



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:08 PM UTC

PDB ID : 7VEA / pdb_00007vea
EMDB ID : EMD-31944
Title : Pentacylindrical allophycocyanin core from *Thermosynechococcus vulcanus*
Authors : Kawakami, K.; Hamaguchi, T.; Hirose, Y.; Kosumi, D.; Miyata, M.; Kamiya, N.; Yonekura, K.
Deposited on : 2021-09-08
Resolution : 3.70 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:

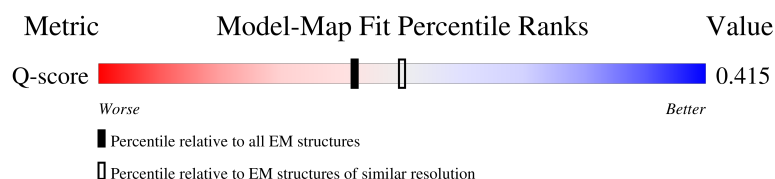
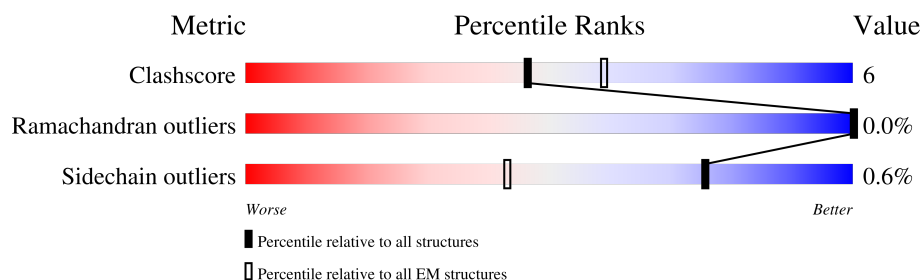
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



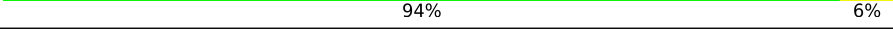
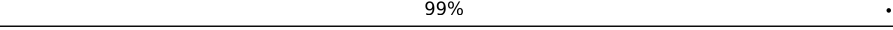
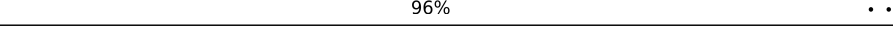
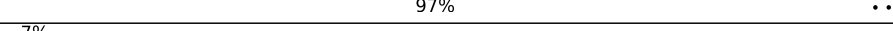
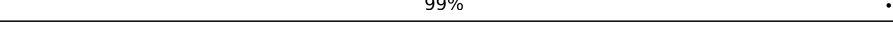
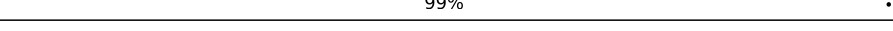
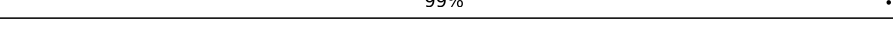
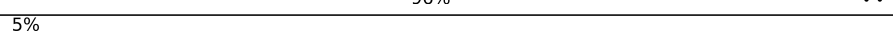
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	aA	161	
1	aC	161	
1	aE	161	
1	aG	161	

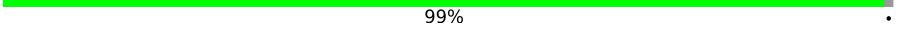
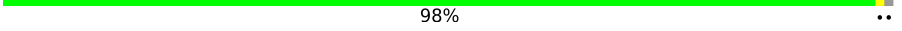
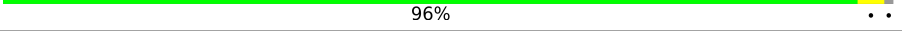
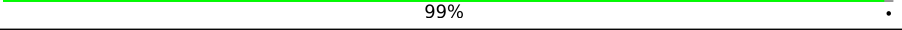
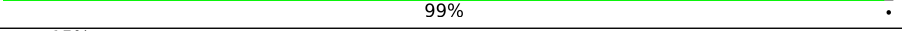
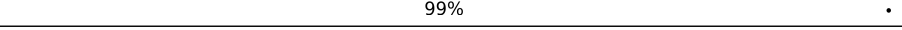
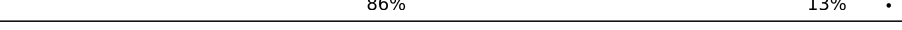
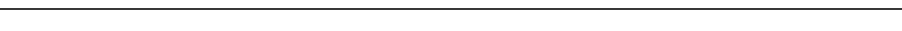
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Mol	Chain	Length	Quality of chain
1	aI	161	 81% 18% .
1	aK	161	 85% 14% .
1	aO	161	 85% 14% .
1	aQ	161	 82% 17% ..
1	bM	161	 83% 17% .
1	bO	161	 89% 9% ..
1	bQ	161	 86% 13% .
1	bS	161	 85% 14% .
1	bU	161	 87% 12% .
1	bW	161	 94% 6% .
1	cA	161	 99% .
1	cC	161	 96% ..
1	cE	161	 97% ..
1	cG	161	 7% 99% .
1	cI	161	 99% .
1	cK	161	 99% .
1	dA	161	 87% 12% .
1	dC	161	 7% 96% ..
1	dE	161	 5% 88% 12% .
1	dG	161	 89% 10% .
1	dI	161	 81% 18% .
1	dK	161	 85% 14% .
1	dO	161	 86% 14% .
1	dQ	161	 81% 17% ..
1	eM	161	 83% 17% .

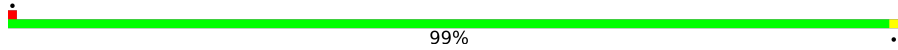
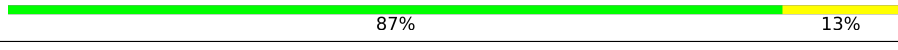
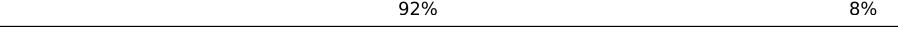
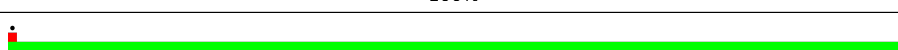
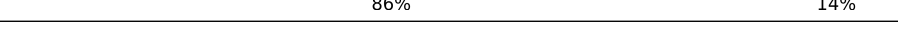
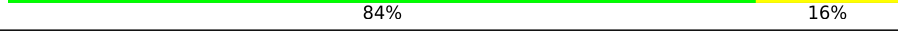
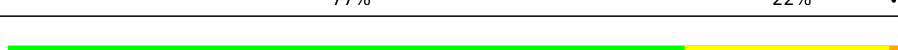
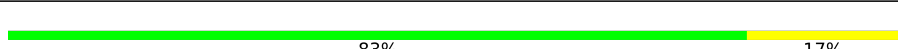
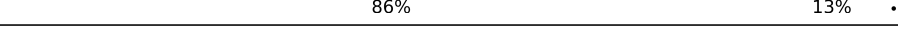
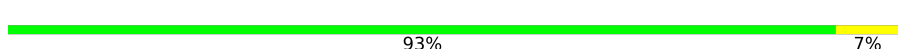
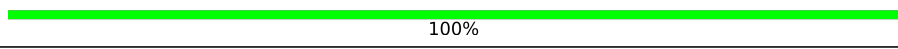
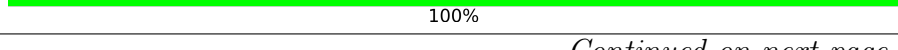
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Mol	Chain	Length	Quality of chain
1	eO	161	 91% 8% ..
1	eQ	161	 86% 13% .
1	eS	161	 86% 13% .
1	eU	161	 85% 14% .
1	eW	161	 94% 5% .
1	fA	161	 99% .
1	fC	161	 16% 98% ..
1	fE	161	 96% ..
1	fG	161	 12% 99% .
1	fI	161	 99% .
1	fK	161	 15% 99% .
2	aB	161	 85% 14% .
2	aD	161	 86% 14% .
2	aF	161	 86% 13% .
2	aH	161	 80% 20% .
2	aJ	161	 79% 20% .
2	aL	161	 87% 12% .
2	aN	161	 78% 22%
2	aP	161	 86% 14%
2	bN	161	 77% 23%
2	bP	161	 76% 24% .
2	bR	161	 81% 19%
2	bT	161	 86% 13% .
2	bV	161	 84% 16%
2	bX	161	 88% 12% .

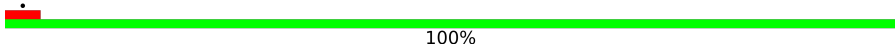
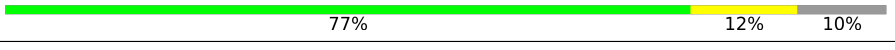
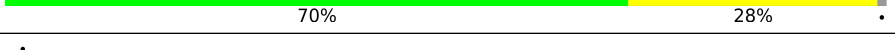
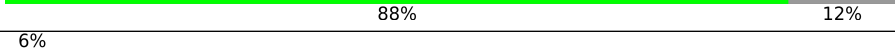
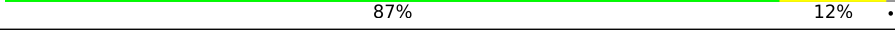
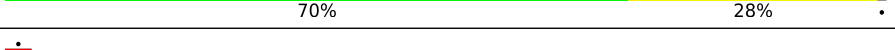
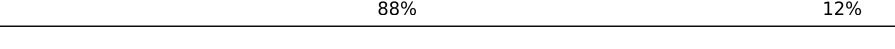
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Mol	Chain	Length	Quality of chain
2	cB	161	 99%
2	cD	161	 87% 13%
2	cF	161	 92% 8%
2	cH	161	 100%
2	cJ	161	 100%
2	cL	161	 100%
2	dB	161	 85% 14%
2	dD	161	 87% 12%
2	dF	161	 86% 14%
2	dH	161	 80% 20%
2	dJ	161	 80% 19%
2	dL	161	 87% 12%
2	dN	161	 80% 20%
2	dP	161	 84% 16%
2	eN	161	 77% 22%
2	eP	161	 76% 23%
2	eR	161	 83% 17%
2	eT	161	 86% 13%
2	eV	161	 84% 16%
2	eX	161	 86% 13%
2	fB	161	 100%
2	fD	161	 86% 14%
2	fF	161	 93% 7%
2	fH	161	 100%
2	fJ	161	100%

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Mol	Chain	Length	Quality of chain
2	fL	161	 100%
3	aM	1139	 77%12%10%
3	dM	1139	 78%12%10%
4	aR	169	 82%17%.
4	dR	169	 83%17%.
5	aS	67	 10%87%12%.
5	bY	67	 70%28%.
5	cM	67	 88%12%
5	dS	67	 6%87%12%.
5	eY	67	 70%28%.
5	fM	67	 88%12%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 111542 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 Allophycocyanin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	160	Total	C	N	O	S	0	0
			1193	749	206	232	6		
1	aC	159	Total	C	N	O	S	0	0
			982	605	177	197	3		
1	aE	160	Total	C	N	O	S	0	0
			1196	750	205	235	6		
1	aG	160	Total	C	N	O	S	0	0
			1202	753	209	234	6		
1	aI	160	Total	C	N	O	S	0	0
			1217	761	212	238	6		
1	aK	160	Total	C	N	O	S	0	0
			1182	742	200	234	6		
1	aO	160	Total	C	N	O	S	0	0
			1191	745	212	229	5		
1	aQ	160	Total	C	N	O	S	0	0
			1216	760	212	238	6		
1	bM	160	Total	C	N	O	S	0	0
			1220	762	212	240	6		
1	bO	160	Total	C	N	O	S	0	0
			1220	762	212	240	6		
1	bQ	160	Total	C	N	O	S	0	0
			1216	760	212	238	6		
1	bS	160	Total	C	N	O	S	0	0
			1202	753	209	234	6		
1	bU	160	Total	C	N	O	S	0	0
			1212	758	212	236	6		
1	bW	160	Total	C	N	O	S	0	0
			1198	751	208	233	6		
1	cA	160	Total	C	N	O		0	0
			809	487	160	162			
1	cC	160	Total	C	N	O		0	0
			843	505	176	162			
1	cE	160	Total	C	N	O	S	0	0
			948	586	187	173	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	cG	160	Total 786	C 466	N 160	O 160		0	0
1	cI	160	Total 800	C 478	N 160	O 162		0	0
1	cK	160	Total 824	C 494	N 165	O 165		0	0
1	dA	160	Total 1193	C 749	N 206	O 232	S 6	0	0
1	dC	159	Total 982	C 605	N 177	O 197	S 3	0	0
1	dE	160	Total 1196	C 750	N 205	O 235	S 6	0	0
1	dG	160	Total 1202	C 753	N 209	O 234	S 6	0	0
1	dI	160	Total 1217	C 761	N 212	O 238	S 6	0	0
1	dK	160	Total 1182	C 742	N 200	O 234	S 6	0	0
1	dO	160	Total 1191	C 745	N 212	O 229	S 5	0	0
1	dQ	160	Total 1216	C 760	N 212	O 238	S 6	0	0
1	eM	160	Total 1220	C 762	N 212	O 240	S 6	0	0
1	eO	160	Total 1220	C 762	N 212	O 240	S 6	0	0
1	eQ	160	Total 1216	C 760	N 212	O 238	S 6	0	0
1	eS	160	Total 1202	C 753	N 209	O 234	S 6	0	0
1	eU	160	Total 1212	C 758	N 212	O 236	S 6	0	0
1	eW	160	Total 1198	C 751	N 208	O 233	S 6	0	0
1	fA	160	Total 809	C 487	N 160	O 162		0	0
1	fC	160	Total 843	C 505	N 176	O 162		0	0
1	fE	160	Total 948	C 586	N 187	O 173	S 2	0	0
1	fG	160	Total 786	C 466	N 160	O 160		0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	fI	160	Total	C	N	O	0	0
			800	478	160	162		
1	fK	160	Total	C	N	O	0	0
			824	494	165	165		

- Molecule 2 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	161	Total 1174	C 741	N 196	O 231	S 6	0	0
2	aD	160	Total 1176	C 742	N 195	O 232	S 7	0	0
2	aF	160	Total 1179	C 744	N 198	O 230	S 7	0	0
2	aH	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	aJ	161	Total 1208	C 764	N 203	O 233	S 8	0	0
2	aL	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	aN	161	Total 1208	C 764	N 203	O 233	S 8	0	0
2	aP	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	bN	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	bP	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	bR	161	Total 1206	C 763	N 200	O 235	S 8	0	0
2	bT	161	Total 1207	C 762	N 203	O 235	S 7	0	0
2	bV	161	Total 1195	C 754	N 200	O 235	S 6	0	0
2	bX	161	Total 1198	C 756	N 202	O 233	S 7	0	0
2	cB	161	Total 808	C 484	N 161	O 163		0	0
2	cD	161	Total 985	C 620	N 180	O 182	S 3	0	0
2	cF	161	Total 983	C 612	N 188	O 182	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	cH	161	Total 794	C 472	N 161	O 161		0	0
2	cJ	161	Total 808	C 484	N 161	O 163		0	0
2	cL	161	Total 800	C 475	N 164	O 161		0	0
2	dB	161	Total 1174	C 741	N 196	O 231	S 6	0	0
2	dD	160	Total 1176	C 742	N 195	O 232	S 7	0	0
2	dF	160	Total 1179	C 744	N 198	O 230	S 7	0	0
2	dH	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	dJ	161	Total 1208	C 764	N 203	O 233	S 8	0	0
2	dL	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	dN	161	Total 1208	C 764	N 203	O 233	S 8	0	0
2	dP	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	eN	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	eP	161	Total 1216	C 768	N 203	O 237	S 8	0	0
2	eR	161	Total 1206	C 763	N 200	O 235	S 8	0	0
2	eT	161	Total 1207	C 762	N 203	O 235	S 7	0	0
2	eV	161	Total 1195	C 754	N 200	O 235	S 6	0	0
2	eX	161	Total 1198	C 756	N 202	O 233	S 7	0	0
2	fB	161	Total 808	C 484	N 161	O 163		0	0
2	fD	161	Total 985	C 620	N 180	O 182	S 3	0	0
2	fF	161	Total 983	C 612	N 188	O 182	S 1	0	0
2	fH	161	Total 794	C 472	N 161	O 161		0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	fJ	161	Total	C	N	O	0	0
			808	484	161	163		
2	fL	161	Total	C	N	O	0	0
			800	475	164	161		

- Molecule 3 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aM	1020	Total	C	N	O	S	0	0
			7856	4993	1409	1443	11		
3	dM	1020	Total	C	N	O	S	0	0
			7856	4993	1409	1443	11		

- Molecule 4 is a protein called Phycobilisome core component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aR	169	Total	C	N	O	S	0	0
			1313	820	234	253	6		
4	dR	169	Total	C	N	O	S	0	0
			1313	820	234	253	6		

- Molecule 5 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aS	66	Total 325	C 193	N 66	O 66		0	0
5	bY	66	Total 513	C 328	N 95	O 88	S 2	0	0
5	cM	59	Total 292	C 174	N 59	O 59		0	0
5	dS	66	Total 325	C 193	N 66	O 66		0	0
5	eY	66	Total 513	C 328	N 95	O 88	S 2	0	0
5	fM	59	Total 292	C 174	N 59	O 59		0	0

- Molecule 6 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms				AltConf
6	aM	1	Total 43	C 33	N 4	O 6	0
6	aN	1	Total 43	C 33	N 4	O 6	0
6	aO	1	Total 43	C 33	N 4	O 6	0
6	aP	1	Total 43	C 33	N 4	O 6	0
6	aQ	1	Total 43	C 33	N 4	O 6	0
6	aR	1	Total 43	C 33	N 4	O 6	0
6	bM	1	Total 43	C 33	N 4	O 6	0
6	bN	1	Total 43	C 33	N 4	O 6	0
6	bO	1	Total 43	C 33	N 4	O 6	0
6	bP	1	Total 43	C 33	N 4	O 6	0
6	bQ	1	Total 43	C 33	N 4	O 6	0
6	bR	1	Total 43	C 33	N 4	O 6	0
6	bS	1	Total 43	C 33	N 4	O 6	0
6	bT	1	Total 43	C 33	N 4	O 6	0
6	bU	1	Total 43	C 33	N 4	O 6	0
6	bV	1	Total 43	C 33	N 4	O 6	0
6	bW	1	Total 43	C 33	N 4	O 6	0
6	bX	1	Total 43	C 33	N 4	O 6	0
6	cB	1	Total 43	C 33	N 4	O 6	0
6	cD	1	Total 43	C 33	N 4	O 6	0
6	cD	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
6	cF	1	Total 43	C 33	N 4	O 6	0
6	cF	1	Total 43	C 33	N 4	O 6	0
6	cG	1	Total 43	C 33	N 4	O 6	0
6	cI	1	Total 43	C 33	N 4	O 6	0
6	cJ	1	Total 43	C 33	N 4	O 6	0
6	cL	1	Total 43	C 33	N 4	O 6	0
6	cM	1	Total 43	C 33	N 4	O 6	0
6	dA	1	Total 43	C 33	N 4	O 6	0
6	dB	1	Total 43	C 33	N 4	O 6	0
6	dC	1	Total 43	C 33	N 4	O 6	0
6	dD	1	Total 43	C 33	N 4	O 6	0
6	dE	1	Total 43	C 33	N 4	O 6	0
6	dF	1	Total 43	C 33	N 4	O 6	0
6	dG	1	Total 43	C 33	N 4	O 6	0
6	dH	1	Total 43	C 33	N 4	O 6	0
6	dI	1	Total 43	C 33	N 4	O 6	0
6	dJ	1	Total 43	C 33	N 4	O 6	0
6	dK	1	Total 43	C 33	N 4	O 6	0
6	dL	1	Total 43	C 33	N 4	O 6	0
6	dM	1	Total 43	C 33	N 4	O 6	0
6	dM	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
6	dM	1	Total 43	C 33	N 4	O 6	0
6	dN	1	Total 43	C 33	N 4	O 6	0
6	dO	1	Total 43	C 33	N 4	O 6	0
6	dP	1	Total 43	C 33	N 4	O 6	0
6	dQ	1	Total 43	C 33	N 4	O 6	0
6	dR	1	Total 43	C 33	N 4	O 6	0
6	eM	1	Total 43	C 33	N 4	O 6	0
6	eN	1	Total 43	C 33	N 4	O 6	0
6	eO	1	Total 43	C 33	N 4	O 6	0
6	eP	1	Total 43	C 33	N 4	O 6	0
6	eQ	1	Total 43	C 33	N 4	O 6	0
6	eR	1	Total 43	C 33	N 4	O 6	0
6	eS	1	Total 43	C 33	N 4	O 6	0
6	eT	1	Total 43	C 33	N 4	O 6	0
6	eU	1	Total 43	C 33	N 4	O 6	0
6	eV	1	Total 43	C 33	N 4	O 6	0
6	eW	1	Total 43	C 33	N 4	O 6	0
6	eX	1	Total 43	C 33	N 4	O 6	0
6	fB	1	Total 43	C 33	N 4	O 6	0
6	fD	1	Total 43	C 33	N 4	O 6	0
6	fD	1	Total 43	C 33	N 4	O 6	0

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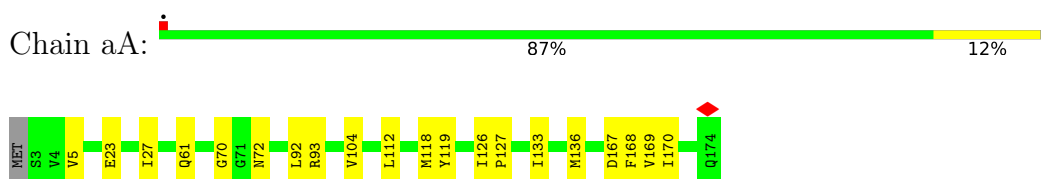
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Mol	Chain	Residues	Atoms				AltConf
6	fF	1	Total 43	C 33	N 4	O 6	0
6	fF	1	Total 43	C 33	N 4	O 6	0
6	fG	1	Total 43	C 33	N 4	O 6	0
6	fI	1	Total 43	C 33	N 4	O 6	0
6	fJ	1	Total 43	C 33	N 4	O 6	0
6	fL	1	Total 43	C 33	N 4	O 6	0
6	fM	1	Total 43	C 33	N 4	O 6	0

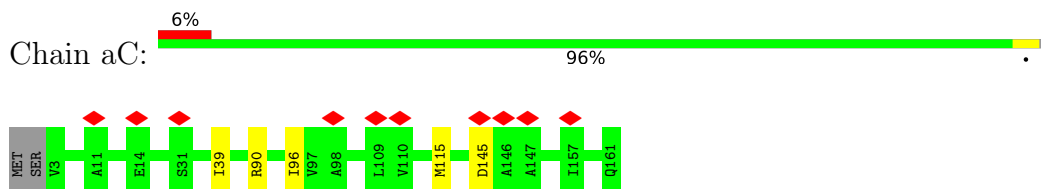
3 Residue-property plots [i](#)

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.

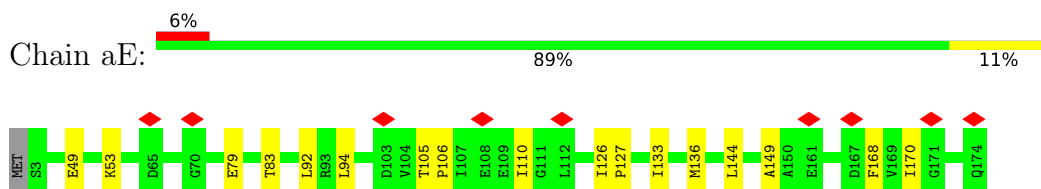
- Molecule 1: Allophycocyanin alpha chain



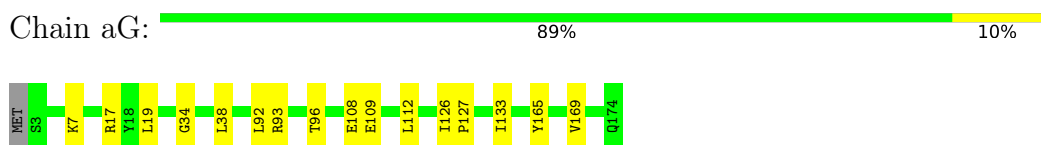
- Molecule 1: Allophycocyanin alpha chain



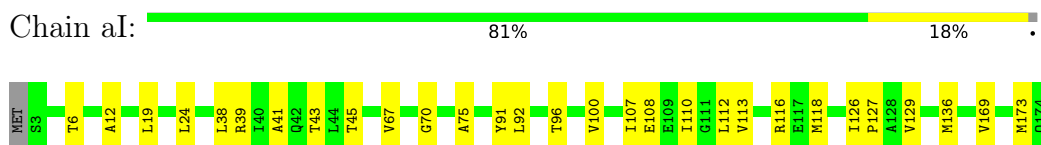
- Molecule 1: Allophycocyanin alpha chain



- Molecule 1: Allophycocyanin alpha chain



- Molecule 1: Allophycocyanin alpha chain



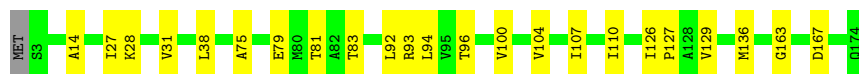
- Molecule 1: Allophycocyanin alpha chain

Chain aK:  85% 14%



- Molecule 1: Allophycocyanin alpha chain

Chain aO:  85% 14%



- Molecule 1: Allophycocyanin alpha chain

Chain aQ:  82% 17%



- Molecule 1: Allophycocyanin alpha chain

Chain bM:  83% 17%



- Molecule 1: Allophycocyanin alpha chain

Chain bO:  89% 9%



- Molecule 1: Allophycocyanin alpha chain

Chain bQ:  86% 13%



- Molecule 1: Allophycocyanin alpha chain

Chain bS:  85% 14%

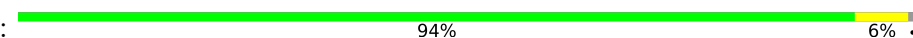


- Molecule 1: Allophycocyanin alpha chain

Chain bU:  87% 12%

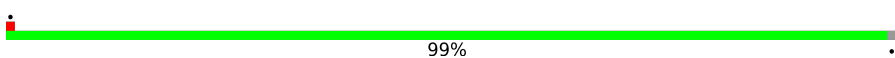


- Molecule 1: Allophycocyanin alpha chain

Chain bW:  94% 6%

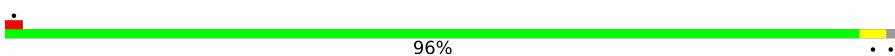


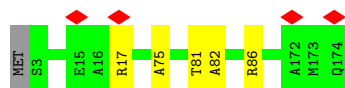
- Molecule 1: Allophycocyanin alpha chain

Chain cA:  99%

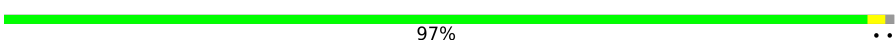


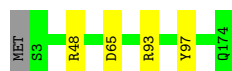
- Molecule 1: Allophycocyanin alpha chain

Chain cC:  96%

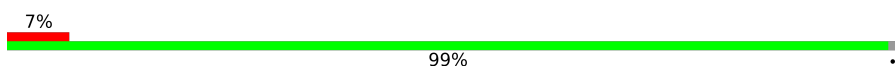


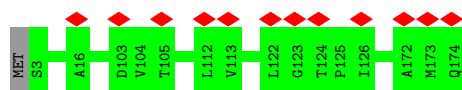
- Molecule 1: Allophycocyanin alpha chain

Chain cE:  97%

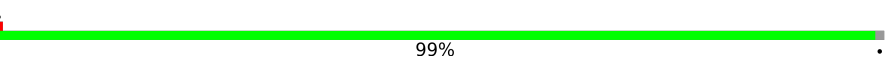


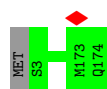
- Molecule 1: Allophycocyanin alpha chain

Chain cG:  7% 99%

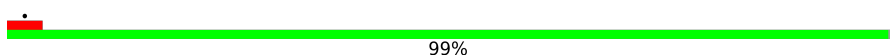


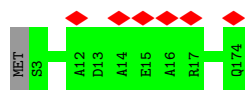
- Molecule 1: Allophycocyanin alpha chain

Chain cI:  99%



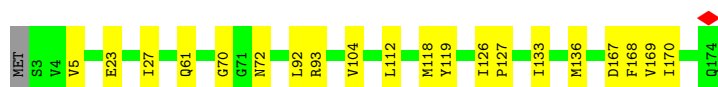
- Molecule 1: Allophycocyanin alpha chain

Chain cK:  99%

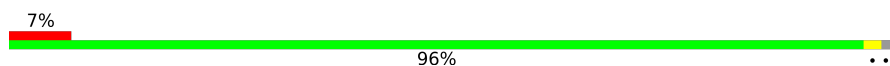


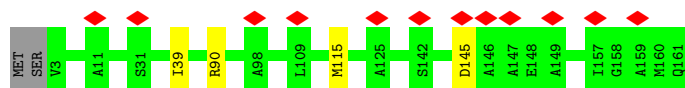
- Molecule 1: Allophycocyanin alpha chain

Chain dA:  87%

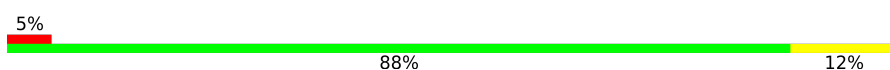


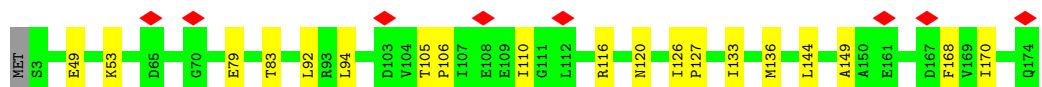
- Molecule 1: Allophycocyanin alpha chain

Chain dC:  96%



- Molecule 1: Allophycocyanin alpha chain

Chain dE:  88%



- Molecule 1: Allophycocyanin alpha chain

Chain dG:  89%



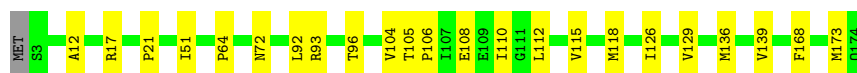
- Molecule 1: Allophycocyanin alpha chain

Chain dI:  81%

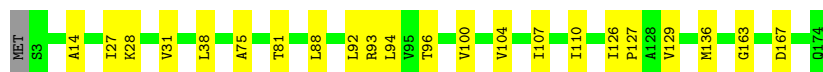


- Molecule 1: Allophycocyanin alpha chain

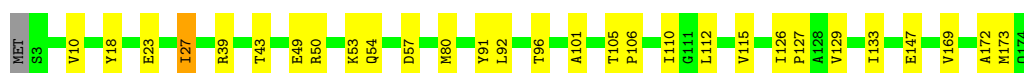
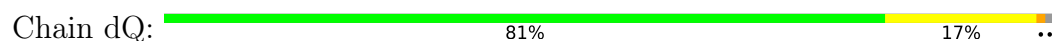
Chain dK:  85%



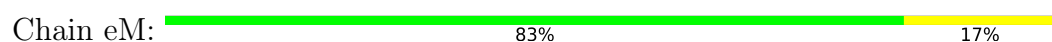
- Molecule 1: Allophycocyanin alpha chain



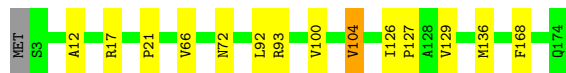
- Molecule 1: Allophycocyanin alpha chain



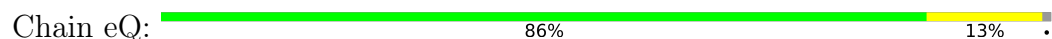
- Molecule 1: Allophycocyanin alpha chain



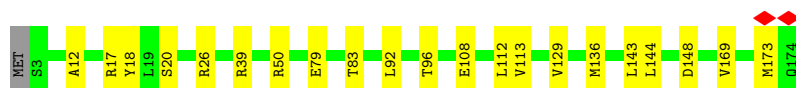
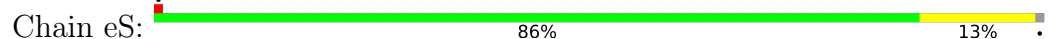
- Molecule 1: Allophycocyanin alpha chain



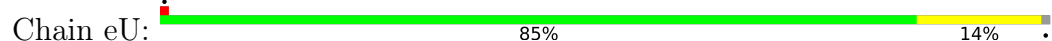
- Molecule 1: Allophycocyanin alpha chain



- Molecule 1: Allophycocyanin alpha chain



- Molecule 1: Allophycocyanin alpha chain





- Molecule 1: Allophycocyanin alpha chain

Chain eW: 94% 5%



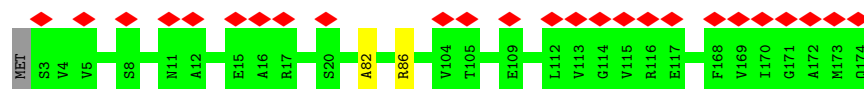
- Molecule 1: Allophycocyanin alpha chain

Chain fA: 99%



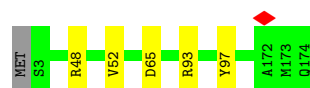
- Molecule 1: Allophycocyanin alpha chain

Chain fC: 16% 98%



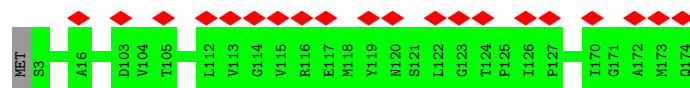
- Molecule 1: Allophycocyanin alpha chain

Chain fE: 96%



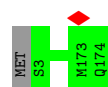
- Molecule 1: Allophycocyanin alpha chain

Chain fG: 12% 99%

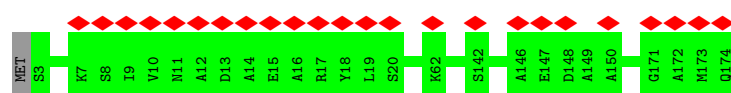


- Molecule 1: Allophycocyanin alpha chain

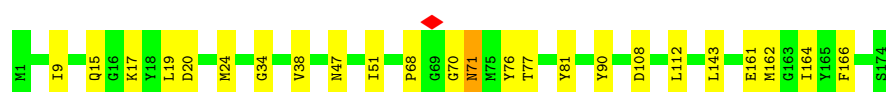
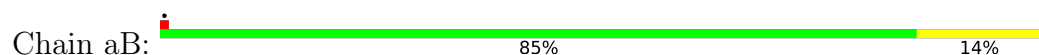
Chain fI: 99%



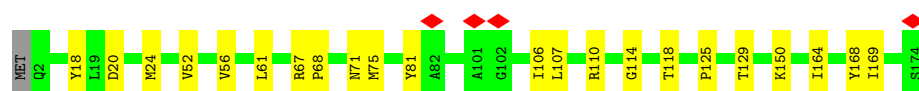
- Molecule 1: Allophycocyanin alpha chain



- Molecule 2: Allophycocyanin beta chain



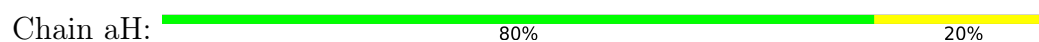
- Molecule 2: Allophycocyanin beta chain



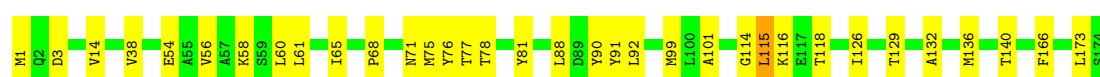
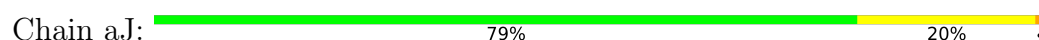
- Molecule 2: Allophycocyanin beta chain



- Molecule 2: Allophycocyanin beta chain



- Molecule 2: Allophycocyanin beta chain

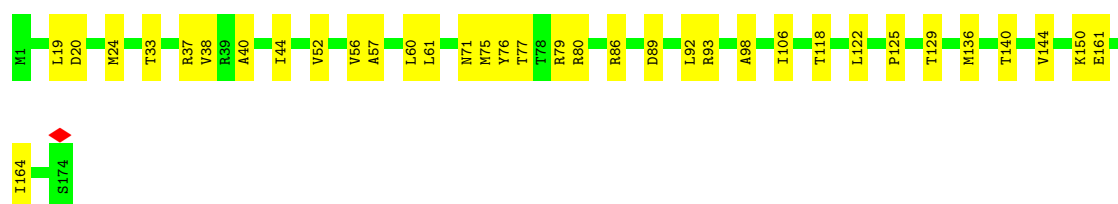


- Molecule 2: Allophycocyanin beta chain



- Molecule 2: Allophycocyanin beta chain

Chain aN:  78% 22%



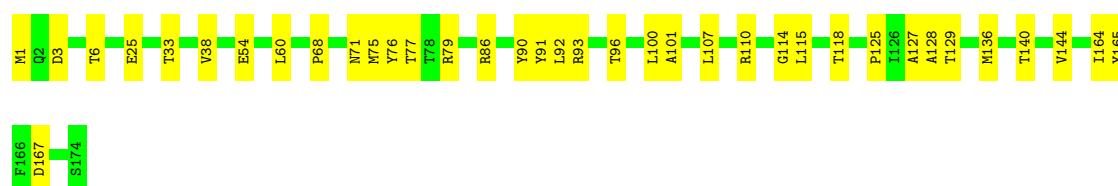
- Molecule 2: Allophycocyanin beta chain

Chain aP:  86% 14%



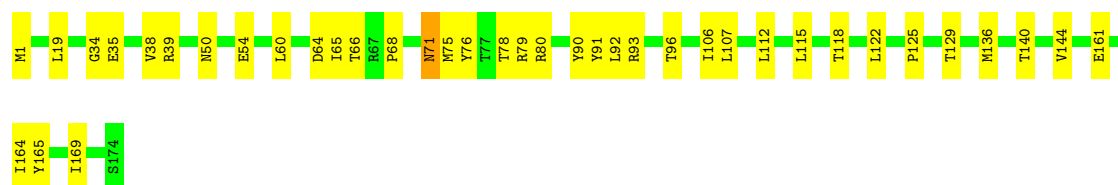
- Molecule 2: Allophycocyanin beta chain

Chain bN:  77% 23%



- Molecule 2: Allophycocyanin beta chain

Chain bP:  76% 24%



- Molecule 2: Allophycocyanin beta chain

Chain bR:  81% 19%



- Molecule 2: Allophycocyanin beta chain

Chain bT:  86% 13%



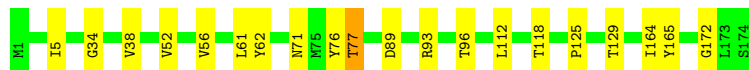
- Molecule 2: Allophycocyanin beta chain

Chain bV:  84% 16%



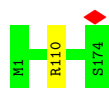
- Molecule 2: Allophycocyanin beta chain

Chain bX:  88% 12%



- Molecule 2: Allophycocyanin beta chain

Chain cB:  99%



- Molecule 2: Allophycocyanin beta chain

Chain cD:  87% 13%

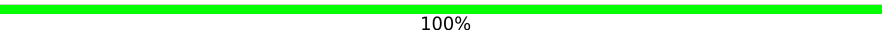


- Molecule 2: Allophycocyanin beta chain

Chain cF:  92% 8%



- Molecule 2: Allophycocyanin beta chain

Chain cH:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Allophycocyanin beta chain

Chain cJ:  100%



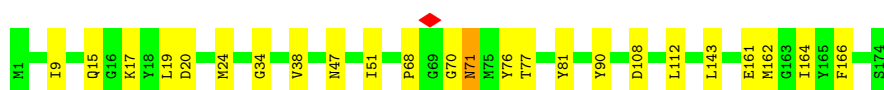
- Molecule 2: Allophycocyanin beta chain

Chain cL:  100%



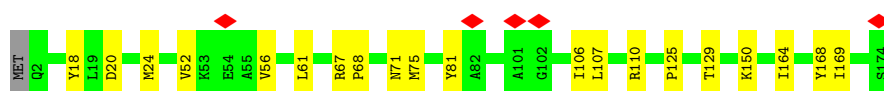
- Molecule 2: Allophycocyanin beta chain

Chain dB:  85% 14%



- Molecule 2: Allophycocyanin beta chain

Chain dD:  87% 12%



- Molecule 2: Allophycocyanin beta chain

Chain dF:  86% 14%



- Molecule 2: Allophycocyanin beta chain

Chain dH:  80% 20%



- Molecule 2: Allophycocyanin beta chain

Chain dJ:  80% 19%



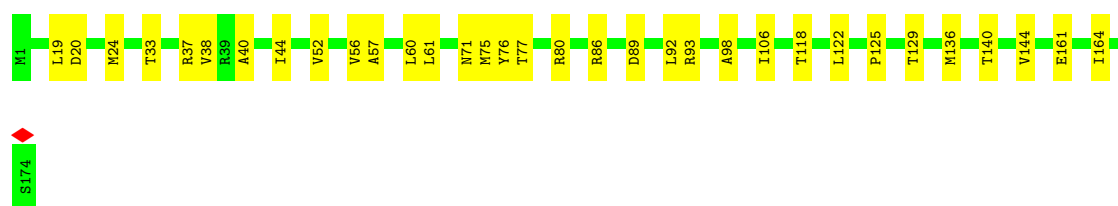
- Molecule 2: Allophycocyanin beta chain

Chain dL:  87% 12%



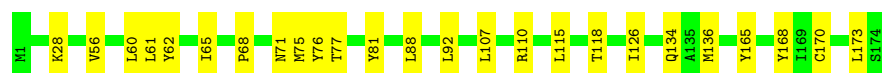
- Molecule 2: Allophycocyanin beta chain

Chain dN:  80% 20%



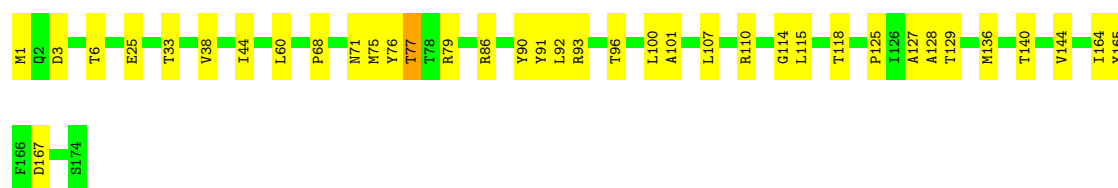
- Molecule 2: Allophycocyanin beta chain

Chain dP:  84% 16%



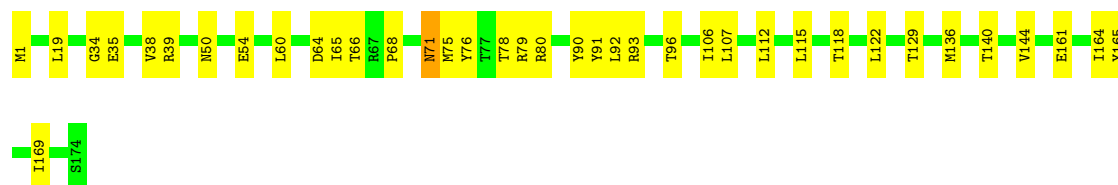
- Molecule 2: Allophycocyanin beta chain

Chain eN:  77% 22%



- Molecule 2: Allophycocyanin beta chain

Chain eP:  76% 23%



- Molecule 2: Allophycocyanin beta chain

Chain eR:  83% 17%



- Molecule 2: Allophycocyanin beta chain

Chain eT:  86% 13%



- Molecule 2: Allophycocyanin beta chain

Chain eV:  84% 16%



- Molecule 2: Allophycocyanin beta chain

Chain eX:  86% 13%



- Molecule 2: Allophycocyanin beta chain

Chain fB:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Allophycocyanin beta chain

Chain fD:  86% 14%

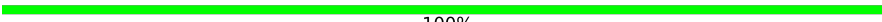


- Molecule 2: Allophycocyanin beta chain

Chain fF:  93% 7%



- Molecule 2: Allophycocyanin beta chain

Chain fH:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Allophycocyanin beta chain

Chain fJ:  100%



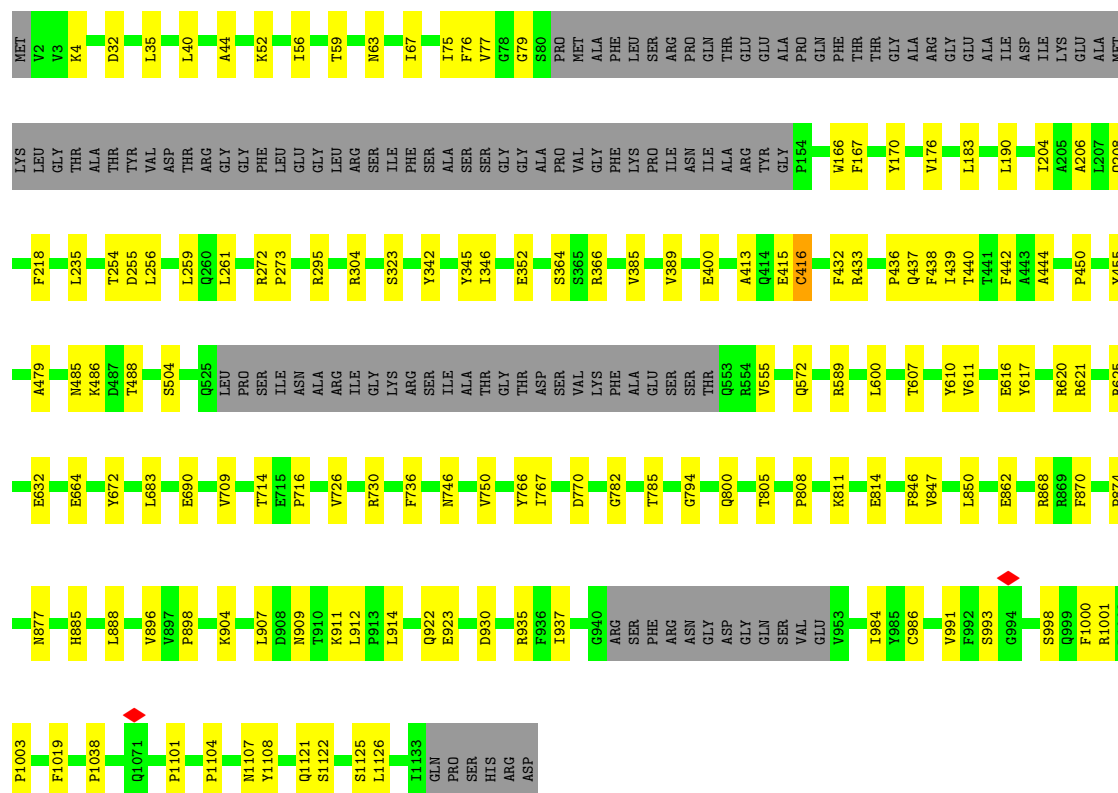
- Molecule 2: Allophycocyanin beta chain

Chain fL:  100%



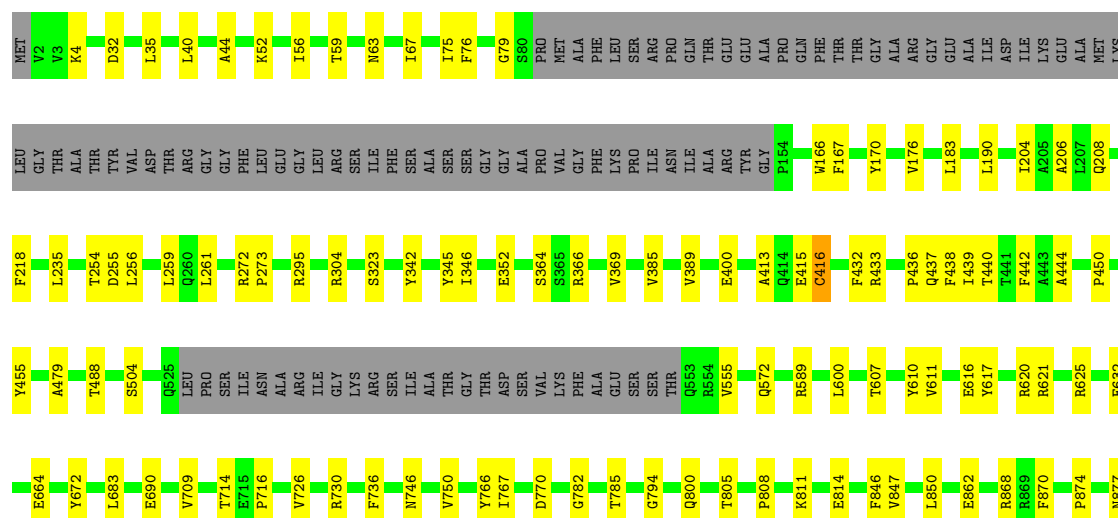
• Molecule 3: Phycobiliprotein ApcE

Chain aM: 77% 12% 10%



• Molecule 3: Phycobiliprotein ApcE

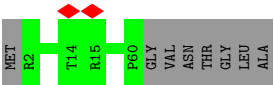
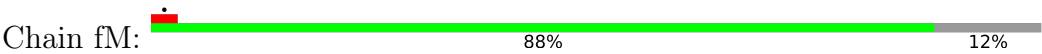
Chain dM: 78% 12% 10%



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25532	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	84.1	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.241	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.00612	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MEN, 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	aA	0.15	0/1209	0.35	0/1640
1	aC	0.11	0/992	0.34	0/1359
1	aE	0.11	0/1212	0.33	0/1644
1	aG	0.14	0/1218	0.32	0/1651
1	aI	0.18	0/1233	0.33	0/1669
1	aK	0.16	0/1198	0.33	0/1628
1	aO	0.15	0/1206	0.34	0/1635
1	aQ	0.18	0/1232	0.34	0/1668
1	bM	0.15	0/1236	0.35	0/1673
1	bO	0.16	0/1236	0.35	0/1673
1	bQ	0.13	0/1232	0.30	0/1668
1	bS	0.12	0/1218	0.32	0/1651
1	bU	0.13	0/1228	0.31	0/1663
1	bW	0.13	0/1214	0.36	0/1646
1	cA	0.07	0/811	0.22	0/1124
1	cC	0.07	0/845	0.21	0/1165
1	cE	0.11	0/957	0.25	0/1306
1	cG	0.06	0/785	0.21	0/1089
1	cI	0.07	0/801	0.22	0/1111
1	cK	0.08	0/826	0.21	0/1141
1	dA	0.15	0/1209	0.35	0/1640
1	dC	0.11	0/992	0.34	0/1359
1	dE	0.11	0/1212	0.33	0/1644
1	dG	0.14	0/1218	0.32	0/1651
1	dI	0.18	0/1233	0.33	0/1669
1	dK	0.15	0/1198	0.32	0/1628
1	dO	0.15	0/1206	0.34	0/1635
1	dQ	0.18	0/1232	0.34	0/1668
1	eM	0.15	0/1236	0.35	0/1673
1	eO	0.16	0/1236	0.35	0/1673
1	eQ	0.13	0/1232	0.30	0/1668
1	eS	0.12	0/1218	0.32	0/1651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	eU	0.13	0/1228	0.31	0/1663
1	eW	0.13	0/1214	0.36	0/1646
1	fA	0.07	0/811	0.22	0/1124
1	fC	0.07	0/845	0.21	0/1165
1	fE	0.11	0/957	0.25	0/1306
1	fG	0.06	0/785	0.20	0/1089
1	fI	0.07	0/801	0.22	0/1111
1	fK	0.07	0/826	0.21	0/1141
2	aB	0.11	0/1180	0.31	0/1603
2	aD	0.11	0/1181	0.30	0/1601
2	aF	0.12	0/1185	0.29	0/1607
2	aH	0.19	0/1222	0.33	0/1653
2	aJ	0.18	0/1214	0.34	0/1643
2	aL	0.16	0/1222	0.31	0/1653
2	aN	0.15	0/1214	0.30	0/1643
2	aP	0.17	0/1222	0.33	0/1653
2	bN	0.20	0/1222	0.37	0/1653
2	bP	0.17	0/1222	0.36	0/1653
2	bR	0.15	0/1212	0.35	0/1641
2	bT	0.12	0/1213	0.32	0/1642
2	bV	0.11	0/1201	0.32	0/1628
2	bX	0.11	0/1203	0.31	0/1629
2	cB	0.08	0/803	0.21	0/1114
2	cD	0.11	0/993	0.29	0/1362
2	cF	0.10	0/988	0.28	0/1351
2	cH	0.07	0/787	0.22	0/1092
2	cJ	0.07	0/803	0.21	0/1114
2	cL	0.07	0/793	0.20	0/1099
2	dB	0.11	0/1180	0.31	0/1603
2	dD	0.11	0/1181	0.30	0/1601
2	dF	0.12	0/1185	0.29	0/1607
2	dH	0.19	0/1222	0.33	0/1653
2	dJ	0.18	0/1214	0.34	0/1643
2	dL	0.16	0/1222	0.31	0/1653
2	dN	0.15	0/1214	0.30	0/1643
2	dP	0.17	0/1222	0.33	0/1653
2	eN	0.20	0/1222	0.37	0/1653
2	eP	0.17	0/1222	0.36	0/1653
2	eR	0.15	0/1212	0.35	0/1641
2	eT	0.12	0/1213	0.32	0/1642
2	eV	0.11	0/1201	0.32	0/1628
2	eX	0.11	0/1203	0.31	0/1629
2	fB	0.08	0/803	0.22	0/1114

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	fD	0.11	0/993	0.29	0/1362
2	fF	0.10	0/988	0.28	0/1351
2	fH	0.07	0/787	0.21	0/1092
2	fJ	0.07	0/803	0.21	0/1114
2	fL	0.07	0/793	0.20	0/1099
3	aM	0.16	0/8018	0.37	0/10878
3	dM	0.16	0/8018	0.37	0/10878
4	aR	0.18	0/1321	0.31	0/1788
4	dR	0.18	0/1321	0.31	0/1788
5	aS	0.10	0/324	0.38	0/449
5	bY	0.13	0/522	0.35	0/703
5	cM	0.07	0/291	0.24	0/404
5	dS	0.10	0/324	0.38	0/449
5	eY	0.13	0/522	0.35	0/703
5	fM	0.07	0/291	0.24	0/404
All	All	0.14	0/108890	0.32	0/148120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	aA	1193	0	1183	13	0
1	aC	982	0	739	4	0
1	aE	1196	0	1183	11	0
1	aG	1202	0	1192	12	0
1	aI	1217	0	1217	21	0
1	aK	1182	0	1155	17	0
1	aO	1191	0	1187	15	0
1	aQ	1216	0	1215	19	0
1	bM	1220	0	1219	22	0
1	bO	1220	0	1219	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	bQ	1216	0	1215	16	0
1	bS	1202	0	1196	19	0
1	bU	1212	0	1211	14	0
1	bW	1198	0	1190	8	0
1	cA	809	0	408	0	0
1	cC	843	0	484	3	0
1	cE	948	0	647	8	0
1	cG	786	0	378	0	0
1	cI	800	0	392	0	0
1	cK	824	0	431	0	0
1	dA	1193	0	1183	14	0
1	dC	982	0	739	3	0
1	dE	1196	0	1183	11	0
1	dG	1202	0	1192	13	0
1	dI	1217	0	1217	21	0
1	dK	1182	0	1155	18	0
1	dO	1191	0	1187	15	0
1	dQ	1216	0	1215	20	0
1	eM	1220	0	1219	22	0
1	eO	1220	0	1219	8	0
1	eQ	1216	0	1215	16	0
1	eS	1202	0	1196	18	0
1	eU	1212	0	1211	16	0
1	eW	1198	0	1190	6	0
1	fA	809	0	408	0	0
1	fC	843	0	484	1	0
1	fE	948	0	647	8	0
1	fG	786	0	378	0	0
1	fI	800	0	392	0	0
1	fK	824	0	431	0	0
2	aB	1174	0	1144	15	0
2	aD	1176	0	1161	13	0
2	aF	1179	0	1159	13	0
2	aH	1216	0	1228	26	0
2	aJ	1208	0	1220	28	0
2	aL	1216	0	1228	18	0
2	aN	1208	0	1220	30	0
2	aP	1216	0	1228	18	0
2	bN	1216	0	1228	30	0
2	bP	1216	0	1228	25	0
2	bR	1206	0	1213	24	0
2	bT	1207	0	1210	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	bV	1195	0	1183	14	0
2	bX	1198	0	1204	11	0
2	cB	808	0	423	1	0
2	cD	985	0	748	20	0
2	cF	983	0	742	12	0
2	cH	794	0	409	0	0
2	cJ	808	0	423	0	0
2	cL	800	0	420	0	0
2	dB	1174	0	1144	15	0
2	dD	1176	0	1161	12	0
2	dF	1179	0	1159	15	0
2	dH	1216	0	1228	26	0
2	dJ	1208	0	1220	29	0
2	dL	1216	0	1228	18	0
2	dN	1208	0	1220	27	0
2	dP	1216	0	1228	20	0
2	eN	1216	0	1228	31	0
2	eP	1216	0	1228	24	0
2	eR	1206	0	1213	21	0
2	eT	1207	0	1210	15	0
2	eV	1195	0	1183	15	0
2	eX	1198	0	1204	12	0
2	fB	808	0	423	0	0
2	fD	985	0	748	19	0
2	fF	983	0	742	11	0
2	fH	794	0	409	0	0
2	fJ	808	0	423	0	0
2	fL	800	0	420	0	0
3	aM	7856	0	7714	115	0
3	dM	7856	0	7714	113	0
4	aR	1313	0	1310	25	0
4	dR	1313	0	1310	24	0
5	aS	325	0	139	6	0
5	bY	513	0	516	13	0
5	cM	292	0	120	0	0
5	dS	325	0	139	6	0
5	eY	513	0	516	13	0
5	fM	292	0	120	0	0
6	aA	43	0	37	2	0
6	aB	43	0	37	2	0
6	aC	43	0	37	2	0
6	aD	43	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	aE	43	0	37	3	0
6	aF	43	0	37	0	0
6	aG	43	0	37	3	0
6	aH	43	0	37	2	0
6	aI	43	0	37	5	0
6	aJ	43	0	37	6	0
6	aK	43	0	37	5	0
6	aL	43	0	37	6	0
6	aM	129	0	112	9	0
6	aN	43	0	37	5	0
6	aO	43	0	37	7	0
6	aP	43	0	37	7	0
6	aQ	43	0	37	5	0
6	aR	43	0	35	8	0
6	bM	43	0	37	2	0
6	bN	43	0	37	4	0
6	bO	43	0	37	4	0
6	bP	43	0	37	4	0
6	bQ	43	0	37	3	0
6	bR	43	0	37	4	0
6	bS	43	0	37	5	0
6	bT	43	0	37	2	0
6	bU	43	0	37	3	0
6	bV	43	0	37	1	0
6	bW	43	0	37	3	0
6	bX	43	0	37	0	0
6	cB	43	0	38	3	0
6	cD	86	0	76	11	0
6	cF	86	0	76	5	0
6	cG	43	0	38	3	0
6	cI	43	0	38	4	0
6	cJ	43	0	38	2	0
6	cL	43	0	38	0	0
6	cM	43	0	38	2	0
6	dA	43	0	37	2	0
6	dB	43	0	37	3	0
6	dC	43	0	37	2	0
6	dD	43	0	37	1	0
6	dE	43	0	37	3	0
6	dF	43	0	37	0	0
6	dG	43	0	37	3	0
6	dH	43	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	dI	43	0	37	5	0
6	dJ	43	0	37	6	0
6	dK	43	0	37	4	0
6	dL	43	0	37	6	0
6	dM	129	0	112	9	0
6	dN	43	0	37	5	0
6	dO	43	0	37	8	0
6	dP	43	0	37	5	0
6	dQ	43	0	37	5	0
6	dR	43	0	35	7	0
6	eM	43	0	37	2	0
6	eN	43	0	37	4	0
6	eO	43	0	37	4	0
6	eP	43	0	37	4	0
6	eQ	43	0	37	3	0
6	eR	43	0	37	4	0
6	eS	43	0	37	5	0
6	eT	43	0	37	2	0
6	eU	43	0	37	3	0
6	eV	43	0	37	1	0
6	eW	43	0	37	3	0
6	eX	43	0	37	0	0
6	fB	43	0	38	3	0
6	fD	86	0	76	10	0
6	fF	86	0	76	4	0
6	fG	43	0	38	3	0
6	fI	43	0	38	4	0
6	fJ	43	0	38	3	0
6	fL	43	0	38	0	0
6	fM	43	0	38	2	0
All	All	111542	0	100884	1287	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 6.

The worst 5 of 1287 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)
6:dR:201:CYC:HC	6:dR:201:CYC:HMD3	1.35	0.90
6:aR:201:CYC:HMD3	6:aR:201:CYC:HC	1.35	0.89
6:dO:201:CYC:HMD1	6:dO:201:CYC:HC	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:aO:201:CYC:HMD1	6:aO:201:CYC:HC	1.37	0.87
6:aJ:201:CYC:HC	6:aJ:201:CYC:HMD1	1.41	0.86

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	aA	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	aC	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
1	aE	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	aG	158/161 (98%)	158 (100%)	0	0	100	100
1	aI	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	aK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	aO	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	aQ	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	bM	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	bO	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	bQ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	bS	158/161 (98%)	158 (100%)	0	0	100	100
1	bU	158/161 (98%)	158 (100%)	0	0	100	100
1	bW	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	cA	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	cC	158/161 (98%)	158 (100%)	0	0	100	100
1	cE	158/161 (98%)	158 (100%)	0	0	100	100
1	cG	158/161 (98%)	158 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	cI	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	cK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	dA	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	dC	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
1	dE	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	dG	158/161 (98%)	158 (100%)	0	0	100	100
1	dI	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	dK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	dO	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	dQ	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	eM	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	eO	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	eQ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	eS	158/161 (98%)	158 (100%)	0	0	100	100
1	eU	158/161 (98%)	158 (100%)	0	0	100	100
1	eW	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	fA	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	fC	158/161 (98%)	158 (100%)	0	0	100	100
1	fE	158/161 (98%)	158 (100%)	0	0	100	100
1	fG	158/161 (98%)	158 (100%)	0	0	100	100
1	fI	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	fK	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	aB	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	aD	157/161 (98%)	157 (100%)	0	0	100	100
2	aF	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
2	aH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	aJ	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	aL	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	aN	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	aP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	bN	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	bP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	bR	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	bT	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	bV	158/161 (98%)	157 (99%)	0	1 (1%)	21	52
2	bX	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	cB	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	cD	158/161 (98%)	158 (100%)	0	0	100	100
2	cF	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	cH	158/161 (98%)	158 (100%)	0	0	100	100
2	cJ	158/161 (98%)	158 (100%)	0	0	100	100
2	cL	158/161 (98%)	158 (100%)	0	0	100	100
2	dB	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	dD	157/161 (98%)	157 (100%)	0	0	100	100
2	dF	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
2	dH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	dJ	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	dL	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	dN	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	dP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	eN	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	52
2	eP	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	eR	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	eT	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
2	eV	158/161 (98%)	157 (99%)	0	1 (1%)	21	52
2	eX	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
2	fB	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	fD	158/161 (98%)	158 (100%)	0	0	100	100
2	fF	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	fH	158/161 (98%)	158 (100%)	0	0	100	100
2	fJ	158/161 (98%)	158 (100%)	0	0	100	100
2	fL	158/161 (98%)	158 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	aM	1012/1139 (89%)	962 (95%)	50 (5%)	0	100	100
3	dM	1012/1139 (89%)	962 (95%)	50 (5%)	0	100	100
4	aR	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
4	dR	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
5	aS	64/67 (96%)	61 (95%)	3 (5%)	0	100	100
5	bY	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
5	cM	57/67 (85%)	57 (100%)	0	0	100	100
5	dS	64/67 (96%)	61 (95%)	3 (5%)	0	100	100
5	eY	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
5	fM	57/67 (85%)	57 (100%)	0	0	100	100
All	All	15360/15898 (97%)	15120 (98%)	236 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	bV	77	THR
2	eV	77	THR
2	bN	77	THR
2	eN	77	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	123/130 (95%)	122 (99%)	1 (1%)	73	76
1	aC	56/130 (43%)	56 (100%)	0	100	100
1	aE	124/130 (95%)	123 (99%)	1 (1%)	73	76
1	aG	124/130 (95%)	123 (99%)	1 (1%)	73	76
1	aI	128/130 (98%)	128 (100%)	0	100	100
1	aK	121/130 (93%)	120 (99%)	1 (1%)	73	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aO	122/130 (94%)	122 (100%)	0	100	100
1	aQ	128/130 (98%)	126 (98%)	2 (2%)	55	68
1	bM	129/130 (99%)	129 (100%)	0	100	100
1	bO	129/130 (99%)	126 (98%)	3 (2%)	44	62
1	bQ	128/130 (98%)	126 (98%)	2 (2%)	55	68
1	bS	125/130 (96%)	125 (100%)	0	100	100
1	bU	127/130 (98%)	127 (100%)	0	100	100
1	bW	124/130 (95%)	123 (99%)	1 (1%)	73	76
1	cA	4/130 (3%)	4 (100%)	0	100	100
1	cC	12/130 (9%)	12 (100%)	0	100	100
1	cE	33/130 (25%)	33 (100%)	0	100	100
1	cI	2/130 (2%)	2 (100%)	0	100	100
1	cK	7/130 (5%)	7 (100%)	0	100	100
1	dA	123/130 (95%)	122 (99%)	1 (1%)	73	76
1	dC	56/130 (43%)	56 (100%)	0	100	100
1	dE	124/130 (95%)	123 (99%)	1 (1%)	73	76
1	dG	124/130 (95%)	123 (99%)	1 (1%)	73	76
1	dI	128/130 (98%)	128 (100%)	0	100	100
1	dK	121/130 (93%)	120 (99%)	1 (1%)	73	76
1	dO	122/130 (94%)	122 (100%)	0	100	100
1	dQ	128/130 (98%)	126 (98%)	2 (2%)	55	68
1	eM	129/130 (99%)	129 (100%)	0	100	100
1	eO	129/130 (99%)	126 (98%)	3 (2%)	44	62
1	eQ	128/130 (98%)	126 (98%)	2 (2%)	55	68
1	eS	125/130 (96%)	125 (100%)	0	100	100
1	eU	127/130 (98%)	127 (100%)	0	100	100
1	eW	124/130 (95%)	123 (99%)	1 (1%)	73	76
1	fA	4/130 (3%)	4 (100%)	0	100	100
1	fC	12/130 (9%)	12 (100%)	0	100	100
1	fE	33/130 (25%)	33 (100%)	0	100	100
1	fI	2/130 (2%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	fK	7/130 (5%)	7 (100%)	0	100	100
2	aB	112/123 (91%)	112 (100%)	0	100	100
2	aD	115/123 (94%)	115 (100%)	0	100	100
2	aF	114/123 (93%)	114 (100%)	0	100	100
2	aH	123/123 (100%)	122 (99%)	1 (1%)	73	76
2	aJ	121/123 (98%)	119 (98%)	2 (2%)	53	67
2	aL	123/123 (100%)	122 (99%)	1 (1%)	73	76
2	aN	121/123 (98%)	121 (100%)	0	100	100
2	aP	123/123 (100%)	123 (100%)	0	100	100
2	bN	123/123 (100%)	123 (100%)	0	100	100
2	bP	123/123 (100%)	122 (99%)	1 (1%)	73	76
2	bR	121/123 (98%)	121 (100%)	0	100	100
2	bT	120/123 (98%)	119 (99%)	1 (1%)	73	76
2	bV	117/123 (95%)	116 (99%)	1 (1%)	70	75
2	bX	119/123 (97%)	118 (99%)	1 (1%)	73	76
2	cB	2/123 (2%)	2 (100%)	0	100	100
2	cD	46/123 (37%)	46 (100%)	0	100	100
2	cF	43/123 (35%)	43 (100%)	0	100	100
2	cJ	2/123 (2%)	2 (100%)	0	100	100
2	cL	1/123 (1%)	1 (100%)	0	100	100
2	dB	112/123 (91%)	112 (100%)	0	100	100
2	dD	115/123 (94%)	115 (100%)	0	100	100
2	dF	114/123 (93%)	114 (100%)	0	100	100
2	dH	123/123 (100%)	122 (99%)	1 (1%)	73	76
2	dJ	121/123 (98%)	119 (98%)	2 (2%)	53	67
2	dL	123/123 (100%)	122 (99%)	1 (1%)	73	76
2	dN	121/123 (98%)	121 (100%)	0	100	100
2	dP	123/123 (100%)	123 (100%)	0	100	100
2	eN	123/123 (100%)	123 (100%)	0	100	100
2	eP	123/123 (100%)	122 (99%)	1 (1%)	73	76
2	eR	121/123 (98%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	eT	120/123 (98%)	119 (99%)	1 (1%)	73	76
2	eV	117/123 (95%)	116 (99%)	1 (1%)	70	75
2	eX	119/123 (97%)	118 (99%)	1 (1%)	73	76
2	fB	2/123 (2%)	2 (100%)	0	100	100
2	fD	46/123 (37%)	46 (100%)	0	100	100
2	fF	43/123 (35%)	43 (100%)	0	100	100
2	fJ	2/123 (2%)	2 (100%)	0	100	100
2	fL	1/123 (1%)	1 (100%)	0	100	100
3	aM	791/956 (83%)	786 (99%)	5 (1%)	78	79
3	dM	791/956 (83%)	786 (99%)	5 (1%)	78	79
4	aR	134/135 (99%)	133 (99%)	1 (1%)	76	77
4	dR	134/135 (99%)	133 (99%)	1 (1%)	76	77
5	bY	51/60 (85%)	51 (100%)	0	100	100
5	eY	51/60 (85%)	51 (100%)	0	100	100
All	All	8982/11916 (75%)	8930 (99%)	52 (1%)	76	79

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	dG	7	LYS
3	dM	555	VAL
2	eV	134	GLN
2	dH	10	ASN
1	dK	72	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	dL	2	GLN
3	dM	752	GLN
2	dL	10	ASN
3	dM	453	HIS
1	dO	174	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	MEN	dD	71	2	7,8,9	1.16	1 (14%)	4,9,11	0.72	0
2	MEN	eR	71	2	7,8,9	1.14	1 (14%)	4,9,11	0.70	0
2	MEN	fD	71	2	3,4,9	0.55	0	2,4,11	0.99	0
2	MEN	aD	71	2	7,8,9	1.16	1 (14%)	4,9,11	0.72	0
2	MEN	bT	71	2	7,8,9	1.16	1 (14%)	4,9,11	0.74	0
2	MEN	cF	71	2	3,4,9	0.54	0	2,4,11	0.99	0
2	MEN	eV	71	2	7,8,9	1.17	1 (14%)	4,9,11	0.83	0
2	MEN	bV	71	2	7,8,9	1.17	1 (14%)	4,9,11	0.83	0
2	MEN	dJ	71	2	7,8,9	1.19	1 (14%)	4,9,11	0.63	0
2	MEN	bN	71	2	7,8,9	1.09	1 (14%)	4,9,11	0.72	0
2	MEN	dL	71	2	7,8,9	1.11	1 (14%)	4,9,11	0.66	0
2	MEN	bX	71	2	7,8,9	1.15	1 (14%)	4,9,11	0.77	0
2	MEN	cH	71	2	3,4,9	0.55	0	2,4,11	0.89	0
2	MEN	cJ	71	2	3,4,9	0.54	0	2,4,11	0.95	0
2	MEN	dP	71	2	7,8,9	1.14	1 (14%)	4,9,11	0.70	0
2	MEN	aL	71	2	7,8,9	1.11	1 (14%)	4,9,11	0.66	0
2	MEN	eN	71	2	7,8,9	1.09	1 (14%)	4,9,11	0.72	0
2	MEN	fF	71	2	3,4,9	0.54	0	2,4,11	0.99	0
2	MEN	cL	71	2	3,4,9	0.55	0	2,4,11	0.95	0
2	MEN	dB	71	2	7,8,9	1.15	1 (14%)	4,9,11	0.63	0
2	MEN	aP	71	2	7,8,9	1.14	1 (14%)	4,9,11	0.70	0
2	MEN	fB	71	2	3,4,9	0.56	0	2,4,11	0.98	0
2	MEN	fH	71	2	3,4,9	0.55	0	2,4,11	0.89	0
2	MEN	dN	71	2	7,8,9	1.12	1 (14%)	4,9,11	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	dF	71	2	7,8,9	1.17	1 (14%)	4,9,11	0.72	0
2	MEN	aJ	71	2	7,8,9	1.19	1 (14%)	4,9,11	0.63	0
2	MEN	aN	71	2	7,8,9	1.12	1 (14%)	4,9,11	0.67	0
2	MEN	dH	71	2	7,8,9	1.12	1 (14%)	4,9,11	0.65	0
2	MEN	aH	71	2	7,8,9	1.12	1 (14%)	4,9,11	0.65	0
2	MEN	aB	71	2	7,8,9	1.15	1 (14%)	4,9,11	0.63	0
2	MEN	eT	71	2	7,8,9	1.16	1 (14%)	4,9,11	0.74	0
2	MEN	cD	71	2	3,4,9	0.55	0	2,4,11	0.99	0
2	MEN	eX	71	2	7,8,9	1.15	1 (14%)	4,9,11	0.77	0
2	MEN	fL	71	2	3,4,9	0.55	0	2,4,11	0.95	0
4	MEN	aR	72	4	7,8,9	1.15	1 (14%)	4,9,11	0.70	0
2	MEN	bR	71	2	7,8,9	1.14	1 (14%)	4,9,11	0.70	0
2	MEN	fJ	71	2	3,4,9	0.54	0	2,4,11	0.95	0
2	MEN	cB	71	2	3,4,9	0.55	0	2,4,11	0.98	0
2	MEN	aF	71	2	7,8,9	1.17	1 (14%)	4,9,11	0.71	0
4	MEN	dR	72	4	7,8,9	1.15	1 (14%)	4,9,11	0.70	0
2	MEN	bP	71	2	7,8,9	1.13	1 (14%)	4,9,11	0.65	0
2	MEN	eP	71	2	7,8,9	1.13	1 (14%)	4,9,11	0.65	0

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
2	MEN	dD	71	2	-	2/7/8/10	-
2	MEN	eR	71	2	-	3/7/8/10	-
2	MEN	fD	71	2	-	1/1/2/10	-
2	MEN	aD	71	2	-	2/7/8/10	-
2	MEN	bT	71	2	-	0/7/8/10	-
2	MEN	cF	71	2	-	1/1/2/10	-
2	MEN	eV	71	2	-	1/7/8/10	-
2	MEN	bV	71	2	-	1/7/8/10	-
2	MEN	dJ	71	2	-	4/7/8/10	-
2	MEN	bN	71	2	-	0/7/8/10	-
2	MEN	dL	71	2	-	5/7/8/10	-
2	MEN	bX	71	2	-	0/7/8/10	-
2	MEN	cH	71	2	-	1/1/2/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	cJ	71	2	-	1/1/2/10	-
2	MEN	dP	71	2	-	2/7/8/10	-
2	MEN	aL	71	2	-	5/7/8/10	-
2	MEN	eN	71	2	-	0/7/8/10	-
2	MEN	fF	71	2	-	1/1/2/10	-
2	MEN	cL	71	2	-	1/1/2/10	-
2	MEN	dB	71	2	-	2/7/8/10	-
2	MEN	aP	71	2	-	2/7/8/10	-
2	MEN	fB	71	2	-	1/1/2/10	-
2	MEN	fH	71	2	-	1/1/2/10	-
2	MEN	dN	71	2	-	5/7/8/10	-
2	MEN	dF	71	2	-	0/7/8/10	-
2	MEN	aJ	71	2	-	4/7/8/10	-
2	MEN	aN	71	2	-	5/7/8/10	-
2	MEN	dH	71	2	-	3/7/8/10	-
2	MEN	aH	71	2	-	3/7/8/10	-
2	MEN	aB	71	2	-	2/7/8/10	-
2	MEN	eT	71	2	-	0/7/8/10	-
2	MEN	cD	71	2	-	1/1/2/10	-
2	MEN	eX	71	2	-	0/7/8/10	-
2	MEN	fL	71	2	-	1/1/2/10	-
4	MEN	aR	72	4	-	4/7/8/10	-
2	MEN	bR	71	2	-	3/7/8/10	-
2	MEN	fJ	71	2	-	1/1/2/10	-
2	MEN	cB	71	2	-	1/1/2/10	-
2	MEN	aF	71	2	-	0/7/8/10	-
4	MEN	dR	72	4	-	4/7/8/10	-
2	MEN	bP	71	2	-	2/7/8/10	-
2	MEN	eP	71	2	-	2/7/8/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	dF	71	MEN	CE2-ND2	2.97	1.50	1.45
2	aF	71	MEN	CE2-ND2	2.96	1.50	1.45
2	bV	71	MEN	CE2-ND2	2.95	1.50	1.45
2	eV	71	MEN	CE2-ND2	2.95	1.50	1.45
2	eT	71	MEN	CE2-ND2	2.92	1.50	1.45

There are no bond angle outliers.

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	aB	71	MEN	C-CA-CB-CG
2	aJ	71	MEN	C-CA-CB-CG
2	aL	71	MEN	O-C-CA-CB
2	aL	71	MEN	C-CA-CB-CG
2	aN	71	MEN	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	dL	71	MEN	2	0
2	aL	71	MEN	2	0
2	dB	71	MEN	1	0
2	aB	71	MEN	1	0
2	bP	71	MEN	1	0
2	eP	71	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

84 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$
6	CYC	bP	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.27	29 (46%)
6	CYC	aF	201	2	46,46,46	2.12	14 (30%)	63,67,67	3.24	24 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	aO	201	1	46,46,46	2.17	14 (30%)	63,67,67	3.24	29 (46%)
6	CYC	dJ	201	2	46,46,46	2.15	14 (30%)	63,67,67	3.49	31 (49%)
6	CYC	cD	201	-	46,46,46	2.13	15 (32%)	63,67,67	3.17	31 (49%)
6	CYC	aG	201	1	46,46,46	2.14	14 (30%)	63,67,67	3.31	26 (41%)
6	CYC	bM	201	1	46,46,46	2.14	14 (30%)	63,67,67	3.27	31 (49%)
6	CYC	aE	201	1	46,46,46	2.17	14 (30%)	63,67,67	3.32	32 (50%)
6	CYC	cM	101	-	46,46,46	2.13	15 (32%)	63,67,67	3.23	30 (47%)
6	CYC	bT	201	2	46,46,46	2.15	14 (30%)	63,67,67	3.29	28 (44%)
6	CYC	fL	201	-	46,46,46	2.14	15 (32%)	63,67,67	3.22	29 (46%)
6	CYC	aD	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.26	26 (41%)
6	CYC	aH	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.31	33 (52%)
6	CYC	aJ	201	2	46,46,46	2.15	14 (30%)	63,67,67	3.49	31 (49%)
6	CYC	cG	201	-	46,46,46	2.16	15 (32%)	63,67,67	3.24	31 (49%)
6	CYC	dI	201	1	46,46,46	2.13	14 (30%)	63,67,67	3.35	28 (44%)
6	CYC	aB	201	2	46,46,46	2.15	15 (32%)	63,67,67	3.26	30 (47%)
6	CYC	aM	1202	-	46,46,46	2.14	15 (32%)	63,67,67	3.22	30 (47%)
6	CYC	dR	201	4	46,46,46	2.22	15 (32%)	63,67,67	3.22	28 (44%)
6	CYC	dO	201	1	46,46,46	2.17	14 (30%)	63,67,67	3.24	29 (46%)
6	CYC	cF	201	-	46,46,46	2.14	15 (32%)	63,67,67	3.27	31 (49%)
6	CYC	aI	201	1	46,46,46	2.13	14 (30%)	63,67,67	3.35	28 (44%)
6	CYC	aA	201	1	46,46,46	2.12	14 (30%)	63,67,67	3.31	28 (44%)
6	CYC	eT	201	2	46,46,46	2.15	14 (30%)	63,67,67	3.30	28 (44%)
6	CYC	aC	201	1	46,46,46	2.14	14 (30%)	63,67,67	3.31	31 (49%)
6	CYC	eW	201	1	46,46,46	2.15	15 (32%)	63,67,67	3.23	31 (49%)
6	CYC	eM	201	1	46,46,46	2.14	14 (30%)	63,67,67	3.27	31 (49%)
6	CYC	dG	201	1	46,46,46	2.14	14 (30%)	63,67,67	3.31	26 (41%)
6	CYC	aM	1203	-	46,46,46	2.13	15 (32%)	63,67,67	3.25	27 (42%)
6	CYC	cD	202	-	46,46,46	2.12	14 (30%)	63,67,67	3.30	33 (52%)
6	CYC	cB	201	-	46,46,46	2.16	15 (32%)	63,67,67	3.22	30 (47%)
6	CYC	dF	201	2	46,46,46	2.12	14 (30%)	63,67,67	3.24	24 (38%)
6	CYC	aK	201	1	46,46,46	2.13	14 (30%)	63,67,67	3.35	31 (49%)
6	CYC	bR	201	2	46,46,46	2.12	14 (30%)	63,67,67	3.33	31 (49%)
6	CYC	eV	201	2	46,46,46	2.14	14 (30%)	63,67,67	3.28	28 (44%)
6	CYC	fD	202	-	46,46,46	2.12	14 (30%)	63,67,67	3.30	33 (52%)
6	CYC	dC	201	1	46,46,46	2.14	14 (30%)	63,67,67	3.31	31 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	dK	201	1	46,46,46	2.13	14 (30%)	63,67,67	3.35	31 (49%)
6	CYC	dQ	201	1	46,46,46	2.14	13 (28%)	63,67,67	3.31	29 (46%)
6	CYC	eR	201	2	46,46,46	2.12	14 (30%)	63,67,67	3.33	30 (47%)
6	CYC	dD	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.26	27 (42%)
6	CYC	aR	201	4	46,46,46	2.22	15 (32%)	63,67,67	3.22	28 (44%)
6	CYC	dH	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.31	33 (52%)
6	CYC	dL	201	2	46,46,46	2.15	13 (28%)	63,67,67	3.33	30 (47%)
6	CYC	dA	201	1	46,46,46	2.12	14 (30%)	63,67,67	3.30	28 (44%)
6	CYC	eQ	201	1	46,46,46	2.13	15 (32%)	63,67,67	3.24	29 (46%)
6	CYC	aL	201	2	46,46,46	2.15	13 (28%)	63,67,67	3.33	30 (47%)
6	CYC	eN	201	2	46,46,46	2.14	13 (28%)	63,67,67	3.33	28 (44%)
6	CYC	bU	201	1	46,46,46	2.17	13 (28%)	63,67,67	3.32	31 (49%)
6	CYC	bO	201	1	46,46,46	2.15	13 (28%)	63,67,67	3.30	29 (46%)
6	CYC	fI	201	-	46,46,46	2.17	14 (30%)	63,67,67	3.24	30 (47%)
6	CYC	dB	201	2	46,46,46	2.14	15 (32%)	63,67,67	3.26	30 (47%)
6	CYC	aQ	201	1	46,46,46	2.14	13 (28%)	63,67,67	3.31	29 (46%)
6	CYC	bV	201	2	46,46,46	2.14	14 (30%)	63,67,67	3.28	28 (44%)
6	CYC	aM	1201	3	46,46,46	2.15	14 (30%)	63,67,67	3.30	31 (49%)
6	CYC	cL	201	-	46,46,46	2.14	15 (32%)	63,67,67	3.22	30 (47%)
6	CYC	eS	201	1	46,46,46	2.15	15 (32%)	63,67,67	3.30	27 (42%)
6	CYC	fF	201	-	46,46,46	2.14	15 (32%)	63,67,67	3.27	31 (49%)
6	CYC	fM	101	-	46,46,46	2.13	15 (32%)	63,67,67	3.23	30 (47%)
6	CYC	eP	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.27	29 (46%)
6	CYC	aP	201	2	46,46,46	2.17	14 (30%)	63,67,67	3.34	31 (49%)
6	CYC	cJ	201	-	46,46,46	2.15	15 (32%)	63,67,67	3.29	31 (49%)
6	CYC	eO	201	1	46,46,46	2.15	13 (28%)	63,67,67	3.30	29 (46%)
6	CYC	bW	201	1	46,46,46	2.15	15 (32%)	63,67,67	3.23	31 (49%)
6	CYC	fG	201	-	46,46,46	2.16	15 (32%)	63,67,67	3.24	31 (49%)
6	CYC	bN	201	2	46,46,46	2.14	13 (28%)	63,67,67	3.34	28 (44%)
6	CYC	eX	201	2	46,46,46	2.13	15 (32%)	63,67,67	3.26	29 (46%)
6	CYC	fF	202	-	46,46,46	2.13	15 (32%)	63,67,67	3.22	29 (46%)
6	CYC	bS	201	1	46,46,46	2.15	15 (32%)	63,67,67	3.30	27 (42%)
6	CYC	dE	201	1	46,46,46	2.17	14 (30%)	63,67,67	3.32	32 (50%)
6	CYC	dP	201	2	46,46,46	2.17	14 (30%)	63,67,67	3.35	31 (49%)
6	CYC	dM	1202	-	46,46,46	2.14	15 (32%)	63,67,67	3.22	30 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CYC	eU	201	1	46,46,46	2.16	13 (28%)	63,67,67	3.32	31 (49%)
6	CYC	dM	1203	-	46,46,46	2.13	15 (32%)	63,67,67	3.25	27 (42%)
6	CYC	fD	201	-	46,46,46	2.13	15 (32%)	63,67,67	3.17	31 (49%)
6	CYC	bX	201	2	46,46,46	2.13	15 (32%)	63,67,67	3.26	29 (46%)
6	CYC	dN	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.30	29 (46%)
6	CYC	cF	202	-	46,46,46	2.13	15 (32%)	63,67,67	3.23	29 (46%)
6	CYC	bQ	201	1	46,46,46	2.13	15 (32%)	63,67,67	3.24	29 (46%)
6	CYC	aN	201	2	46,46,46	2.13	14 (30%)	63,67,67	3.30	30 (47%)
6	CYC	fB	201	-	46,46,46	2.16	15 (32%)	63,67,67	3.22	30 (47%)
6	CYC	fJ	201	-	46,46,46	2.15	15 (32%)	63,67,67	3.29	31 (49%)
6	CYC	dM	1201	3	46,46,46	2.15	14 (30%)	63,67,67	3.30	31 (49%)
6	CYC	cI	201	-	46,46,46	2.17	14 (30%)	63,67,67	3.23	30 (47%)

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
6	CYC	bP	201	2	-	10/26/74/74	0/4/4/4
6	CYC	aF	201	2	-	11/26/74/74	0/4/4/4
6	CYC	aO	201	1	-	9/26/74/74	0/4/4/4
6	CYC	dJ	201	2	-	14/26/74/74	0/4/4/4
6	CYC	cD	201	-	-	10/26/74/74	0/4/4/4
6	CYC	aG	201	1	-	12/26/74/74	0/4/4/4
6	CYC	bM	201	1	-	11/26/74/74	0/4/4/4
6	CYC	aE	201	1	-	11/26/74/74	0/4/4/4
6	CYC	cM	101	-	-	11/26/74/74	0/4/4/4
6	CYC	bT	201	2	-	11/26/74/74	0/4/4/4
6	CYC	fL	201	-	-	11/26/74/74	0/4/4/4
6	CYC	aD	201	2	-	7/26/74/74	0/4/4/4
6	CYC	aH	201	2	-	9/26/74/74	0/4/4/4
6	CYC	aJ	201	2	-	14/26/74/74	0/4/4/4
6	CYC	cG	201	-	-	10/26/74/74	0/4/4/4
6	CYC	dI	201	1	-	9/26/74/74	0/4/4/4
6	CYC	aB	201	2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	aM	1202	-	-	10/26/74/74	0/4/4/4
6	CYC	dR	201	4	-	9/26/74/74	0/4/4/4
6	CYC	dO	201	1	-	9/26/74/74	0/4/4/4
6	CYC	cF	201	-	-	12/26/74/74	0/4/4/4
6	CYC	aI	201	1	-	9/26/74/74	0/4/4/4
6	CYC	aA	201	1	-	10/26/74/74	0/4/4/4
6	CYC	eT	201	2	-	11/26/74/74	0/4/4/4
6	CYC	aC	201	1	-	9/26/74/74	0/4/4/4
6	CYC	eW	201	1	-	10/26/74/74	0/4/4/4
6	CYC	eM	201	1	-	11/26/74/74	0/4/4/4
6	CYC	dG	201	1	-	12/26/74/74	0/4/4/4
6	CYC	aM	1203	-	-	8/26/74/74	0/4/4/4
6	CYC	cD	202	-	-	10/26/74/74	0/4/4/4
6	CYC	cB	201	-	-	11/26/74/74	0/4/4/4
6	CYC	dF	201	2	-	11/26/74/74	0/4/4/4
6	CYC	aK	201	1	-	11/26/74/74	0/4/4/4
6	CYC	bR	201	2	-	10/26/74/74	0/4/4/4
6	CYC	eV	201	2	-	8/26/74/74	0/4/4/4
6	CYC	fD	202	-	-	10/26/74/74	0/4/4/4
6	CYC	dC	201	1	-	9/26/74/74	0/4/4/4
6	CYC	dK	201	1	-	11/26/74/74	0/4/4/4
6	CYC	dQ	201	1	-	10/26/74/74	0/4/4/4
6	CYC	eR	201	2	-	10/26/74/74	0/4/4/4
6	CYC	dD	201	2	-	7/26/74/74	0/4/4/4
6	CYC	aR	201	4	-	9/26/74/74	0/4/4/4
6	CYC	dH	201	2	-	9/26/74/74	0/4/4/4
6	CYC	dL	201	2	-	7/26/74/74	0/4/4/4
6	CYC	dA	201	1	-	10/26/74/74	0/4/4/4
6	CYC	eQ	201	1	-	10/26/74/74	0/4/4/4
6	CYC	aL	201	2	-	7/26/74/74	0/4/4/4
6	CYC	eN	201	2	-	9/26/74/74	0/4/4/4
6	CYC	bU	201	1	-	10/26/74/74	0/4/4/4
6	CYC	bO	201	1	-	8/26/74/74	0/4/4/4
6	CYC	fI	201	-	-	12/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	dB	201	2	-	8/26/74/74	0/4/4/4
6	CYC	aQ	201	1	-	10/26/74/74	0/4/4/4
6	CYC	bV	201	2	-	8/26/74/74	0/4/4/4
6	CYC	aM	1201	3	-	11/26/74/74	0/4/4/4
6	CYC	cL	201	-	-	11/26/74/74	0/4/4/4
6	CYC	eS	201	1	-	14/26/74/74	0/4/4/4
6	CYC	fF	201	-	-	12/26/74/74	0/4/4/4
6	CYC	fM	101	-	-	11/26/74/74	0/4/4/4
6	CYC	eP	201	2	-	10/26/74/74	0/4/4/4
6	CYC	aP	201	2	-	11/26/74/74	0/4/4/4
6	CYC	cJ	201	-	-	9/26/74/74	0/4/4/4
6	CYC	eO	201	1	-	8/26/74/74	0/4/4/4
6	CYC	bW	201	1	-	10/26/74/74	0/4/4/4
6	CYC	fG	201	-	-	10/26/74/74	0/4/4/4
6	CYC	bN	201	2	-	9/26/74/74	0/4/4/4
6	CYC	eX	201	2	-	7/26/74/74	0/4/4/4
6	CYC	fF	202	-	-	12/26/74/74	0/4/4/4
6	CYC	bS	201	1	-	14/26/74/74	0/4/4/4
6	CYC	dE	201	1	-	11/26/74/74	0/4/4/4
6	CYC	dP	201	2	-	11/26/74/74	0/4/4/4
6	CYC	dM	1202	-	-	10/26/74/74	0/4/4/4
6	CYC	eU	201	1	-	10/26/74/74	0/4/4/4
6	CYC	dM	1203	-	-	8/26/74/74	0/4/4/4
6	CYC	fD	201	-	-	10/26/74/74	0/4/4/4
6	CYC	bX	201	2	-	7/26/74/74	0/4/4/4
6	CYC	dN	201	2	-	9/26/74/74	0/4/4/4
6	CYC	cF	202	-	-	12/26/74/74	0/4/4/4
6	CYC	bQ	201	1	-	10/26/74/74	0/4/4/4
6	CYC	aN	201	2	-	9/26/74/74	0/4/4/4
6	CYC	fB	201	-	-	11/26/74/74	0/4/4/4
6	CYC	fJ	201	-	-	9/26/74/74	0/4/4/4
6	CYC	dM	1201	3	-	11/26/74/74	0/4/4/4
6	CYC	cI	201	-	-	12/26/74/74	0/4/4/4

The worst 5 of 1198 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	dE	201	CYC	OB-C4B	7.08	1.37	1.23
6	aE	201	CYC	OB-C4B	7.07	1.37	1.23
6	fB	201	CYC	OB-C4B	7.07	1.37	1.23
6	cI	201	CYC	OB-C4B	7.07	1.37	1.23
6	fI	201	CYC	OB-C4B	7.07	1.37	1.23

The worst 5 of 2482 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	aJ	201	CYC	C3B-C4B-NB	13.24	117.32	106.77
6	dJ	201	CYC	C3B-C4B-NB	13.24	117.32	106.77
6	eR	201	CYC	C3B-C4B-NB	12.89	117.05	106.77
6	bR	201	CYC	C3B-C4B-NB	12.88	117.04	106.77
6	fF	201	CYC	C3B-C4B-NB	12.80	116.98	106.77

There are no chirality outliers.

5 of 842 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	aB	201	CYC	NA-C4A-CHB-C1B
6	aB	201	CYC	C3A-C4A-CHB-C1B
6	aC	201	CYC	C2D-C1D-CHD-C4C
6	aD	201	CYC	NA-C4A-CHB-C1B
6	aD	201	CYC	C3A-C4A-CHB-C1B

There are no ring outliers.

76 monomers are involved in 283 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	bP	201	CYC	4	0
6	aO	201	CYC	7	0
6	dJ	201	CYC	6	0
6	cD	201	CYC	7	0
6	aG	201	CYC	3	0
6	bM	201	CYC	2	0
6	aE	201	CYC	3	0
6	cM	101	CYC	2	0
6	bT	201	CYC	2	0
6	aD	201	CYC	1	0
6	aH	201	CYC	2	0
6	aJ	201	CYC	6	0
6	cG	201	CYC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	dI	201	CYC	5	0
6	aB	201	CYC	2	0
6	aM	1202	CYC	1	0
6	dR	201	CYC	7	0
6	dO	201	CYC	8	0
6	cF	201	CYC	3	0
6	aI	201	CYC	5	0
6	aA	201	CYC	2	0
6	eT	201	CYC	2	0
6	aC	201	CYC	2	0
6	eW	201	CYC	3	0
6	eM	201	CYC	2	0
6	dG	201	CYC	3	0
6	cD	202	CYC	4	0
6	cB	201	CYC	3	0
6	aK	201	CYC	5	0
6	bR	201	CYC	4	0
6	eV	201	CYC	1	0
6	fD	202	CYC	4	0
6	dC	201	CYC	2	0
6	dK	201	CYC	4	0
6	dQ	201	CYC	5	0
6	eR	201	CYC	4	0
6	dD	201	CYC	1	0
6	aR	201	CYC	8	0
6	dH	201	CYC	2	0
6	dL	201	CYC	6	0
6	dA	201	CYC	2	0
6	eQ	201	CYC	3	0
6	aL	201	CYC	6	0
6	eN	201	CYC	4	0
6	bU	201	CYC	3	0
6	bO	201	CYC	4	0
6	fI	201	CYC	4	0
6	dB	201	CYC	3	0
6	aQ	201	CYC	5	0
6	bV	201	CYC	1	0
6	aM	1201	CYC	8	0
6	eS	201	CYC	5	0
6	fF	201	CYC	2	0
6	fM	101	CYC	2	0
6	eP	201	CYC	4	0

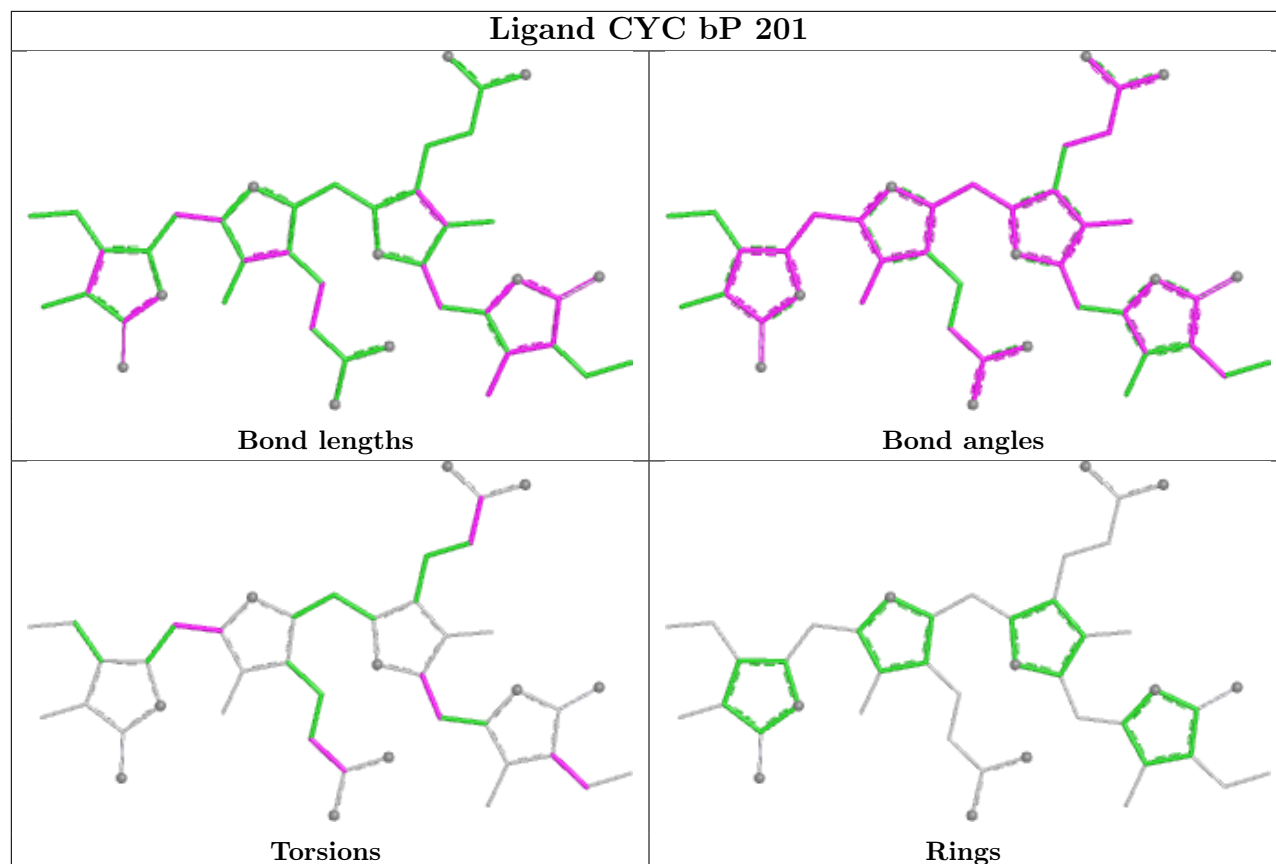
Continued on next page...

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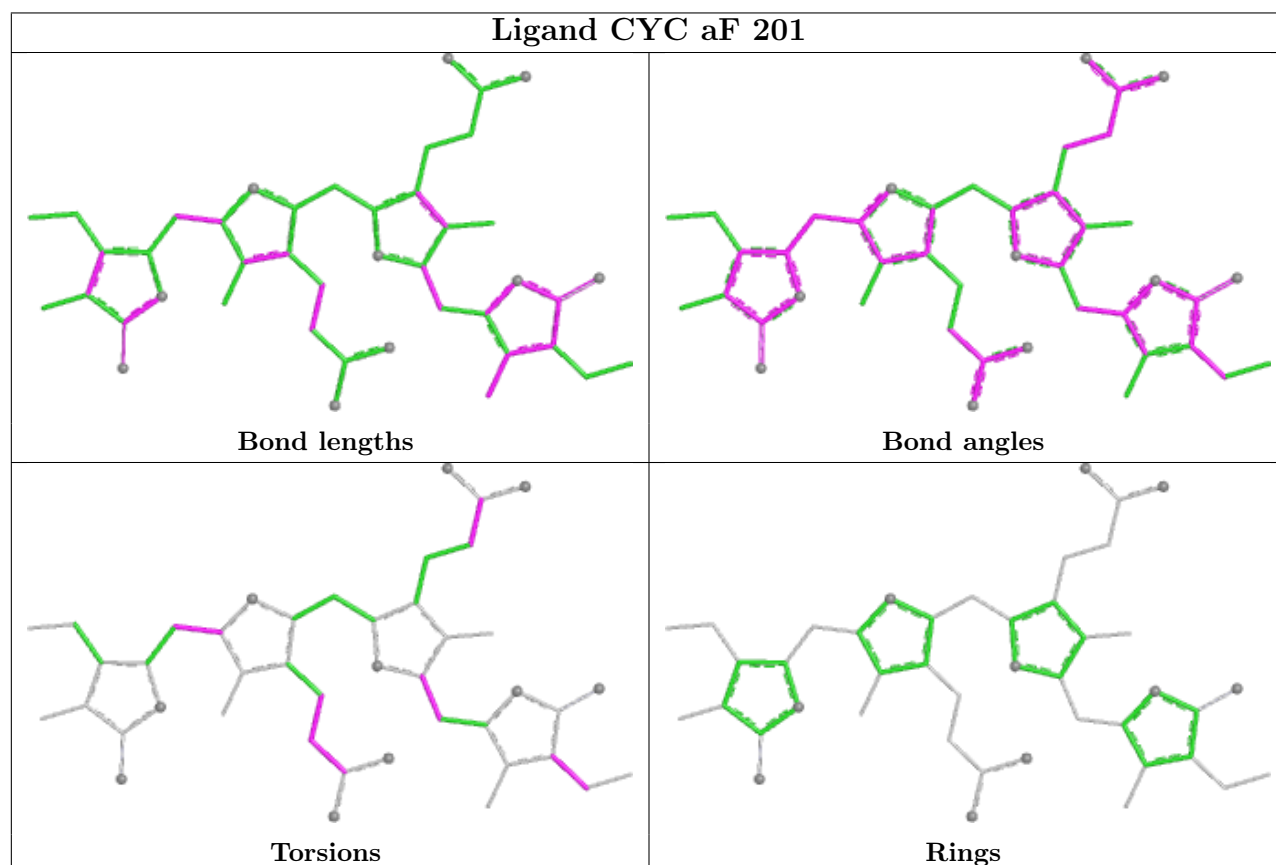
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	aP	201	CYC	7	0
6	cJ	201	CYC	2	0
6	eO	201	CYC	4	0
6	bW	201	CYC	3	0
6	fG	201	CYC	3	0
6	bN	201	CYC	4	0
6	fF	202	CYC	2	0
6	bS	201	CYC	5	0
6	dE	201	CYC	3	0
6	dP	201	CYC	5	0
6	dM	1202	CYC	1	0
6	eU	201	CYC	3	0
6	fD	201	CYC	6	0
6	dN	201	CYC	5	0
6	cF	202	CYC	2	0
6	bQ	201	CYC	3	0
6	aN	201	CYC	5	0
6	fB	201	CYC	3	0
6	fJ	201	CYC	3	0
6	dM	1201	CYC	8	0
6	cI	201	CYC	4	0

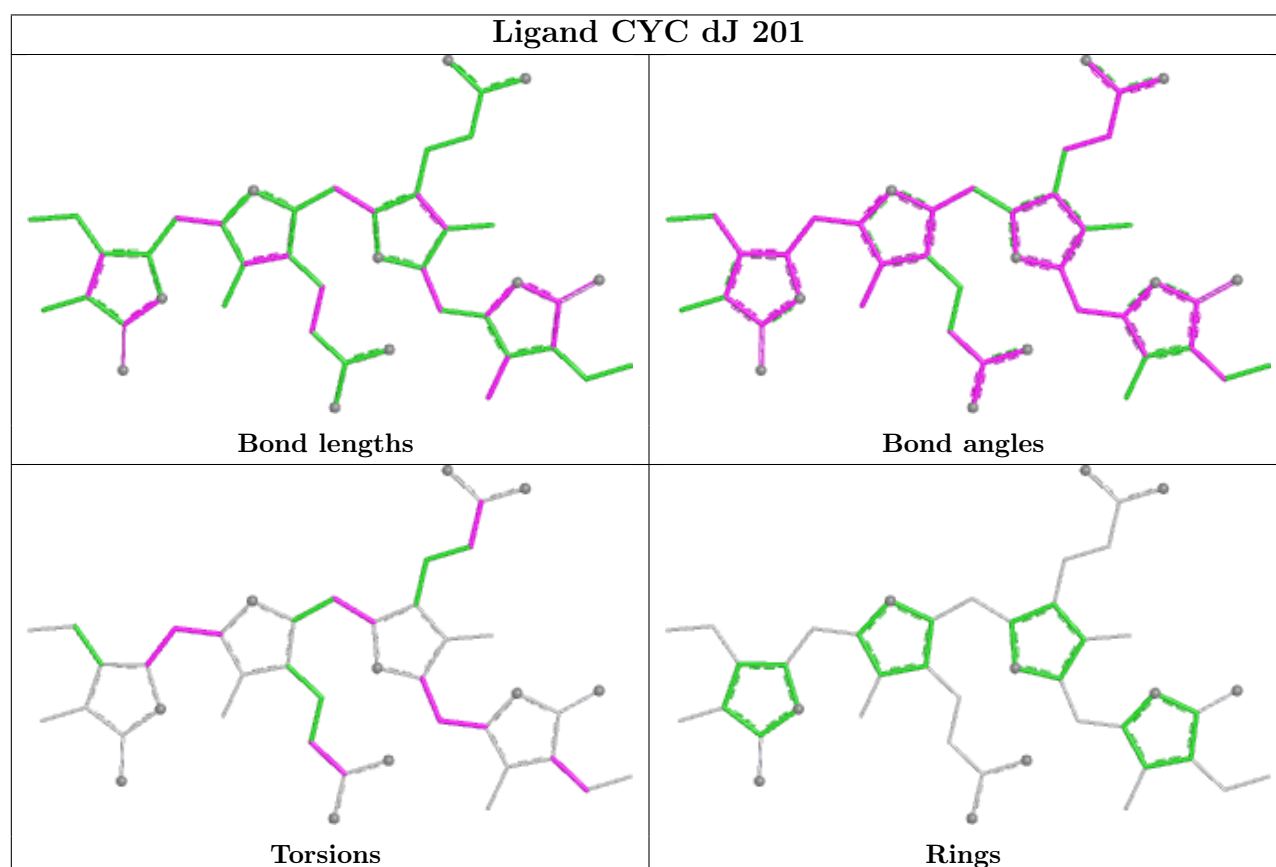
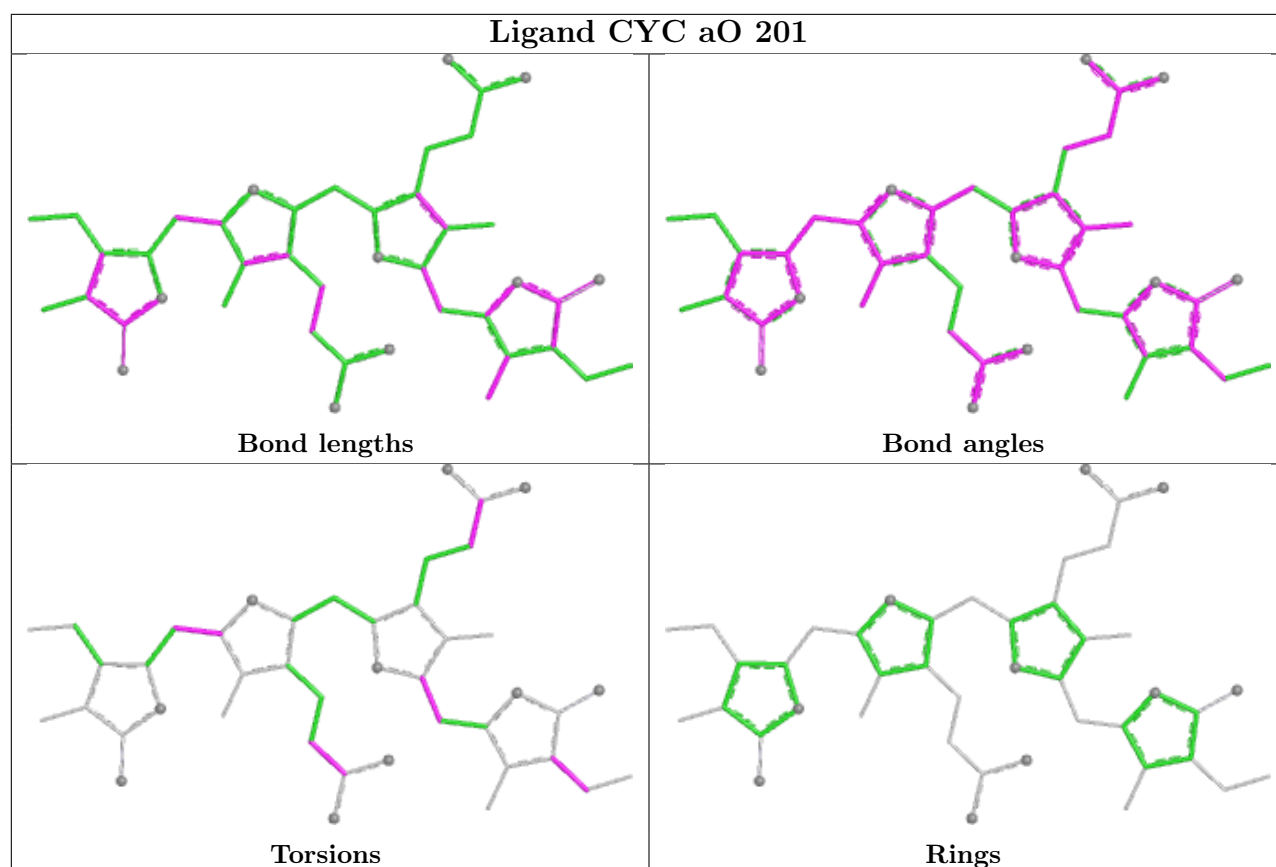
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

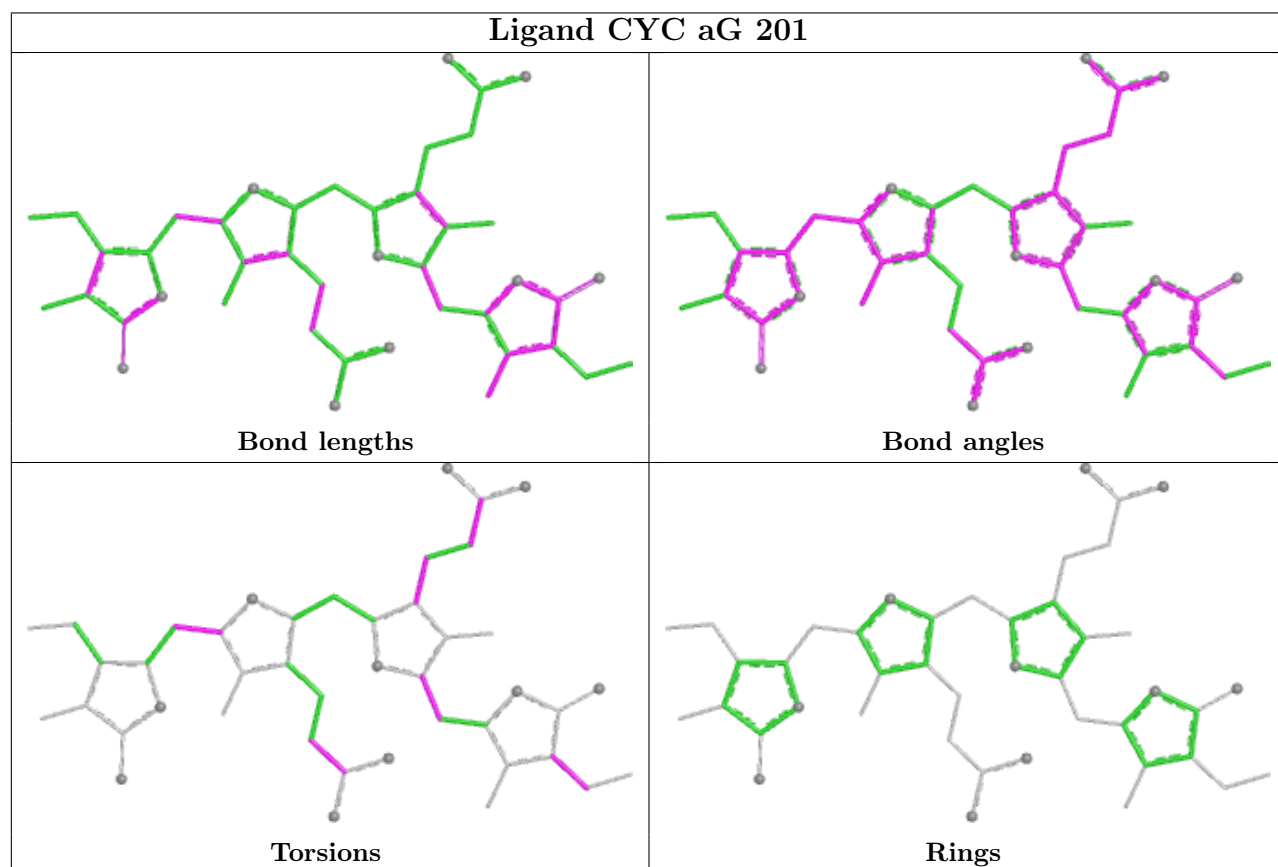
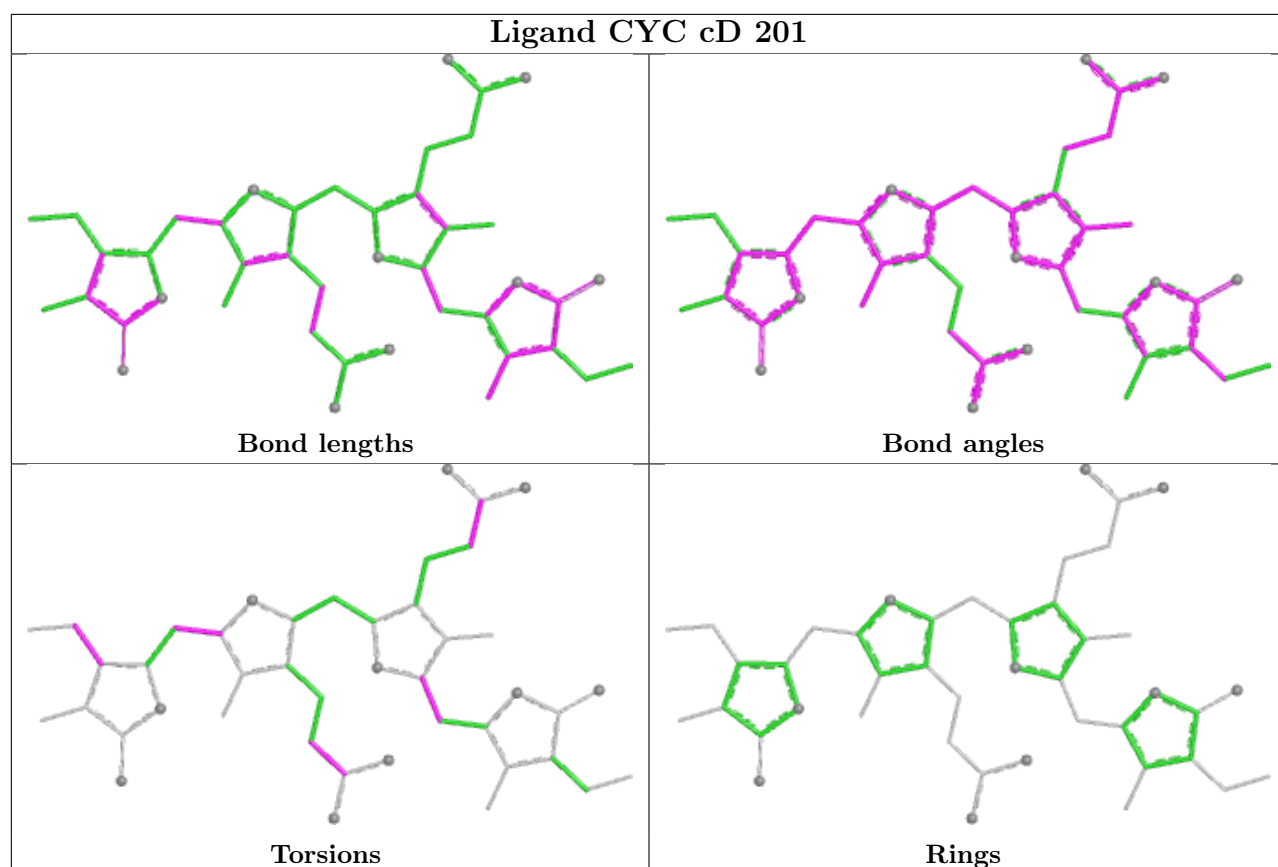
Ligand CYC bP 201



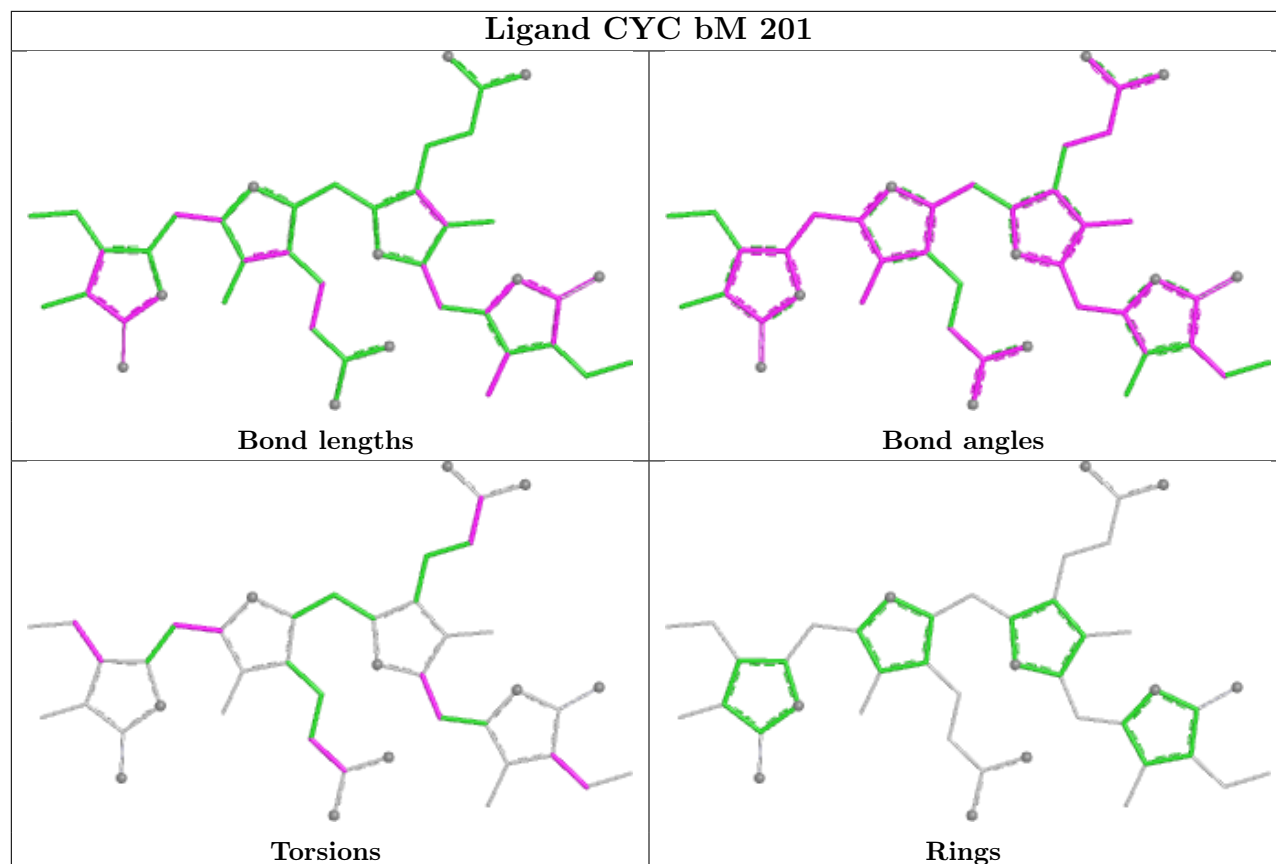
Ligand CYC aF 201



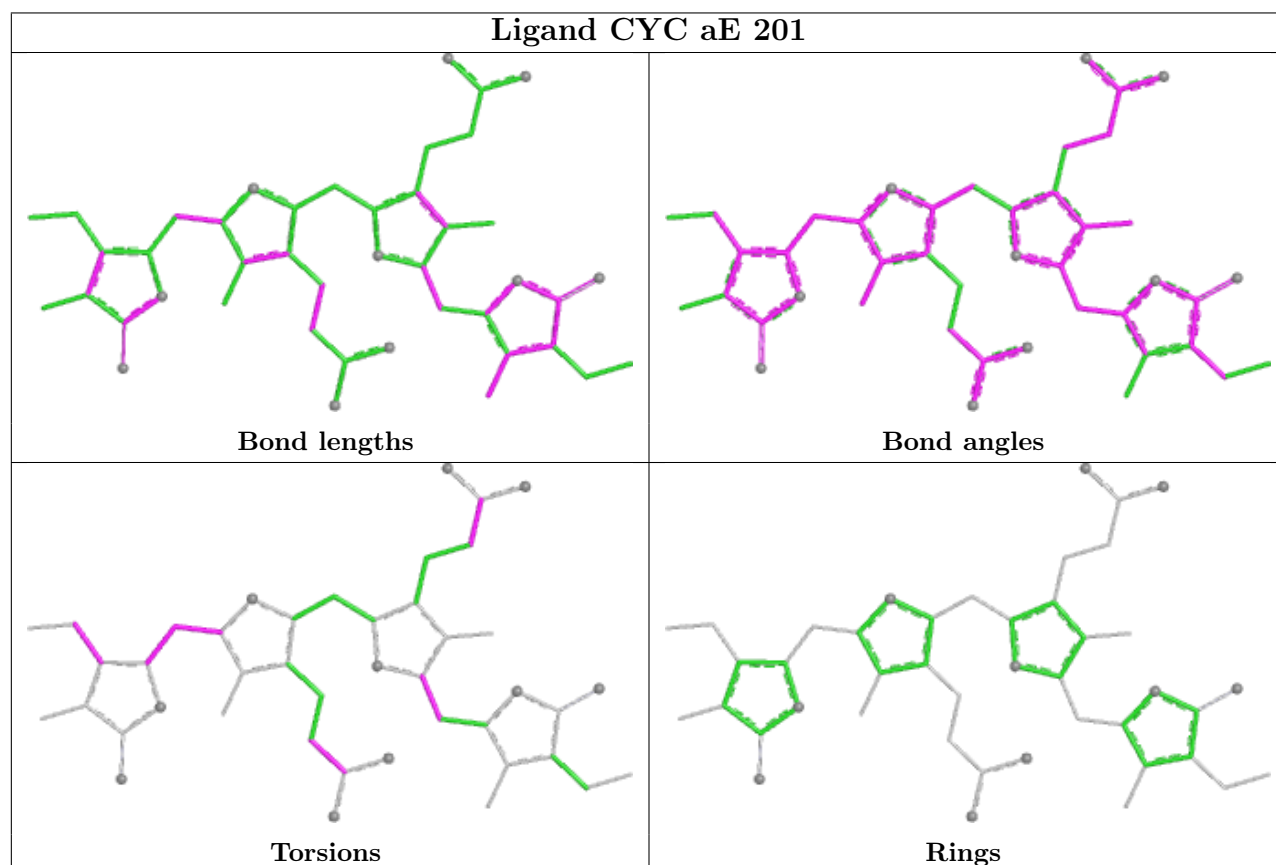


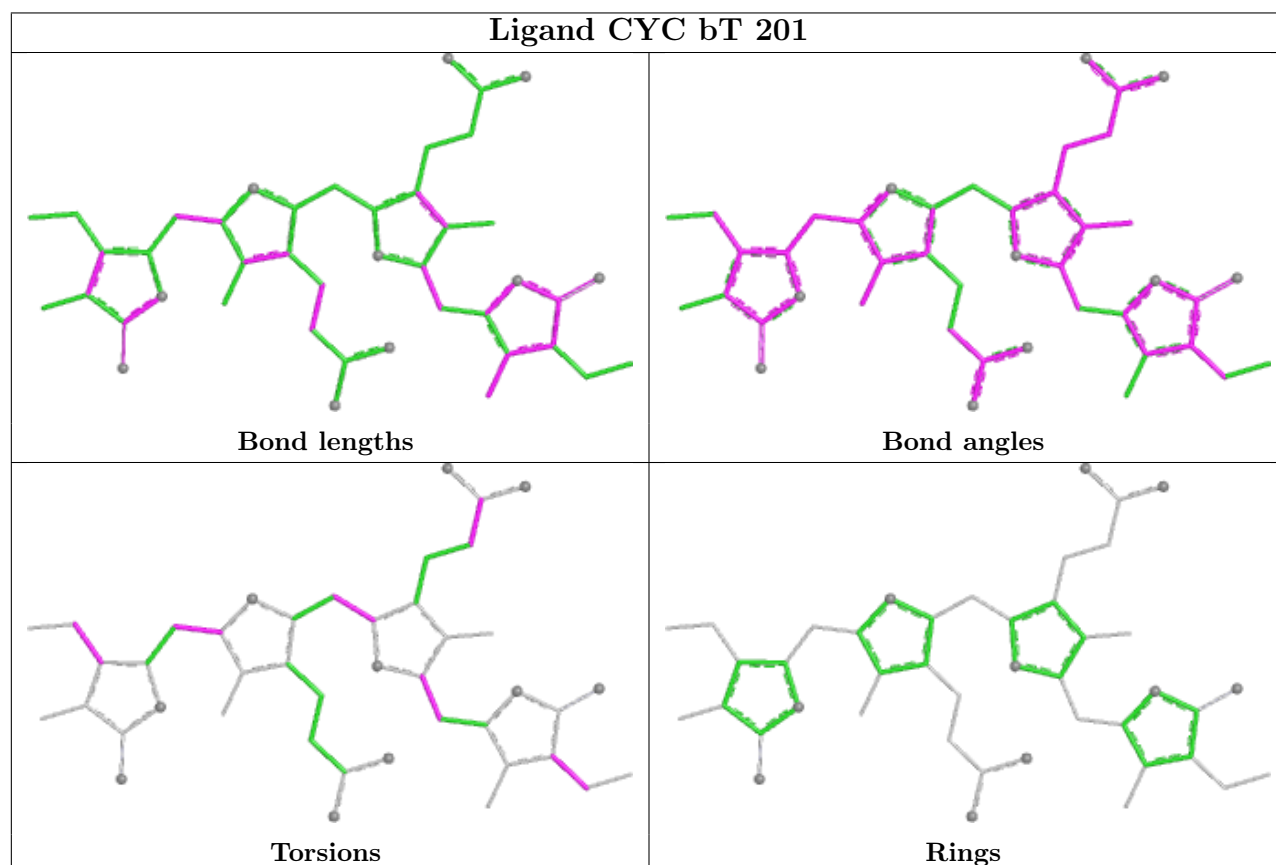
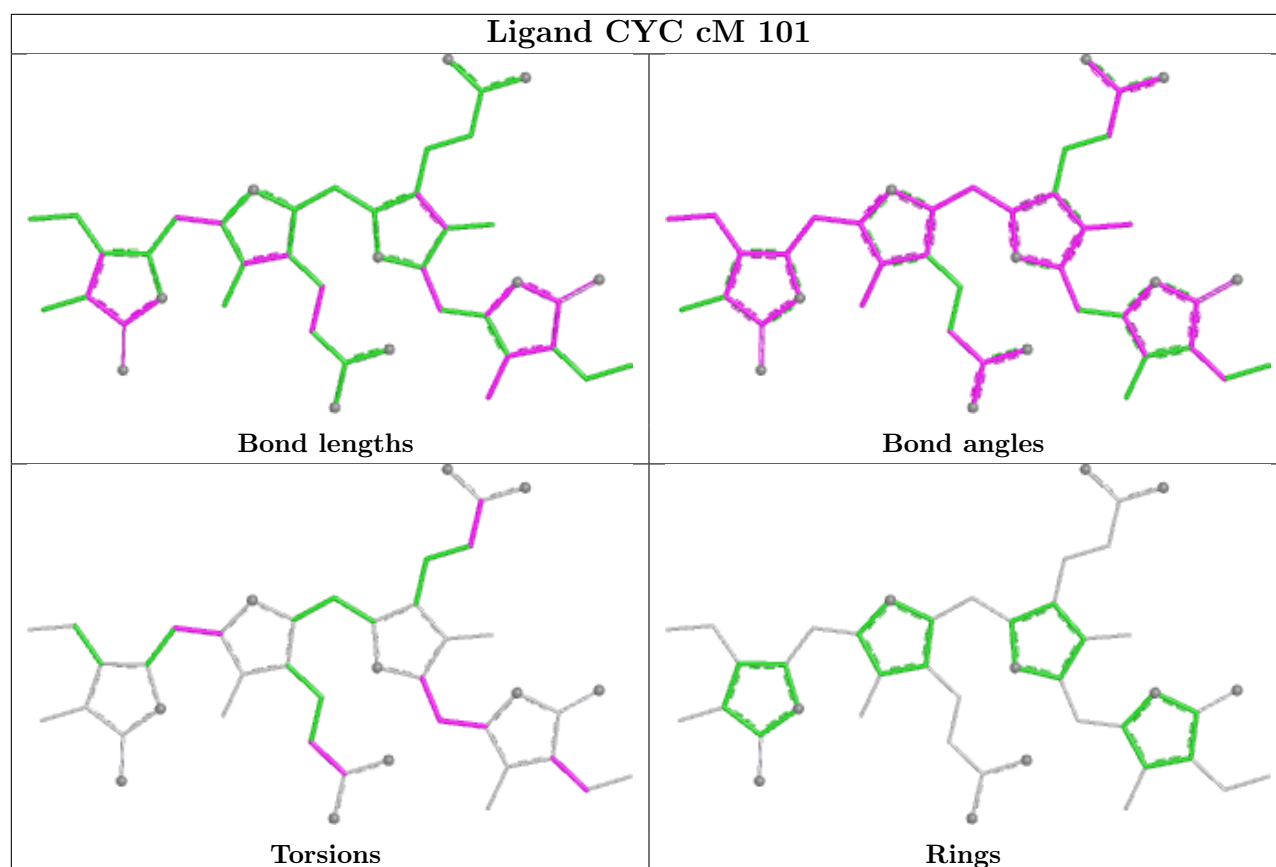


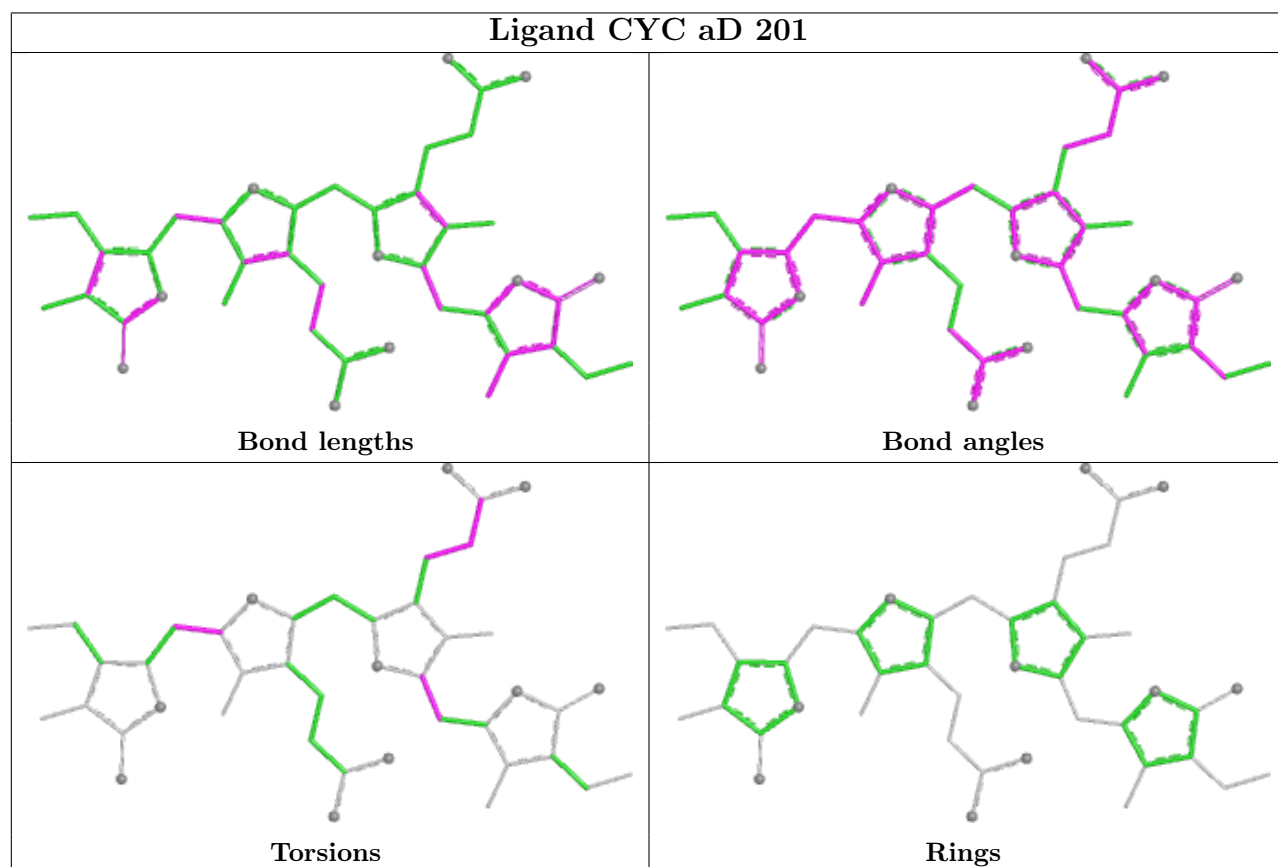
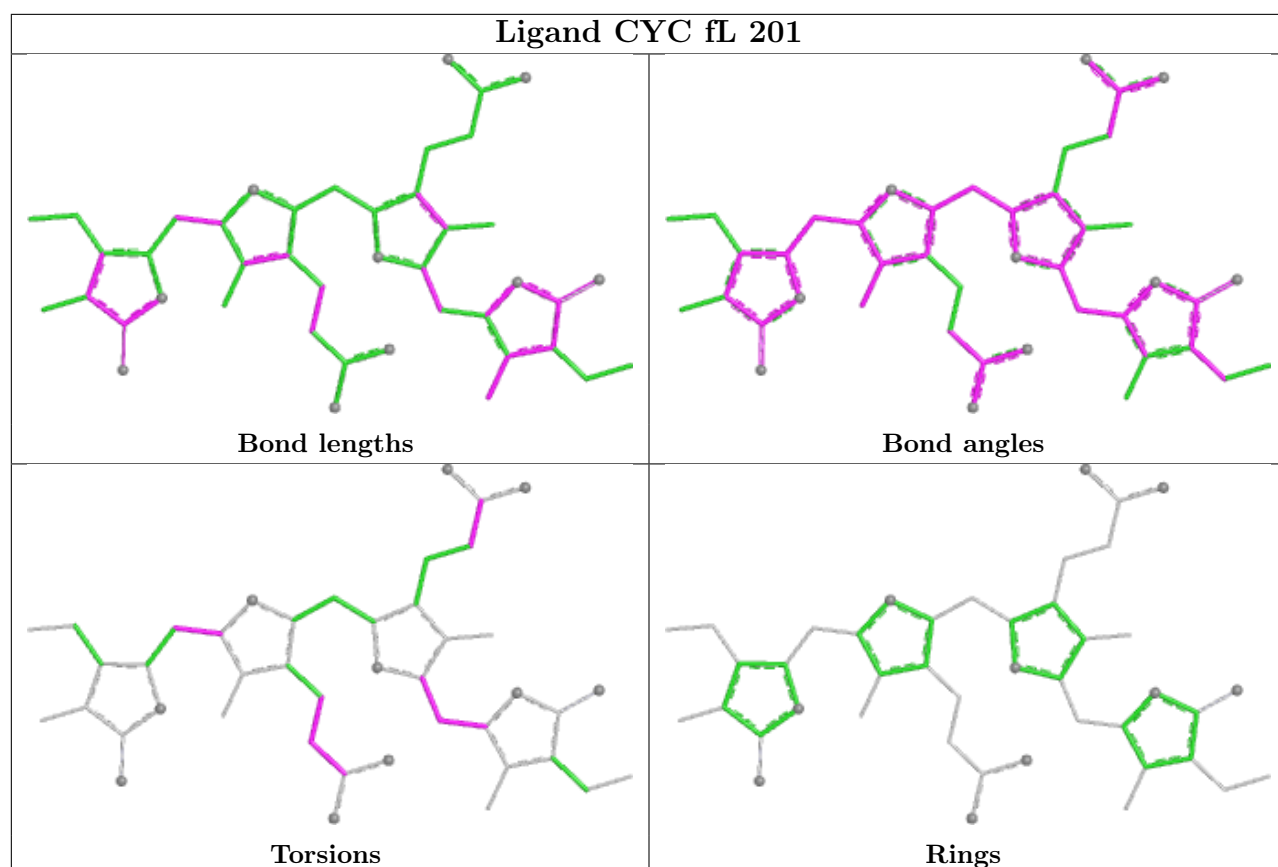
Ligand CYC bM 201

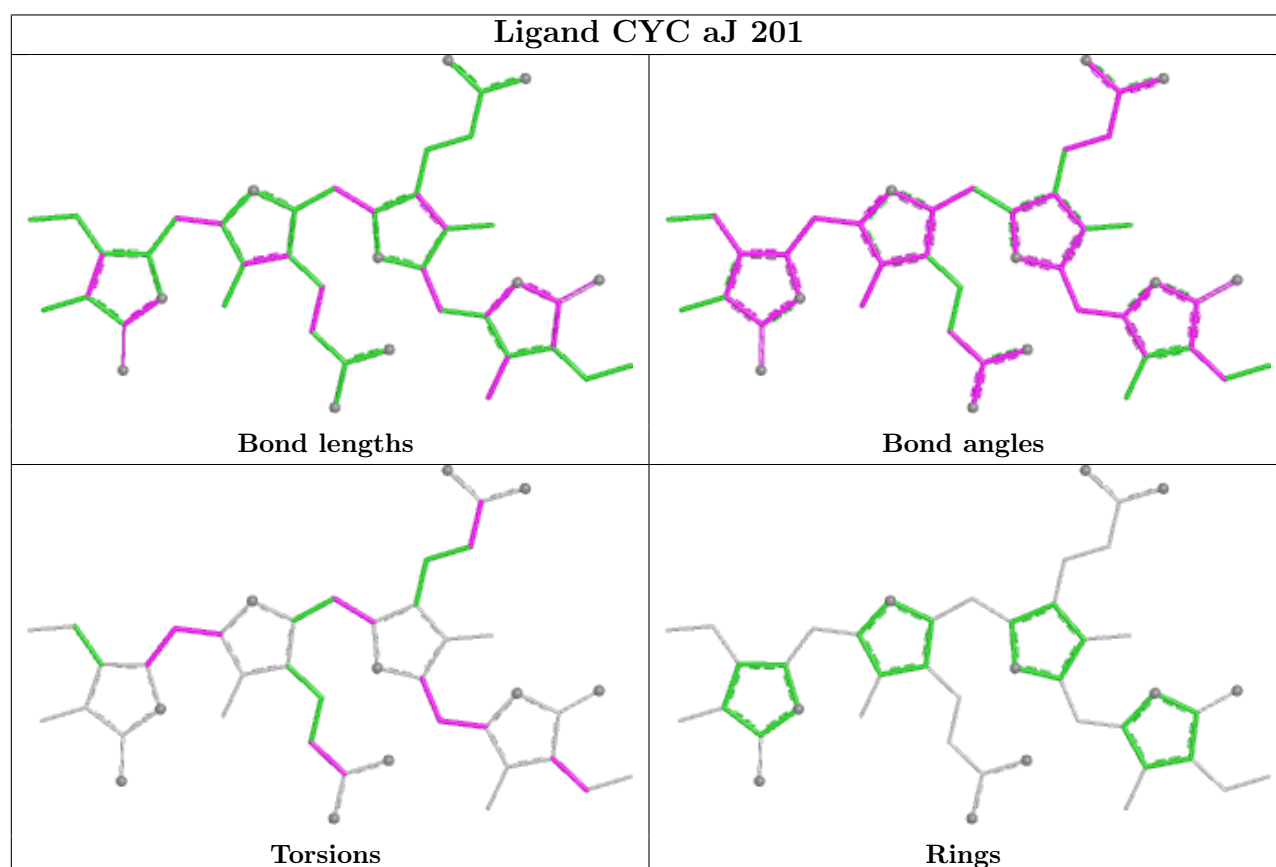
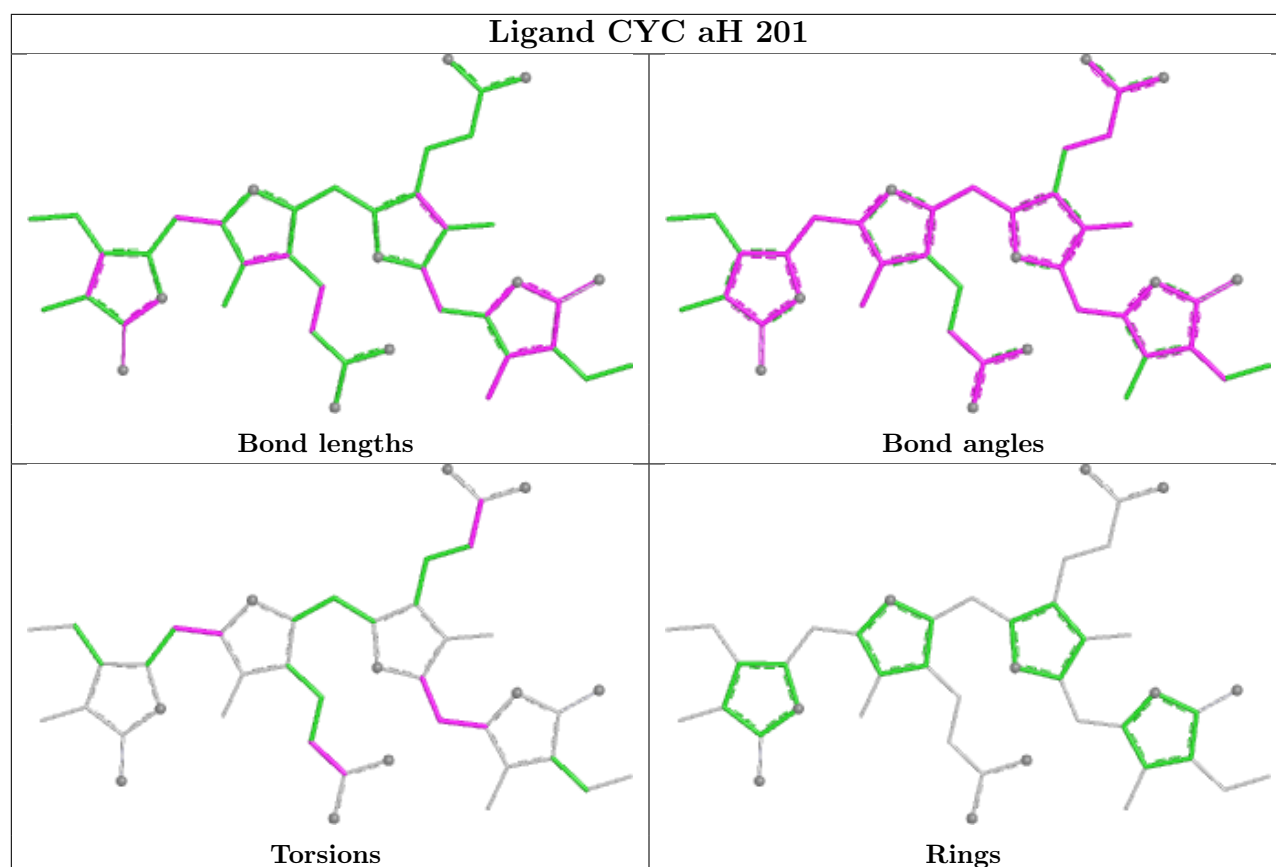


Ligand CYC aE 201

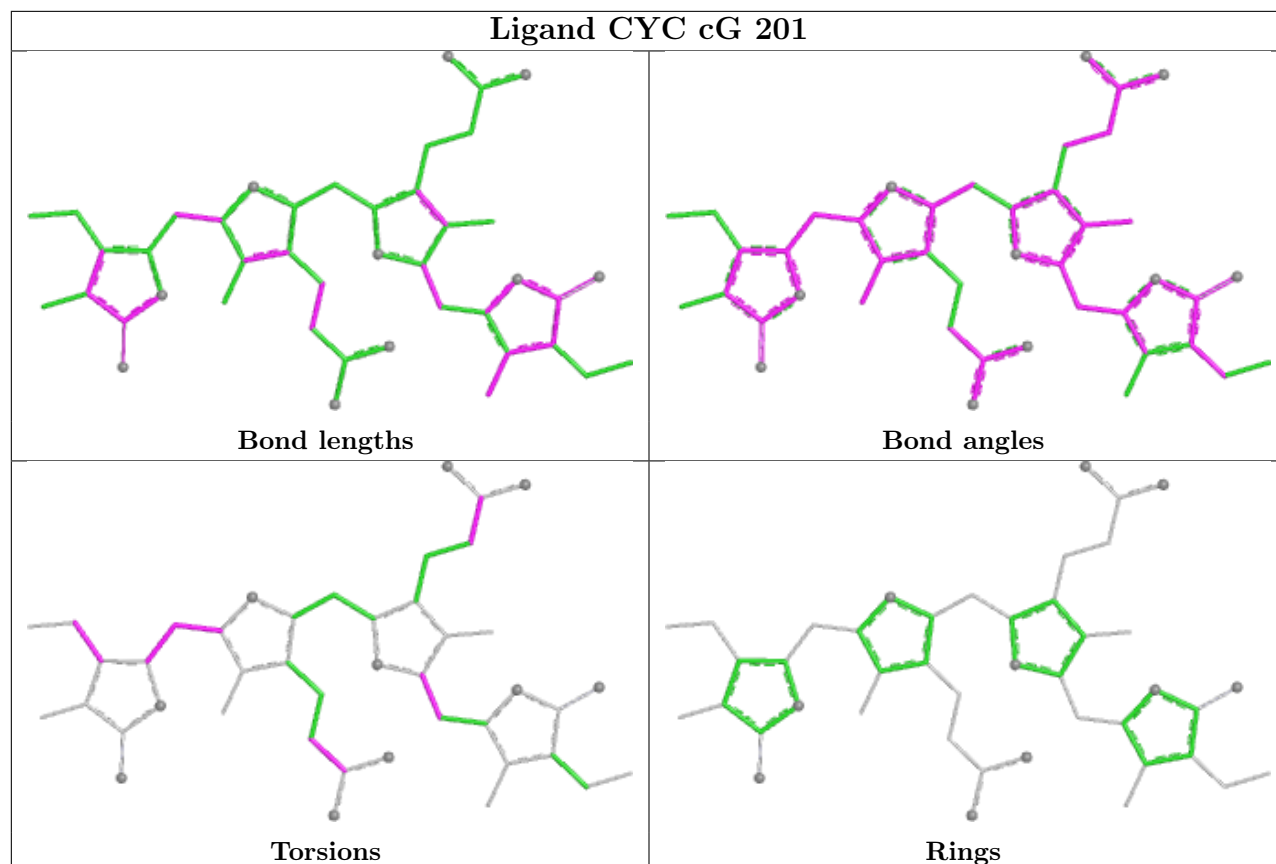




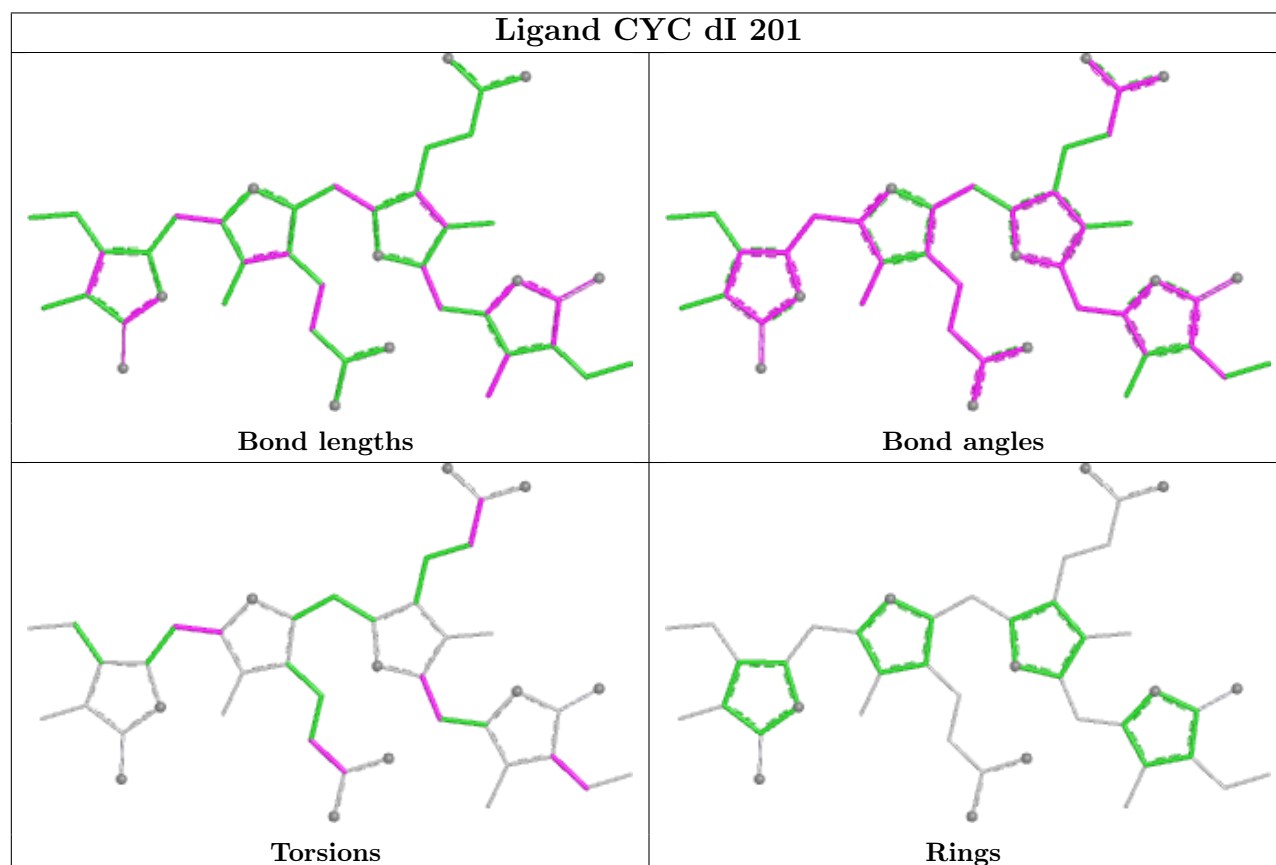


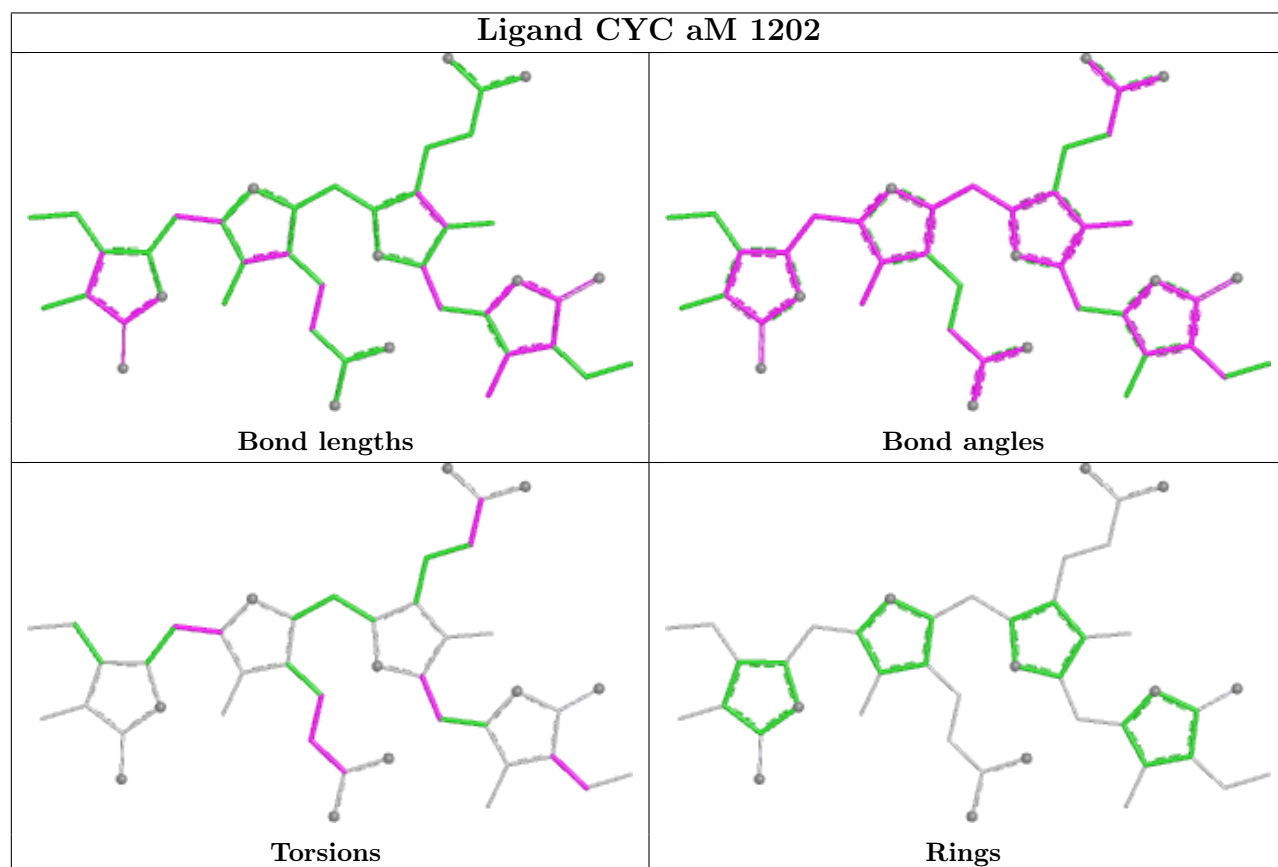
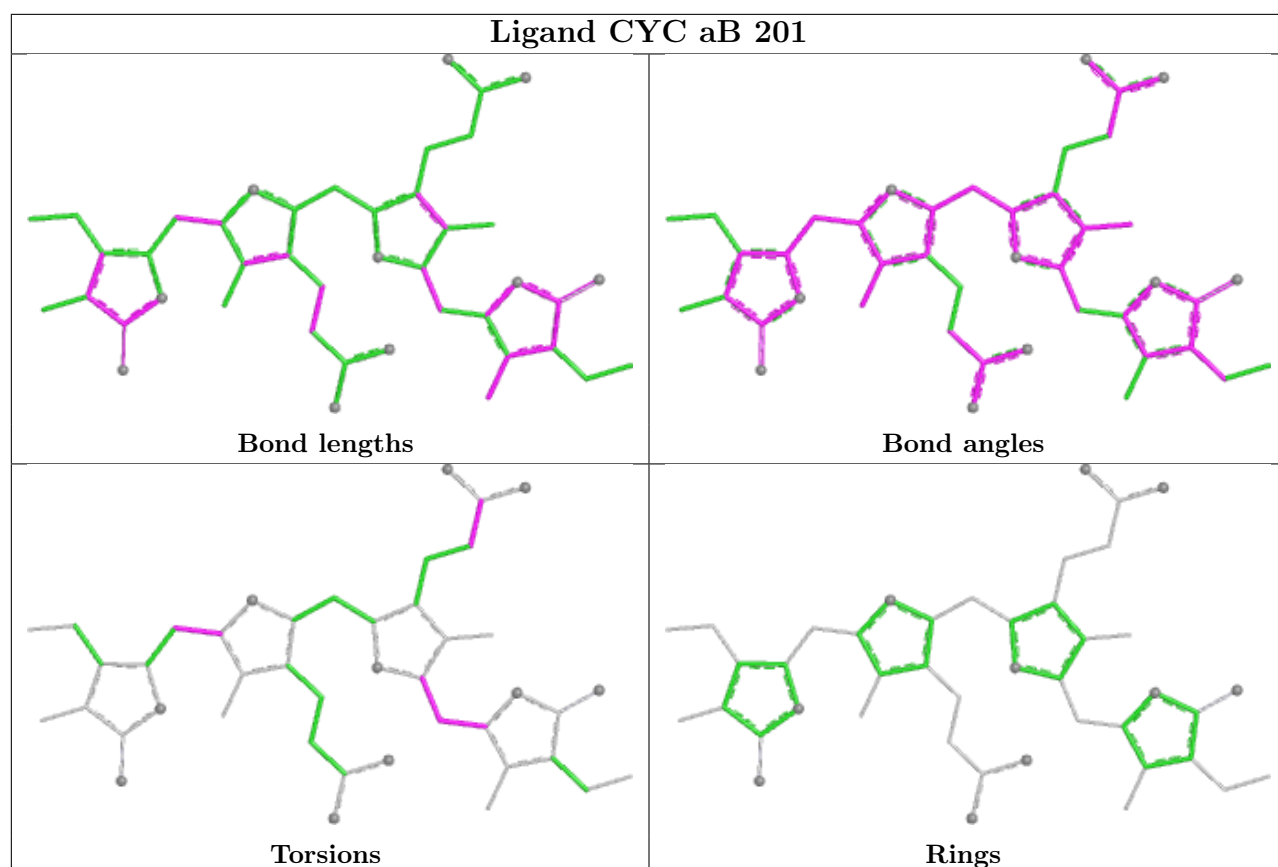


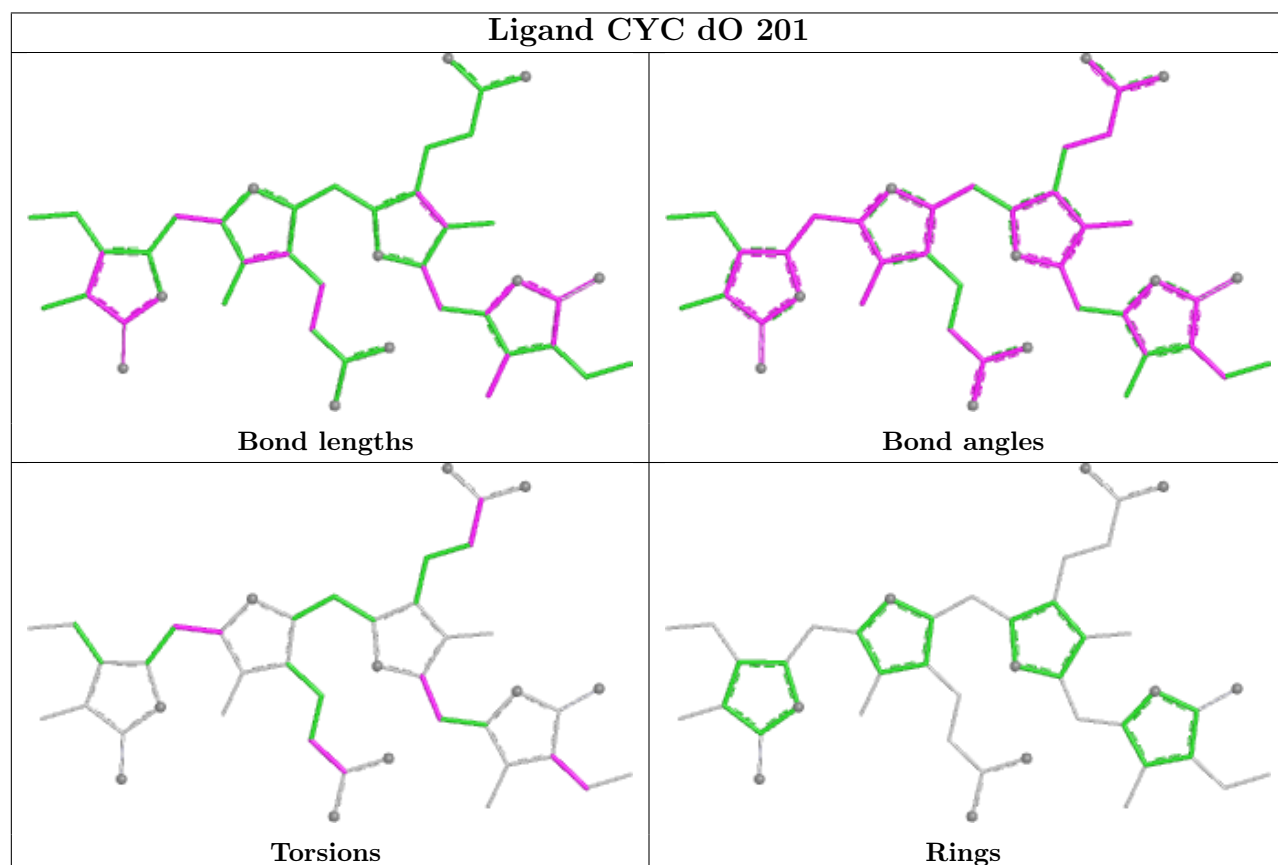
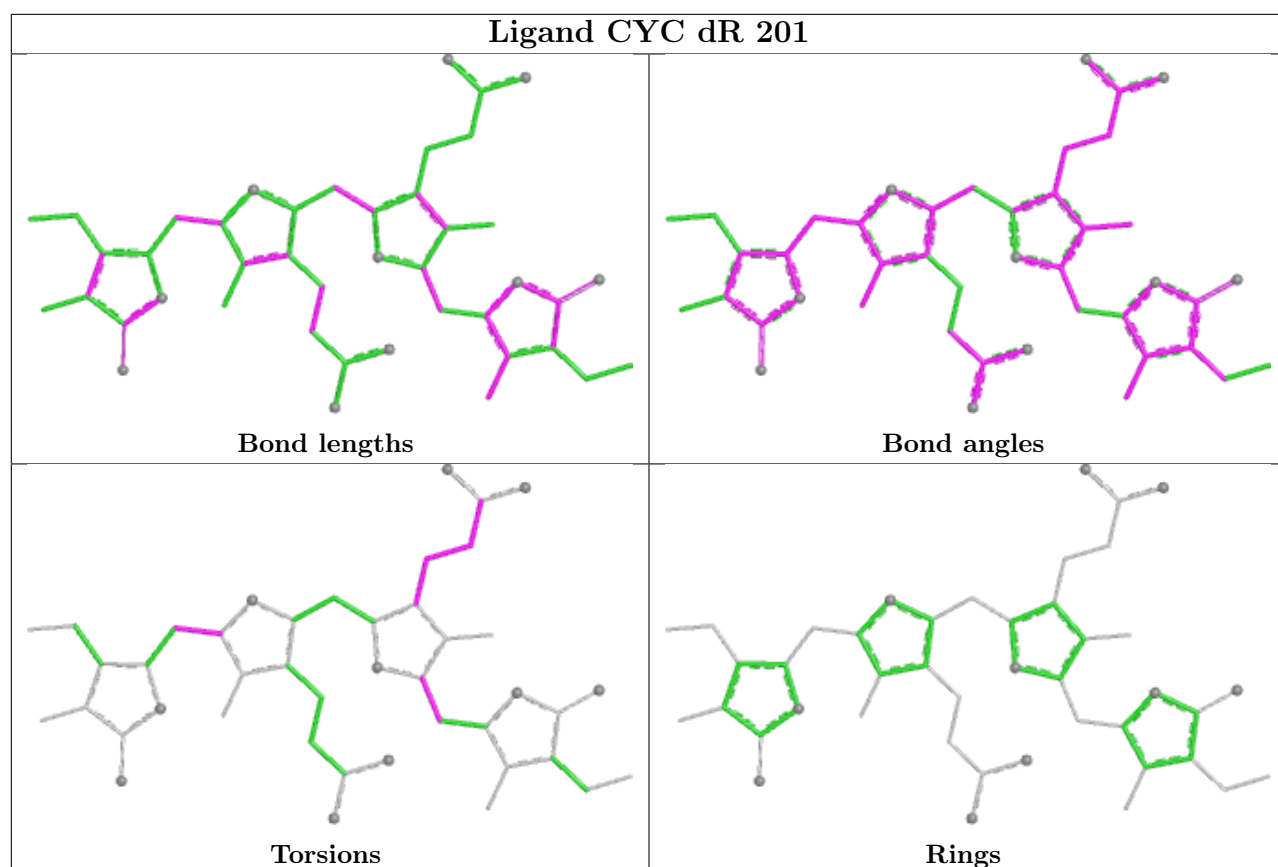
Ligand CYC cG 201

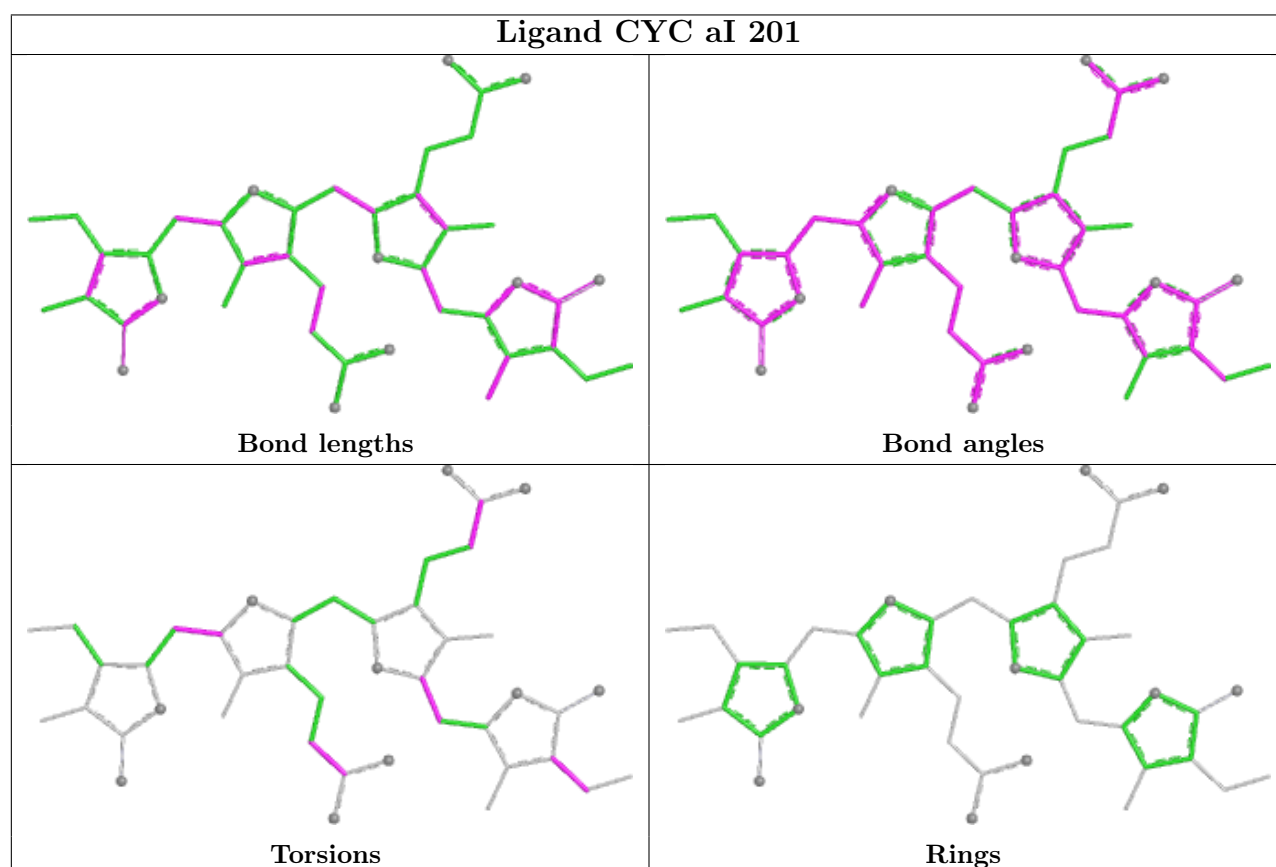
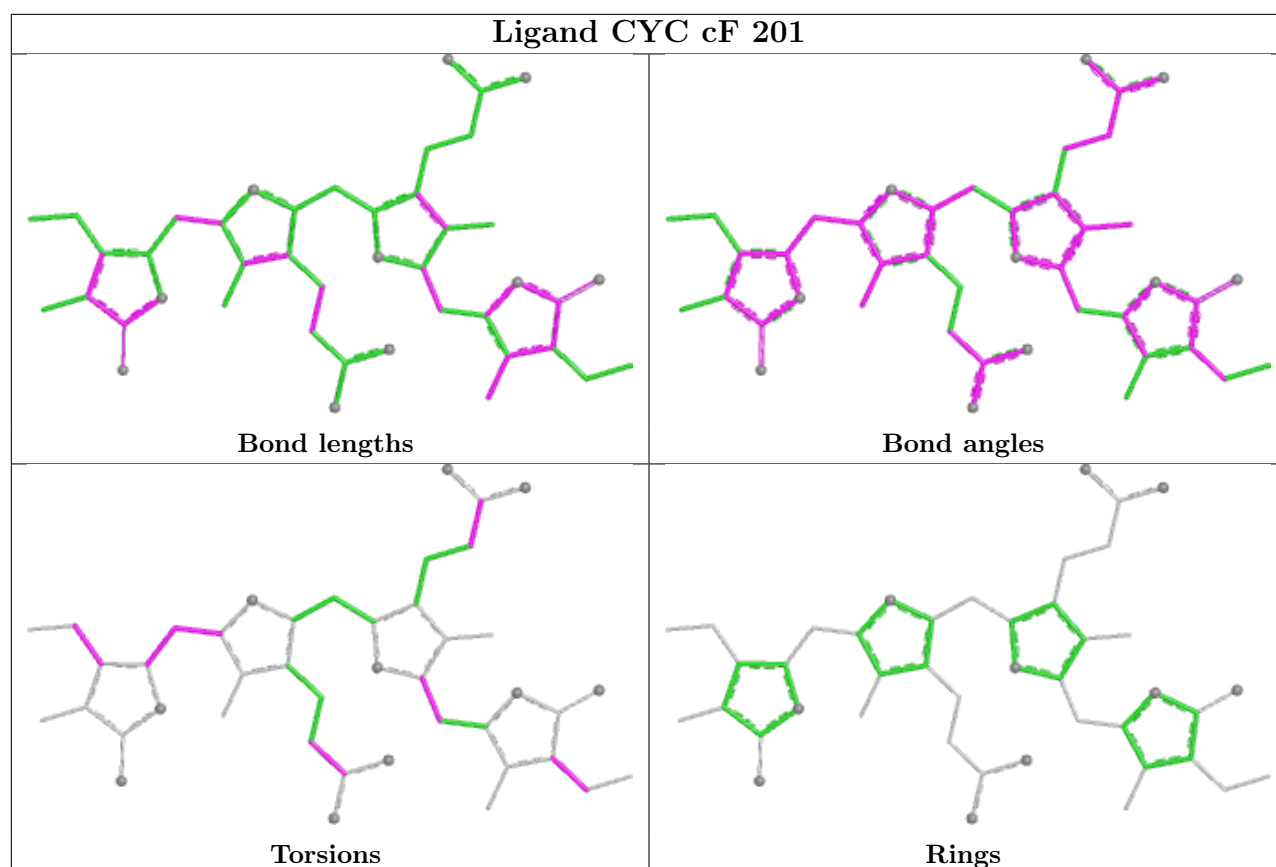


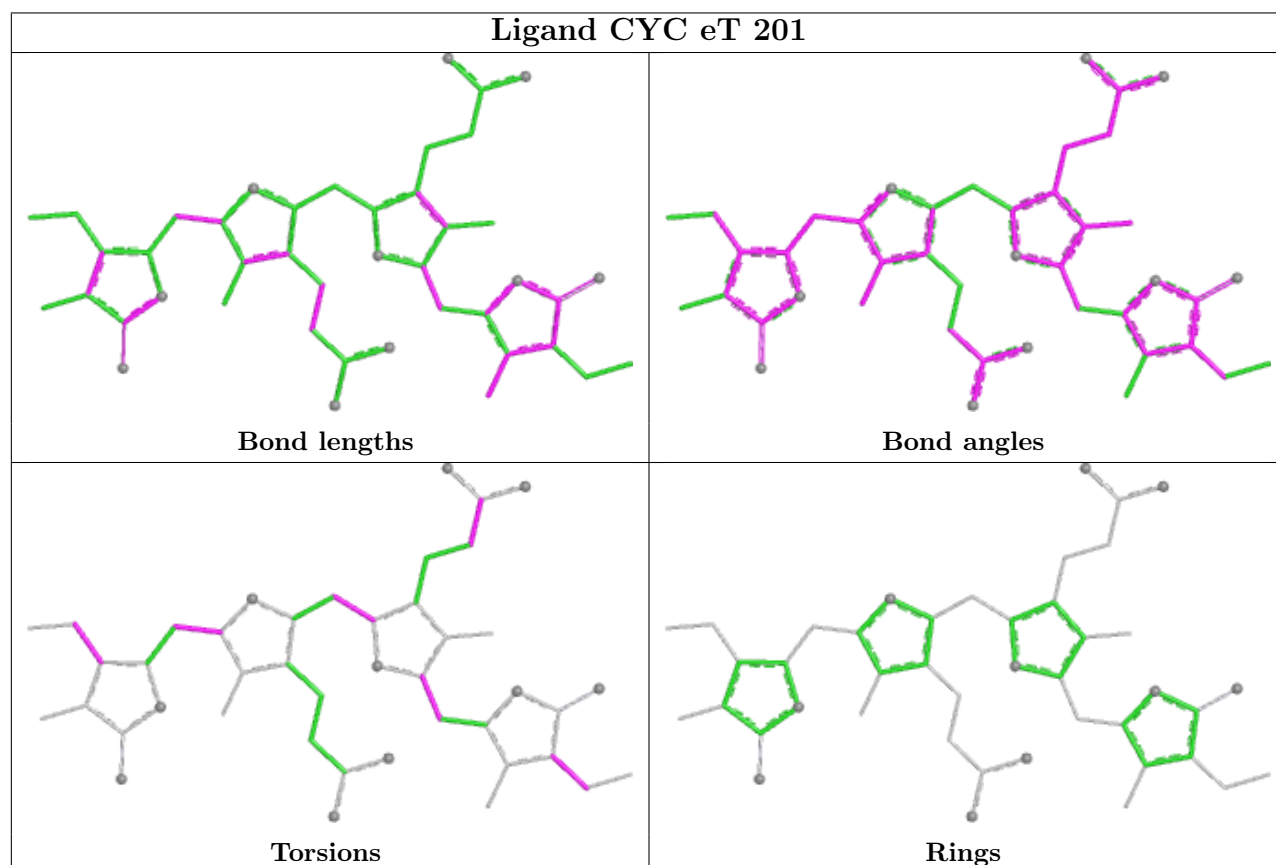
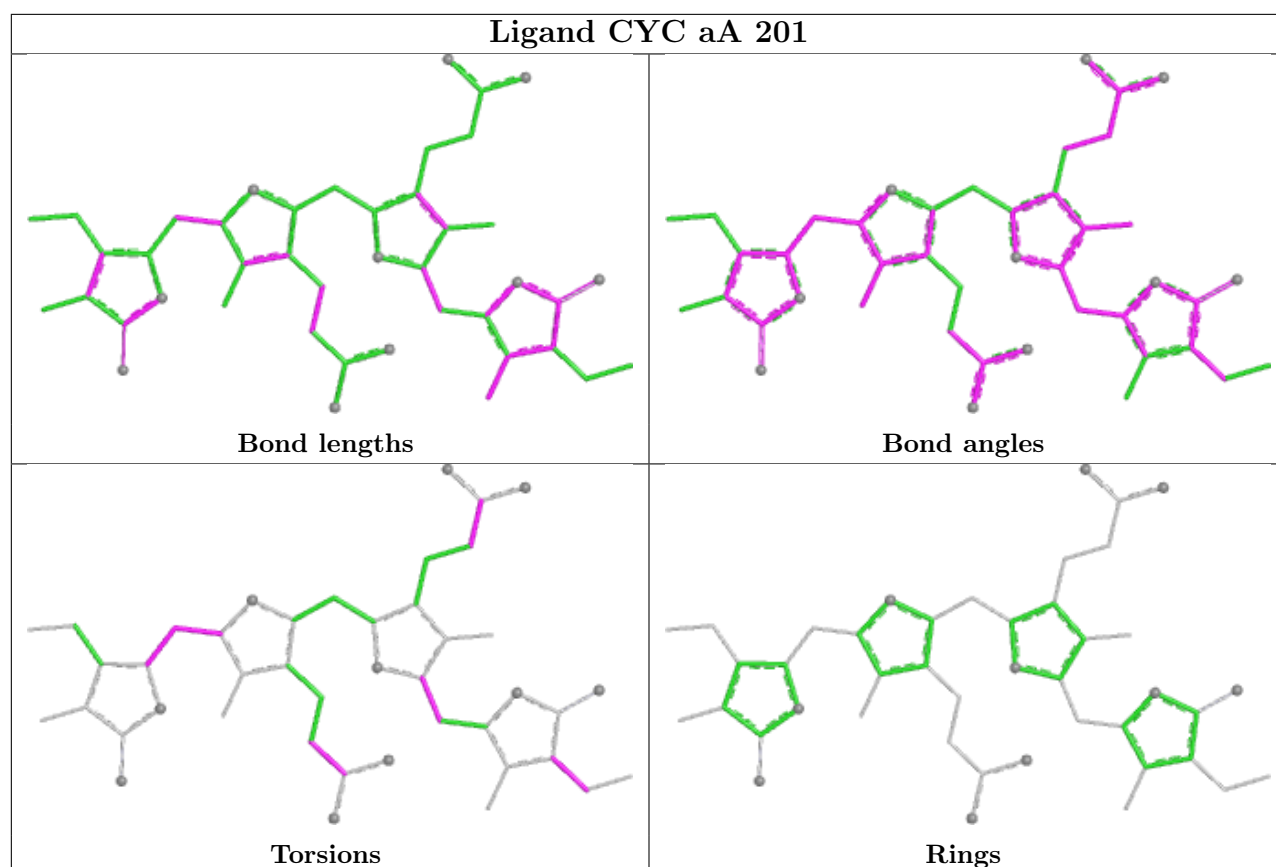
Ligand CYC dI 201

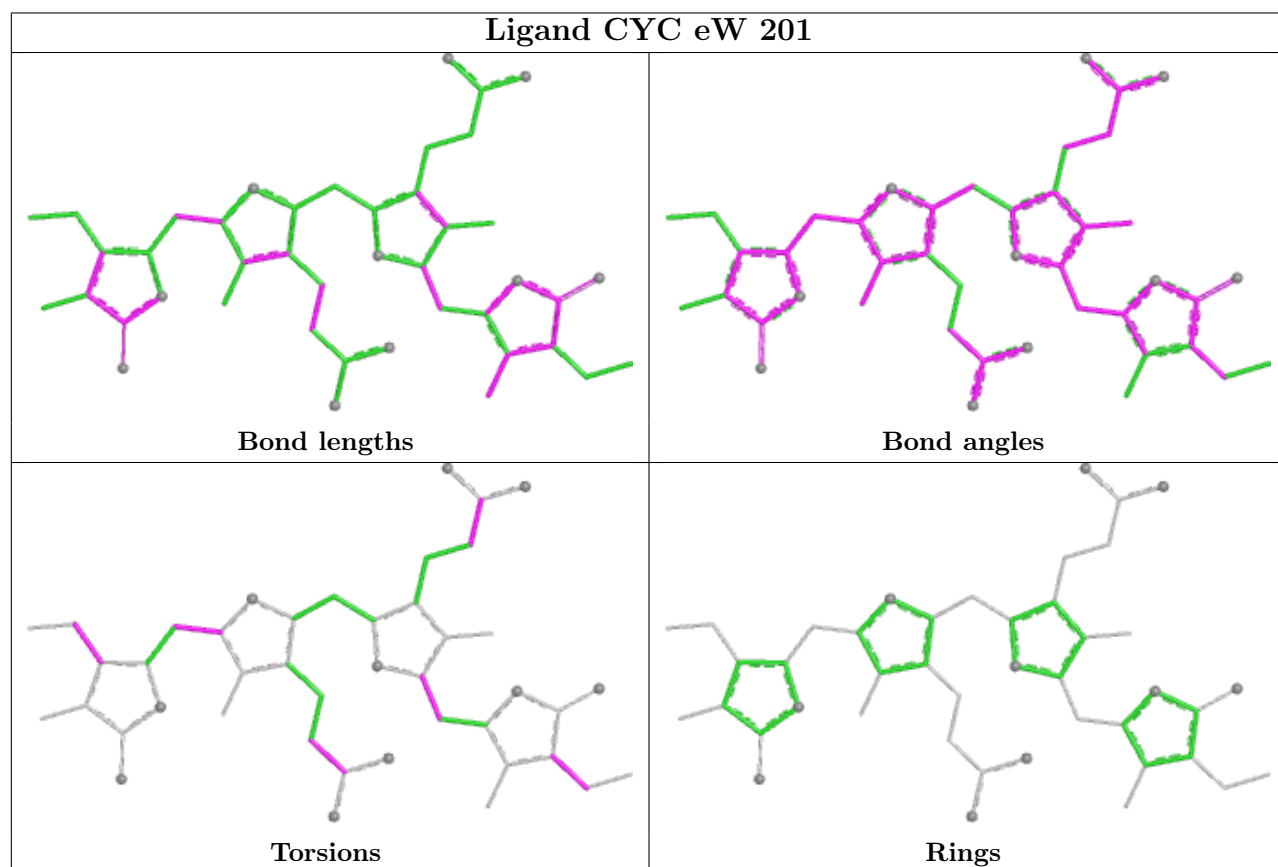
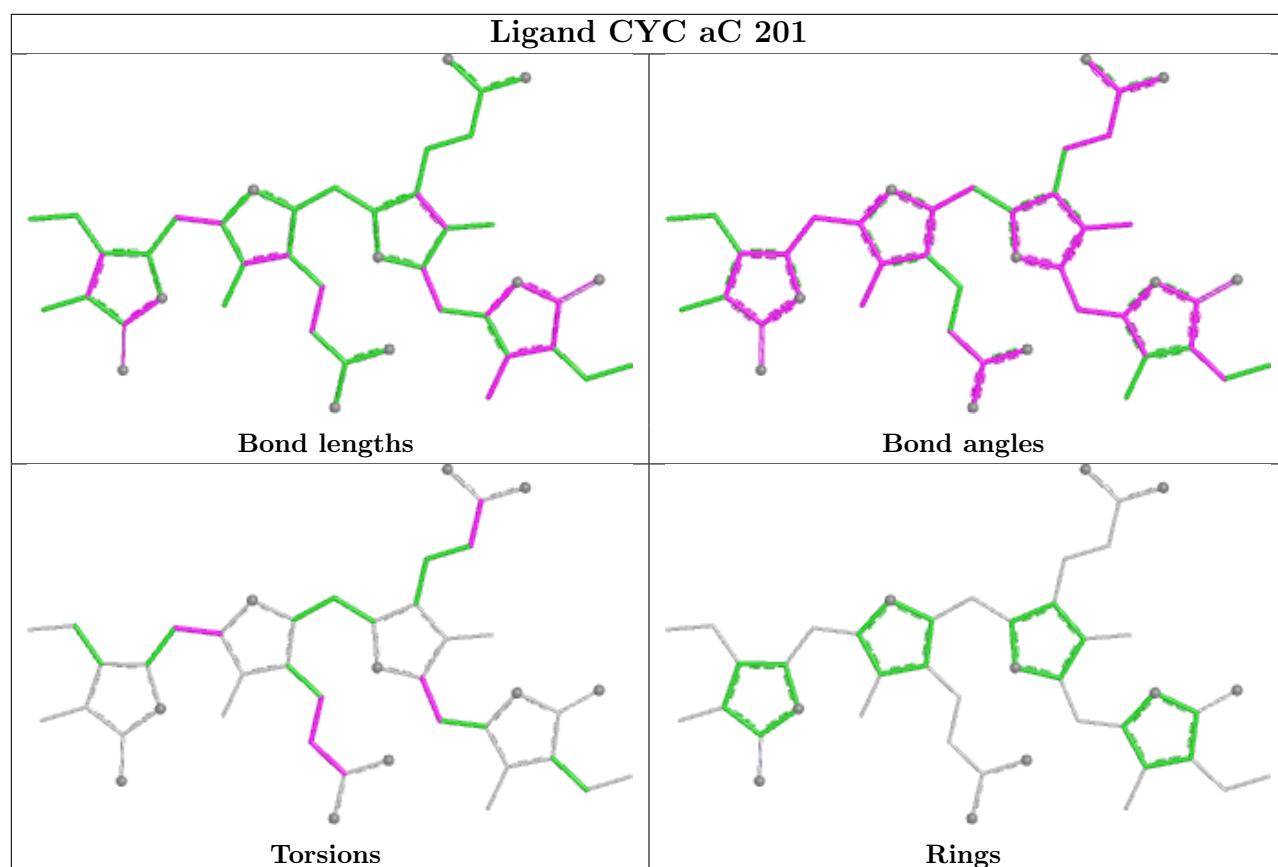


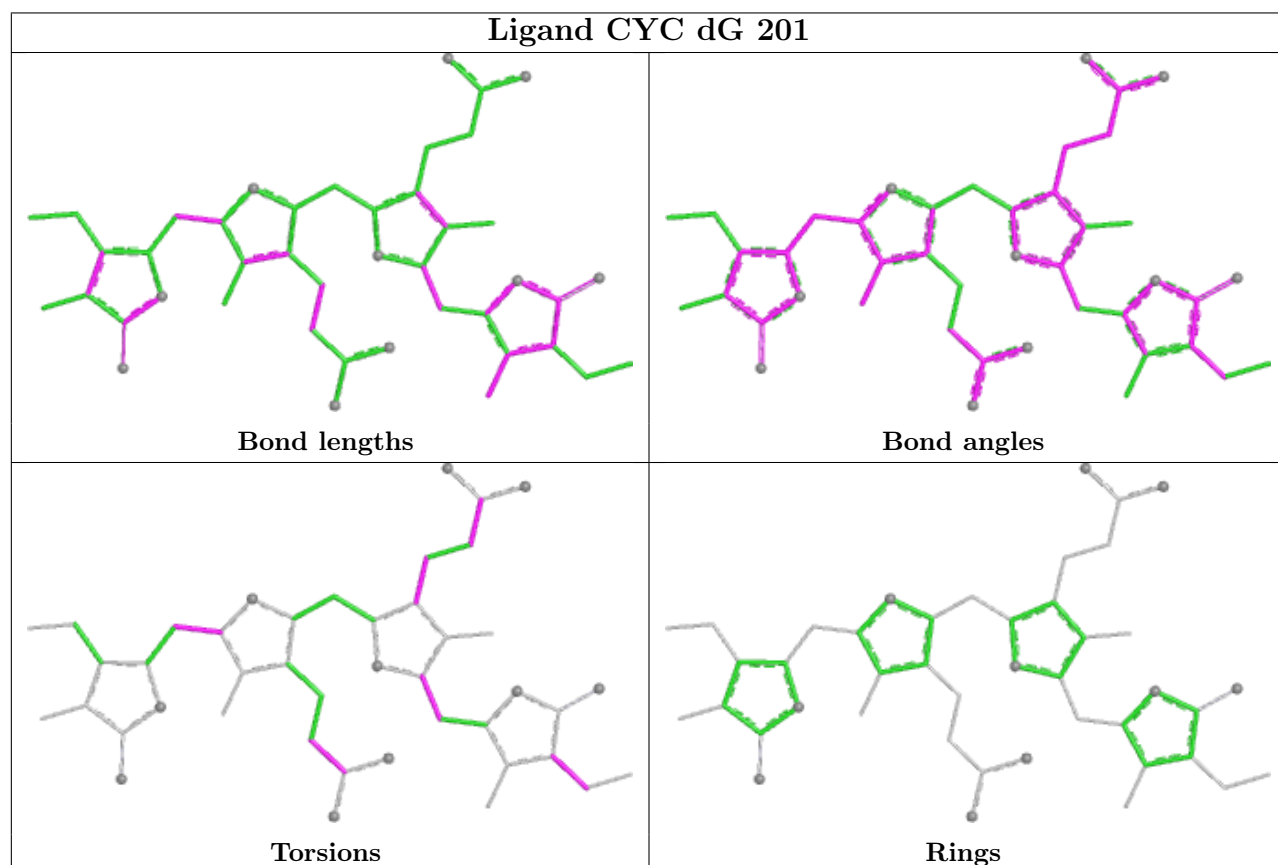
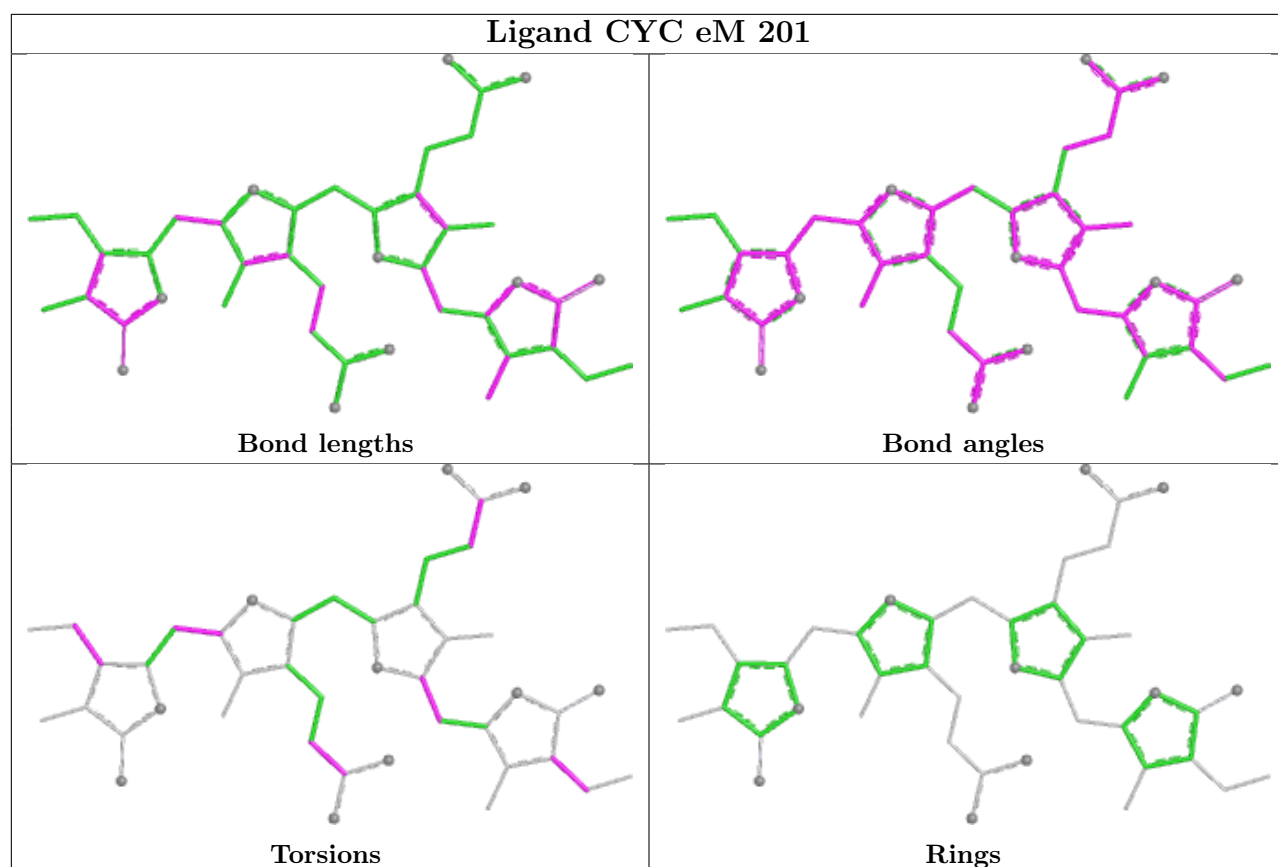




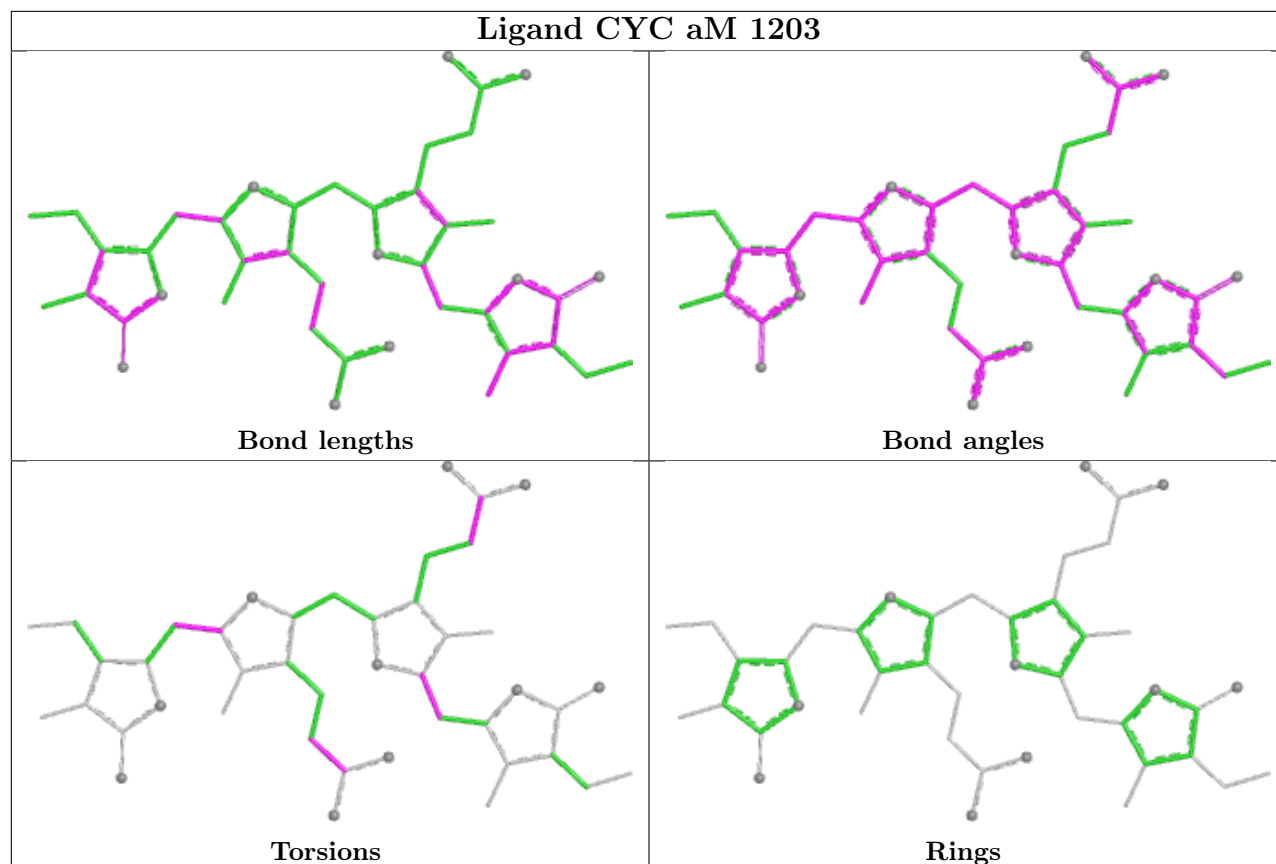




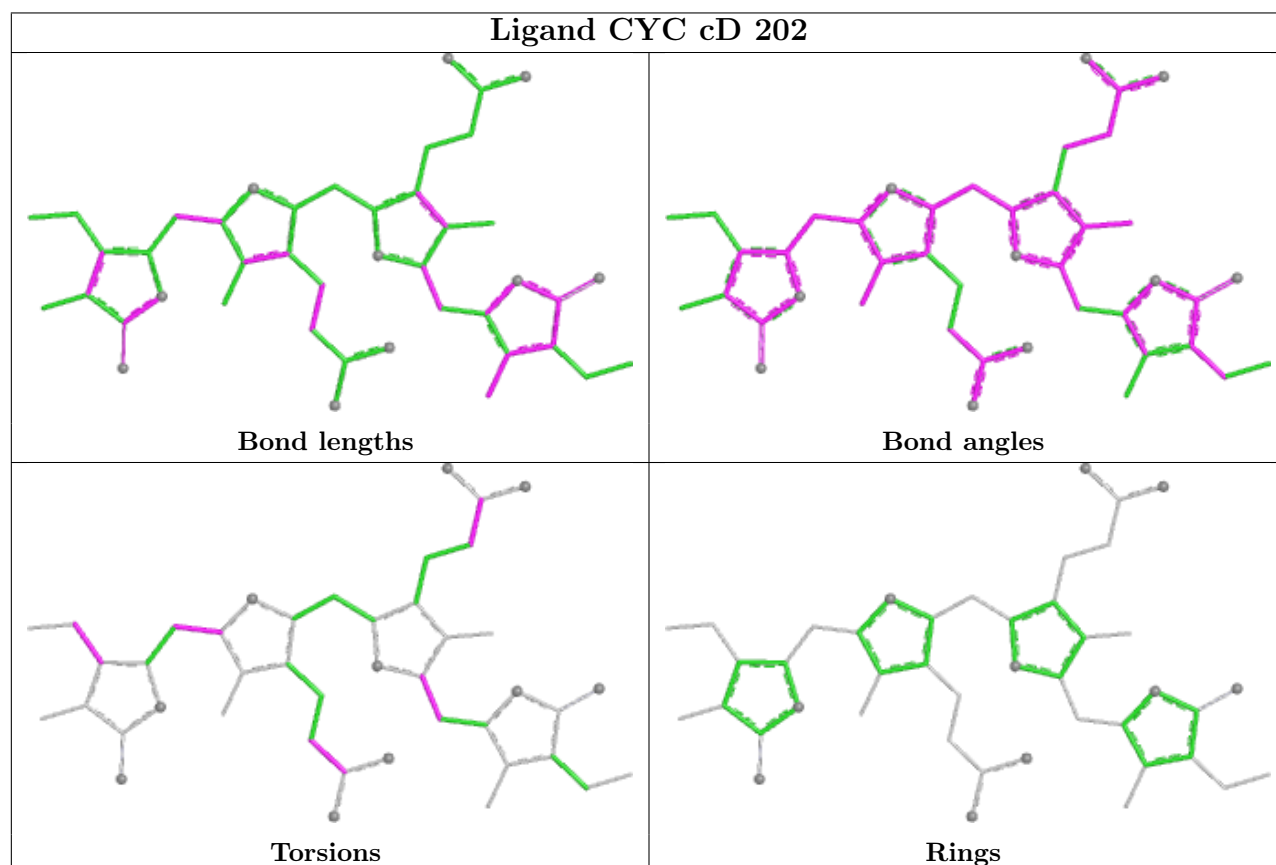


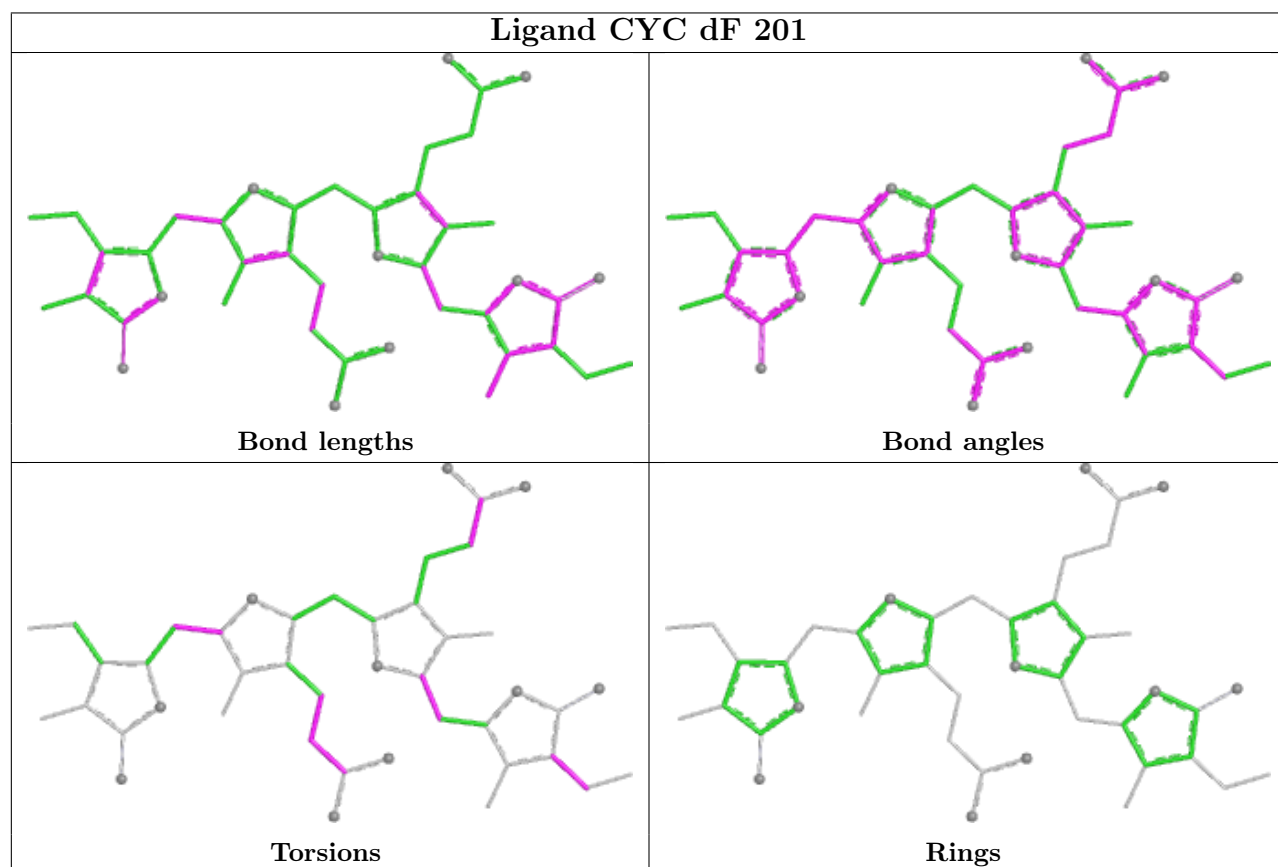
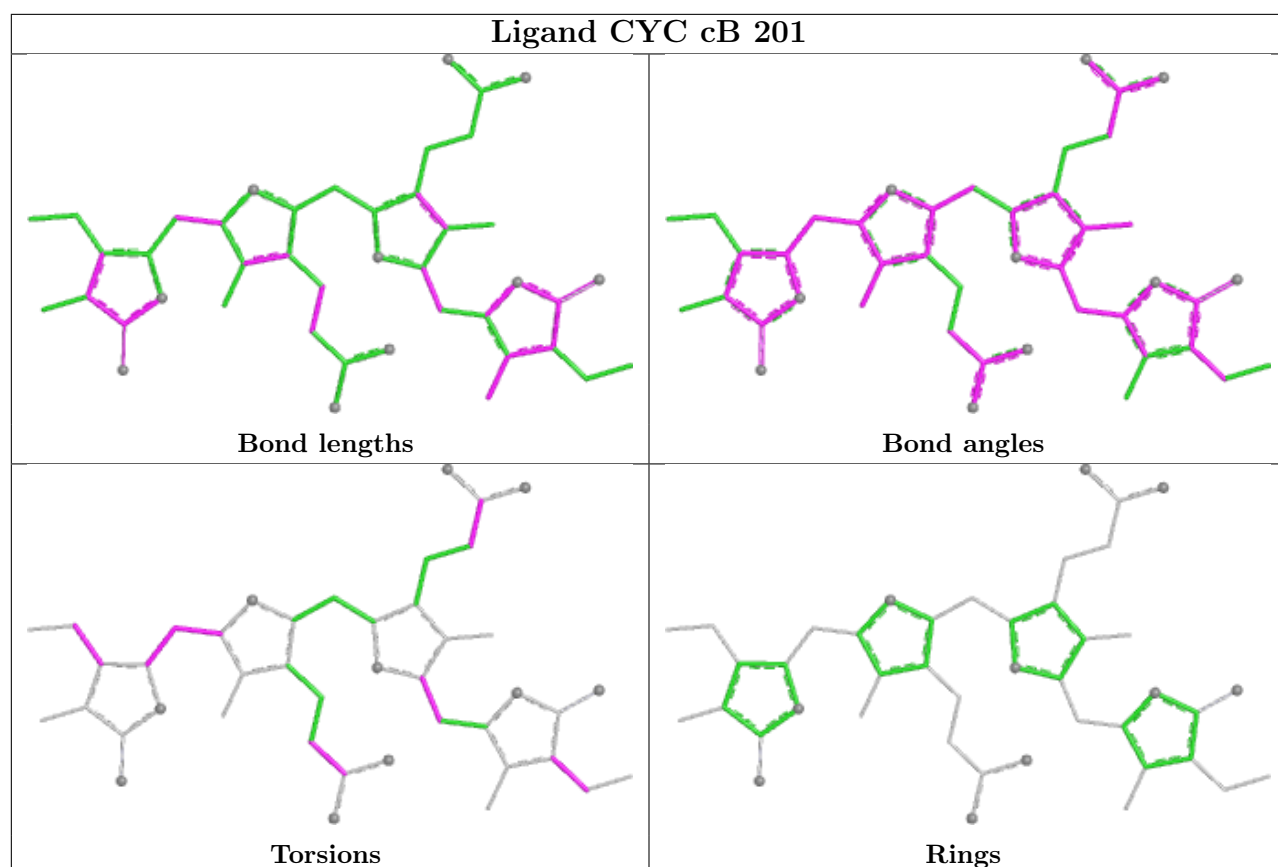


Ligand CYC aM 1203

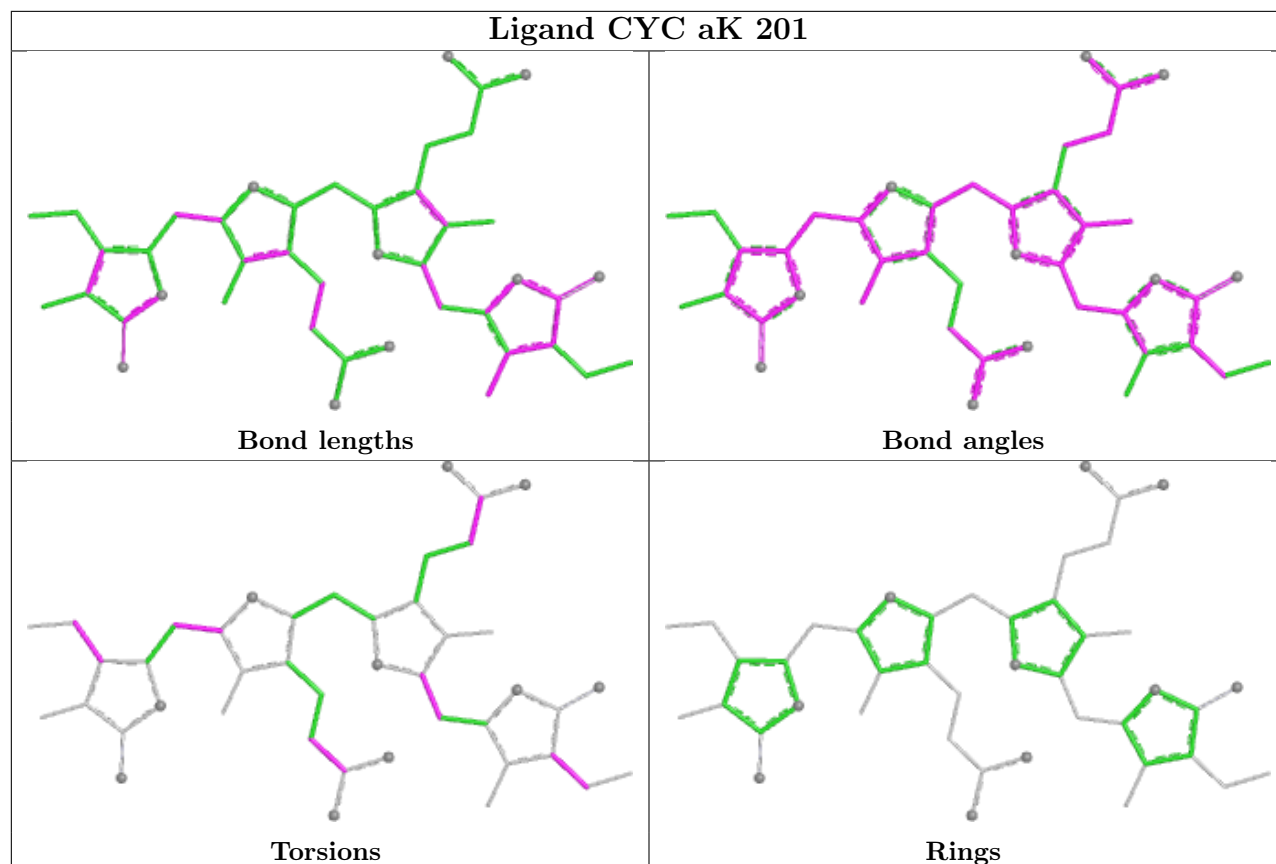


Ligand CYC cD 202

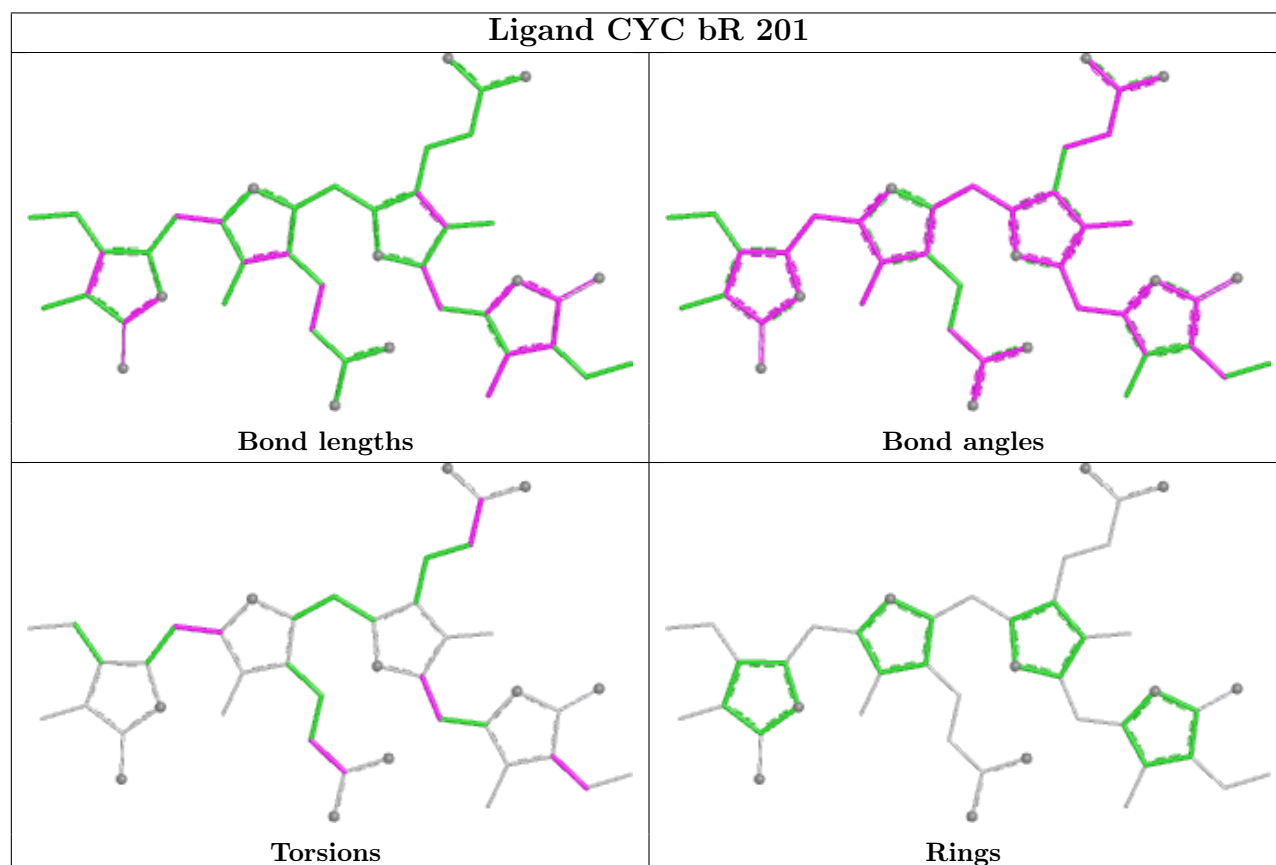


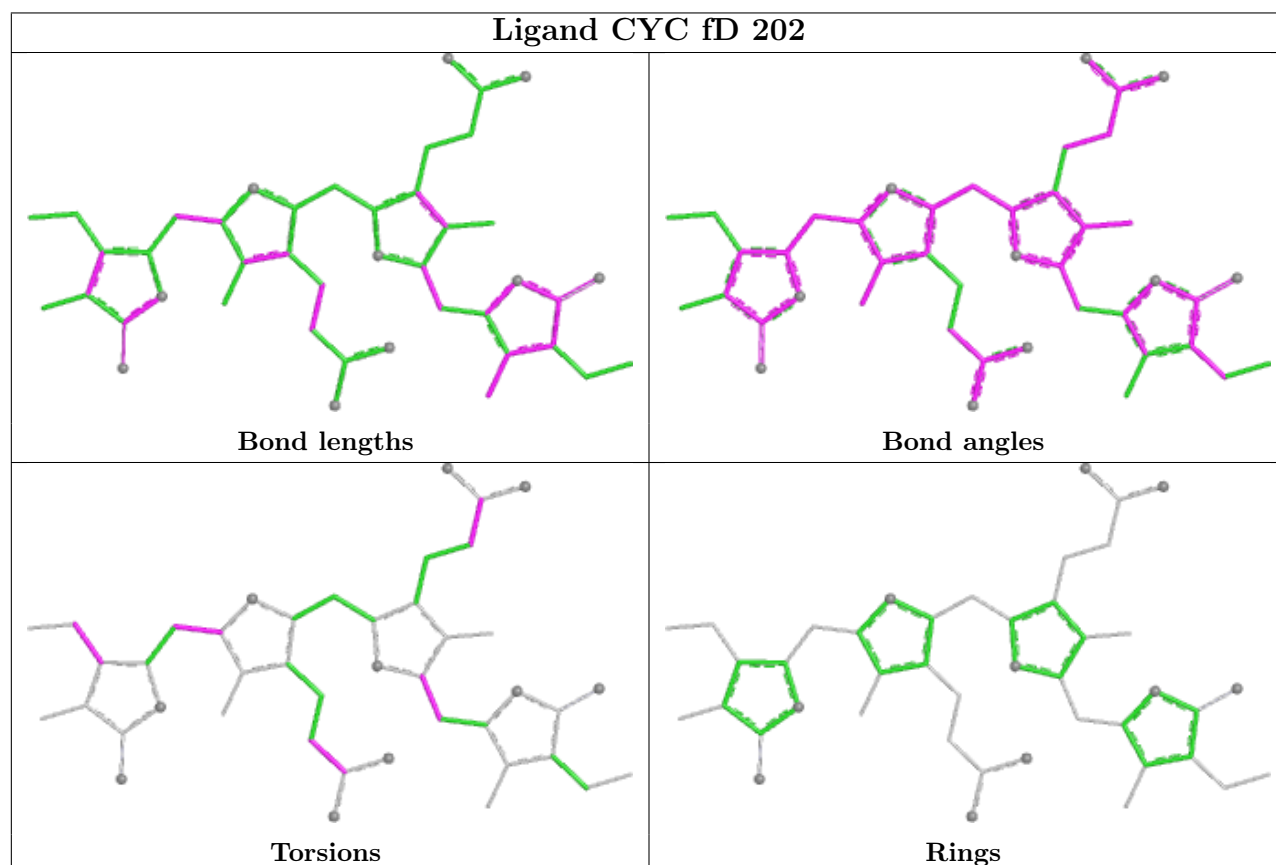
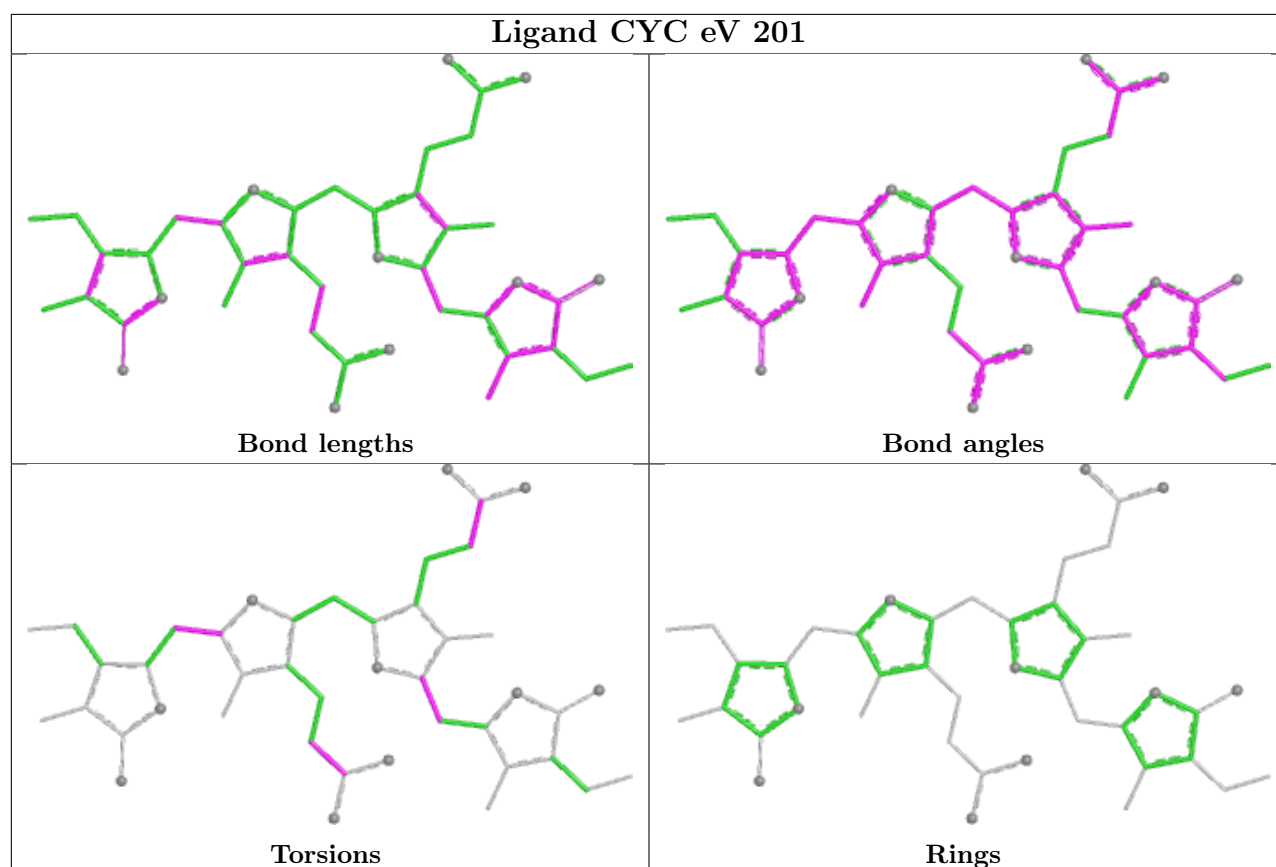


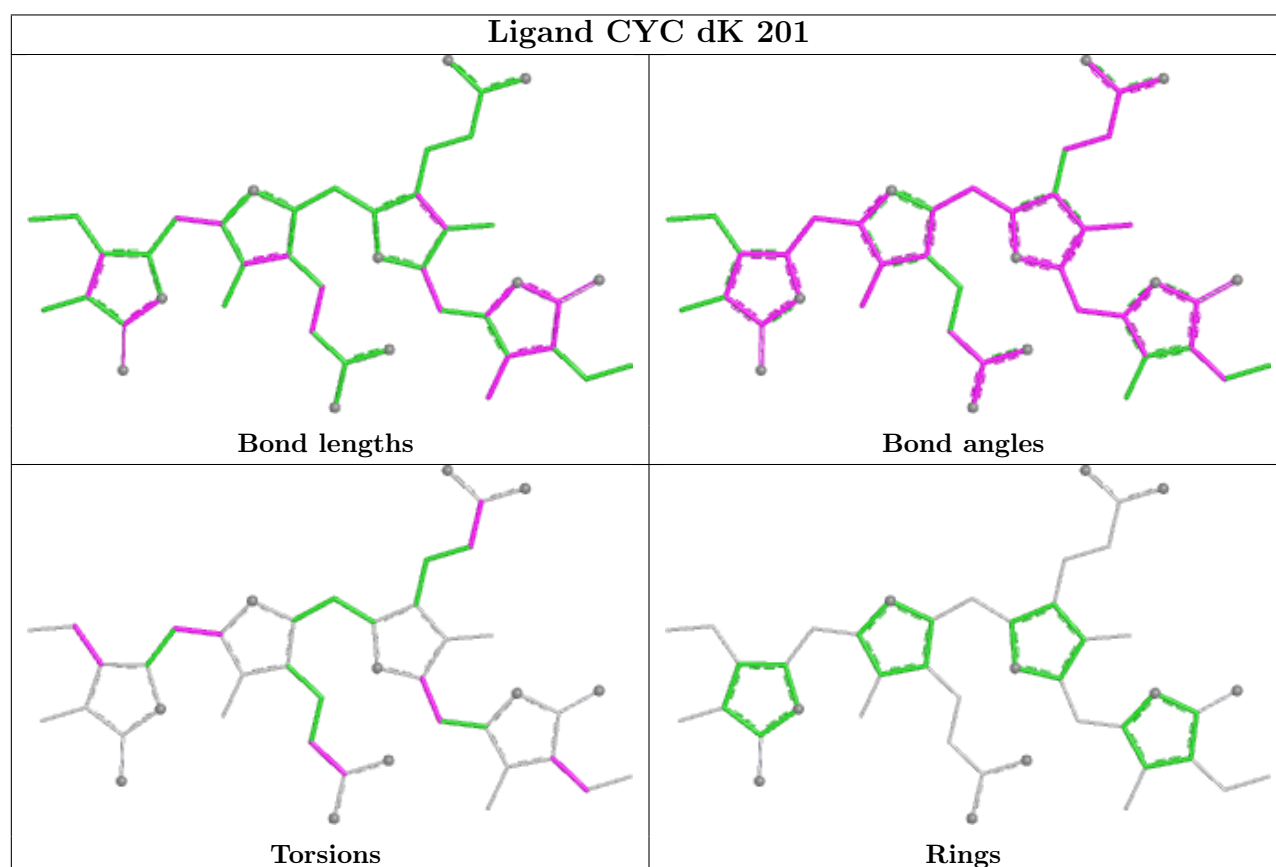
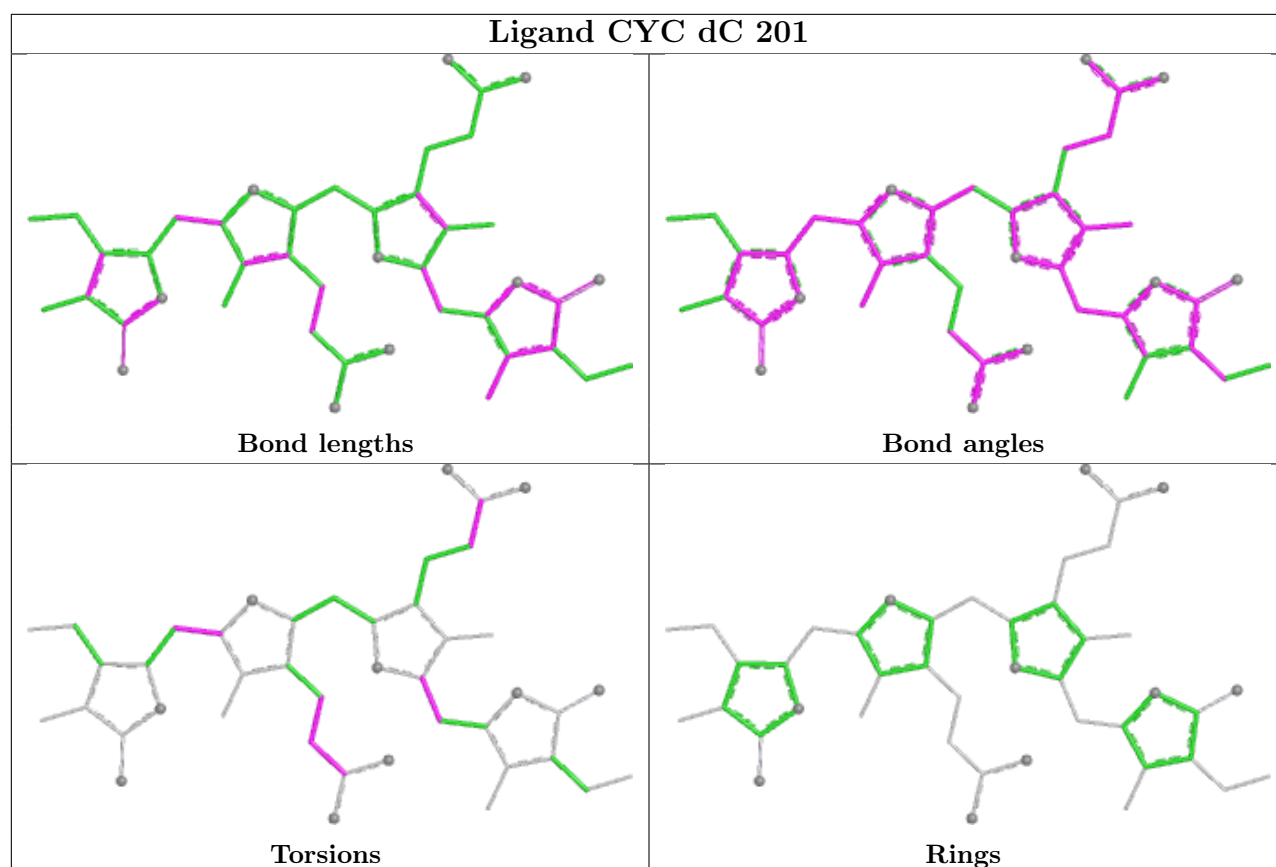
Ligand CYC aK 201

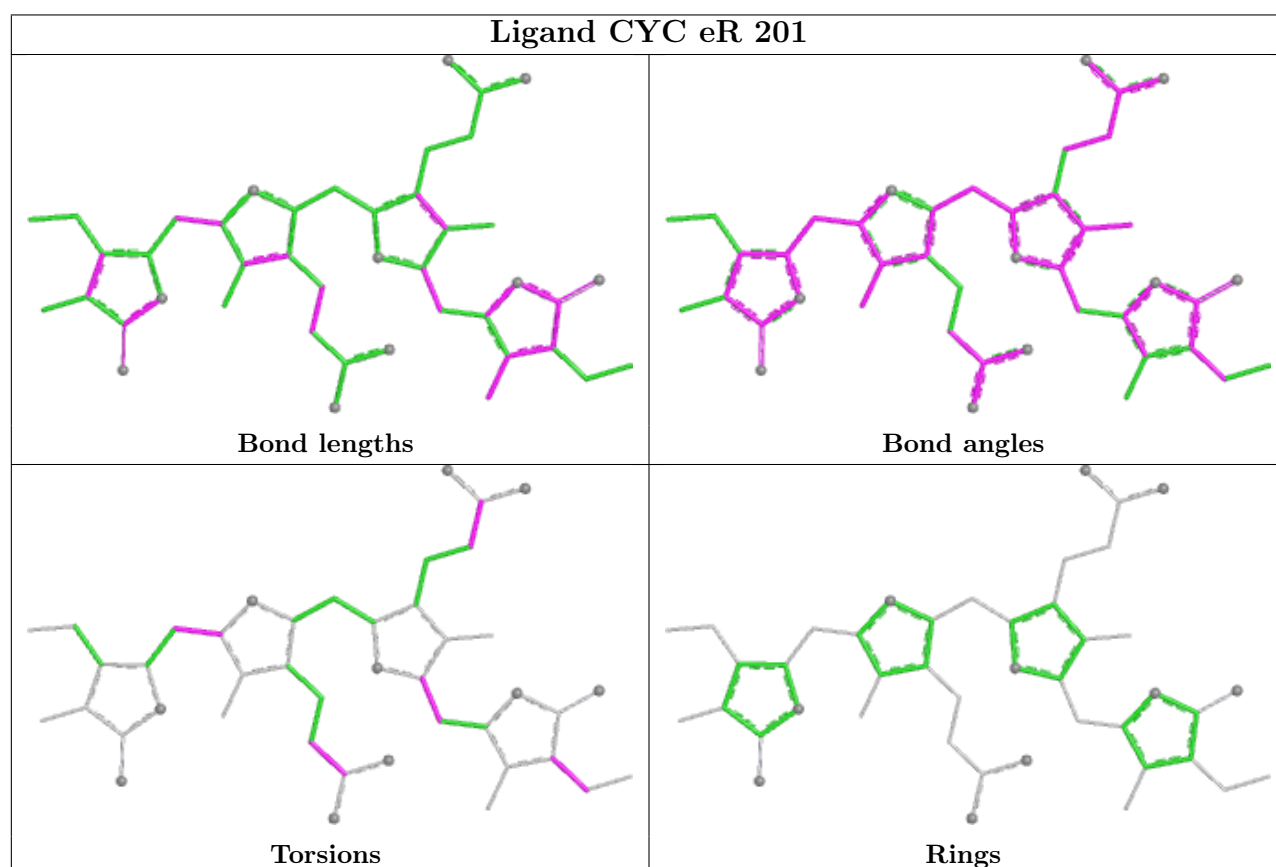
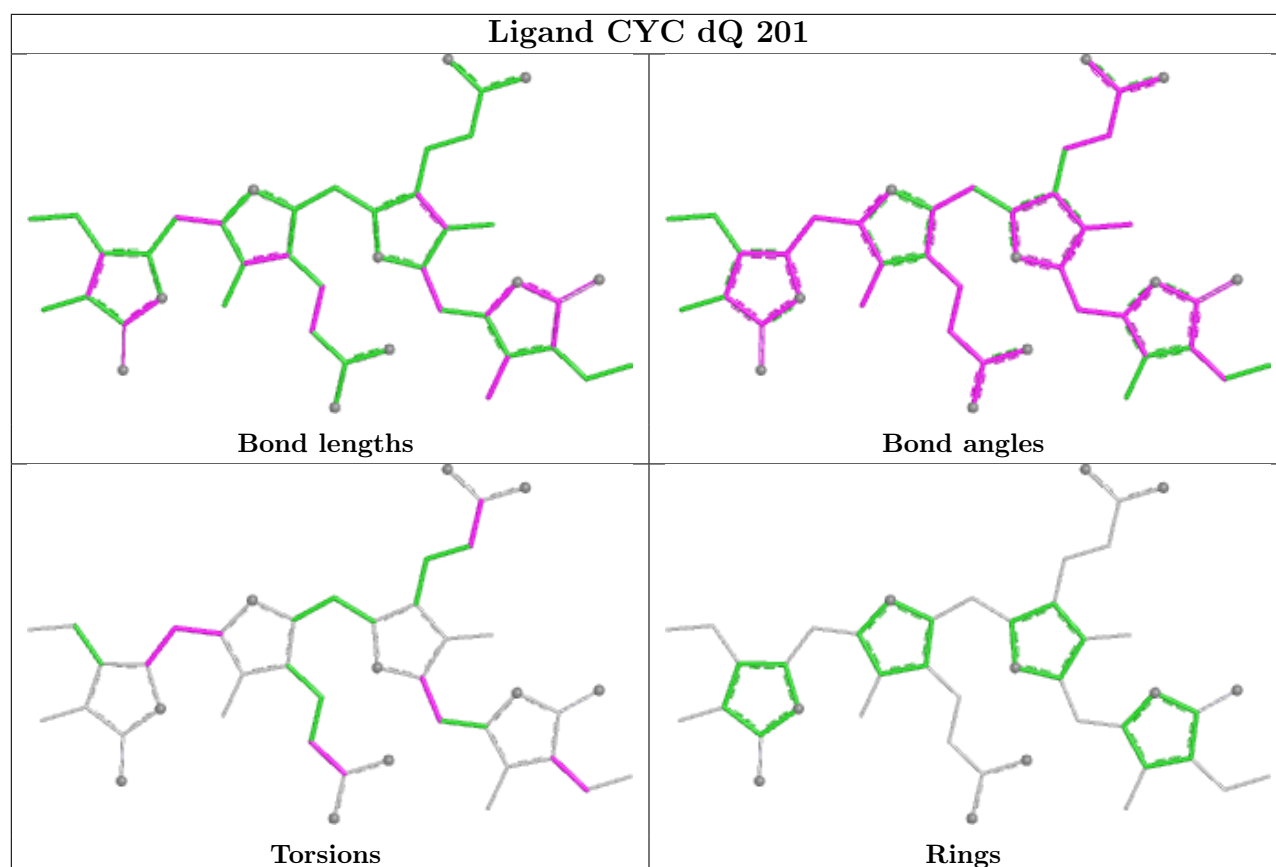


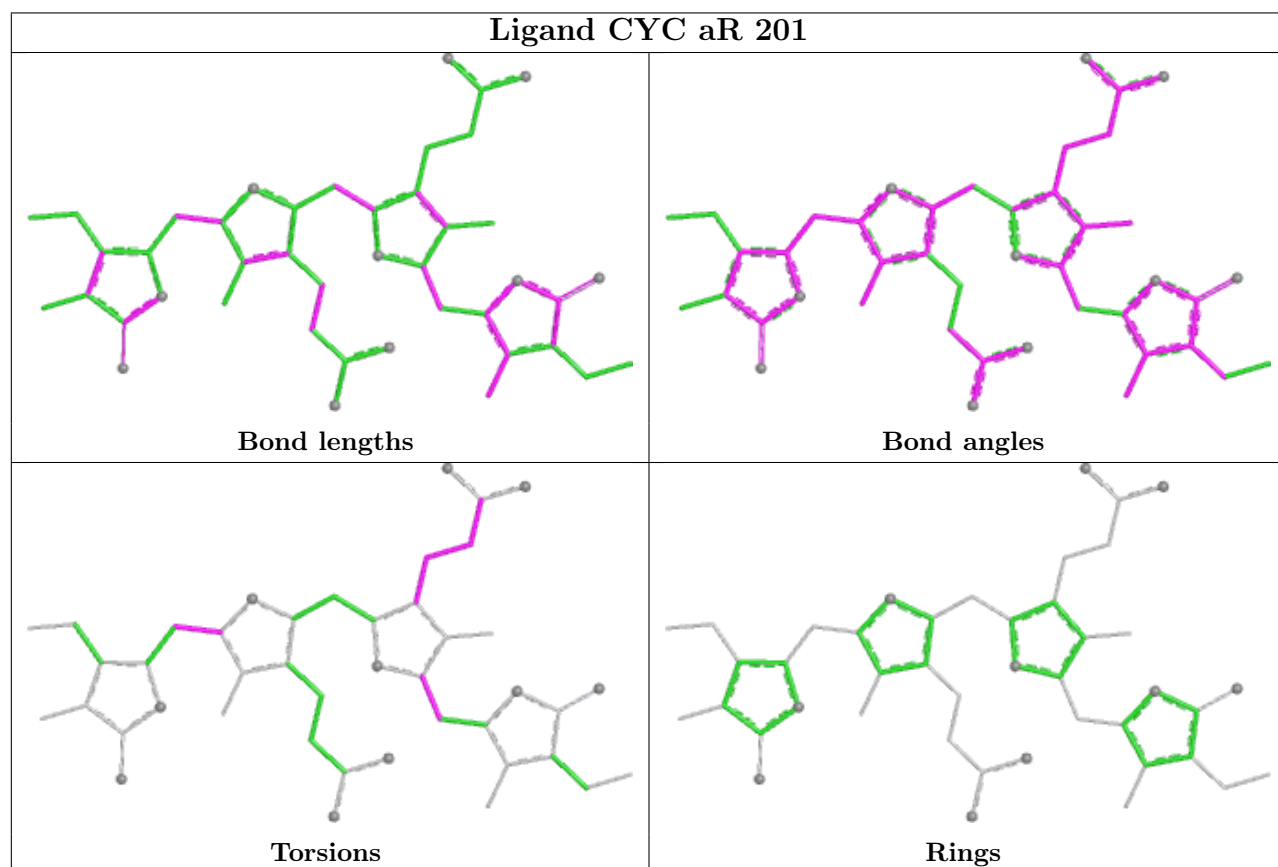
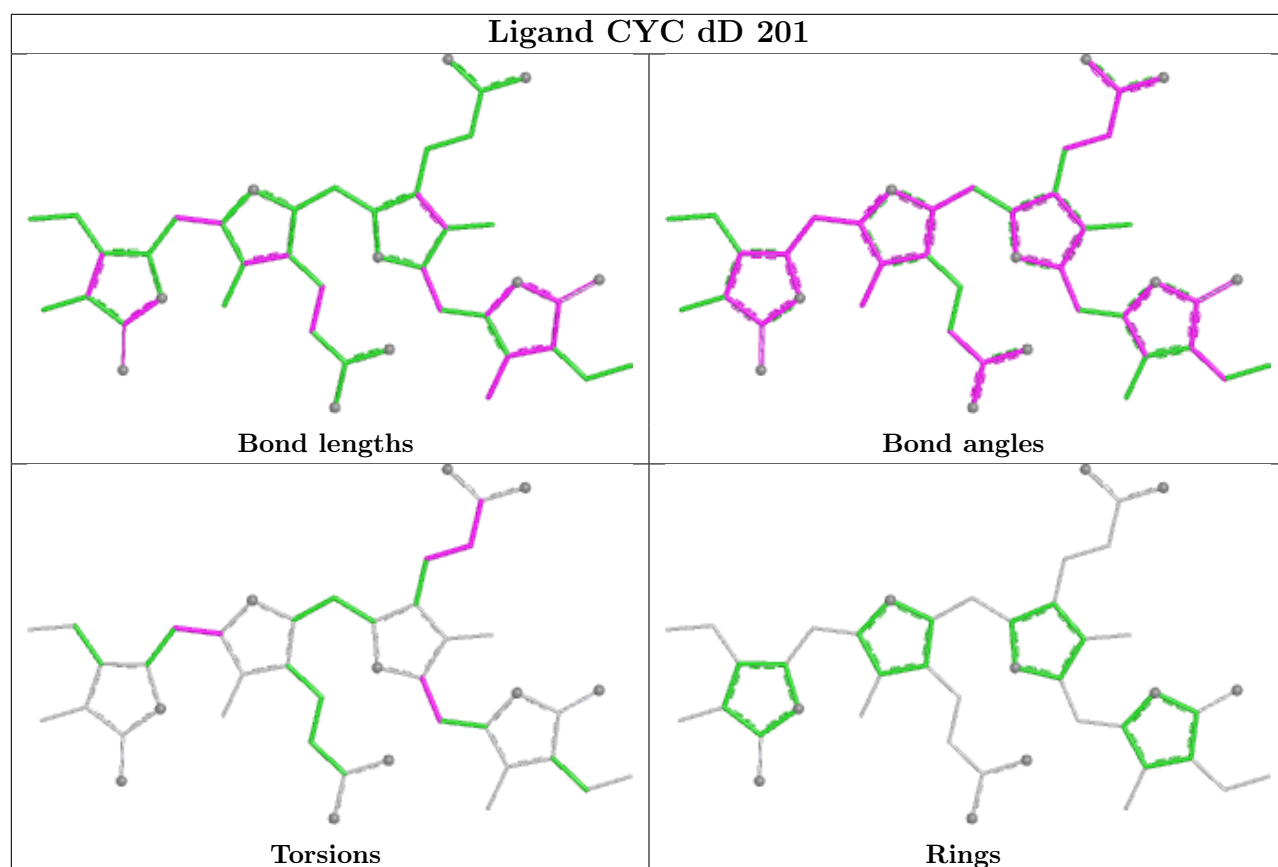
Ligand CYC bR 201

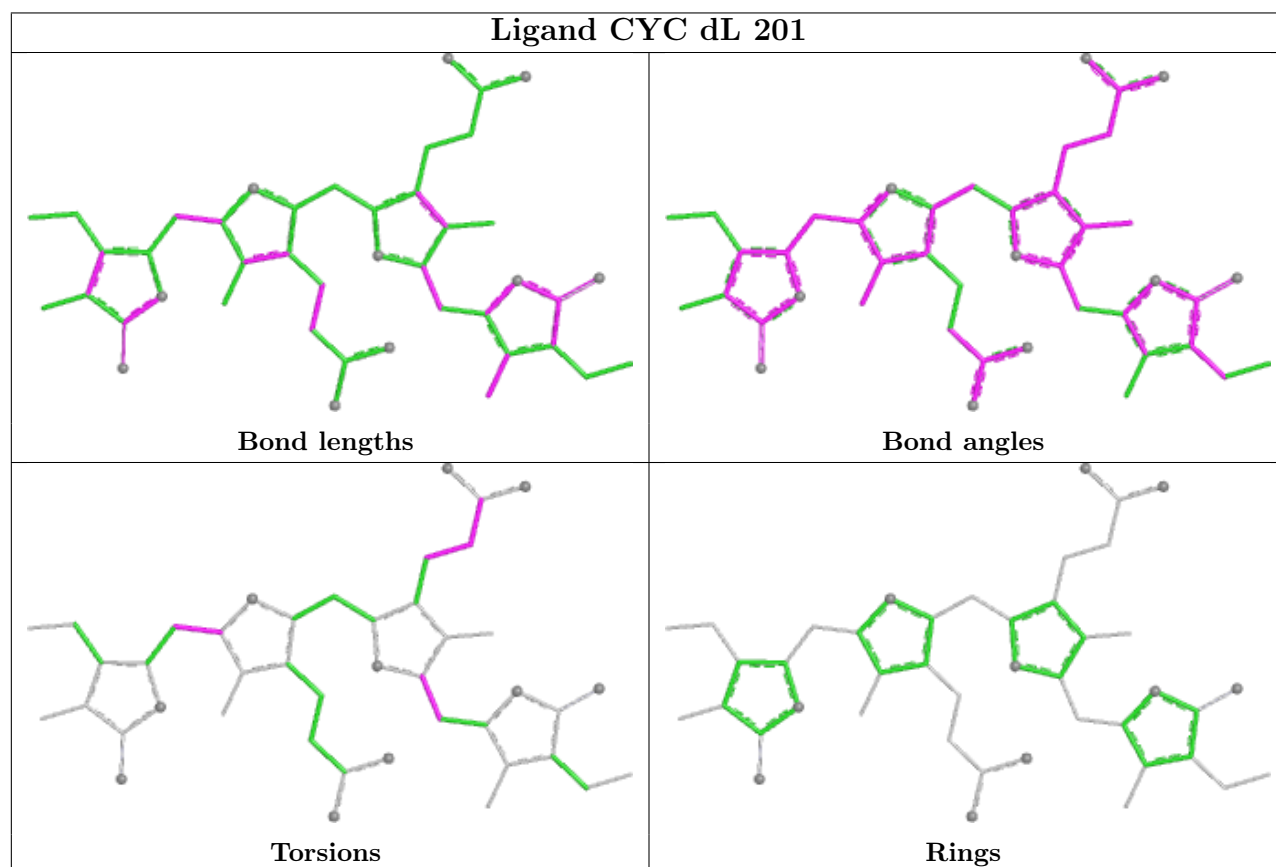
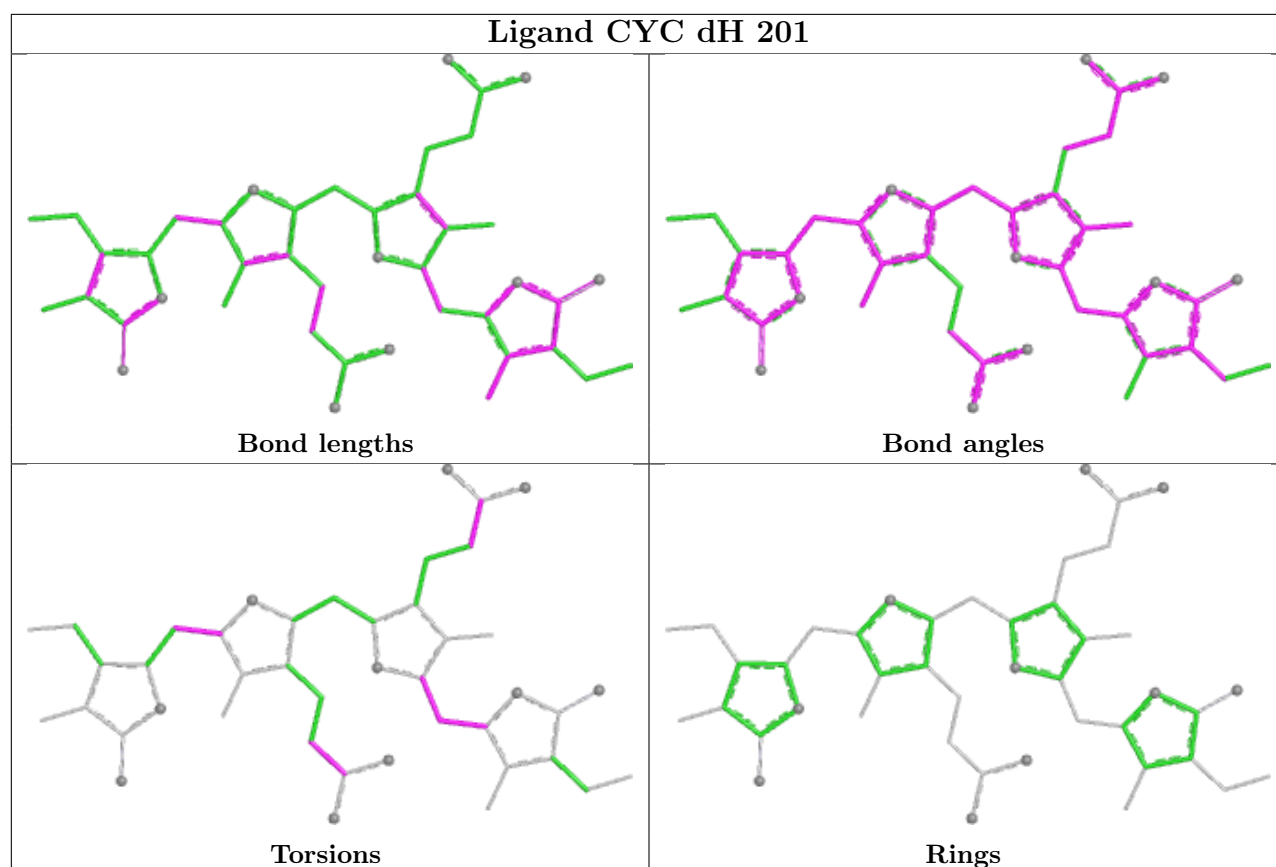


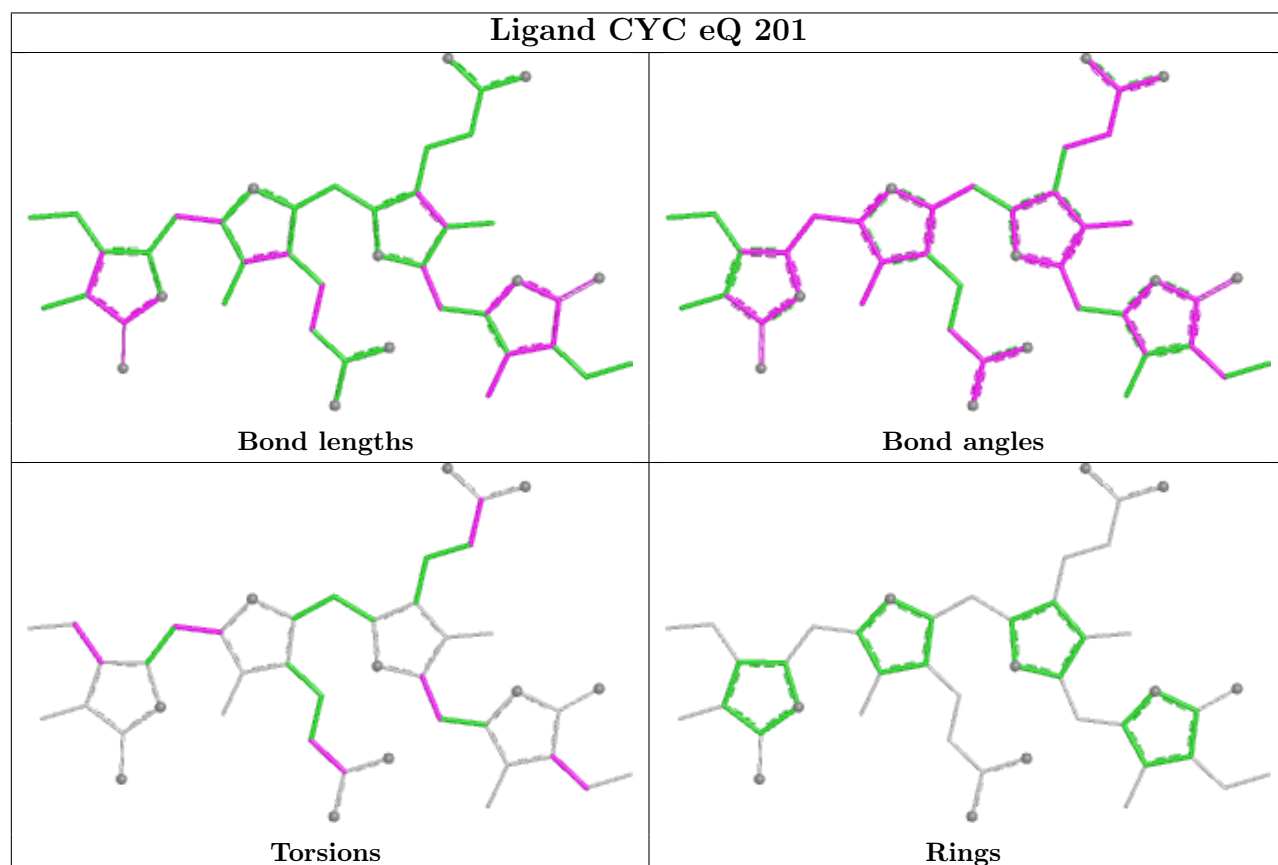
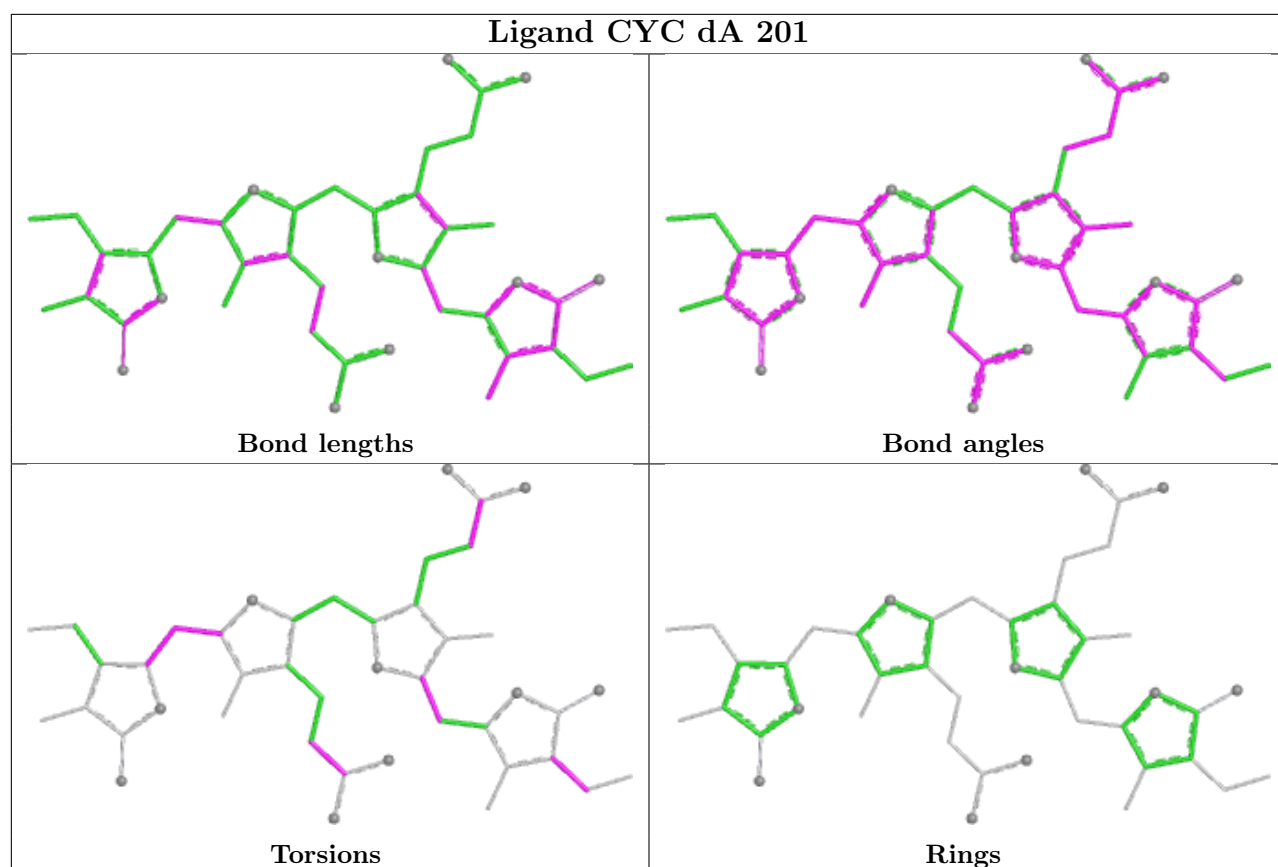


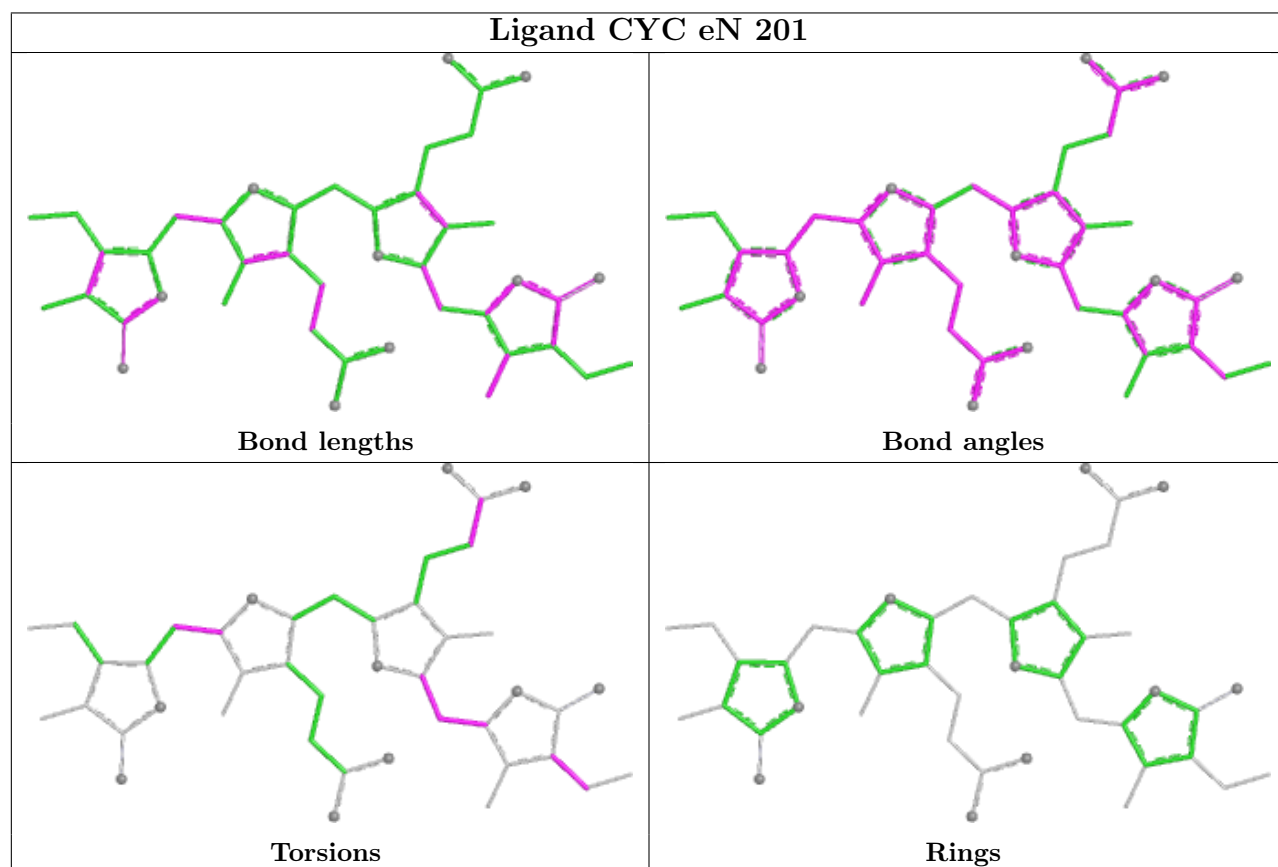
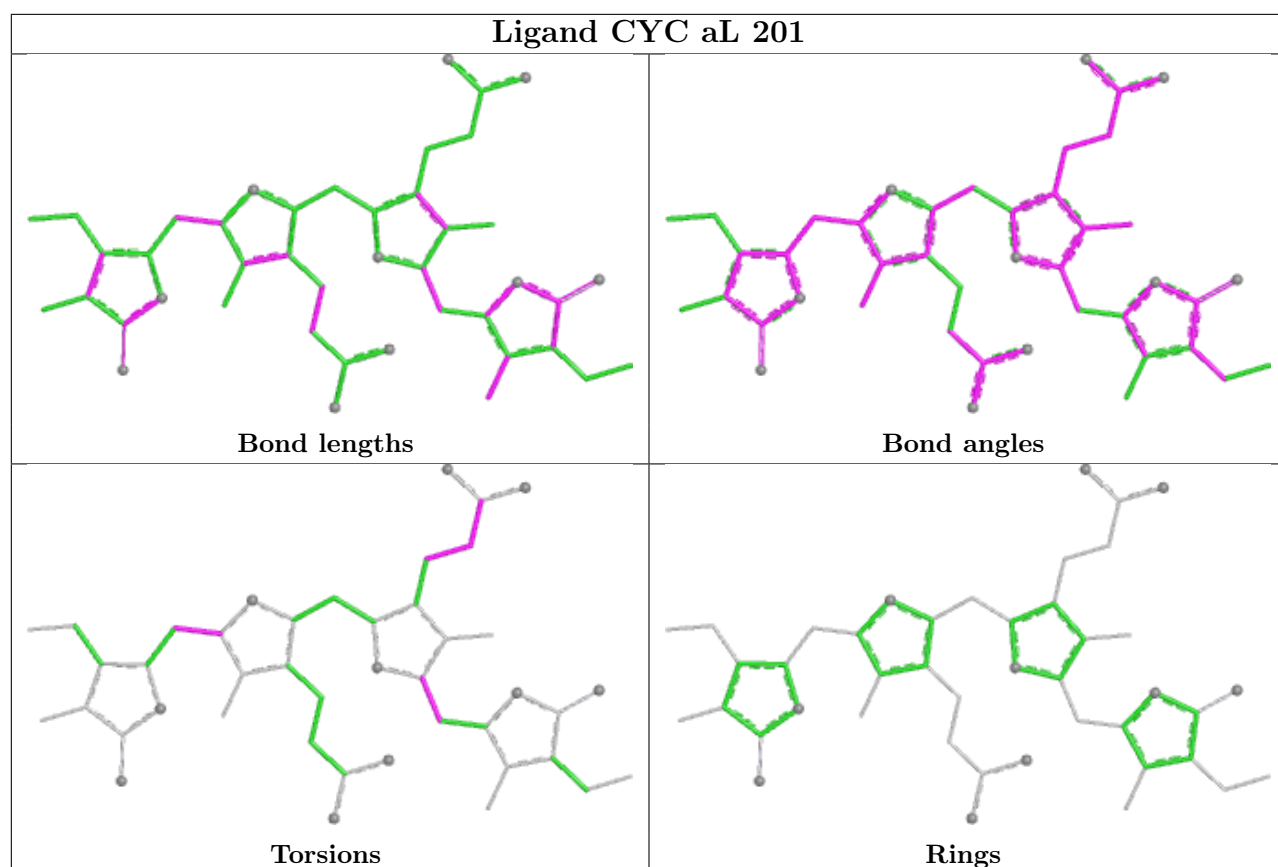


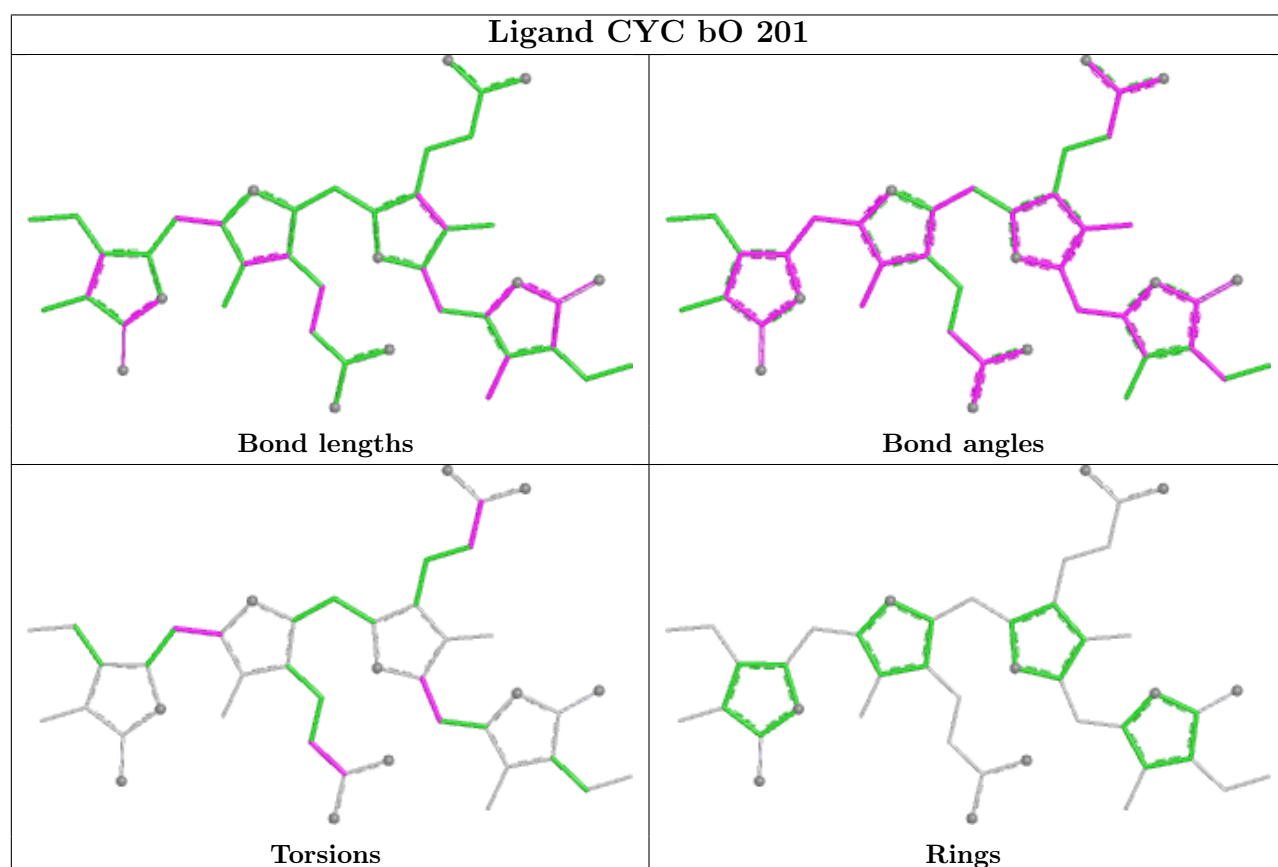
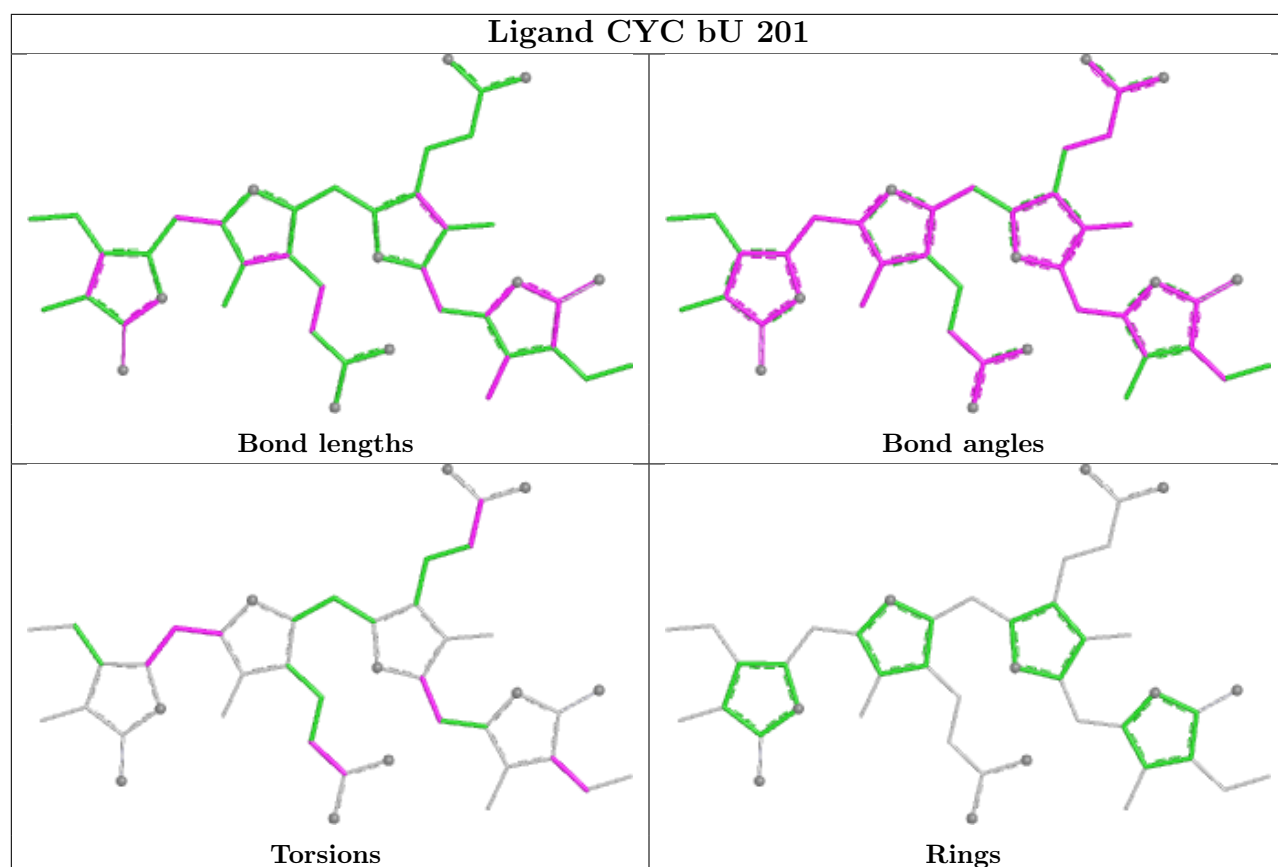


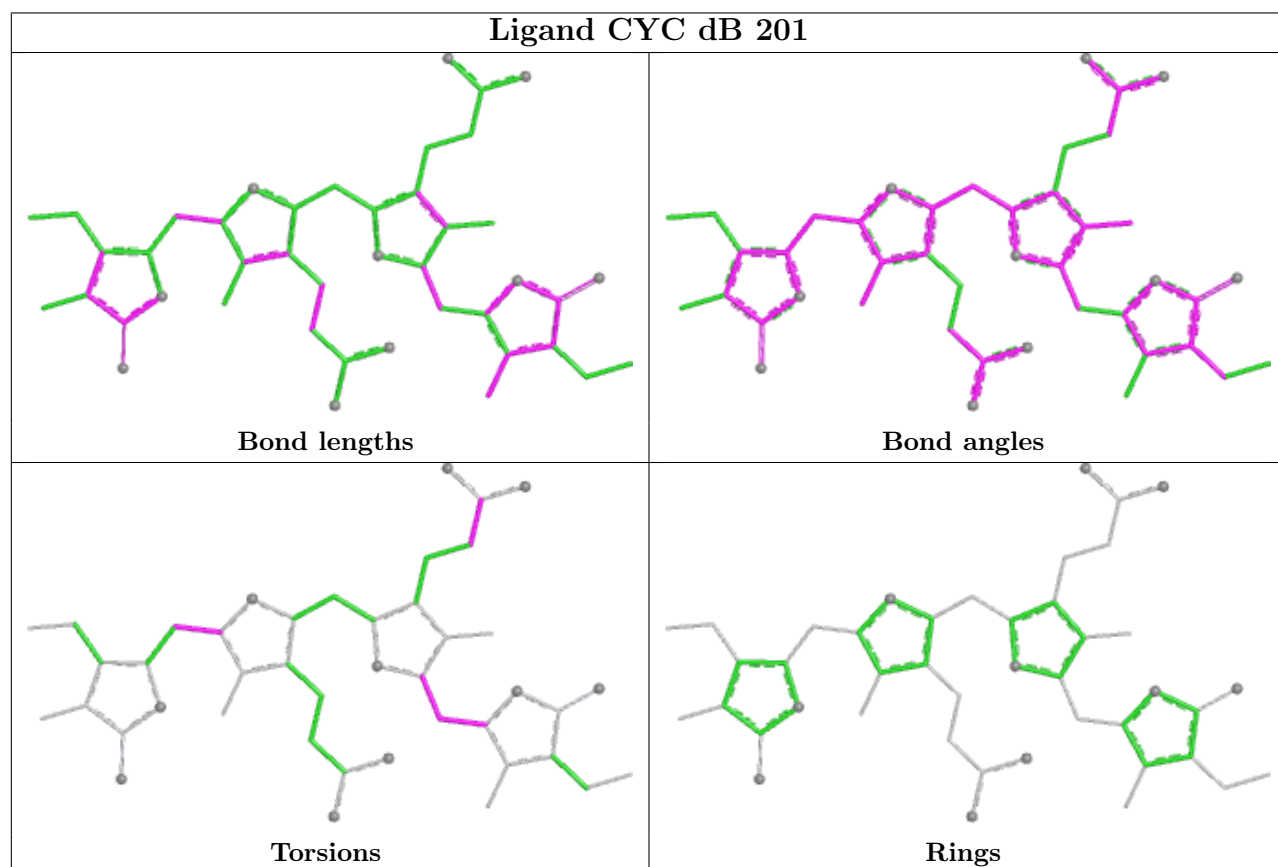
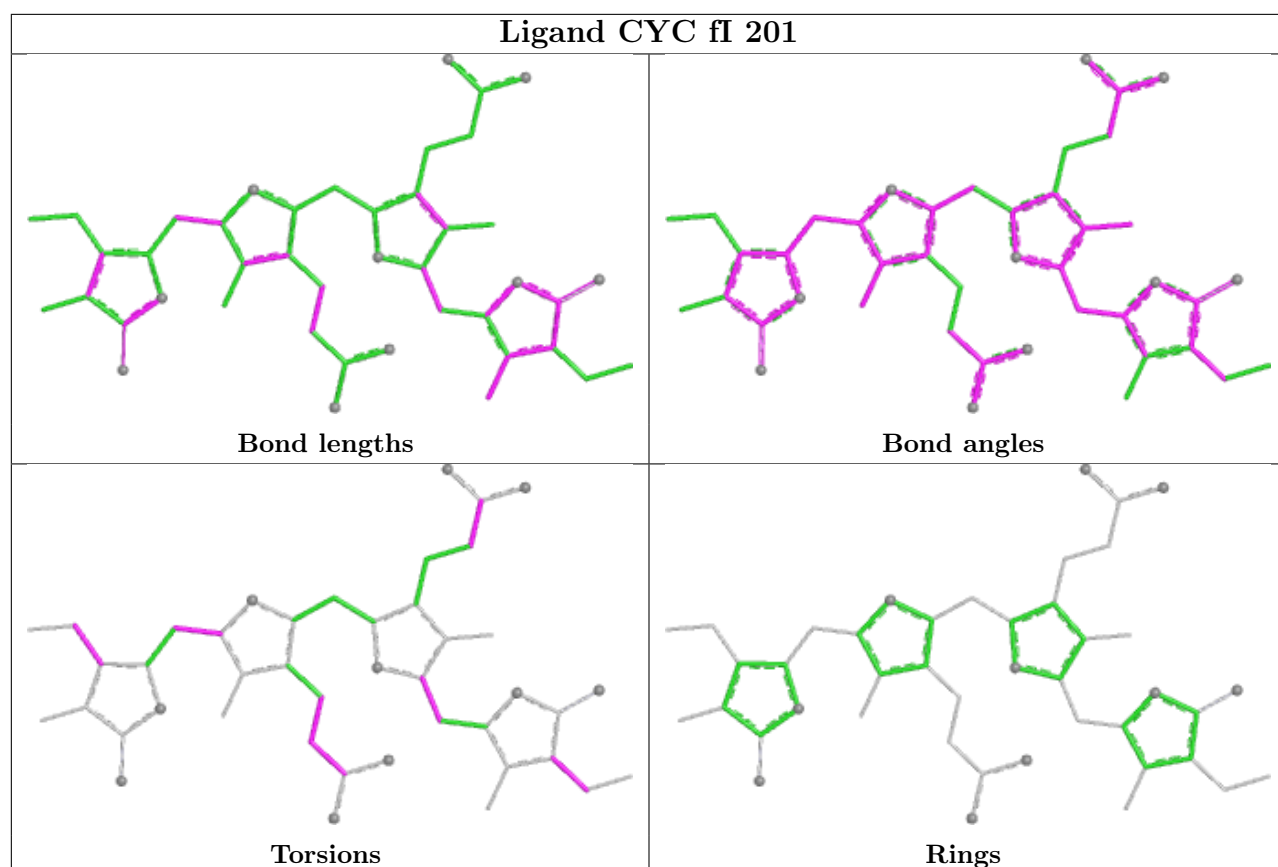


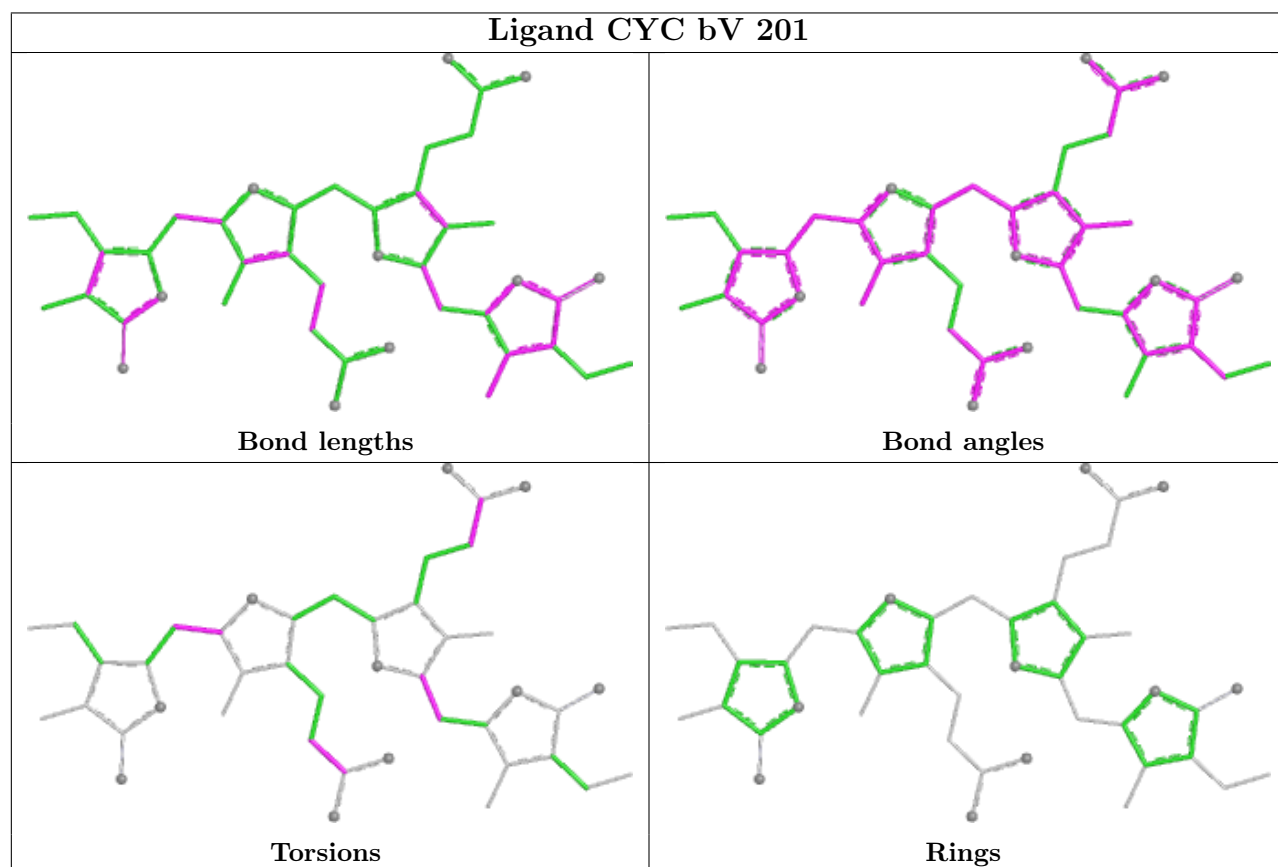
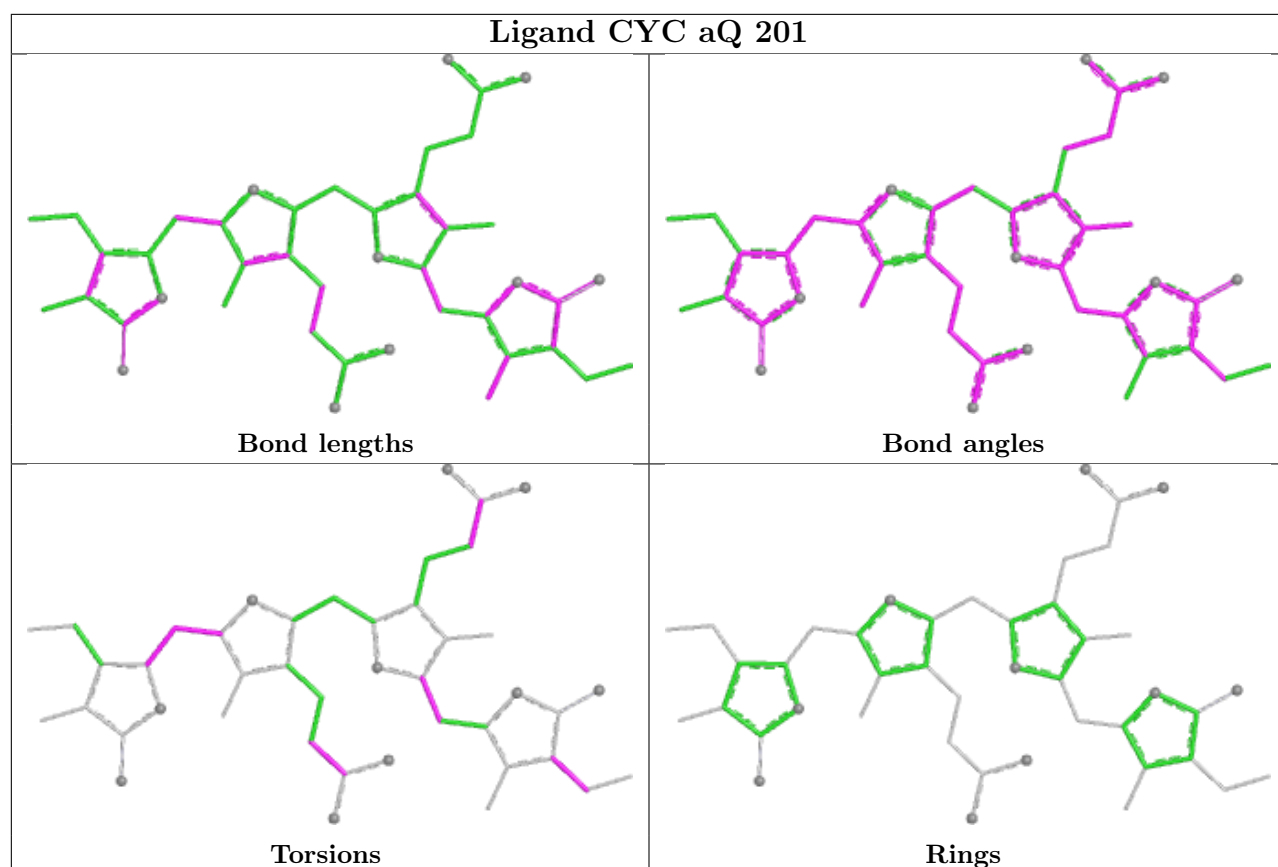




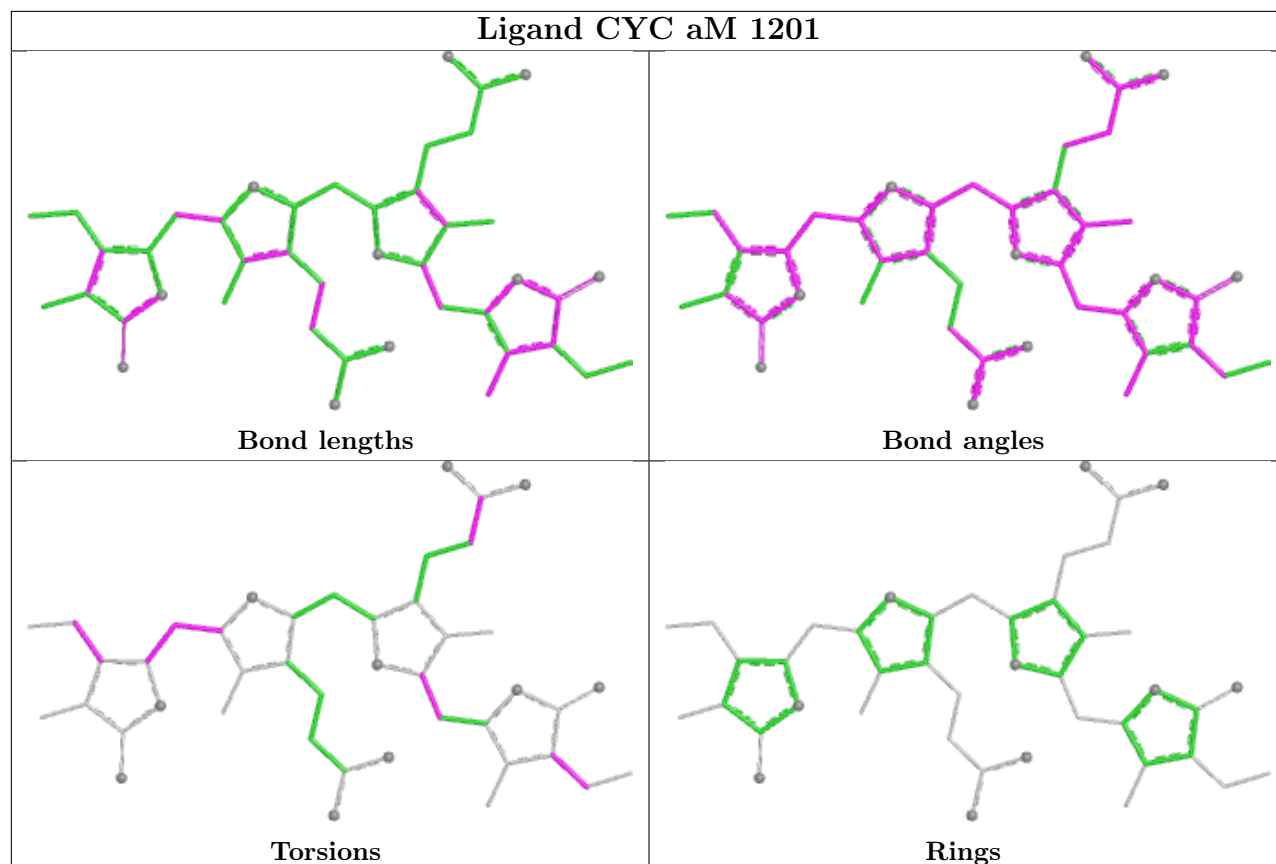




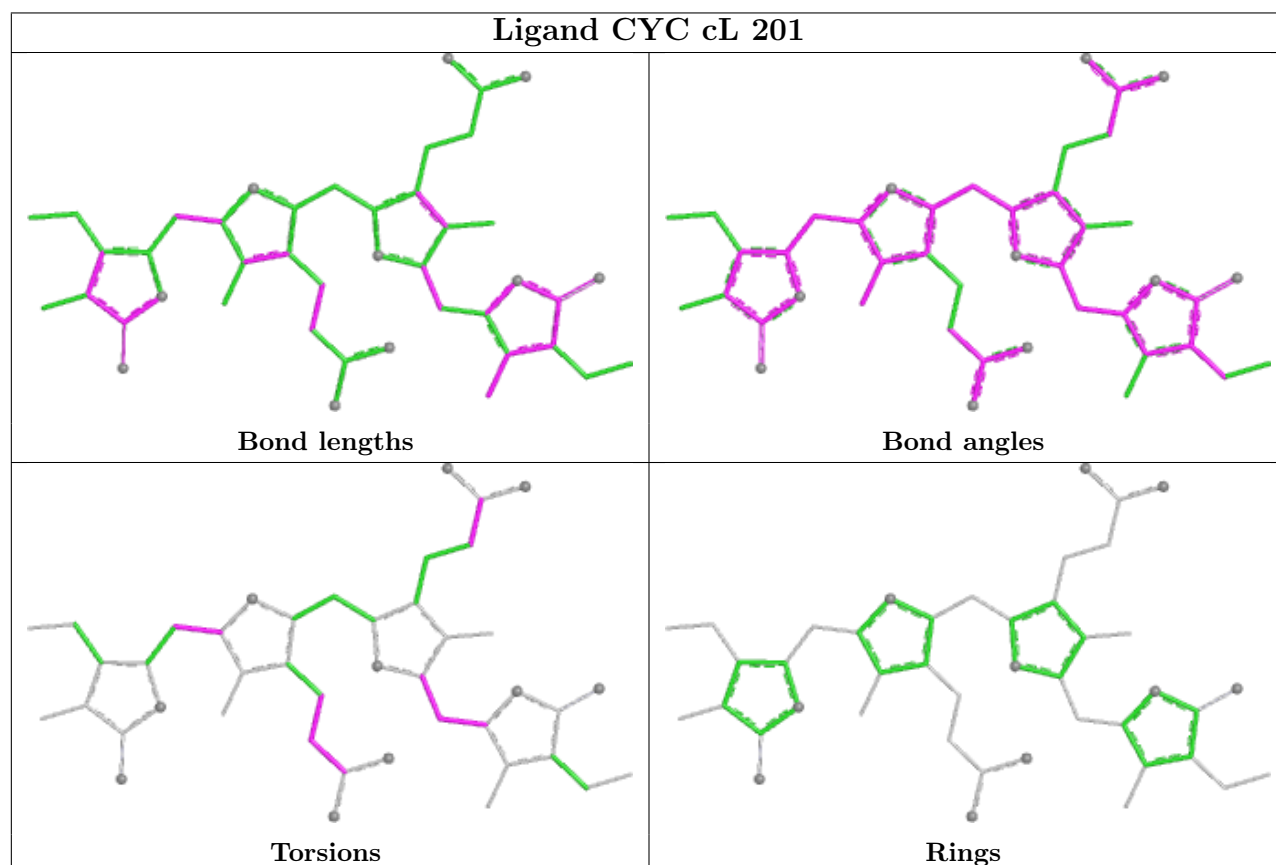


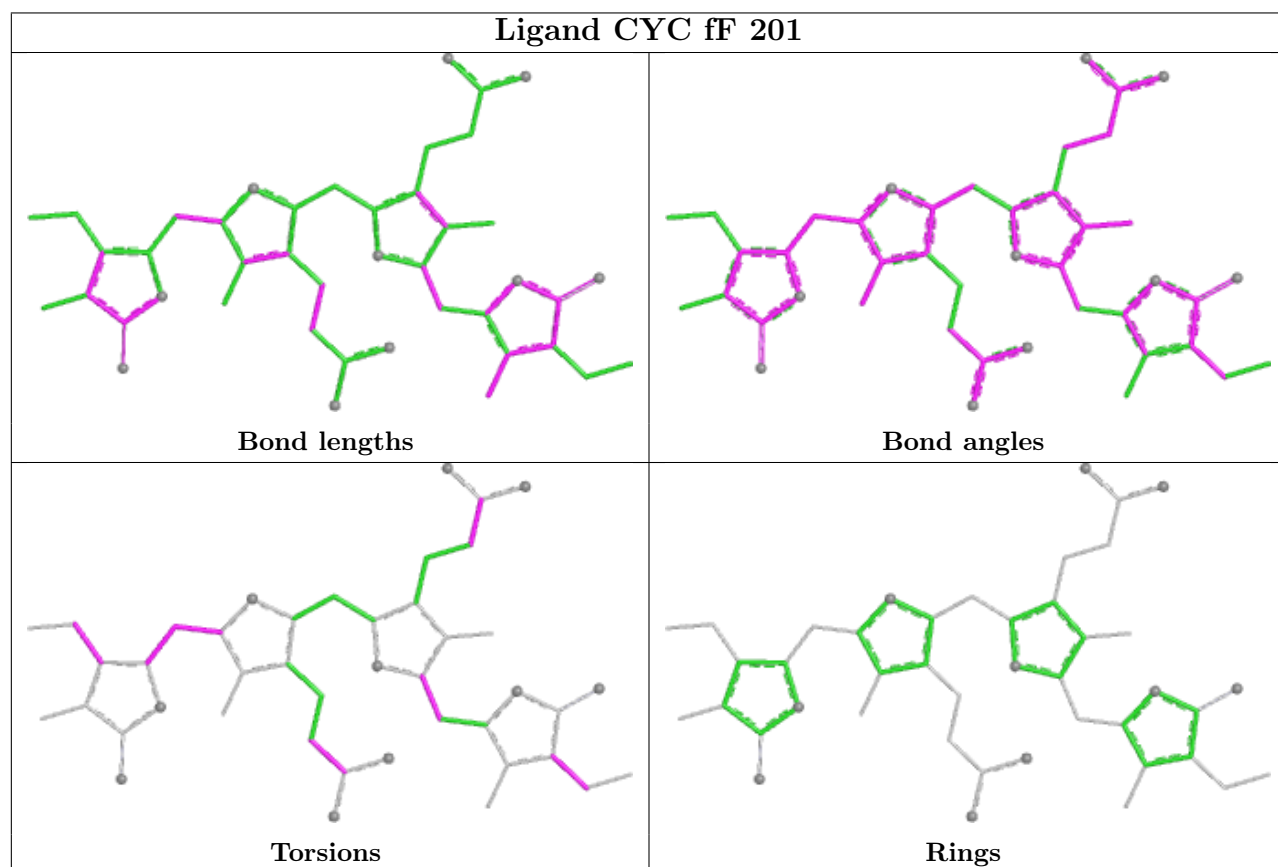
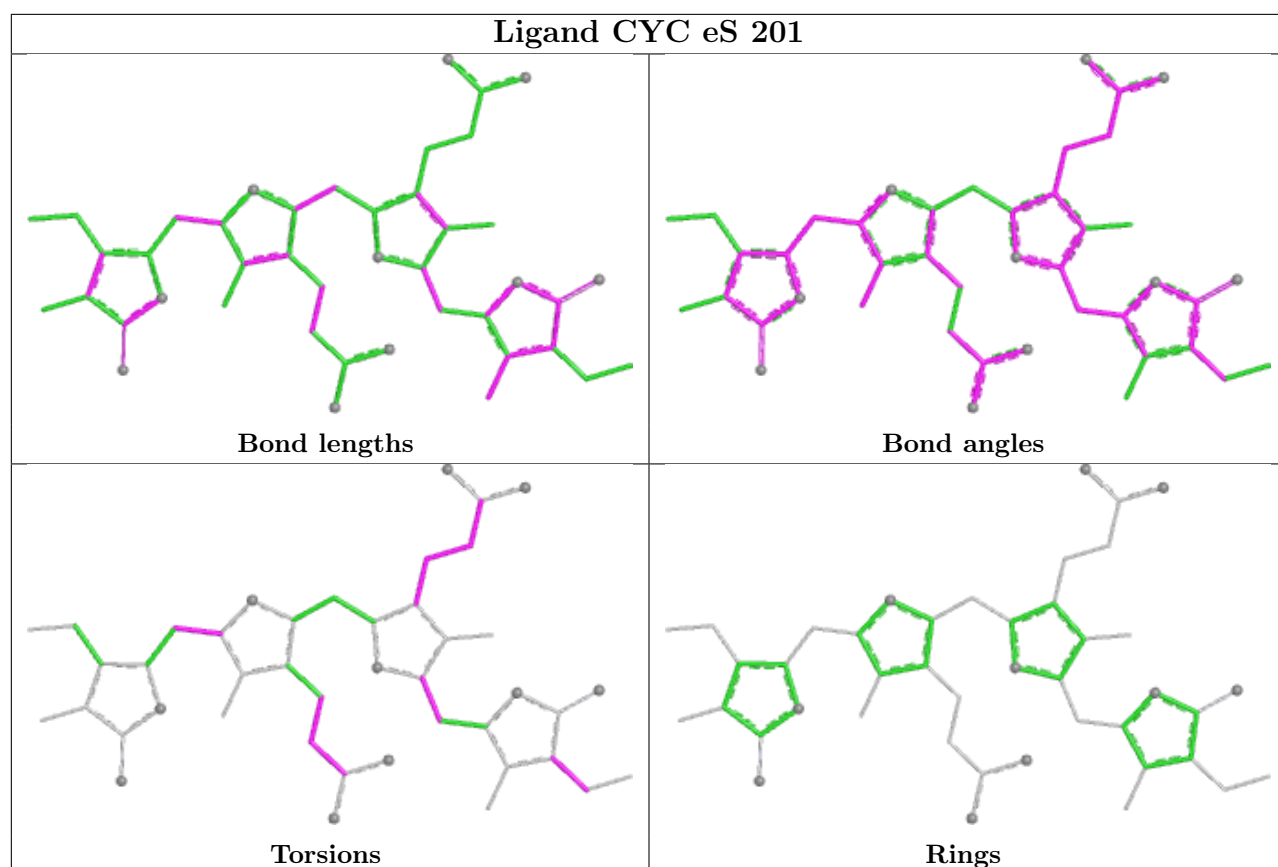


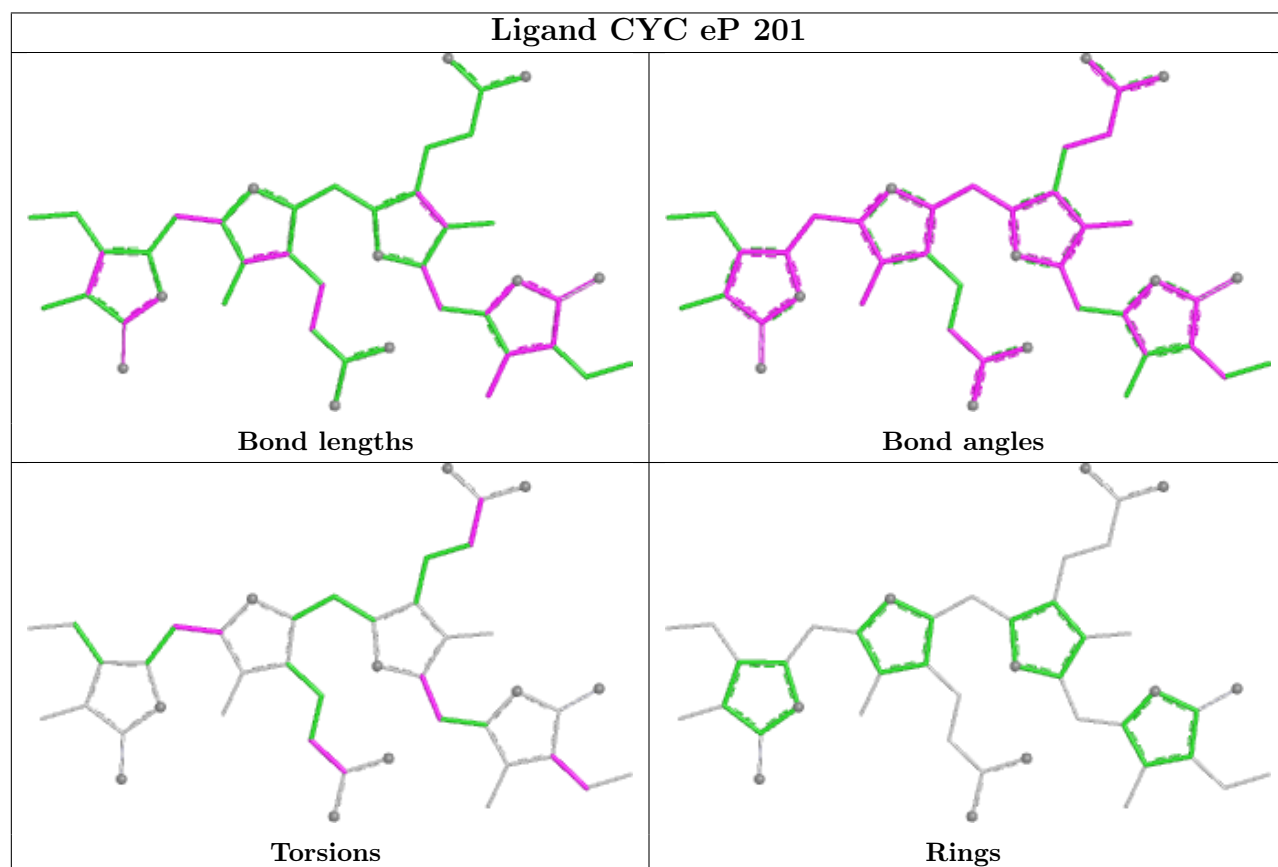
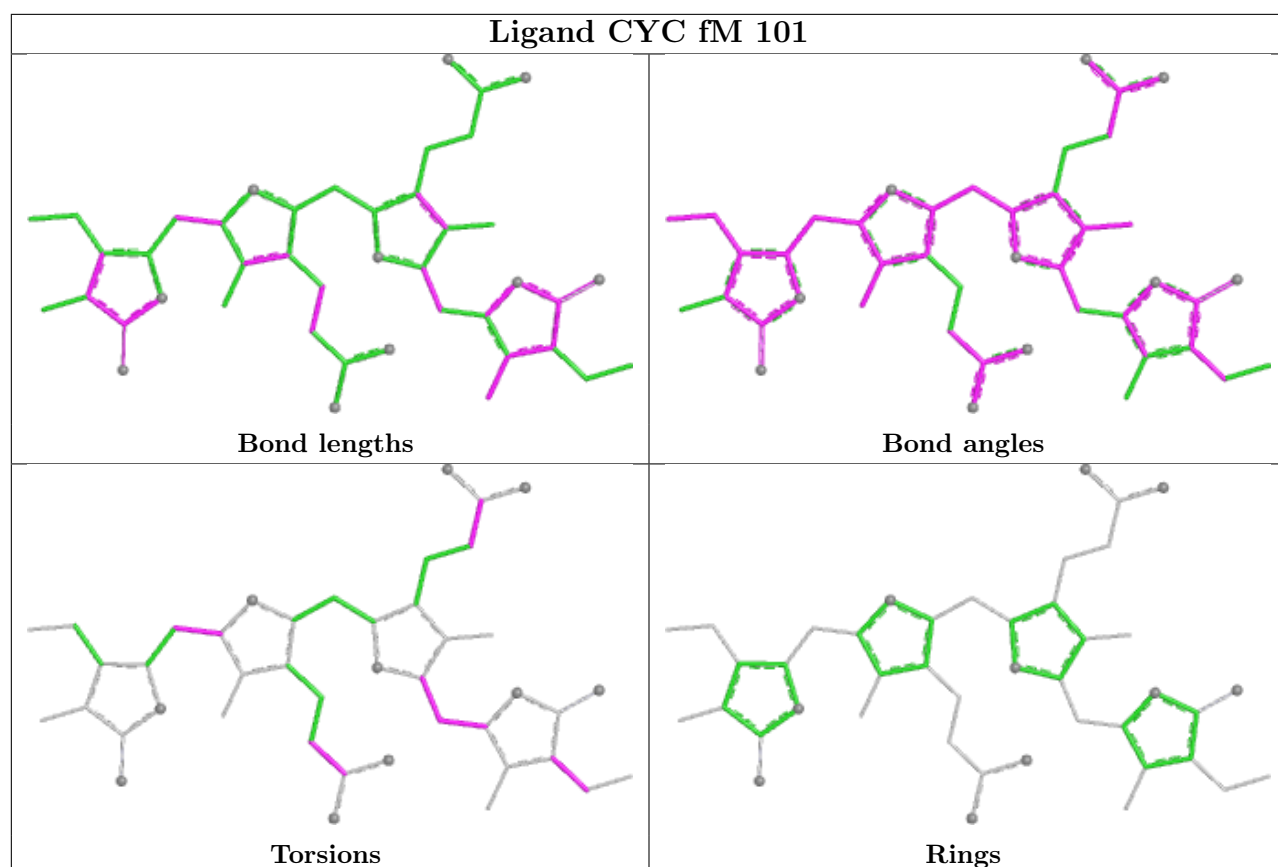
Ligand CYC aM 1201

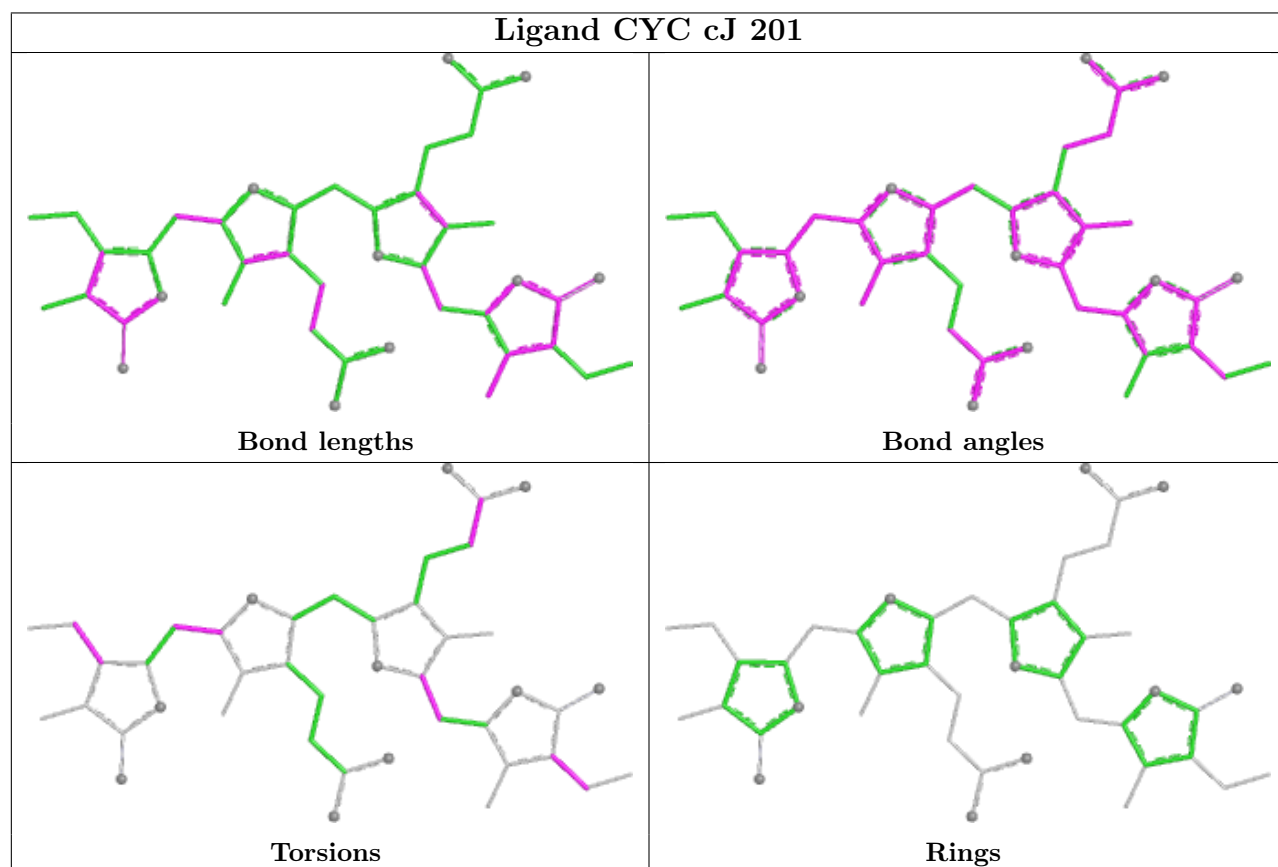
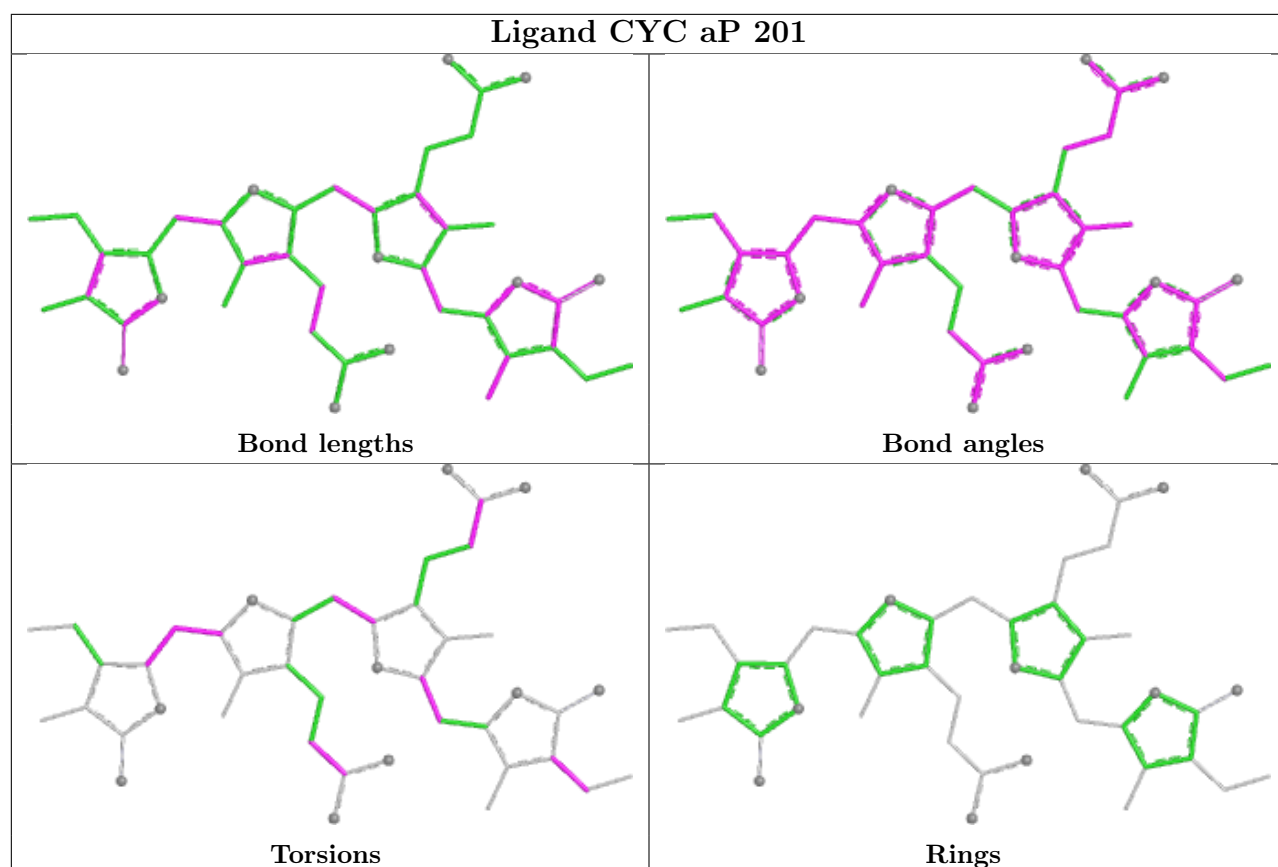


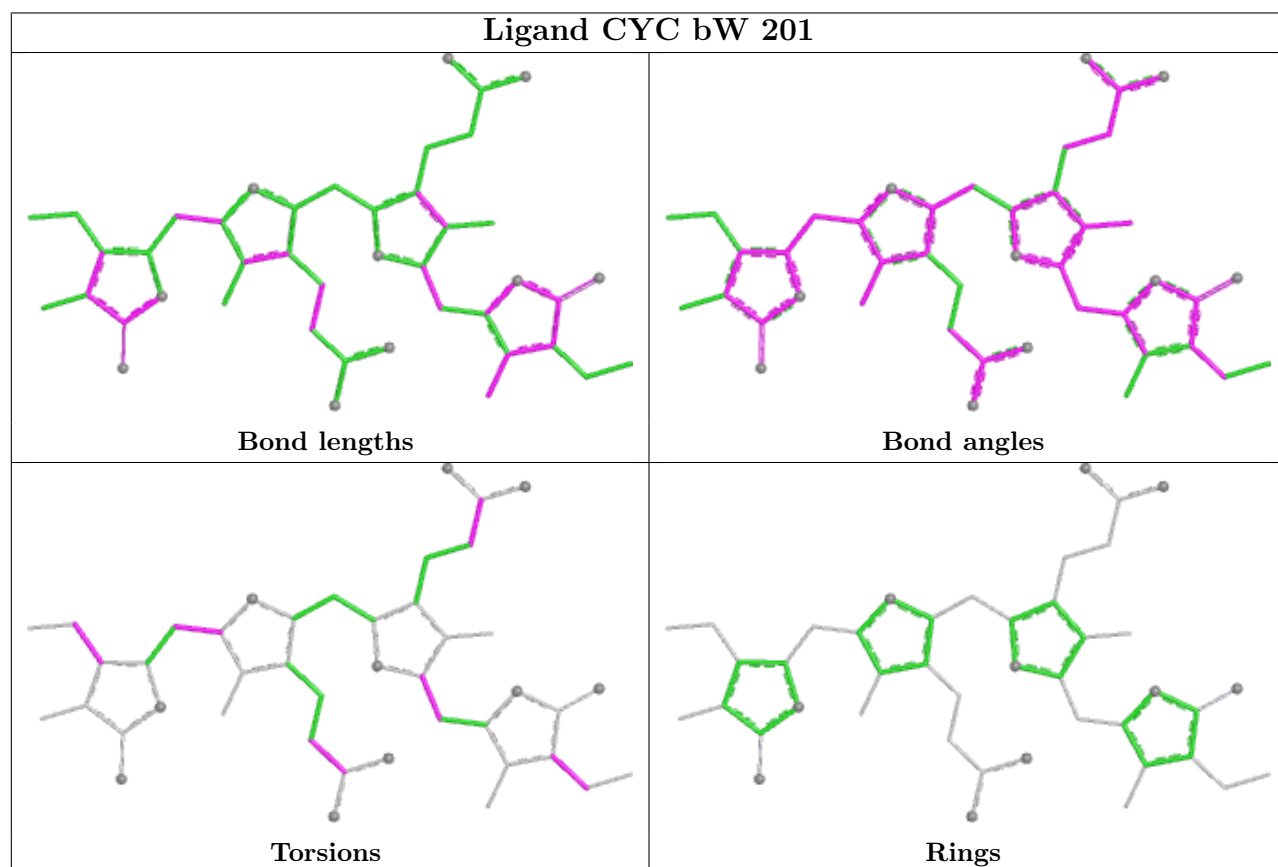
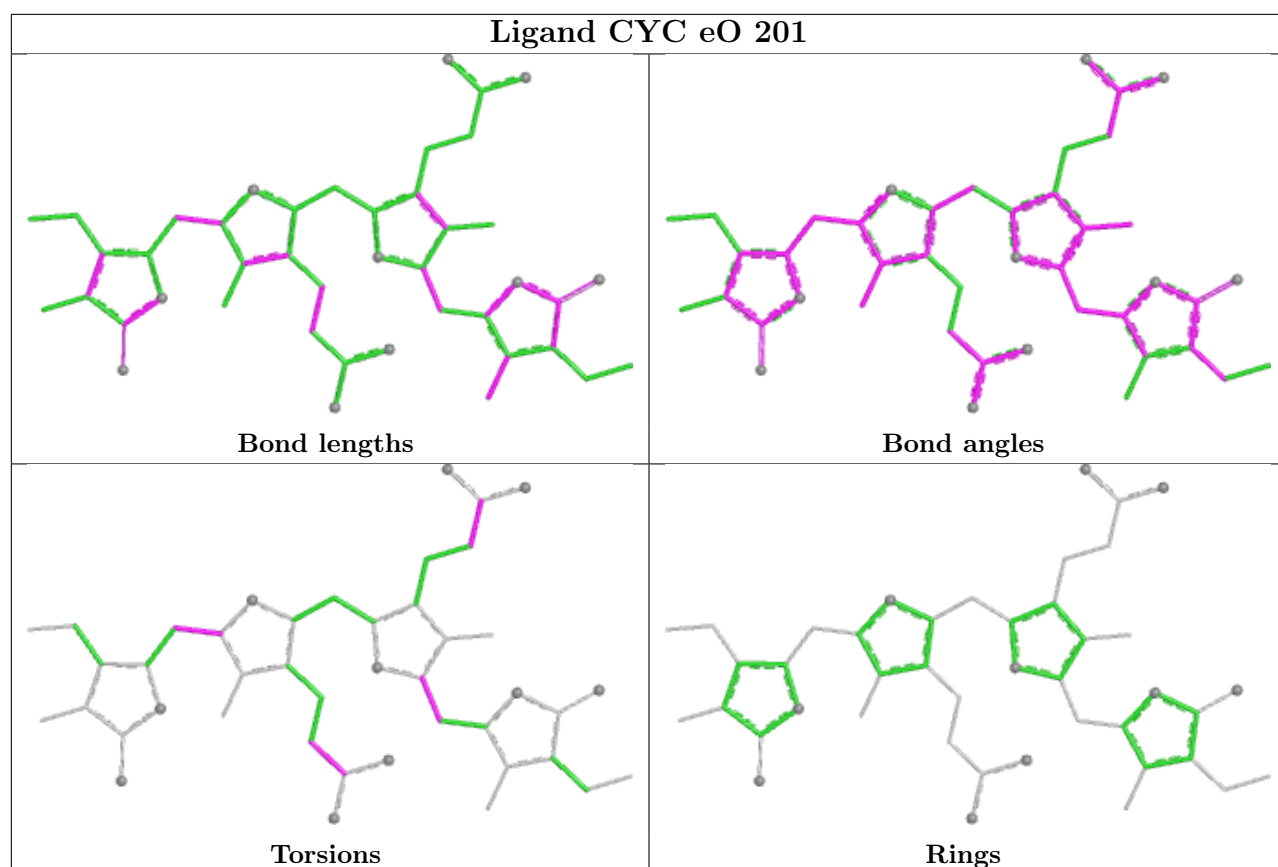
Ligand CYC cL 201

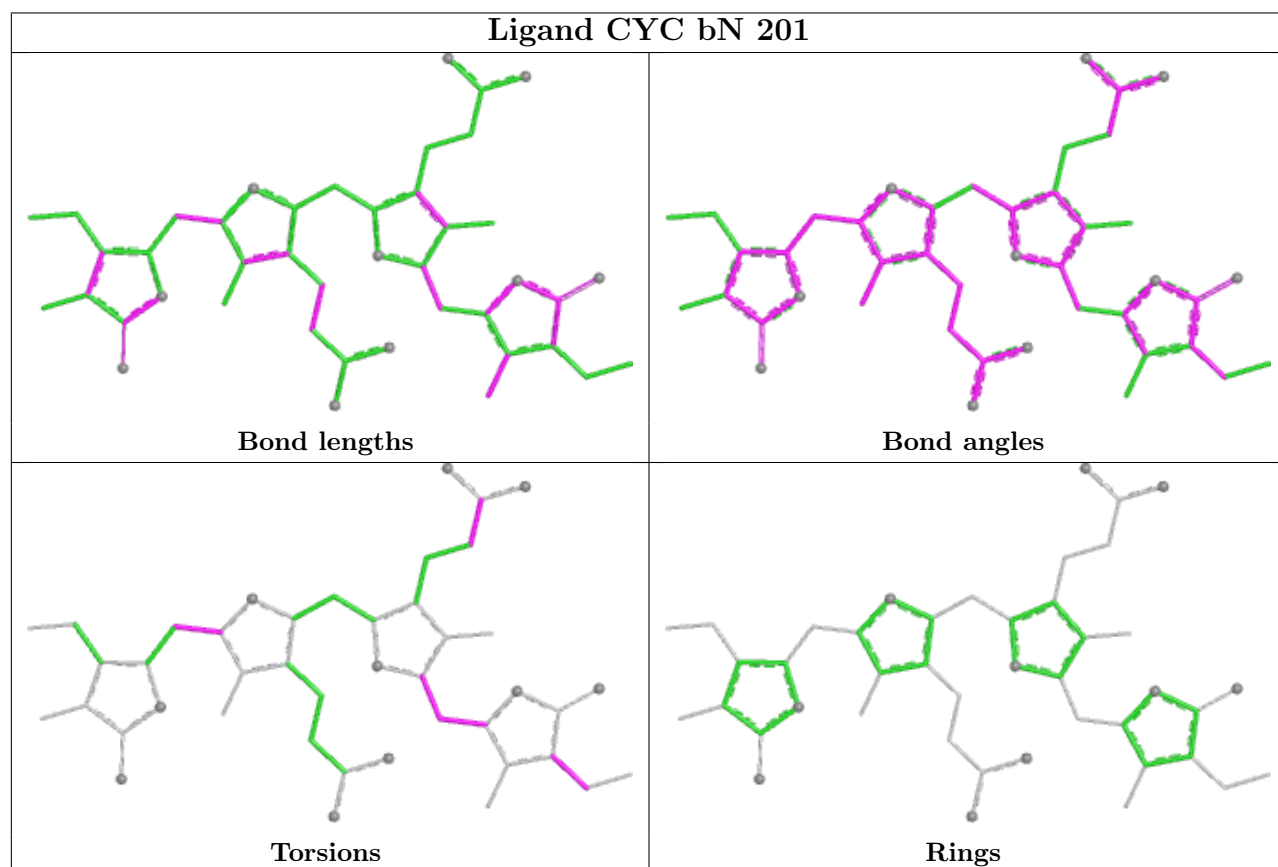
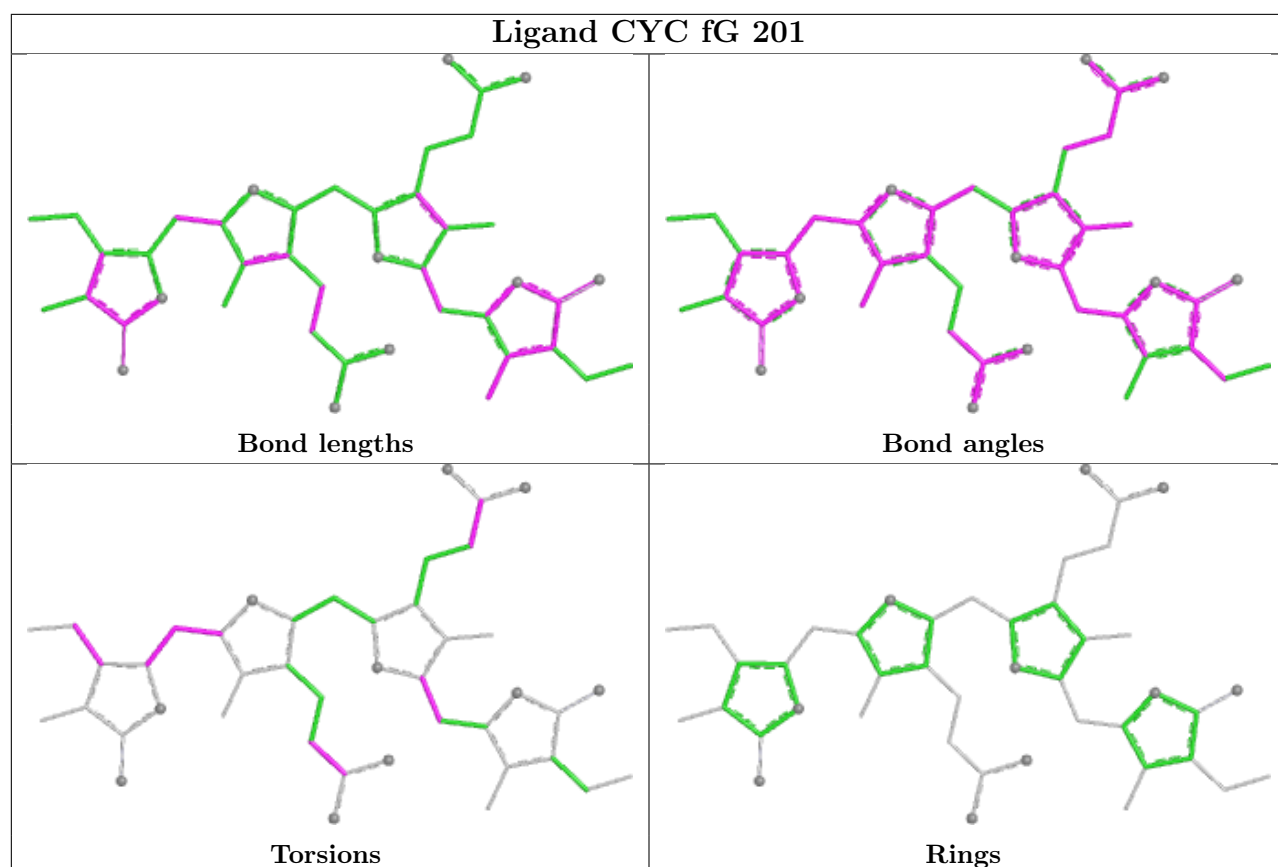




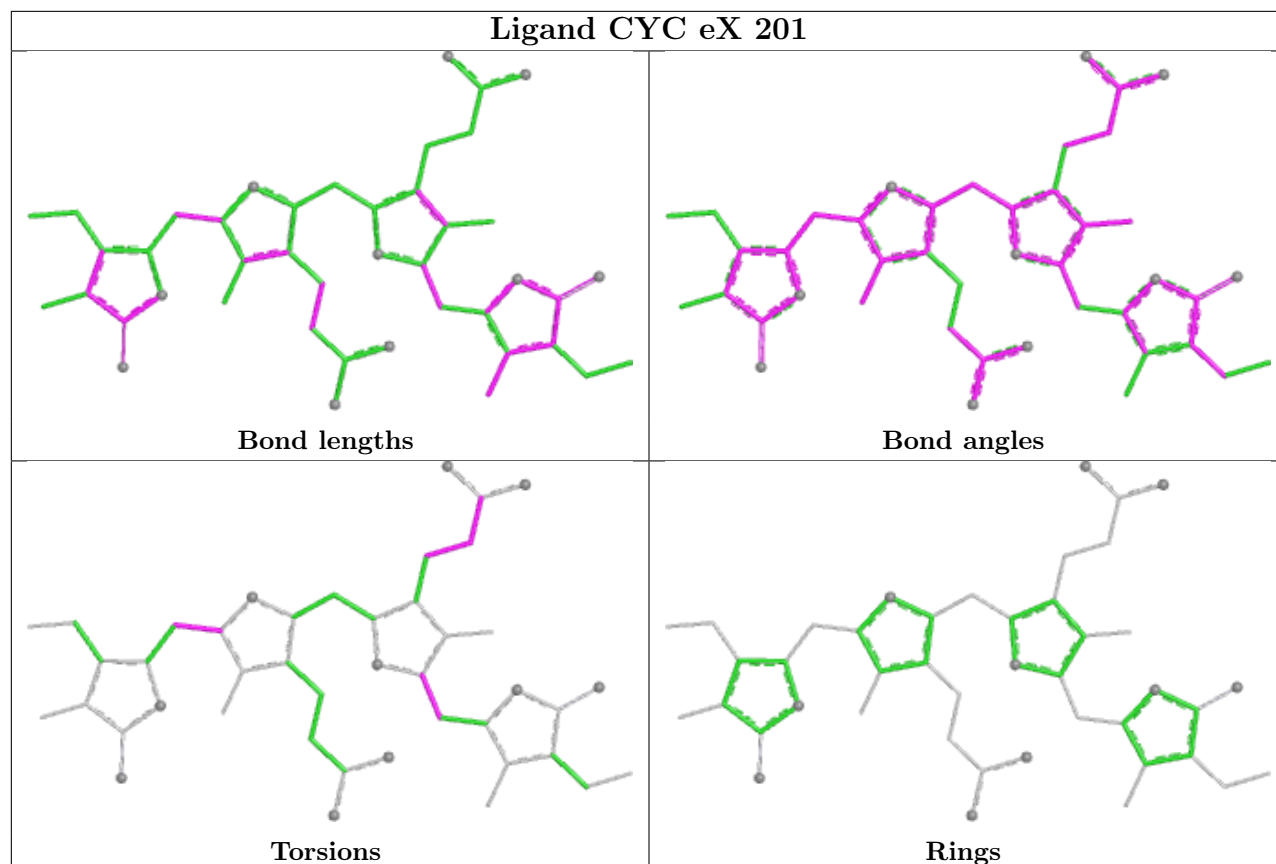




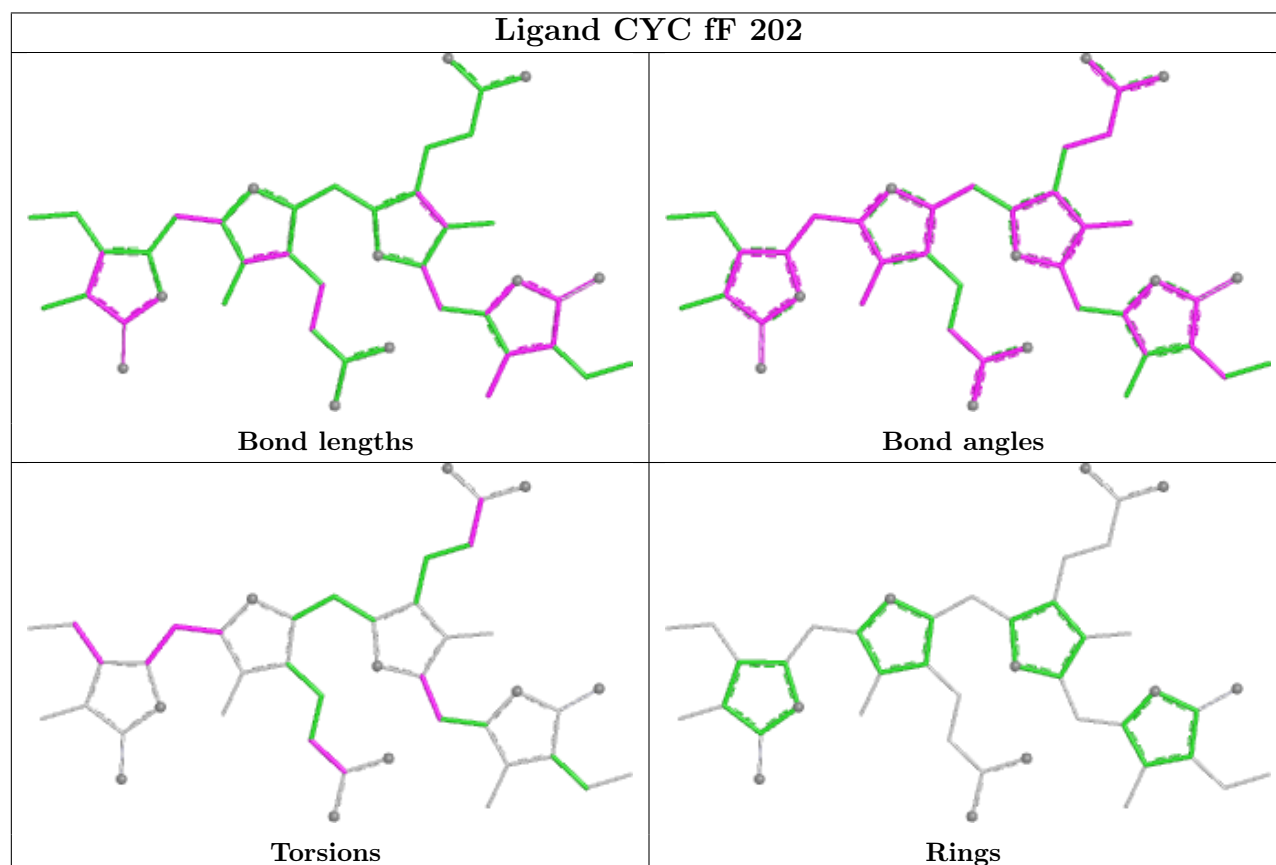


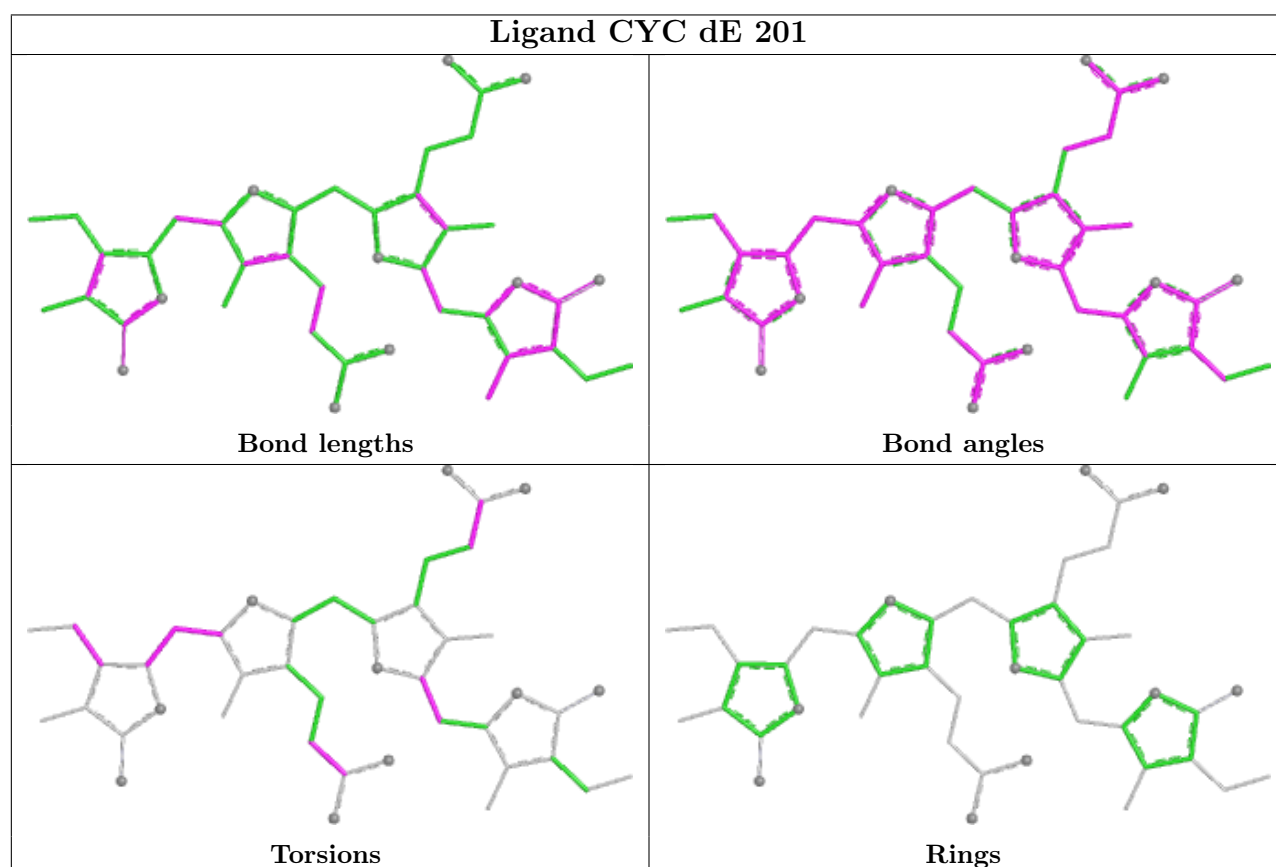
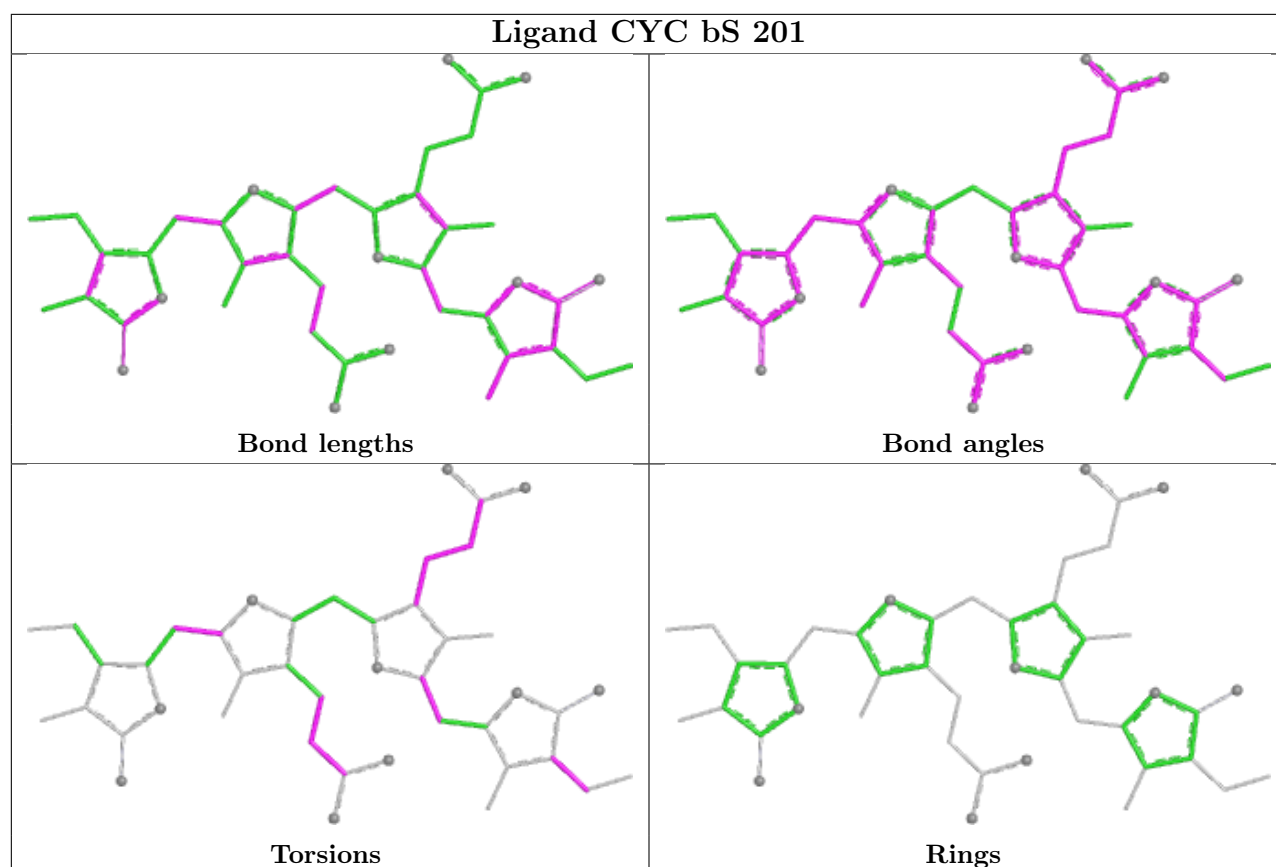


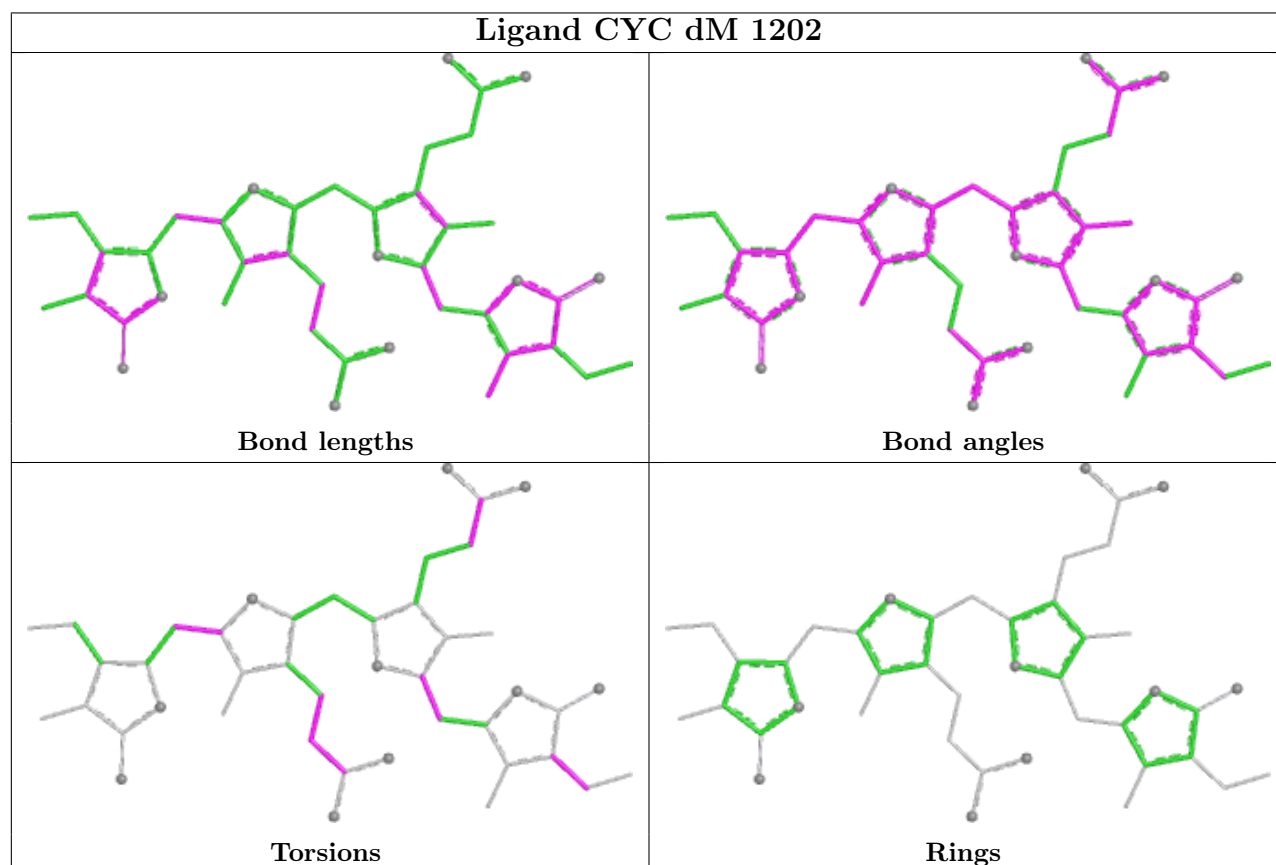
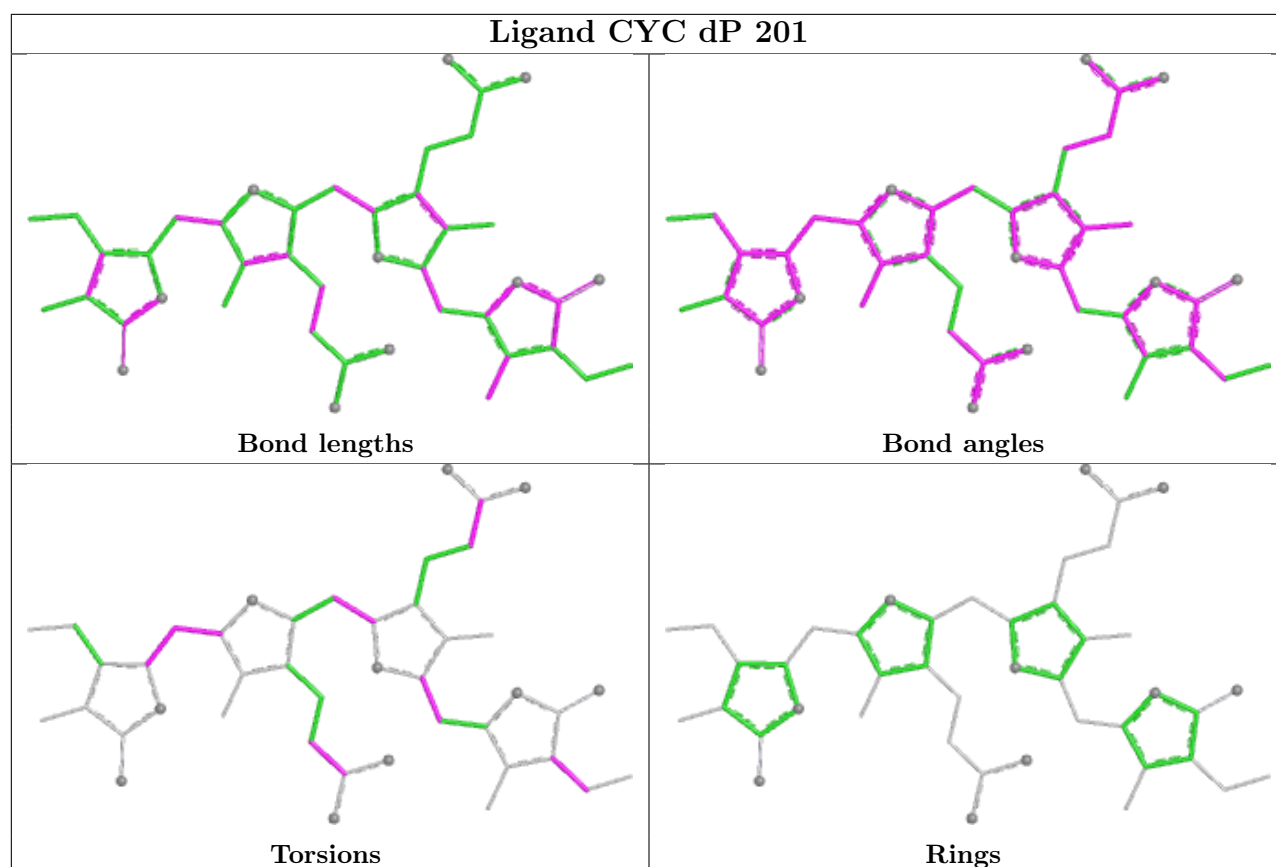
Ligand CYC eX 201



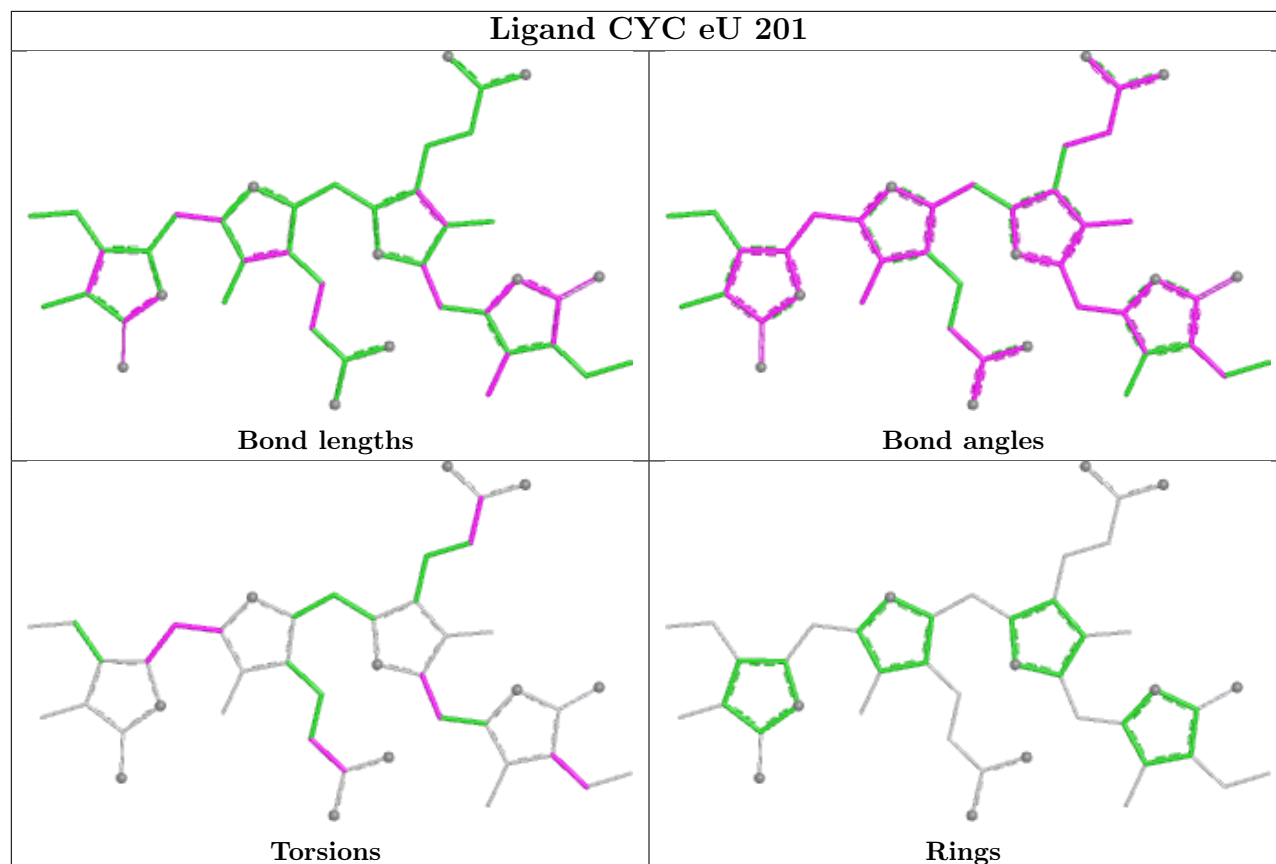
Ligand CYC fF 202



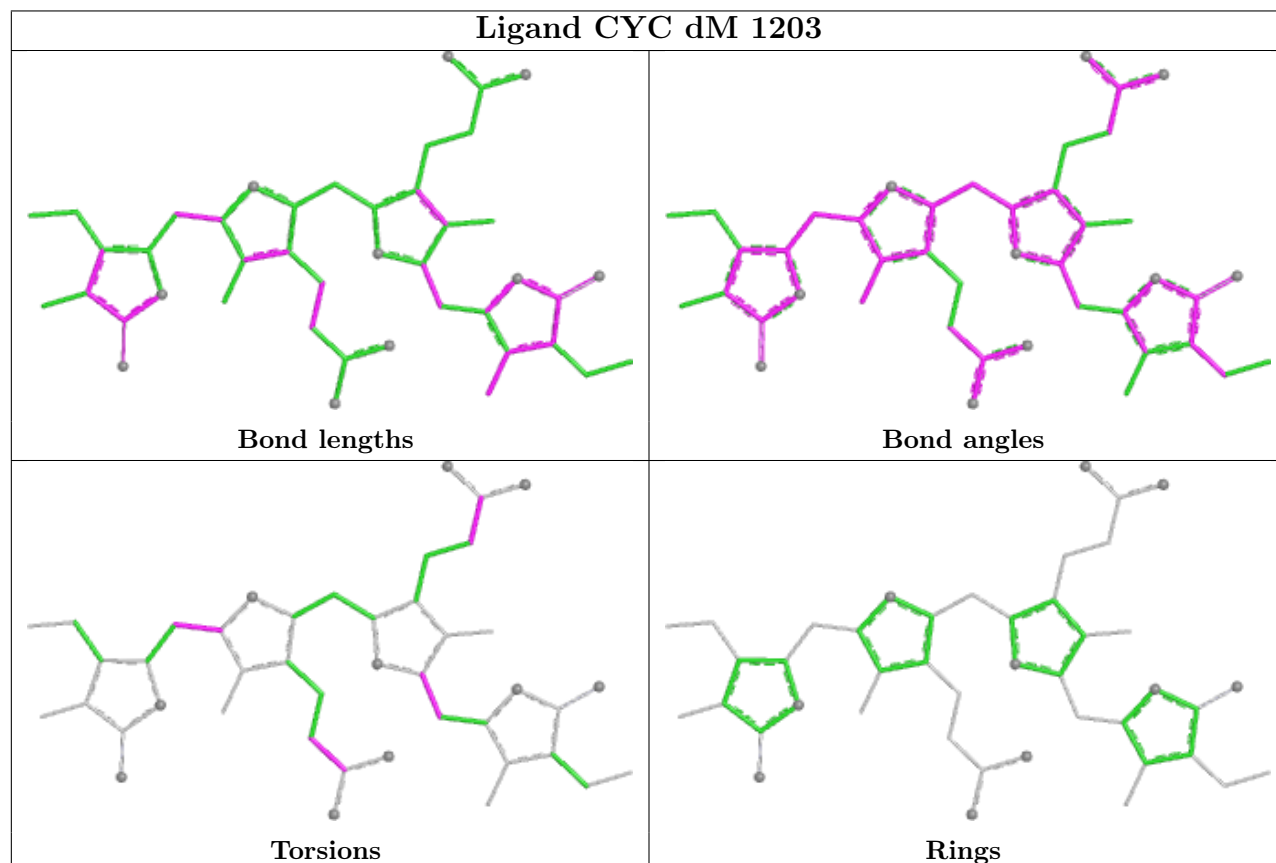


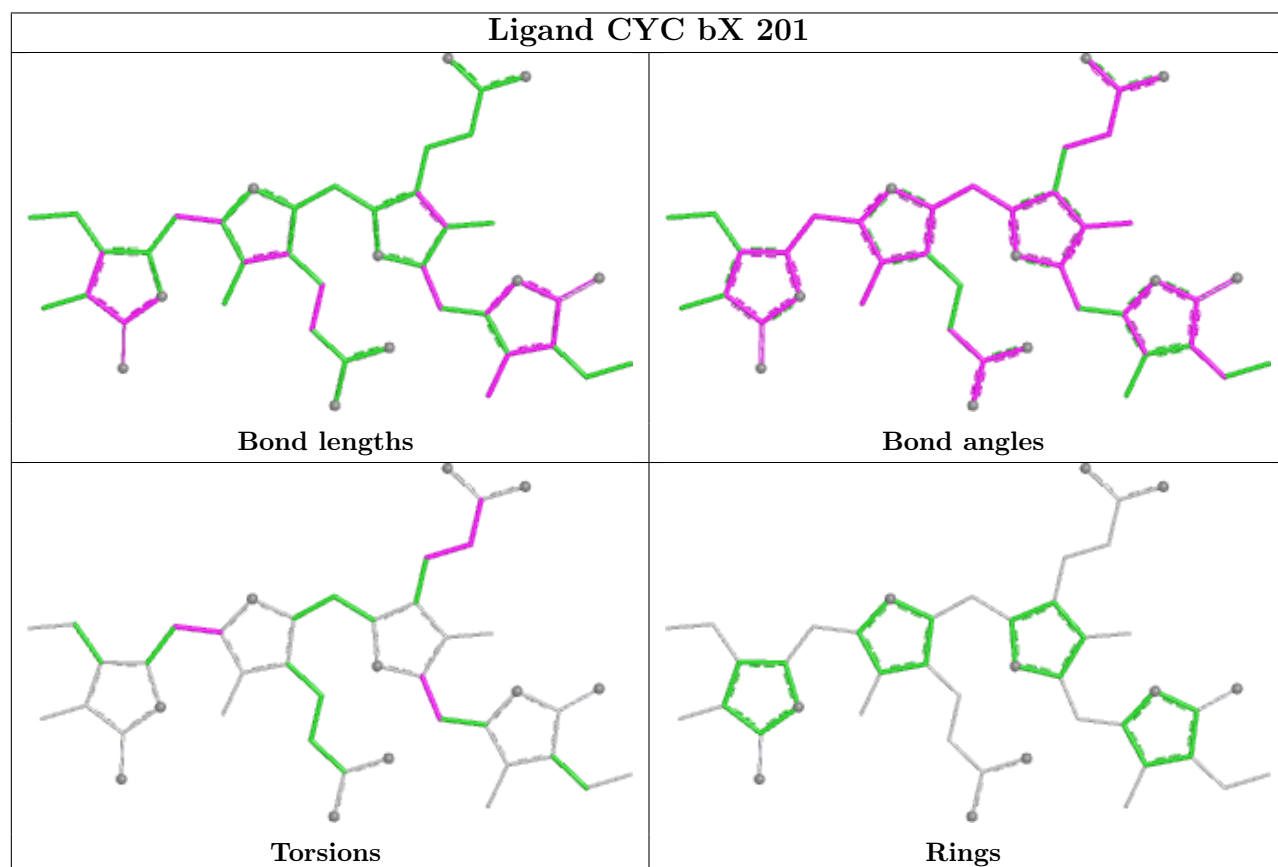
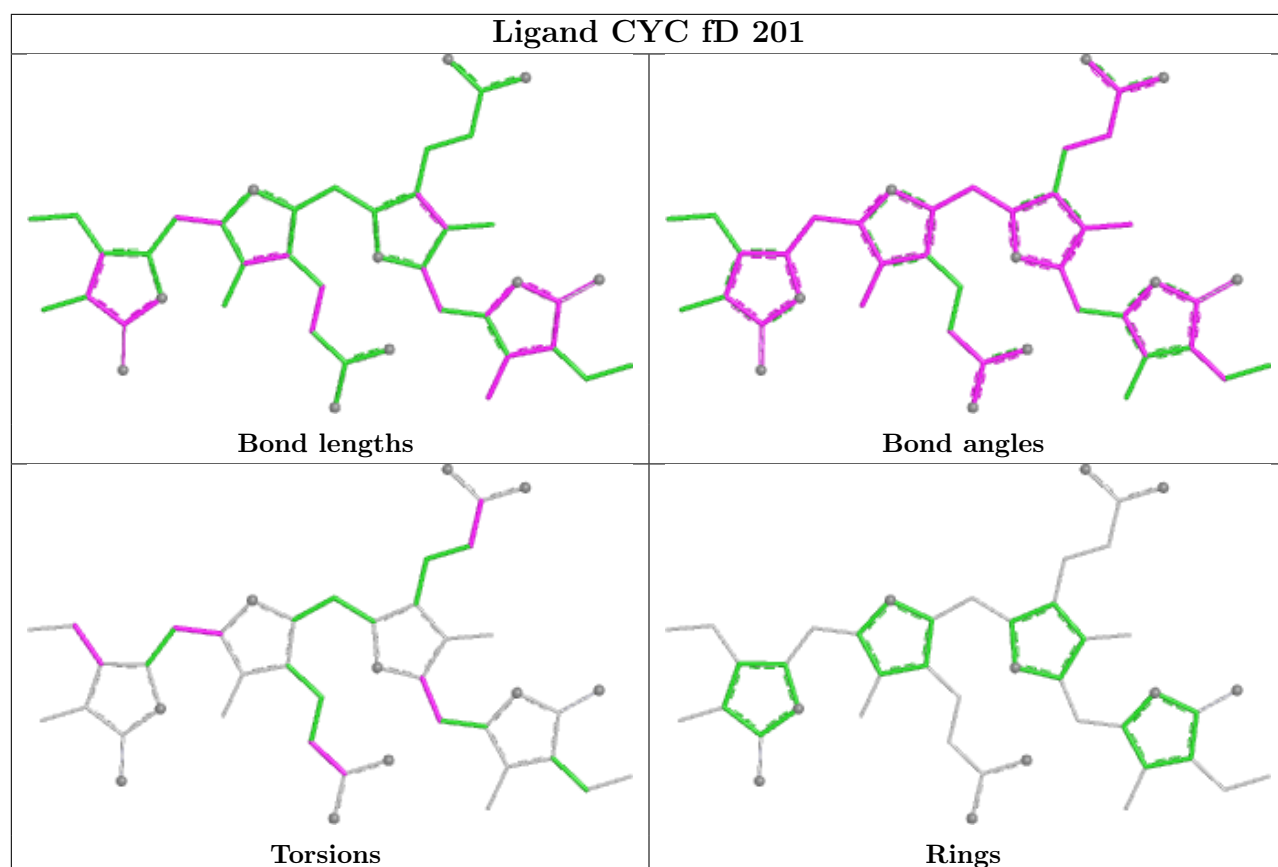


Ligand CYC eU 201

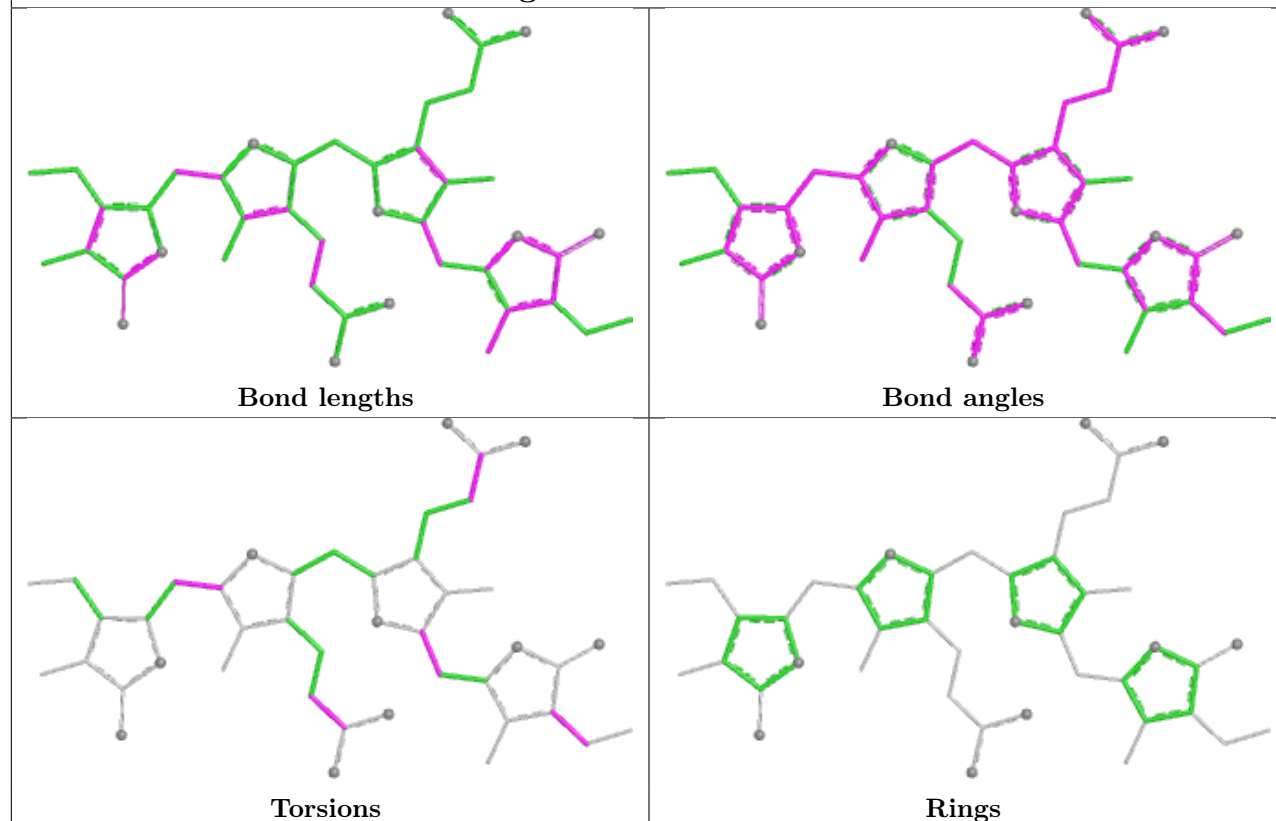


Ligand CYC dM 1203

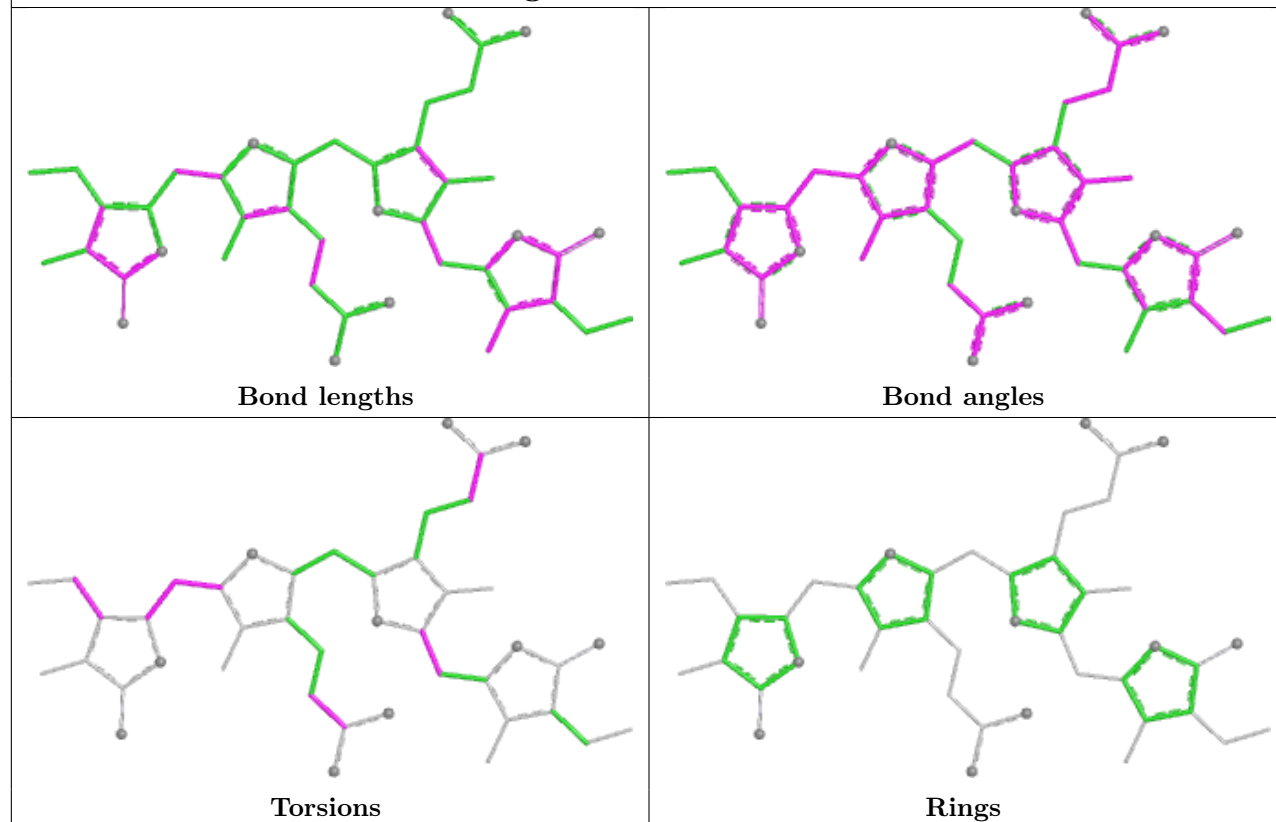


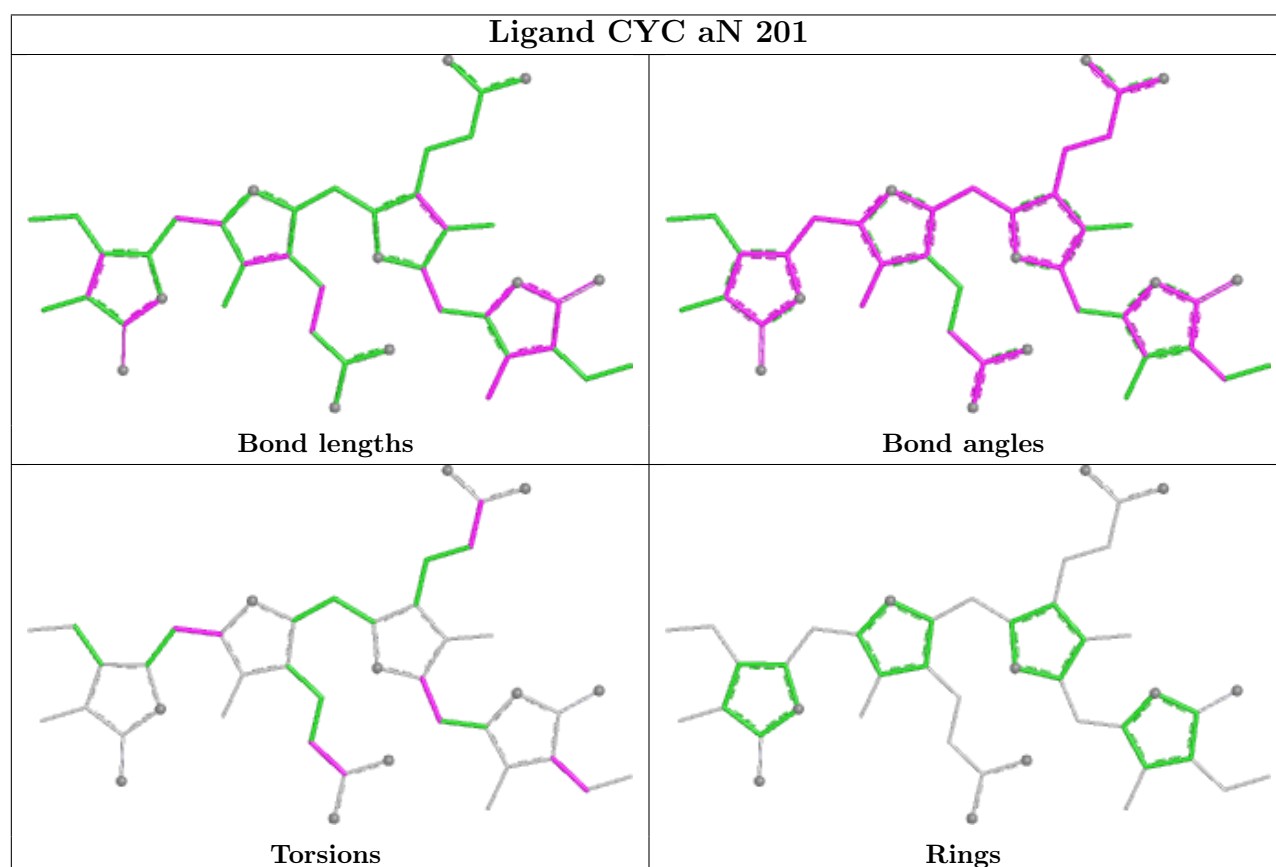
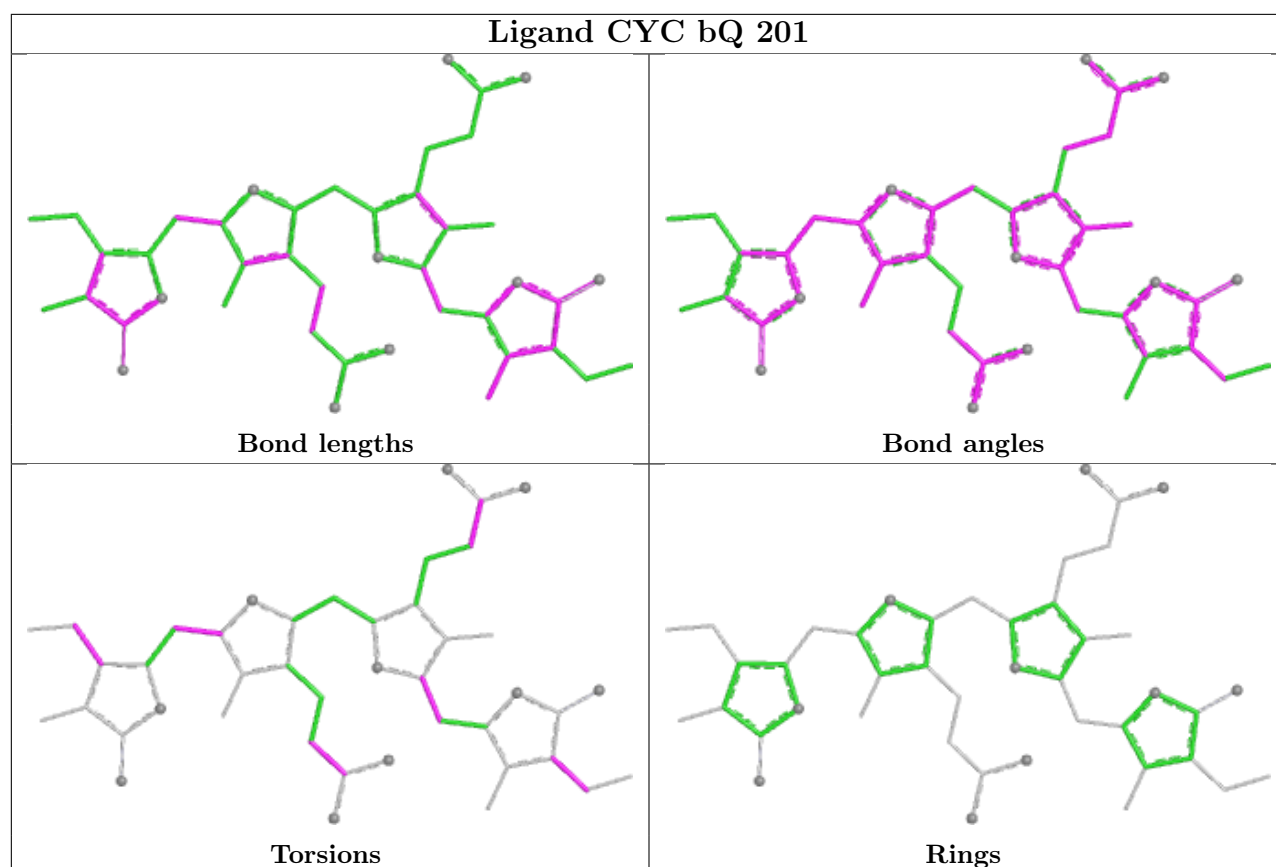


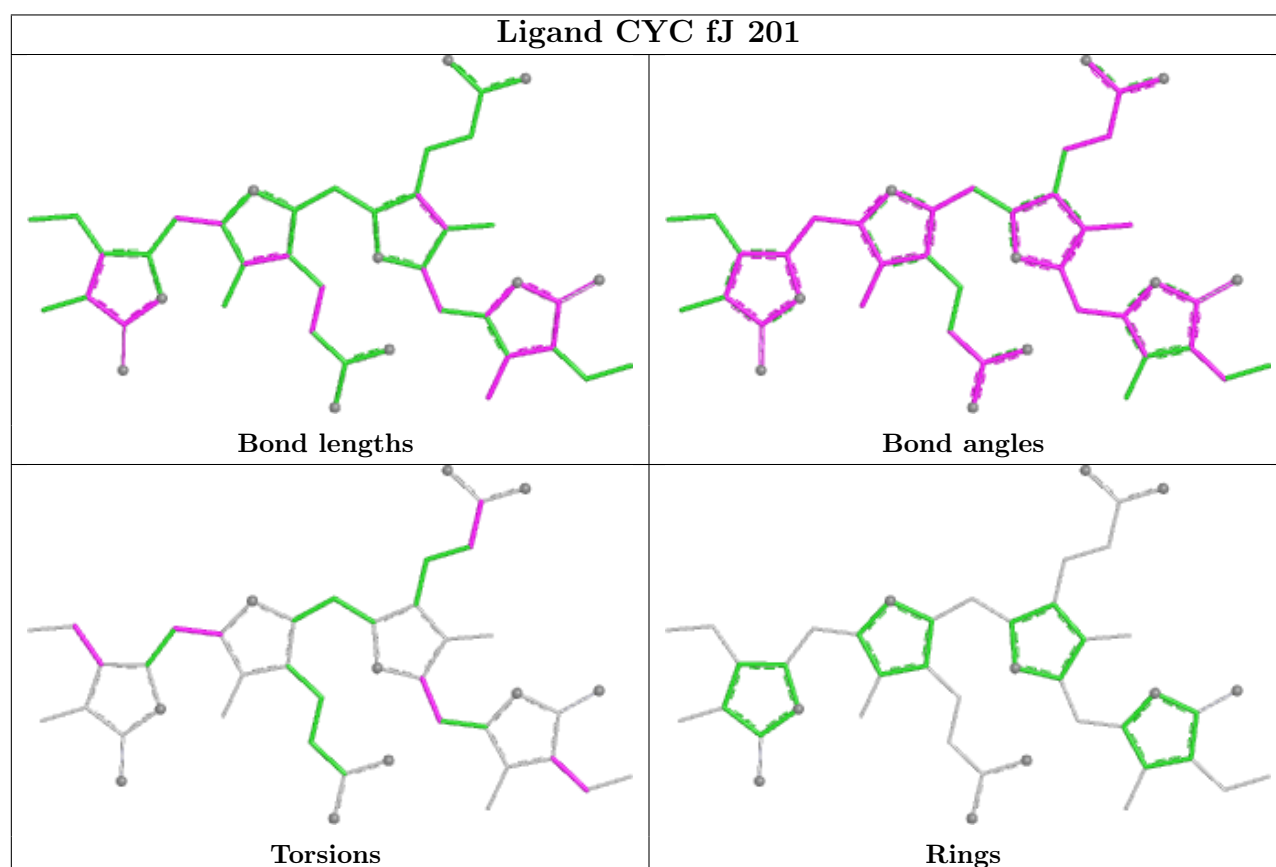
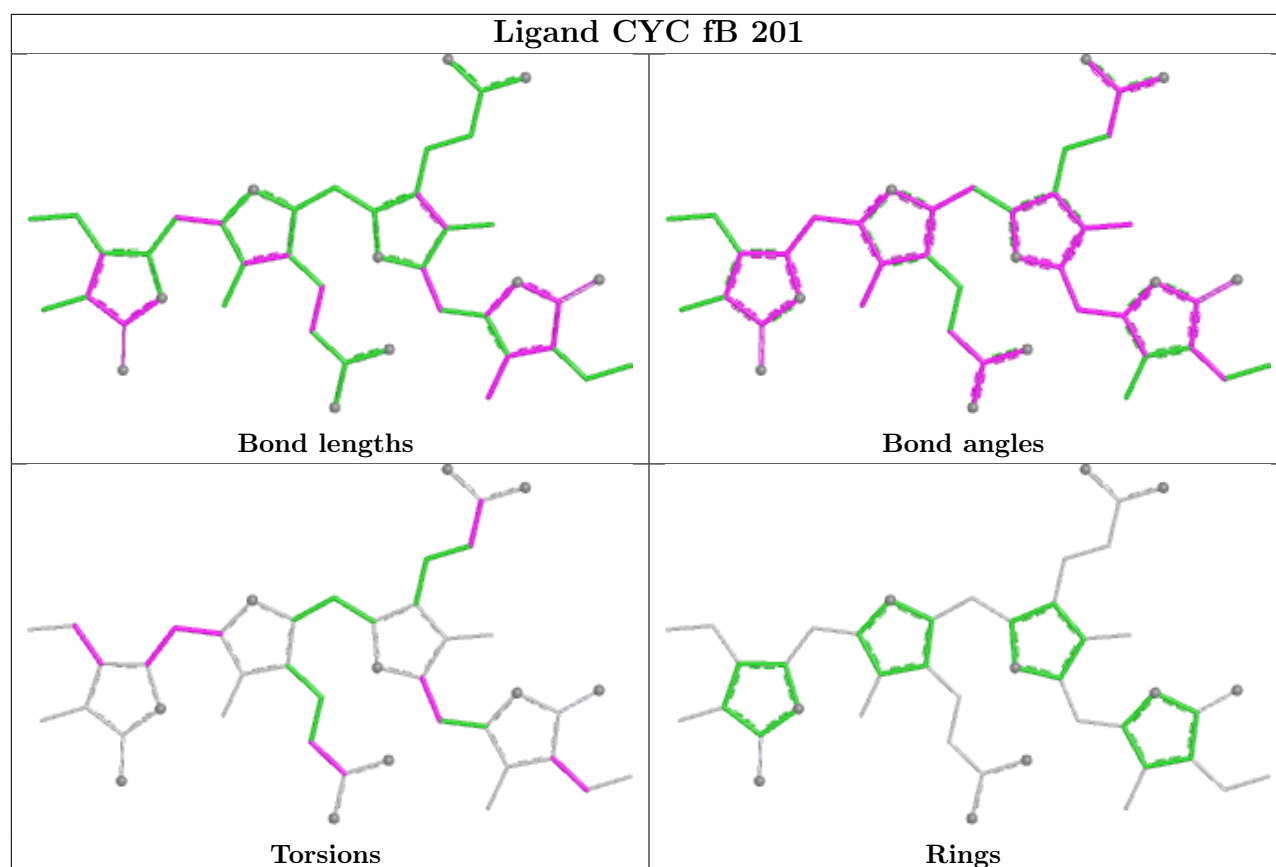
Ligand CYC dN 201



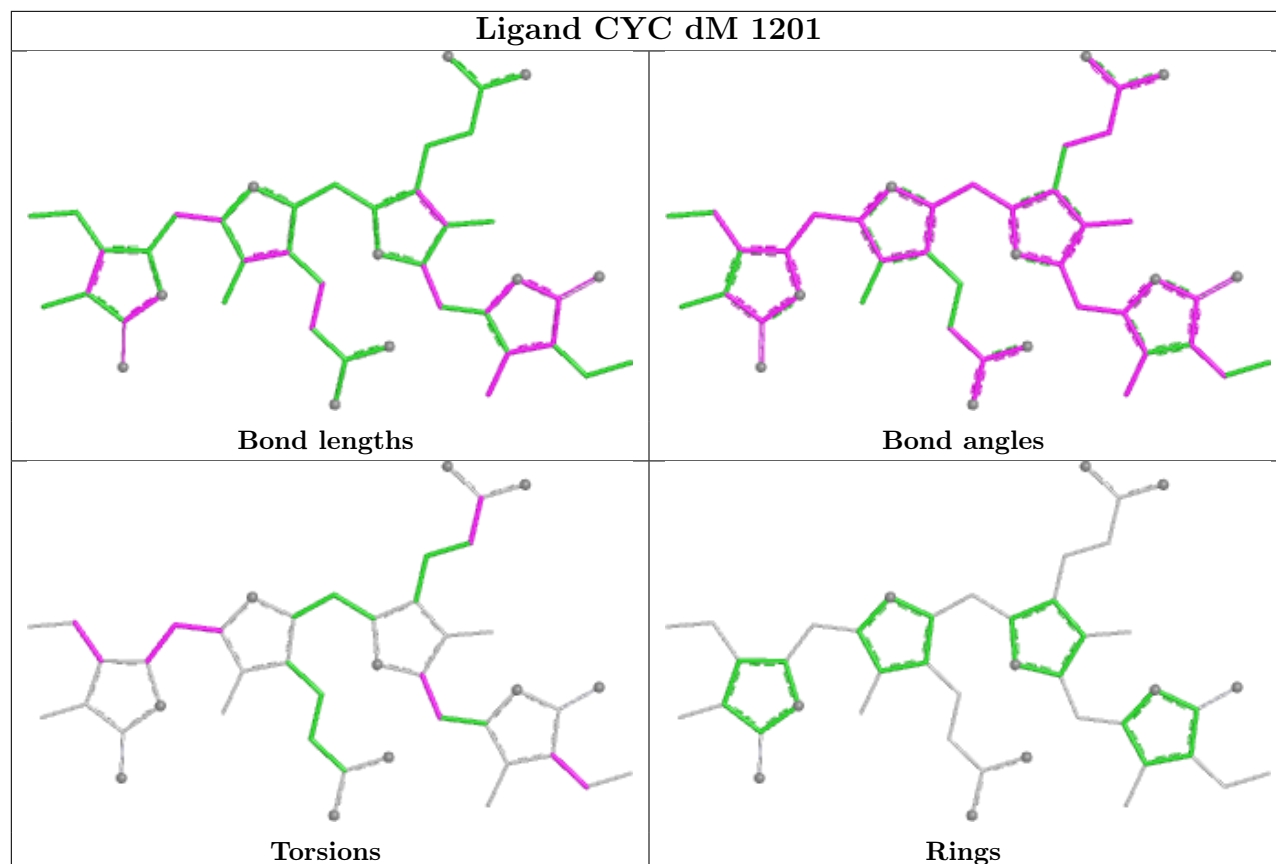
Ligand CYC cF 202



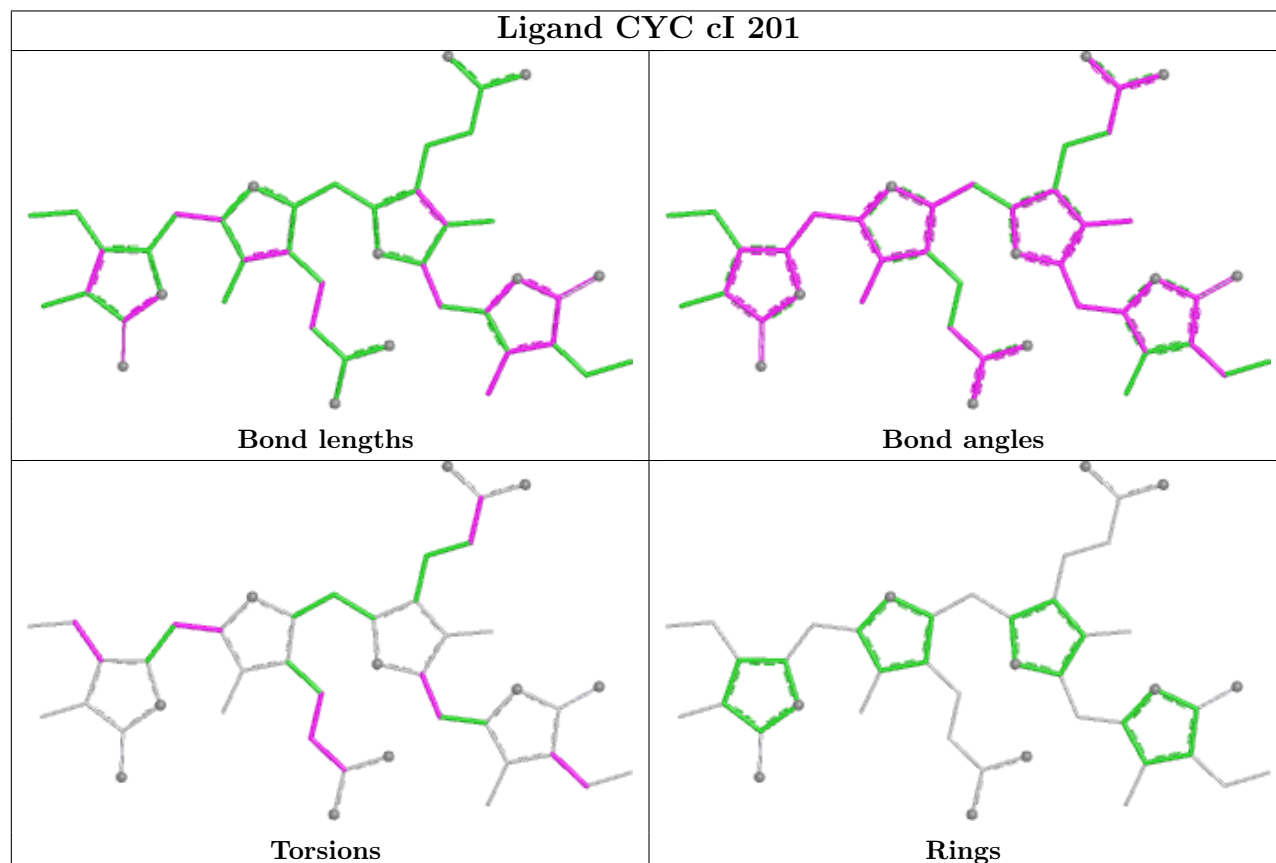




Ligand CYC dM 1201



Ligand CYC cI 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.

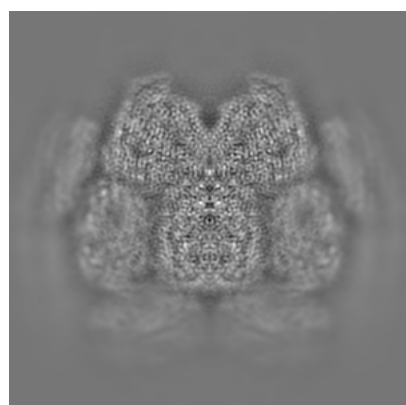
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31944. These allow visual inspection of the internal detail of the map and identification of artifacts.

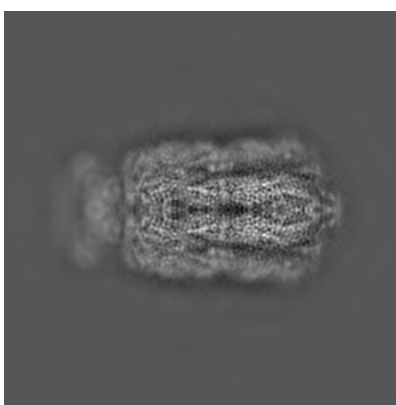
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

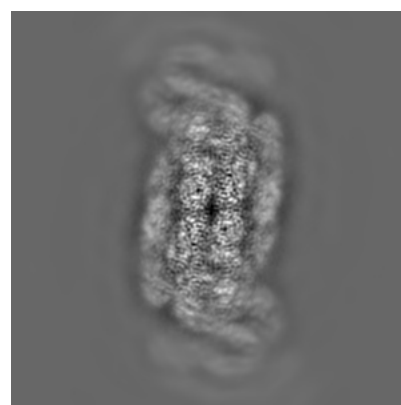
6.1.1 Primary map



X



Y

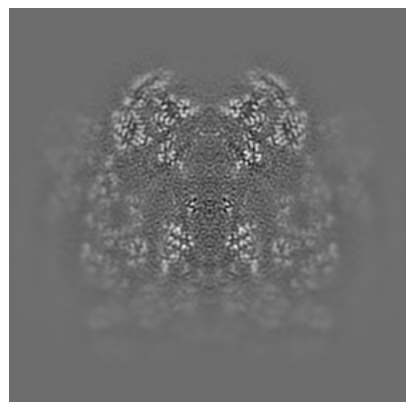


Z

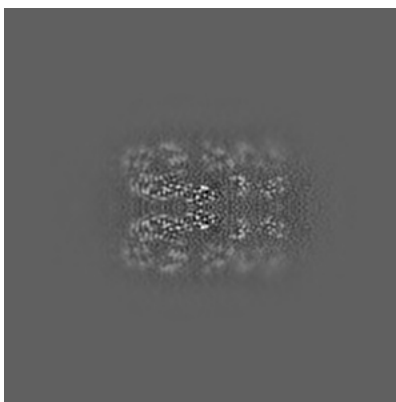
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

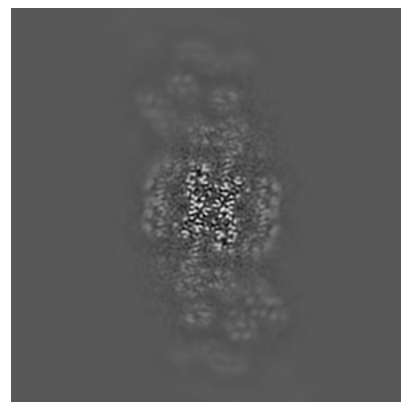
6.2.1 Primary map



X Index: 150



Y Index: 150

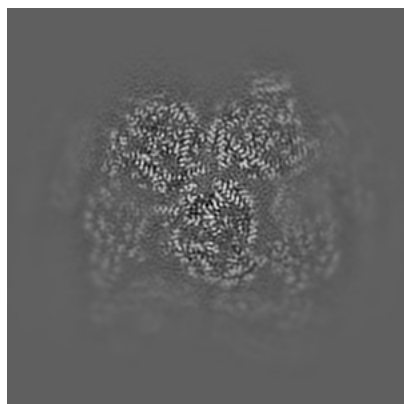


Z Index: 150

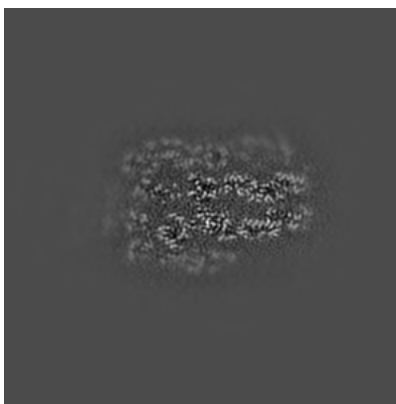
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

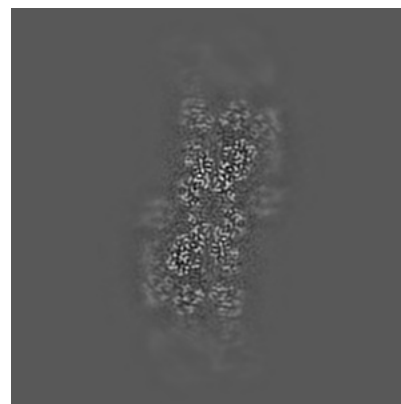
6.3.1 Primary map



X Index: 138



Y Index: 160

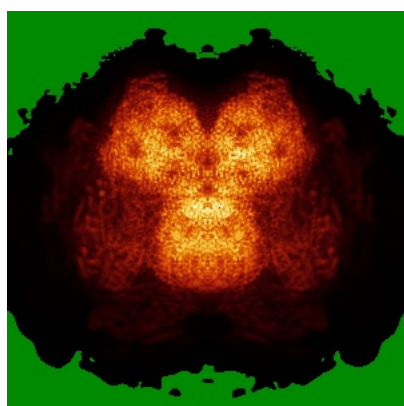


Z Index: 194

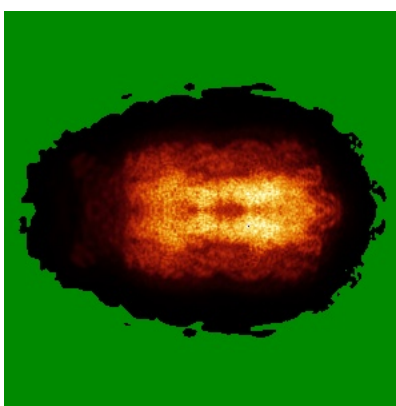
The images above show the largest variance slices of the map in three orthogonal directions.

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

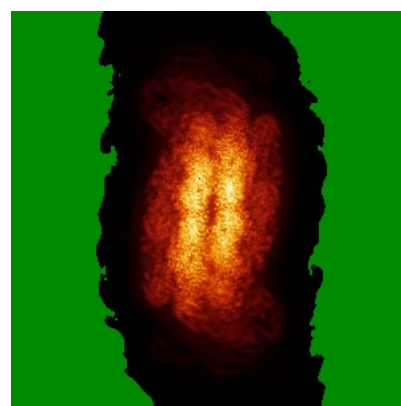
6.4.1 Primary map



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.

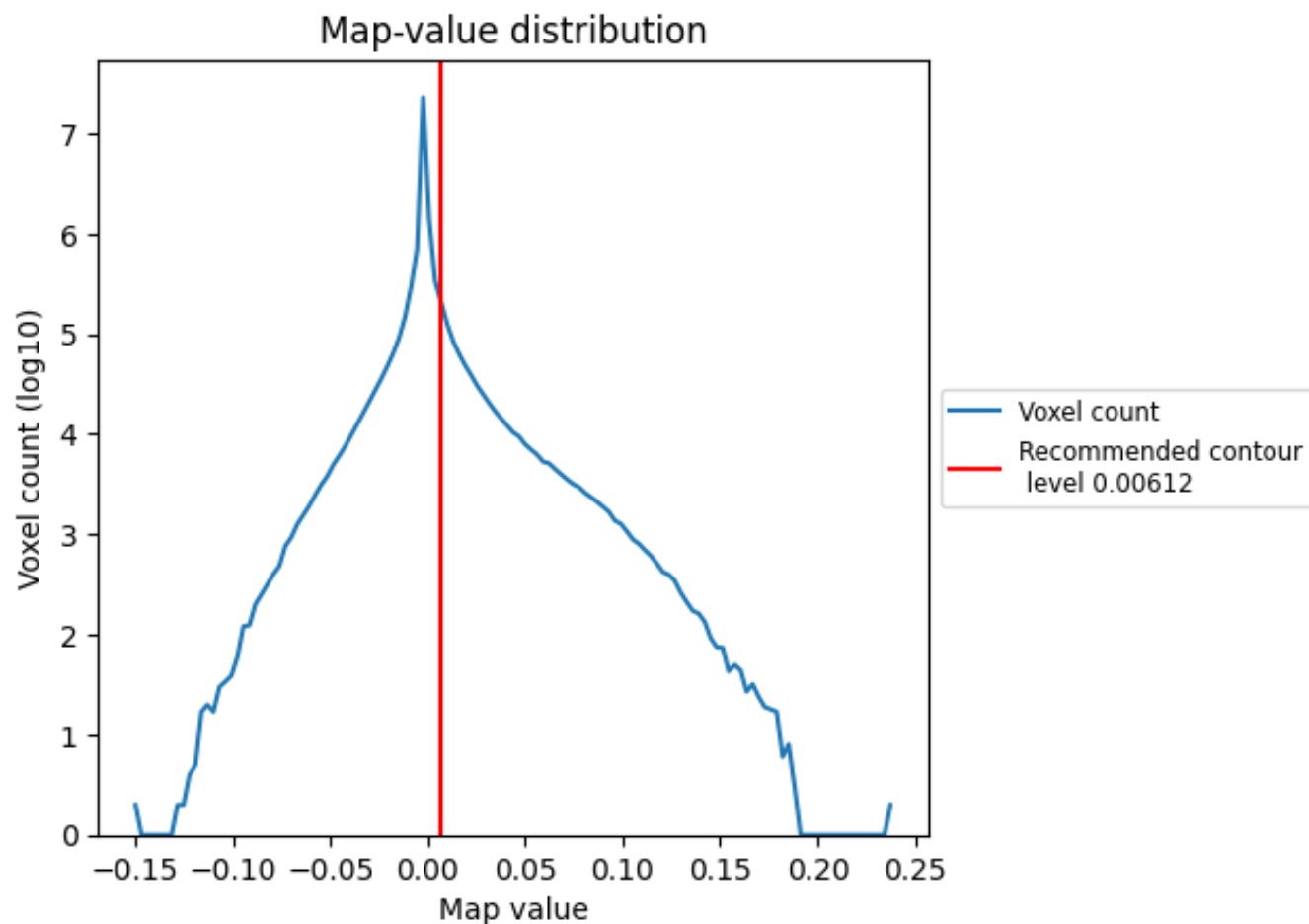
6.6 Mask visualisation

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

7 Map analysis [i](#)

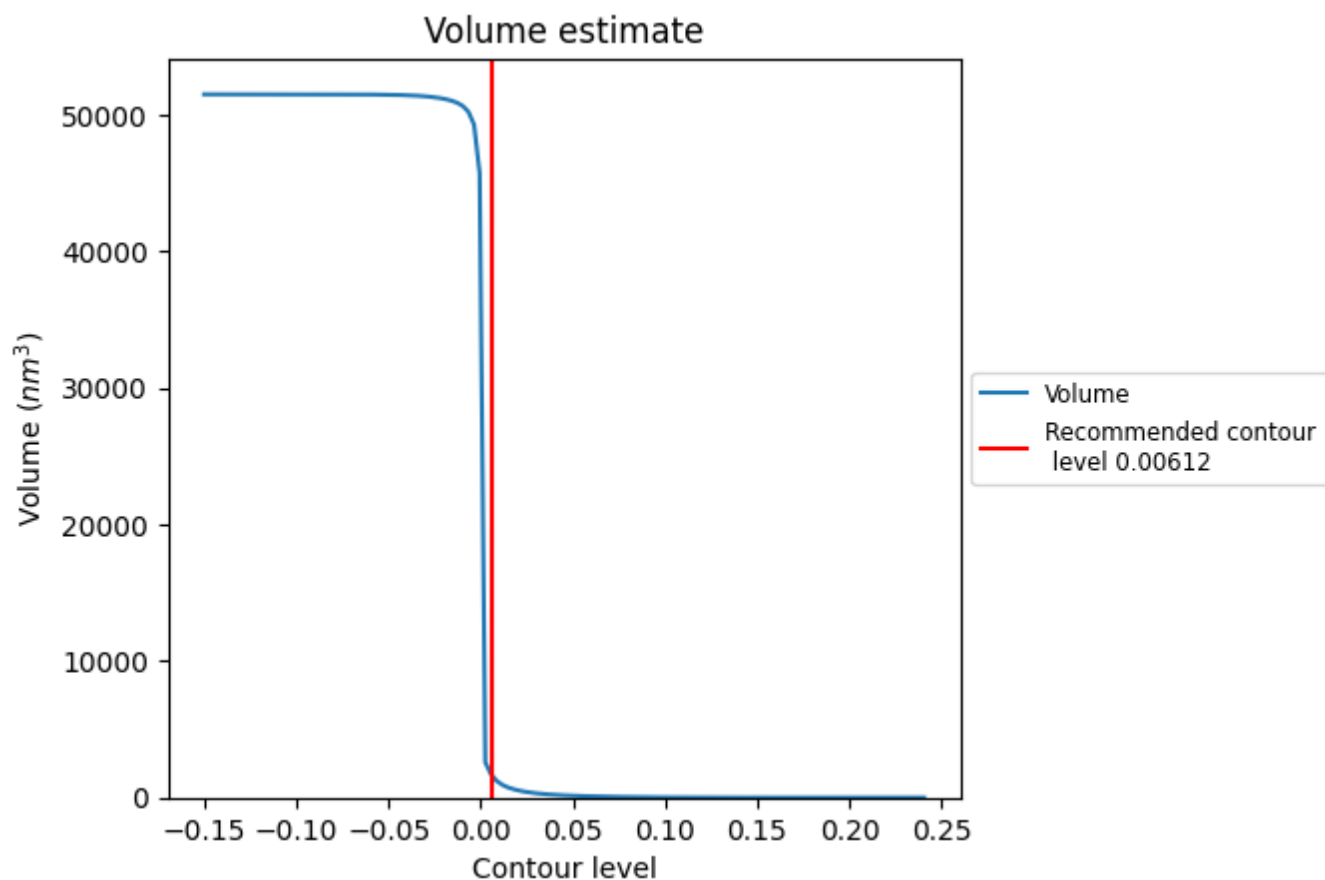
This section contains the results of statistical analysis of the map.

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.

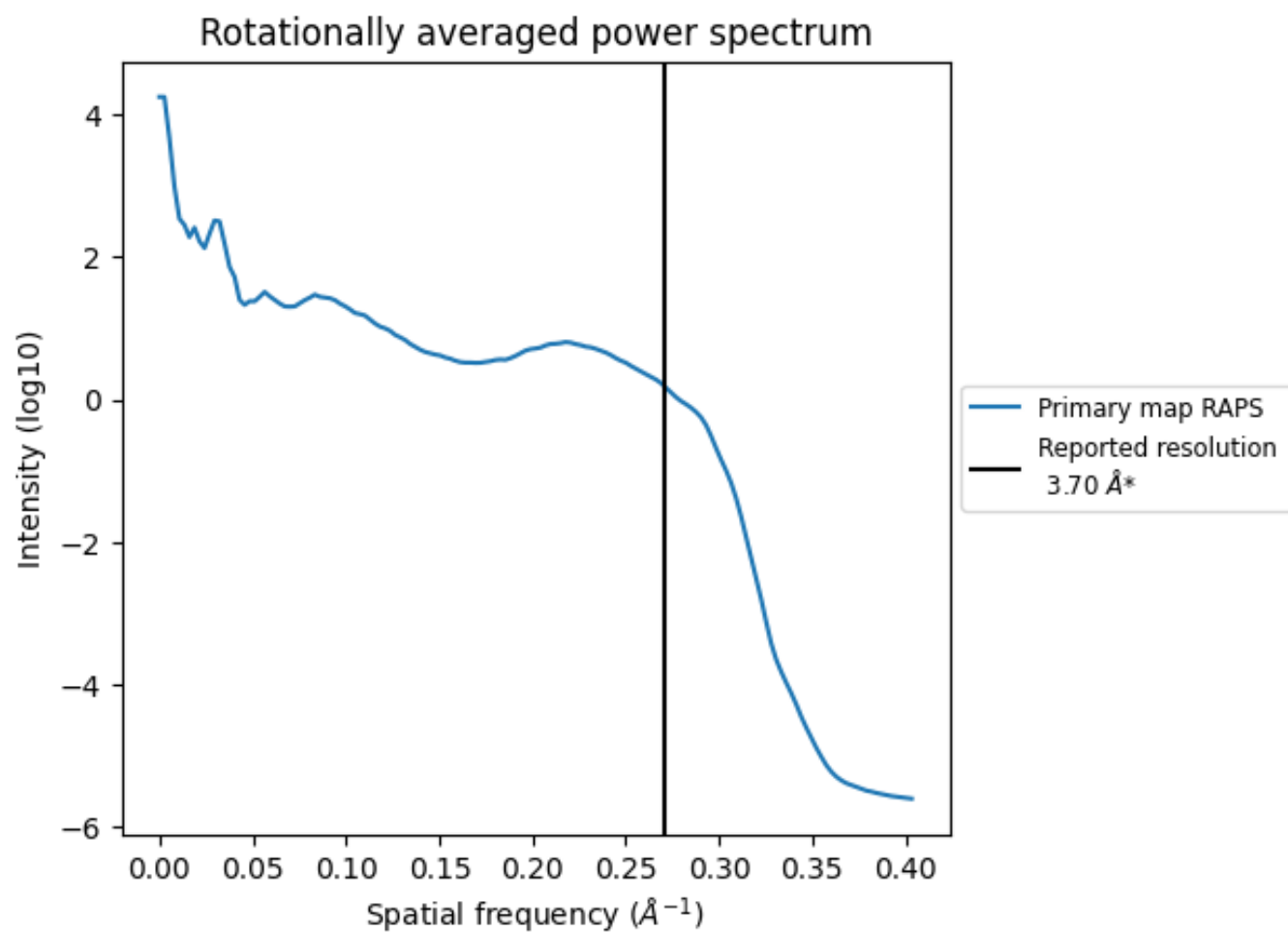
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1627 nm^3 ; this corresponds to an approximate mass of 1470 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 ⓘ

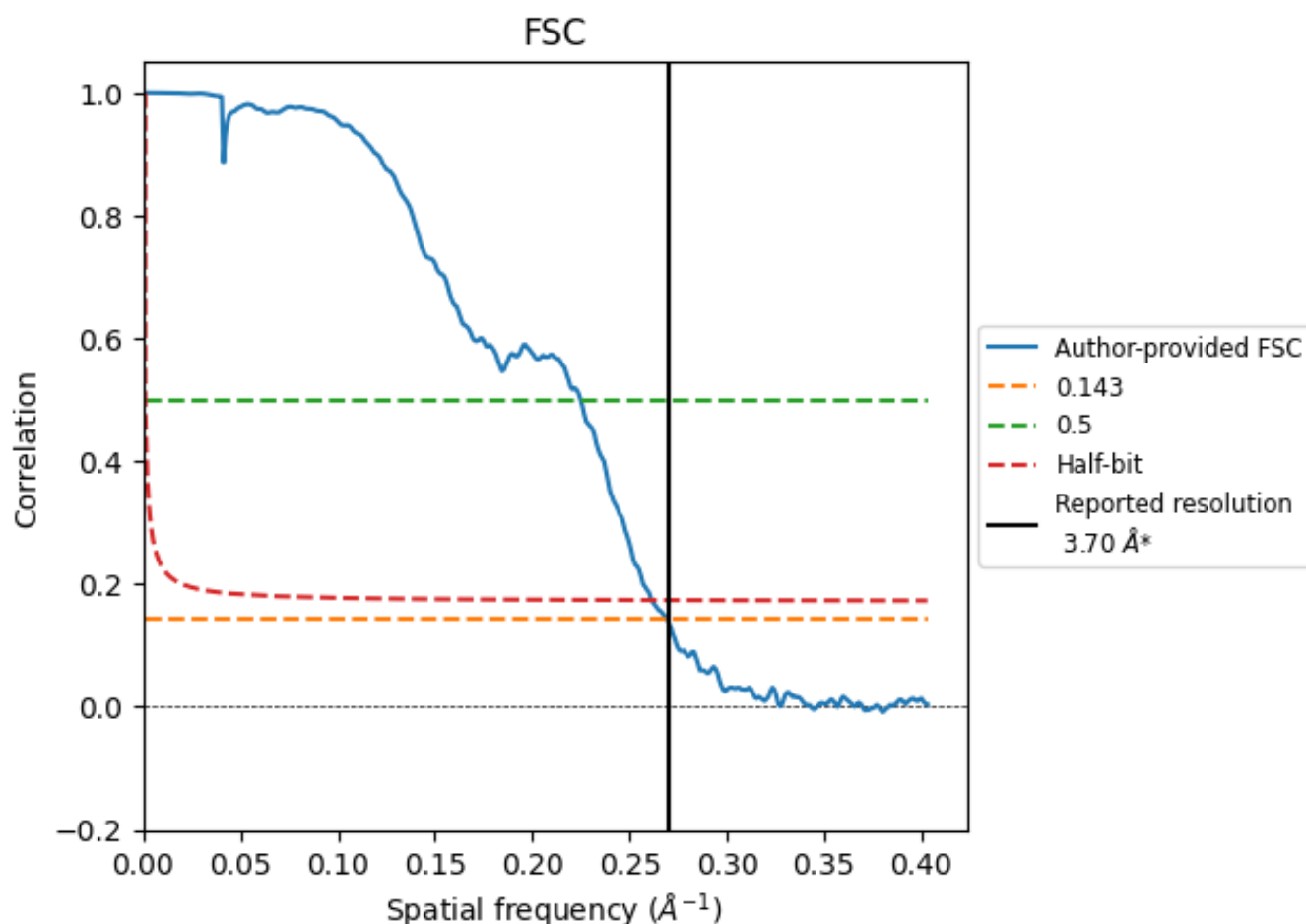


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.45	3.82
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

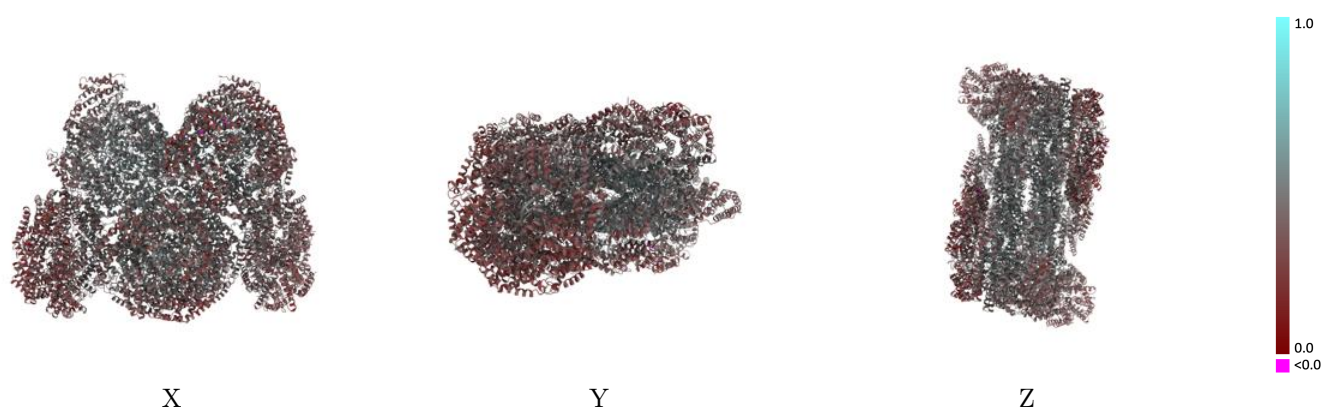
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31944 and PDB model 7VEA. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)

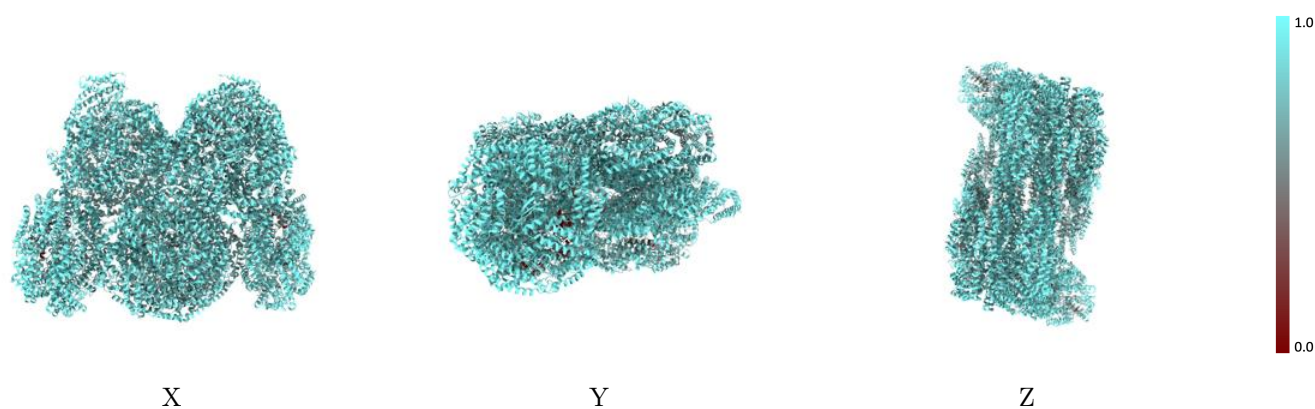
This section was not generated.

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



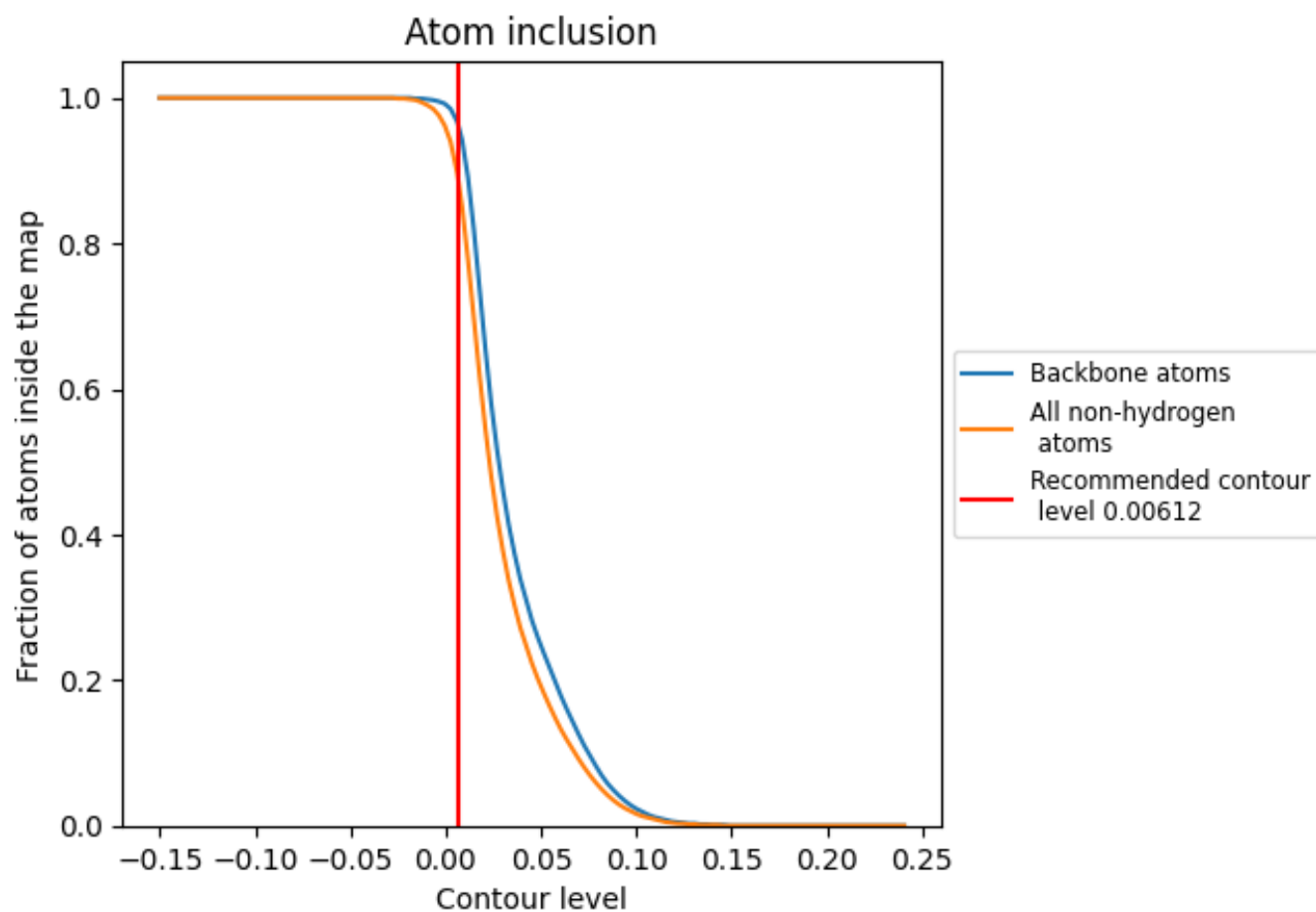
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00612).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.00612) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.4150
aA	 0.8290	 0.4300
aB	 0.8810	 0.3300
aC	 0.8110	 0.3300
aD	 0.8490	 0.3070
aE	 0.7970	 0.3490
aF	 0.8960	 0.3490
aG	 0.9250	 0.4410
aH	 0.9190	 0.5100
aI	 0.9340	 0.5070
aJ	 0.9100	 0.4930
aK	 0.8970	 0.4460
aL	 0.8940	 0.4680
aM	 0.9050	 0.4640
aN	 0.9020	 0.4320
aO	 0.9040	 0.4180
aP	 0.9070	 0.4950
aQ	 0.9410	 0.4940
aR	 0.9110	 0.4680
aS	 0.8620	 0.3530
bM	 0.8990	 0.4330
bN	 0.9190	 0.4960
bO	 0.9340	 0.4880
bP	 0.9020	 0.4690
bQ	 0.8530	 0.3970
bR	 0.8880	 0.4370
bS	 0.8160	 0.3310
bT	 0.8890	 0.3810
bU	 0.8230	 0.4050
bV	 0.8850	 0.3580
bW	 0.8690	 0.3790
bX	 0.8900	 0.3660
bY	 0.8700	 0.4530
cA	 0.9430	 0.3300
cB	 0.9540	 0.3280



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Chain	Atom inclusion	Q-score
cC	 0.9040	 0.3350
cD	 0.9410	 0.4200
cE	 0.9370	 0.4090
cF	 0.9340	 0.4040
cG	 0.8520	 0.2840
cH	 0.9580	 0.2960
cI	 0.9190	 0.3210
cJ	 0.9700	 0.3600
cK	 0.9110	 0.3890
cL	 0.9480	 0.3180
cM	 0.8850	 0.4150
dA	 0.8360	 0.4320
dB	 0.8880	 0.3320
dC	 0.8180	 0.3270
dD	 0.8560	 0.3110
dE	 0.8250	 0.3470
dF	 0.8930	 0.3530
dG	 0.9260	 0.4430
dH	 0.9160	 0.5110
dI	 0.9360	 0.5110
dJ	 0.9130	 0.4970
dK	 0.8940	 0.4460
dL	 0.8970	 0.4670
dM	 0.9050	 0.4660
dN	 0.9060	 0.4330
dO	 0.9090	 0.4210
dP	 0.9110	 0.4990
dQ	 0.9400	 0.4940
dR	 0.9110	 0.4700
dS	 0.8860	 0.3480
eM	 0.9000	 0.4320
eN	 0.9180	 0.4960
eO	 0.9320	 0.4870
eP	 0.9050	 0.4750
eQ	 0.8510	 0.3970
eR	 0.8870	 0.4350
eS	 0.8150	 0.3260
eT	 0.8870	 0.3780
eU	 0.8310	 0.4070
eV	 0.8790	 0.3530
eW	 0.8690	 0.3790
eX	 0.8880	 0.3620

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Chain	Atom inclusion	Q-score
eY	 0.8740	 0.4520
fA	 0.9440	 0.3300
fB	 0.9680	 0.3290
fC	 0.8000	 0.3180
fD	 0.9400	 0.4170
fE	 0.9190	 0.4070
fF	 0.9340	 0.4030
fG	 0.8270	 0.2770
fH	 0.9600	 0.2970
fI	 0.9150	 0.3140
fJ	 0.9790	 0.3500
fK	 0.7840	 0.3830
fL	 0.9100	 0.2950
fM	 0.8820	 0.4070