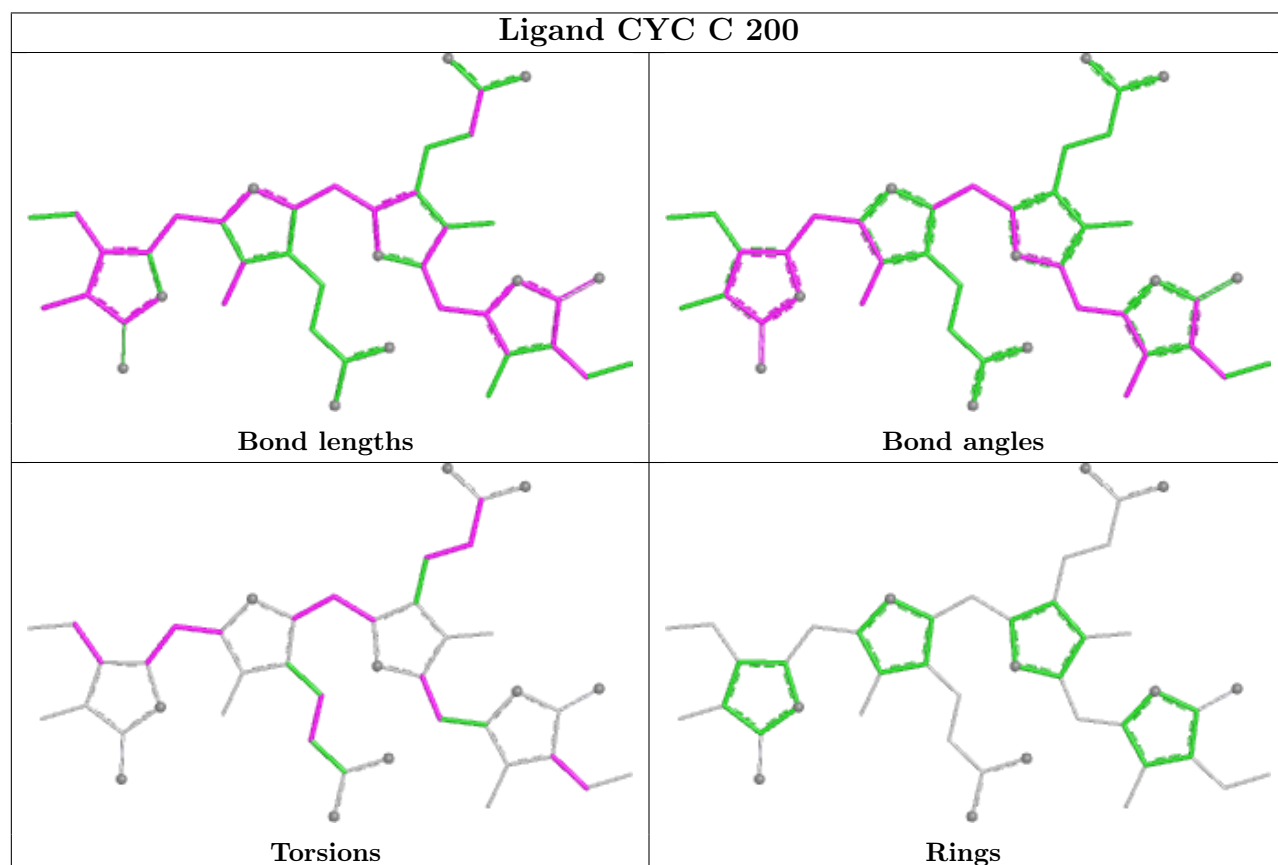
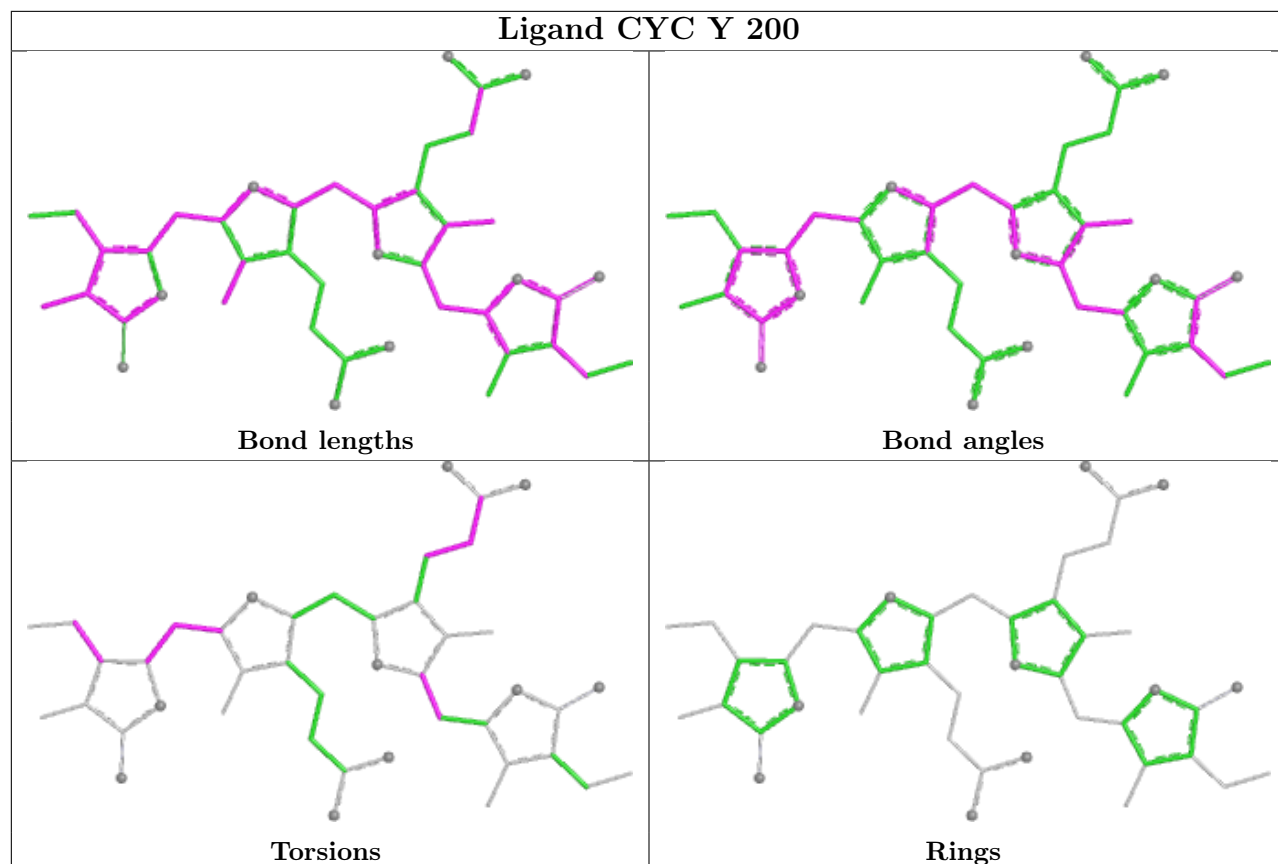


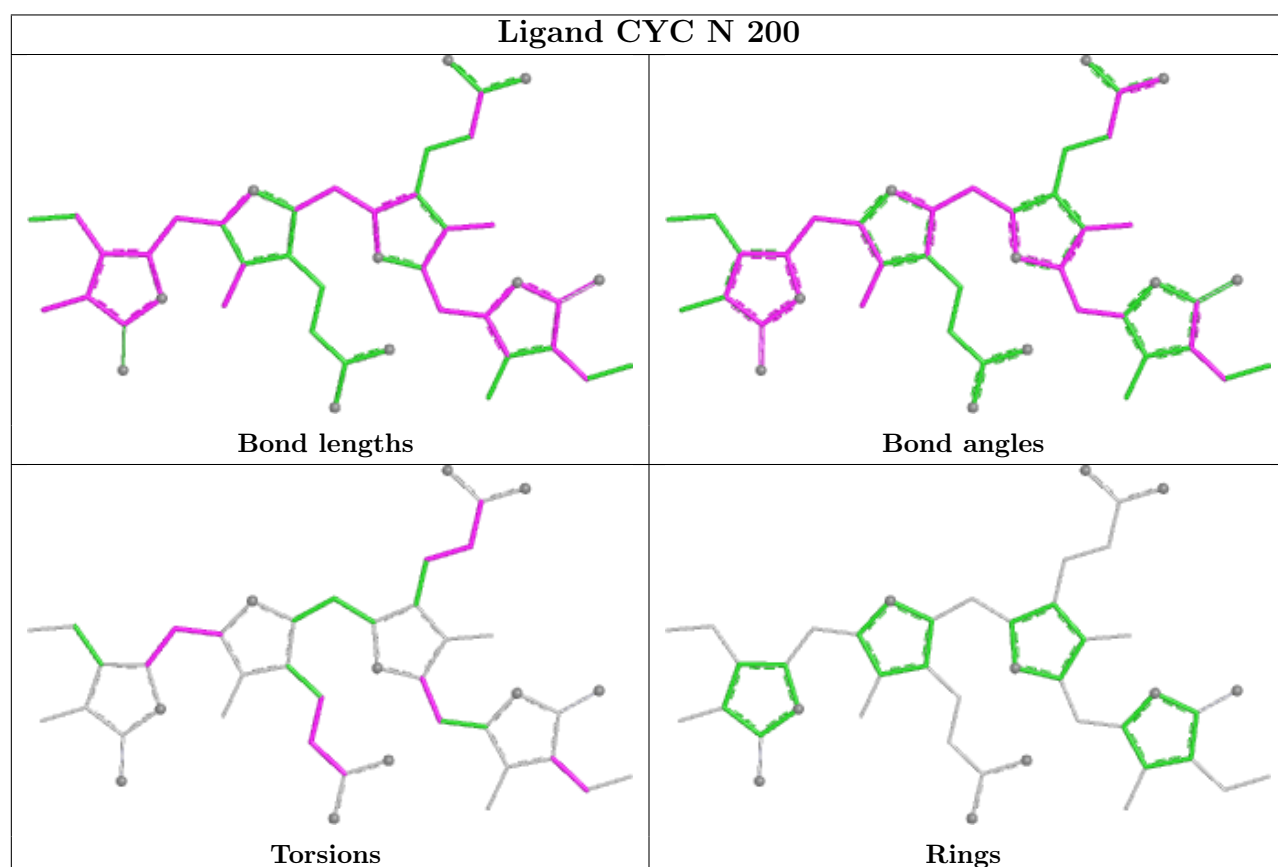
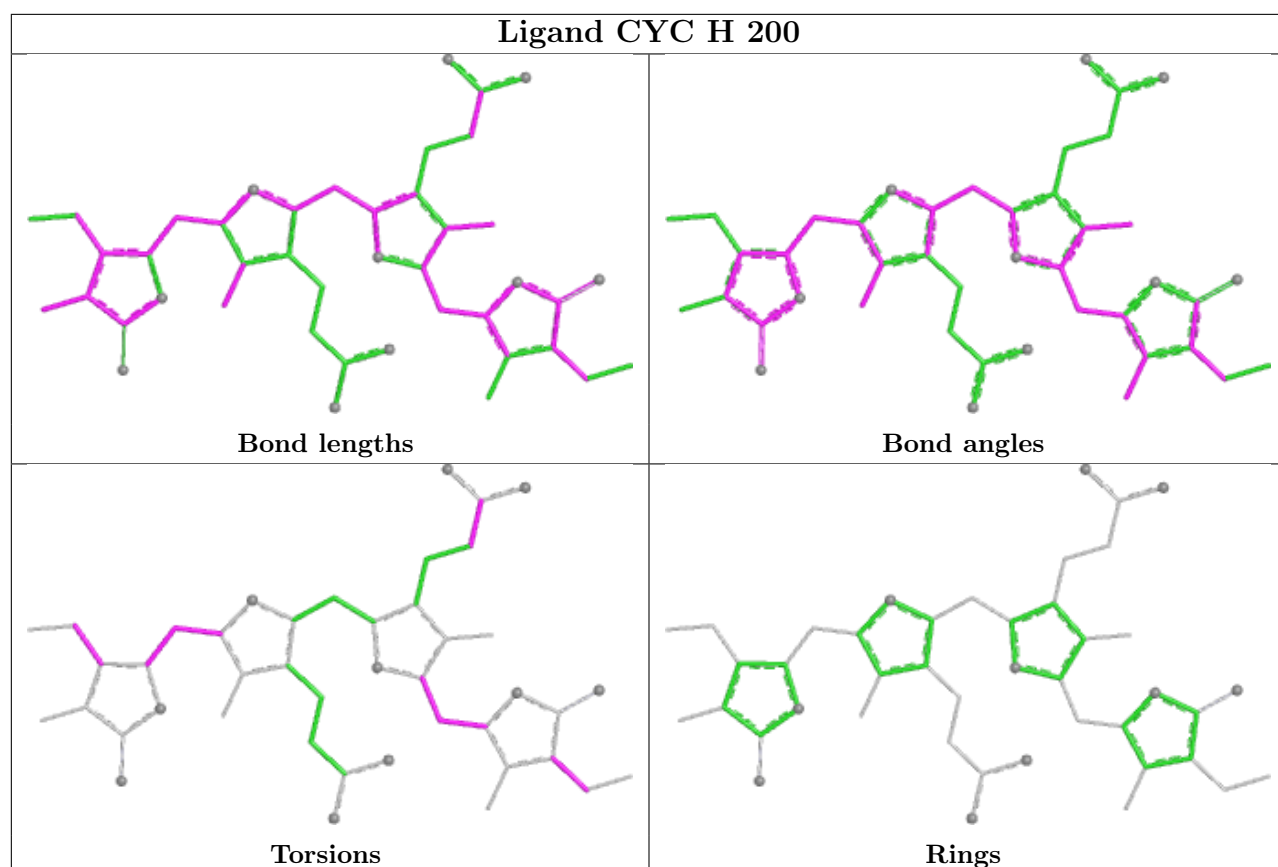
Ligand CYC a 200

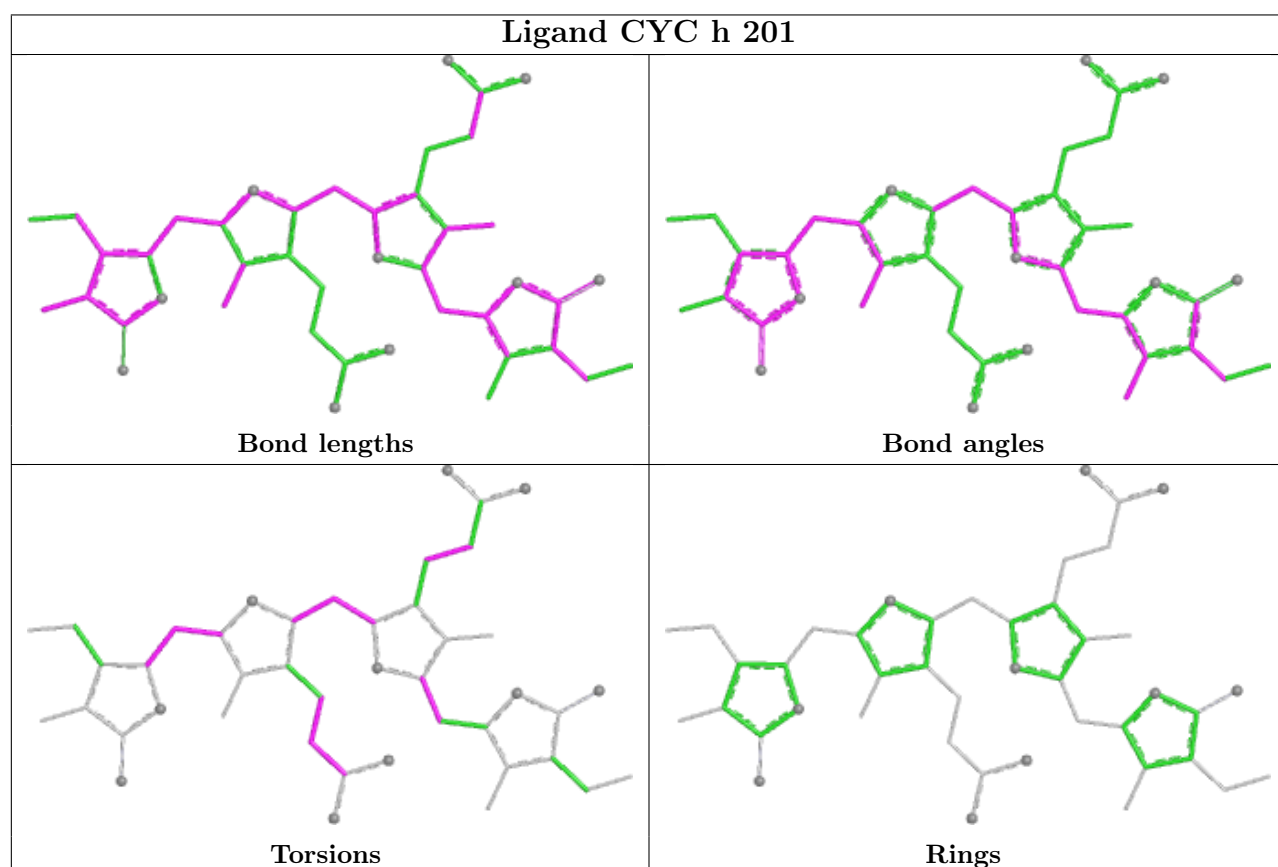
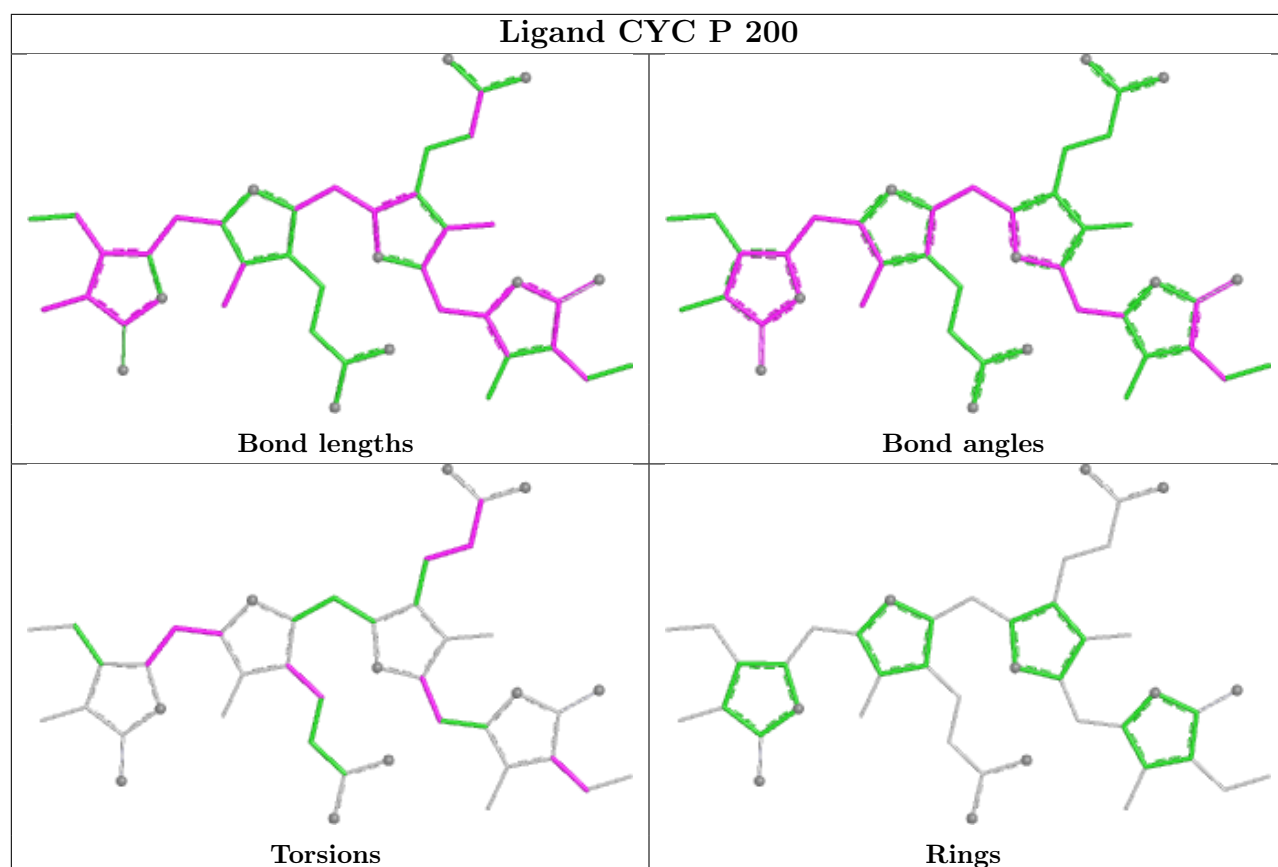


Ligand CYC g 201

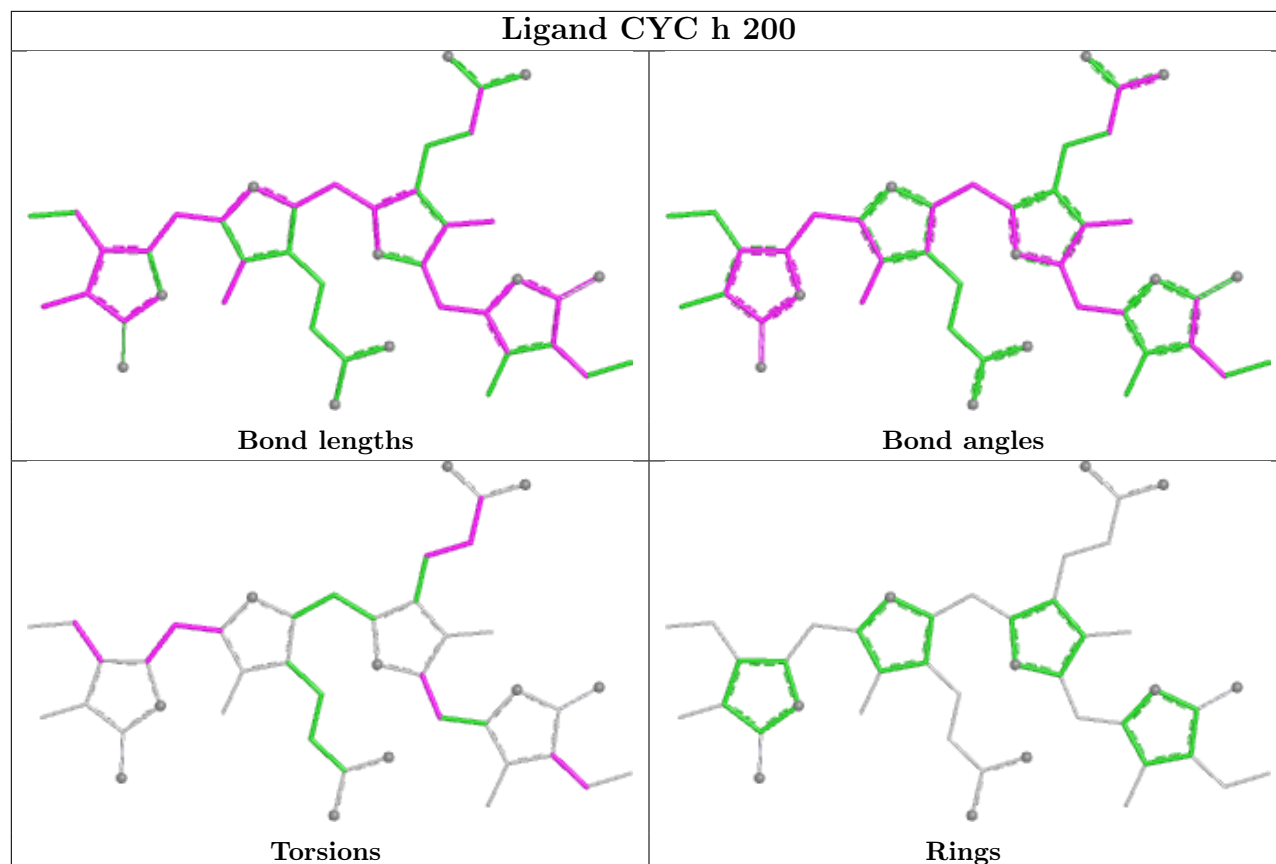




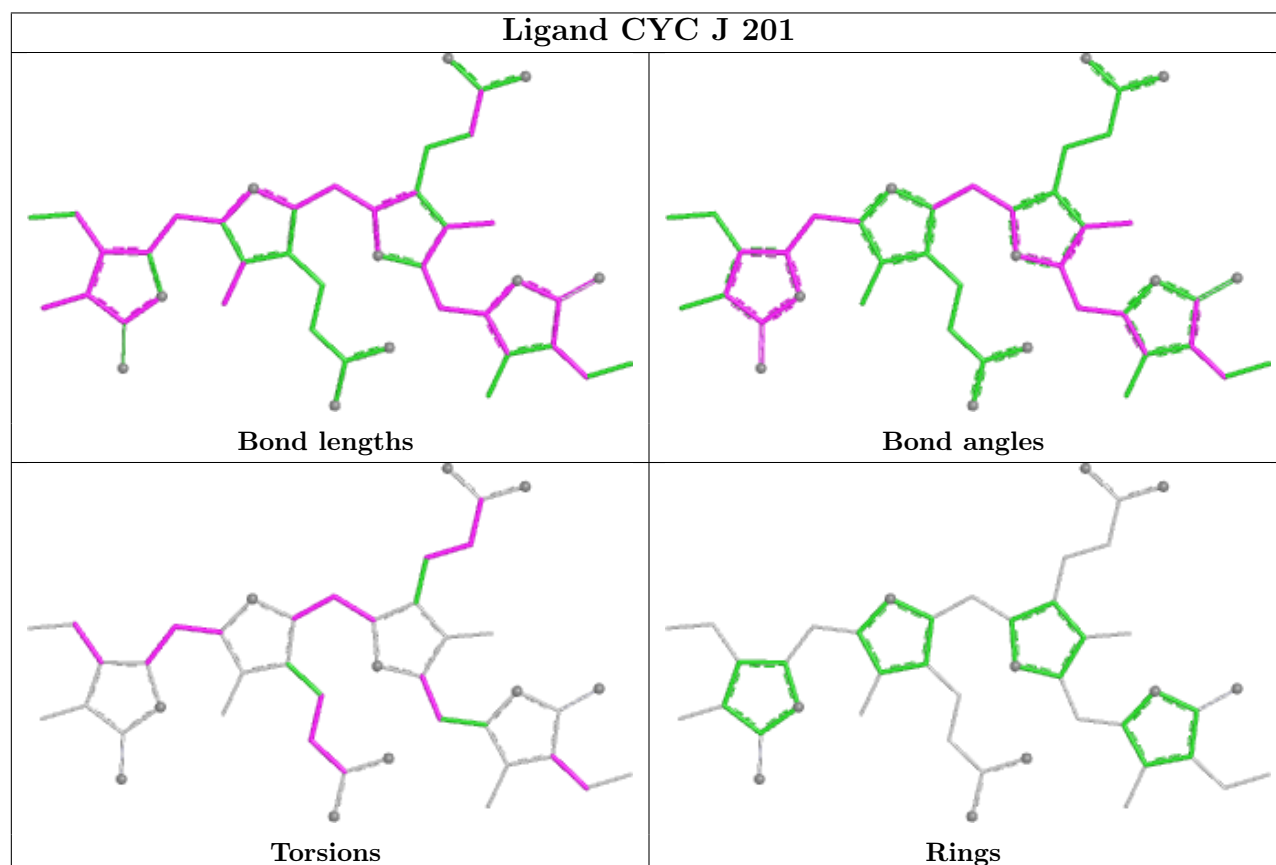




Ligand CYC h 200



Ligand CYC J 201



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.

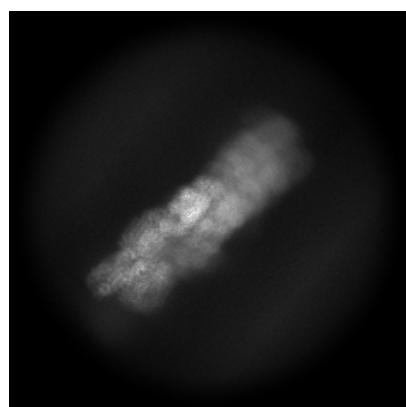
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35570. These allow visual inspection of the internal detail of the map and identification of artifacts.

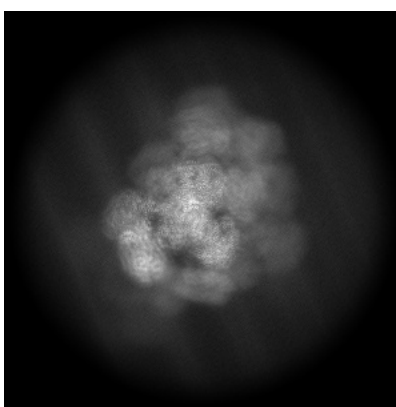
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

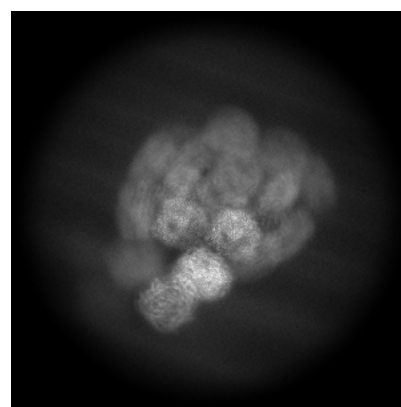
6.1.1 Primary map



X



Y

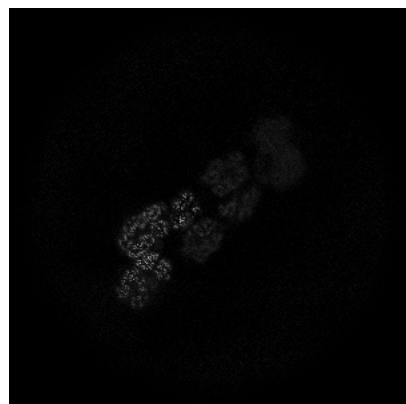


Z

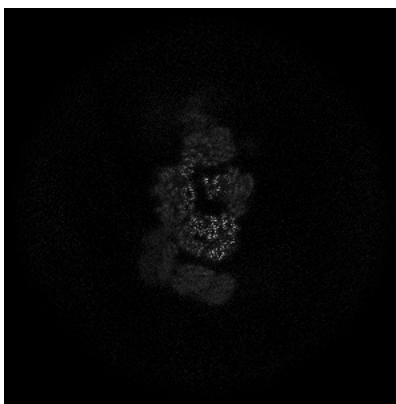
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

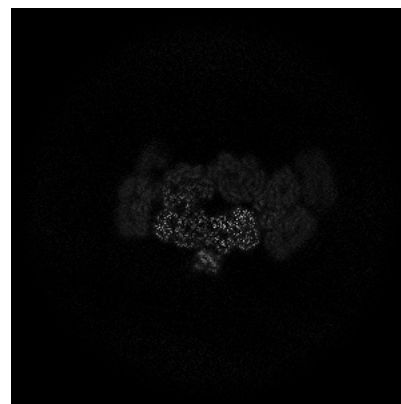
6.2.1 Primary map



X Index: 340



Y Index: 340

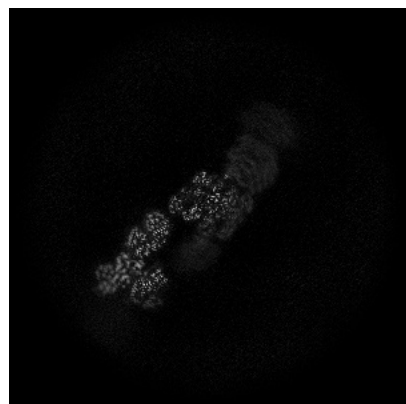


Z Index: 340

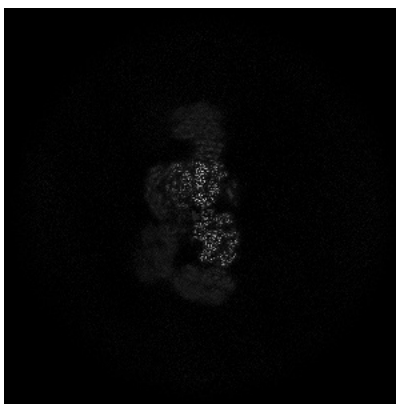
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

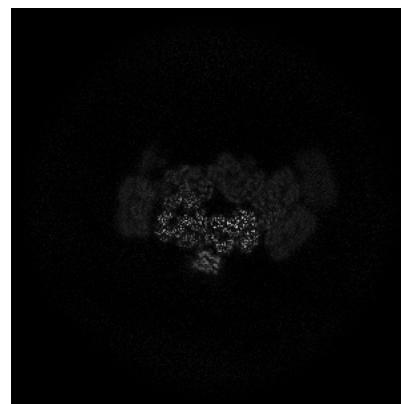
6.3.1 Primary map



X Index: 298



Y Index: 320



Z Index: 337

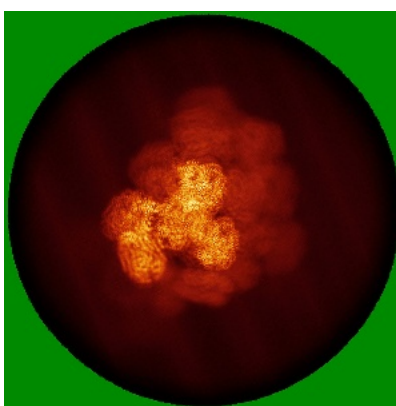
The images above show the largest variance slices of the map in three orthogonal directions.

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

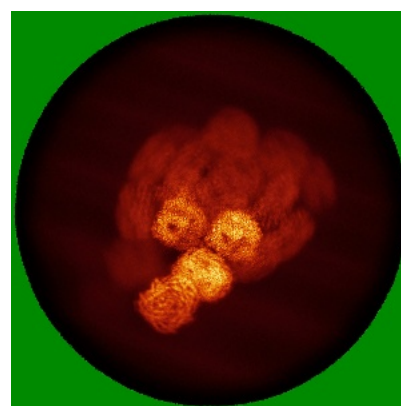
6.4.1 Primary map



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.

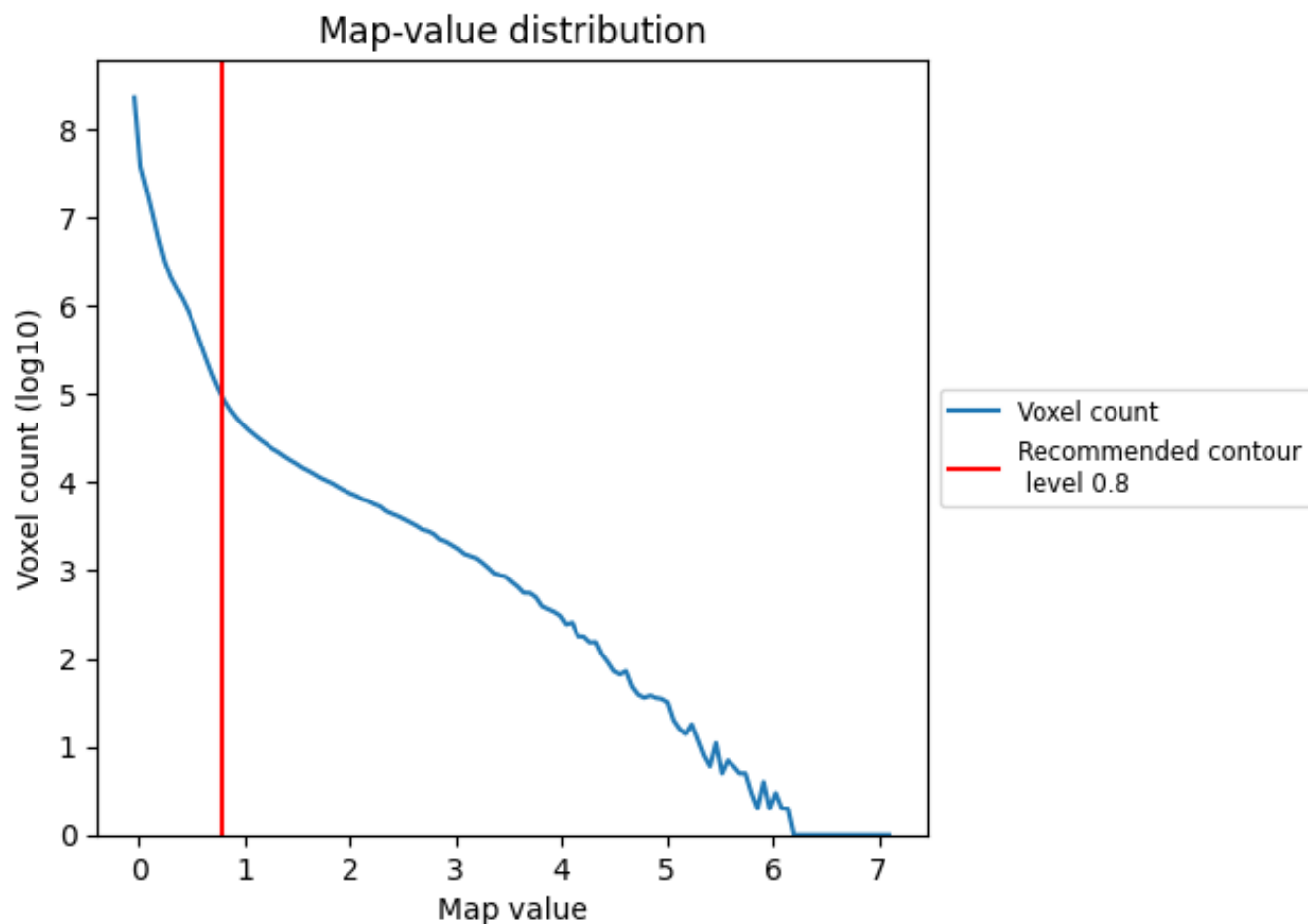
6.6 Mask visualisation

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

7 Map analysis [i](#)

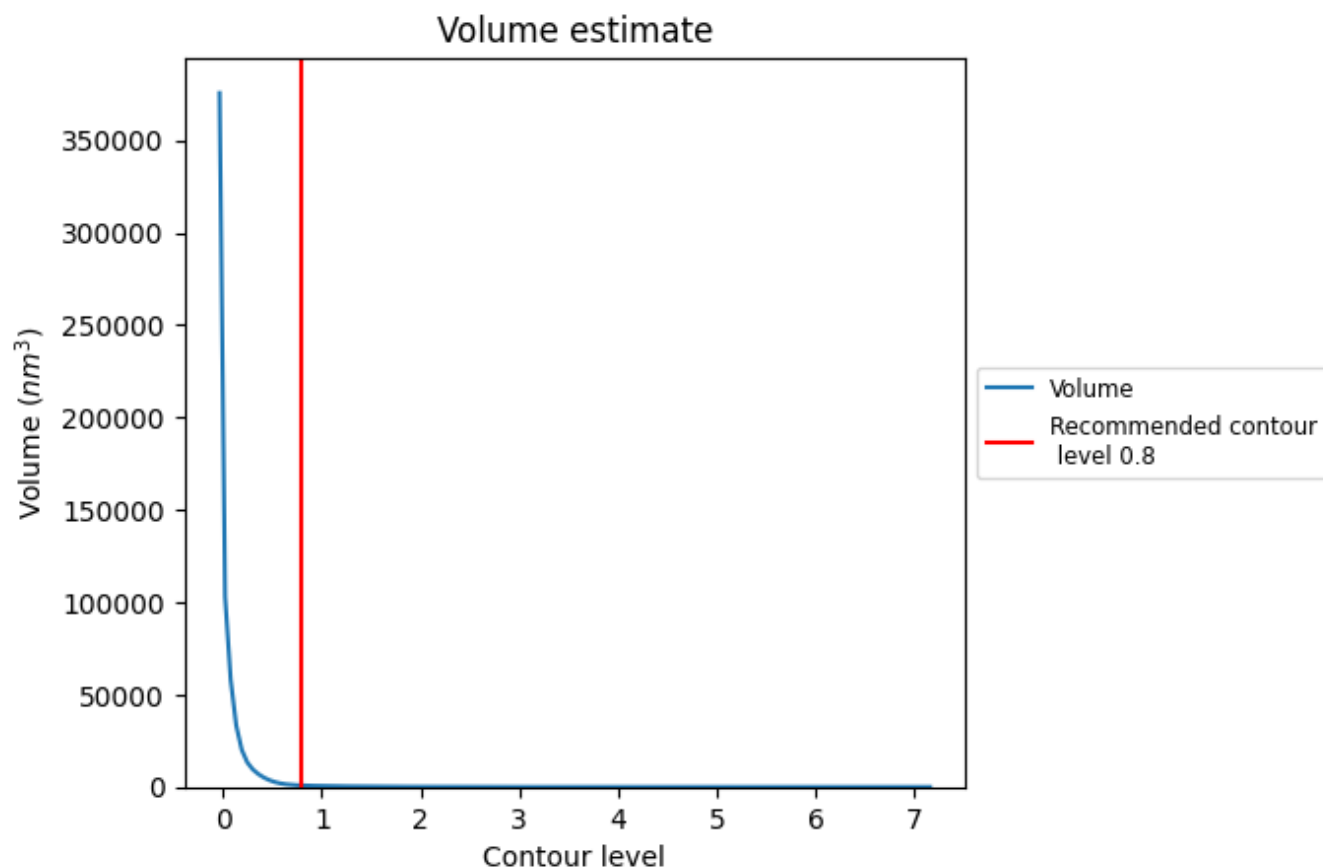
This section contains the results of statistical analysis of the map.

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.

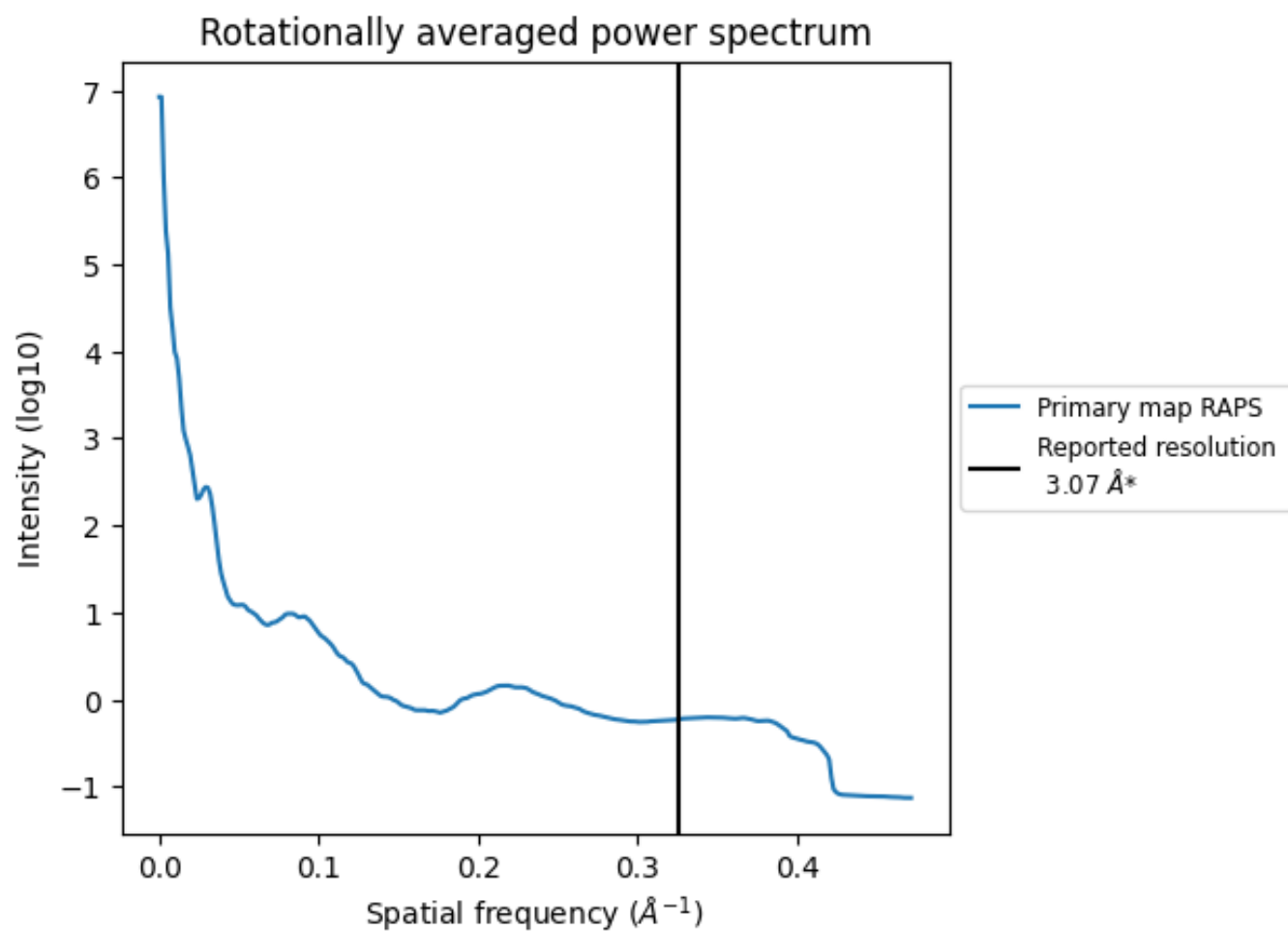
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 815 nm^3 ; this corresponds to an approximate mass of 736 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 0.326 Å⁻¹

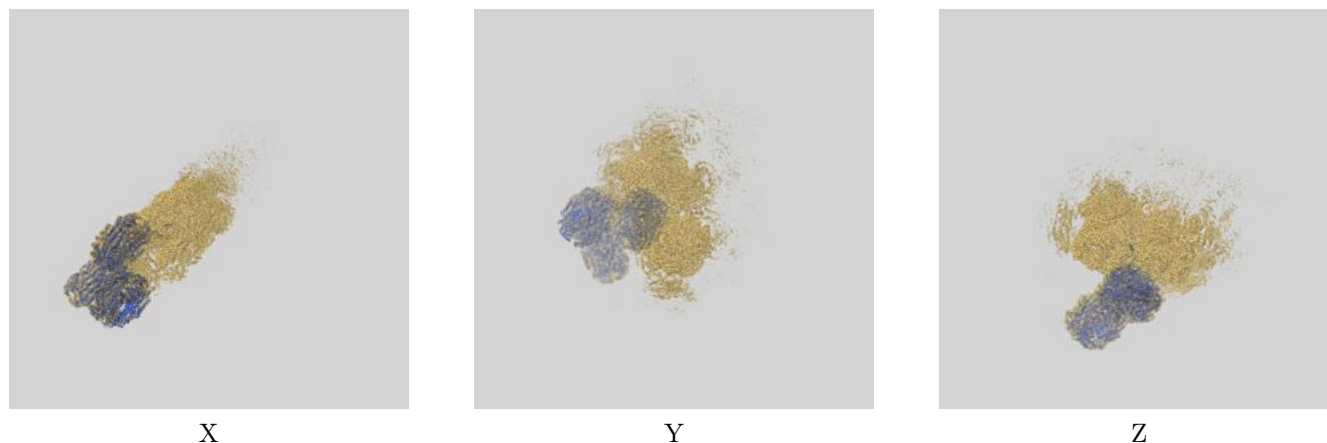
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

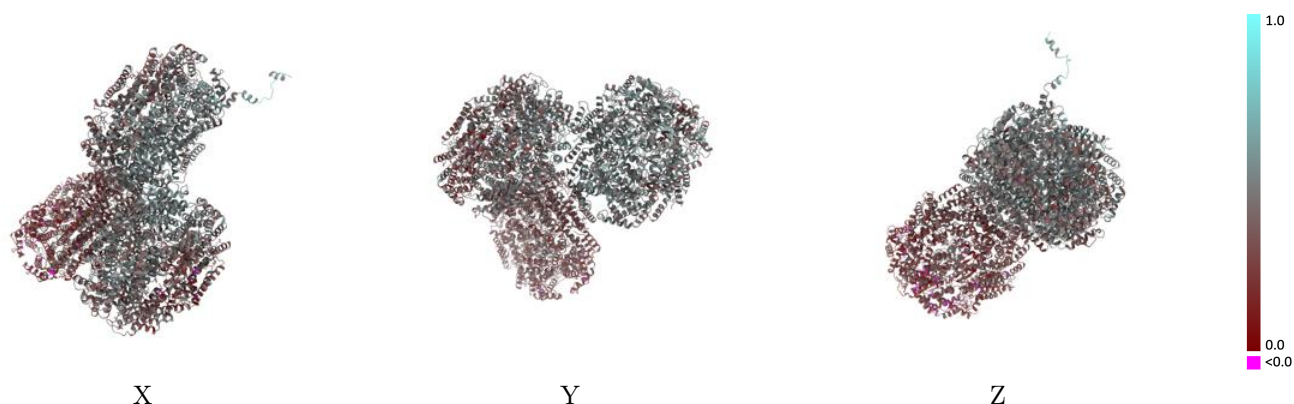
This section contains information regarding the fit between EMDB map EMD-35570 and PDB model 8IMN. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.8 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](#)

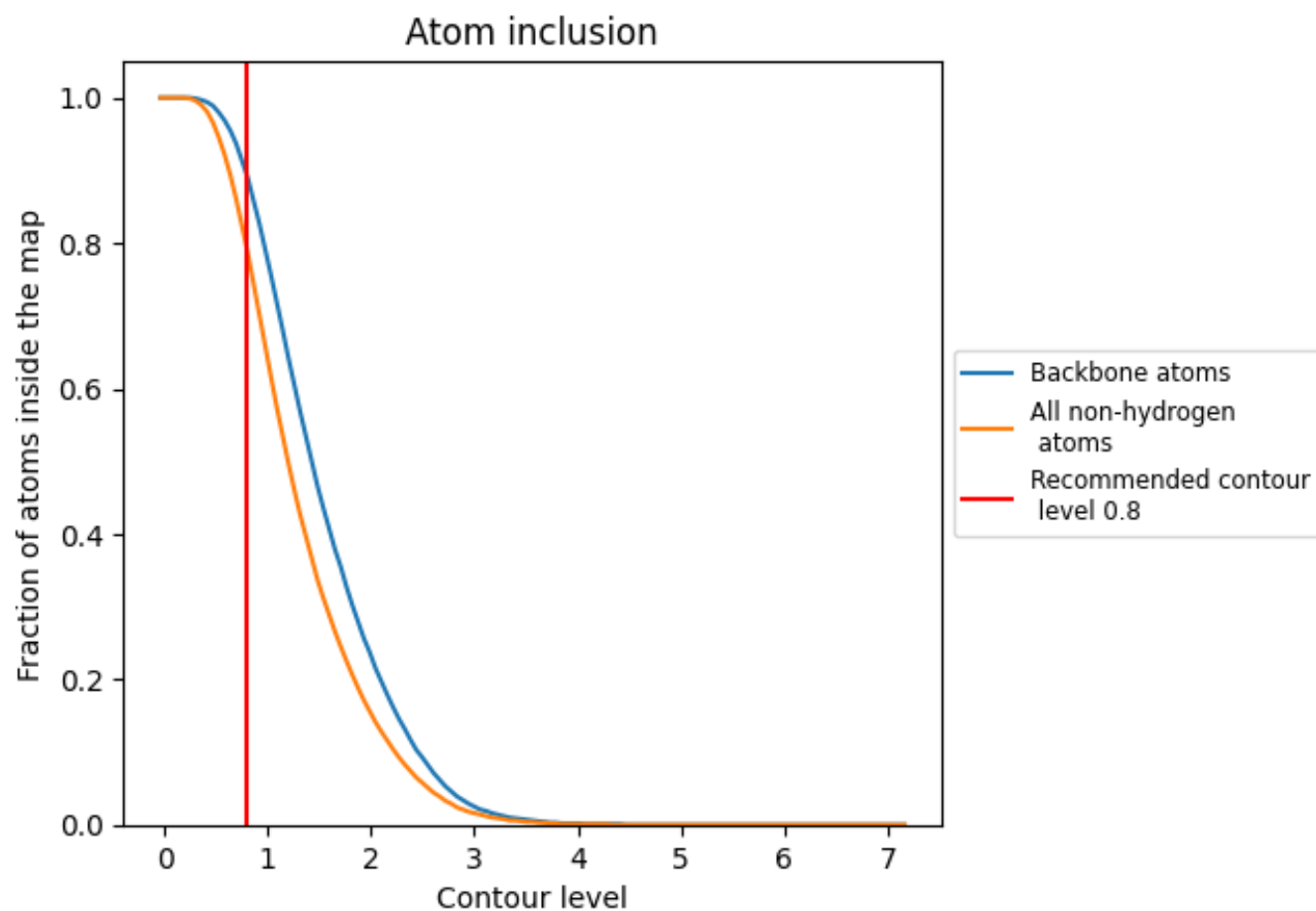


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7910	 0.3970
5	 0.8500	 0.4540
A	 0.9390	 0.4340
B	 0.9400	 0.4870
C	 0.8590	 0.4420
D	 0.9220	 0.5150
E	 0.9220	 0.4720
F	 0.9100	 0.5040
G	 0.9210	 0.4320
H	 0.8160	 0.4020
I	 0.8720	 0.4500
J	 0.9170	 0.5150
K	 0.9180	 0.5200
L	 0.8680	 0.5080
M	 0.5730	 0.3850
N	 0.7860	 0.4440
O	 0.7730	 0.4600
P	 0.2910	 0.3400
Q	 0.7440	 0.4660
R	 0.6520	 0.4330
S	 0.9270	 0.5170
T	 0.7730	 0.4070
U	 0.4110	 0.3550
V	 0.4600	 0.3910
W	 0.9250	 0.5130
X	 0.7780	 0.4660
Y	 0.8300	 0.4950
Z	 0.0700	 0.3000
a	 0.8620	 0.2810
b	 0.8270	 0.2670
c	 0.6320	 0.2060
d	 0.8700	 0.2620
e	 0.8890	 0.2670
f	 0.9300	 0.3340
g	 0.8680	 0.2740



Continued on next page...

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Chain	Atom inclusion	Q-score
h	 0.6360	 0.2190
i	 0.6710	 0.2130
j	 0.7710	 0.2990
k	 0.8330	 0.2670
l	 0.8970	 0.3290
m	 0.2480	 0.1930