



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:09 PM UTC

PDB ID : 8IMK / pdb_00008imk
EMDB ID : EMD-35567
Title : D3-D4, D1-D2, D'3-D'4, D'1-D'2 cylinder in cyanobacterial phycobilisome from *Anthocerotibacter panamensis* (Cluster C)
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 : 2.48 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

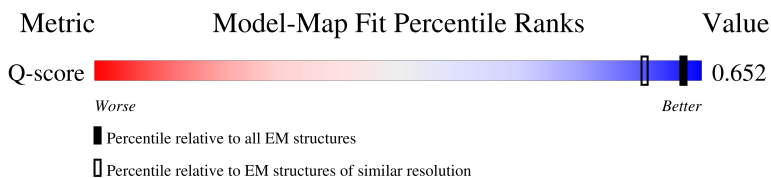
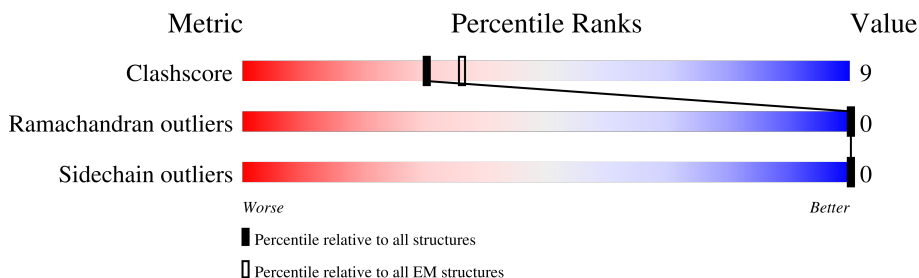
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.48 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.



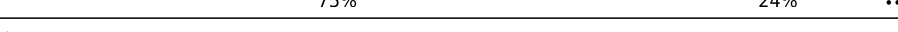
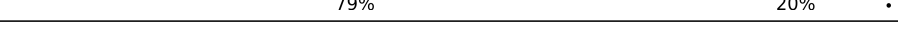
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6178 (1.98 - 2.98)

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	1	431	 81% 19%
1	2	431	 83% 17%
2	A	161	 84% 15% .
2	C	161	 81% 18% .

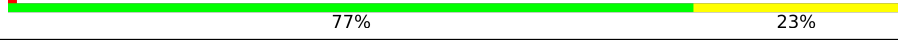
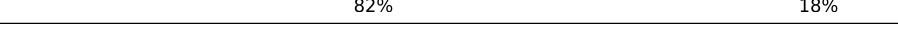
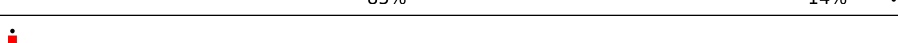
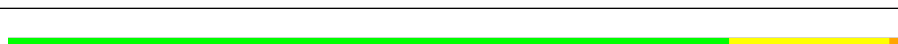
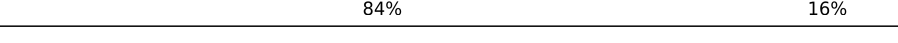
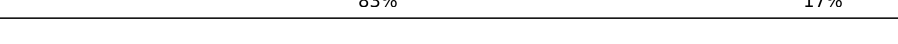
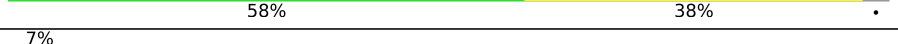
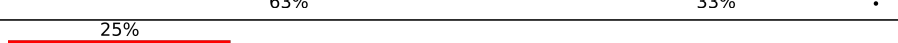
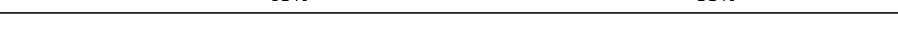
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Mol	Chain	Length	Quality of chain
2	E	161	 88% 11% .
2	N	161	 78% 22% .
2	O	161	 85% 14% .
2	P	161	 79% 20% .
2	Q	161	 84% 16% .
2	R	161	 78% 22% .
2	S	161	 71% 27% ..
2	a	161	 84% 15% .
2	c	161	 83% 16% .
2	e	161	 87% 12% .
2	n	161	 83% 16% .
2	o	161	 82% 17% .
2	p	161	 81% 18% .
2	q	161	 89% 11% .
2	r	161	 71% 28% .
2	s	161	 75% 24% ..
3	B	161	 79% 20% .
3	D	161	 78% 22% .
3	F	161	 78% 21% .
3	b	161	 75% 24% .
3	d	161	 80% 20% .
3	f	161	 84% 15% .
4	G	158	 82% 18%
4	H	158	 83% 17%
4	I	158	 85% 14% .

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Mol	Chain	Length	Quality of chain
4	T	158	 73%27%
4	U	158	 78%22%
4	V	158	 77%23%
4	W	158	 83%17%
4	X	158	 82%18%
4	Y	158	 85%14%
4	g	158	 81%19%
4	h	158	 81%18%
4	i	158	 81%18%
4	t	158	 70%30%
4	u	158	 78%22%
4	v	158	 85%15%
4	w	158	 80%20%
4	x	158	 84%16%
4	y	158	 83%17%
5	J	162	 84%16%
5	K	162	 79%20%
5	L	162	 83%17%
5	j	162	 85%15%
5	k	162	 86%14%
5	l	162	 90%10%
6	M	60	 12%63%33%
6	Z	60	 32%58%38%
6	m	60	 7%63%33%
6	z	60	 25%63%33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 68842 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 ApcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	431	Total	C	N	O	S	0	0
			3445	2185	615	642	3		
1	2	431	Total	C	N	O	S	0	0
			3445	2185	615	642	3		

- Molecule 2 is a protein called ApcA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	C	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	E	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	N	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	O	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	P	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	Q	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	R	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	S	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	a	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	c	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	e	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	n	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	o	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	p	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	q	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	r	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		
2	s	160	Total	C	N	O	S	0	0
			1207	762	208	234	3		

- Molecule 3 is a protein called ApcA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
3	D	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
3	F	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
3	b	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
3	d	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		
3	f	160	Total	C	N	O	S	0	0
			1218	766	211	237	4		

- Molecule 4 is a protein called ApcB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	H	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	I	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	T	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	U	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	V	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	X	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	Y	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	g	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	h	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	i	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	t	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	u	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	v	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	w	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	x	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		
4	y	158	Total	C	N	O	S	0	0
			1201	755	207	233	6		

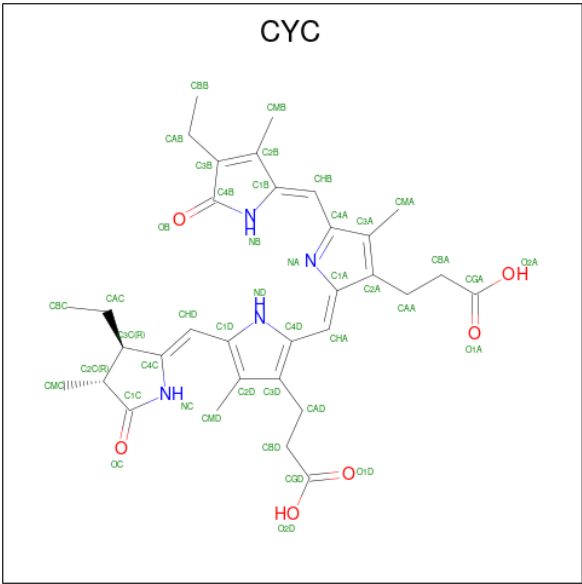
- Molecule 5 is a protein called ApcB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
5	K	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
5	L	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
5	j	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
5	k	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		
5	l	162	Total	C	N	O	S	0	0
			1230	774	205	245	6		

- Molecule 6 is a protein called ApcC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	58	Total	C	N	O	S	0	0
			464	288	90	83	3		
6	Z	58	Total	C	N	O	S	0	0
			464	288	90	83	3		
6	m	58	Total	C	N	O	S	0	0
			464	288	90	83	3		
6	z	58	Total	C	N	O	S	0	0
			464	288	90	83	3		

- Molecule 7 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			43	33	4	6	
7	B	1	Total	C	N	O	0
			43	33	4	6	
7	C	1	Total	C	N	O	0
			43	33	4	6	
7	D	1	Total	C	N	O	0
			43	33	4	6	
7	E	1	Total	C	N	O	0
			43	33	4	6	
7	F	1	Total	C	N	O	0
			43	33	4	6	
7	G	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
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	K	1	Total 43	C 33	N 4	O 6	0
7	L	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
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	S	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	W	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	a	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

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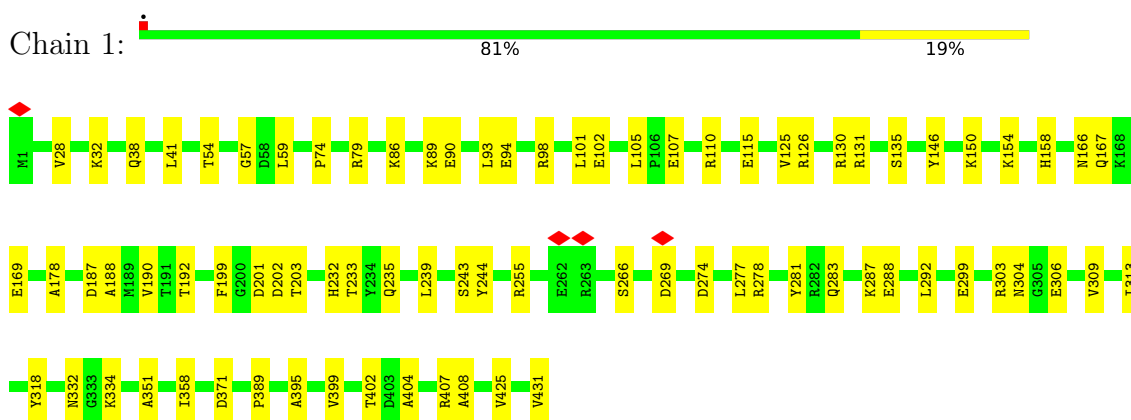
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Mol	Chain	Residues	Atoms				AltConf
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7	f	1	Total 43	C 33	N 4	O 6	0
7	g	1	Total 43	C 33	N 4	O 6	0
7	h	1	Total 43	C 33	N 4	O 6	0
7	i	1	Total 43	C 33	N 4	O 6	0
7	j	1	Total 43	C 33	N 4	O 6	0
7	k	1	Total 43	C 33	N 4	O 6	0
7	l	1	Total 43	C 33	N 4	O 6	0
7	n	1	Total 43	C 33	N 4	O 6	0
7	o	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	s	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	w	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

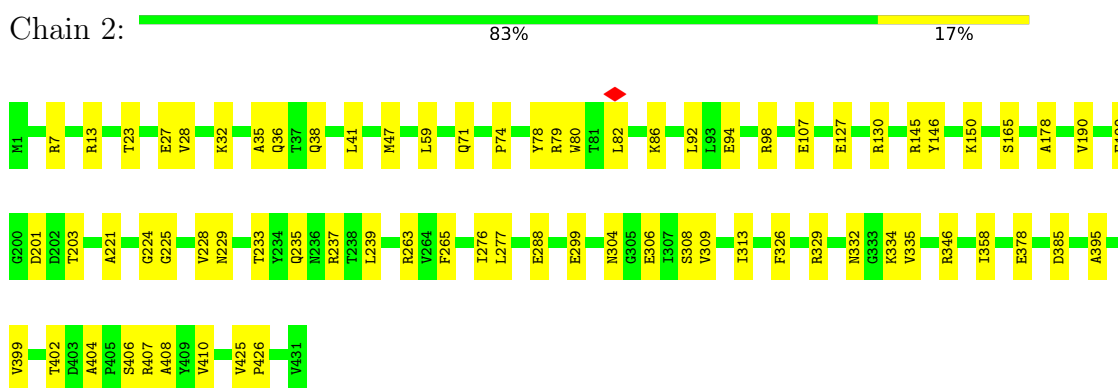
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

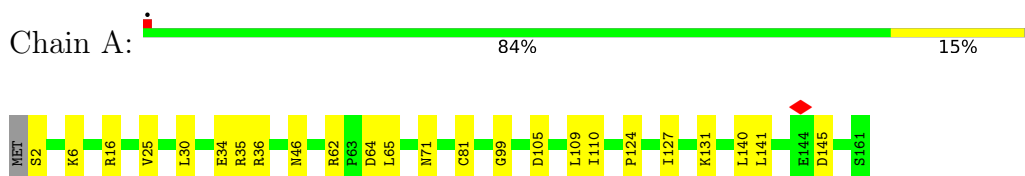
- Molecule 1: ApcH



- Molecule 1: ApcH



- Molecule 2: ApcA1



- Molecule 2: ApcA1

Chain C:  81% 18%



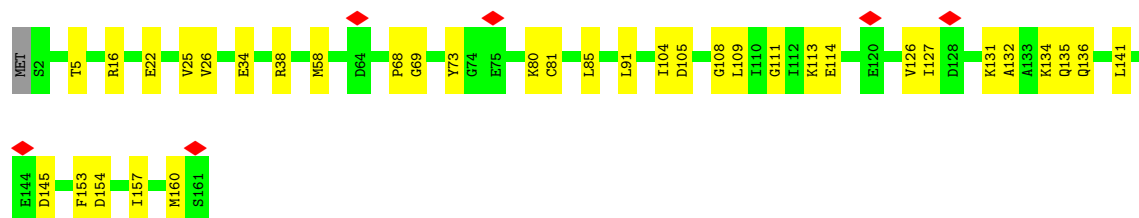
• Molecule 2: ApcA1

Chain E:  88% 11%



• Molecule 2: ApcA1

Chain N:  78% 22%



• Molecule 2: ApcA1

Chain O:  85% 14%



• Molecule 2: ApcA1

Chain P:  79% 20%



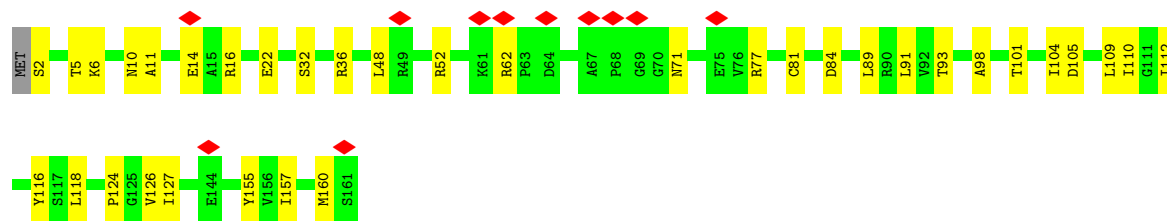
• Molecule 2: ApcA1

Chain Q:  84% 16%

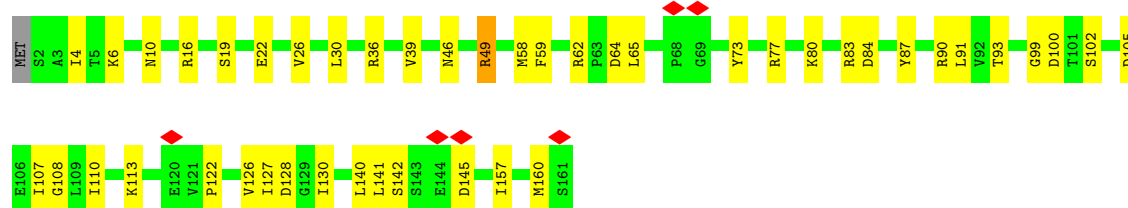


• Molecule 2: ApcA1

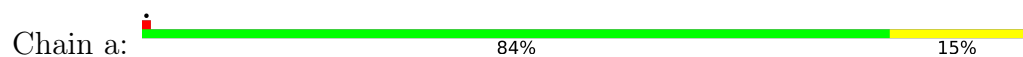
Chain R:  78% 22%



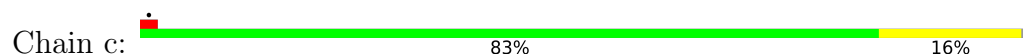
• Molecule 2: ApcA1



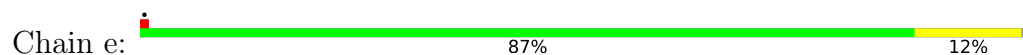
• Molecule 2: ApcA1



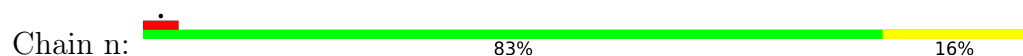
• Molecule 2: ApcA1



• Molecule 2: ApcA1

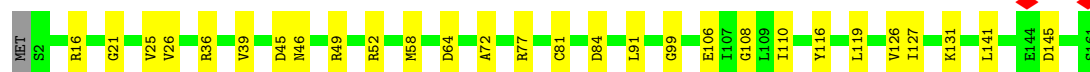


• Molecule 2: ApcA1



• Molecule 2: ApcA1

Chain o:  82% 17%



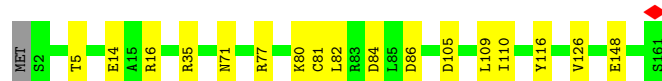
- Molecule 2: ApcA1

Chain p:  81% 18%



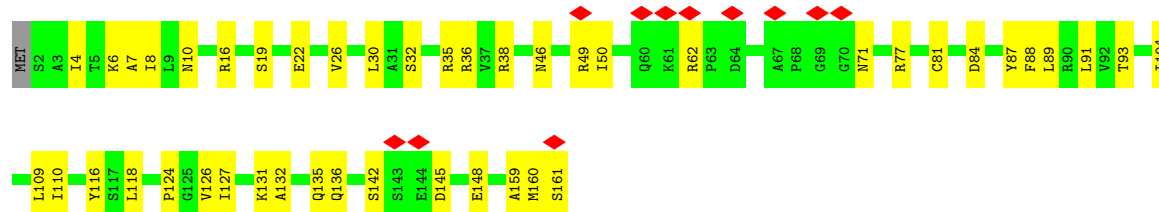
- Molecule 2: ApcA1

Chain q:  89% 11%



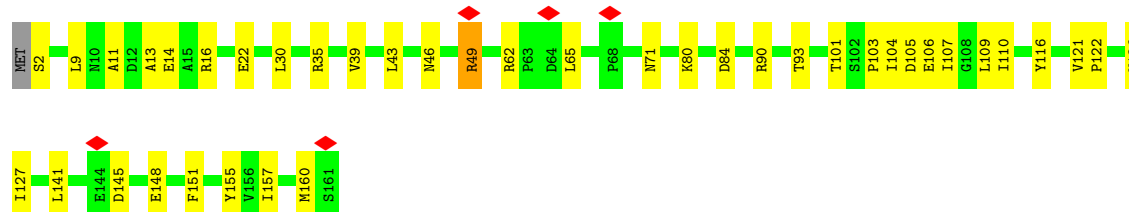
- Molecule 2: ApcA1

Chain r:  7% 71% 28%



- Molecule 2: ApcA1

Chain s:  75% 24%



- Molecule 3: ApcA2

Chain B:  79% 20%

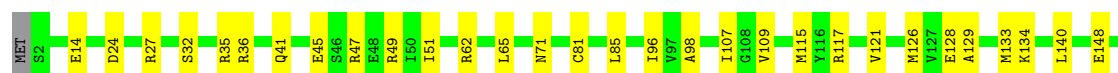


A161

- Molecule 3: ApcA2

Chain D:  78% 22%

- Molecule 3: ApcA2

Chain F:  78% 21%F153
D154
A159
L160
A161

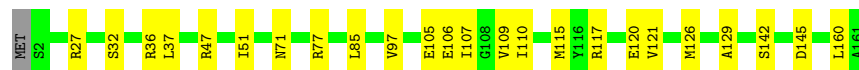
- Molecule 3: ApcA2

Chain b:  75% 24%D145
E148
V149
F153
L160
A161

- Molecule 3: ApcA2

Chain d:  80% 20%L160
A161

- Molecule 3: ApcA2

Chain f:  84% 15%

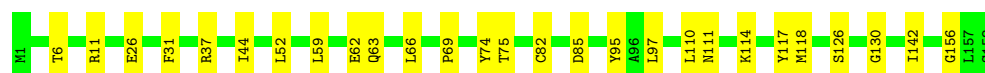
- Molecule 4: ApcB1

Chain G:  82% 18%



• Molecule 4: ApcB1

Chain H:  83% 17%



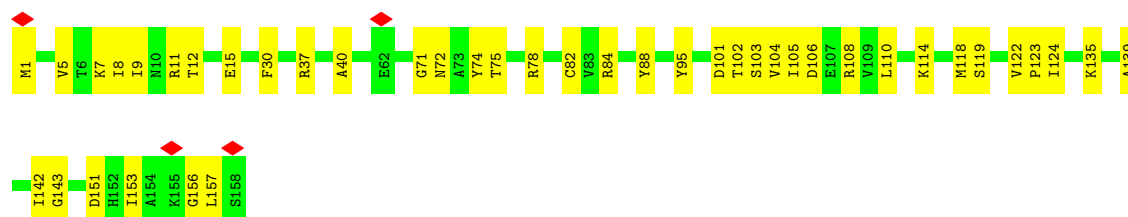
• Molecule 4: ApcB1

Chain I:  85% 14%



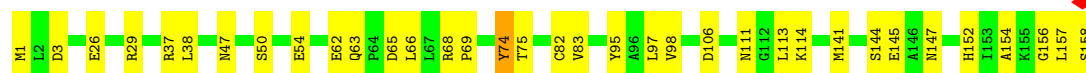
• Molecule 4: ApcB1

Chain T:  73% 27%



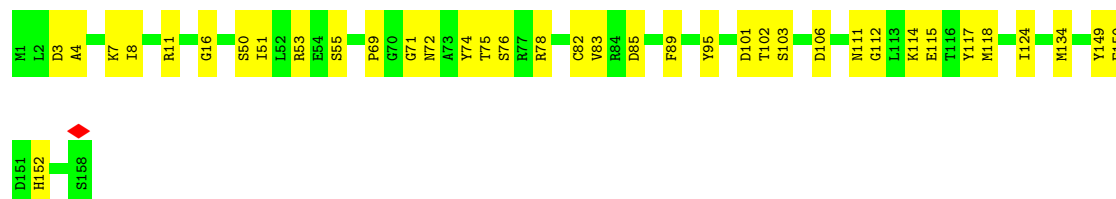
• Molecule 4: ApcB1

Chain U:  78% 22%



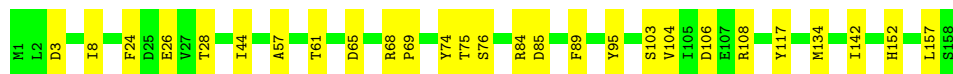
• Molecule 4: ApcB1

Chain V:  77% 23%



- Molecule 4: ApcB1

Chain W:  83% 17%



- Molecule 4: ApcB1

Chain X:  82% 18%



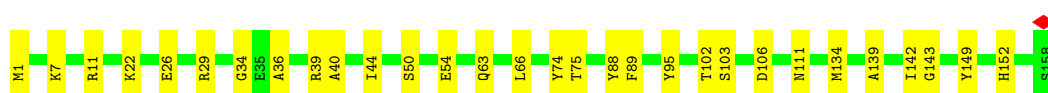
- Molecule 4: ApcB1

Chain Y:  85% 14%



- Molecule 4: ApcB1

Chain g:  81% 19%



- Molecule 4: ApcB1

Chain h:  81% 18%



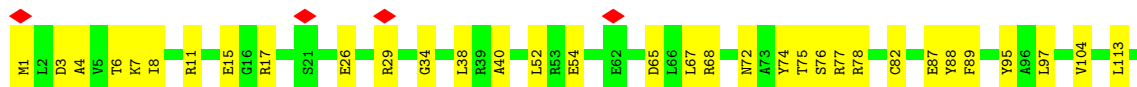
- Molecule 4: ApcB1

Chain i:  81% 18%



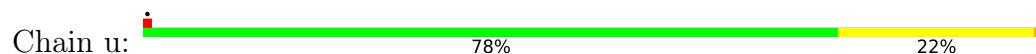
- Molecule 4: ApcB1

Chain t:  70% 30%

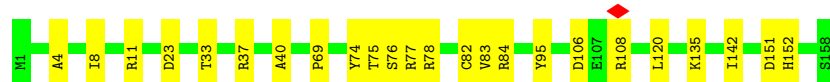
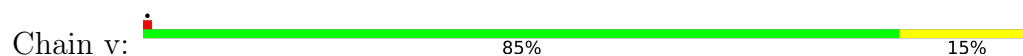




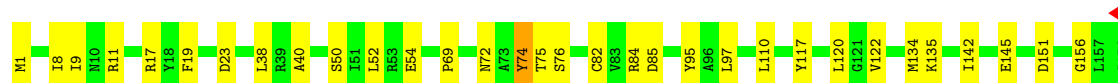
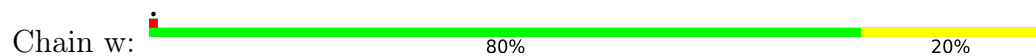
• Molecule 4: ApcB1



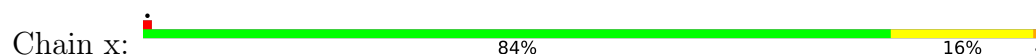
• Molecule 4: ApcB1



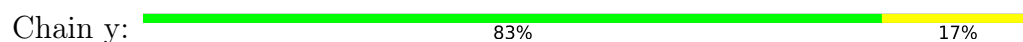
• Molecule 4: ApcB1



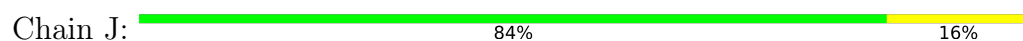
• Molecule 4: ApcB1



• Molecule 4: ApcB1

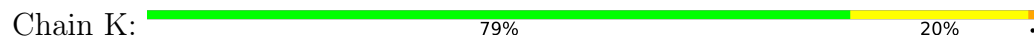


• Molecule 5: ApcB2

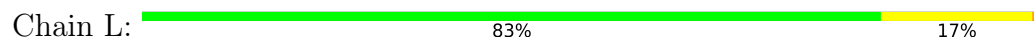




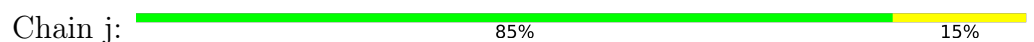
- Molecule 5: ApcB2



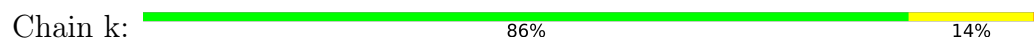
- Molecule 5: ApcB2



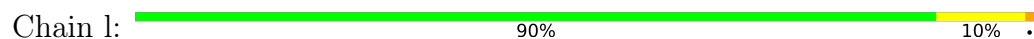
- Molecule 5: ApcB2



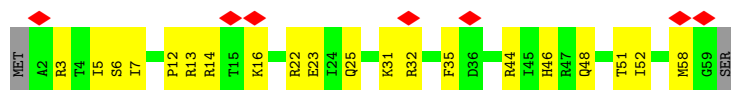
- Molecule 5: ApcB2



- Molecule 5: ApcB2

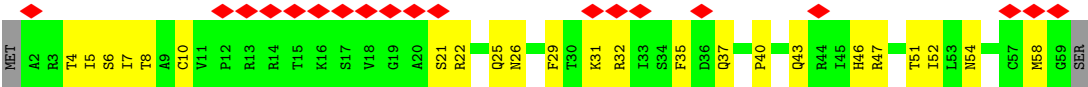


- Molecule 6: ApcC1

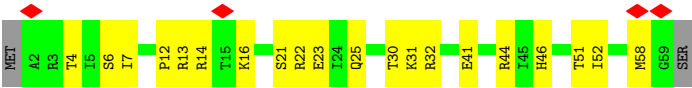


- Molecule 6: ApcC1

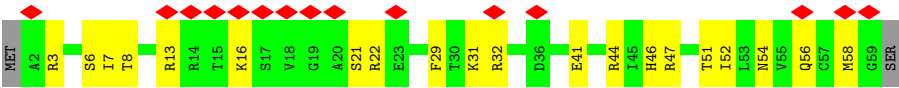




• Molecule 6: ApcC1



• Molecule 6: ApcC1



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	7.699	Depositor
Minimum map value	-0.284	Depositor
Average map value	0.074	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	1	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

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	1	0.29	0/3518	0.45	0/4767
1	2	0.29	0/3518	0.45	0/4767
2	A	0.27	0/1224	0.40	0/1657
2	C	0.25	0/1224	0.41	0/1657
2	E	0.26	0/1224	0.39	0/1657
2	N	0.22	0/1224	0.39	0/1657
2	O	0.27	0/1224	0.44	0/1657
2	P	0.26	0/1224	0.44	0/1657
2	Q	0.28	0/1224	0.44	0/1657
2	R	0.21	0/1224	0.40	0/1657
2	S	0.24	0/1224	0.46	1/1657 (0.1%)
2	a	0.26	0/1224	0.39	0/1657
2	c	0.24	0/1224	0.44	0/1657
2	e	0.24	0/1224	0.38	0/1657
2	n	0.21	0/1224	0.43	0/1657
2	o	0.26	0/1224	0.45	0/1657
2	p	0.26	0/1224	0.42	0/1657
2	q	0.27	0/1224	0.40	0/1657
2	r	0.23	0/1224	0.44	0/1657
2	s	0.25	0/1224	0.49	1/1657 (0.1%)
3	B	0.28	0/1235	0.47	0/1668
3	D	0.30	0/1235	0.48	0/1668
3	F	0.28	0/1235	0.50	0/1668
3	b	0.27	0/1235	0.47	0/1668
3	d	0.34	0/1235	0.56	0/1668
3	f	0.28	0/1235	0.51	0/1668
4	G	0.25	0/1220	0.45	0/1650
4	H	0.27	0/1220	0.45	0/1650
4	I	0.27	0/1220	0.50	0/1650
4	T	0.22	0/1220	0.43	0/1650
4	U	0.24	0/1220	0.43	0/1650
4	V	0.25	0/1220	0.46	0/1650

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	W	0.25	0/1220	0.46	0/1650
4	X	0.28	0/1220	0.44	0/1650
4	Y	0.27	0/1220	0.43	0/1650
4	g	0.26	0/1220	0.49	0/1650
4	h	0.27	0/1220	0.51	0/1650
4	i	0.27	0/1220	0.49	0/1650
4	t	0.23	0/1220	0.44	0/1650
4	u	0.25	0/1220	0.44	0/1650
4	v	0.26	0/1220	0.44	0/1650
4	w	0.26	0/1220	0.51	0/1650
4	x	0.31	0/1220	0.46	0/1650
4	y	0.28	0/1220	0.46	0/1650
5	J	0.27	0/1249	0.45	0/1688
5	K	0.29	0/1249	0.50	0/1688
5	L	0.29	0/1249	0.49	0/1688
5	j	0.27	0/1249	0.45	0/1688
5	k	0.32	0/1249	0.51	0/1688
5	l	0.30	0/1249	0.47	0/1688
6	M	0.25	0/471	0.55	0/633
6	Z	0.20	0/471	0.46	0/633
6	m	0.22	0/471	0.48	0/633
6	z	0.18	0/471	0.49	0/633
All	All	0.27	0/67816	0.46	2/91728 (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
4	I	0	1
4	U	0	1
4	Y	0	1
4	h	0	1
4	i	0	1
4	u	0	1
4	w	0	1
4	x	0	1
5	K	0	1
5	L	0	1
5	k	0	1
5	l	0	1
All	All	0	12

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	49	ARG	CB-CG-CD	-5.96	97.60	111.30
2	s	49	ARG	CB-CG-CD	-5.81	97.94	111.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	74	TYR	Peptide
5	K	74	TYR	Peptide
5	L	74	TYR	Peptide
4	U	74	TYR	Peptide
4	Y	74	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3445	0	3468	49	0
1	2	3445	0	3468	54	0
2	A	1207	0	1222	17	0
2	C	1207	0	1222	21	0
2	E	1207	0	1222	16	0
2	N	1207	0	1222	28	0
2	O	1207	0	1222	16	0
2	P	1207	0	1222	29	0
2	Q	1207	0	1222	24	0
2	R	1207	0	1222	23	0
2	S	1207	0	1222	40	0
2	a	1207	0	1222	22	0
2	c	1207	0	1222	24	0
2	e	1207	0	1222	16	0
2	n	1207	0	1222	24	0
2	o	1207	0	1222	20	0
2	p	1207	0	1222	22	0
2	q	1207	0	1222	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	r	1207	0	1222	35	0
2	s	1207	0	1222	36	0
3	B	1218	0	1229	24	0
3	D	1218	0	1229	26	0
3	F	1218	0	1229	26	0
3	b	1218	0	1229	31	0
3	d	1218	0	1229	32	0
3	f	1218	0	1229	20	0
4	G	1201	0	1196	19	0
4	H	1201	0	1196	21	0
4	I	1201	0	1196	19	0
4	T	1201	0	1196	31	0
4	U	1201	0	1196	27	0
4	V	1201	0	1196	28	0
4	W	1201	0	1196	17	0
4	X	1201	0	1196	24	0
4	Y	1201	0	1196	18	0
4	g	1201	0	1196	20	0
4	h	1201	0	1196	28	0
4	i	1201	0	1196	25	0
4	t	1201	0	1196	37	0
4	u	1201	0	1196	28	0
4	v	1201	0	1196	20	0
4	w	1201	0	1196	24	0
4	x	1201	0	1196	24	0
4	y	1201	0	1196	23	0
5	J	1230	0	1219	22	0
5	K	1230	0	1219	33	0
5	L	1230	0	1219	22	0
5	j	1230	0	1219	21	0
5	k	1230	0	1219	26	0
5	l	1230	0	1219	17	0
6	M	464	0	471	18	0
6	Z	464	0	471	18	0
6	m	464	0	471	20	0
6	z	464	0	471	17	0
7	A	43	0	37	4	0
7	B	43	0	38	5	0
7	C	43	0	38	1	0
7	D	43	0	38	7	0
7	E	43	0	38	6	0
7	F	43	0	37	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	43	0	38	2	0
7	H	43	0	38	5	0
7	I	43	0	38	3	0
7	J	43	0	38	3	0
7	K	43	0	37	8	0
7	L	43	0	38	8	0
7	N	43	0	38	3	0
7	O	43	0	38	2	0
7	P	43	0	38	4	0
7	Q	43	0	38	4	0
7	R	43	0	38	2	0
7	S	43	0	38	10	0
7	T	43	0	38	5	0
7	U	43	0	37	4	0
7	V	43	0	37	5	0
7	W	43	0	38	4	0
7	X	43	0	37	6	0
7	Y	43	0	37	5	0
7	a	43	0	38	7	0
7	b	43	0	37	4	0
7	c	43	0	38	4	0
7	d	43	0	37	6	0
7	e	43	0	38	7	0
7	f	43	0	38	7	0
7	g	43	0	38	1	0
7	h	43	0	37	4	0
7	i	43	0	37	5	0
7	j	43	0	38	5	0
7	k	43	0	38	5	0
7	l	43	0	38	4	0
7	n	43	0	38	4	0
7	o	43	0	37	4	0
7	p	43	0	37	3	0
7	q	43	0	38	3	0
7	r	43	0	38	5	0
7	s	43	0	38	8	0
7	t	43	0	38	8	0
7	u	43	0	37	7	0
7	v	43	0	38	6	0
7	w	43	0	38	7	0
7	x	43	0	37	7	0
7	y	43	0	37	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	68842	0	68840	1237	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 9.

The worst 5 of 1237 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)
7:K:200:CYC:HMD1	7:K:200:CYC:HC	1.26	0.97
7:k:200:CYC:HMD1	7:k:200:CYC:HC	1.31	0.94
2:P:80:LYS:HZ1	7:P:200:CYC:HAD2	1.35	0.91
4:V:114:LYS:HG3	4:V:118:MET:HE2	1.55	0.89
4:u:15:GLU:OE1	4:u:17:ARG:NH2	2.06	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	1	429/431 (100%)	421 (98%)	8 (2%)	0	100	100
1	2	429/431 (100%)	419 (98%)	10 (2%)	0	100	100
2	A	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	C	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	E	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	N	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	O	158/161 (98%)	158 (100%)	0	0	100	100
2	P	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	Q	158/161 (98%)	158 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	158/161 (98%)	158 (100%)	0	0	100	100
2	S	158/161 (98%)	158 (100%)	0	0	100	100
2	a	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	c	158/161 (98%)	158 (100%)	0	0	100	100
2	e	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	n	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	o	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	p	158/161 (98%)	158 (100%)	0	0	100	100
2	q	158/161 (98%)	158 (100%)	0	0	100	100
2	r	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	s	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
3	B	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
3	D	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
3	F	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
3	b	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
3	d	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
3	f	158/161 (98%)	158 (100%)	0	0	100	100
4	G	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
4	H	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	I	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
4	T	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
4	U	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	V	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	W	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	X	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
4	Y	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
4	g	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
4	h	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	i	156/158 (99%)	153 (98%)	3 (2%)	0	100	100
4	t	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
4	u	156/158 (99%)	153 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	v	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
4	w	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
4	x	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
4	y	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
5	J	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
5	K	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
5	L	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
5	j	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
5	k	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
5	l	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
6	M	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
6	Z	56/60 (93%)	55 (98%)	1 (2%)	0	100	100
6	m	56/60 (93%)	56 (100%)	0	0	100	100
6	z	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
All	All	8642/8782 (98%)	8541 (99%)	101 (1%)	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	1	367/367 (100%)	367 (100%)	0	100	100
1	2	367/367 (100%)	367 (100%)	0	100	100
2	A	124/125 (99%)	124 (100%)	0	100	100
2	C	124/125 (99%)	124 (100%)	0	100	100
2	E	124/125 (99%)	124 (100%)	0	100	100
2	N	124/125 (99%)	124 (100%)	0	100	100
2	O	124/125 (99%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	124/125 (99%)	124 (100%)	0	100	100
2	Q	124/125 (99%)	124 (100%)	0	100	100
2	R	124/125 (99%)	124 (100%)	0	100	100
2	S	124/125 (99%)	124 (100%)	0	100	100
2	a	124/125 (99%)	124 (100%)	0	100	100
2	c	124/125 (99%)	124 (100%)	0	100	100
2	e	124/125 (99%)	124 (100%)	0	100	100
2	n	124/125 (99%)	124 (100%)	0	100	100
2	o	124/125 (99%)	124 (100%)	0	100	100
2	p	124/125 (99%)	124 (100%)	0	100	100
2	q	124/125 (99%)	124 (100%)	0	100	100
2	r	124/125 (99%)	124 (100%)	0	100	100
2	s	124/125 (99%)	124 (100%)	0	100	100
3	B	127/128 (99%)	127 (100%)	0	100	100
3	D	127/128 (99%)	127 (100%)	0	100	100
3	F	127/128 (99%)	127 (100%)	0	100	100
3	b	127/128 (99%)	127 (100%)	0	100	100
3	d	127/128 (99%)	127 (100%)	0	100	100
3	f	127/128 (99%)	127 (100%)	0	100	100
4	G	123/123 (100%)	123 (100%)	0	100	100
4	H	123/123 (100%)	123 (100%)	0	100	100
4	I	123/123 (100%)	123 (100%)	0	100	100
4	T	123/123 (100%)	123 (100%)	0	100	100
4	U	123/123 (100%)	123 (100%)	0	100	100
4	V	123/123 (100%)	123 (100%)	0	100	100
4	W	123/123 (100%)	123 (100%)	0	100	100
4	X	123/123 (100%)	123 (100%)	0	100	100
4	Y	123/123 (100%)	123 (100%)	0	100	100
4	g	123/123 (100%)	123 (100%)	0	100	100
4	h	123/123 (100%)	123 (100%)	0	100	100
4	i	123/123 (100%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	t	123/123 (100%)	123 (100%)	0	100	100
4	u	123/123 (100%)	123 (100%)	0	100	100
4	v	123/123 (100%)	123 (100%)	0	100	100
4	w	123/123 (100%)	123 (100%)	0	100	100
4	x	123/123 (100%)	123 (100%)	0	100	100
4	y	123/123 (100%)	123 (100%)	0	100	100
5	J	128/128 (100%)	128 (100%)	0	100	100
5	K	128/128 (100%)	128 (100%)	0	100	100
5	L	128/128 (100%)	128 (100%)	0	100	100
5	j	128/128 (100%)	128 (100%)	0	100	100
5	k	128/128 (100%)	128 (100%)	0	100	100
5	l	128/128 (100%)	128 (100%)	0	100	100
6	M	51/53 (96%)	51 (100%)	0	100	100
6	Z	51/53 (96%)	51 (100%)	0	100	100
6	m	51/53 (96%)	51 (100%)	0	100	100
6	z	51/53 (96%)	51 (100%)	0	100	100
All	All	6914/6946 (100%)	6914 (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 49 such sidechains are listed below:

Mol	Chain	Res	Type
4	V	147	ASN
5	k	62	ASN
4	X	47	ASN
4	h	47	ASN
5	l	47	ASN

5.3.3 RNA ⓘ

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](#)

48 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	e	200	-	46,46,46	5.27	27 (58%)	63,67,67	3.97	20 (31%)
7	CYC	n	200	-	46,46,46	5.27	26 (56%)	63,67,67	4.04	14 (22%)
7	CYC	N	200	-	46,46,46	5.26	26 (56%)	63,67,67	4.05	12 (19%)
7	CYC	i	200	-	46,46,46	5.20	27 (58%)	63,67,67	3.81	18 (28%)
7	CYC	a	200	-	46,46,46	5.19	27 (58%)	63,67,67	4.07	16 (25%)
7	CYC	P	200	-	46,46,46	5.32	27 (58%)	63,67,67	4.12	22 (34%)
7	CYC	H	200	-	46,46,46	5.23	27 (58%)	63,67,67	3.80	17 (26%)
7	CYC	j	200	-	46,46,46	5.20	28 (60%)	63,67,67	4.05	17 (26%)
7	CYC	U	200	-	46,46,46	5.19	27 (58%)	63,67,67	4.05	20 (31%)
7	CYC	X	200	-	46,46,46	5.16	27 (58%)	63,67,67	3.94	20 (31%)
7	CYC	f	200	-	46,46,46	5.22	27 (58%)	63,67,67	4.01	18 (28%)
7	CYC	v	200	-	46,46,46	5.21	27 (58%)	63,67,67	4.05	19 (30%)
7	CYC	D	200	-	46,46,46	5.29	27 (58%)	63,67,67	3.77	18 (28%)
7	CYC	o	200	-	46,46,46	5.21	26 (56%)	63,67,67	4.02	15 (23%)
7	CYC	C	200	-	46,46,46	5.29	26 (56%)	63,67,67	4.02	17 (26%)
7	CYC	k	200	-	46,46,46	5.19	27 (58%)	63,67,67	4.11	23 (36%)
7	CYC	l	200	-	46,46,46	5.25	27 (58%)	63,67,67	3.81	18 (28%)
7	CYC	V	200	-	46,46,46	5.20	27 (58%)	63,67,67	4.05	18 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CYC	F	200	-	46,46,46	5.23	27 (58%)	63,67,67	3.88	18 (28%)
7	CYC	p	200	-	46,46,46	5.33	27 (58%)	63,67,67	3.92	18 (28%)
7	CYC	r	200	-	46,46,46	5.30	26 (56%)	63,67,67	4.04	12 (19%)
7	CYC	S	200	-	46,46,46	5.29	26 (56%)	63,67,67	4.02	14 (22%)
7	CYC	B	200	-	46,46,46	5.22	27 (58%)	63,67,67	4.17	22 (34%)
7	CYC	s	200	-	46,46,46	5.31	26 (56%)	63,67,67	3.91	14 (22%)
7	CYC	t	200	-	46,46,46	5.26	26 (56%)	63,67,67	3.94	18 (28%)
7	CYC	y	200	-	46,46,46	5.17	27 (58%)	63,67,67	4.02	18 (28%)
7	CYC	A	200	-	46,46,46	5.25	27 (58%)	63,67,67	3.94	14 (22%)
7	CYC	E	200	-	46,46,46	5.26	26 (56%)	63,67,67	3.93	15 (23%)
7	CYC	G	200	-	46,46,46	5.31	27 (58%)	63,67,67	3.99	18 (28%)
7	CYC	W	200	-	46,46,46	5.18	27 (58%)	63,67,67	4.18	19 (30%)
7	CYC	u	200	-	46,46,46	5.22	26 (56%)	63,67,67	3.95	18 (28%)
7	CYC	d	200	-	46,46,46	5.28	28 (60%)	63,67,67	3.85	17 (26%)
7	CYC	b	200	-	46,46,46	5.24	27 (58%)	63,67,67	3.91	17 (26%)
7	CYC	g	200	-	46,46,46	5.28	27 (58%)	63,67,67	4.13	19 (30%)
7	CYC	I	200	-	46,46,46	5.19	27 (58%)	63,67,67	4.05	18 (28%)
7	CYC	q	200	-	46,46,46	5.20	26 (56%)	63,67,67	4.03	16 (25%)
7	CYC	R	200	-	46,46,46	5.29	26 (56%)	63,67,67	4.09	14 (22%)
7	CYC	c	200	-	46,46,46	5.22	27 (58%)	63,67,67	4.12	18 (28%)
7	CYC	L	200	-	46,46,46	5.27	26 (56%)	63,67,67	3.80	20 (31%)
7	CYC	T	200	-	46,46,46	5.24	26 (56%)	63,67,67	4.02	16 (25%)
7	CYC	Y	200	-	46,46,46	5.17	27 (58%)	63,67,67	3.89	18 (28%)
7	CYC	w	200	-	46,46,46	5.23	28 (60%)	63,67,67	4.06	18 (28%)
7	CYC	O	200	-	46,46,46	5.21	27 (58%)	63,67,67	4.14	16 (25%)
7	CYC	x	200	-	46,46,46	5.17	26 (56%)	63,67,67	4.05	17 (26%)
7	CYC	Q	200	-	46,46,46	5.24	26 (56%)	63,67,67	3.97	16 (25%)
7	CYC	K	200	-	46,46,46	5.18	27 (58%)	63,67,67	4.11	19 (30%)
7	CYC	J	200	-	46,46,46	5.20	28 (60%)	63,67,67	4.02	21 (33%)
7	CYC	h	200	-	46,46,46	5.28	27 (58%)	63,67,67	3.77	18 (28%)

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	e	200	-	-	9/26/74/74	0/4/4/4
7	CYC	n	200	-	-	10/26/74/74	0/4/4/4
7	CYC	N	200	-	-	9/26/74/74	0/4/4/4
7	CYC	i	200	-	-	9/26/74/74	0/4/4/4
7	CYC	a	200	-	-	7/26/74/74	0/4/4/4
7	CYC	P	200	-	-	11/26/74/74	0/4/4/4
7	CYC	H	200	-	-	8/26/74/74	0/4/4/4
7	CYC	j	200	-	-	9/26/74/74	0/4/4/4
7	CYC	U	200	-	-	6/26/74/74	0/4/4/4
7	CYC	X	200	-	-	11/26/74/74	0/4/4/4
7	CYC	f	200	-	-	10/26/74/74	0/4/4/4
7	CYC	v	200	-	-	11/26/74/74	0/4/4/4
7	CYC	D	200	-	-	6/26/74/74	0/4/4/4
7	CYC	o	200	-	-	12/26/74/74	0/4/4/4
7	CYC	C	200	-	-	11/26/74/74	0/4/4/4
7	CYC	k	200	-	-	9/26/74/74	0/4/4/4
7	CYC	l	200	-	-	7/26/74/74	0/4/4/4
7	CYC	V	200	-	-	10/26/74/74	0/4/4/4
7	CYC	F	200	-	-	8/26/74/74	0/4/4/4
7	CYC	p	200	-	-	12/26/74/74	0/4/4/4
7	CYC	r	200	-	-	11/26/74/74	0/4/4/4
7	CYC	S	200	-	-	13/26/74/74	0/4/4/4
7	CYC	B	200	-	-	8/26/74/74	0/4/4/4
7	CYC	s	200	-	-	10/26/74/74	0/4/4/4
7	CYC	t	200	-	-	9/26/74/74	0/4/4/4
7	CYC	y	200	-	-	6/26/74/74	0/4/4/4
7	CYC	A	200	-	-	8/26/74/74	0/4/4/4
7	CYC	E	200	-	-	9/26/74/74	0/4/4/4
7	CYC	G	200	-	-	12/26/74/74	0/4/4/4
7	CYC	W	200	-	-	12/26/74/74	0/4/4/4
7	CYC	u	200	-	-	7/26/74/74	0/4/4/4
7	CYC	d	200	-	-	10/26/74/74	0/4/4/4
7	CYC	b	200	-	-	7/26/74/74	0/4/4/4
7	CYC	g	200	-	-	9/26/74/74	0/4/4/4
7	CYC	I	200	-	-	9/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CYC	q	200	-	-	11/26/74/74	0/4/4/4
7	CYC	R	200	-	-	7/26/74/74	0/4/4/4
7	CYC	c	200	-	-	12/26/74/74	0/4/4/4
7	CYC	L	200	-	-	7/26/74/74	0/4/4/4
7	CYC	T	200	-	-	11/26/74/74	0/4/4/4
7	CYC	Y	200	-	-	8/26/74/74	0/4/4/4
7	CYC	w	200	-	-	7/26/74/74	0/4/4/4
7	CYC	O	200	-	-	11/26/74/74	0/4/4/4
7	CYC	x	200	-	-	8/26/74/74	0/4/4/4
7	CYC	Q	200	-	-	10/26/74/74	0/4/4/4
7	CYC	K	200	-	-	8/26/74/74	0/4/4/4
7	CYC	J	200	-	-	10/26/74/74	0/4/4/4
7	CYC	h	200	-	-	7/26/74/74	0/4/4/4

The worst 5 of 1284 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	200	CYC	C2C-C1C	14.04	1.64	1.52
7	p	200	CYC	C2C-C1C	14.01	1.64	1.52
7	G	200	CYC	C2C-C1C	13.53	1.64	1.52
7	C	200	CYC	C2C-C1C	13.50	1.64	1.52
7	E	200	CYC	C2C-C1C	13.44	1.64	1.52

The worst 5 of 838 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	n	200	CYC	OC-C1C-C2C	-21.22	109.30	126.17
7	T	200	CYC	OC-C1C-C2C	-21.13	109.38	126.17
7	q	200	CYC	OC-C1C-C2C	-20.91	109.55	126.17
7	K	200	CYC	OC-C1C-C2C	-20.85	109.60	126.17
7	d	200	CYC	OC-C1C-C2C	-20.84	109.60	126.17

There are no chirality outliers.

5 of 442 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	200	CYC	NA-C4A-CHB-C1B
7	A	200	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
7	A	200	CYC	NC-C4C-CHD-C1D
7	B	200	CYC	C2C-C3C-CAC-CBC
7	B	200	CYC	NC-C4C-CHD-C1D

There are no ring outliers.

48 monomers are involved in 237 short contacts:

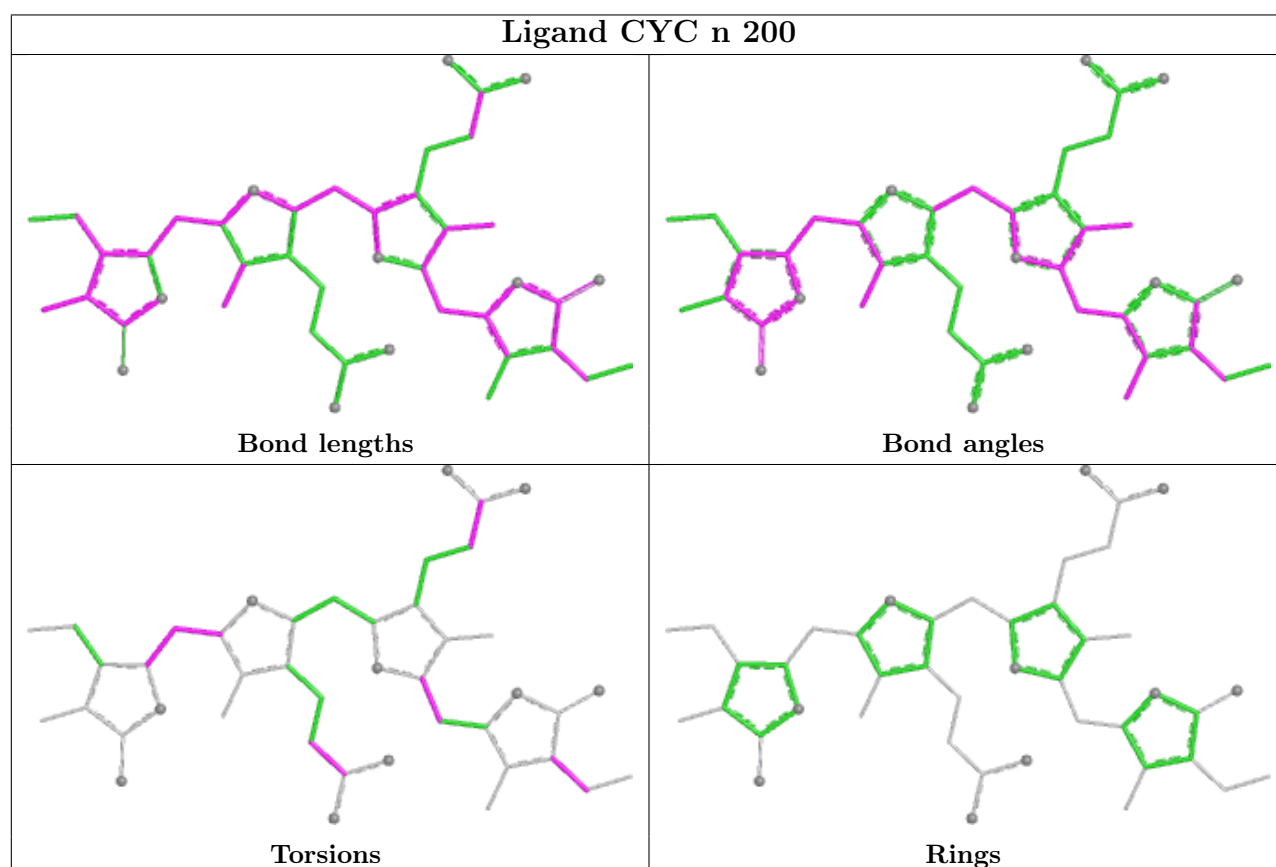
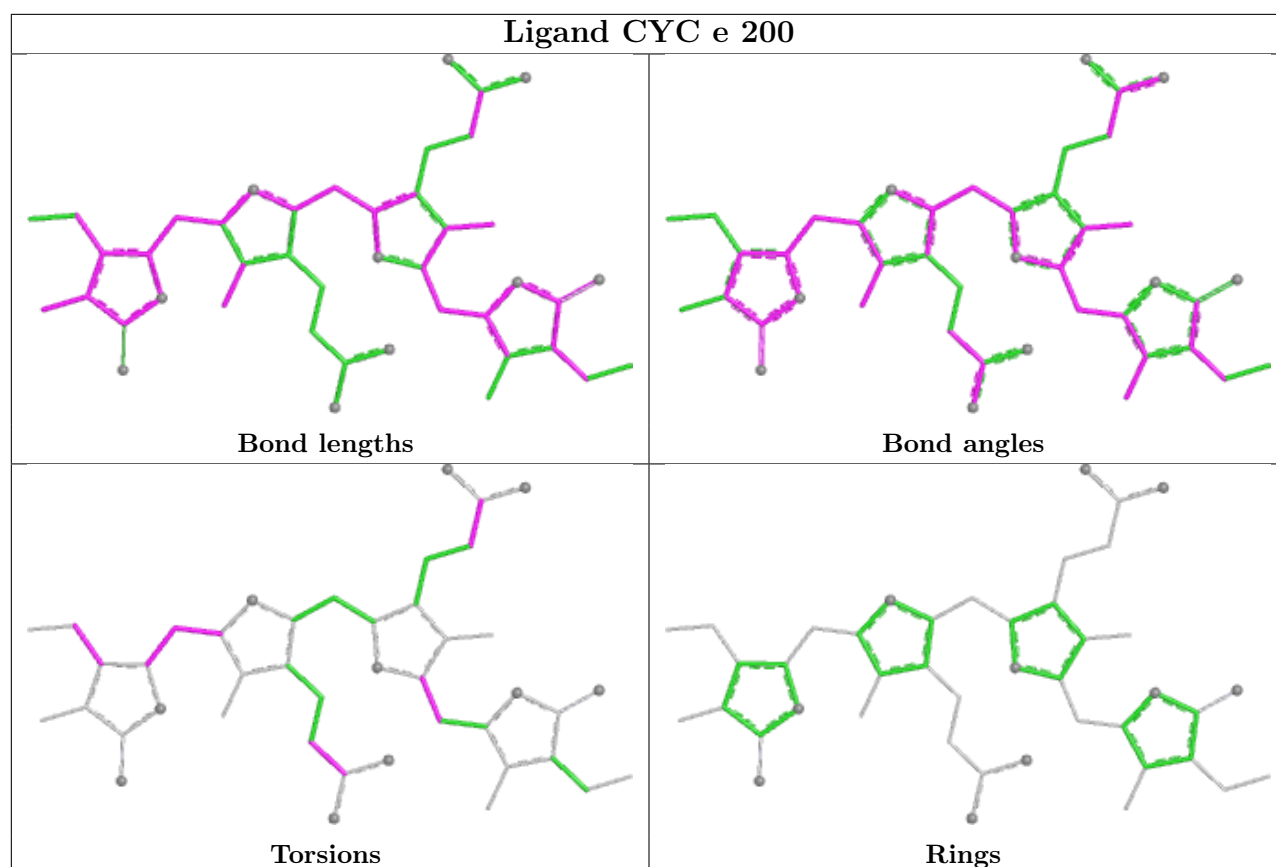
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	e	200	CYC	7	0
7	n	200	CYC	4	0
7	N	200	CYC	3	0
7	i	200	CYC	5	0
7	a	200	CYC	7	0
7	P	200	CYC	4	0
7	H	200	CYC	5	0
7	j	200	CYC	5	0
7	U	200	CYC	4	0
7	X	200	CYC	6	0
7	f	200	CYC	7	0
7	v	200	CYC	6	0
7	D	200	CYC	7	0
7	o	200	CYC	4	0
7	C	200	CYC	1	0
7	k	200	CYC	5	0
7	l	200	CYC	4	0
7	V	200	CYC	5	0
7	F	200	CYC	5	0
7	p	200	CYC	3	0
7	r	200	CYC	5	0
7	S	200	CYC	10	0
7	B	200	CYC	5	0
7	s	200	CYC	8	0
7	t	200	CYC	8	0
7	y	200	CYC	5	0
7	A	200	CYC	4	0
7	E	200	CYC	6	0
7	G	200	CYC	2	0
7	W	200	CYC	4	0
7	u	200	CYC	7	0
7	d	200	CYC	6	0
7	b	200	CYC	4	0
7	g	200	CYC	1	0

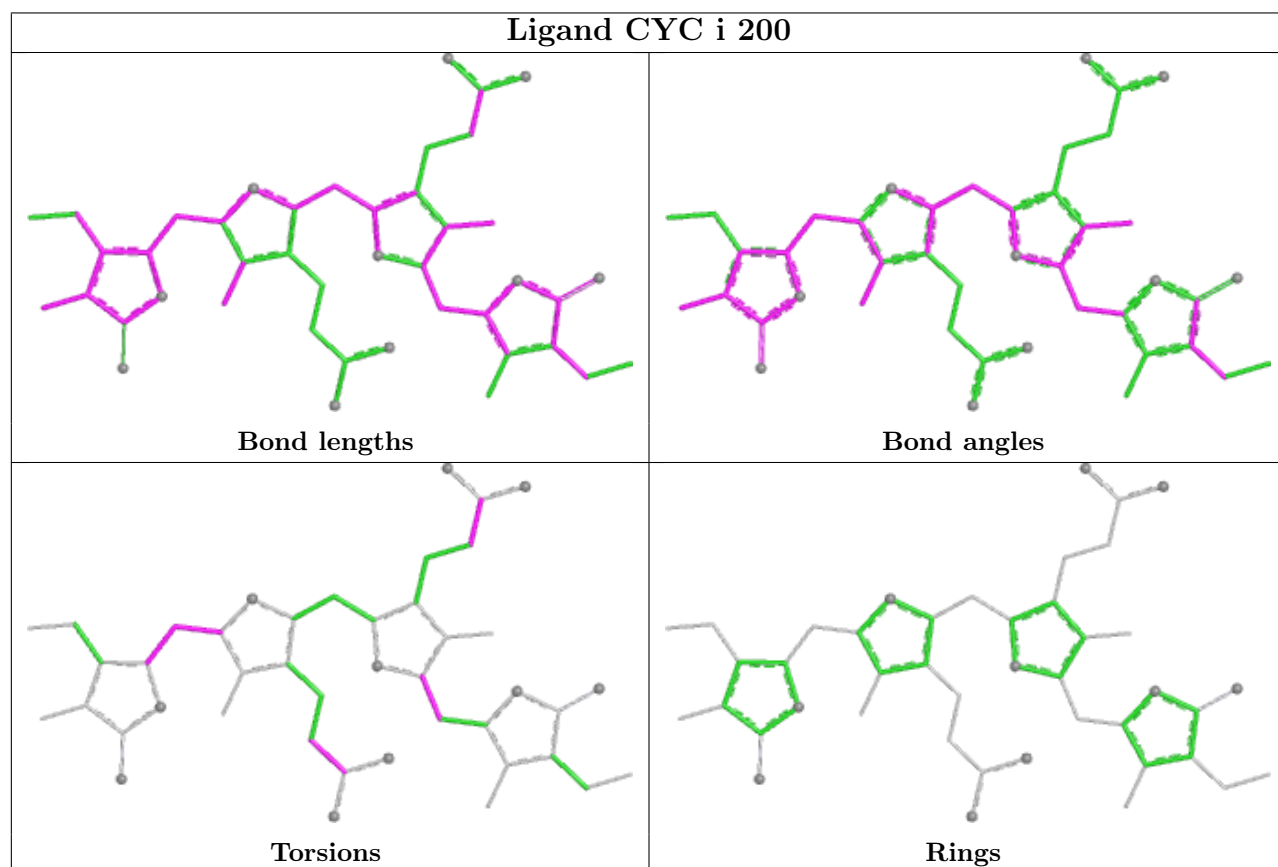
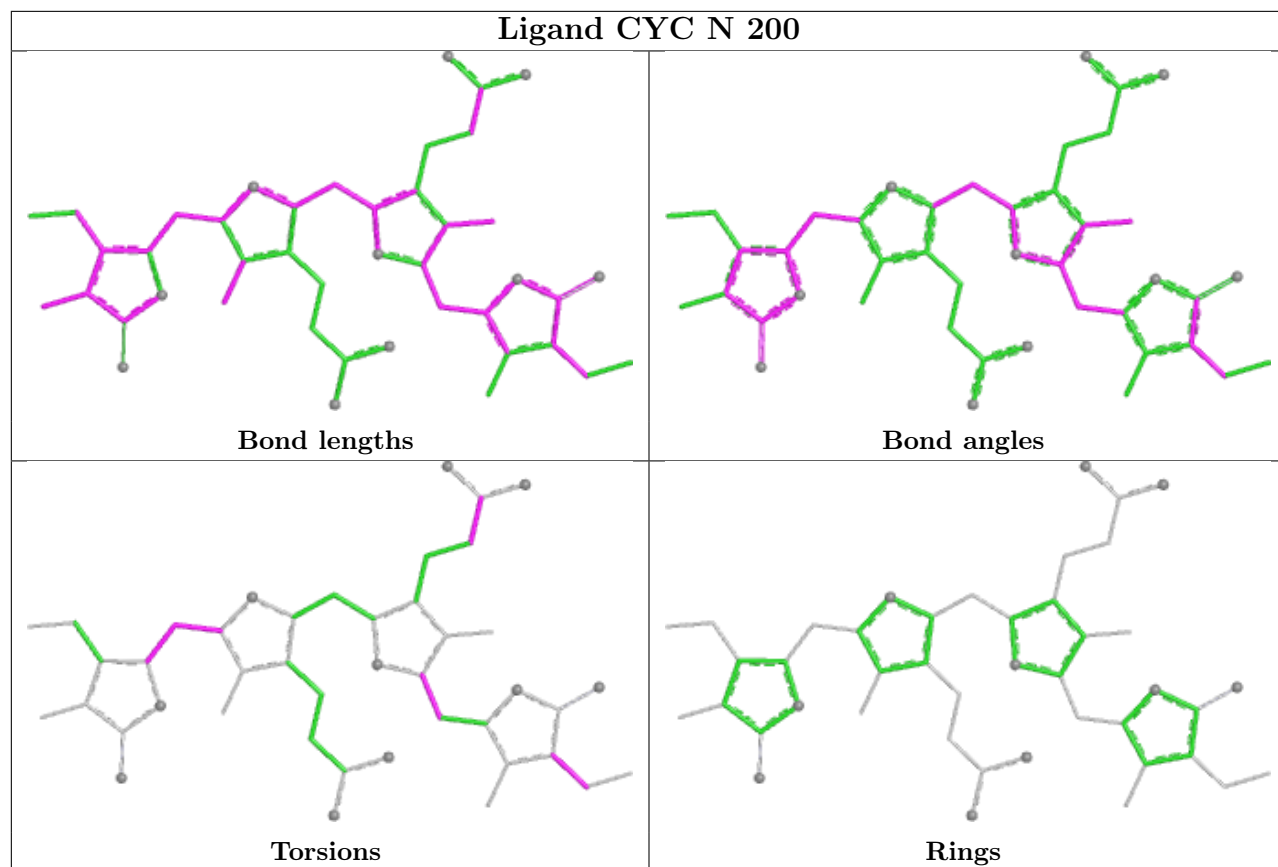
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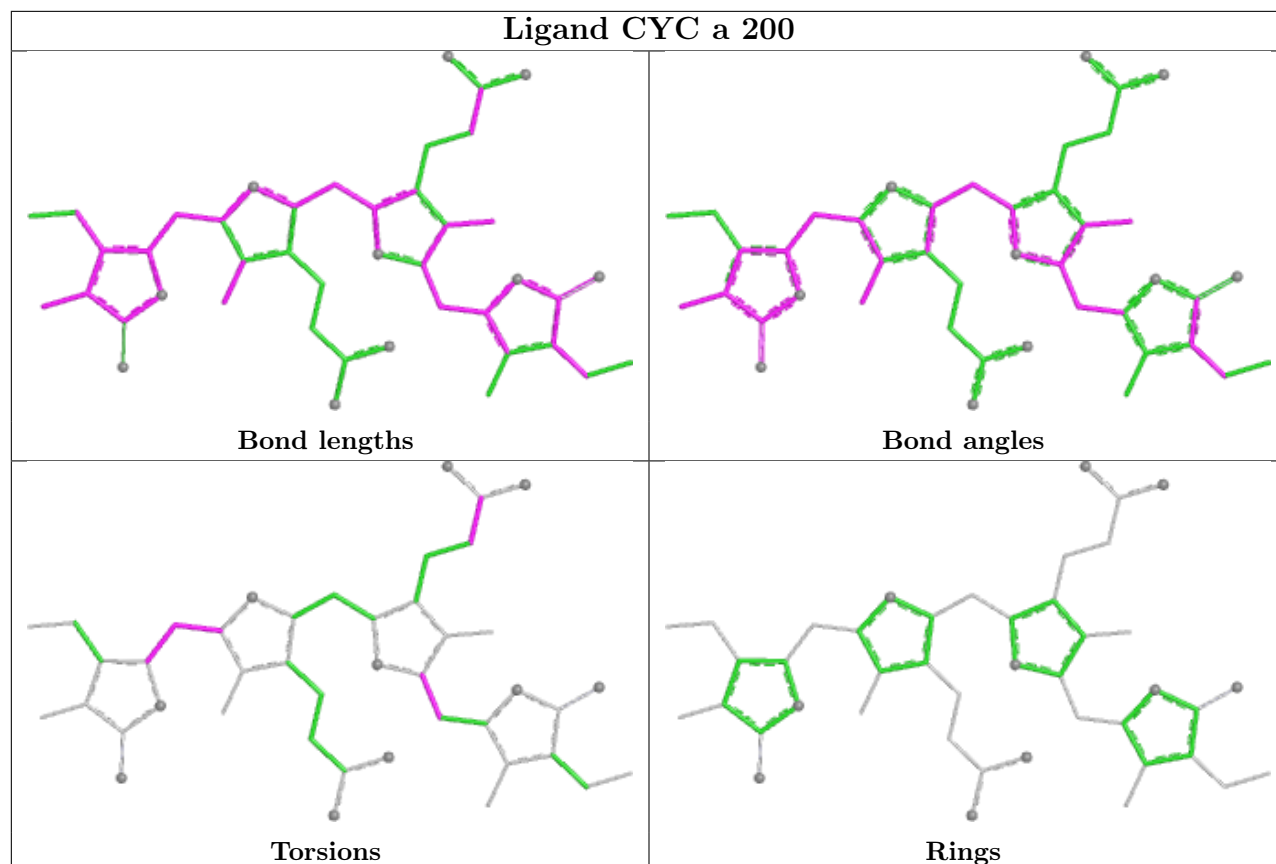
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	200	CYC	3	0
7	q	200	CYC	3	0
7	R	200	CYC	2	0
7	c	200	CYC	4	0
7	L	200	CYC	8	0
7	T	200	CYC	5	0
7	Y	200	CYC	5	0
7	w	200	CYC	7	0
7	O	200	CYC	2	0
7	x	200	CYC	7	0
7	Q	200	CYC	4	0
7	K	200	CYC	8	0
7	J	200	CYC	3	0
7	h	200	CYC	4	0

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.

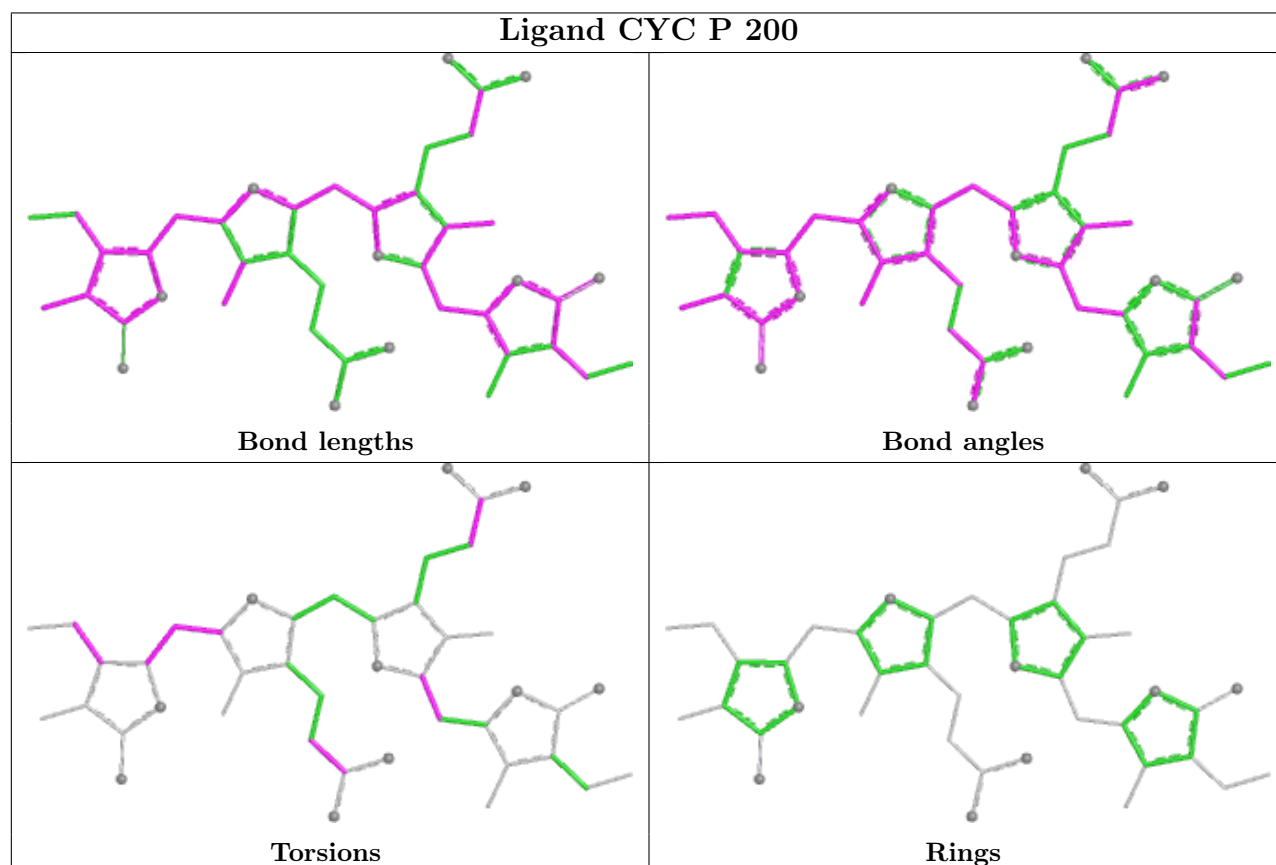


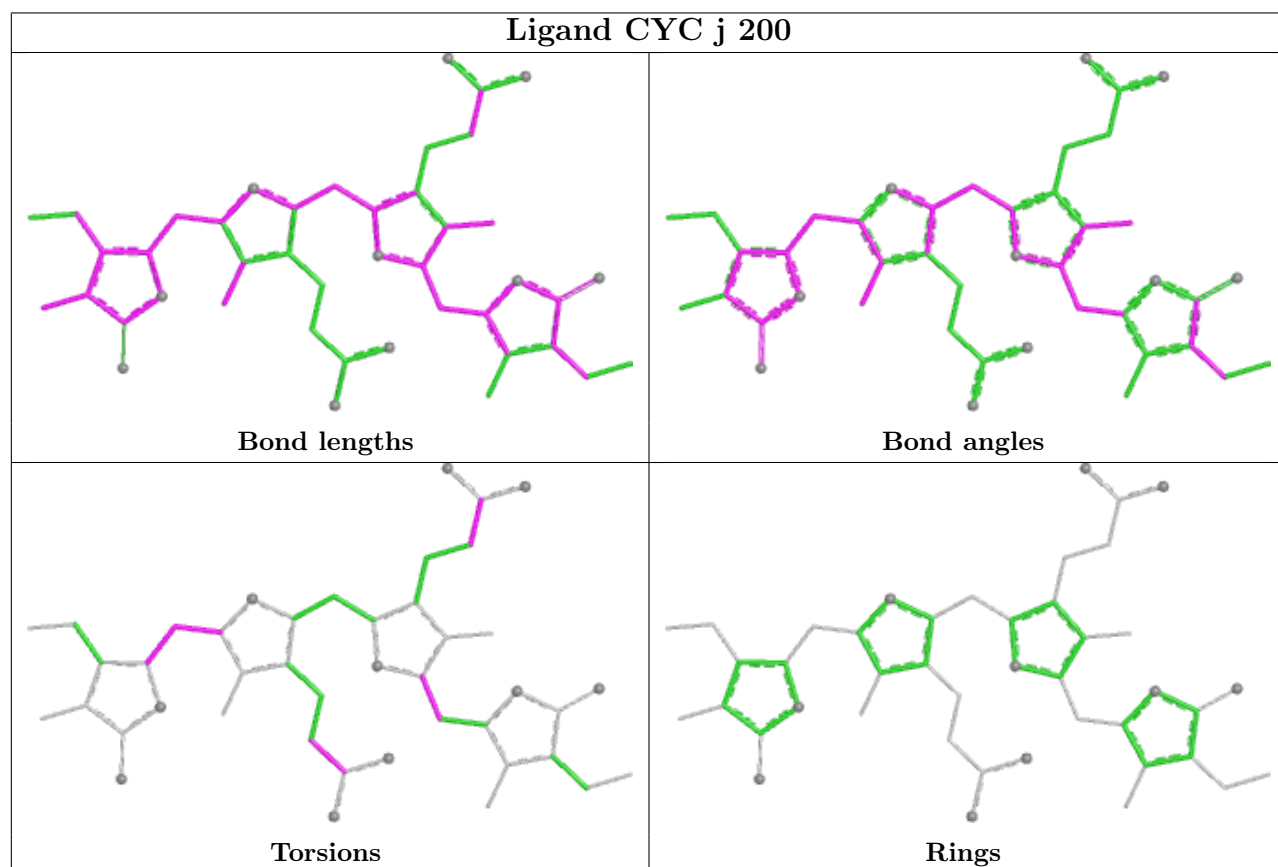
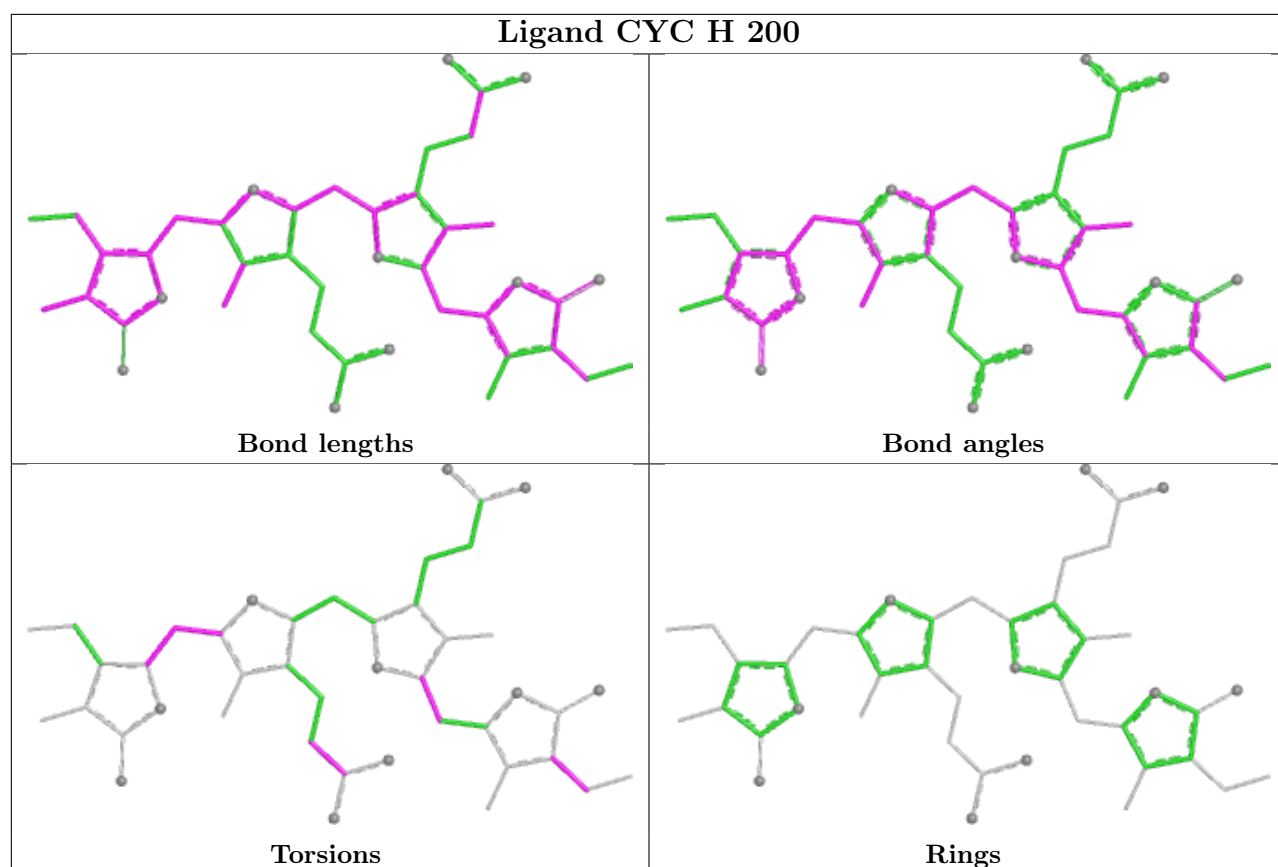


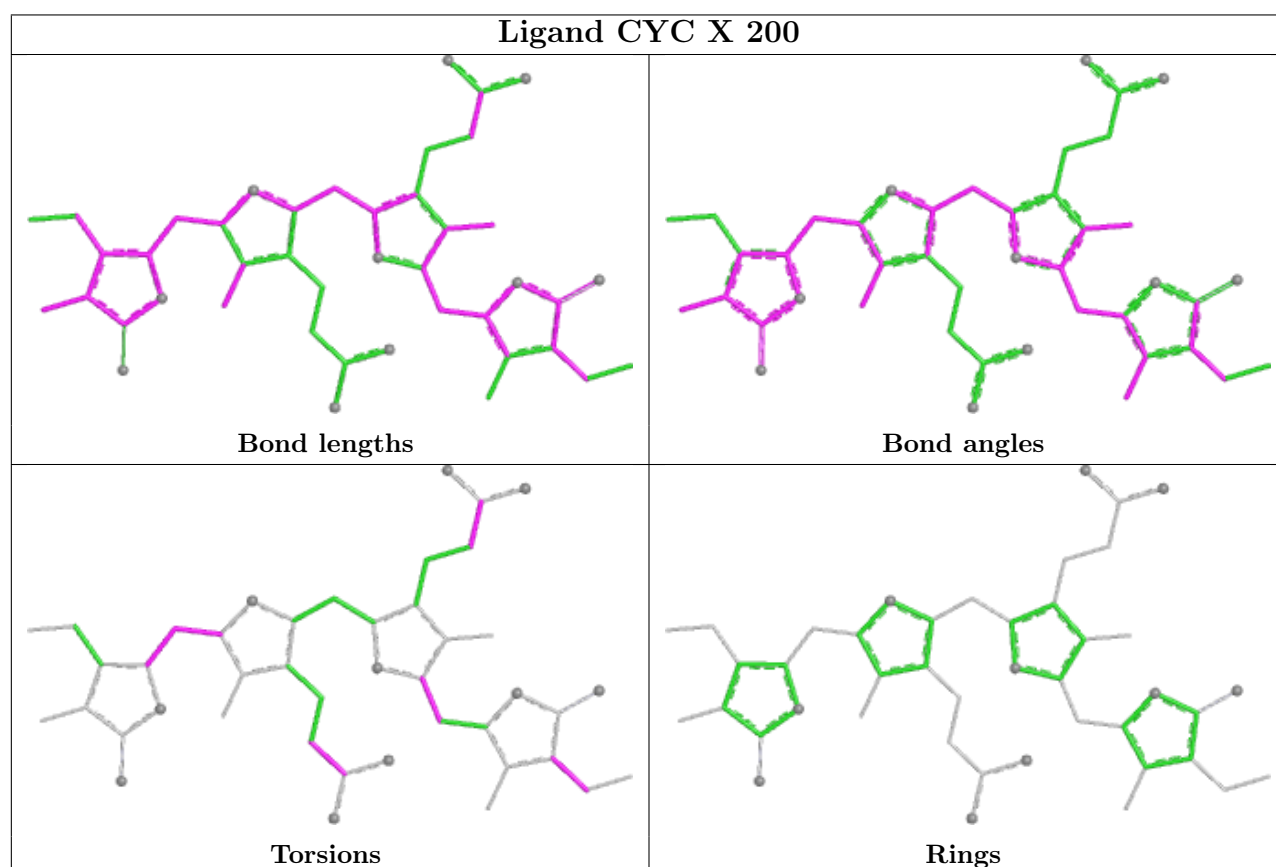
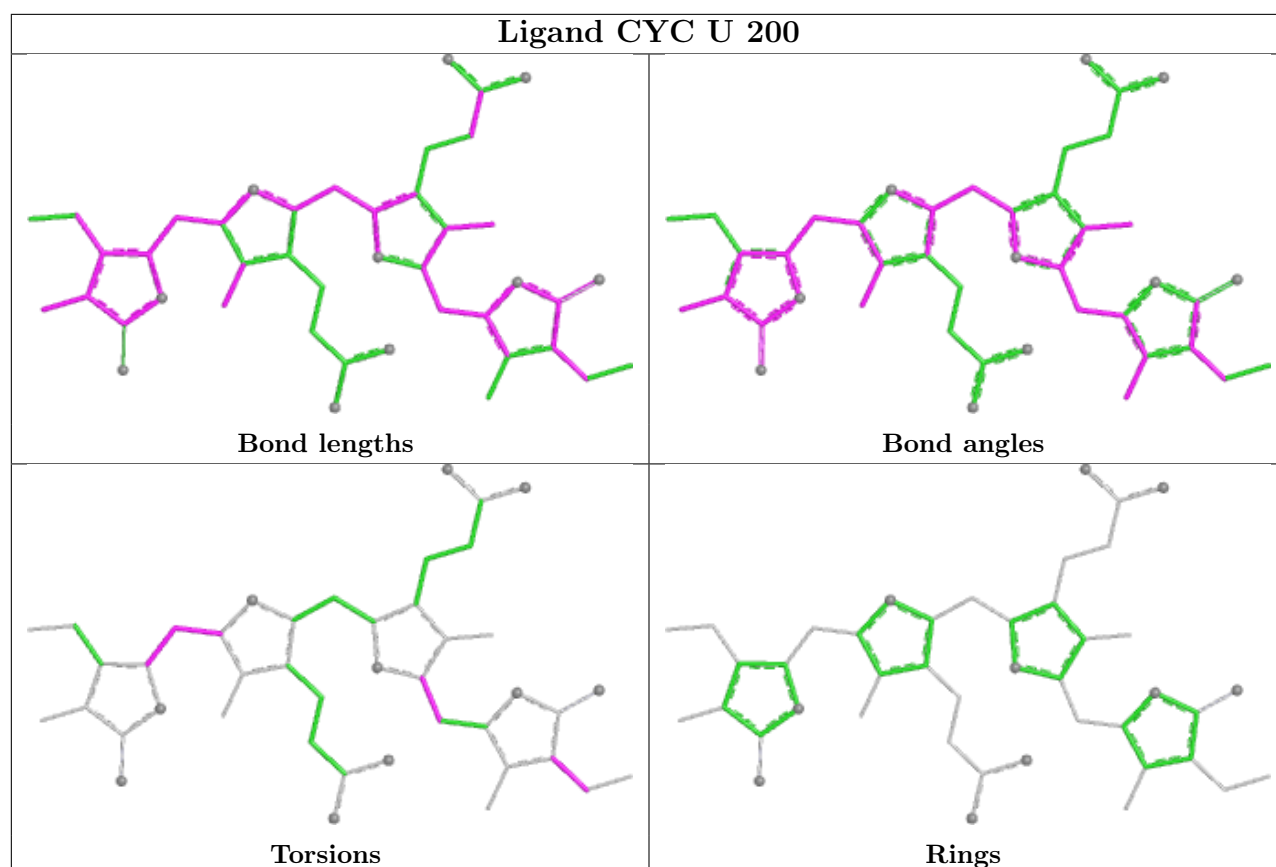
Ligand CYC a 200

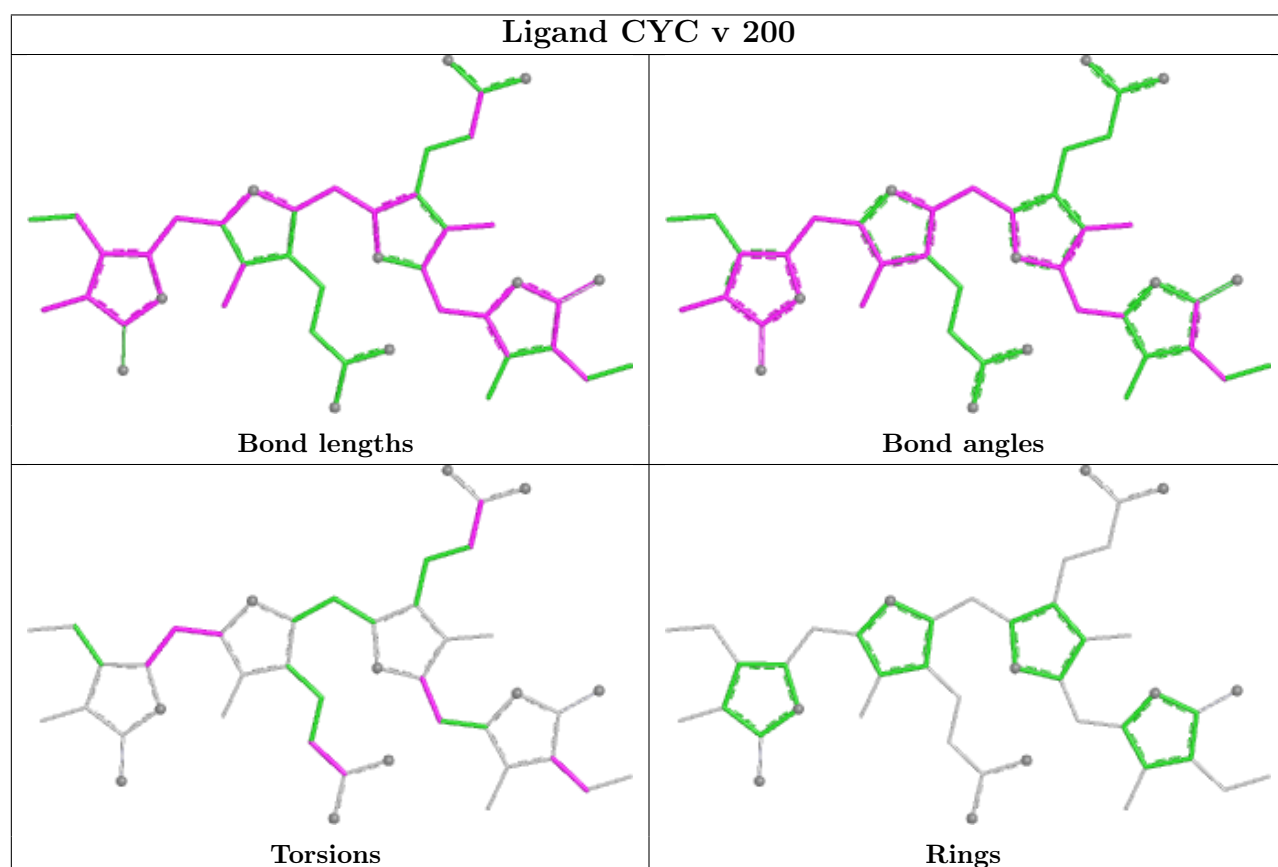
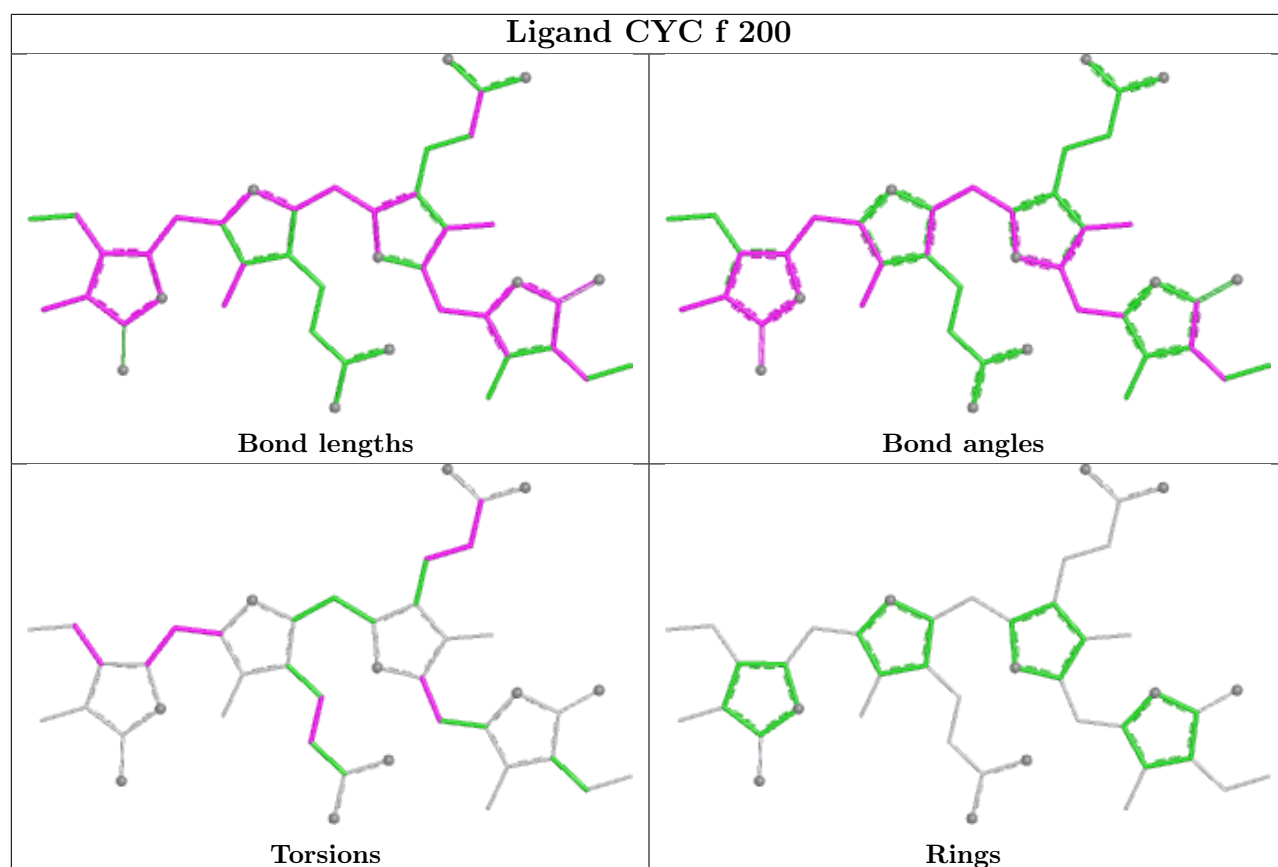


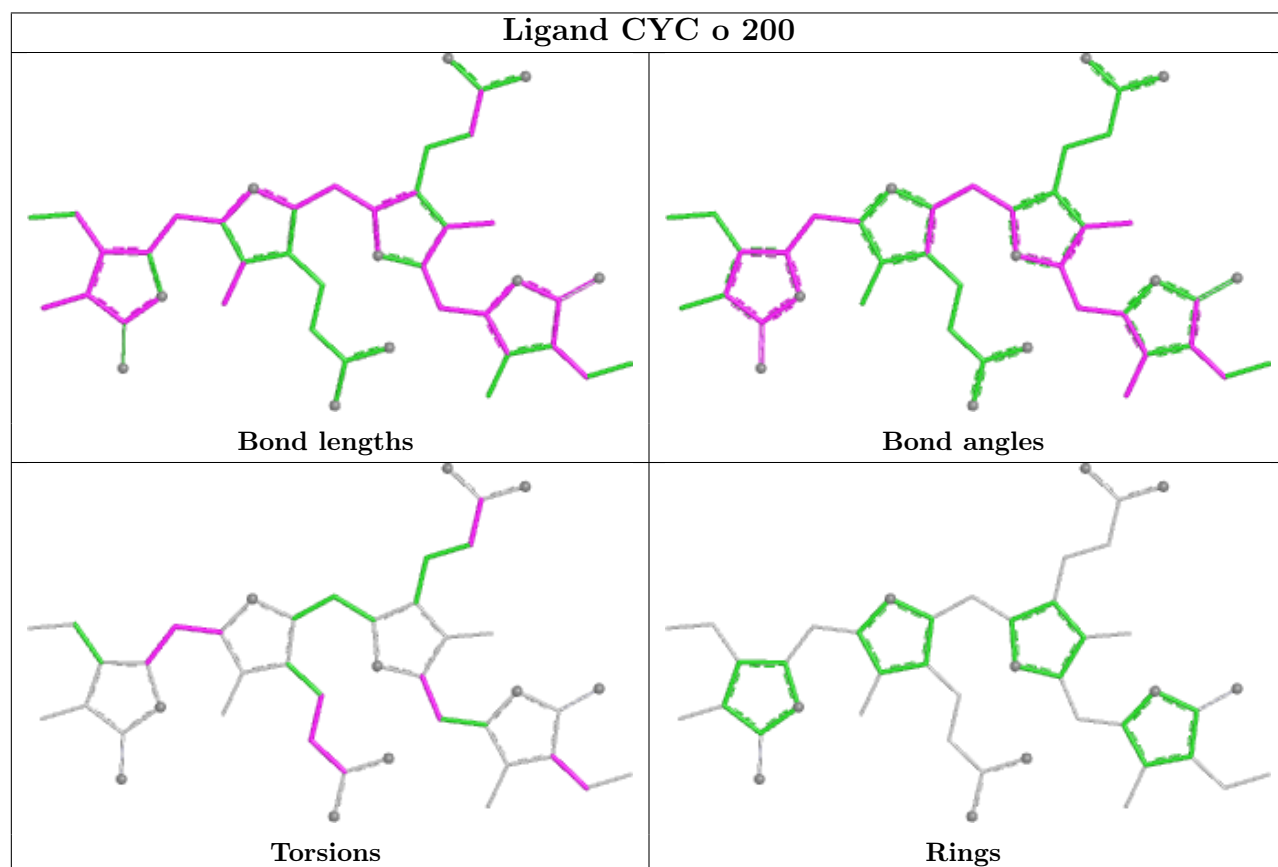
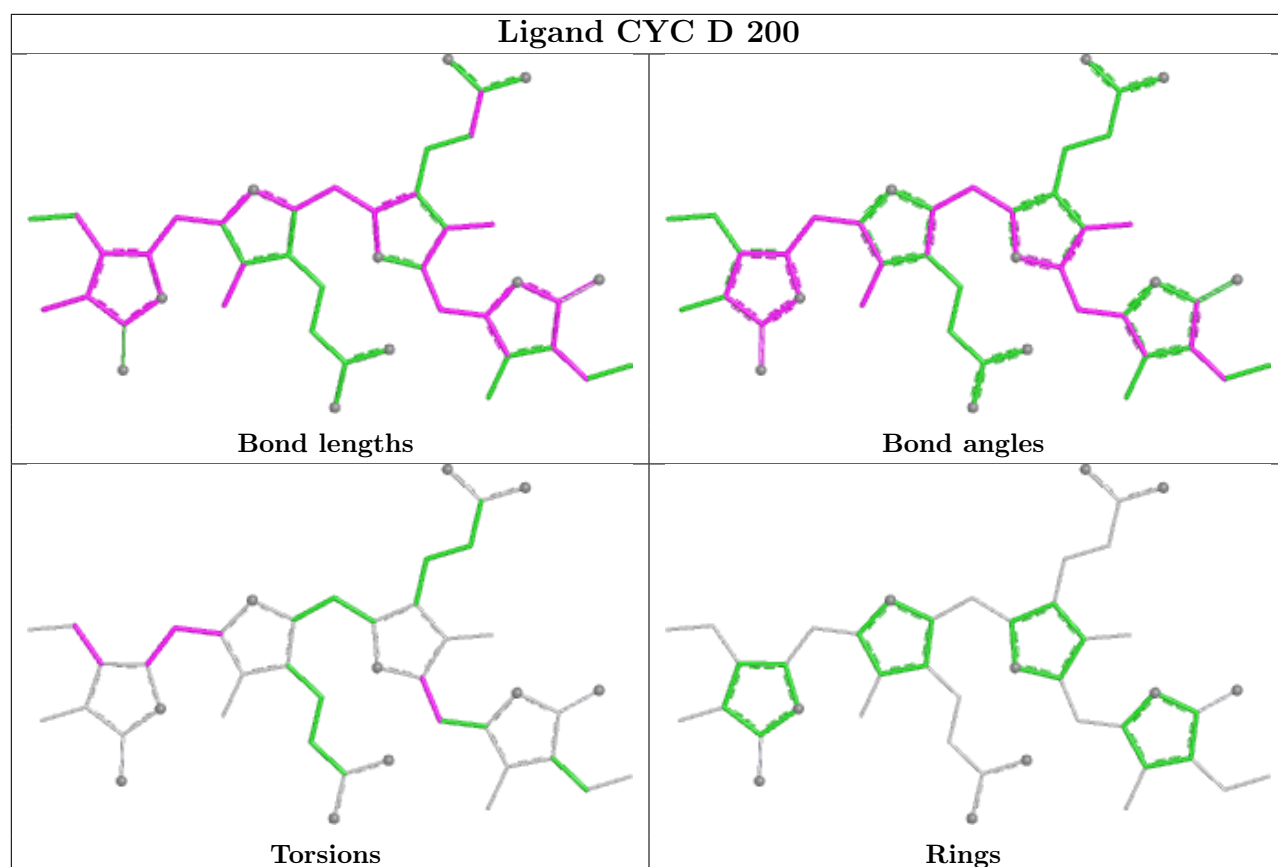
Ligand CYC P 200

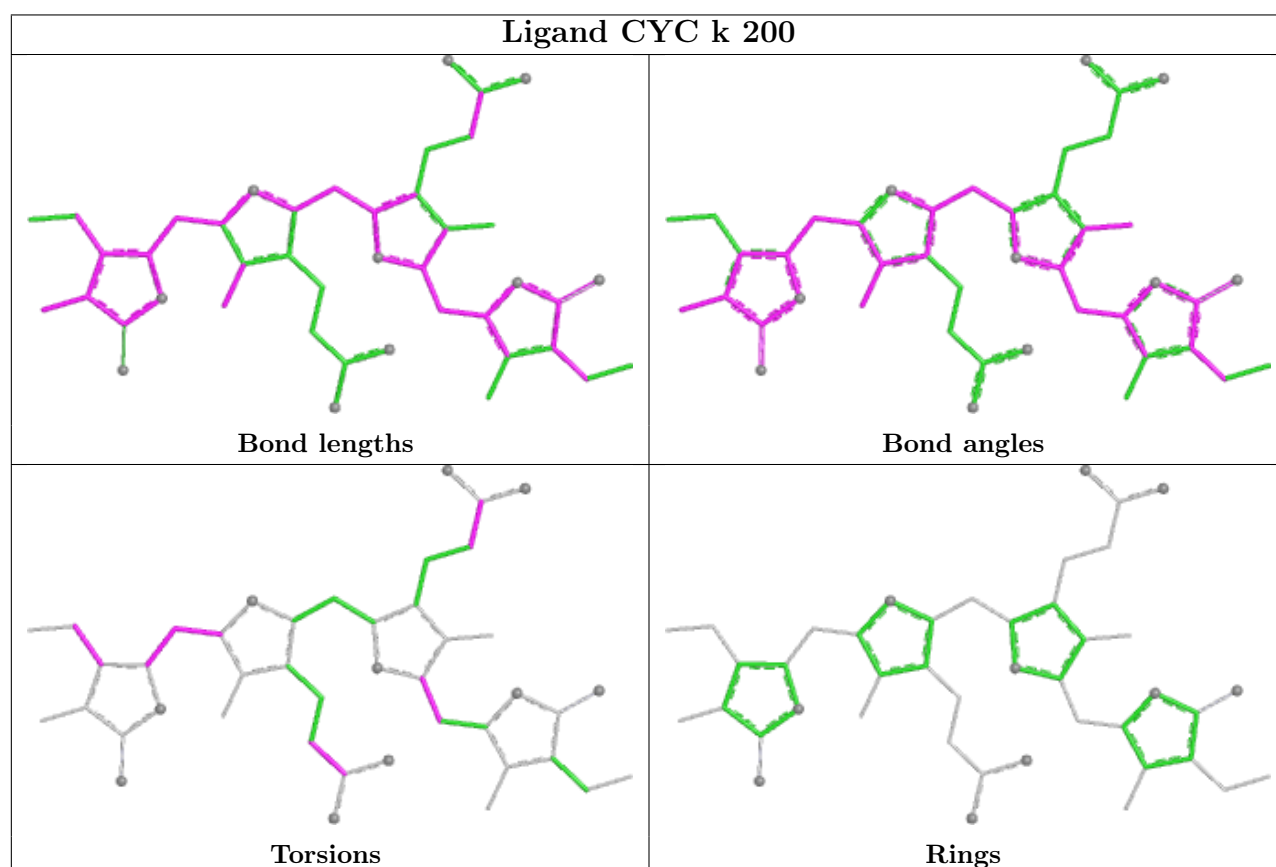
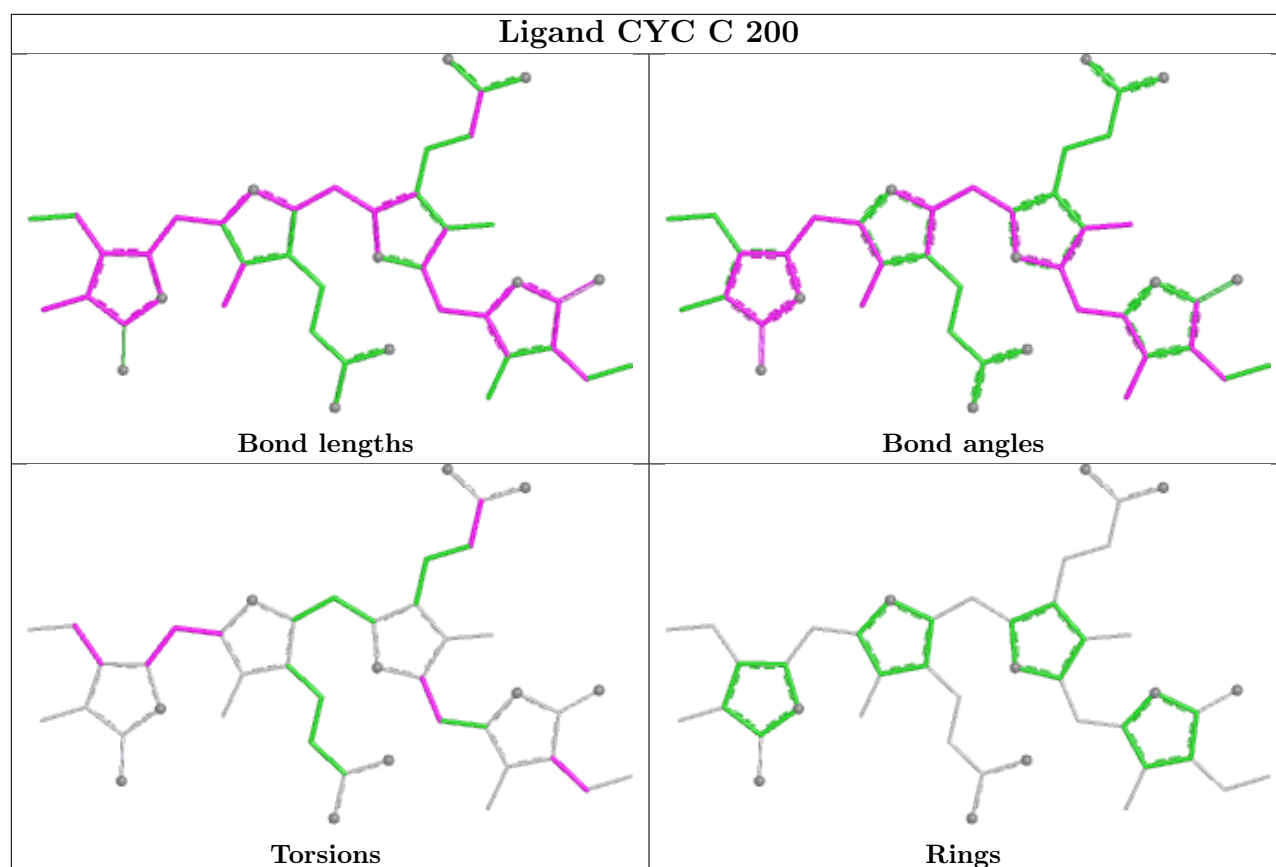




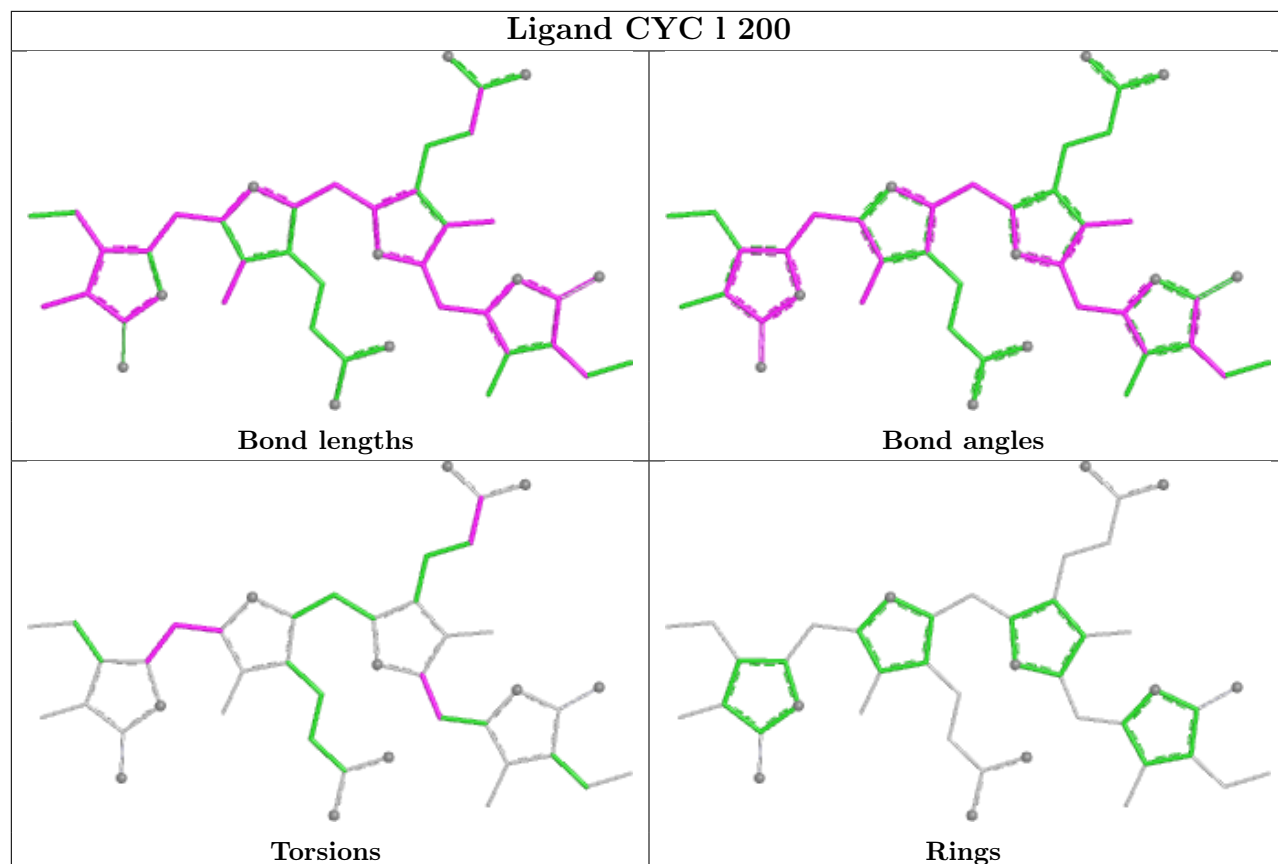




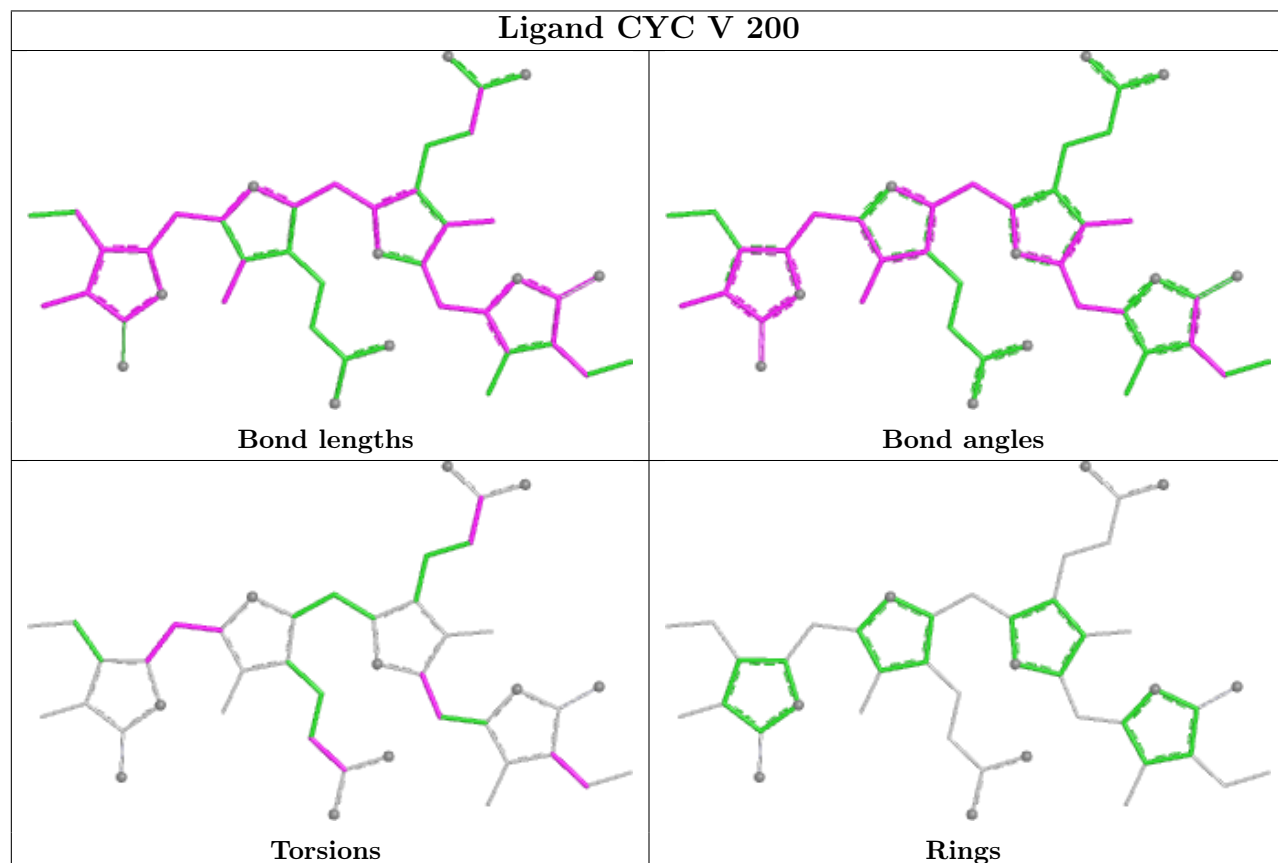


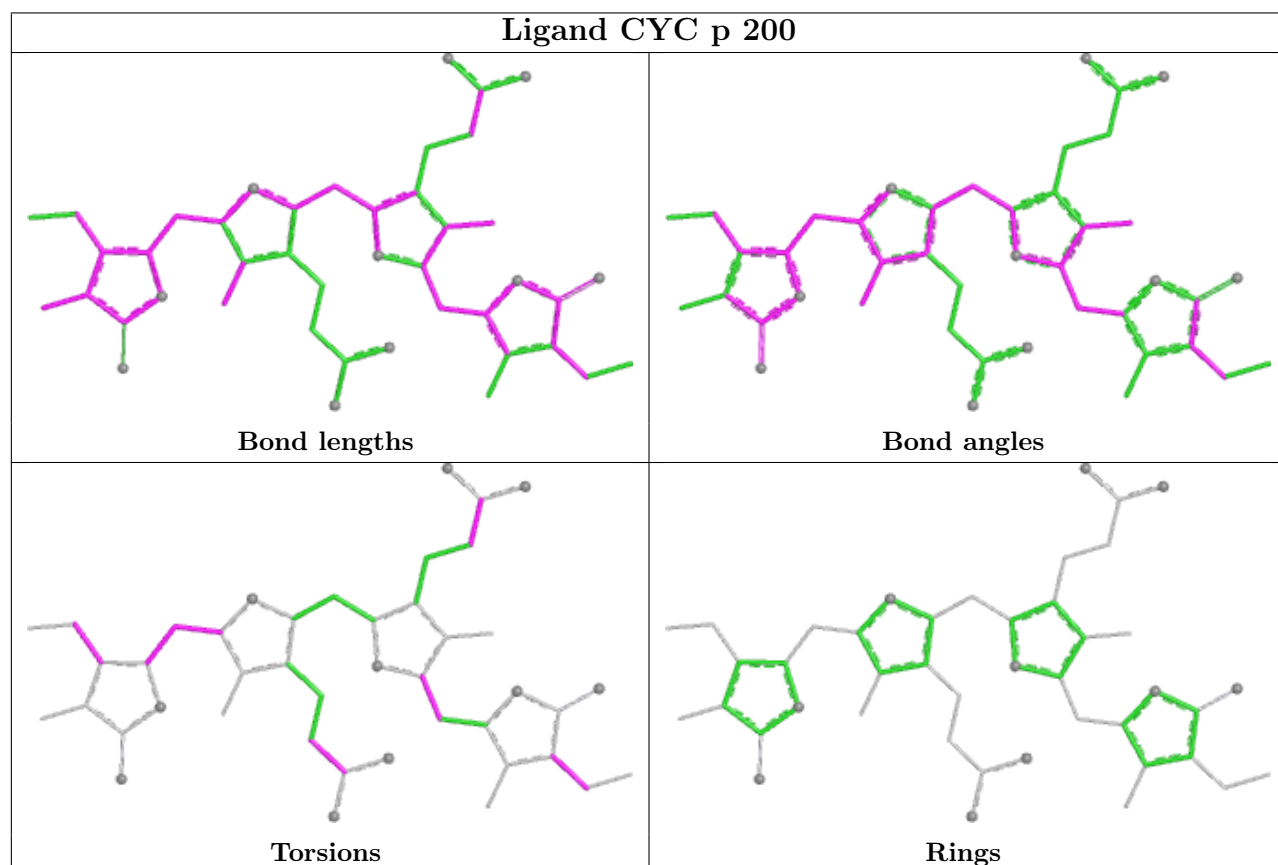
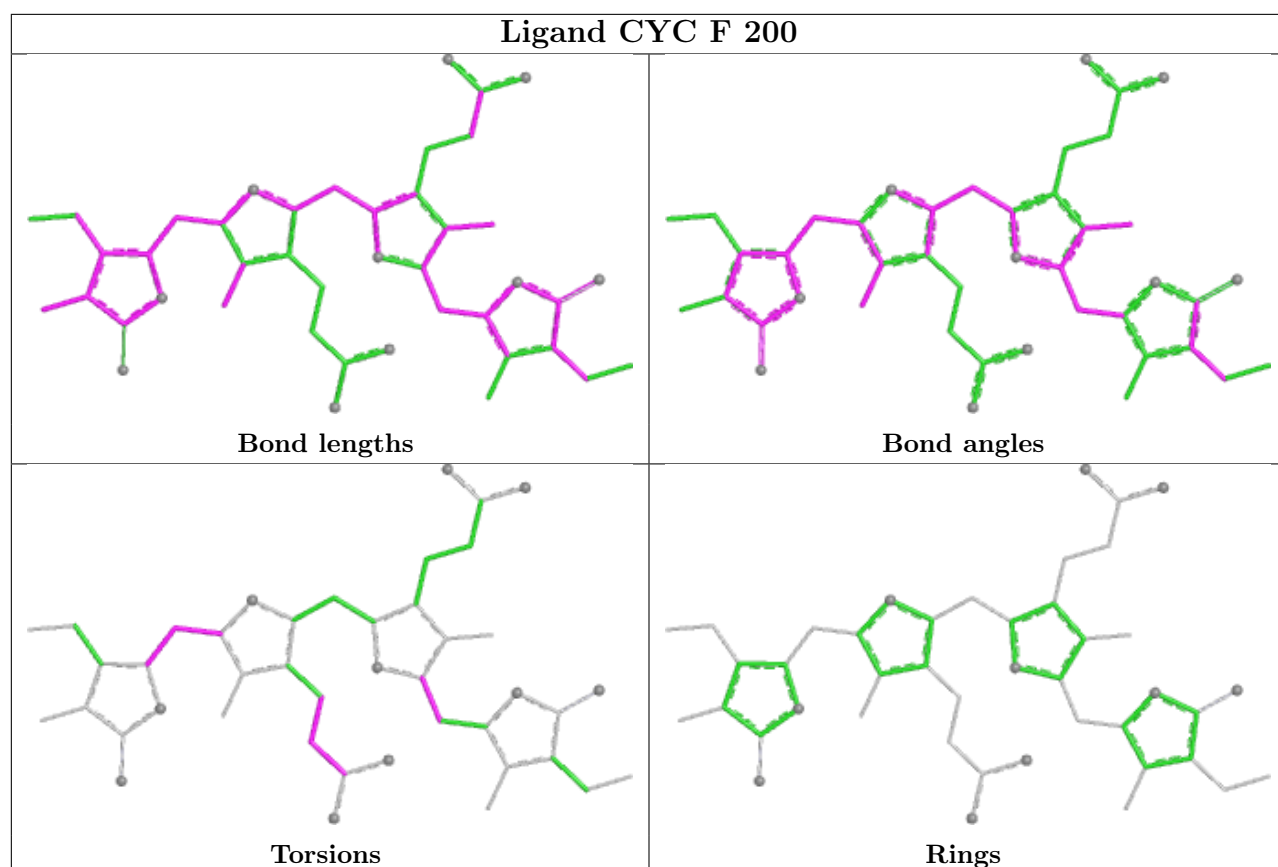


Ligand CYC 1 200

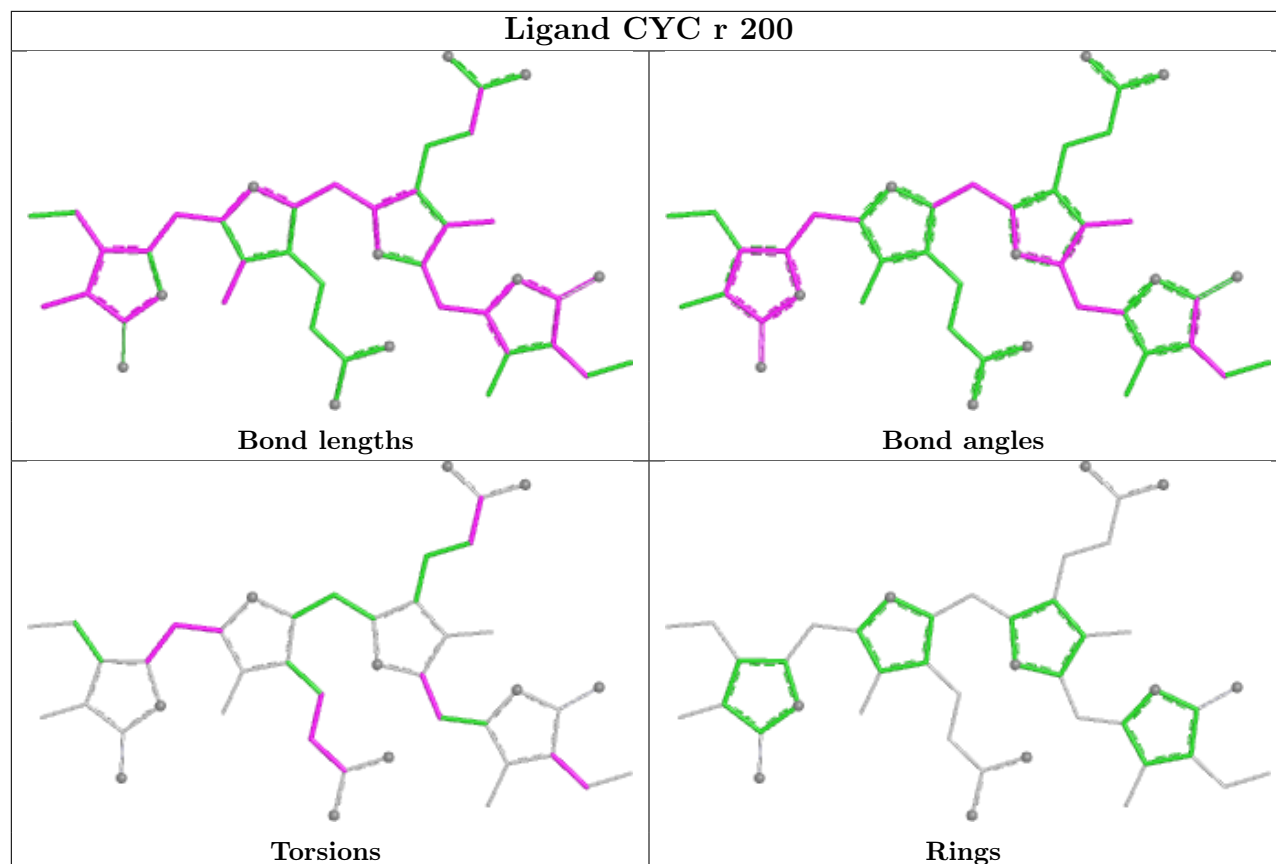


Ligand CYC V 200

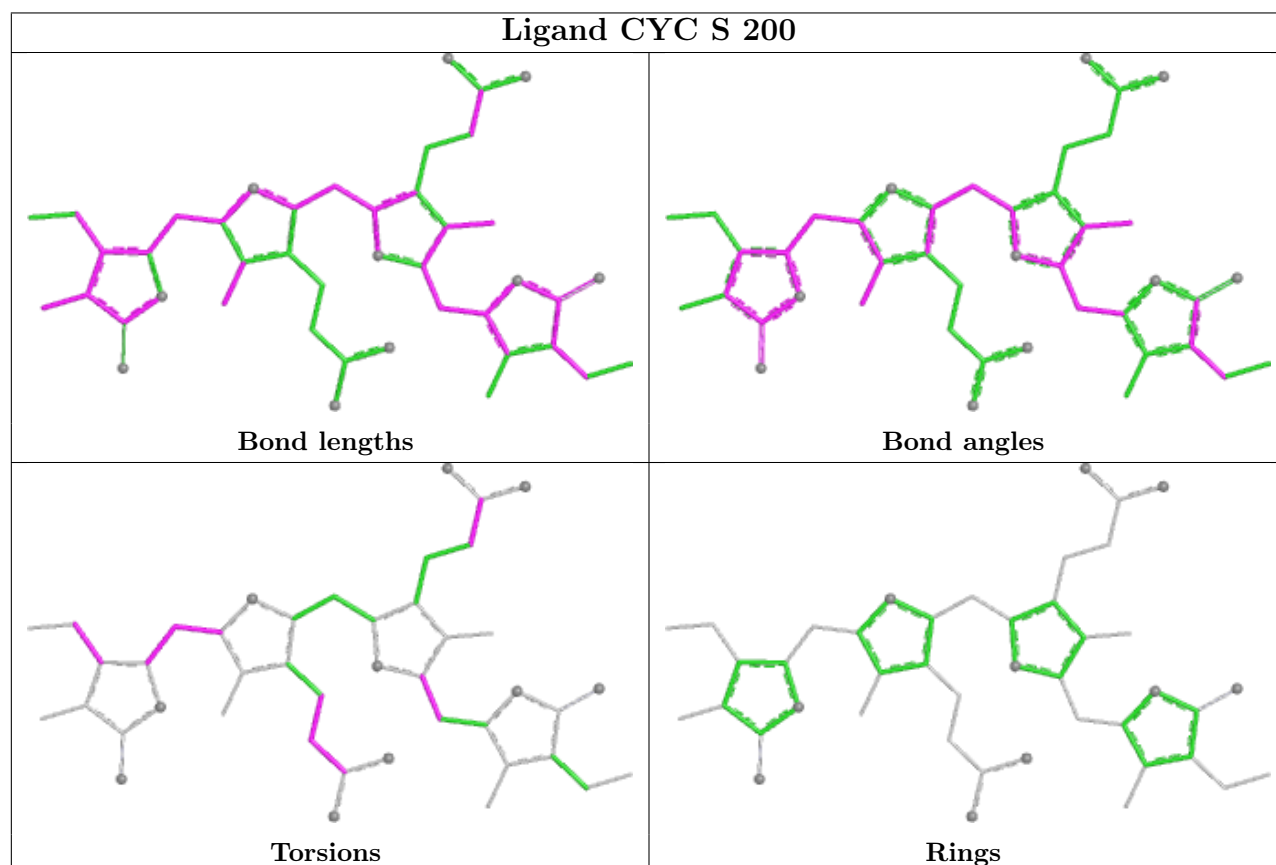


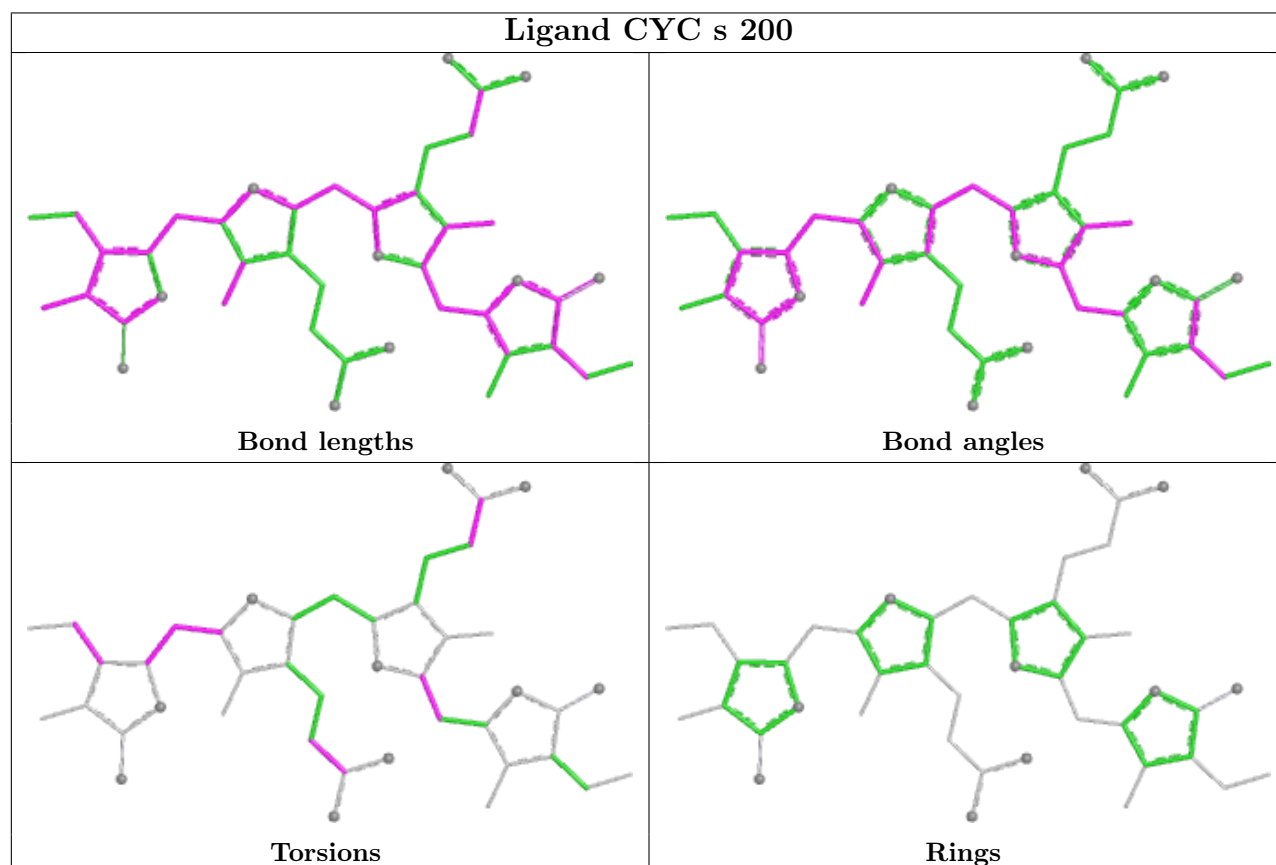
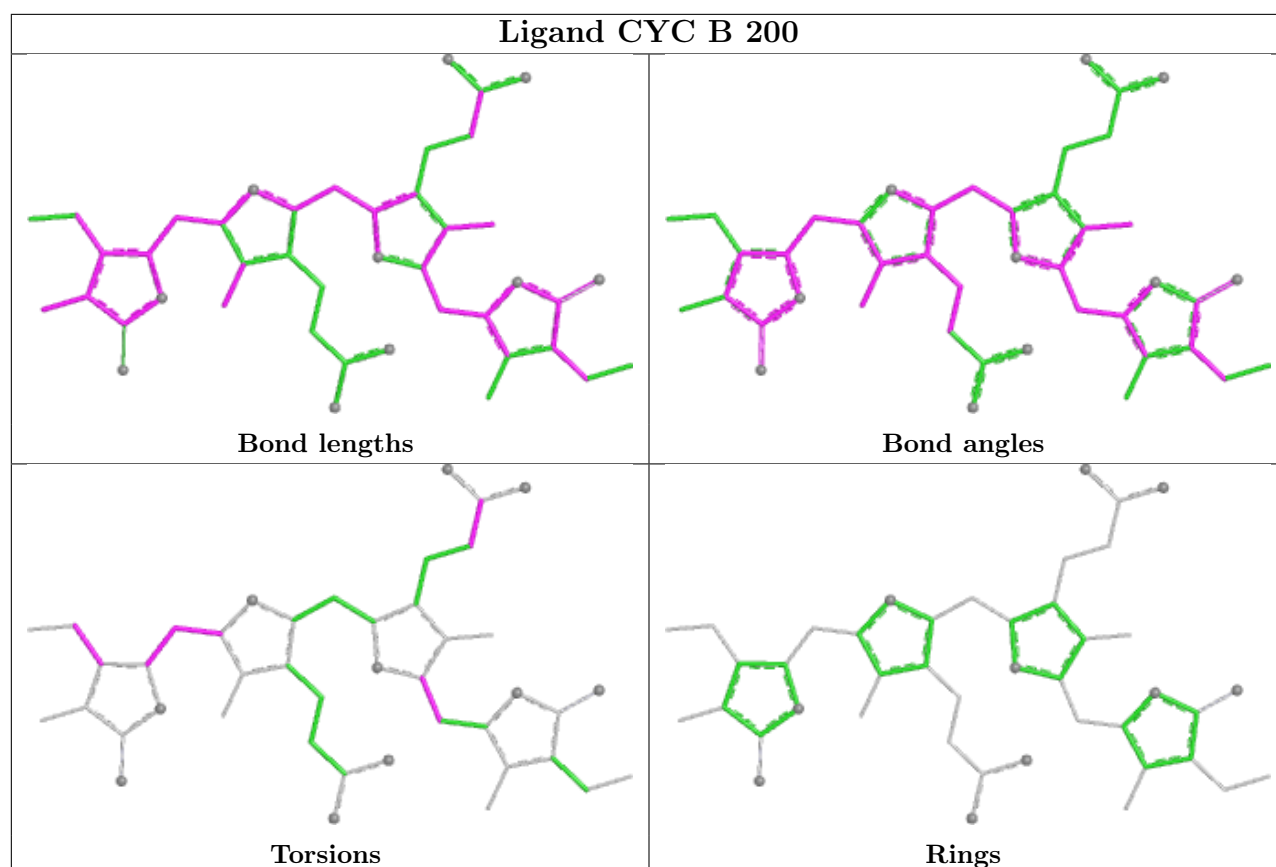


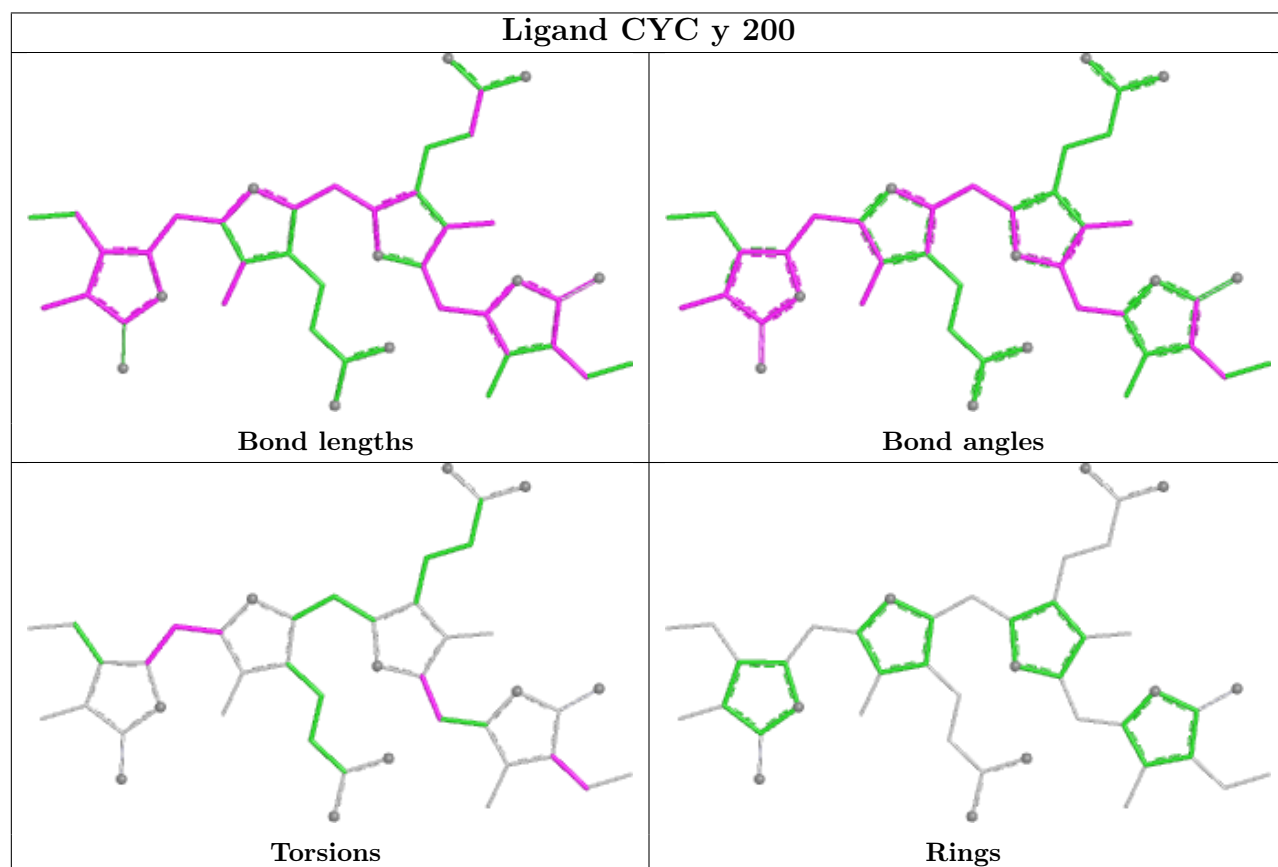
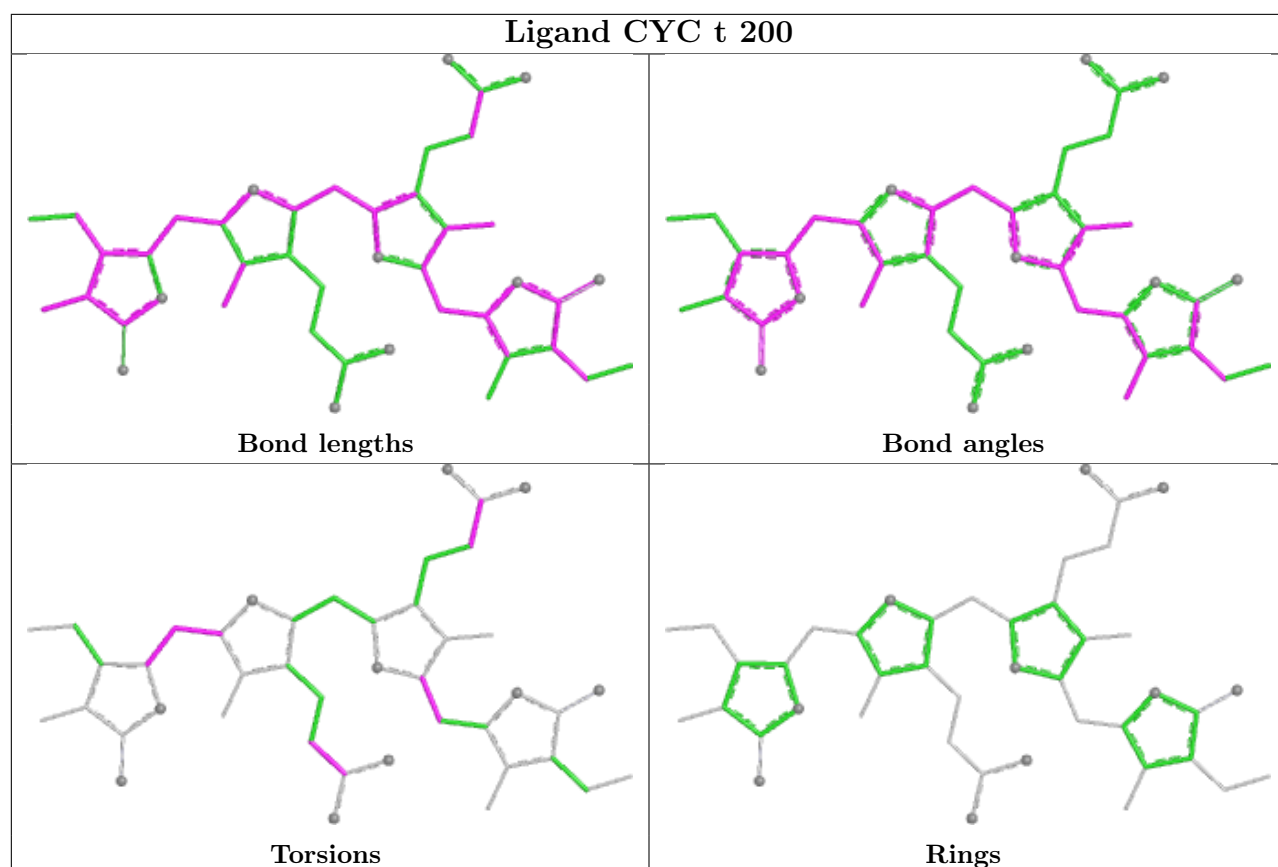
Ligand CYC r 200

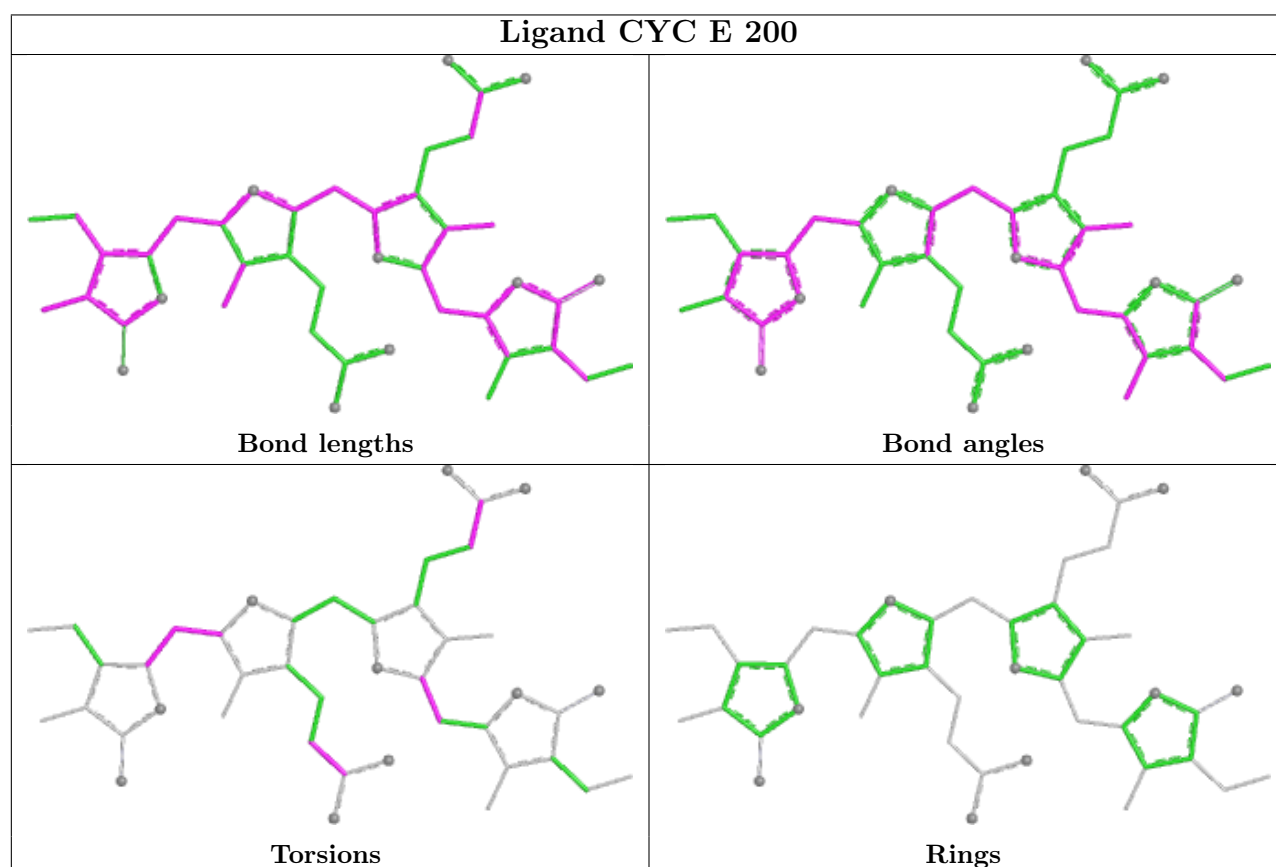
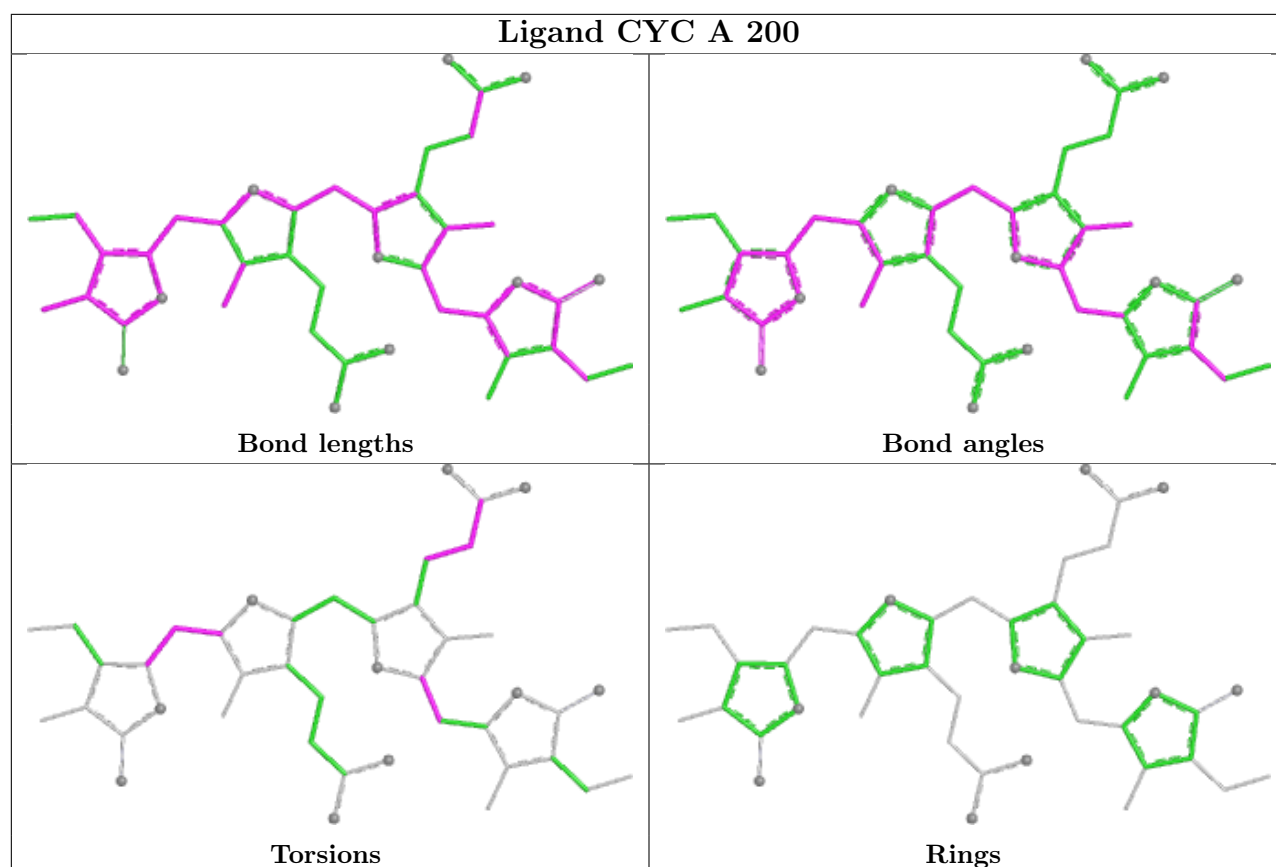


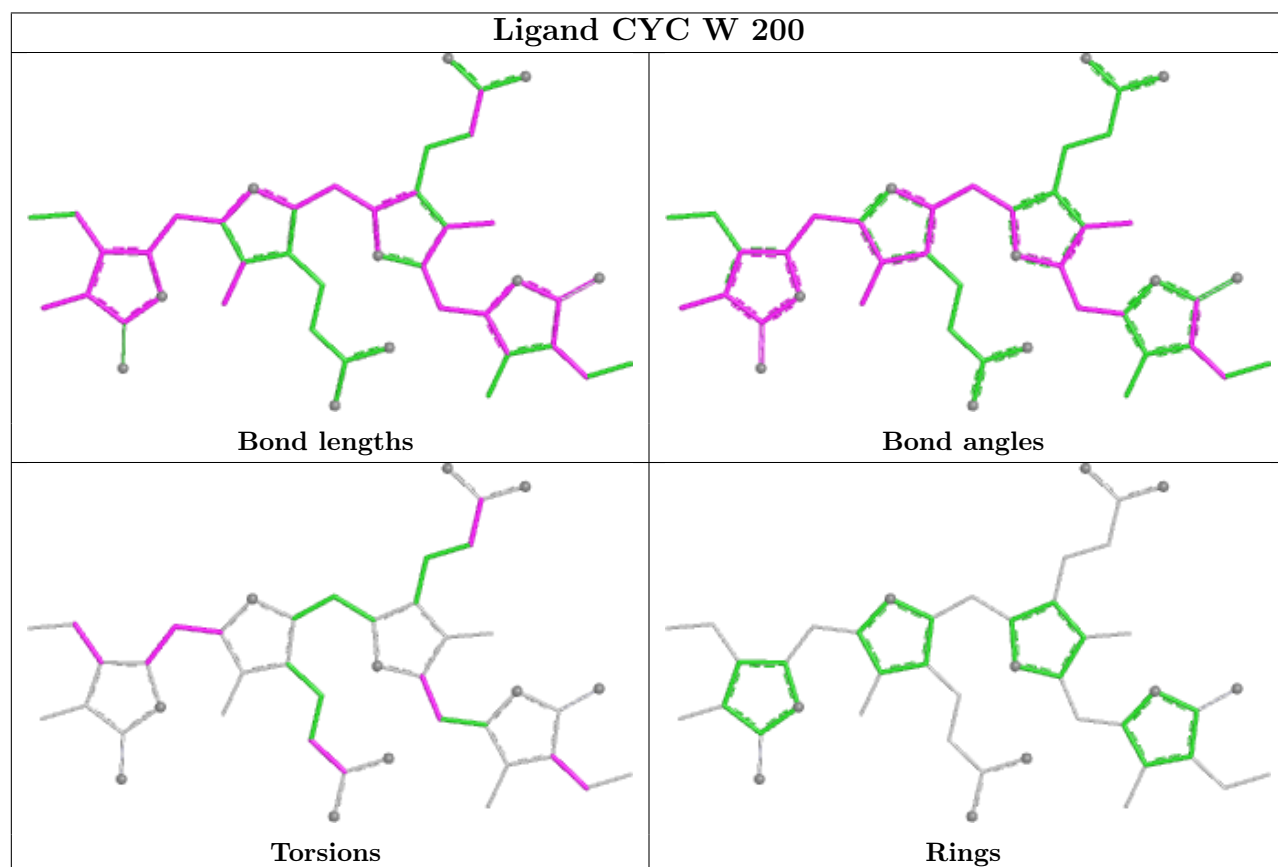
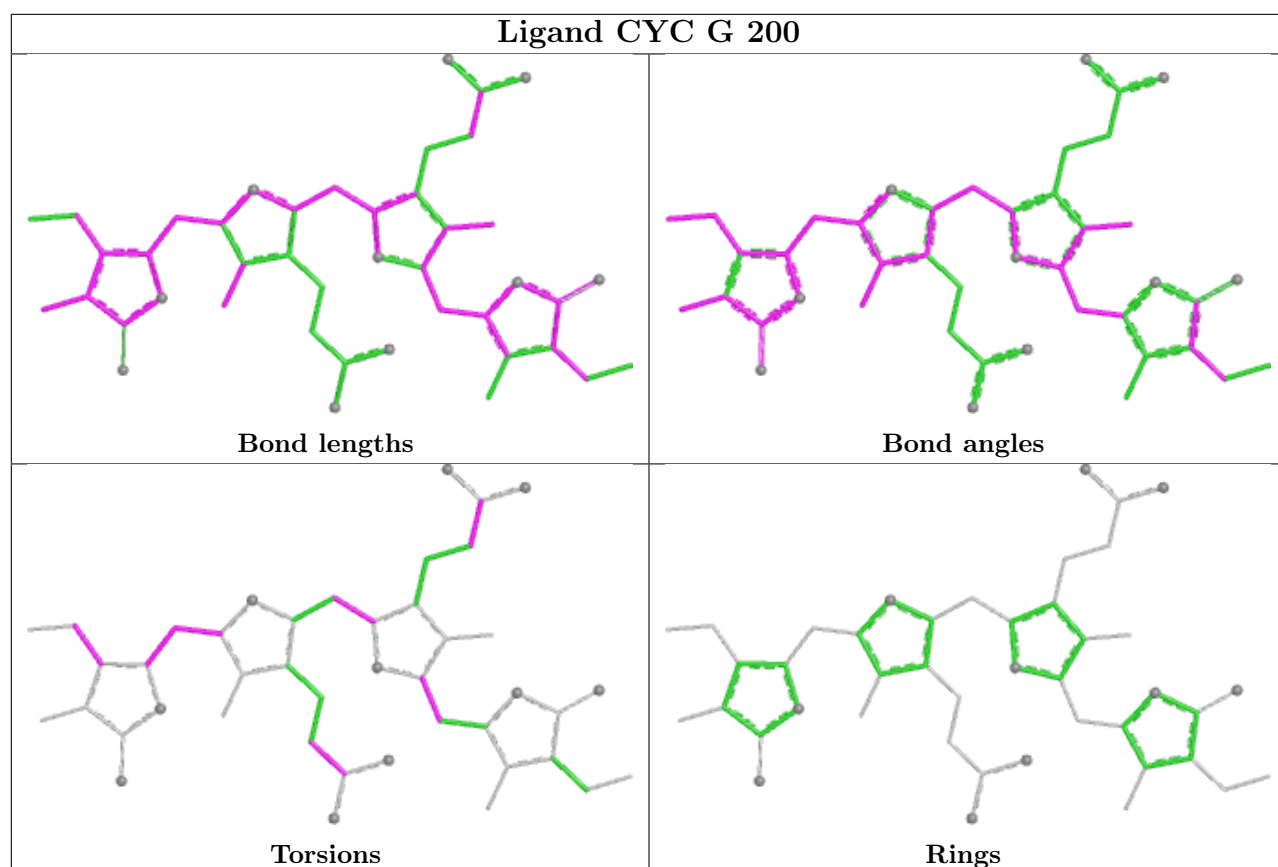
Ligand CYC S 200

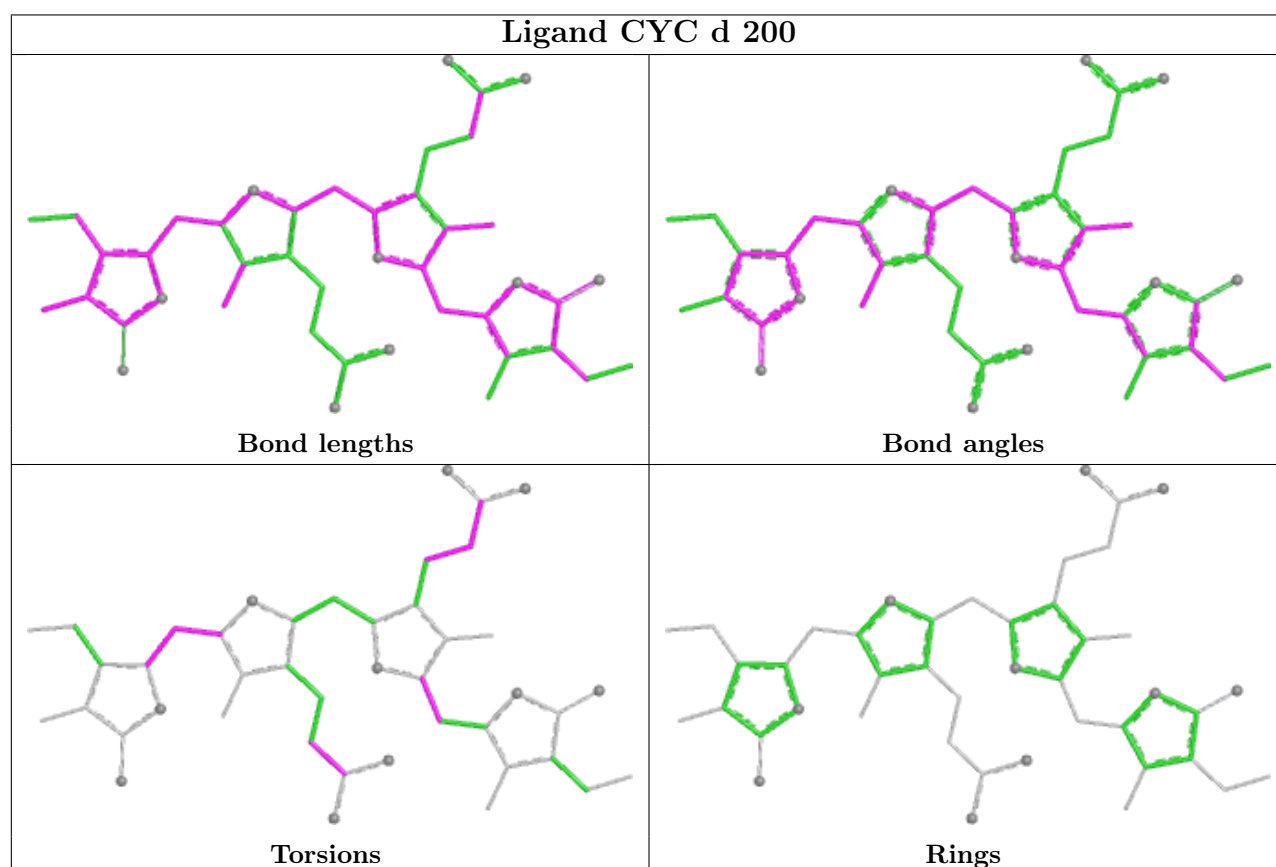
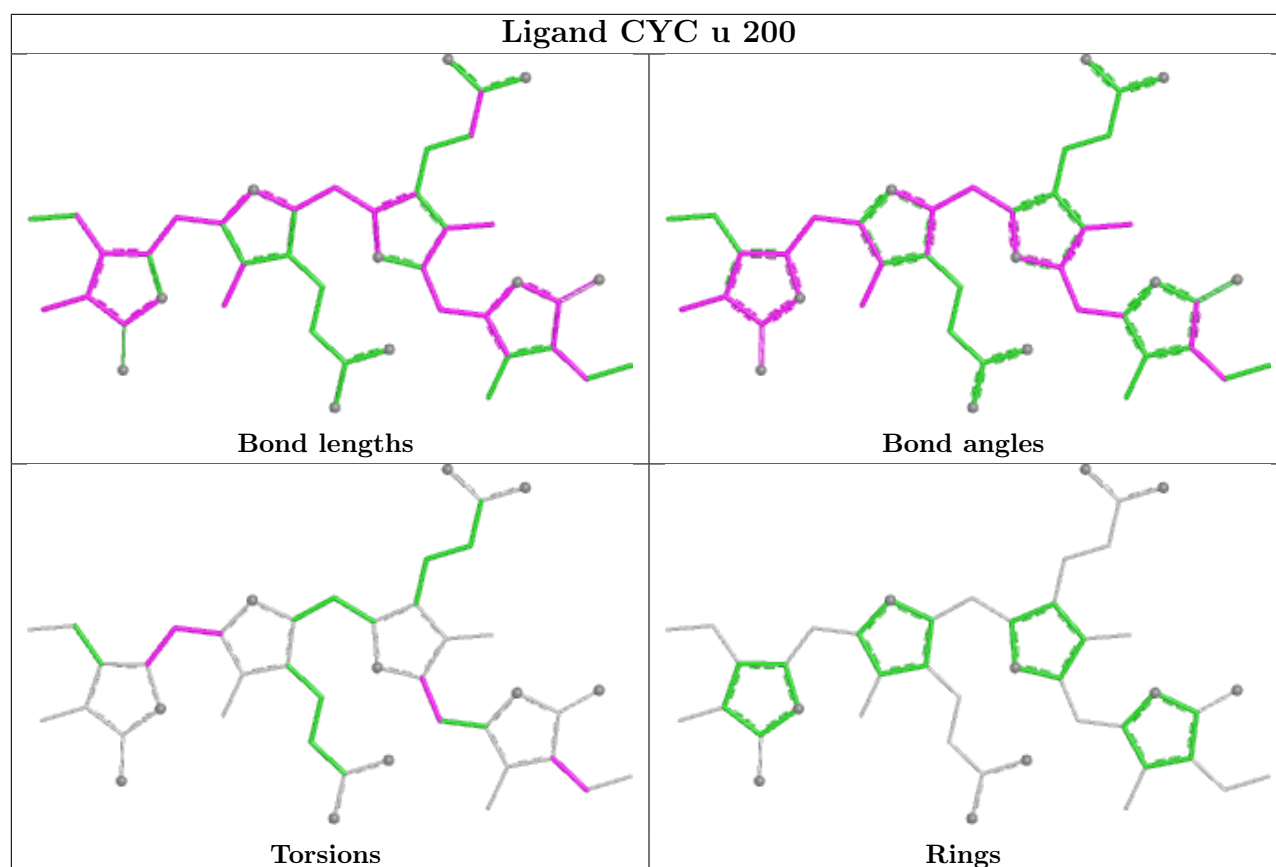


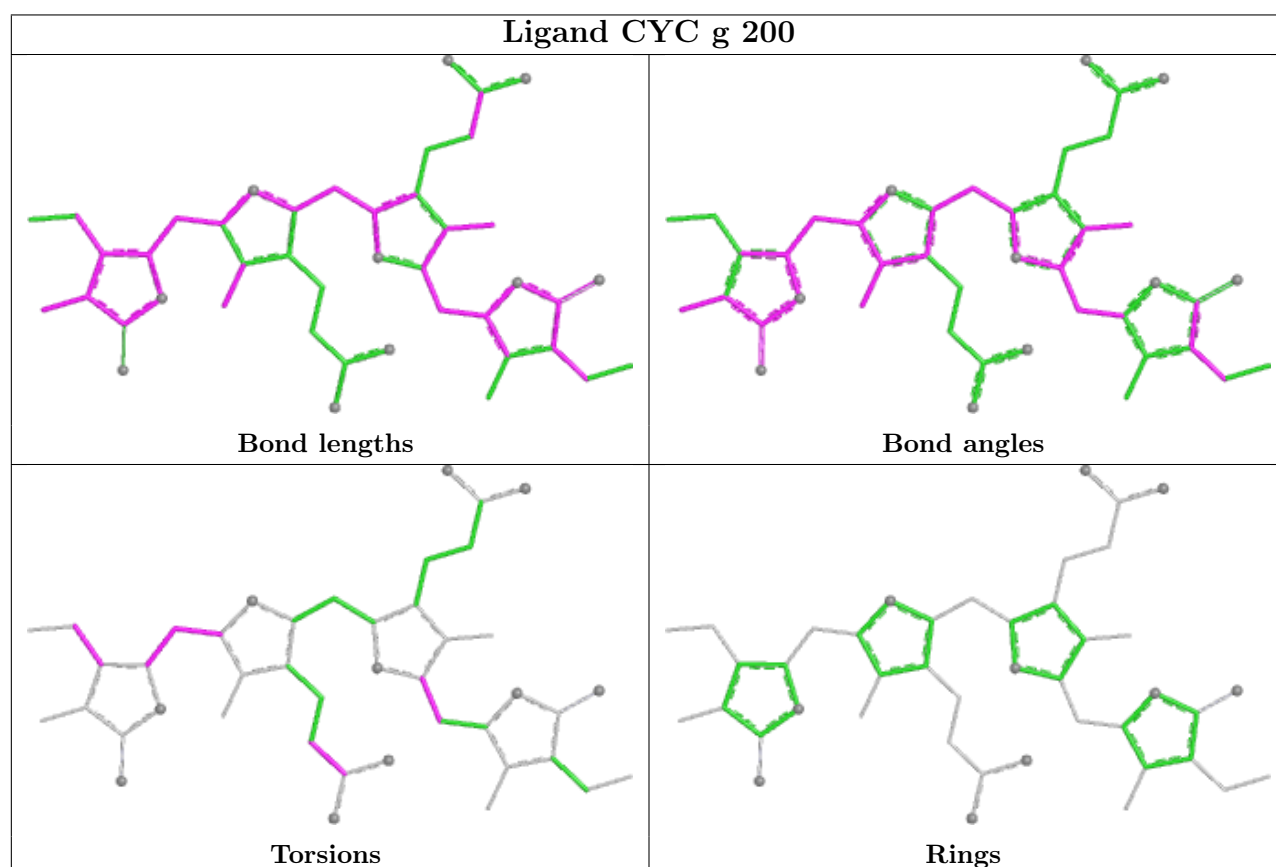
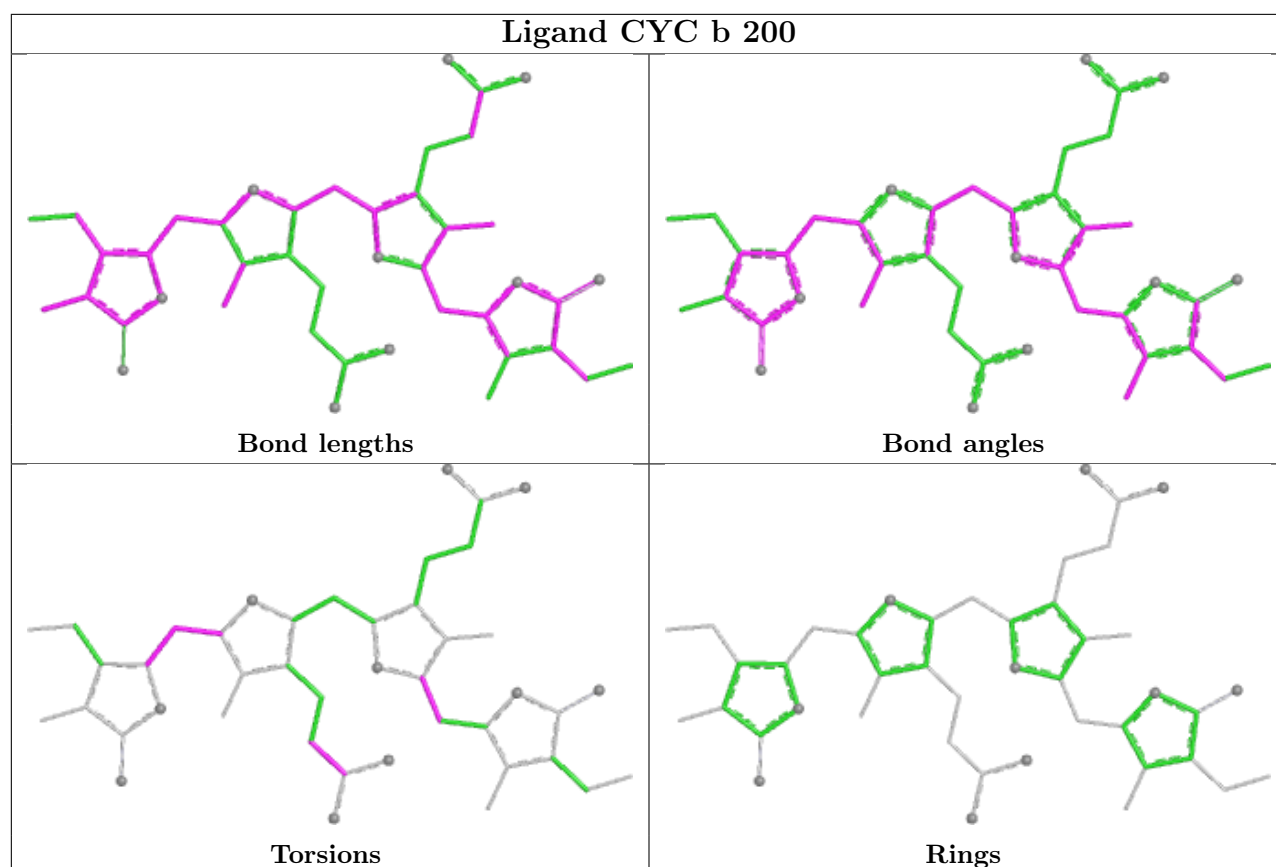


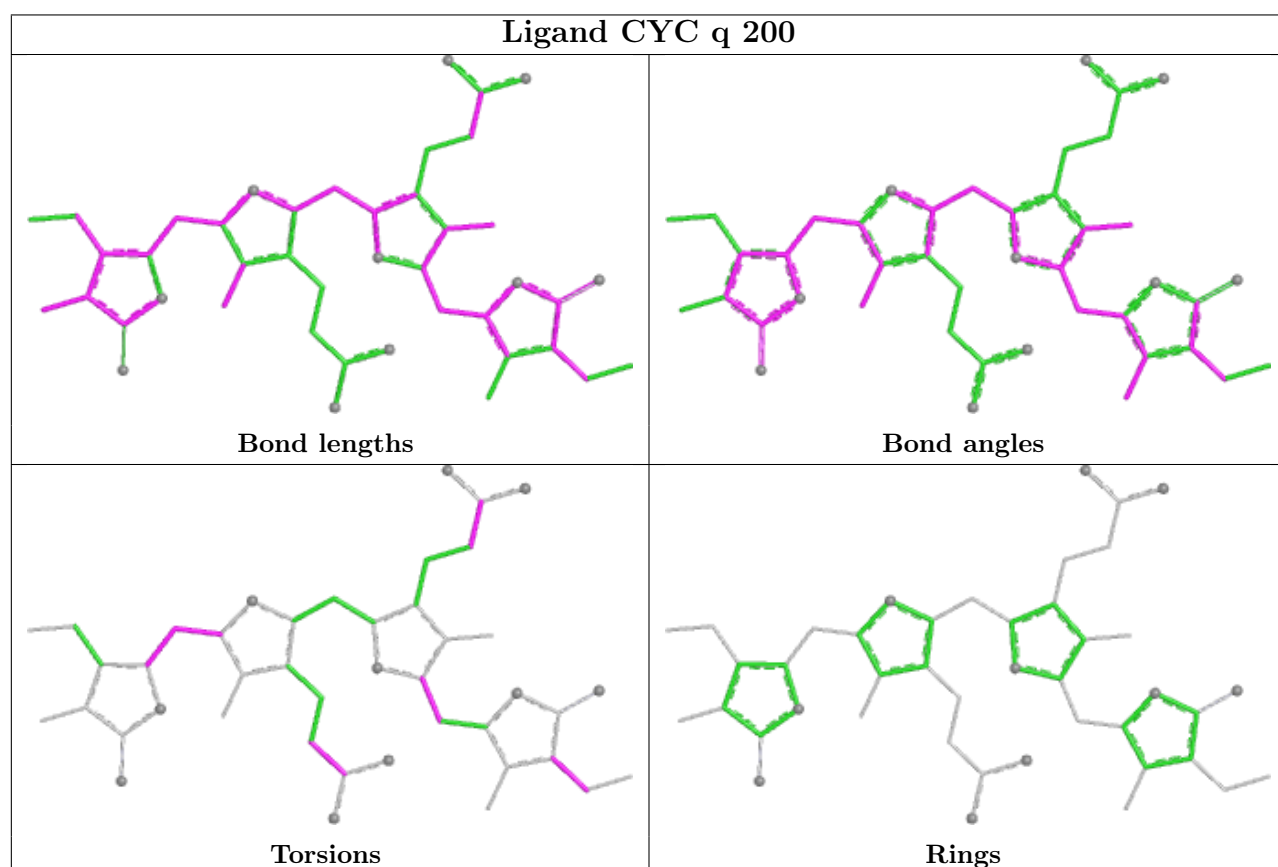
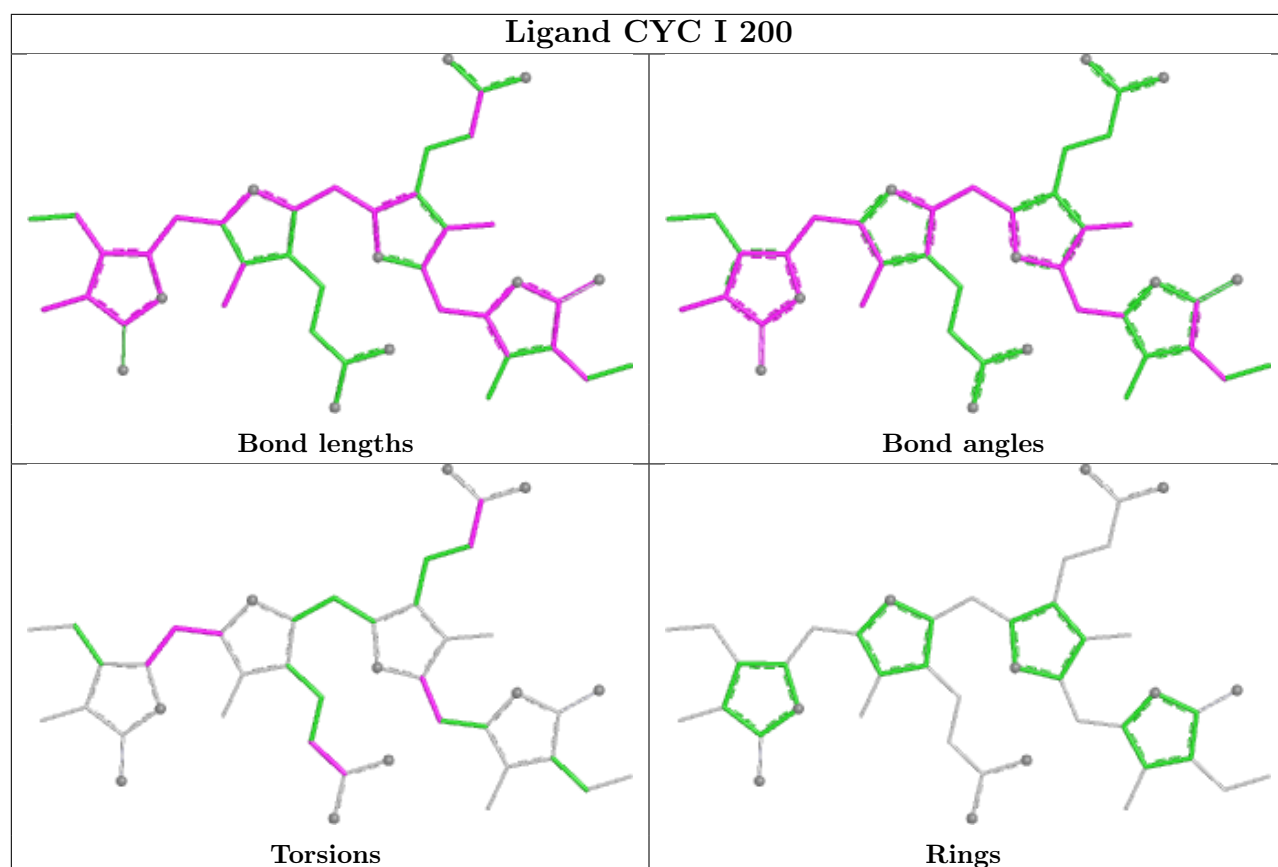


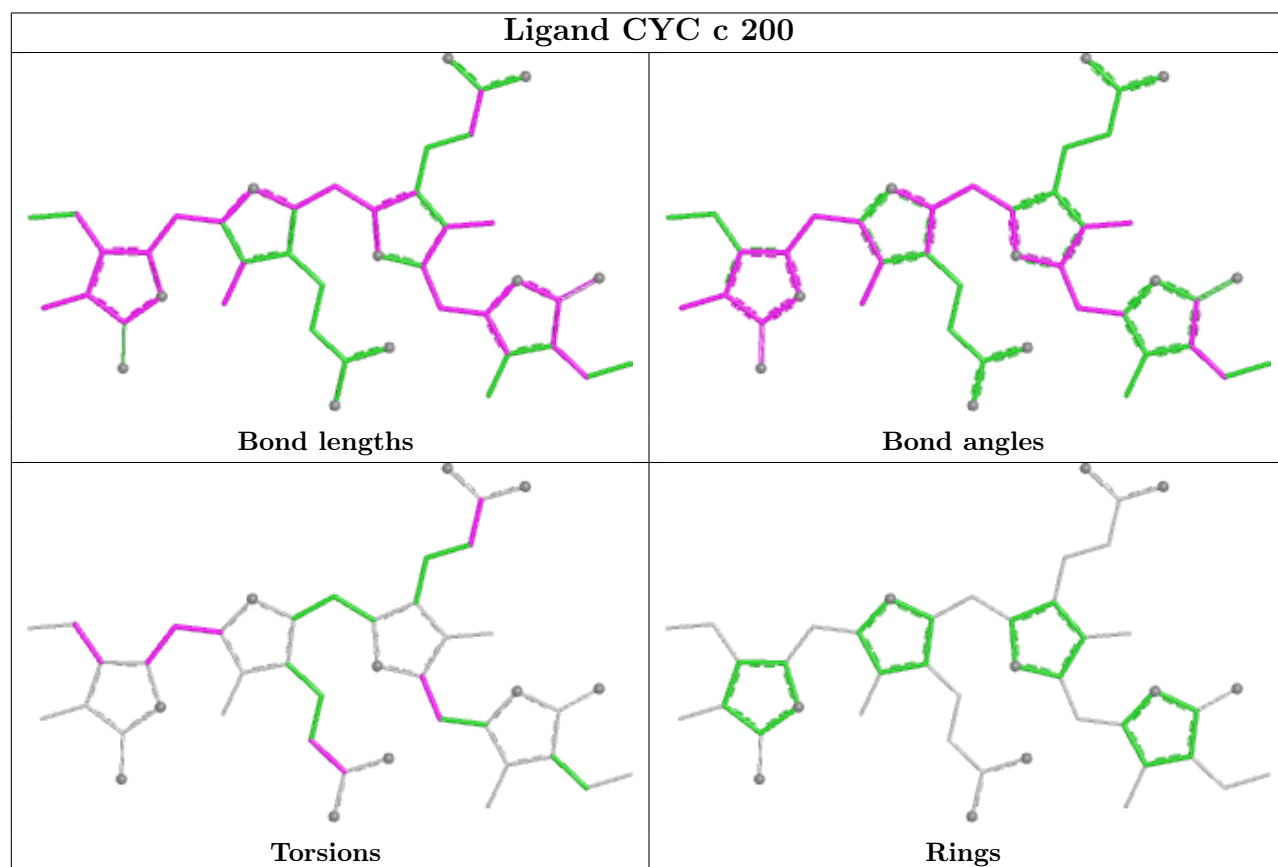
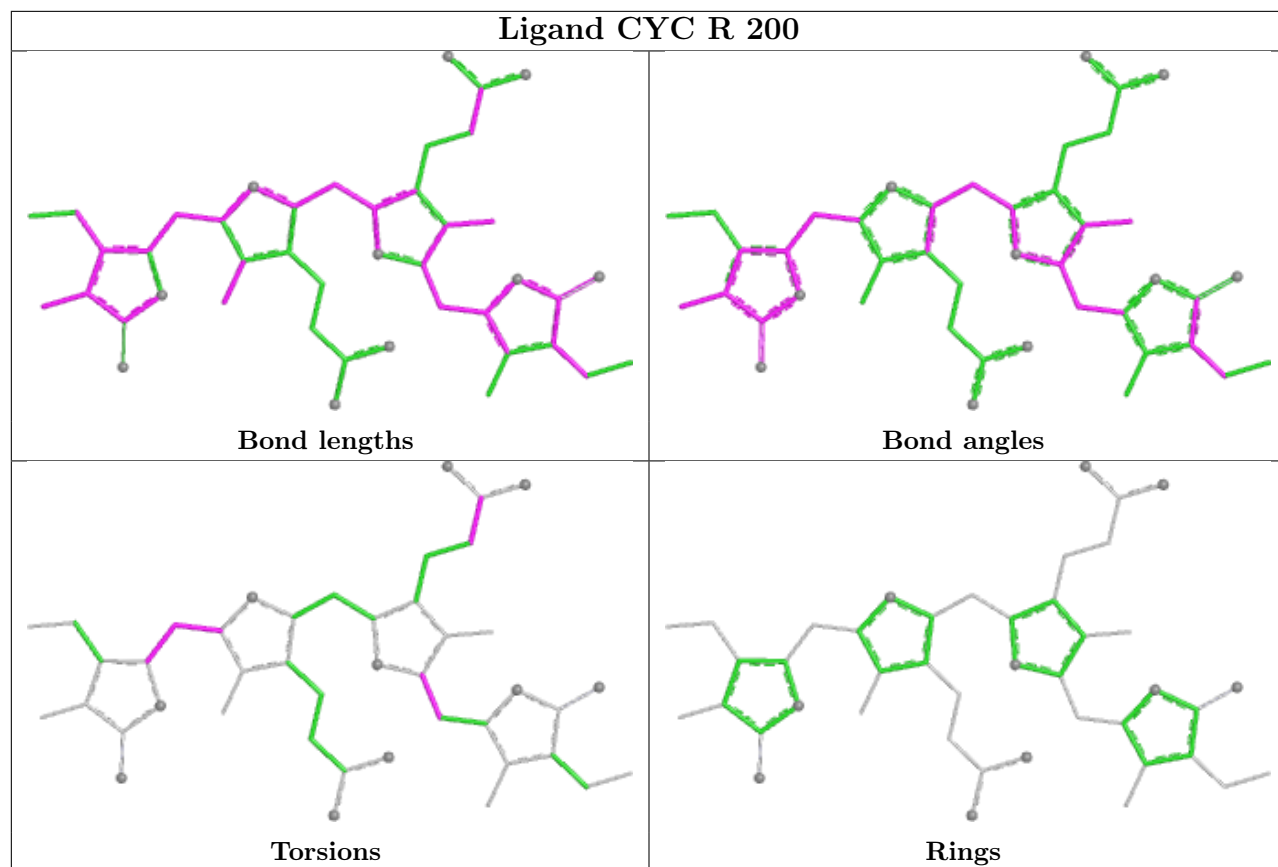




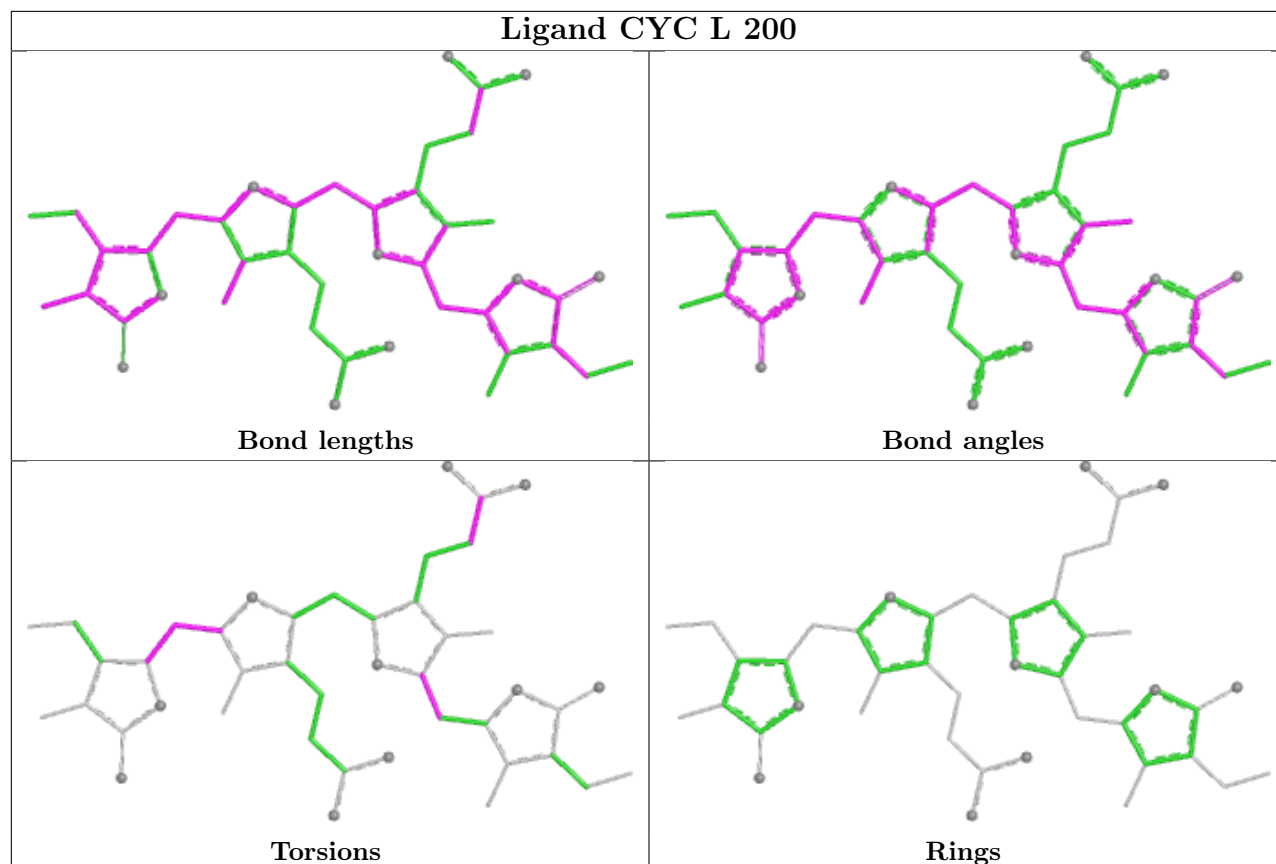




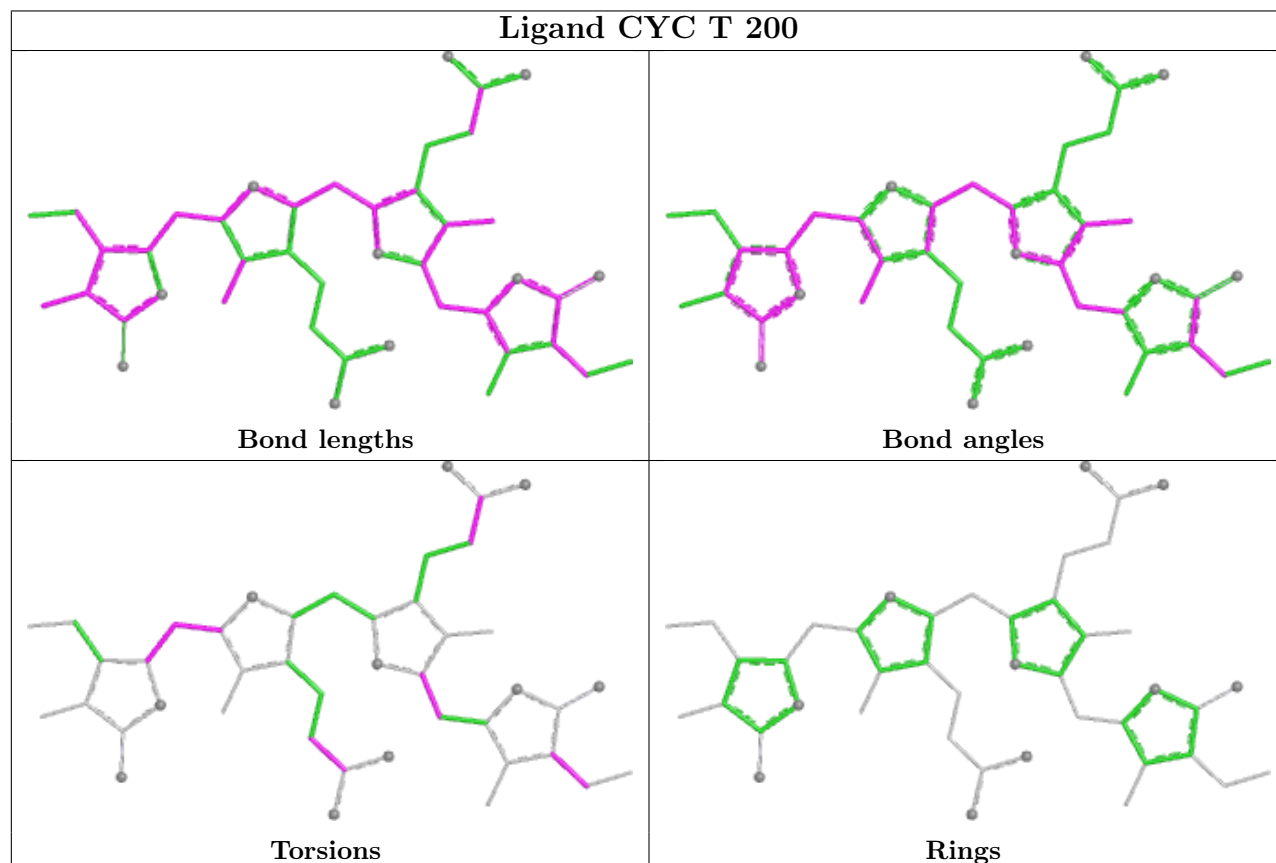


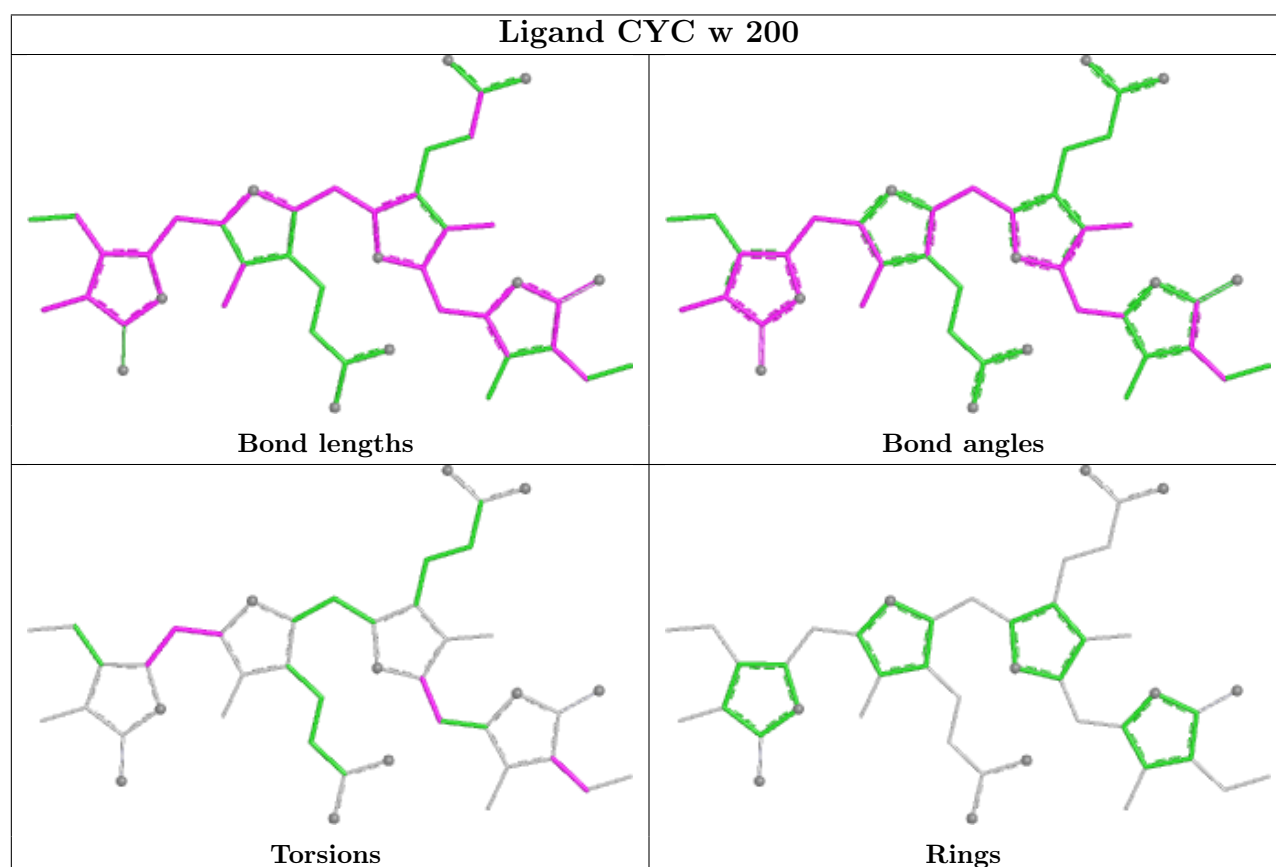
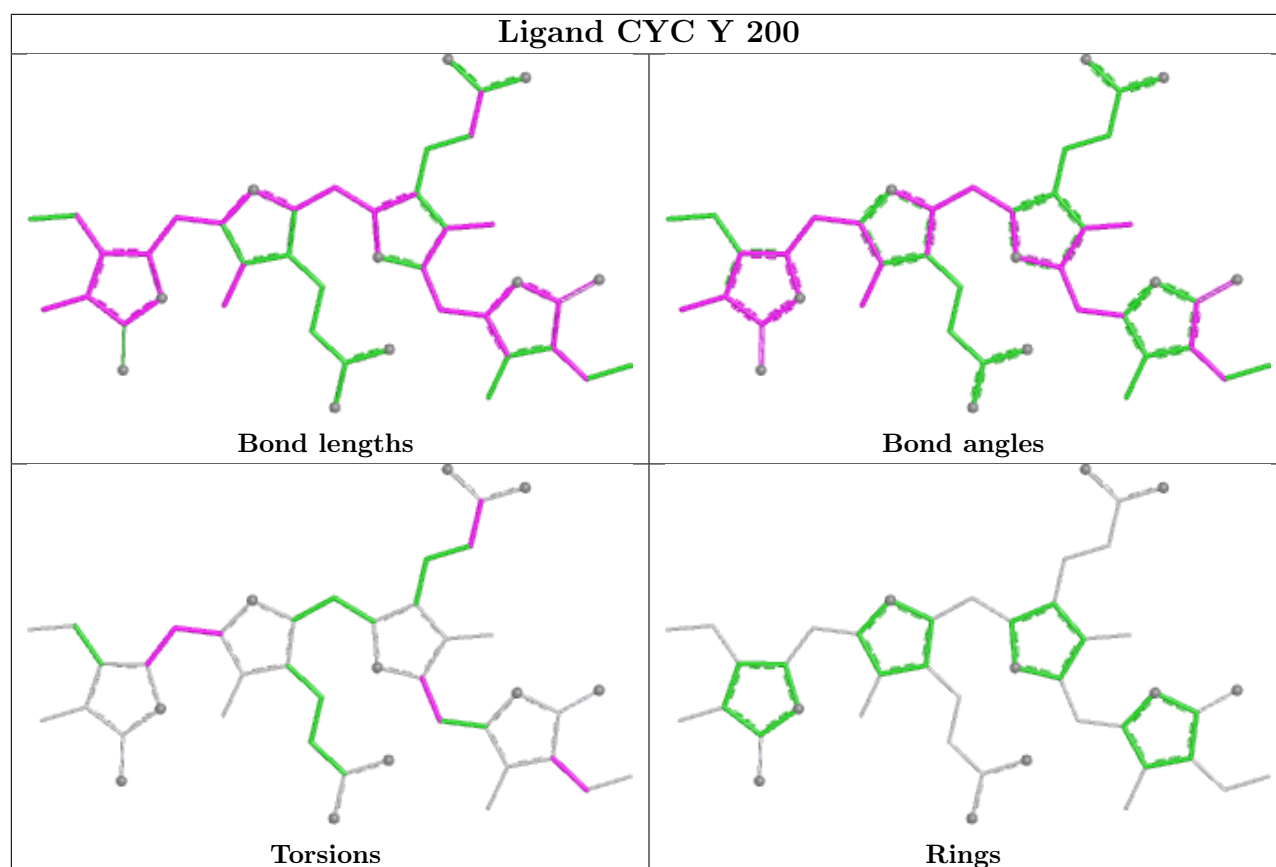


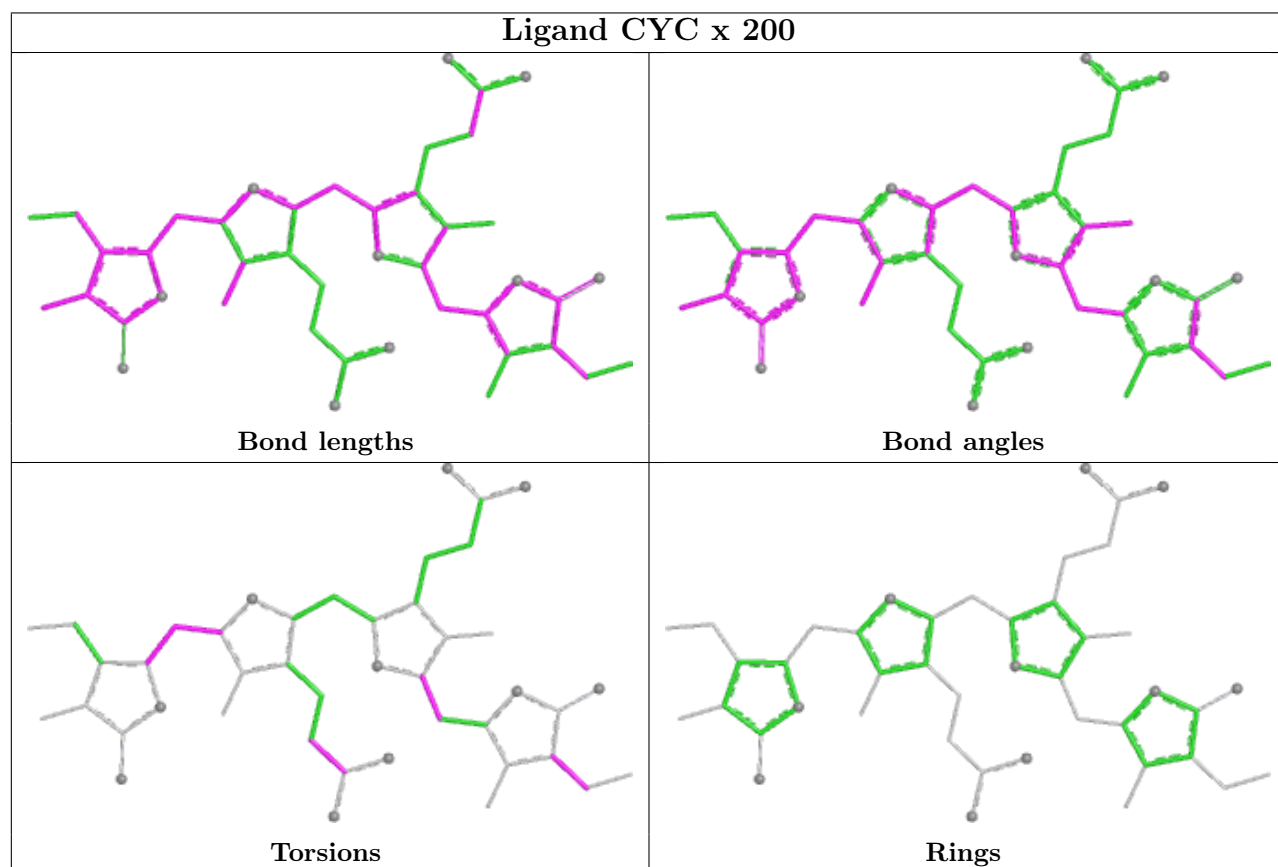
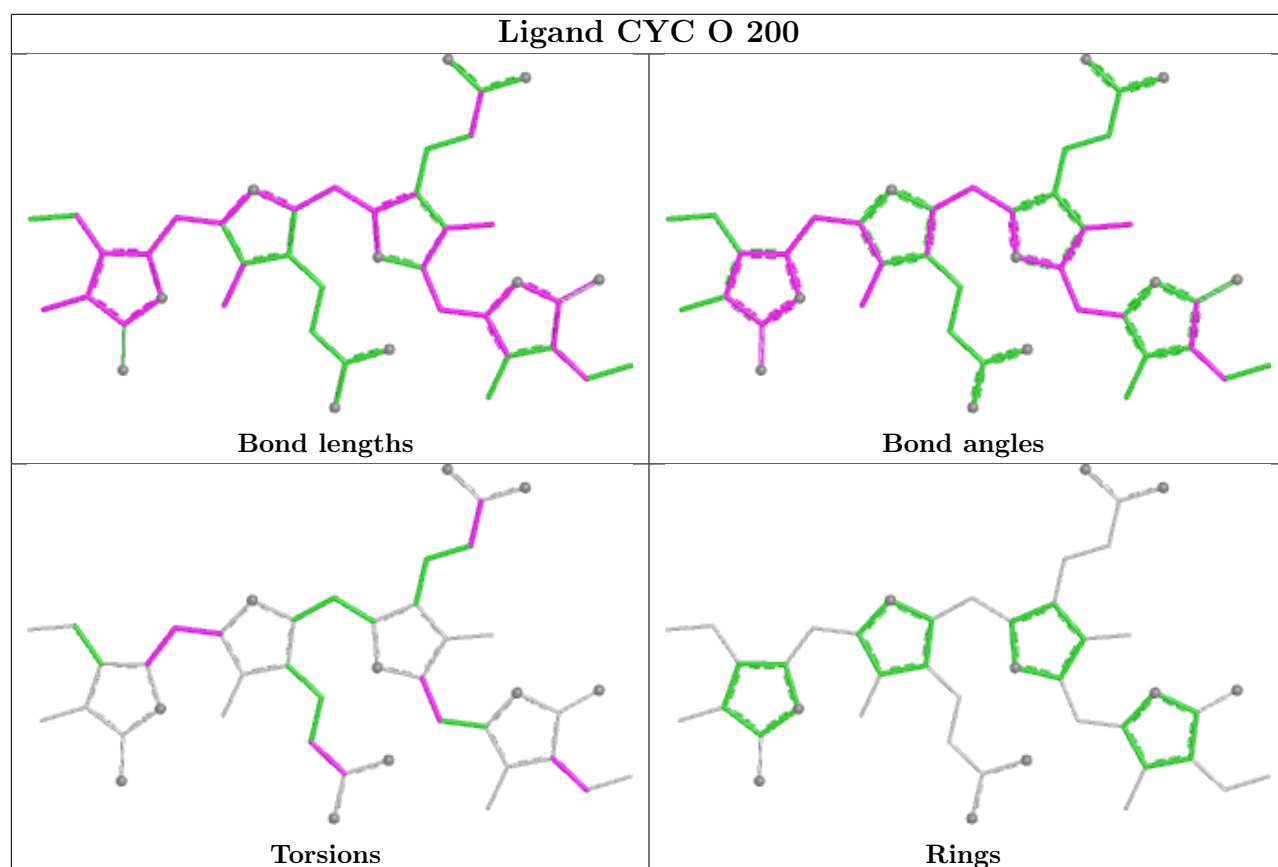
Ligand CYC L 200

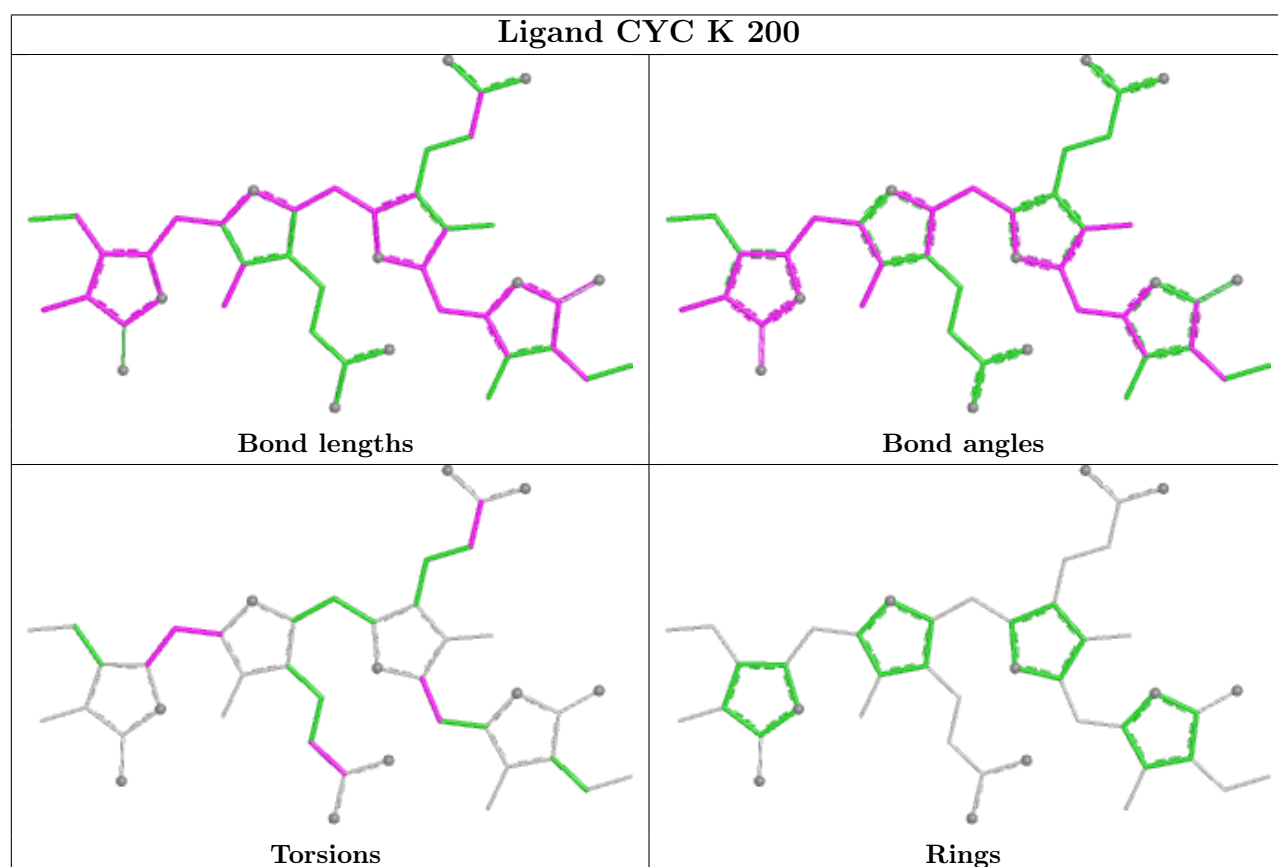
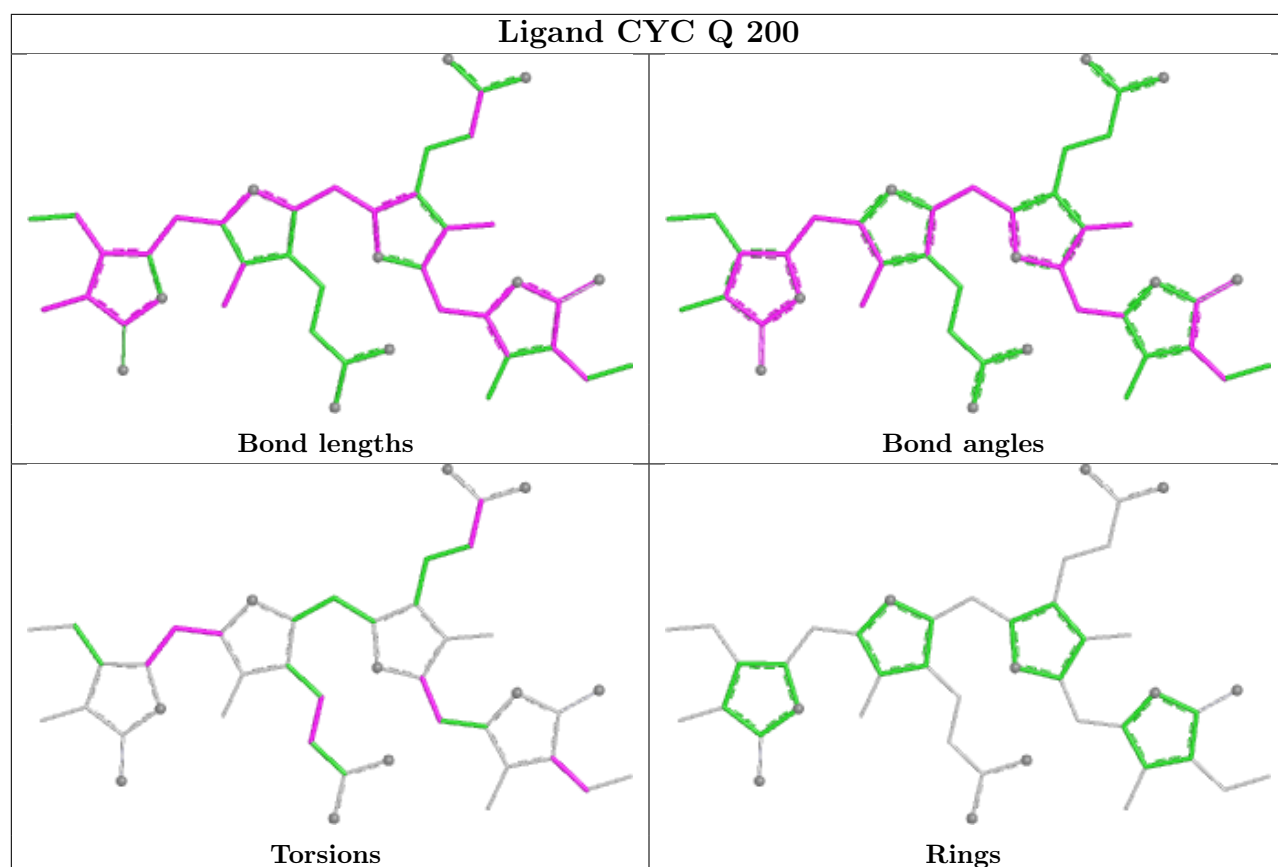


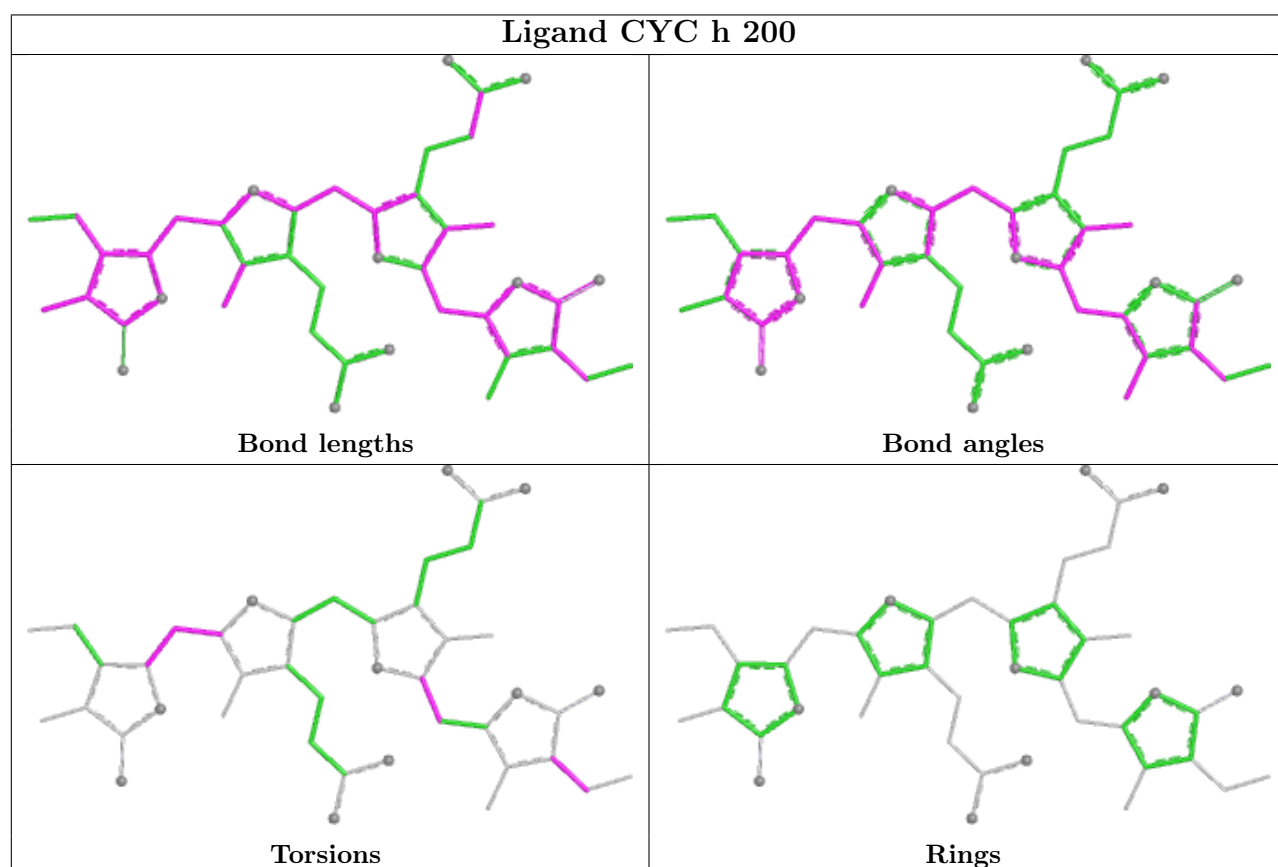
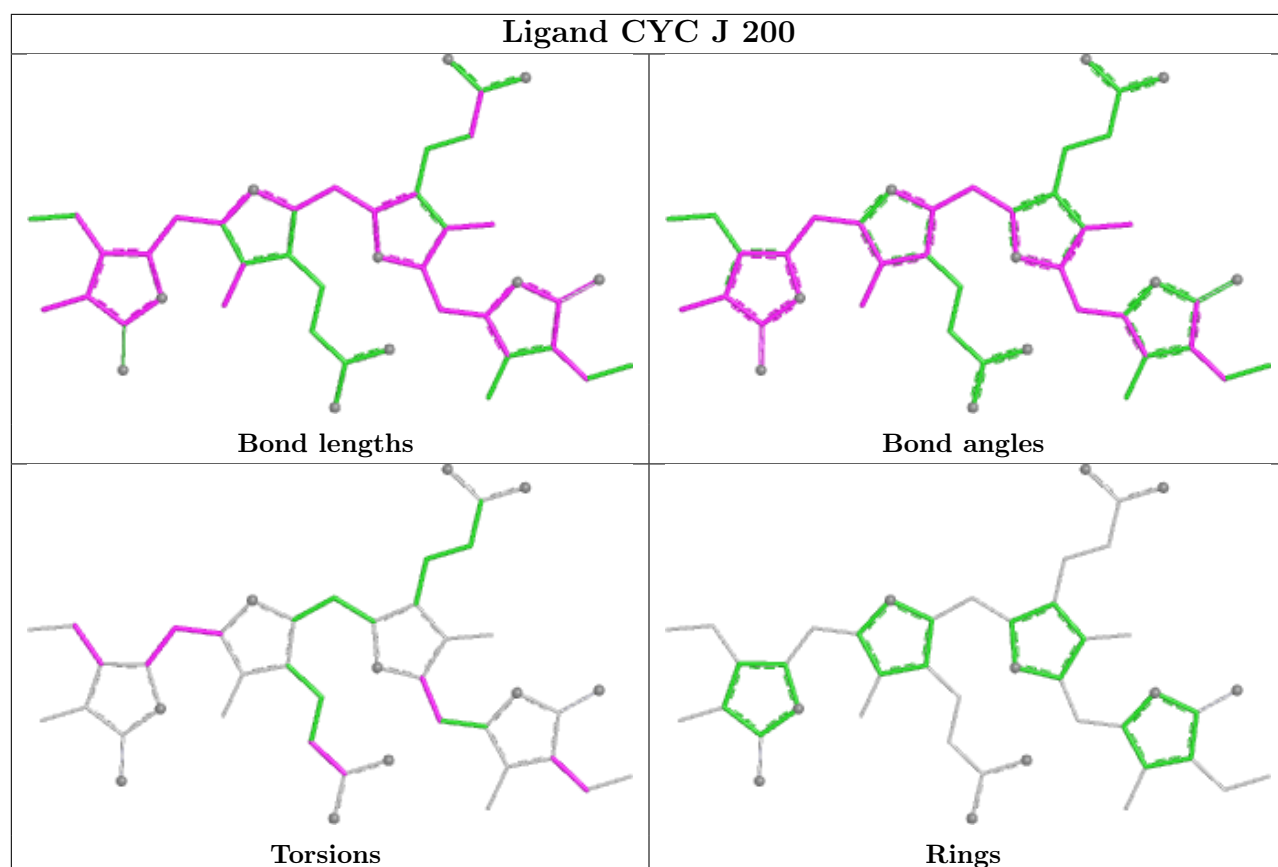
Ligand CYC T 200











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.

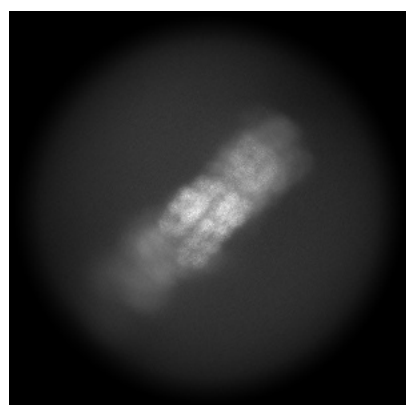
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35567. These allow visual inspection of the internal detail of the map and identification of artifacts.

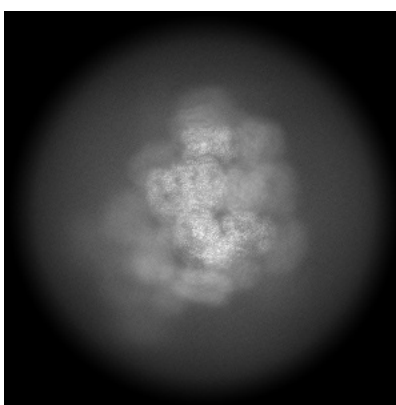
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

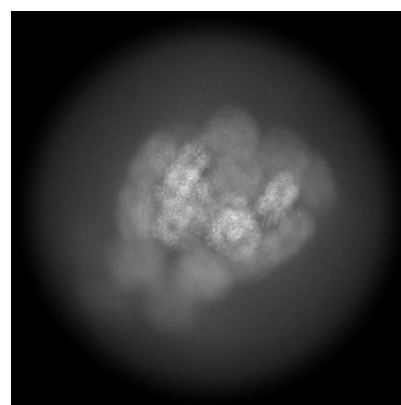
6.1.1 Primary map



X



Y

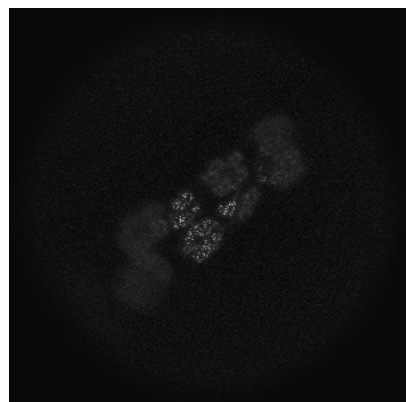


Z

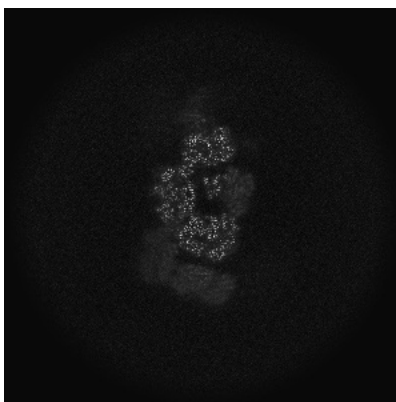
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

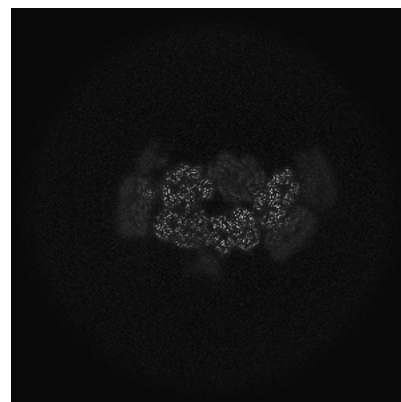
6.2.1 Primary map



X Index: 340



Y Index: 340

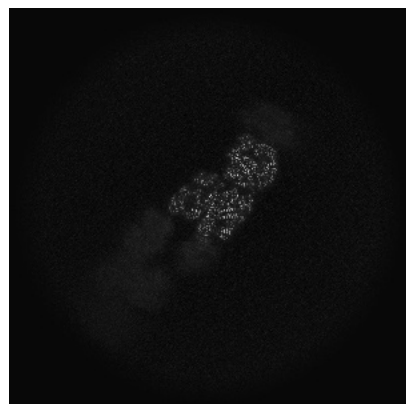


Z Index: 340

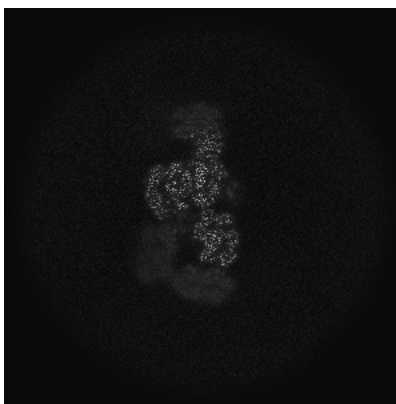
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

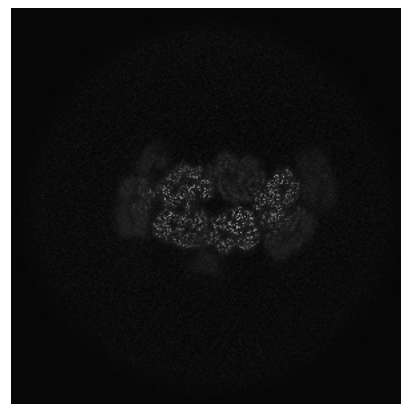
6.3.1 Primary map



X Index: 300



Y Index: 320

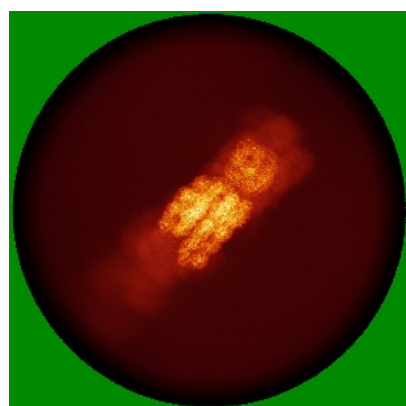


Z Index: 341

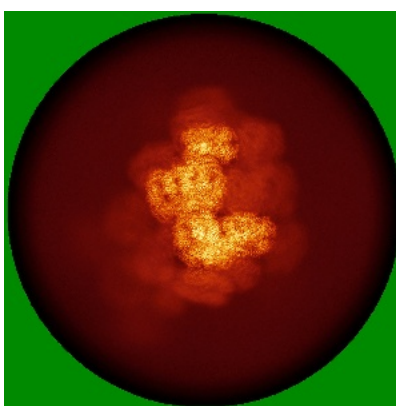
The images above show the largest variance slices of the map in three orthogonal directions.

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

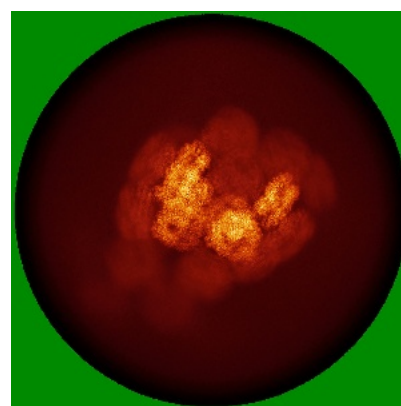
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

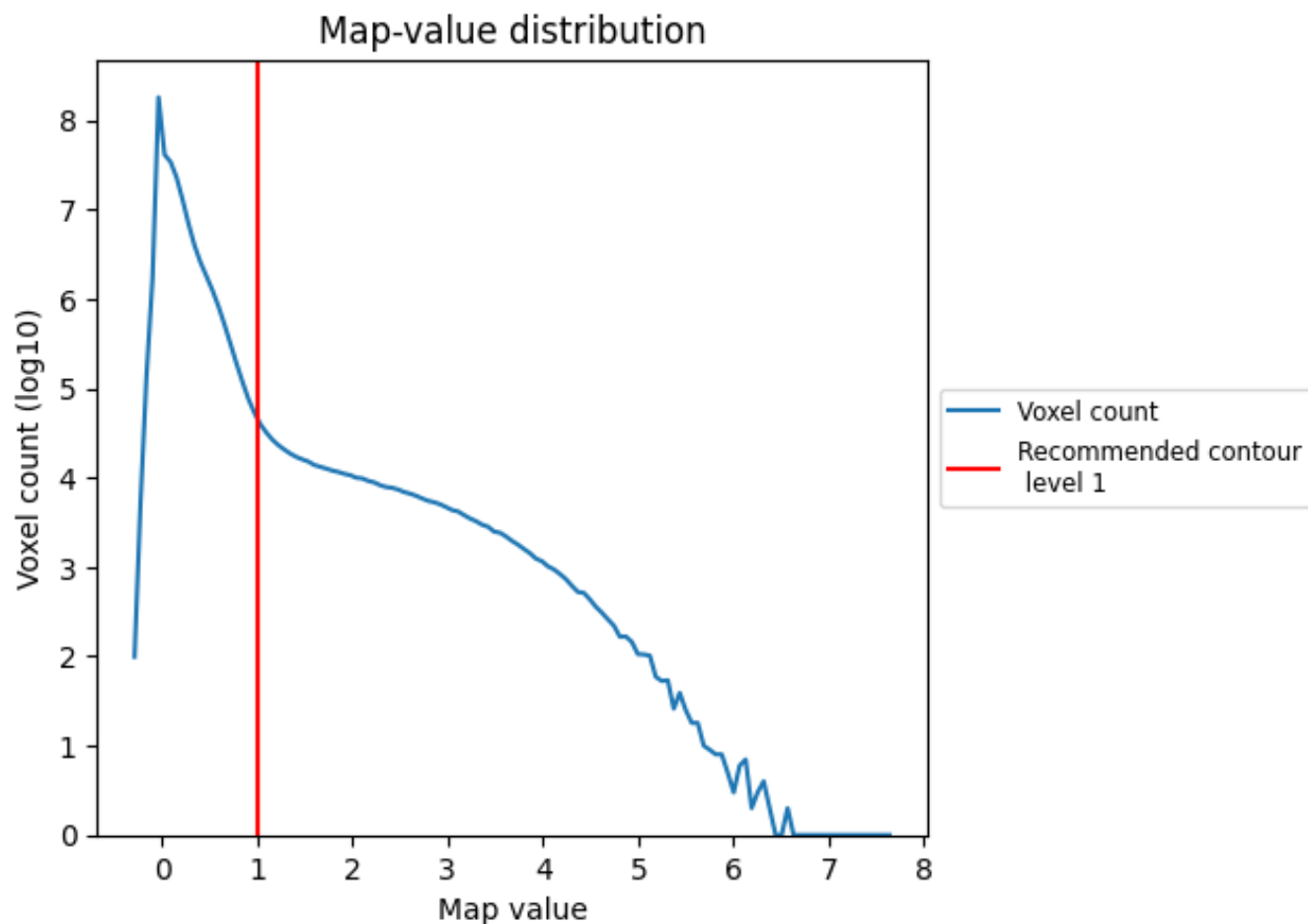
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

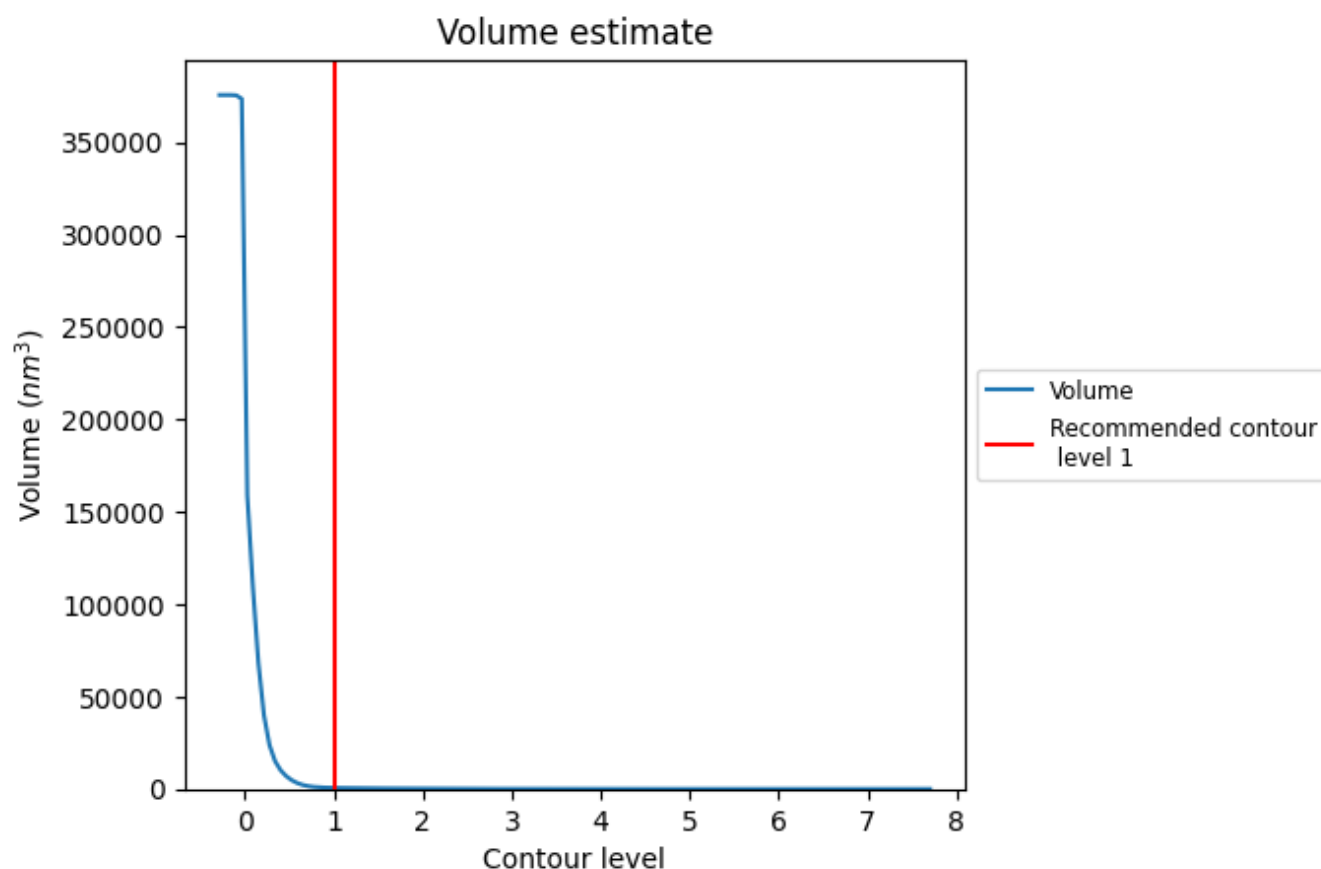
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

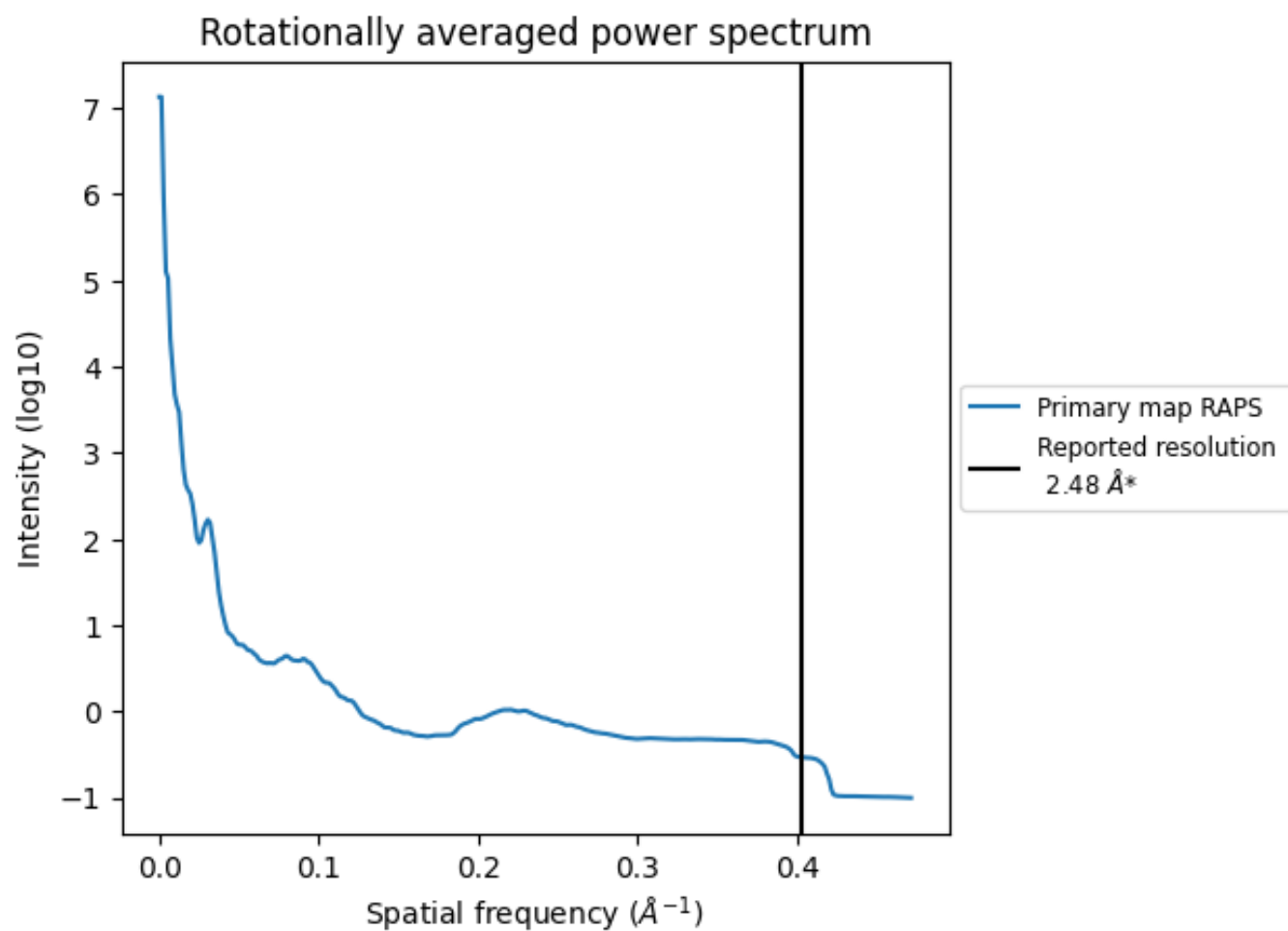
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 584 nm^3 ; this corresponds to an approximate mass of 528 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 0.403 Å⁻¹

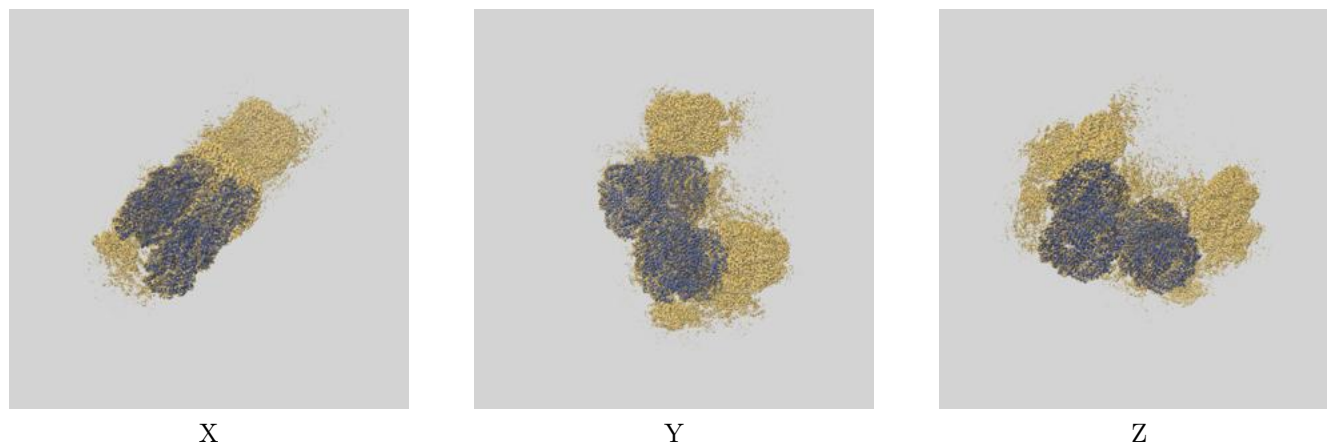
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

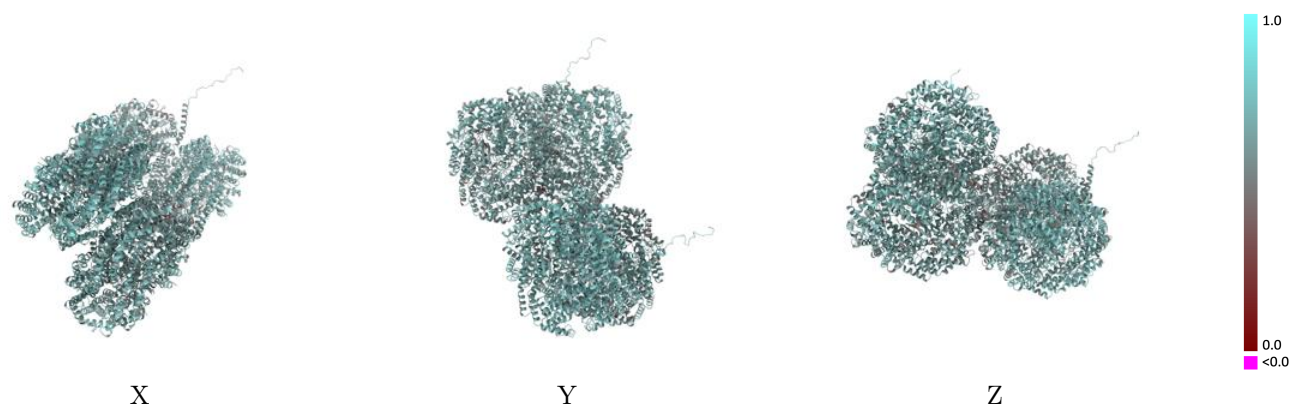
This section contains information regarding the fit between EMDB map EMD-35567 and PDB model 8IMK. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



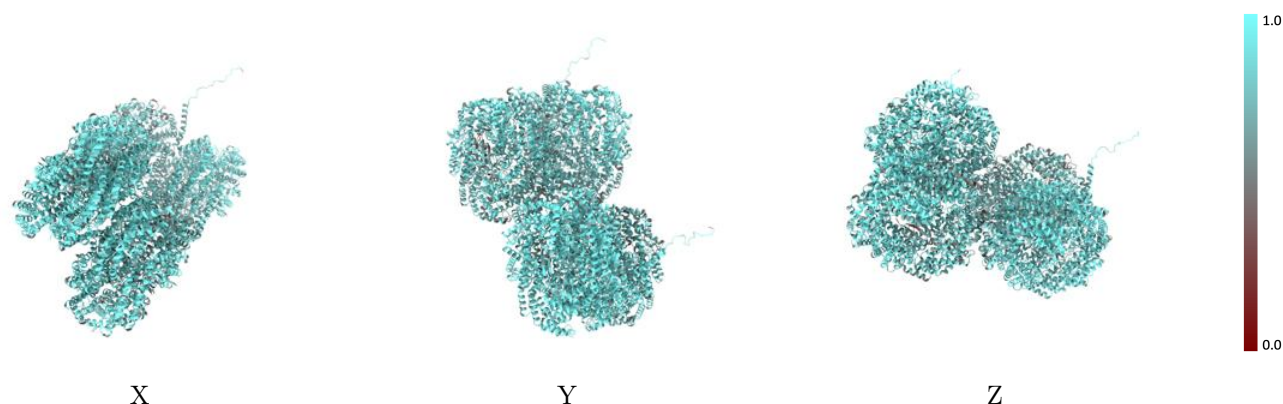
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



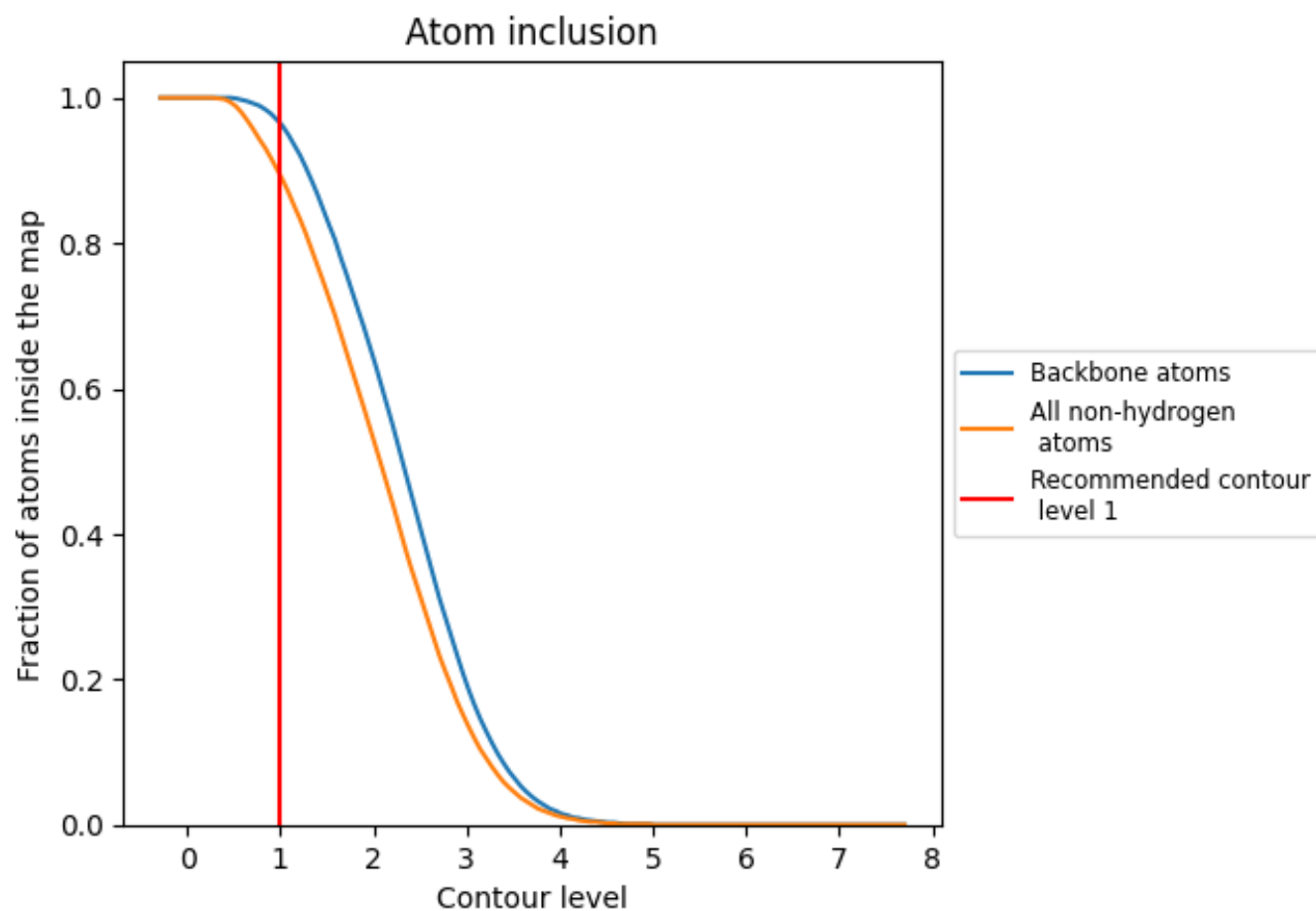
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.6520
1	 0.9230	 0.6760
2	 0.9190	 0.6750
A	 0.9240	 0.6660
B	 0.9150	 0.6590
C	 0.9010	 0.6550
D	 0.9250	 0.6730
E	 0.9200	 0.6700
F	 0.9280	 0.6700
G	 0.9160	 0.6690
H	 0.9360	 0.6700
I	 0.9300	 0.6830
J	 0.9270	 0.6760
K	 0.9440	 0.6890
L	 0.9500	 0.7020
M	 0.7610	 0.6120
N	 0.7990	 0.6020
O	 0.8870	 0.6340
P	 0.8900	 0.6290
Q	 0.9170	 0.6470
R	 0.7730	 0.5860
S	 0.8250	 0.6050
T	 0.8210	 0.6080
U	 0.8690	 0.6300
V	 0.8930	 0.6380
W	 0.9060	 0.6420
X	 0.9350	 0.6610
Y	 0.9290	 0.6580
Z	 0.5620	 0.5520
a	 0.9180	 0.6640
b	 0.9030	 0.6540
c	 0.8860	 0.6490
d	 0.9190	 0.6730
e	 0.9140	 0.6700
f	 0.9270	 0.6790



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Chain	Atom inclusion	Q-score
g	 0.9130	 0.6670
h	 0.9320	 0.6790
i	 0.9170	 0.6710
j	 0.9290	 0.6850
k	 0.9360	 0.6880
l	 0.9450	 0.7030
m	 0.7750	 0.6060
n	 0.7960	 0.6020
o	 0.8890	 0.6380
p	 0.9070	 0.6480
q	 0.9180	 0.6550
r	 0.7670	 0.5780
s	 0.8290	 0.5880
t	 0.8220	 0.6110
u	 0.8730	 0.6280
v	 0.8970	 0.6430
w	 0.8920	 0.6390
x	 0.9320	 0.6640
y	 0.9300	 0.6630
z	 0.5760	 0.5420