



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 06:30 PM EDT

PDB ID : 7SC7
EMDB ID : EMD-25028
Title : Synechocystis PCC 6803 Phycobilisome core from up-down rod conformation
Authors : Sauer, P.V.; Sutter, M.; Dominguez-Martin, M.A.; Kirst, H.; Kerfeld, C.A.
Deposited on : 2021-09-27
Resolution : 2.80 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

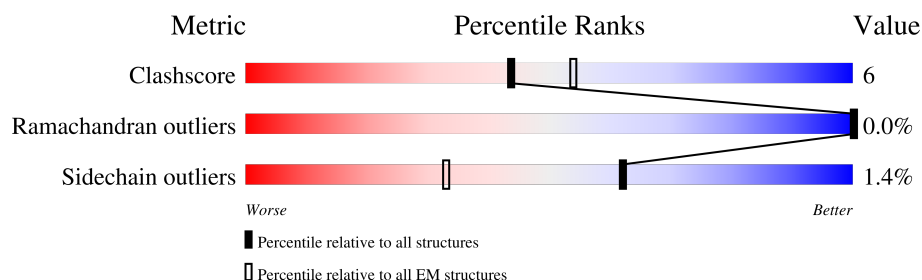
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.









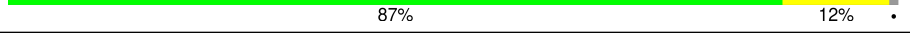
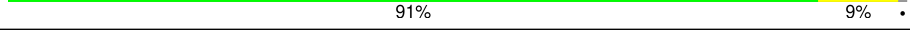
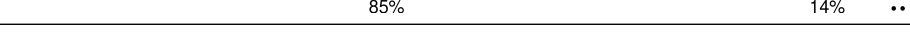
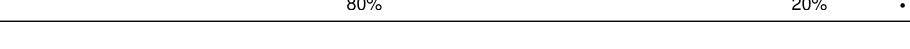
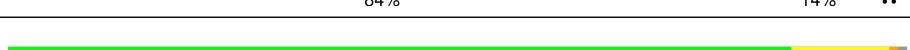

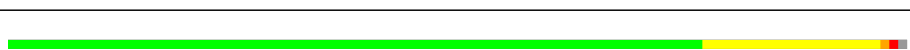

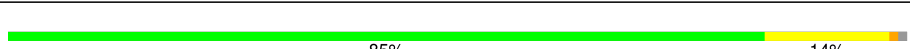





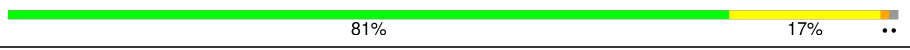
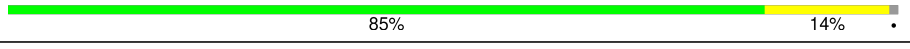



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	AH	161	
1	AJ	161	
1	AN	161	
1	AP	161	
1	AR	161	
1	AV	161	













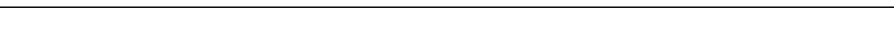

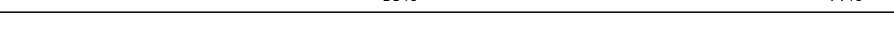

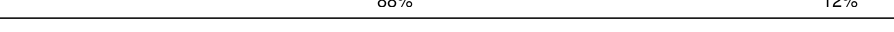








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Mol	Chain	Length	Quality of chain
1	AX	161	
1	AZ	161	
1	BH	161	
1	BJ	161	
1	BO	161	
1	BQ	161	
1	BU	161	
1	BW	161	
1	BY	161	
1	CB	161	
1	CD	161	
1	CF	161	
1	CP	161	
1	CR	161	
1	CT	161	
1	CW	161	
1	CY	161	
1	DA	161	
1	DG	161	
1	DI	161	
1	DK	161	
1	DN	161	
1	DP	161	
1	DR	161	
2	AB	161	











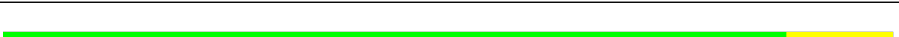


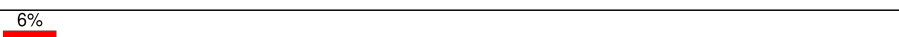
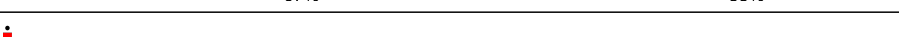
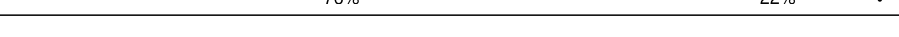



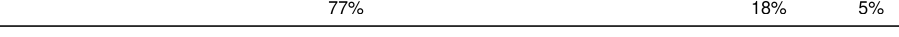





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Mol	Chain	Length	Quality of chain
2	AD	161	 84%16%
2	AF	161	 77%22%.
2	AI	161	 89%11%
2	AL	161	 84%16%
2	AO	161	 87%13%
2	AQ	161	 91%9%
2	AS	161	 86%14%
2	AU	161	 87%13%
2	AW	161	 80%20%.
2	AY	161	 83%17%
2	BI	161	 86%14%
2	BK	161	 90%10%
2	BM	161	 80%20%.
2	BP	161	 89%11%
2	BS	161	 83%16%.
2	BV	161	 88%12%
2	BX	161	 92%8%
2	BZ	161	 87%13%
2	CC	161	 85%15%
2	CE	161	 81%19%
2	CG	161	 86%14%
2	CQ	161	 84%16%
2	CS	161	 89%11%
2	CU	161	 85%15%
2	CX	161	 79%20%.




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Mol	Chain	Length	Quality of chain
2	CZ	161	 84% 16%
2	DB	161	 91% 9%
2	DH	161	 86% 14%
2	DJ	161	 86% 14%
2	DL	161	 89% 11%
2	DO	161	 80% 20%
2	DQ	161	 76% 22%
2	DS	161	 84% 16%
3	AE	161	 83% 16%
3	BL	161	 83% 17%
4	AK	169	 88% 12%
4	BR	169	 82% 18%
5	BA	67	 72% 27%
5	BB	67	 67% 33% 6%
5	CI	67	 76% 22%
5	CJ	67	 81% 19%
5	DD	67	 81% 19%
5	DU	67	 79% 21%
6	BD	896	 77% 18% 5%
6	CL	896	 78% 17% 5%
7	BF	249	 18% 77%
7	CN	249	 19% 77%
7	DE	249	 17% 78%
7	DF	249	 18% 78%
7	DV	249	 18% 78%

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Mol	Chain	Length	Quality of chain
7	DW	249	 18% 78%
8	BG	121	 26% 70%
8	CO	121	 22% 7% 70%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 107930 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
			1210	754	207	242	7		
1	AC	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AH	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AJ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AN	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AP	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AR	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AV	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AX	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	AZ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BH	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BJ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BO	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BQ	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BU	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BW	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	BY	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CB	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CD	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CF	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CP	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CR	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CT	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CW	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	CY	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DA	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DG	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DI	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DK	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DN	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DP	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		
1	DR	160	Total	C	N	O	S	0	0
			1210	754	207	242	7		

- Molecule 2 is a protein called Allophycocyanin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AD	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AF	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AI	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AL	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AO	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AQ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AS	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AU	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AW	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	AY	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BI	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BK	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BM	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BP	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BS	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BV	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BX	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	BZ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CC	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CE	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CG	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CQ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CS	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CU	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CX	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	CZ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DB	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DH	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DJ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DL	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DO	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DQ	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		
2	DS	161	Total	C	N	O	S	0	0
			1206	757	202	240	7		

- Molecule 3 is a protein called Allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AE	160	Total	C	N	O	S	0	0
			1254	797	212	241	4		
3	BL	160	Total	C	N	O	S	0	0
			1254	797	212	241	4		

- Molecule 4 is a protein called Allophycocyanin subunit beta-18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AK	169	Total	C	N	O	S	0	0
			1322	825	229	259	9		
4	BR	169	Total	C	N	O	S	0	0
			1322	825	229	259	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	67	Total	C	N	O	S	0	0
			546	343	104	94	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	CI	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	CJ	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	DD	67	Total	C	N	O	S	0	0
			546	343	104	94	5		
5	DU	67	Total	C	N	O	S	0	0
			546	343	104	94	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	36	TRP	SER	conflict	UNP Q01950
BB	36	TRP	SER	conflict	UNP Q01950
CI	36	TRP	SER	conflict	UNP Q01950
CJ	36	TRP	SER	conflict	UNP Q01950
DD	36	TRP	SER	conflict	UNP Q01950
DU	36	TRP	SER	conflict	UNP Q01950

- Molecule 6 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BD	850	Total	C	N	O	S	0	0
			6761	4299	1183	1262	17		
6	CL	850	Total	C	N	O	S	0	0
			6761	4299	1183	1262	17		

- Molecule 7 is a protein called Phycobilisome rod-core linker polypeptide CpcG.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BF	57	Total	C	N	O	S	0	0
			451	282	87	80	2		
7	CN	57	Total	C	N	O	S	0	0
			451	282	87	80	2		
7	DE	54	Total	C	N	O	S	0	0
			426	266	83	75	2		
7	DF	54	Total	C	N	O	S	0	0
			426	266	83	75	2		
7	DV	54	Total	C	N	O	S	0	0
			426	266	83	75	2		

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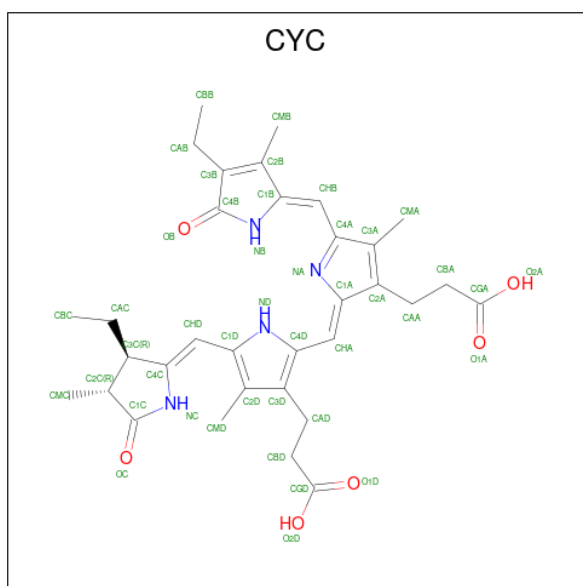
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Mol	Chain	Residues	Atoms					AltConf	Trace
7	DW	54	Total	C	N	O	S	0	0
			426	266	83	75	2		

- Molecule 8 is a protein called Sll1873 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BG	36	Total	C	N	O	S	0	0
			277	172	55	49	1		
8	CO	36	Total	C	N	O	S	0	0
			277	172	55	49	1		

- Molecule 9 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	AA	1	Total	C	N	O	0
			43	33	4	6	
9	AB	1	Total	C	N	O	0
			43	33	4	6	
9	AC	1	Total	C	N	O	0
			43	33	4	6	
9	AD	1	Total	C	N	O	0
			43	33	4	6	
9	AE	1	Total	C	N	O	0
			43	33	4	6	
9	AH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
9	AI	1	Total 43	C 33	N 4	O 6	0
9	AJ	1	Total 43	C 33	N 4	O 6	0
9	AK	1	Total 43	C 33	N 4	O 6	0
9	AL	1	Total 43	C 33	N 4	O 6	0
9	AN	1	Total 43	C 33	N 4	O 6	0
9	AO	1	Total 43	C 33	N 4	O 6	0
9	AP	1	Total 43	C 33	N 4	O 6	0
9	AQ	1	Total 43	C 33	N 4	O 6	0
9	AR	1	Total 43	C 33	N 4	O 6	0
9	AU	1	Total 43	C 33	N 4	O 6	0
9	AV	1	Total 43	C 33	N 4	O 6	0
9	AW	1	Total 43	C 33	N 4	O 6	0
9	AX	1	Total 43	C 33	N 4	O 6	0
9	AY	1	Total 43	C 33	N 4	O 6	0
9	AZ	1	Total 43	C 33	N 4	O 6	0
9	BA	1	Total 43	C 33	N 4	O 6	0
9	BD	1	Total 43	C 33	N 4	O 6	0
9	BD	1	Total 43	C 33	N 4	O 6	0
9	BH	1	Total 43	C 33	N 4	O 6	0
9	BI	1	Total 43	C 33	N 4	O 6	0
9	BJ	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
9	BK	1	Total 43	C 33	N 4	O 6	0
9	BL	1	Total 43	C 33	N 4	O 6	0
9	BO	1	Total 43	C 33	N 4	O 6	0
9	BP	1	Total 43	C 33	N 4	O 6	0
9	BQ	1	Total 43	C 33	N 4	O 6	0
9	BR	1	Total 43	C 33	N 4	O 6	0
9	BS	1	Total 43	C 33	N 4	O 6	0
9	BU	1	Total 43	C 33	N 4	O 6	0
9	BV	1	Total 43	C 33	N 4	O 6	0
9	BW	1	Total 43	C 33	N 4	O 6	0
9	BX	1	Total 43	C 33	N 4	O 6	0
9	BY	1	Total 43	C 33	N 4	O 6	0
9	CB	1	Total 43	C 33	N 4	O 6	0
9	CC	1	Total 43	C 33	N 4	O 6	0
9	CD	1	Total 43	C 33	N 4	O 6	0
9	CE	1	Total 43	C 33	N 4	O 6	0
9	CF	1	Total 43	C 33	N 4	O 6	0
9	CG	1	Total 43	C 33	N 4	O 6	0
9	CI	1	Total 43	C 33	N 4	O 6	0
9	CL	1	Total 43	C 33	N 4	O 6	0
9	CL	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
9	CP	1	Total 43	C 33	N 4	O 6	0
9	CQ	1	Total 43	C 33	N 4	O 6	0
9	CR	1	Total 43	C 33	N 4	O 6	0
9	CS	1	Total 43	C 33	N 4	O 6	0
9	CT	1	Total 43	C 33	N 4	O 6	0
9	CU	1	Total 43	C 33	N 4	O 6	0
9	CW	1	Total 43	C 33	N 4	O 6	0
9	CX	1	Total 43	C 33	N 4	O 6	0
9	CY	1	Total 43	C 33	N 4	O 6	0
9	CZ	1	Total 43	C 33	N 4	O 6	0
9	DA	1	Total 43	C 33	N 4	O 6	0
9	DB	1	Total 43	C 33	N 4	O 6	0
9	DG	1	Total 43	C 33	N 4	O 6	0
9	DH	1	Total 43	C 33	N 4	O 6	0
9	DI	1	Total 43	C 33	N 4	O 6	0
9	DJ	1	Total 43	C 33	N 4	O 6	0
9	DK	1	Total 43	C 33	N 4	O 6	0
9	DL	1	Total 43	C 33	N 4	O 6	0
9	DN	1	Total 43	C 33	N 4	O 6	0
9	DO	1	Total 43	C 33	N 4	O 6	0
9	DP	1	Total 43	C 33	N 4	O 6	0

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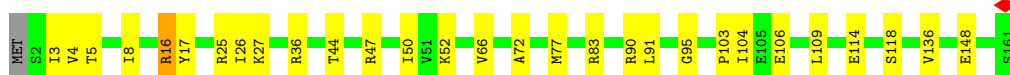
Mol	Chain	Residues	Atoms				AltConf
9	DQ	1	Total	C	N	O	0
			43	33	4	6	
9	DR	1	Total	C	N	O	0
			43	33	4	6	
9	DS	1	Total	C	N	O	0
			43	33	4	6	

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.

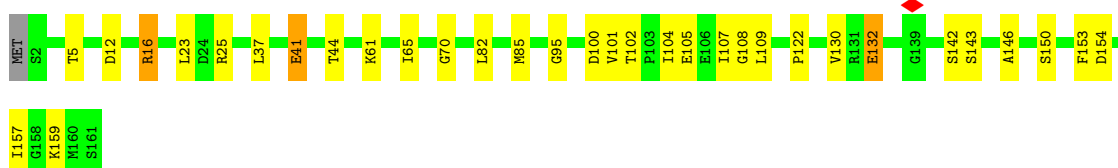
- Molecule 1: Allophycocyanin alpha chain

Chain AA: 




- Molecule 1: Allophycocyanin alpha chain

Chain AC: 




- Molecule 1: Allophycocyanin alpha chain

Chain AH: 




- Molecule 1: Allophycocyanin alpha chain

Chain AJ: 



- Molecule 1: Allophycocyanin alpha chain

Chain AN: 



- Molecule 1: Allophycocyanin alpha chain

Chain AP: 90% 9% .



- Molecule 1: Allophycocyanin alpha chain

Chain AR: 91% 9% .



- Molecule 1: Allophycocyanin alpha chain

Chain AV: 81% 17% ..



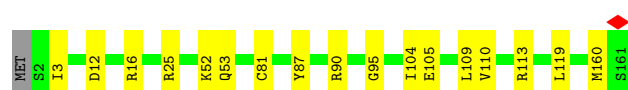
- Molecule 1: Allophycocyanin alpha chain

Chain AX: 86% 13% ..



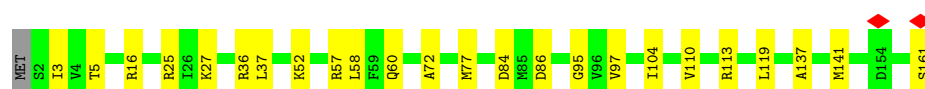
- Molecule 1: Allophycocyanin alpha chain

Chain AZ: 89% 11% .




- Molecule 1: Allophycocyanin alpha chain


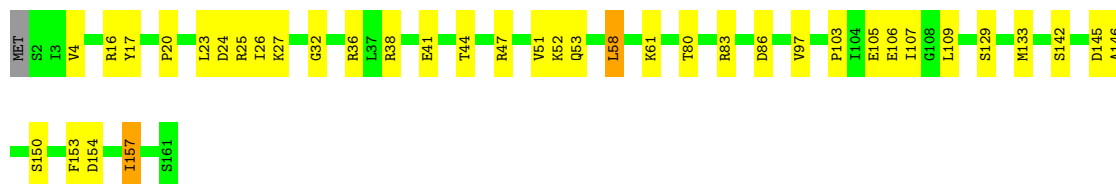
Chain BH: 84% 15% .




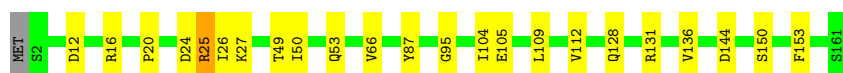
• Molecule 1: Allophycocyanin alpha chain

Chain BJ:  84% 14% ..

• Molecule 1: Allophycocyanin alpha chain

Chain BO:  76% 22% ..

• Molecule 1: Allophycocyanin alpha chain

Chain BQ:  85% 14% ..


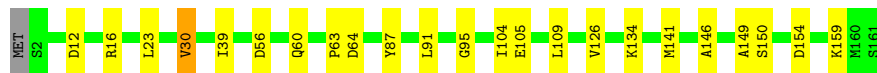
• Molecule 1: Allophycocyanin alpha chain

Chain BU:  87% 12% .


• Molecule 1: Allophycocyanin alpha chain

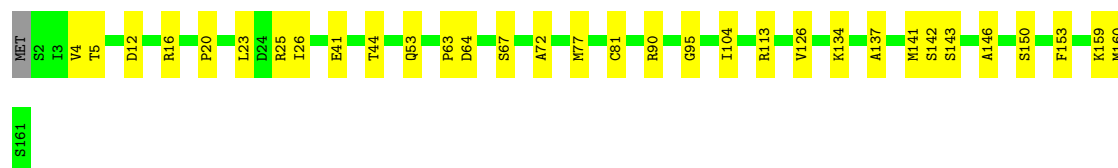
Chain BW:  91% 9% .

• Molecule 1: Allophycocyanin alpha chain

Chain BY:  85% 14% ..

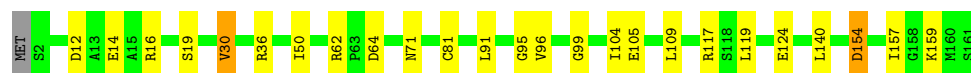
• Molecule 1: Allophycocyanin alpha chain

Chain CB:  80% 20% .



- Molecule 1: Allophycocyanin alpha chain

Chain CD: 84% 14% ..



- Molecule 1: Allophycocyanin alpha chain

Chain CF: 88% 11% ..



- Molecule 1: Allophycocyanin alpha chain

Chain CP: 83% 15% ..



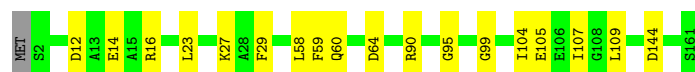
- Molecule 1: Allophycocyanin alpha chain

Chain CR: 78% 20% ...



- Molecule 1: Allophycocyanin alpha chain

Chain CT: 88% 11% .



- Molecule 1: Allophycocyanin alpha chain

Chain CW: 85% 14% ..



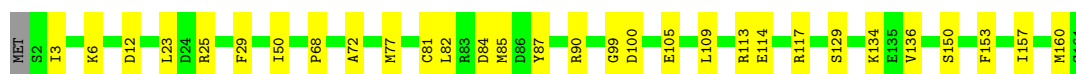
- Molecule 1: Allophycocyanin alpha chain

Chain CY: 83% 16% ..



- Molecule 1: Allophycocyanin alpha chain

Chain DA: 81% 19% .



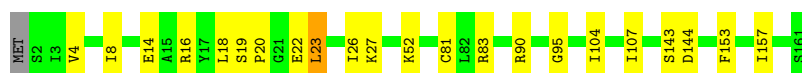
- Molecule 1: Allophycocyanin alpha chain

Chain DG: 73% 25% ..



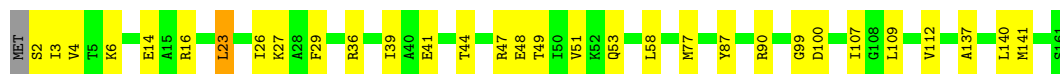
- Molecule 1: Allophycocyanin alpha chain

Chain DI: 86% 13% ..



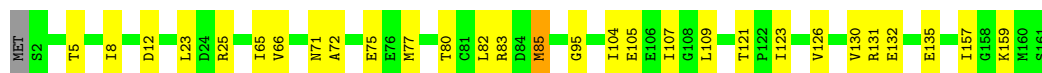
- Molecule 1: Allophycocyanin alpha chain

Chain DK: 80% 19% ..




- Molecule 1: Allophycocyanin alpha chain

Chain DN: 81% 17% ..



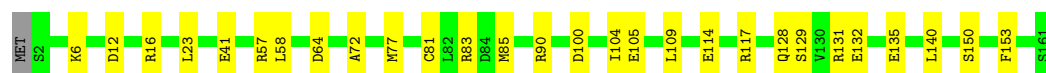
- Molecule 1: Allophycocyanin alpha chain

Chain DP:  85% 14%




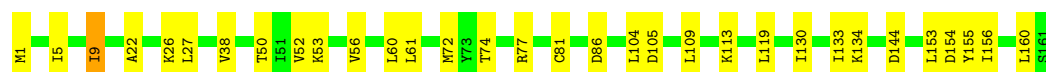
- Molecule 1: Allophycocyanin alpha chain

Chain DR:  82% 17%



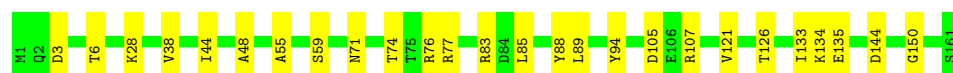
- Molecule 2: Allophycocyanin beta chain

Chain AB:  80% 19%




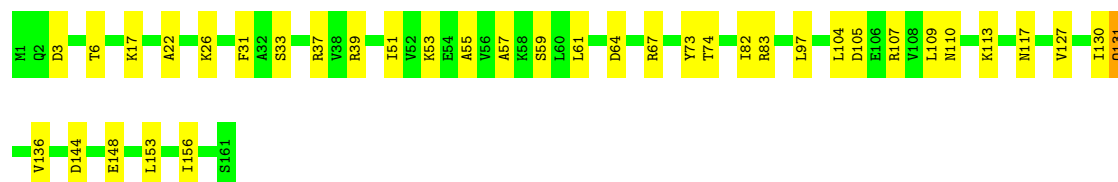
- Molecule 2: Allophycocyanin beta chain

Chain AD:  84% 16%



- Molecule 2: Allophycocyanin beta chain

Chain AF:  77% 22%




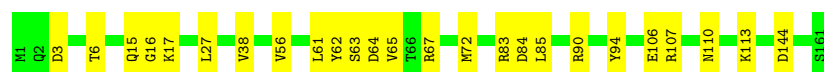
- Molecule 2: Allophycocyanin beta chain

Chain AI:  89% 11%




- Molecule 2: Allophycocyanin beta chain

Chain AL:  84% 16%




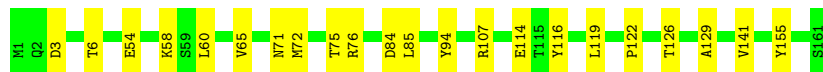
• Molecule 2: Allophycocyanin beta chain

Chain AO:  87% 13%


• Molecule 2: Allophycocyanin beta chain

Chain AQ:  91% 9%


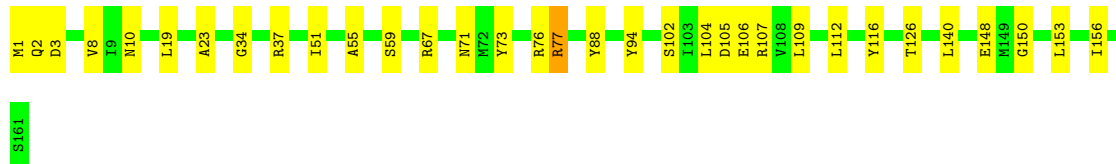
• Molecule 2: Allophycocyanin beta chain

Chain AS:  86% 14%


• Molecule 2: Allophycocyanin beta chain

Chain AU:  87% 13%


• Molecule 2: Allophycocyanin beta chain

Chain AW:  80% 20%

• Molecule 2: Allophycocyanin beta chain

Chain AY:  83% 17%

• Molecule 2: Allophycocyanin beta chain

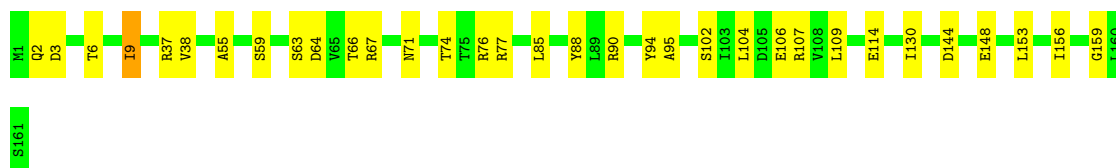
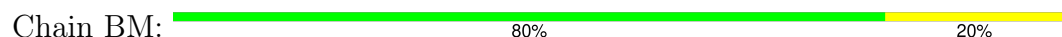
Chain BI:  86% 14%



- Molecule 2: Allophycocyanin beta chain



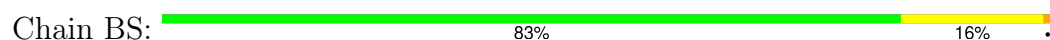
- Molecule 2: Allophycocyanin beta chain



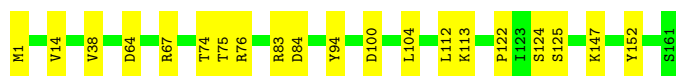
- Molecule 2: Allophycocyanin beta chain



- Molecule 2: Allophycocyanin beta chain




- Molecule 2: Allophycocyanin beta chain



- Molecule 2: Allophycocyanin beta chain




- Molecule 2: Allophycocyanin beta chain

Chain BZ:  87% 13%




- Molecule 2: Allophycocyanin beta chain

Chain CC:  85% 15%




- Molecule 2: Allophycocyanin beta chain

Chain CE:  81% 19%



- Molecule 2: Allophycocyanin beta chain

Chain CG:  86% 14%



- Molecule 2: Allophycocyanin beta chain

Chain CQ:  84% 16%




- Molecule 2: Allophycocyanin beta chain

Chain CS:  89% 11%




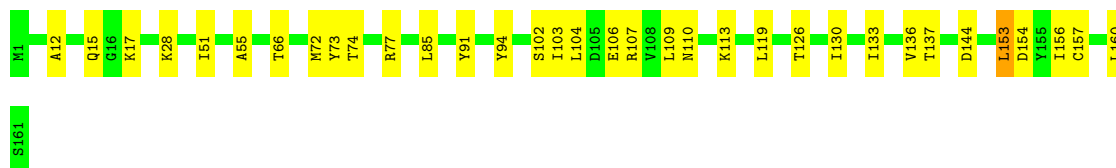
- Molecule 2: Allophycocyanin beta chain

Chain CU:  85% 15%




- Molecule 2: Allophycocyanin beta chain

Chain CX:  79% 20%



- Molecule 2: Allophycocyanin beta chain

Chain CZ:  84% 16%




- Molecule 2: Allophycocyanin beta chain

Chain DB:  91% 9%




- Molecule 2: Allophycocyanin beta chain

Chain DH:  86% 14%



- Molecule 2: Allophycocyanin beta chain

Chain DJ:  86% 14%




- Molecule 2: Allophycocyanin beta chain

Chain DL:  89% 11%



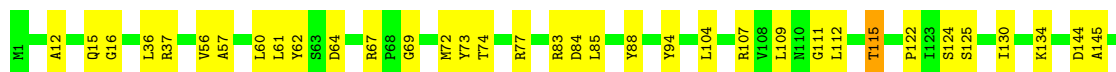
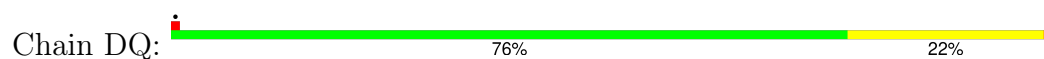
- Molecule 2: Allophycocyanin beta chain

Chain DO:  80% 20%

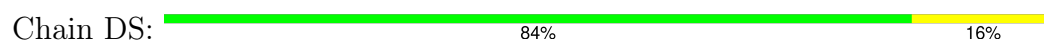




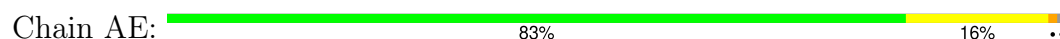
- Molecule 2: Allophycocyanin beta chain



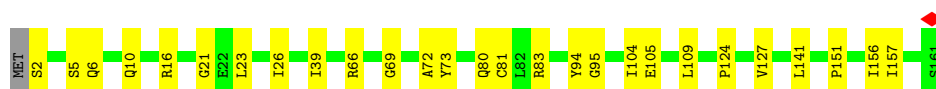
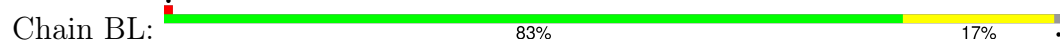
- Molecule 2: Allophycocyanin beta chain



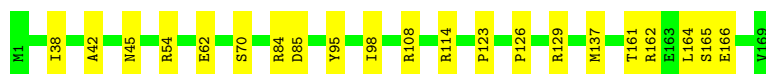
- Molecule 3: Allophycocyanin subunit alpha-B



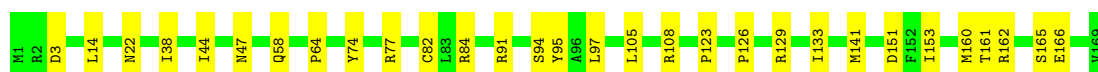
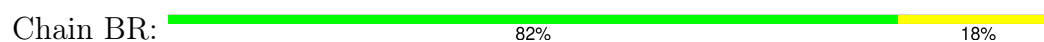
- Molecule 3: Allophycocyanin subunit alpha-B




- Molecule 4: Allophycocyanin subunit beta-18



- Molecule 4: Allophycocyanin subunit beta-18



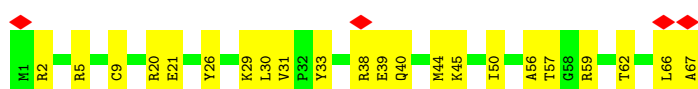
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain BA:  72% 27%




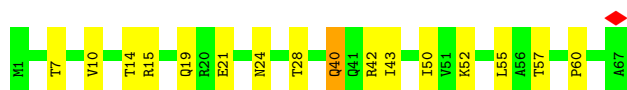
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain BB:  6% 67% 33%




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

Chain CI:  76% 22%




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

Chain CJ:  81% 19%




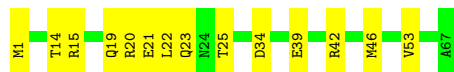
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain DD:  81% 19%




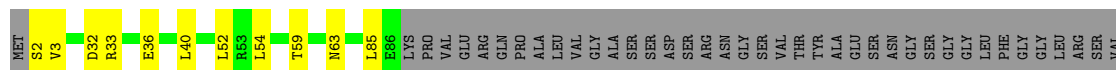
- Molecule 5: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

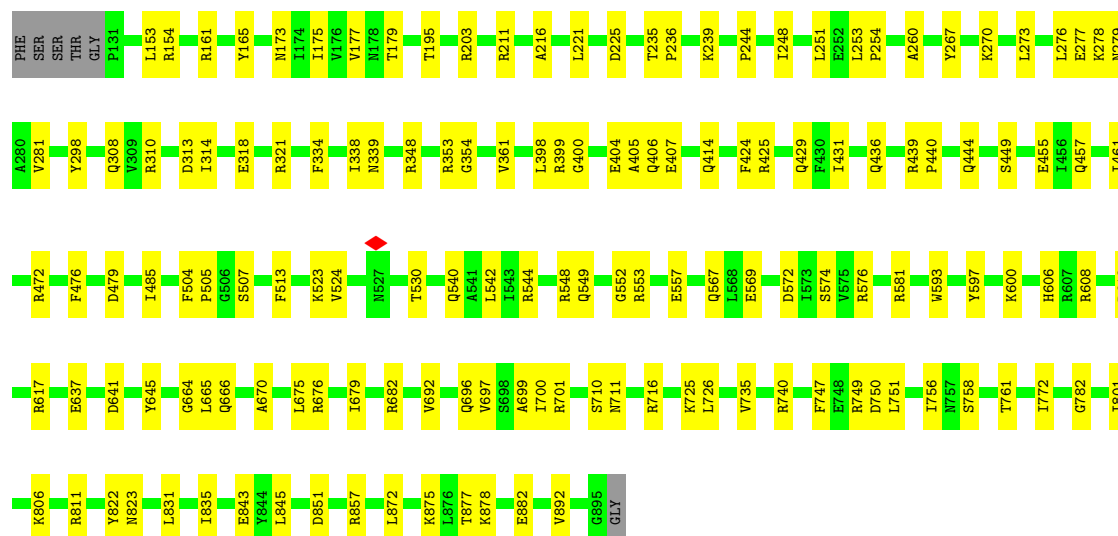
Chain DU:  79% 21%



- Molecule 6: Phycobiliprotein ApcE

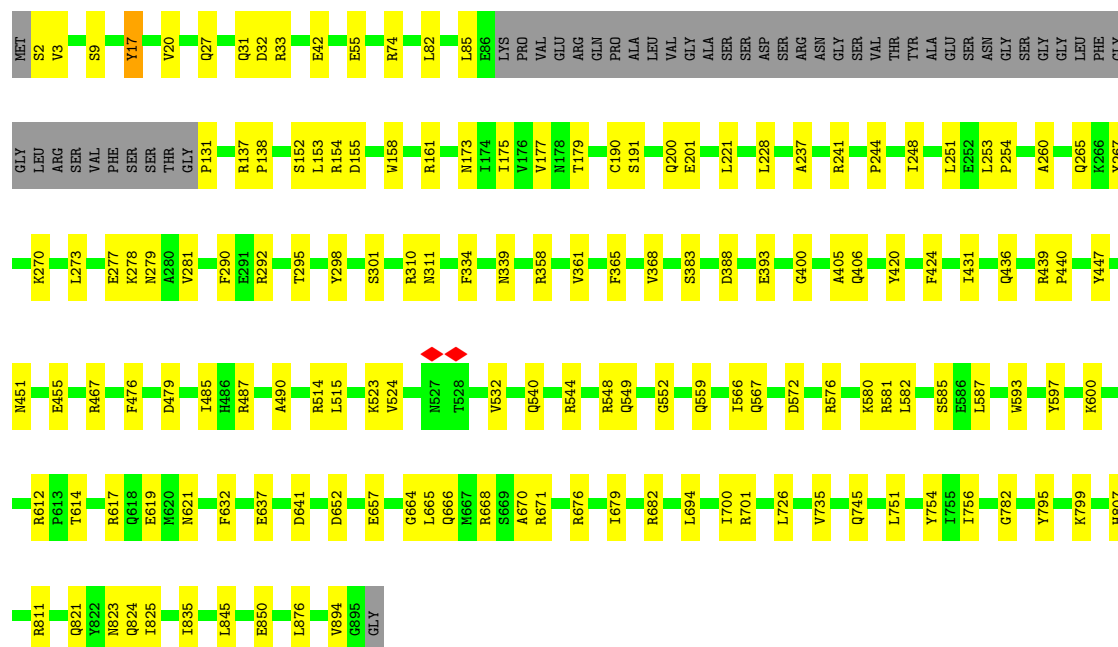
Chain BD:  77% 18% 5%





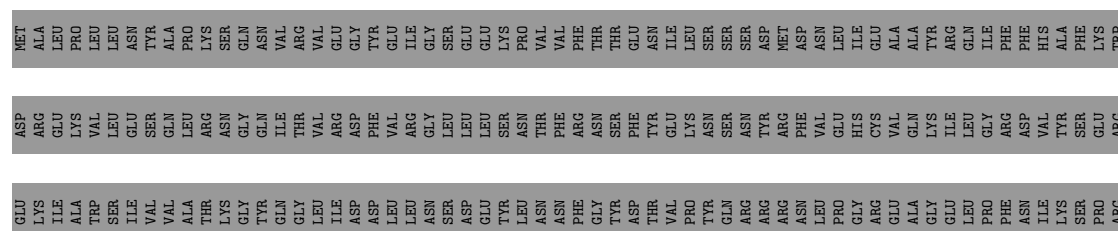
• Molecule 6: Phycobiliprotein ApcE

Chain CL: 78% 17% 5%



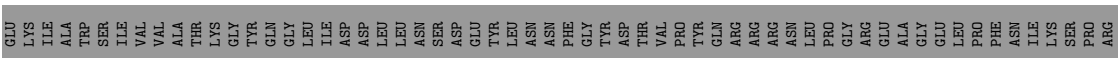
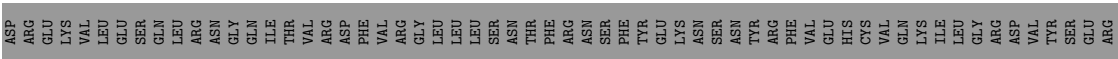
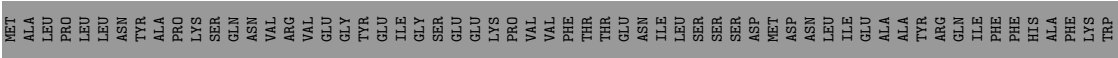
• Molecule 7: Phycobilisome rod-core linker polypeptide CpcG

Chain BF: 18% 77% 5%

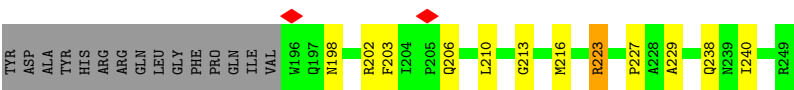
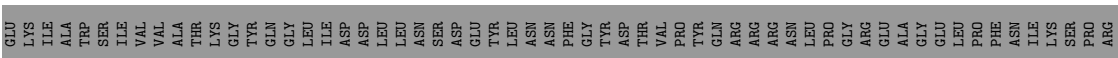
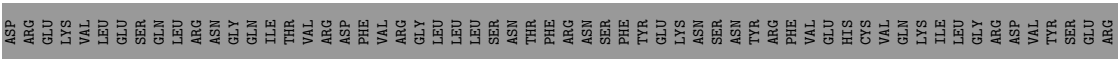
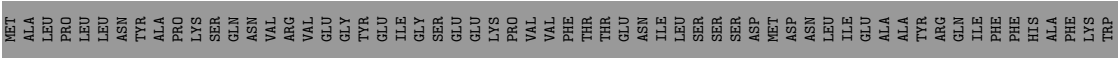




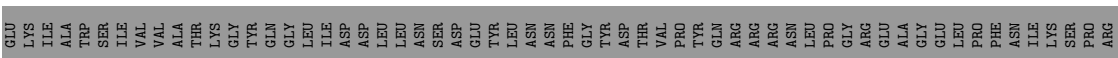
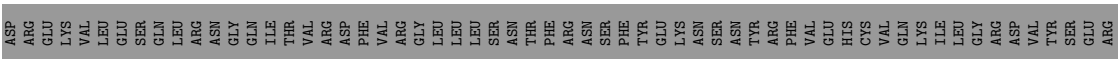
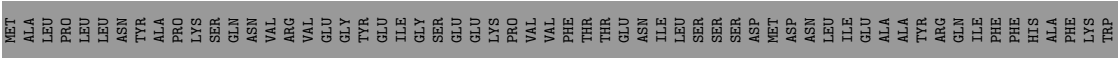
● Molecule 7: Phycobilisome rod-core linker polypeptide CpcG



● Molecule 7: Phycobilisome rod-core linker polypeptide CpcG



● Molecule 7: Phycobilisome rod-core linker polypeptide CpcG



● Molecule 7: Phycobilisome rod-core linker polypeptide CpcG



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202719	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.268	Depositor
Minimum map value	-0.884	Depositor
Average map value	0.045	Depositor
Map value standard deviation	0.159	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	223.65, 324.44998, 435.74997	wwPDB
Map dimensions	213, 309, 415	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.28	0/1225	0.59	0/1652
1	AC	0.32	0/1225	0.69	2/1652 (0.1%)
1	AH	0.29	0/1225	0.57	0/1652
1	AJ	0.28	0/1225	0.52	0/1652
1	AN	0.31	0/1225	0.63	0/1652
1	AP	0.28	0/1225	0.53	0/1652
1	AR	0.28	0/1225	0.57	1/1652 (0.1%)
1	AV	0.29	0/1225	0.58	0/1652
1	AX	0.28	0/1225	0.60	1/1652 (0.1%)
1	AZ	0.27	0/1225	0.57	0/1652
1	BH	0.28	0/1225	0.62	1/1652 (0.1%)
1	BJ	0.30	0/1225	0.64	0/1652
1	BO	0.29	0/1225	0.60	0/1652
1	BQ	0.28	0/1225	0.53	0/1652
1	BU	0.28	0/1225	0.57	1/1652 (0.1%)
1	BW	0.29	0/1225	0.56	0/1652
1	BY	0.29	0/1225	0.55	0/1652
1	CB	0.28	0/1225	0.58	0/1652
1	CD	0.28	0/1225	0.59	1/1652 (0.1%)
1	CF	0.31	0/1225	0.60	0/1652
1	CP	0.31	0/1225	0.62	1/1652 (0.1%)
1	CR	0.30	0/1225	0.65	2/1652 (0.1%)
1	CT	0.29	0/1225	0.55	0/1652
1	CW	0.31	0/1225	0.65	1/1652 (0.1%)
1	CY	0.29	0/1225	0.57	0/1652
1	DA	0.30	0/1225	0.60	1/1652 (0.1%)
1	DG	0.30	0/1225	0.65	1/1652 (0.1%)
1	DI	0.28	0/1225	0.58	0/1652
1	DK	0.29	0/1225	0.59	1/1652 (0.1%)
1	DN	0.33	0/1225	0.66	1/1652 (0.1%)
1	DP	0.29	0/1225	0.61	0/1652
1	DR	0.29	0/1225	0.55	0/1652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	AB	0.27	0/1220	0.55	0/1650
2	AD	0.29	0/1220	0.57	0/1650
2	AF	0.28	0/1220	0.54	0/1650
2	AI	0.29	0/1220	0.51	0/1650
2	AL	0.30	0/1220	0.54	0/1650
2	AO	0.28	0/1220	0.51	0/1650
2	AQ	0.28	0/1220	0.53	0/1650
2	AS	0.27	0/1220	0.52	0/1650
2	AU	0.29	0/1220	0.61	0/1650
2	AW	0.25	0/1220	0.51	0/1650
2	AY	0.27	0/1220	0.54	0/1650
2	BI	0.28	0/1220	0.57	0/1650
2	BK	0.30	0/1220	0.56	0/1650
2	BM	0.27	0/1220	0.61	1/1650 (0.1%)
2	BP	0.28	0/1220	0.53	0/1650
2	BS	0.28	0/1220	0.58	1/1650 (0.1%)
2	BV	0.28	0/1220	0.51	0/1650
2	BX	0.27	0/1220	0.50	0/1650
2	BZ	0.27	0/1220	0.51	0/1650
2	CC	0.30	0/1220	0.60	0/1650
2	CE	0.28	0/1220	0.55	0/1650
2	CG	0.28	0/1220	0.56	1/1650 (0.1%)
2	CQ	0.28	0/1220	0.56	0/1650
2	CS	0.27	0/1220	0.51	0/1650
2	CU	0.27	0/1220	0.53	0/1650
2	CX	0.28	0/1220	0.60	0/1650
2	CZ	0.30	0/1220	0.60	1/1650 (0.1%)
2	DB	0.28	0/1220	0.58	0/1650
2	DH	0.27	0/1220	0.57	0/1650
2	DJ	0.28	0/1220	0.52	0/1650
2	DL	0.27	0/1220	0.52	0/1650
2	DO	0.28	0/1220	0.62	1/1650 (0.1%)
2	DQ	0.27	0/1220	0.55	0/1650
2	DS	0.27	0/1220	0.56	0/1650
3	AE	0.30	0/1277	0.59	0/1730
3	BL	0.30	0/1277	0.59	0/1730
4	AK	0.29	0/1341	0.54	0/1813
4	BR	0.27	0/1341	0.55	0/1813
5	BA	0.28	0/555	0.63	0/743
5	BB	0.26	0/555	0.62	0/743
5	CI	0.27	0/555	0.65	0/743
5	CJ	0.28	0/555	0.62	0/743
5	DD	0.27	0/555	0.60	0/743

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	DU	0.28	0/555	0.66	1/743 (0.1%)
6	BD	0.29	0/6907	0.56	1/9337 (0.0%)
6	CL	0.29	0/6907	0.58	1/9337 (0.0%)
7	BF	0.25	0/459	0.56	0/620
7	CN	0.27	0/459	0.55	0/620
7	DE	0.28	0/434	0.63	0/587
7	DF	0.28	0/434	0.60	0/587
7	DV	0.29	0/434	0.61	0/587
7	DW	0.30	0/434	0.59	0/587
8	BG	0.30	0/283	0.60	0/381
8	CO	0.27	0/283	0.60	0/381
All	All	0.29	0/106280	0.57	23/143532 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	BJ	0	1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BM	9	ILE	CG1-CB-CG2	-9.15	91.27	111.40
1	CD	154	ASP	CB-CG-OD1	7.36	124.92	118.30
1	BH	58	LEU	CA-CB-CG	6.82	130.98	115.30
2	DO	27	LEU	CA-CB-CG	6.51	130.28	115.30
1	DK	140	LEU	CA-CB-CG	6.48	130.20	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BJ	108	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1210	0	1210	19	0
1	AC	1210	0	1210	22	0
1	AH	1210	0	1210	19	0
1	AJ	1210	0	1210	13	0
1	AN	1210	0	1210	28	0
1	AP	1210	0	1210	10	0
1	AR	1210	0	1211	10	0
1	AV	1210	0	1210	23	0
1	AX	1210	0	1210	19	0
1	AZ	1210	0	1210	14	0
1	BH	1210	0	1210	17	0
1	BJ	1210	0	1210	17	0
1	BO	1210	0	1210	26	0
1	BQ	1210	0	1210	15	0
1	BU	1210	0	1210	17	0
1	BW	1210	0	1210	9	0
1	BY	1210	0	1210	17	0
1	CB	1210	0	1210	23	0
1	CD	1210	0	1210	21	0
1	CF	1210	0	1210	15	0
1	CP	1210	0	1210	20	0
1	CR	1210	0	1210	22	0
1	CT	1210	0	1210	13	0
1	CW	1210	0	1210	17	0
1	CY	1210	0	1210	17	0
1	DA	1210	0	1210	19	0
1	DG	1210	0	1210	30	0
1	DI	1210	0	1210	17	0
1	DK	1210	0	1210	20	0
1	DN	1210	0	1210	23	0
1	DP	1210	0	1210	16	0
1	DR	1210	0	1210	18	0
2	AB	1206	0	1218	21	0
2	AD	1206	0	1218	20	0
2	AF	1206	0	1218	25	0
2	AI	1206	0	1218	16	0
2	AL	1206	0	1218	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AO	1206	0	1218	17	0
2	AQ	1206	0	1218	12	0
2	AS	1206	0	1218	16	0
2	AU	1206	0	1218	14	0
2	AW	1206	0	1218	24	0
2	AY	1206	0	1218	25	0
2	BI	1206	0	1218	17	0
2	BK	1206	0	1218	9	0
2	BM	1206	0	1218	20	0
2	BP	1206	0	1218	14	0
2	BS	1206	0	1218	19	0
2	BV	1206	0	1218	18	0
2	BX	1206	0	1218	10	0
2	BZ	1206	0	1218	18	0
2	CC	1206	0	1218	16	0
2	CE	1206	0	1218	19	0
2	CG	1206	0	1218	17	0
2	CQ	1206	0	1218	20	0
2	CS	1206	0	1218	13	0
2	CU	1206	0	1218	17	0
2	CX	1206	0	1218	24	0
2	CZ	1206	0	1218	16	0
2	DB	1206	0	1218	12	0
2	DH	1206	0	1218	19	0
2	DJ	1206	0	1218	16	0
2	DL	1206	0	1218	12	0
2	DO	1206	0	1218	24	0
2	DQ	1206	0	1218	28	0
2	DS	1206	0	1218	21	0
3	AE	1254	0	1250	18	0
3	BL	1254	0	1250	18	0
4	AK	1322	0	1311	16	0
4	BR	1322	0	1311	24	0
5	BA	546	0	568	13	0
5	BB	546	0	568	17	0
5	CI	546	0	568	12	0
5	CJ	546	0	568	9	0
5	DD	546	0	568	10	0
5	DU	546	0	568	10	0
6	BD	6761	0	6739	100	0
6	CL	6761	0	6739	98	0
7	BF	451	0	465	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	CN	451	0	465	5	0
7	DE	426	0	437	10	0
7	DF	426	0	437	5	0
7	DV	426	0	437	9	0
7	DW	426	0	437	7	0
8	BG	277	0	283	3	0
8	CO	277	0	283	8	0
9	AA	43	0	37	2	0
9	AB	43	0	37	2	0
9	AC	43	0	37	3	0
9	AD	43	0	37	3	0
9	AE	43	0	37	2	0
9	AH	43	0	37	0	0
9	AI	43	0	37	2	0
9	AJ	43	0	37	1	0
9	AK	43	0	37	0	0
9	AL	43	0	37	4	0
9	AN	43	0	37	3	0
9	AO	43	0	37	2	0
9	AP	43	0	37	2	0
9	AQ	43	0	37	3	0
9	AR	43	0	38	1	0
9	AU	43	0	37	3	0
9	AV	43	0	37	3	0
9	AW	43	0	37	6	0
9	AX	43	0	37	4	0
9	AY	43	0	37	7	0
9	AZ	43	0	37	4	0
9	BA	43	0	37	2	0
9	BD	86	0	74	6	0
9	BH	43	0	37	3	0
9	BI	43	0	37	6	0
9	BJ	43	0	37	2	0
9	BK	43	0	37	1	0
9	BL	43	0	37	1	0
9	BO	43	0	37	2	0
9	BP	43	0	37	3	0
9	BQ	43	0	37	1	0
9	BR	43	0	37	2	0
9	BS	43	0	37	4	0
9	BU	43	0	37	2	0
9	BV	43	0	37	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	BW	43	0	37	2	0
9	BX	43	0	37	4	0
9	BY	43	0	37	3	0
9	CB	43	0	37	2	0
9	CC	43	0	37	4	0
9	CD	43	0	37	3	0
9	CE	43	0	37	3	0
9	CF	43	0	37	2	0
9	CG	43	0	37	4	0
9	CI	43	0	37	2	0
9	CL	86	0	74	6	0
9	CP	43	0	37	1	0
9	CQ	43	0	37	3	0
9	CR	43	0	37	2	0
9	CS	43	0	37	5	0
9	CT	43	0	37	4	0
9	CU	43	0	37	6	0
9	CW	43	0	37	2	0
9	CX	43	0	37	7	0
9	CY	43	0	37	1	0
9	CZ	43	0	37	1	0
9	DA	43	0	37	2	0
9	DB	43	0	37	5	0
9	DG	43	0	37	4	0
9	DH	43	0	37	1	0
9	DI	43	0	37	1	0
9	DJ	43	0	37	1	0
9	DK	43	0	37	3	0
9	DL	43	0	37	5	0
9	DN	43	0	37	6	0
9	DO	43	0	37	4	0
9	DP	43	0	37	0	0
9	DQ	43	0	37	4	0
9	DR	43	0	37	2	0
9	DS	43	0	37	5	0
All	All	107930	0	108050	1357	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 1357 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)
5:BB:40:GLN:O	5:BB:44:MET:HB2	1.87	0.75
6:CL:548:ARG:O	6:CL:552:GLY:HA2	1.87	0.72
1:CF:83:ARG:HH22	9:CF:200:CYC:HBA2	1.55	0.71
6:BD:548:ARG:O	6:BD:552:GLY:HA2	1.90	0.70
3:BL:2:SER:N	3:BL:5:SER:HG	1.89	0.70

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%)	157 (99%)	1 (1%)	0	100	100
1	AC	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	AH	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	AJ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	AN	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	AP	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	AR	158/161 (98%)	158 (100%)	0	0	100	100
1	AV	158/161 (98%)	158 (100%)	0	0	100	100
1	AX	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	AZ	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	BH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	BJ	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	BO	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	BQ	158/161 (98%)	158 (100%)	0	0	100	100
1	BU	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	BW	158/161 (98%)	157 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BY	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	CB	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	CD	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	CF	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	CP	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	CR	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
1	CT	158/161 (98%)	158 (100%)	0	0	100	100
1	CW	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	CY	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
1	DA	158/161 (98%)	158 (100%)	0	0	100	100
1	DG	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	DI	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
1	DK	158/161 (98%)	158 (100%)	0	0	100	100
1	DN	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	DP	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
1	DR	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
2	AB	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AD	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	AF	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	AI	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AL	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AO	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
2	AQ	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	AS	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	AU	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	AW	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	AY	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	BI	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	BK	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	BM	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	BP	159/161 (99%)	154 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BS	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	BV	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	BX	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
2	BZ	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	CC	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	CE	159/161 (99%)	158 (99%)	1 (1%)	0	100	100
2	CG	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	CQ	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	CS	159/161 (99%)	157 (99%)	2 (1%)	0	100	100
2	CU	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	CX	159/161 (99%)	151 (95%)	8 (5%)	0	100	100
2	CZ	159/161 (99%)	153 (96%)	5 (3%)	1 (1%)	22	51
2	DB	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	DH	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
2	DJ	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	DL	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
2	DO	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
2	DQ	159/161 (99%)	153 (96%)	6 (4%)	0	100	100
2	DS	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
3	AE	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
3	BL	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
4	AK	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
4	BR	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
5	BA	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
5	BB	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
5	CI	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
5	CJ	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
5	DD	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
5	DU	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
6	BD	846/896 (94%)	803 (95%)	43 (5%)	0	100	100
6	CL	846/896 (94%)	792 (94%)	54 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BF	55/249 (22%)	52 (94%)	3 (6%)	0	100	100
7	CN	55/249 (22%)	52 (94%)	3 (6%)	0	100	100
7	DE	52/249 (21%)	46 (88%)	6 (12%)	0	100	100
7	DF	52/249 (21%)	45 (86%)	7 (14%)	0	100	100
7	DV	52/249 (21%)	43 (83%)	9 (17%)	0	100	100
7	DW	52/249 (21%)	45 (86%)	7 (14%)	0	100	100
8	BG	34/121 (28%)	31 (91%)	3 (9%)	0	100	100
8	CO	34/121 (28%)	33 (97%)	1 (3%)	0	100	100
All	All	13580/15216 (89%)	13253 (98%)	326 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CZ	75	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	128/129 (99%)	125 (98%)	3 (2%)	45	78
1	AC	128/129 (99%)	123 (96%)	5 (4%)	27	61
1	AH	128/129 (99%)	128 (100%)	0	100	100
1	AJ	128/129 (99%)	128 (100%)	0	100	100
1	AN	128/129 (99%)	125 (98%)	3 (2%)	45	78
1	AP	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	AR	128/129 (99%)	128 (100%)	0	100	100
1	AV	128/129 (99%)	126 (98%)	2 (2%)	58	85
1	AX	128/129 (99%)	128 (100%)	0	100	100
1	AZ	128/129 (99%)	126 (98%)	2 (2%)	58	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BH	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	BJ	128/129 (99%)	125 (98%)	3 (2%)	45	78
1	BO	128/129 (99%)	124 (97%)	4 (3%)	35	69
1	BQ	128/129 (99%)	125 (98%)	3 (2%)	45	78
1	BU	128/129 (99%)	128 (100%)	0	100	100
1	BW	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	BY	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	CB	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	CD	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	CF	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	CP	128/129 (99%)	125 (98%)	3 (2%)	45	78
1	CR	128/129 (99%)	124 (97%)	4 (3%)	35	69
1	CT	128/129 (99%)	126 (98%)	2 (2%)	58	85
1	CW	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	CY	128/129 (99%)	125 (98%)	3 (2%)	45	78
1	DA	128/129 (99%)	126 (98%)	2 (2%)	58	85
1	DG	128/129 (99%)	124 (97%)	4 (3%)	35	69
1	DI	128/129 (99%)	124 (97%)	4 (3%)	35	69
1	DK	128/129 (99%)	126 (98%)	2 (2%)	58	85
1	DN	128/129 (99%)	127 (99%)	1 (1%)	79	93
1	DP	128/129 (99%)	126 (98%)	2 (2%)	58	85
1	DR	128/129 (99%)	126 (98%)	2 (2%)	58	85
2	AB	125/125 (100%)	123 (98%)	2 (2%)	58	85
2	AD	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	AF	125/125 (100%)	123 (98%)	2 (2%)	58	85
2	AI	125/125 (100%)	125 (100%)	0	100	100
2	AL	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	AO	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	AQ	125/125 (100%)	125 (100%)	0	100	100
2	AS	125/125 (100%)	123 (98%)	2 (2%)	58	85
2	AU	125/125 (100%)	121 (97%)	4 (3%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AW	125/125 (100%)	122 (98%)	3 (2%)	44	77
2	AY	125/125 (100%)	125 (100%)	0	100	100
2	BI	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	BK	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	BM	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	BP	125/125 (100%)	125 (100%)	0	100	100
2	BS	125/125 (100%)	121 (97%)	4 (3%)	34	68
2	BV	125/125 (100%)	125 (100%)	0	100	100
2	BX	125/125 (100%)	125 (100%)	0	100	100
2	BZ	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	CC	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	CE	125/125 (100%)	121 (97%)	4 (3%)	34	68
2	CG	125/125 (100%)	125 (100%)	0	100	100
2	CQ	125/125 (100%)	123 (98%)	2 (2%)	58	85
2	CS	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	CU	125/125 (100%)	122 (98%)	3 (2%)	44	77
2	CX	125/125 (100%)	123 (98%)	2 (2%)	58	85
2	CZ	125/125 (100%)	122 (98%)	3 (2%)	44	77
2	DB	125/125 (100%)	125 (100%)	0	100	100
2	DH	125/125 (100%)	125 (100%)	0	100	100
2	DJ	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	DL	125/125 (100%)	124 (99%)	1 (1%)	79	93
2	DO	125/125 (100%)	122 (98%)	3 (2%)	44	77
2	DQ	125/125 (100%)	122 (98%)	3 (2%)	44	77
2	DS	125/125 (100%)	123 (98%)	2 (2%)	58	85
3	AE	132/133 (99%)	129 (98%)	3 (2%)	45	78
3	BL	132/133 (99%)	131 (99%)	1 (1%)	79	93
4	AK	140/140 (100%)	140 (100%)	0	100	100
4	BR	140/140 (100%)	140 (100%)	0	100	100
5	BA	58/58 (100%)	57 (98%)	1 (2%)	56	84
5	BB	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CI	58/58 (100%)	57 (98%)	1 (2%)	56	84
5	CJ	58/58 (100%)	56 (97%)	2 (3%)	32	66
5	DD	58/58 (100%)	58 (100%)	0	100	100
5	DU	58/58 (100%)	56 (97%)	2 (3%)	32	66
6	BD	719/753 (96%)	707 (98%)	12 (2%)	56	84
6	CL	719/753 (96%)	709 (99%)	10 (1%)	62	87
7	BF	49/221 (22%)	49 (100%)	0	100	100
7	CN	49/221 (22%)	48 (98%)	1 (2%)	50	81
7	DE	46/221 (21%)	45 (98%)	1 (2%)	47	79
7	DF	46/221 (21%)	45 (98%)	1 (2%)	47	79
7	DV	46/221 (21%)	45 (98%)	1 (2%)	47	79
7	DW	46/221 (21%)	45 (98%)	1 (2%)	47	79
8	BG	30/98 (31%)	29 (97%)	1 (3%)	33	67
8	CO	30/98 (31%)	29 (97%)	1 (3%)	33	67
All	All	11018/12300 (90%)	10867 (99%)	151 (1%)	62	87

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CZ	27	LEU
1	DR	81	CYS
1	DA	157	ILE
2	DJ	15	GLN
7	DW	249	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	CE	131	GLN
6	CL	451	ASN
1	CT	60	GLN
6	CL	846	GLN
2	AY	71	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

72 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	$\# Z > 2$
9	CYC	DH	200	2	42,46,46	1.70	9 (21%)	52,67,67	2.22	11 (21%)
9	CYC	DN	200	1	42,46,46	1.68	8 (19%)	52,67,67	2.32	14 (26%)
9	CYC	AL	200	2	42,46,46	1.71	10 (23%)	52,67,67	2.19	12 (23%)
9	CYC	AV	200	1	42,46,46	1.67	10 (23%)	52,67,67	2.12	12 (23%)
9	CYC	CF	200	1	42,46,46	1.64	9 (21%)	52,67,67	2.25	12 (23%)
9	CYC	BO	200	1	42,46,46	1.70	10 (23%)	52,67,67	2.21	12 (23%)
9	CYC	CD	200	1	42,46,46	1.69	10 (23%)	52,67,67	2.21	14 (26%)
9	CYC	BJ	200	1	42,46,46	1.71	9 (21%)	52,67,67	2.07	12 (23%)
9	CYC	BR	200	4	42,46,46	1.69	8 (19%)	52,67,67	2.29	13 (25%)
9	CYC	BP	200	2	42,46,46	1.64	9 (21%)	52,67,67	2.36	14 (26%)
9	CYC	CU	200	2	42,46,46	1.72	8 (19%)	52,67,67	2.27	13 (25%)
9	CYC	AP	200	1	42,46,46	1.65	8 (19%)	52,67,67	2.31	14 (26%)
9	CYC	BH	200	1	42,46,46	1.71	9 (21%)	52,67,67	2.16	11 (21%)
9	CYC	BK	200	2	42,46,46	1.67	9 (21%)	52,67,67	2.26	17 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CYC	DG	200	1	42,46,46	1.70	9 (21%)	52,67,67	2.03	13 (25%)
9	CYC	CX	200	2	42,46,46	1.67	8 (19%)	52,67,67	2.16	14 (26%)
9	CYC	AA	200	1	42,46,46	1.67	9 (21%)	52,67,67	2.10	9 (17%)
9	CYC	AJ	200	1	42,46,46	1.63	8 (19%)	52,67,67	2.29	14 (26%)
9	CYC	AC	200	1	42,46,46	1.70	9 (21%)	52,67,67	2.02	12 (23%)
9	CYC	BL	200	3	42,46,46	1.71	9 (21%)	52,67,67	2.21	15 (28%)
9	CYC	CP	200	1	42,46,46	1.66	10 (23%)	52,67,67	2.21	12 (23%)
9	CYC	CZ	200	2	42,46,46	1.68	9 (21%)	52,67,67	2.36	12 (23%)
9	CYC	DJ	200	2	42,46,46	1.63	9 (21%)	52,67,67	2.43	15 (28%)
9	CYC	AR	200	-	42,46,46	1.70	10 (23%)	52,67,67	2.11	13 (25%)
9	CYC	DB	200	2	42,46,46	1.69	9 (21%)	52,67,67	2.08	14 (26%)
9	CYC	DQ	200	2	42,46,46	1.68	9 (21%)	52,67,67	2.33	14 (26%)
9	CYC	BY	200	1	42,46,46	1.70	9 (21%)	52,67,67	2.18	13 (25%)
9	CYC	BQ	200	1	42,46,46	1.66	8 (19%)	52,67,67	2.23	11 (21%)
9	CYC	CR	200	1	42,46,46	1.69	9 (21%)	52,67,67	1.96	10 (19%)
9	CYC	DO	200	2	42,46,46	1.65	9 (21%)	52,67,67	2.36	15 (28%)
9	CYC	CG	200	2	42,46,46	1.65	9 (21%)	52,67,67	2.20	14 (26%)
9	CYC	AY	200	2	42,46,46	1.67	9 (21%)	52,67,67	2.13	16 (30%)
9	CYC	AQ	200	2	42,46,46	1.67	9 (21%)	52,67,67	2.26	14 (26%)
9	CYC	DP	200	1	42,46,46	1.70	10 (23%)	52,67,67	2.19	13 (25%)
9	CYC	AI	200	2	42,46,46	1.66	8 (19%)	52,67,67	2.41	15 (28%)
9	CYC	CE	200	2	42,46,46	1.69	8 (19%)	52,67,67	2.56	17 (32%)
9	CYC	BW	200	1	42,46,46	1.65	8 (19%)	52,67,67	2.31	14 (26%)
9	CYC	CC	200	2	42,46,46	1.72	9 (21%)	52,67,67	2.24	17 (32%)
9	CYC	BS	200	2	42,46,46	1.70	8 (19%)	52,67,67	2.16	12 (23%)
9	CYC	CS	200	2	42,46,46	1.64	9 (21%)	52,67,67	2.26	15 (28%)
9	CYC	AH	200	1	42,46,46	1.67	10 (23%)	52,67,67	2.11	13 (25%)
9	CYC	BD	902	6	42,46,46	1.68	9 (21%)	52,67,67	2.18	14 (26%)
9	CYC	BV	200	2	42,46,46	1.65	8 (19%)	52,67,67	2.34	14 (26%)
9	CYC	CT	200	1	42,46,46	1.68	9 (21%)	52,67,67	2.17	13 (25%)
9	CYC	CY	200	1	42,46,46	1.66	9 (21%)	52,67,67	2.27	14 (26%)
9	CYC	DL	200	2	42,46,46	1.71	9 (21%)	52,67,67	2.29	13 (25%)
9	CYC	AE	200	3	42,46,46	1.72	9 (21%)	52,67,67	2.35	15 (28%)
9	CYC	DR	200	1	42,46,46	1.72	8 (19%)	52,67,67	2.25	17 (32%)
9	CYC	CB	200	1	42,46,46	1.67	10 (23%)	52,67,67	2.10	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CYC	AO	200	2	42,46,46	1.67	9 (21%)	52,67,67	2.34	15 (28%)
9	CYC	BA	200	2	42,46,46	1.70	9 (21%)	52,67,67	2.05	11 (21%)
9	CYC	AD	200	2	42,46,46	1.67	9 (21%)	52,67,67	2.16	17 (32%)
9	CYC	AU	200	2	42,46,46	1.68	9 (21%)	52,67,67	2.30	17 (32%)
9	CYC	CI	200	2	42,46,46	1.69	9 (21%)	52,67,67	2.11	11 (21%)
9	CYC	CL	901	2	42,46,46	1.66	9 (21%)	52,67,67	2.12	15 (28%)
9	CYC	DA	200	1	42,46,46	1.68	9 (21%)	52,67,67	2.29	17 (32%)
9	CYC	AK	200	4	42,46,46	1.67	9 (21%)	52,67,67	2.22	11 (21%)
9	CYC	BU	200	1	42,46,46	1.68	9 (21%)	52,67,67	2.18	14 (26%)
9	CYC	AW	200	2	42,46,46	1.66	9 (21%)	52,67,67	2.19	14 (26%)
9	CYC	AX	200	1	42,46,46	1.69	9 (21%)	52,67,67	2.12	9 (17%)
9	CYC	BX	200	2	42,46,46	1.67	9 (21%)	52,67,67	2.26	17 (32%)
9	CYC	AN	200	1	42,46,46	1.68	9 (21%)	52,67,67	2.19	14 (26%)
9	CYC	BD	901	2	42,46,46	1.66	9 (21%)	52,67,67	2.08	16 (30%)
9	CYC	AZ	200	1	42,46,46	1.70	8 (19%)	52,67,67	2.14	14 (26%)
9	CYC	DS	200	2	42,46,46	1.67	9 (21%)	52,67,67	2.30	16 (30%)
9	CYC	CQ	200	2	42,46,46	1.75	9 (21%)	52,67,67	2.19	12 (23%)
9	CYC	AB	200	2	42,46,46	1.66	8 (19%)	52,67,67	2.37	15 (28%)
9	CYC	DK	200	1	42,46,46	1.70	9 (21%)	52,67,67	2.20	14 (26%)
9	CYC	DI	200	1	42,46,46	1.66	10 (23%)	52,67,67	1.95	12 (23%)
9	CYC	CW	200	1	42,46,46	1.69	8 (19%)	52,67,67	2.26	11 (21%)
9	CYC	CL	902	6	42,46,46	1.68	9 (21%)	52,67,67	2.22	15 (28%)
9	CYC	BI	200	2	42,46,46	1.66	9 (21%)	52,67,67	2.33	17 (32%)

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
9	CYC	DH	200	2	-	13/25/74/74	0/4/4/4
9	CYC	DN	200	1	-	11/25/74/74	0/4/4/4
9	CYC	AL	200	2	-	18/25/74/74	0/4/4/4
9	CYC	AV	200	1	-	11/25/74/74	0/4/4/4
9	CYC	CF	200	1	-	10/25/74/74	0/4/4/4
9	CYC	BO	200	1	-	6/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CYC	CD	200	1	-	12/25/74/74	0/4/4/4
9	CYC	BJ	200	1	-	12/25/74/74	0/4/4/4
9	CYC	BR	200	4	-	12/25/74/74	0/4/4/4
9	CYC	BP	200	2	-	15/25/74/74	0/4/4/4
9	CYC	CU	200	2	-	8/25/74/74	0/4/4/4
9	CYC	AP	200	1	-	7/25/74/74	0/4/4/4
9	CYC	BH	200	1	-	7/25/74/74	0/4/4/4
9	CYC	BK	200	2	-	13/25/74/74	0/4/4/4
9	CYC	DG	200	1	-	10/25/74/74	0/4/4/4
9	CYC	CX	200	2	-	12/25/74/74	0/4/4/4
9	CYC	AA	200	1	-	12/25/74/74	0/4/4/4
9	CYC	AJ	200	1	-	8/25/74/74	0/4/4/4
9	CYC	AC	200	1	-	7/25/74/74	0/4/4/4
9	CYC	BL	200	3	-	6/25/74/74	0/4/4/4
9	CYC	CP	200	1	-	7/25/74/74	0/4/4/4
9	CYC	CZ	200	2	-	15/25/74/74	0/4/4/4
9	CYC	DJ	200	2	-	16/25/74/74	0/4/4/4
9	CYC	AR	200	-	-	11/25/74/74	0/4/4/4
9	CYC	DB	200	2	-	9/25/74/74	0/4/4/4
9	CYC	DQ	200	2	-	11/25/74/74	0/4/4/4
9	CYC	BY	200	1	-	9/25/74/74	0/4/4/4
9	CYC	BQ	200	1	-	9/25/74/74	0/4/4/4
9	CYC	CR	200	1	-	15/25/74/74	0/4/4/4
9	CYC	DO	200	2	-	19/25/74/74	0/4/4/4
9	CYC	CG	200	2	-	15/25/74/74	0/4/4/4
9	CYC	AY	200	2	-	15/25/74/74	0/4/4/4
9	CYC	AQ	200	2	-	17/25/74/74	0/4/4/4
9	CYC	DP	200	1	-	9/25/74/74	0/4/4/4
9	CYC	AI	200	2	-	16/25/74/74	0/4/4/4
9	CYC	CE	200	2	-	18/25/74/74	0/4/4/4
9	CYC	BW	200	1	-	7/25/74/74	0/4/4/4
9	CYC	CC	200	2	-	10/25/74/74	0/4/4/4
9	CYC	BS	200	2	-	14/25/74/74	0/4/4/4
9	CYC	CS	200	2	-	13/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CYC	AH	200	1	-	11/25/74/74	0/4/4/4
9	CYC	BD	902	6	-	15/25/74/74	0/4/4/4
9	CYC	BV	200	2	-	10/25/74/74	0/4/4/4
9	CYC	CT	200	1	-	12/25/74/74	0/4/4/4
9	CYC	CY	200	1	-	6/25/74/74	0/4/4/4
9	CYC	DL	200	2	-	11/25/74/74	0/4/4/4
9	CYC	AE	200	3	-	8/25/74/74	0/4/4/4
9	CYC	DR	200	1	-	5/25/74/74	0/4/4/4
9	CYC	CB	200	1	-	6/25/74/74	0/4/4/4
9	CYC	AO	200	2	-	12/25/74/74	0/4/4/4
9	CYC	BA	200	2	-	8/25/74/74	0/4/4/4
9	CYC	AD	200	2	-	12/25/74/74	0/4/4/4
9	CYC	AU	200	2	-	10/25/74/74	0/4/4/4
9	CYC	CI	200	2	-	12/25/74/74	0/4/4/4
9	CYC	CL	901	2	-	12/25/74/74	0/4/4/4
9	CYC	DA	200	1	-	10/25/74/74	0/4/4/4
9	CYC	AK	200	4	-	12/25/74/74	0/4/4/4
9	CYC	BU	200	1	-	9/25/74/74	0/4/4/4
9	CYC	AW	200	2	-	12/25/74/74	0/4/4/4
9	CYC	AX	200	1	-	10/25/74/74	0/4/4/4
9	CYC	BX	200	2	-	15/25/74/74	0/4/4/4
9	CYC	AN	200	1	-	11/25/74/74	0/4/4/4
9	CYC	BD	901	2	-	11/25/74/74	0/4/4/4
9	CYC	AZ	200	1	-	4/25/74/74	0/4/4/4
9	CYC	DS	200	2	-	12/25/74/74	0/4/4/4
9	CYC	CQ	200	2	-	15/25/74/74	0/4/4/4
9	CYC	AB	200	2	-	18/25/74/74	0/4/4/4
9	CYC	DK	200	1	-	7/25/74/74	0/4/4/4
9	CYC	DI	200	1	-	12/25/74/74	0/4/4/4
9	CYC	CW	200	1	-	10/25/74/74	0/4/4/4
9	CYC	CL	902	6	-	8/25/74/74	0/4/4/4
9	CYC	BI	200	2	-	17/25/74/74	0/4/4/4

The worst 5 of 642 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	CQ	200	CYC	CHA-C1A	5.80	1.40	1.35
9	CC	200	CYC	CHA-C1A	5.58	1.40	1.35
9	CE	200	CYC	CHA-C1A	5.53	1.40	1.35
9	CU	200	CYC	CHA-C1A	5.53	1.40	1.35
9	DR	200	CYC	CHA-C1A	5.45	1.40	1.35

The worst 5 of 984 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CZ	200	CYC	OC-C1C-C2C	-7.89	119.90	126.17
9	BI	200	CYC	C1D-CHD-C4C	7.48	138.74	128.47
9	DJ	200	CYC	C1D-CHD-C4C	7.48	138.74	128.47
9	BK	200	CYC	OC-C1C-C2C	-7.31	120.36	126.17
9	BP	200	CYC	CAB-C3B-C4B	7.10	132.35	121.37

There are no chirality outliers.

5 of 808 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AA	200	CYC	ND-C4D-CHA-C1A
9	AA	200	CYC	C3D-C4D-CHA-C1A
9	AA	200	CYC	NA-C4A-CHB-C1B
9	AA	200	CYC	C3A-C4A-CHB-C1B
9	AA	200	CYC	C4C-C3C-CAC-CBC

There are no ring outliers.

69 monomers are involved in 205 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	DH	200	CYC	1	0
9	DN	200	CYC	6	0
9	AL	200	CYC	4	0
9	AV	200	CYC	3	0
9	CF	200	CYC	2	0
9	BO	200	CYC	2	0
9	CD	200	CYC	3	0
9	BJ	200	CYC	2	0
9	BR	200	CYC	2	0
9	BP	200	CYC	3	0
9	CU	200	CYC	6	0
9	AP	200	CYC	2	0
9	BH	200	CYC	3	0

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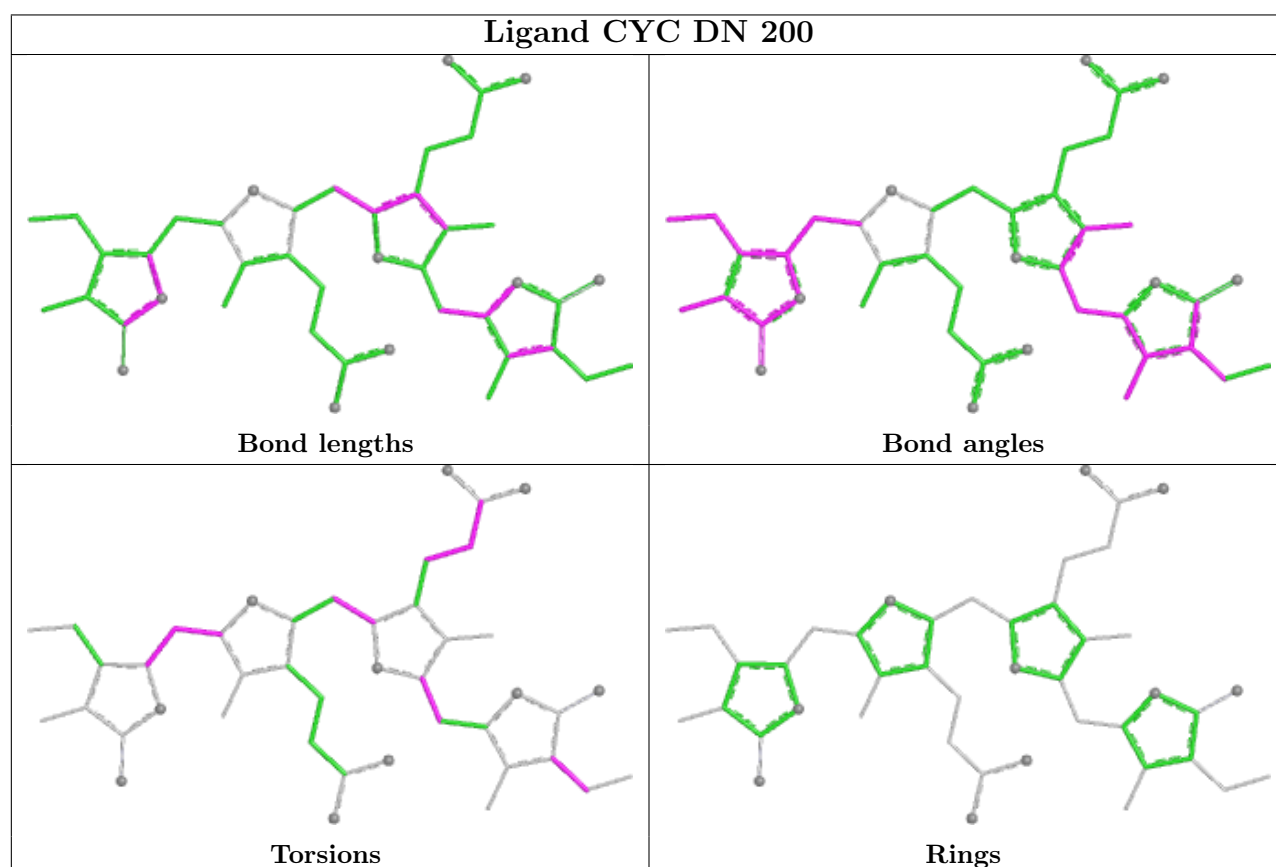
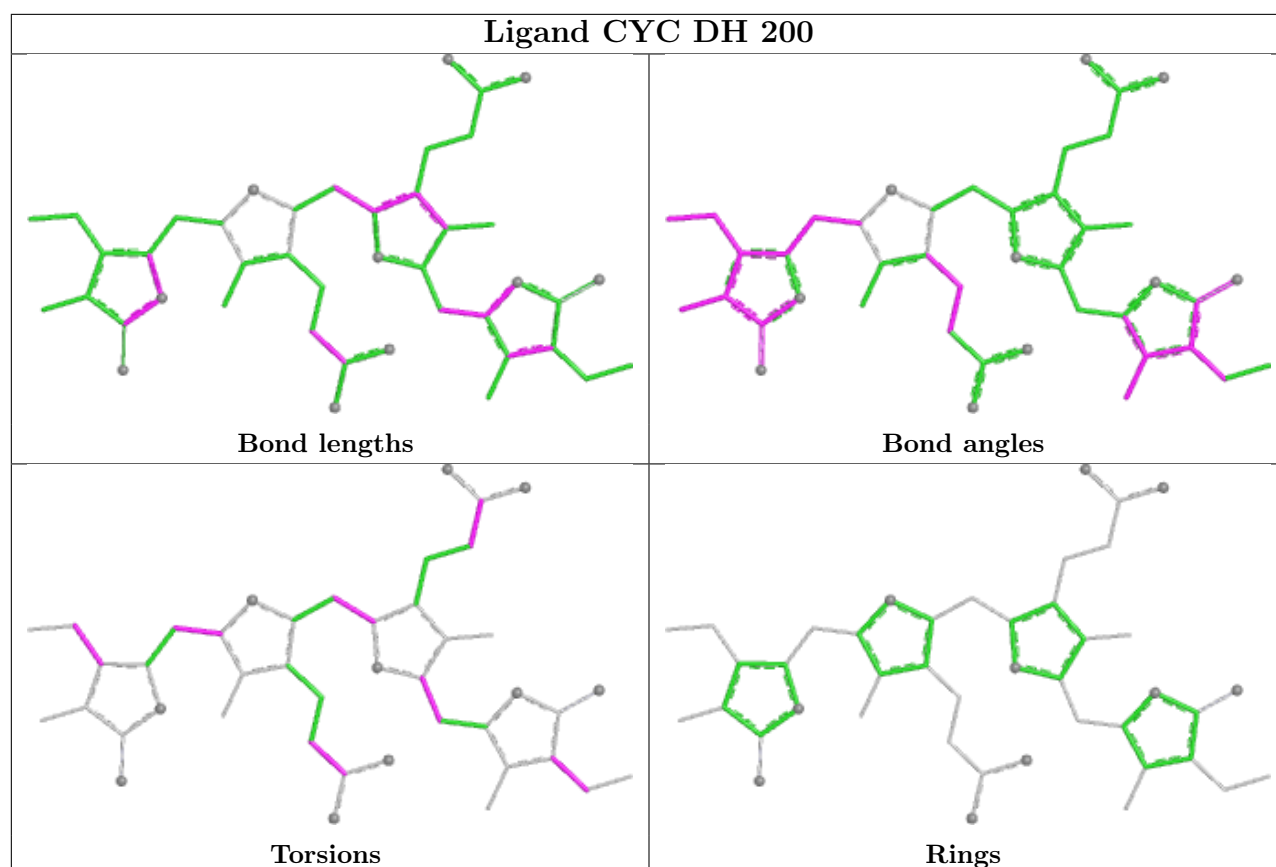
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	BK	200	CYC	1	0
9	DG	200	CYC	4	0
9	CX	200	CYC	7	0
9	AA	200	CYC	2	0
9	AJ	200	CYC	1	0
9	AC	200	CYC	3	0
9	BL	200	CYC	1	0
9	CP	200	CYC	1	0
9	CZ	200	CYC	1	0
9	DJ	200	CYC	1	0
9	AR	200	CYC	1	0
9	DB	200	CYC	5	0
9	DQ	200	CYC	4	0
9	BY	200	CYC	3	0
9	BQ	200	CYC	1	0
9	CR	200	CYC	2	0
9	DO	200	CYC	4	0
9	CG	200	CYC	4	0
9	AY	200	CYC	7	0
9	AQ	200	CYC	3	0
9	AI	200	CYC	2	0
9	CE	200	CYC	3	0
9	BW	200	CYC	2	0
9	CC	200	CYC	4	0
9	BS	200	CYC	4	0
9	CS	200	CYC	5	0
9	BD	902	CYC	3	0
9	BV	200	CYC	3	0
9	CT	200	CYC	4	0
9	CY	200	CYC	1	0
9	DL	200	CYC	5	0
9	AE	200	CYC	2	0
9	DR	200	CYC	2	0
9	CB	200	CYC	2	0
9	AO	200	CYC	2	0
9	BA	200	CYC	2	0
9	AD	200	CYC	3	0
9	AU	200	CYC	3	0
9	CI	200	CYC	2	0
9	CL	901	CYC	3	0
9	DA	200	CYC	2	0
9	BU	200	CYC	2	0

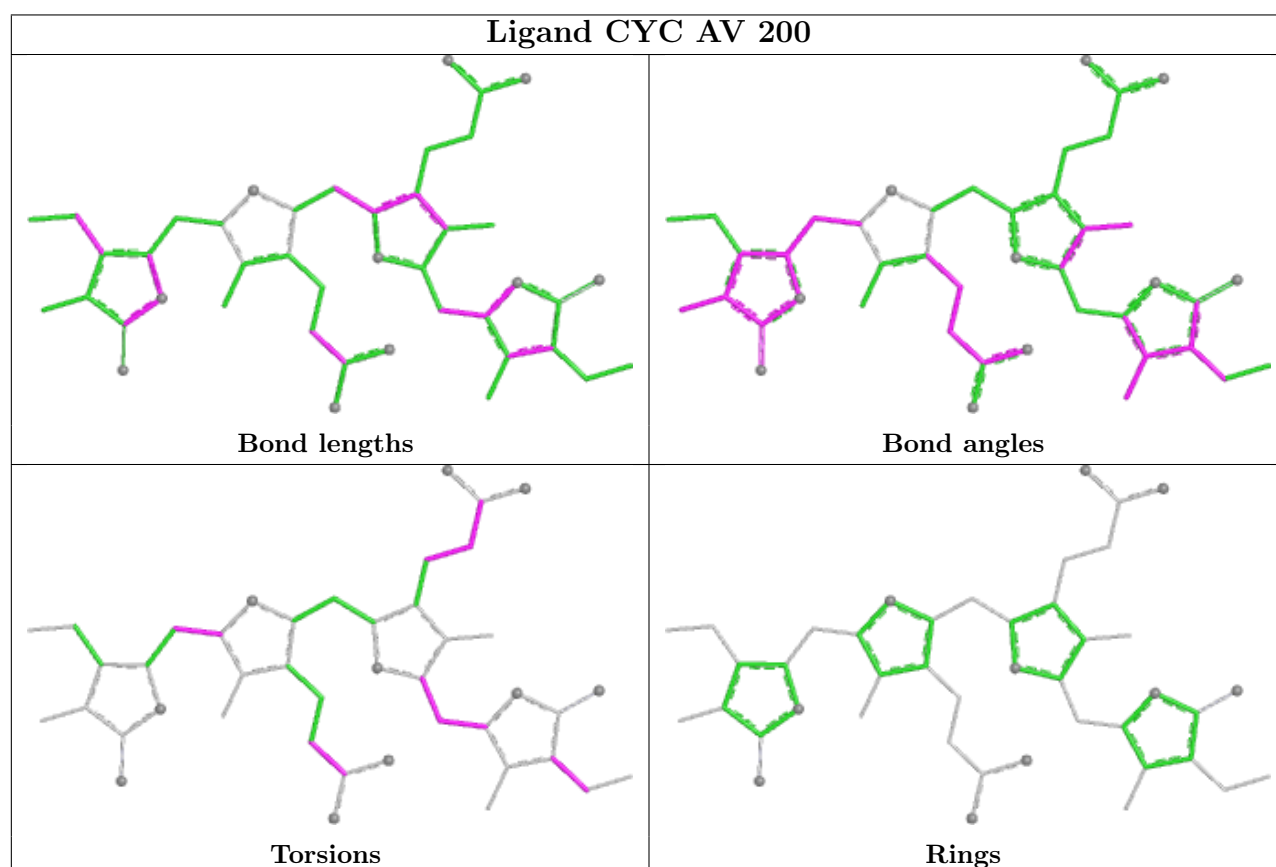
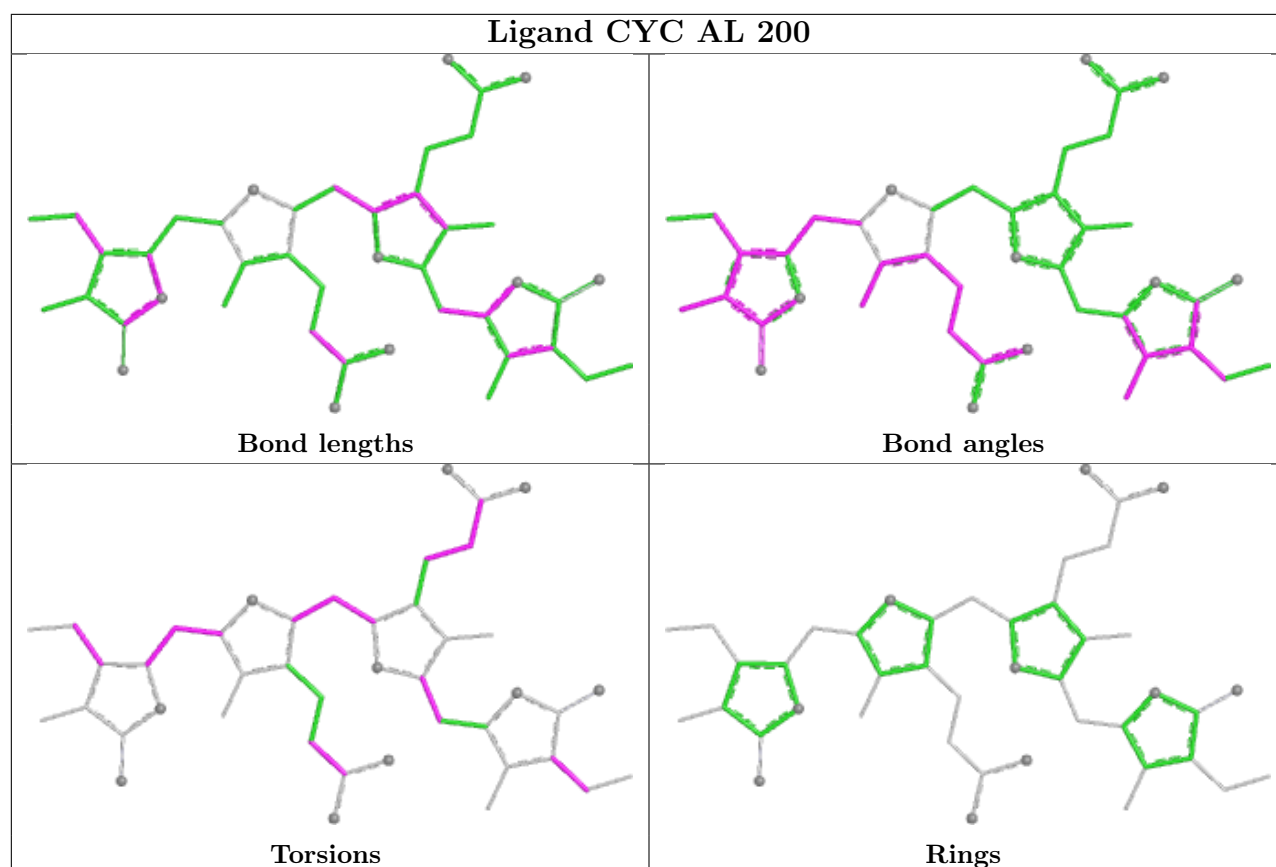
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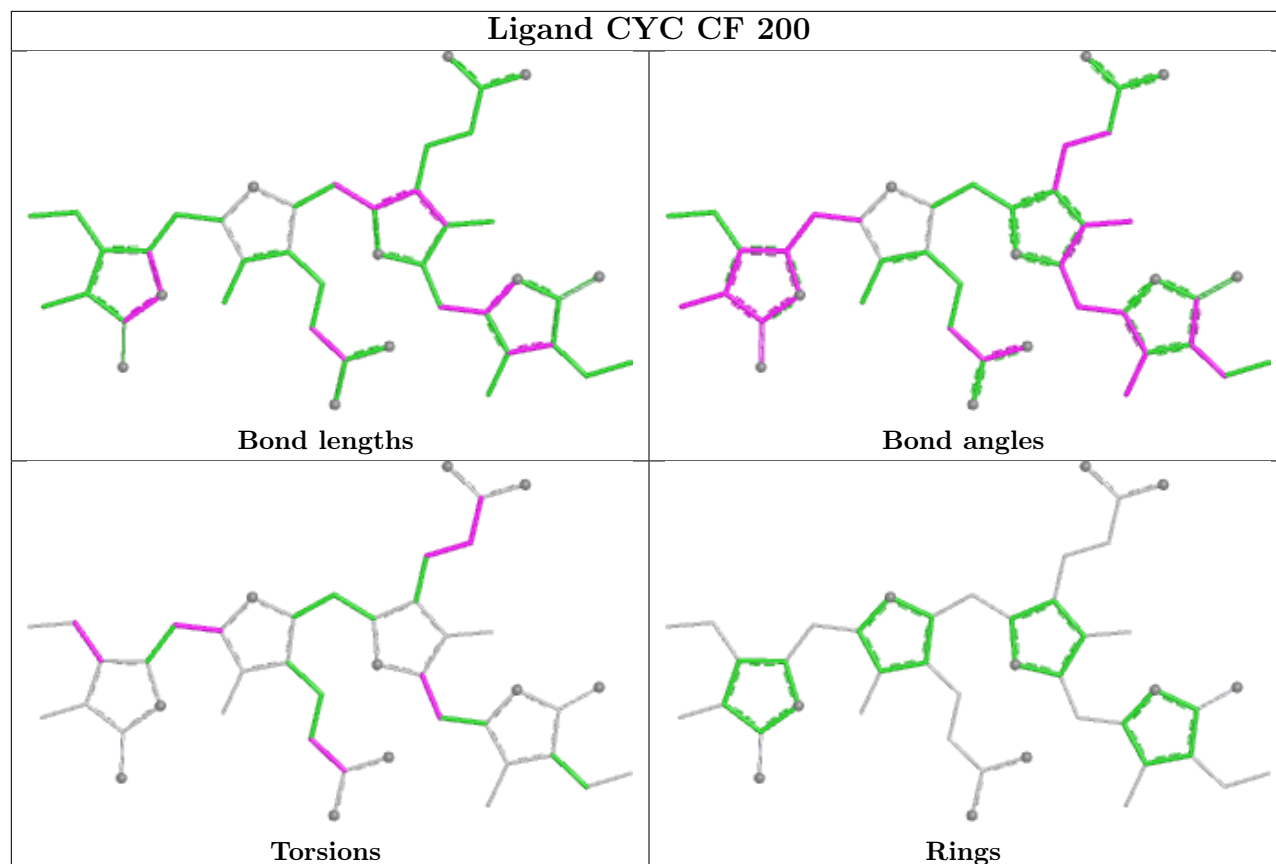
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	AW	200	CYC	6	0
9	AX	200	CYC	4	0
9	BX	200	CYC	4	0
9	AN	200	CYC	3	0
9	BD	901	CYC	3	0
9	AZ	200	CYC	4	0
9	DS	200	CYC	5	0
9	CQ	200	CYC	3	0
9	AB	200	CYC	2	0
9	DK	200	CYC	3	0
9	DI	200	CYC	1	0
9	CW	200	CYC	2	0
9	CL	902	CYC	3	0
9	BI	200	CYC	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

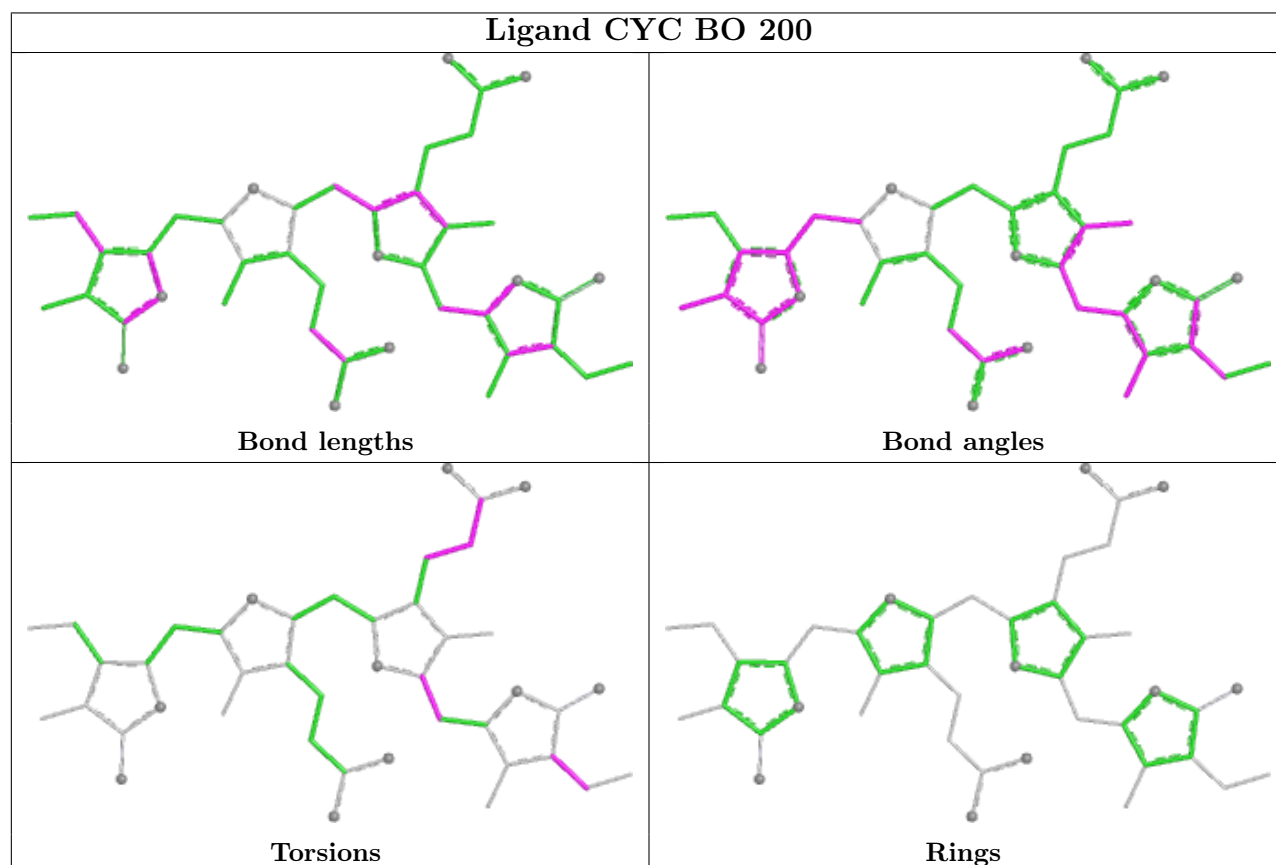




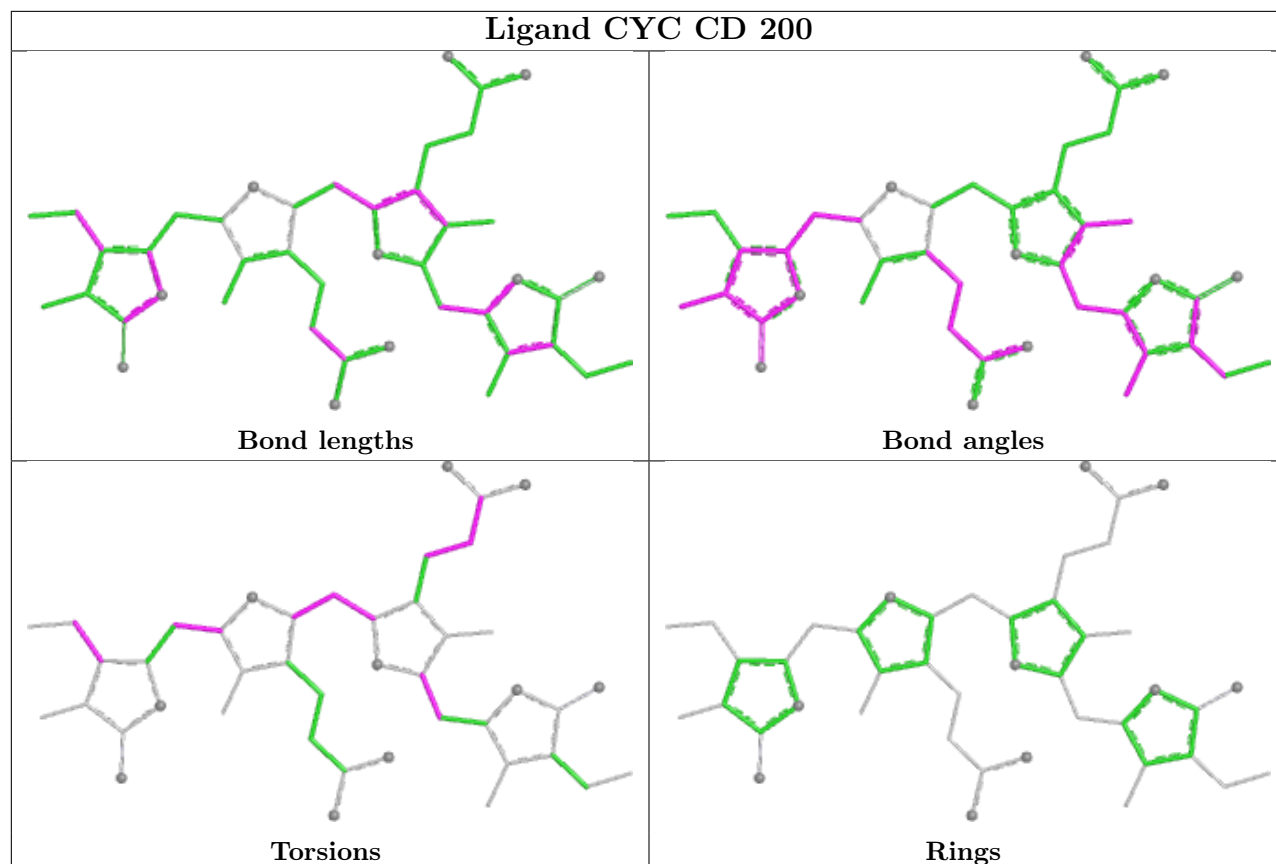
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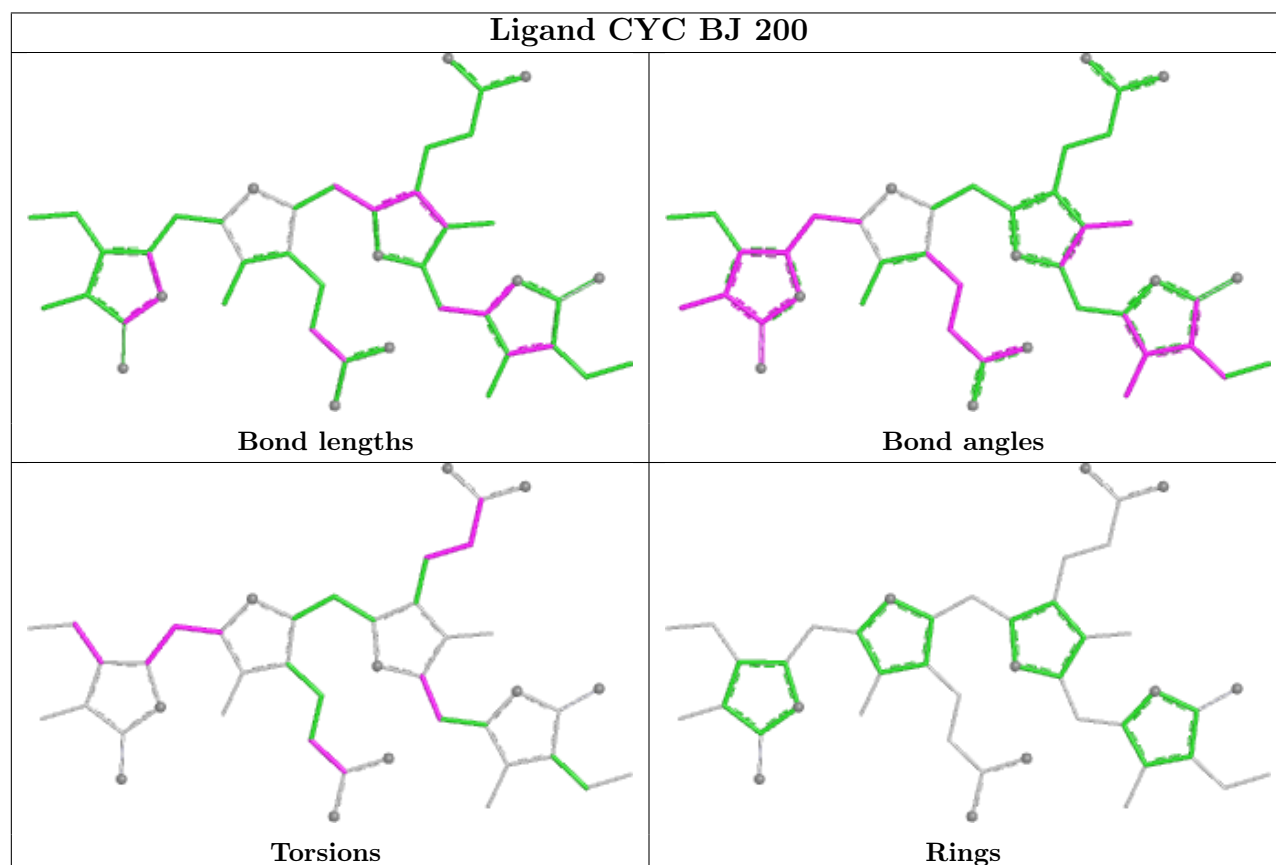
Ligand CYC BO 200

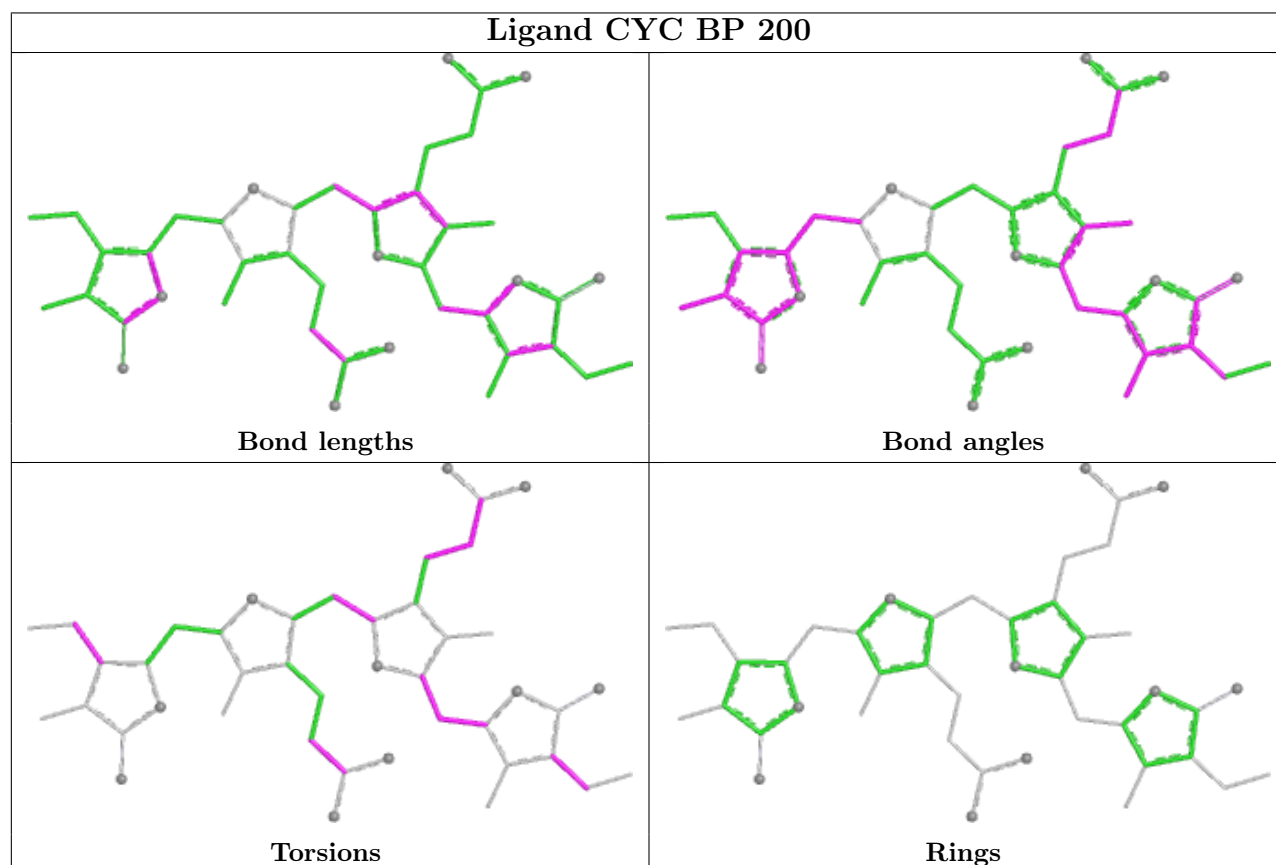
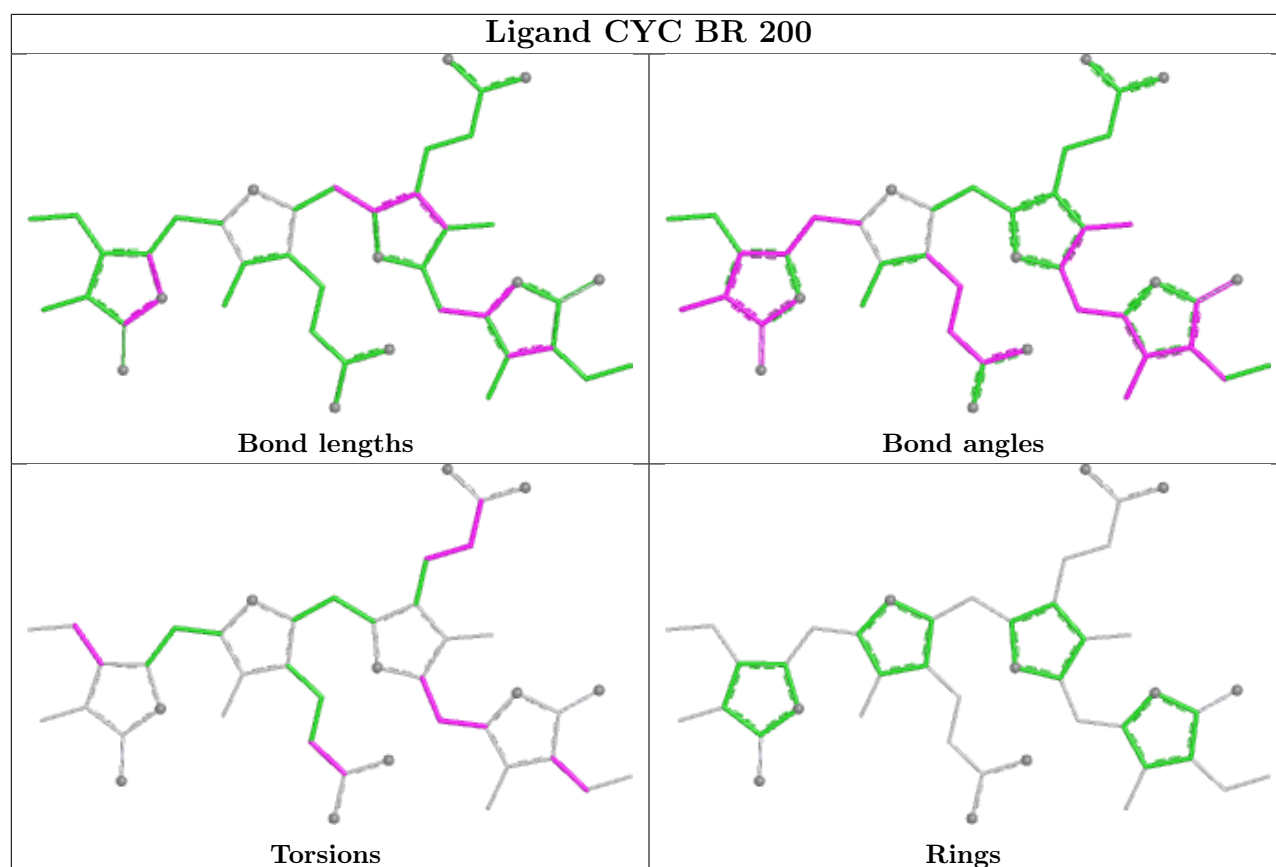


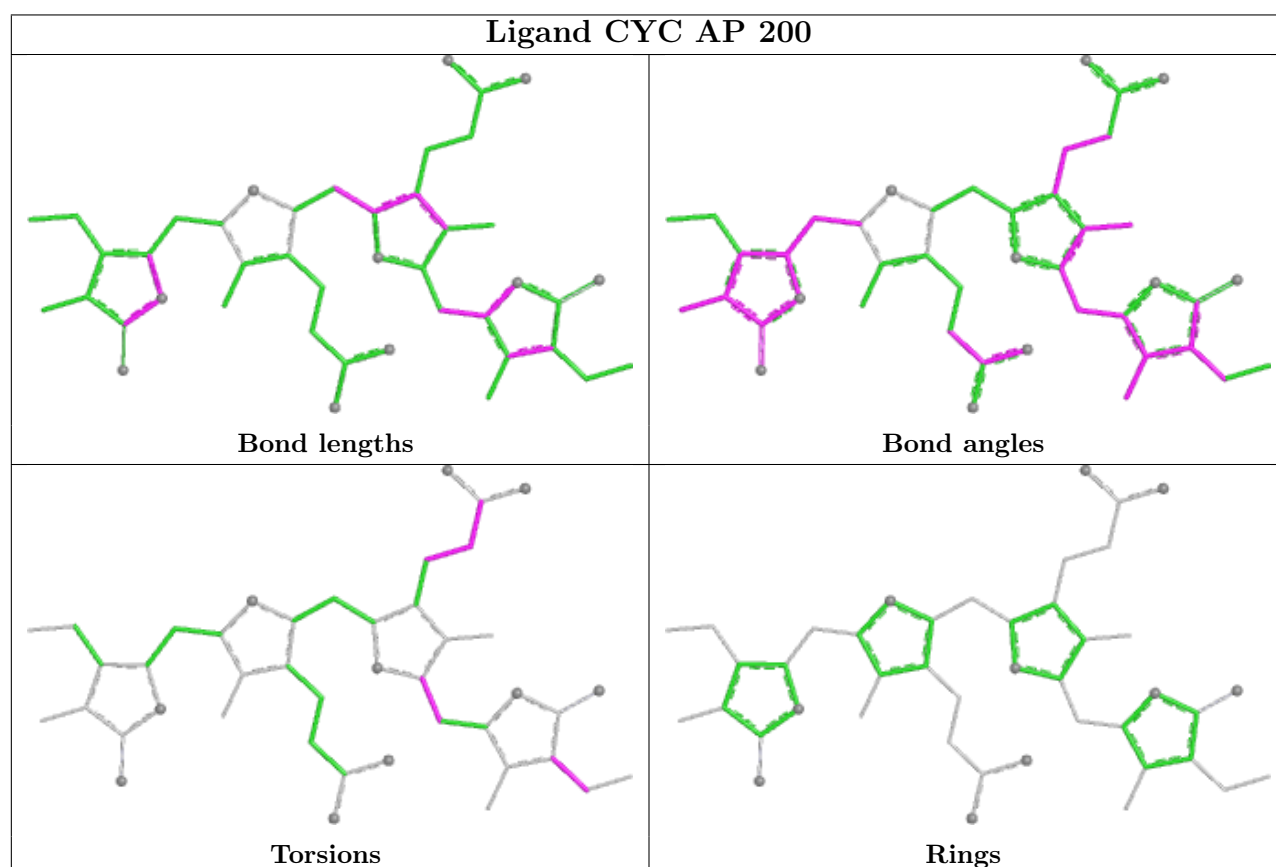
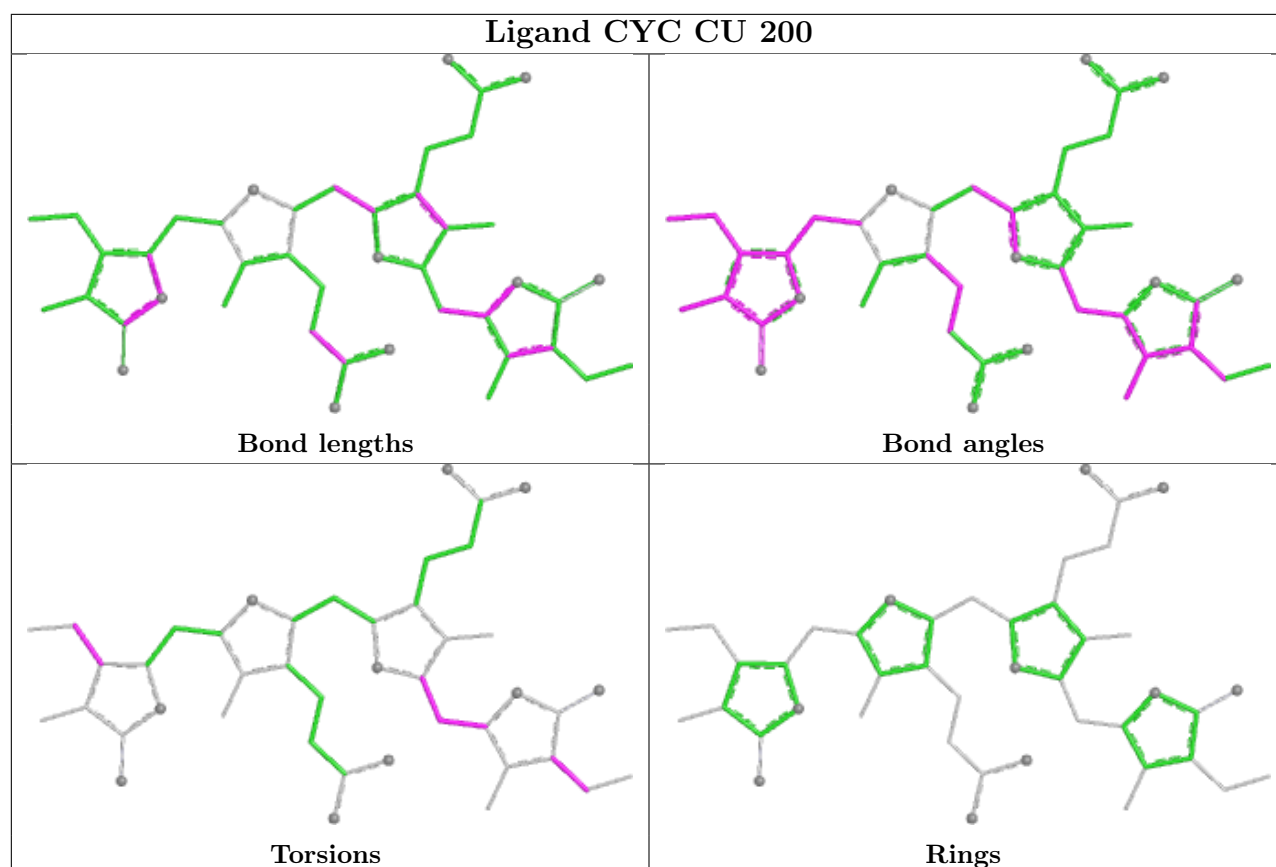
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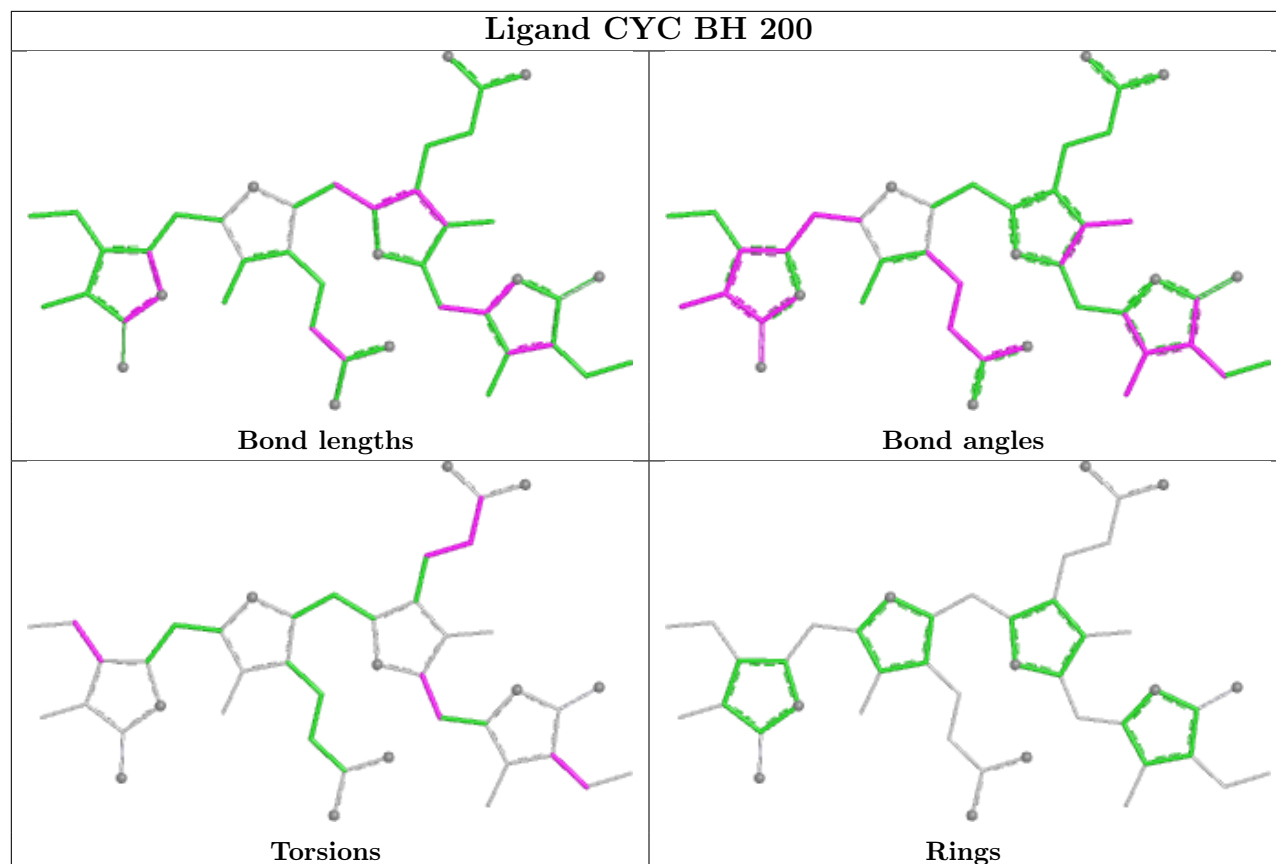
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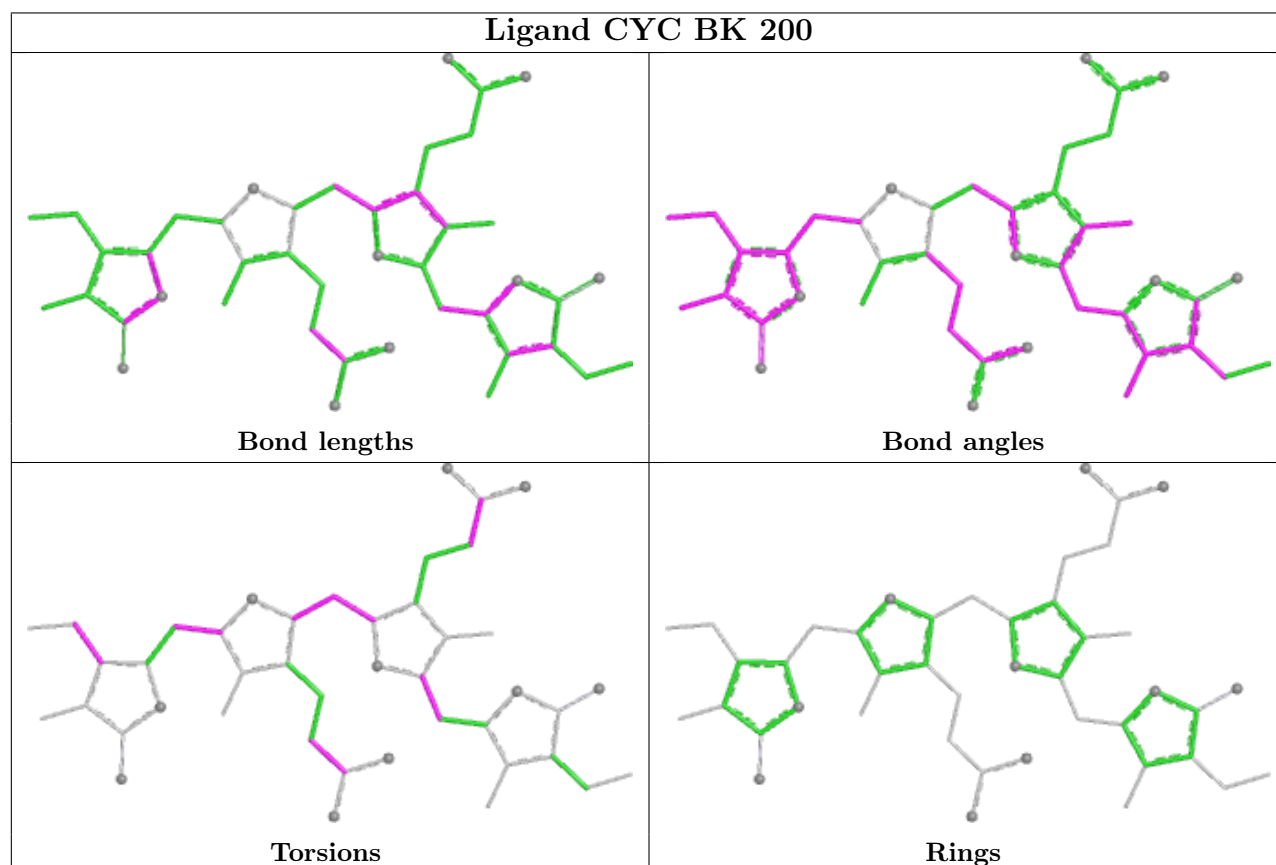




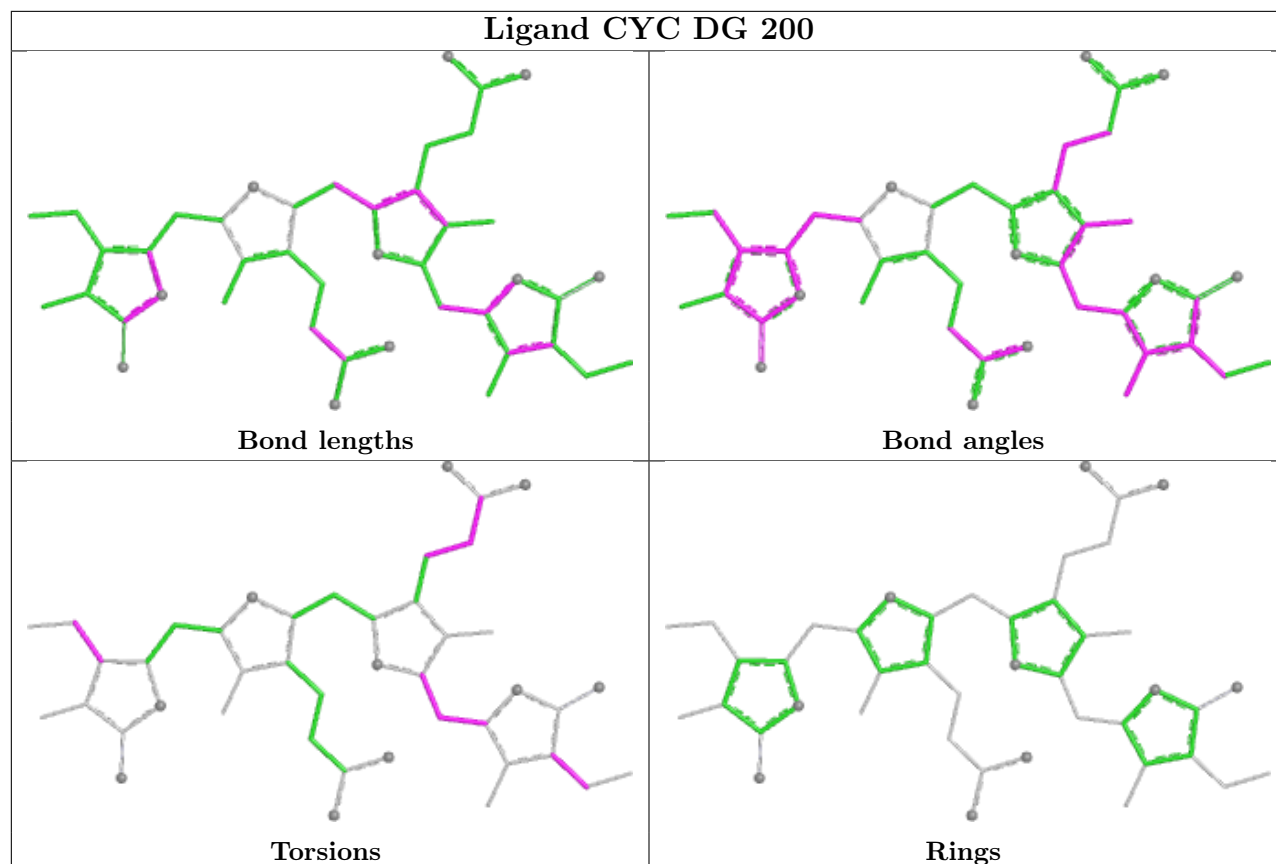
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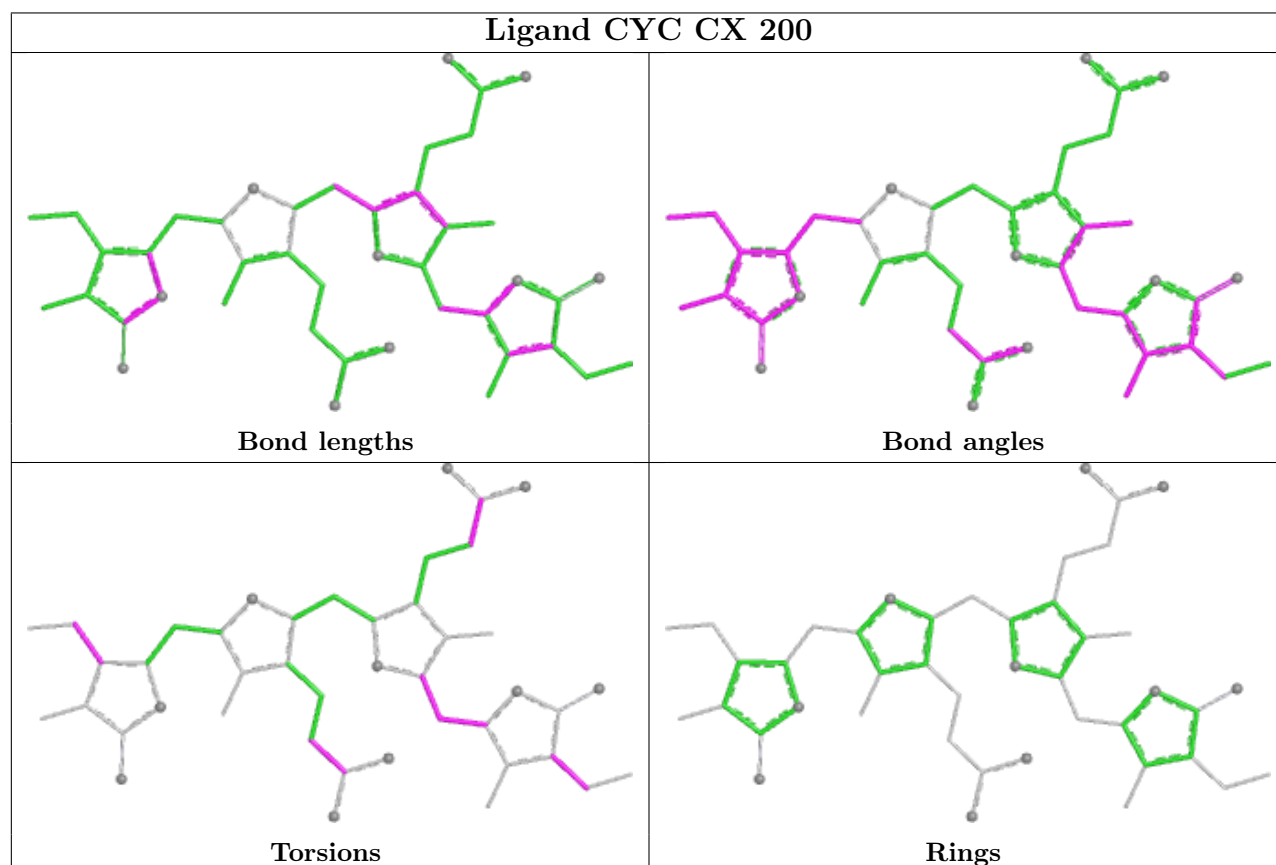
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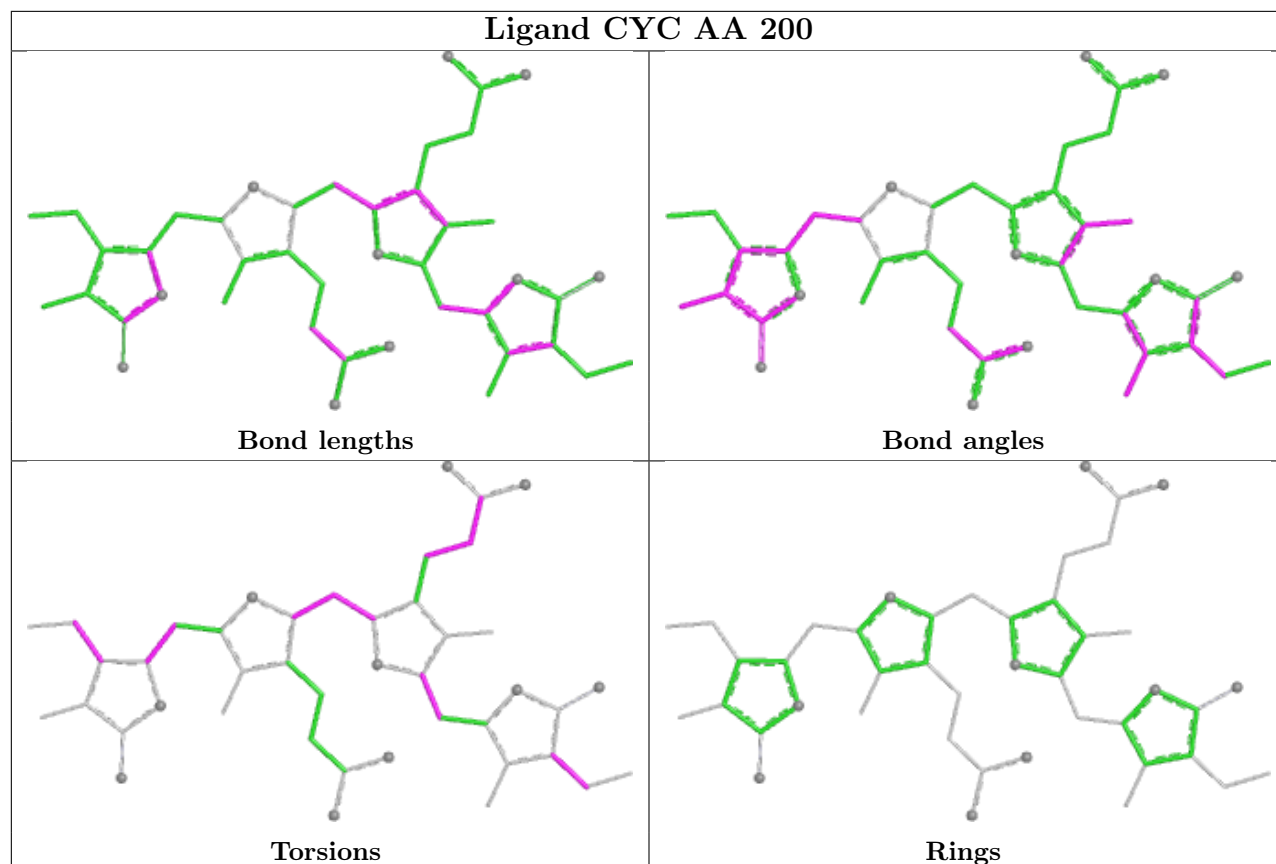
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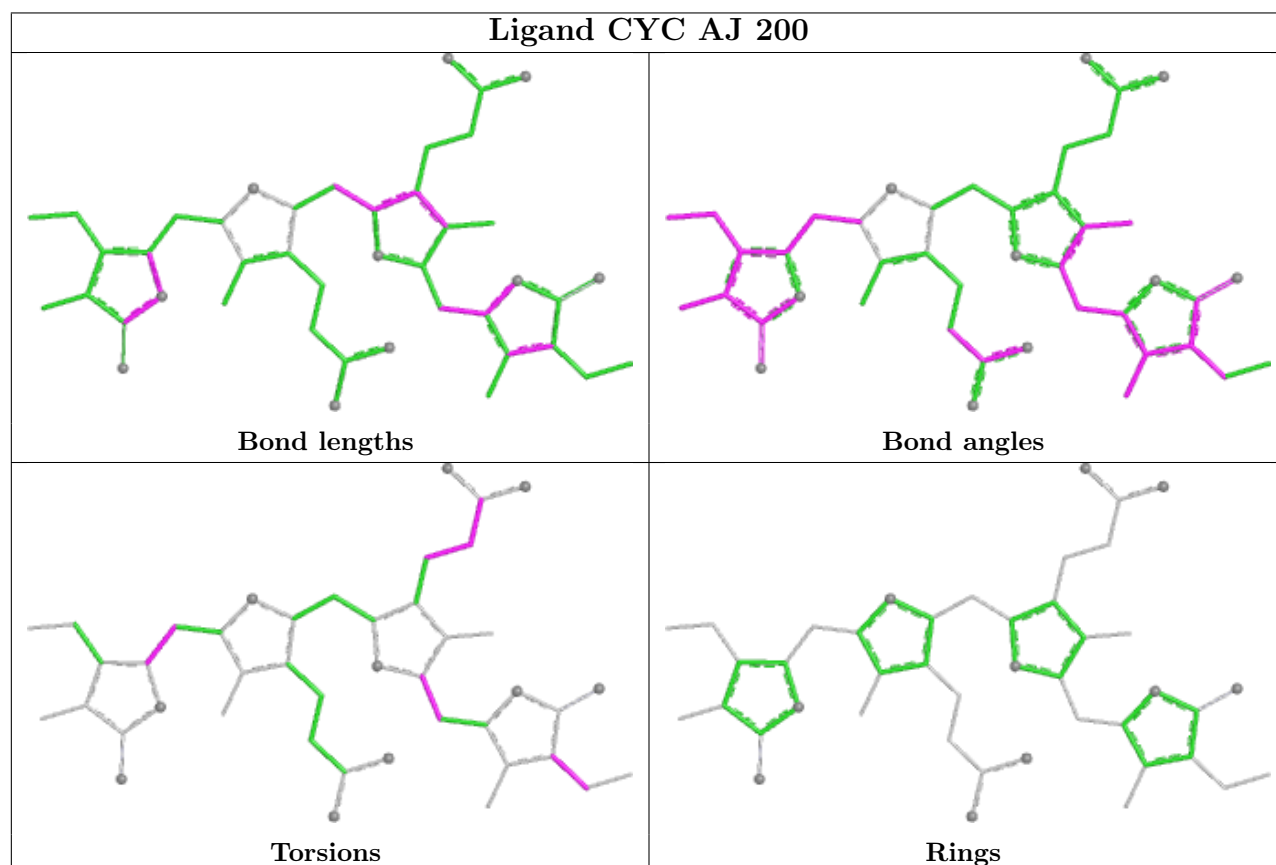
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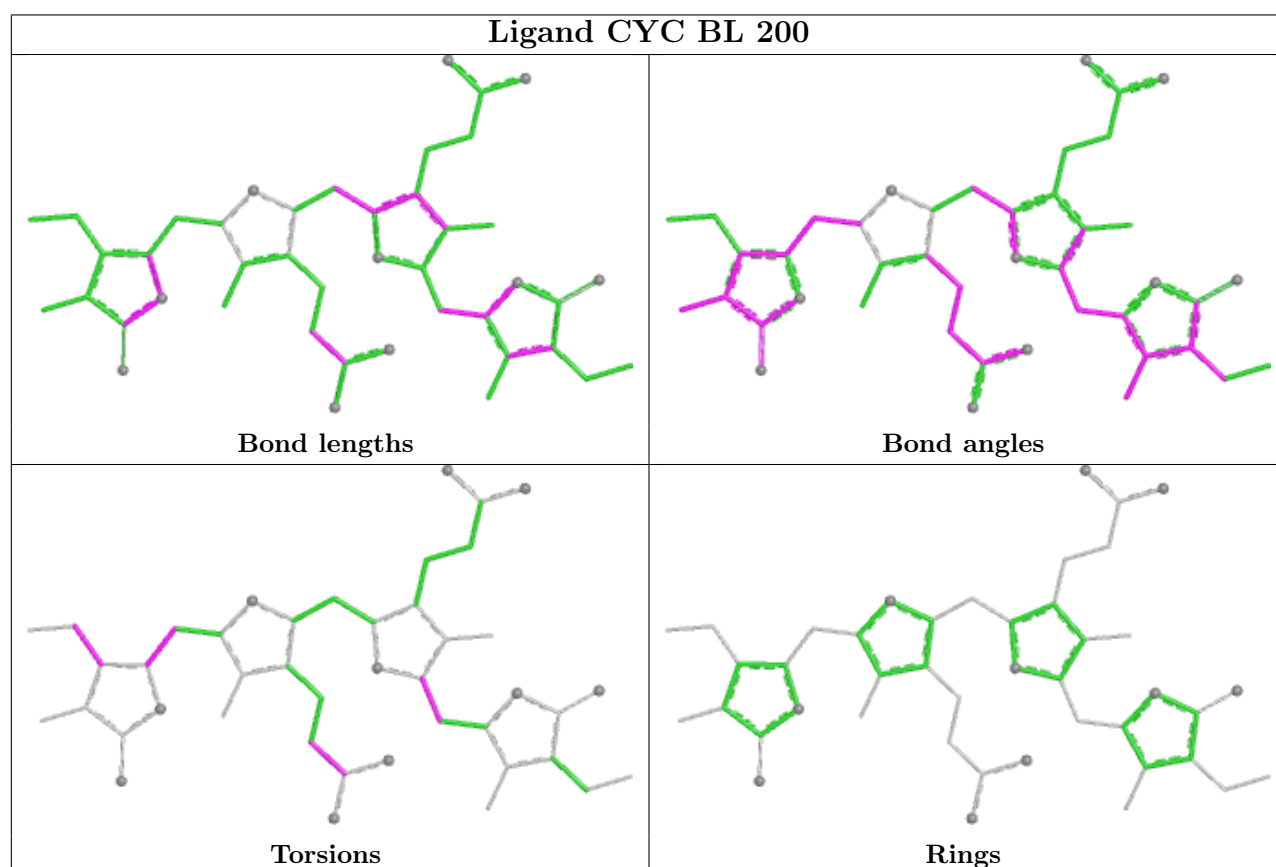
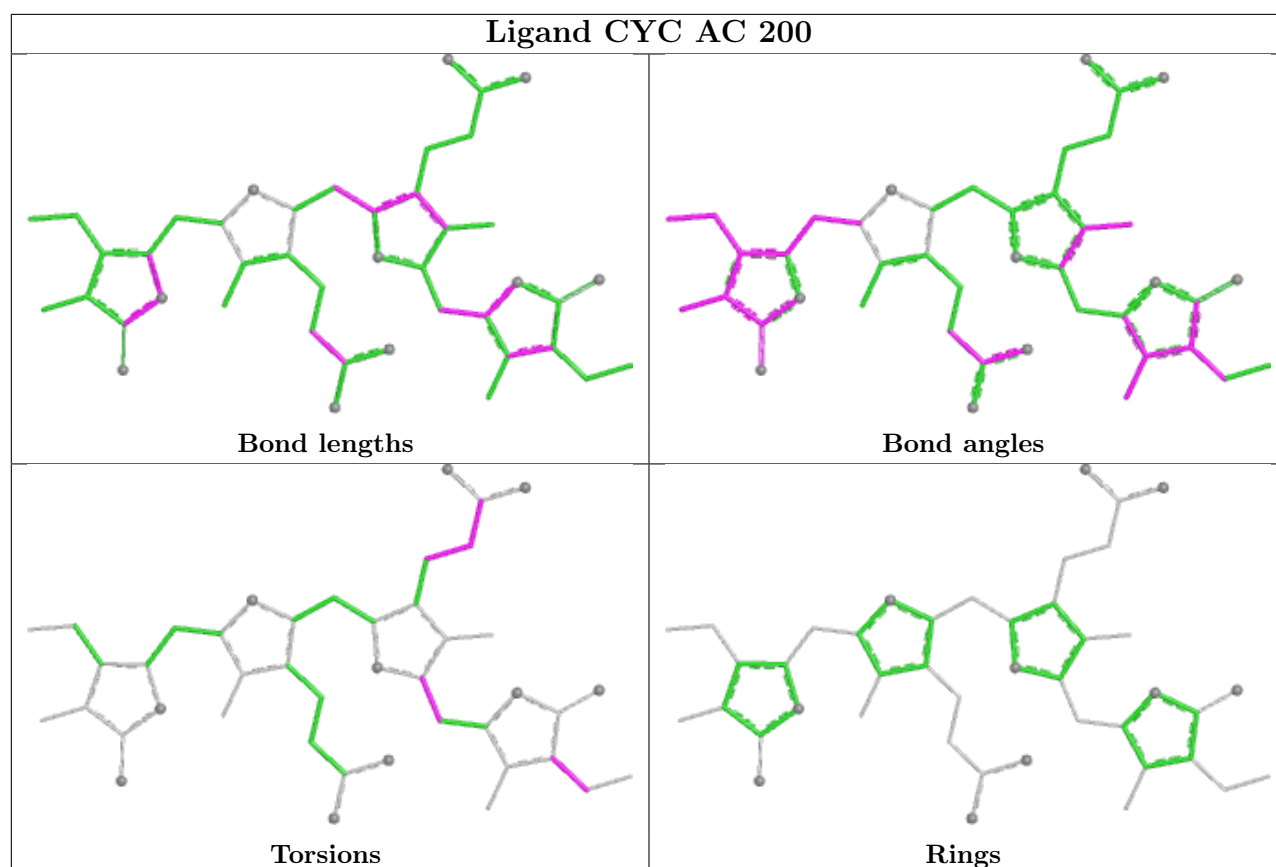


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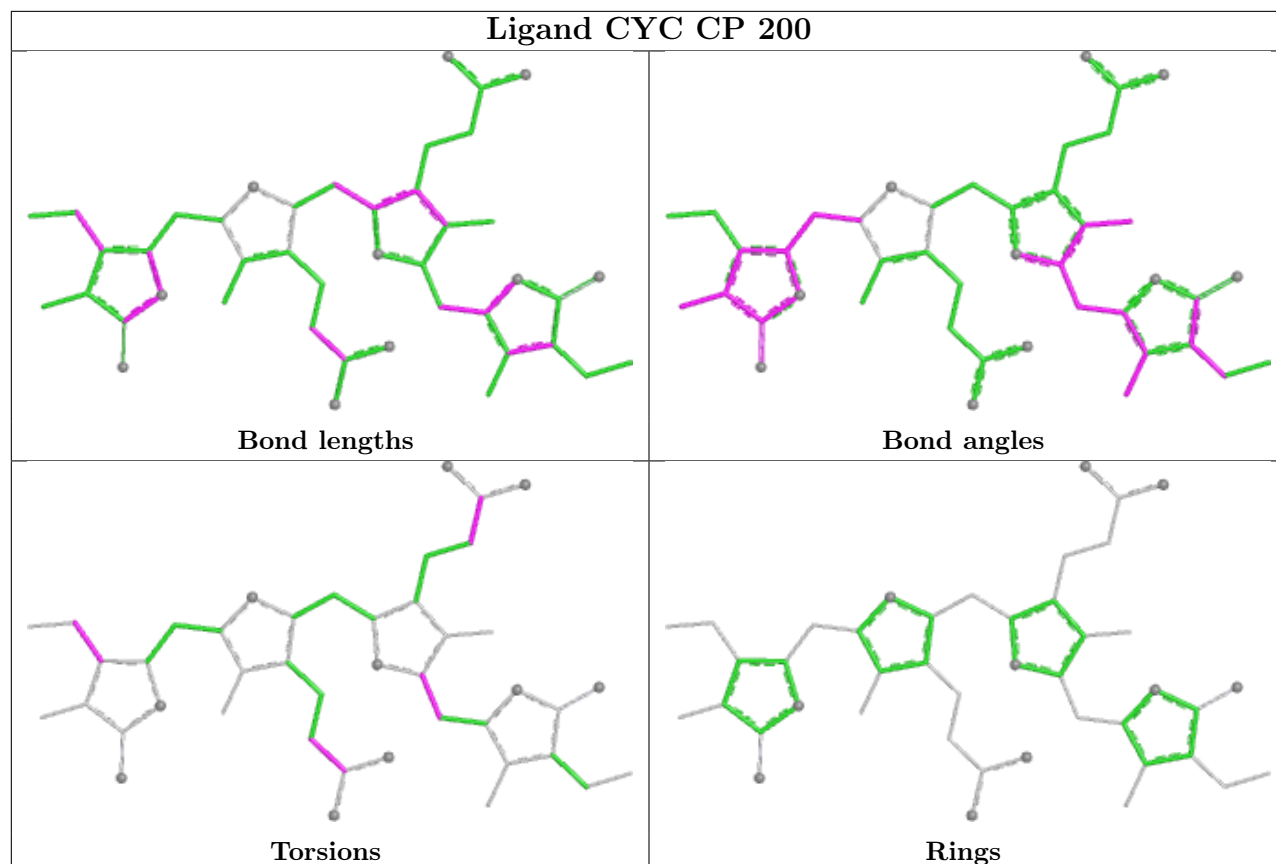


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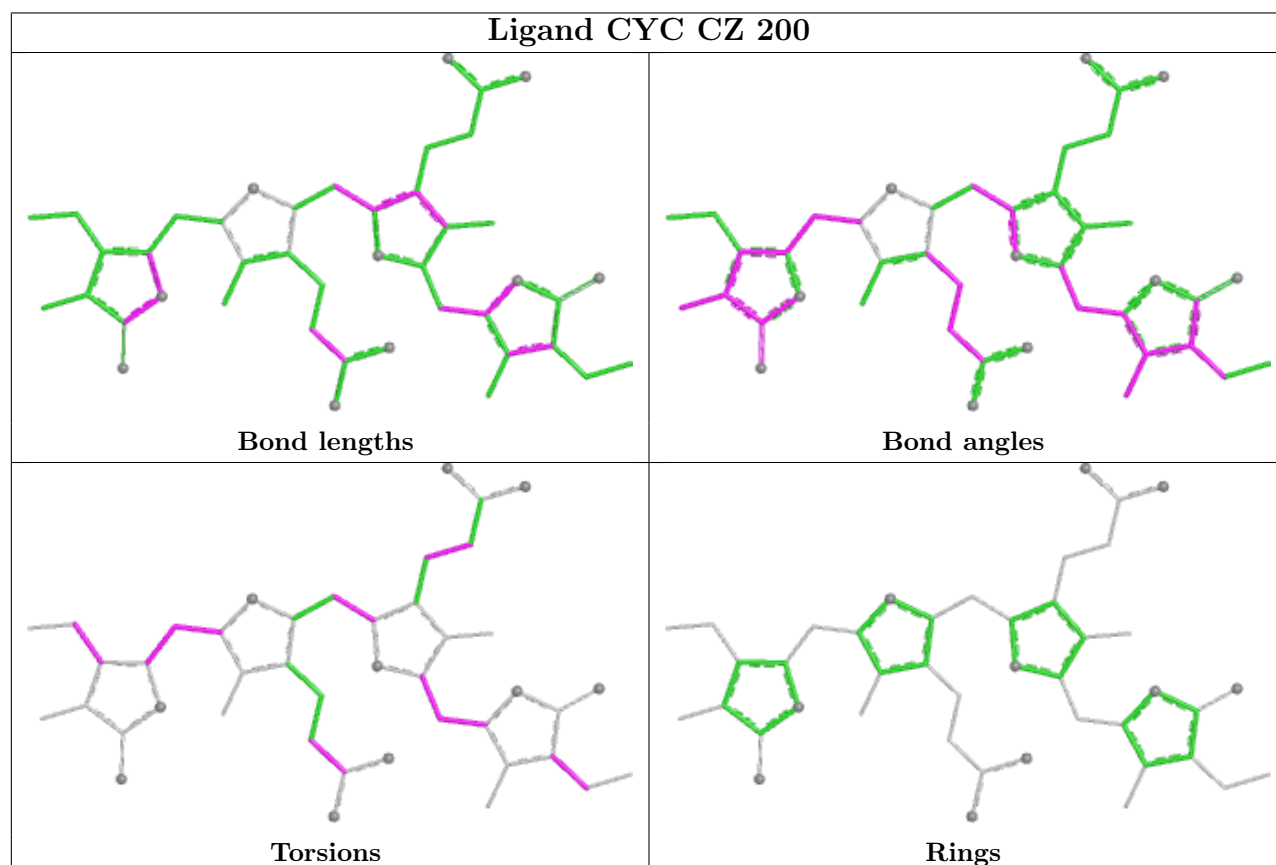


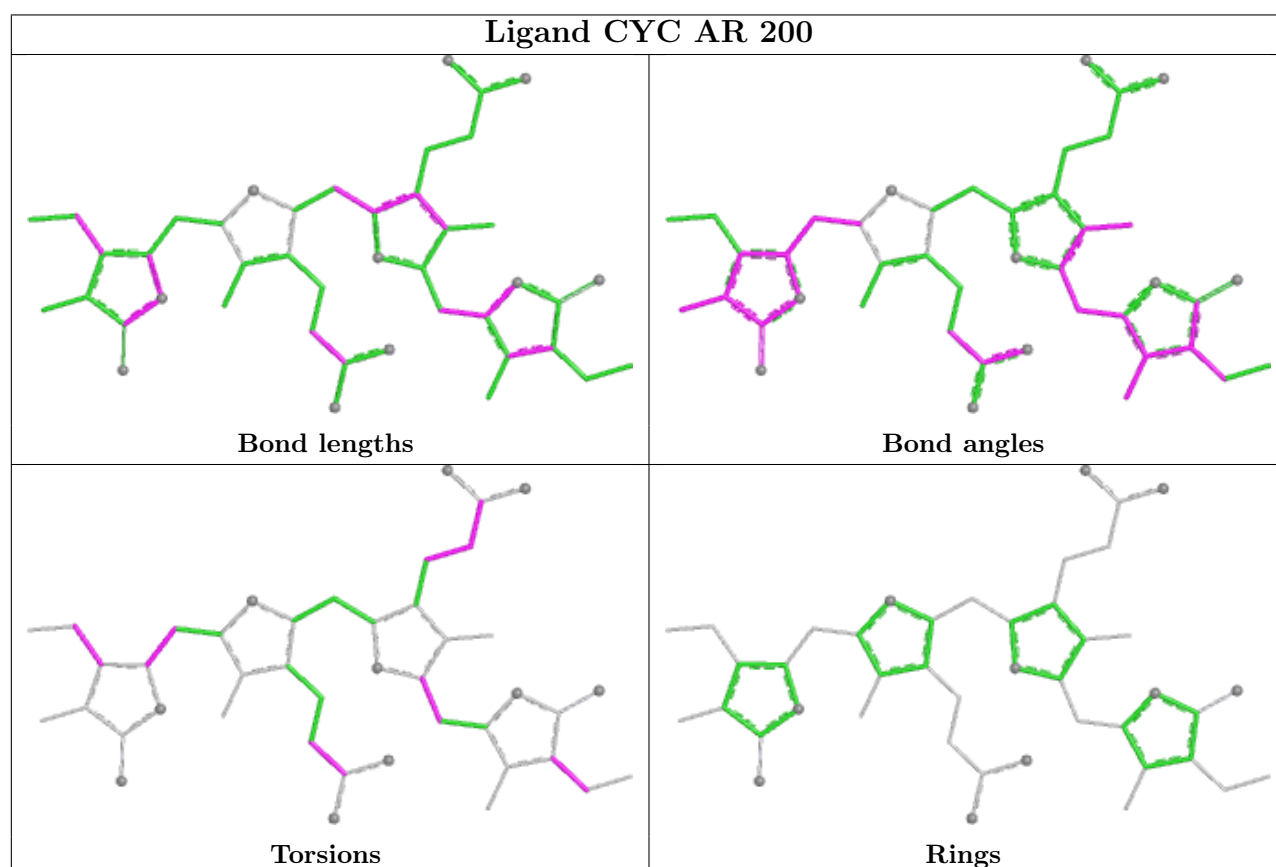
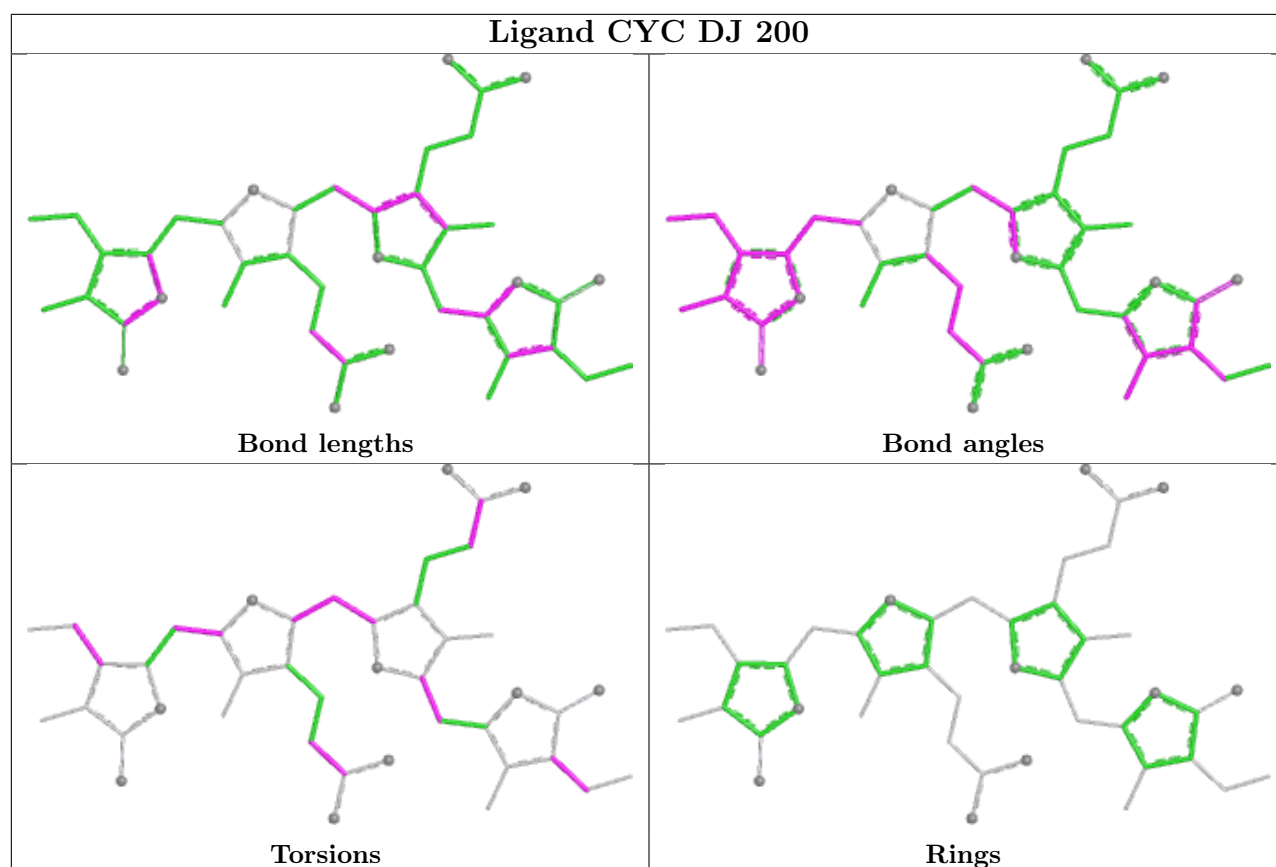


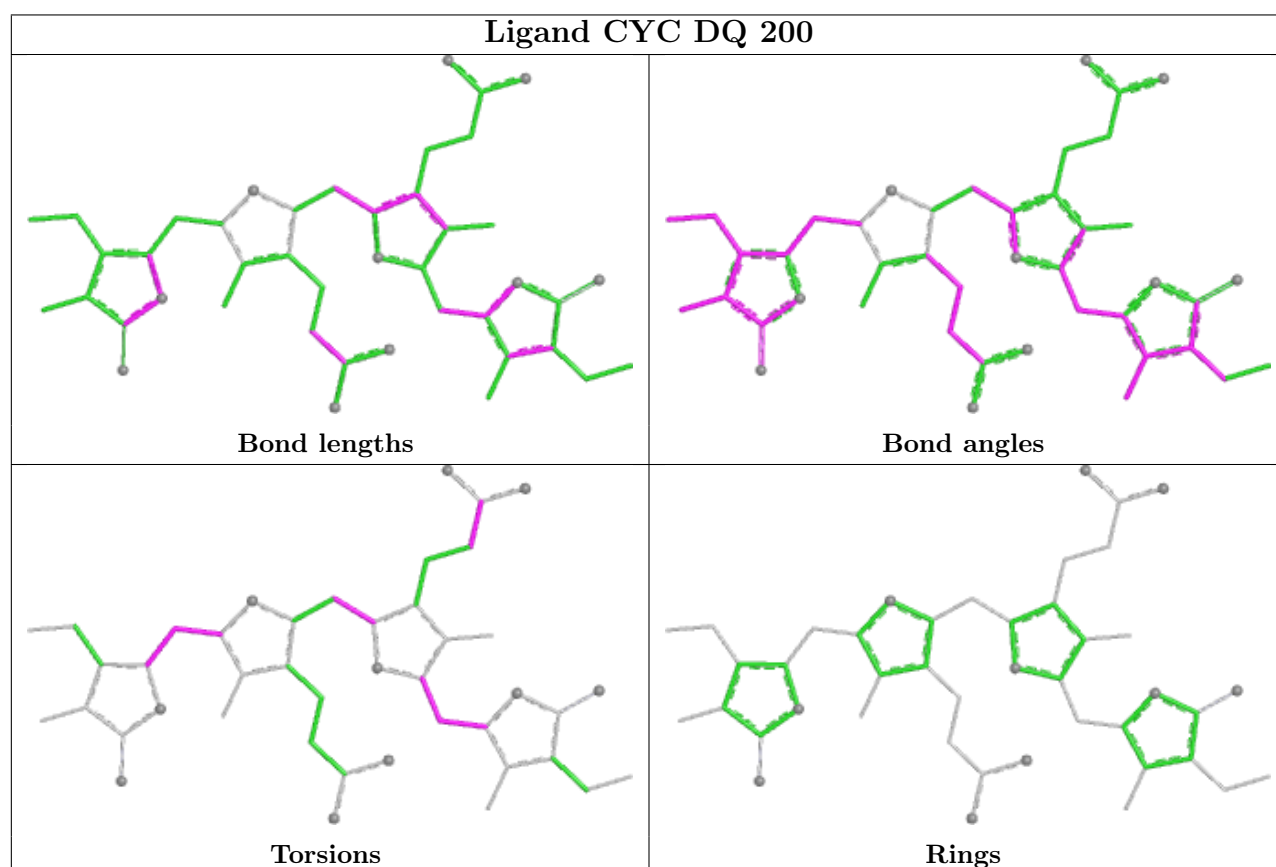
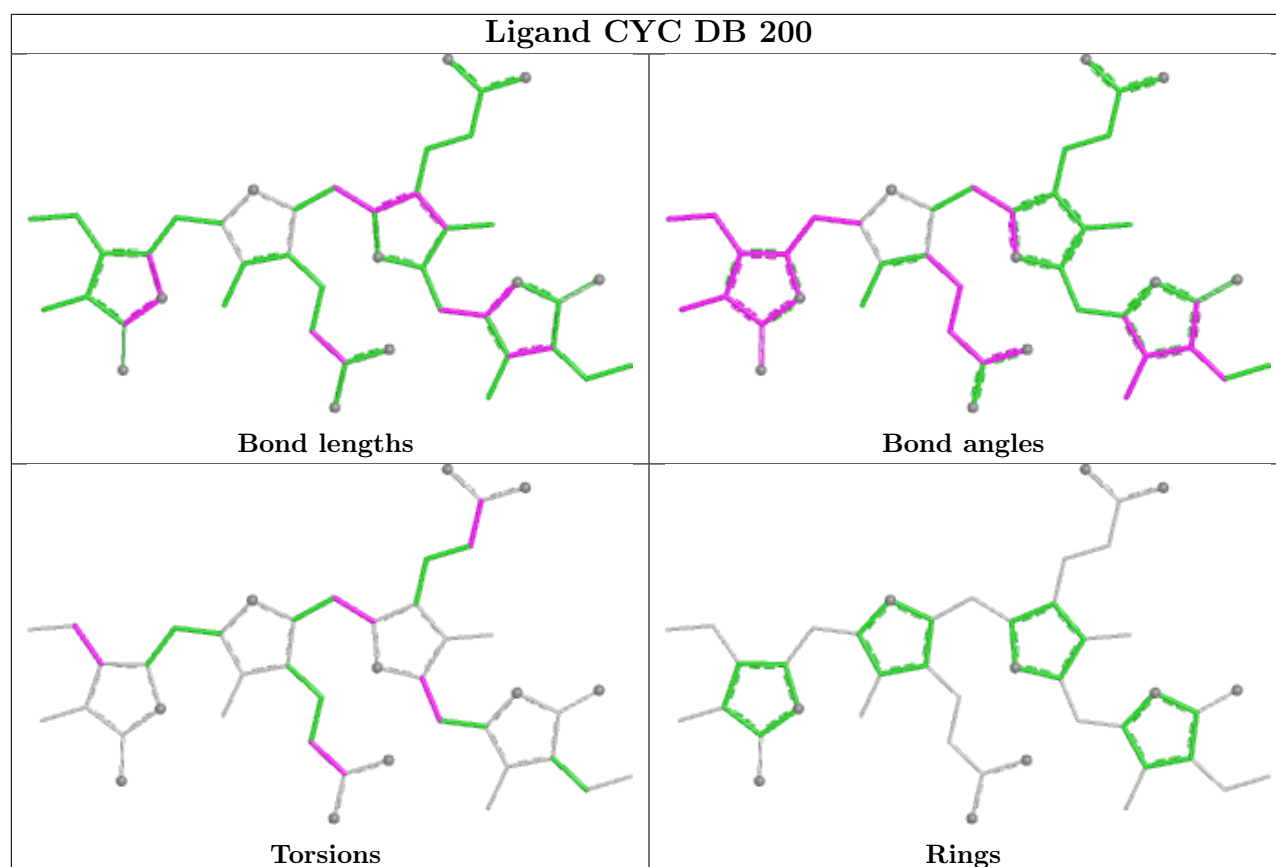
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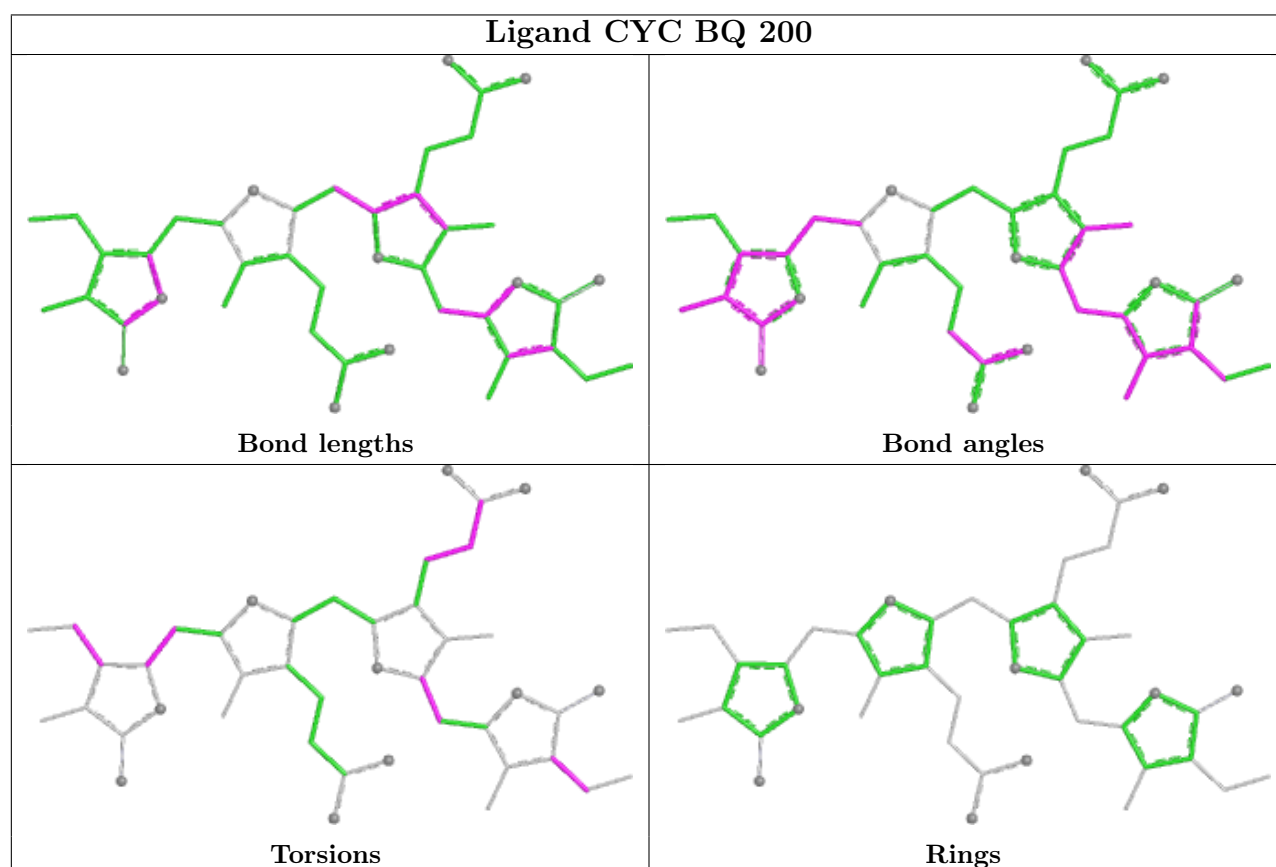
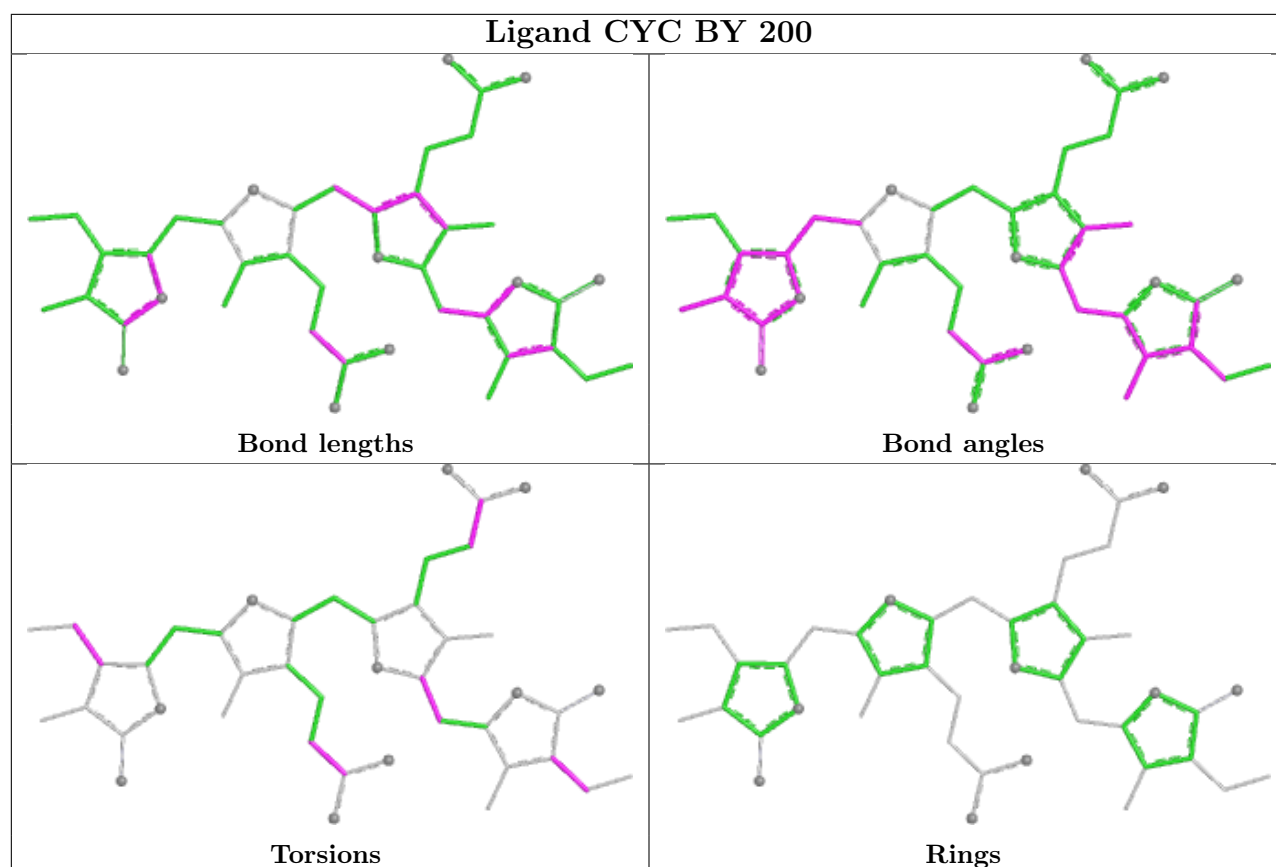


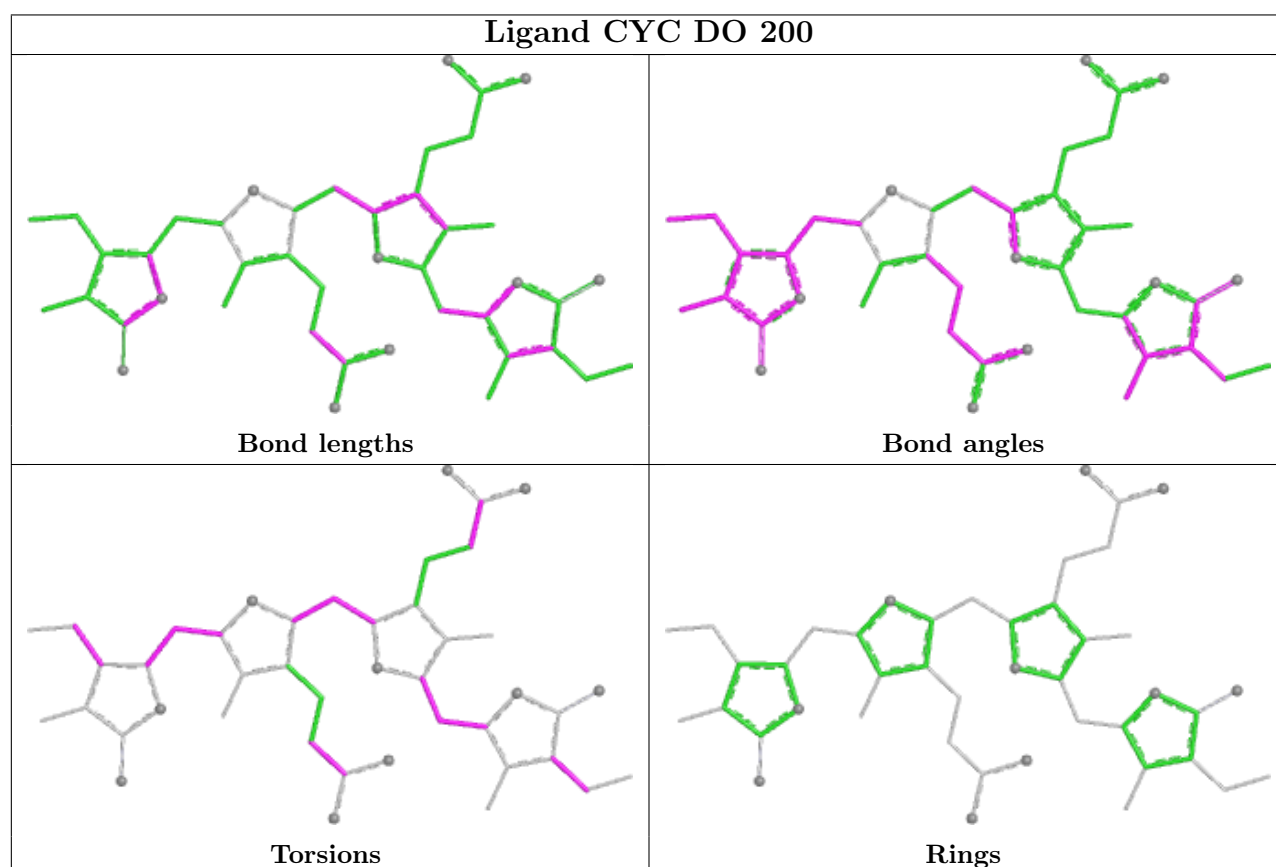
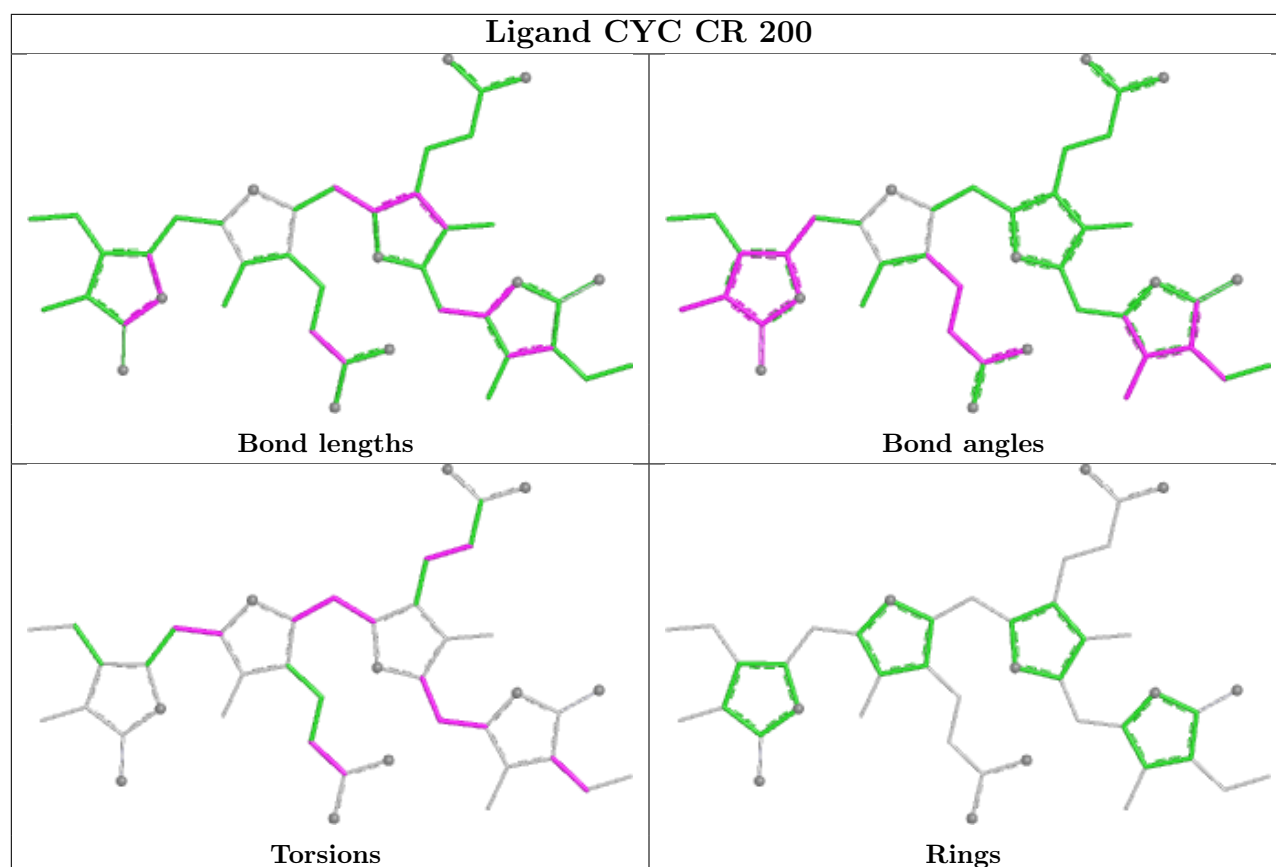
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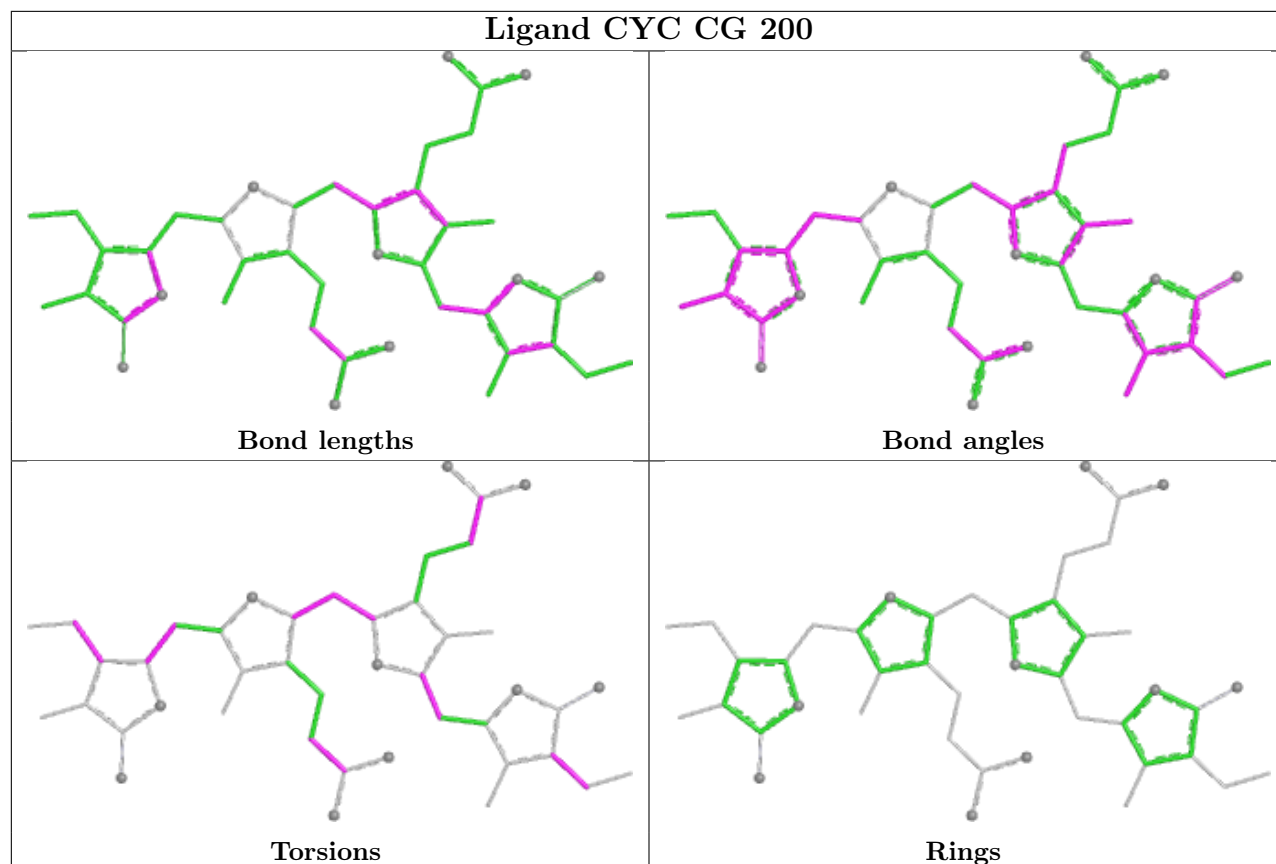




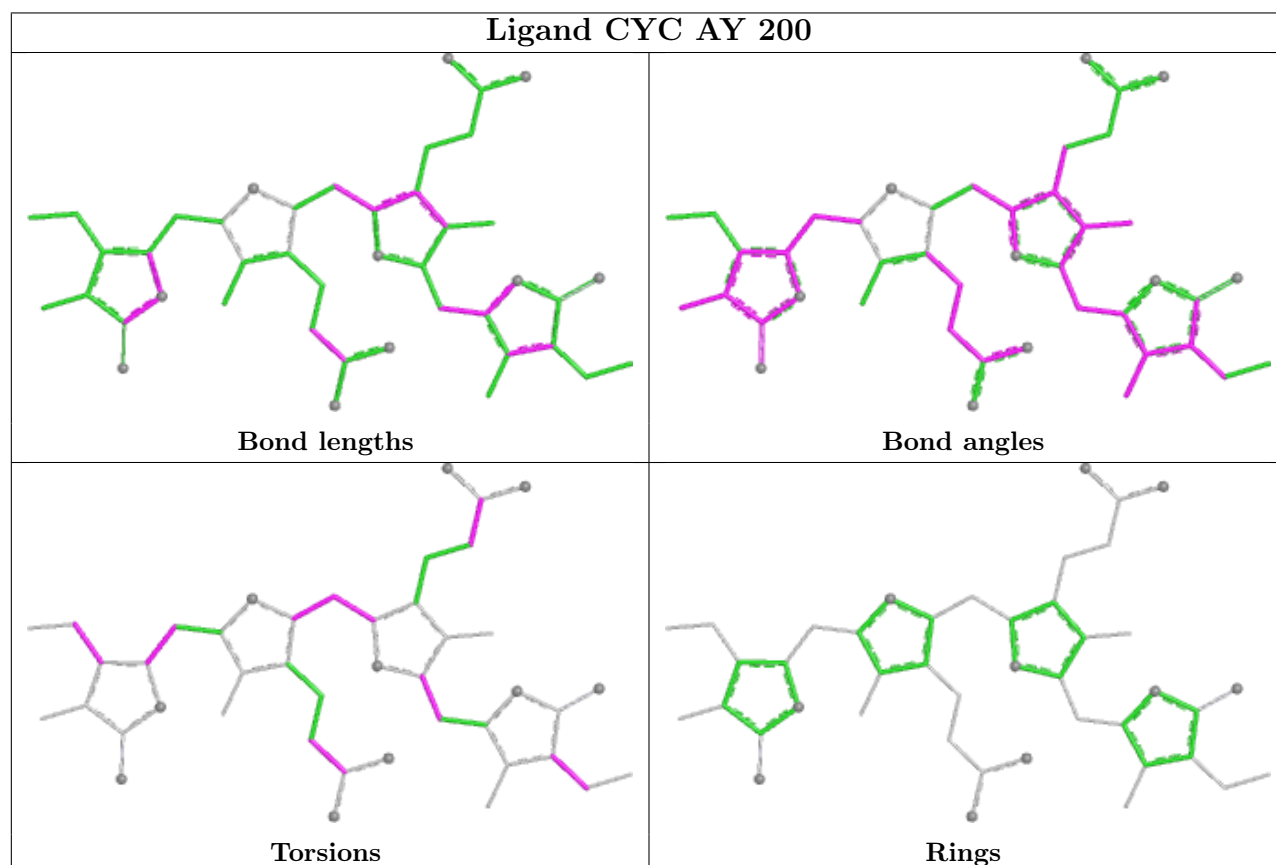


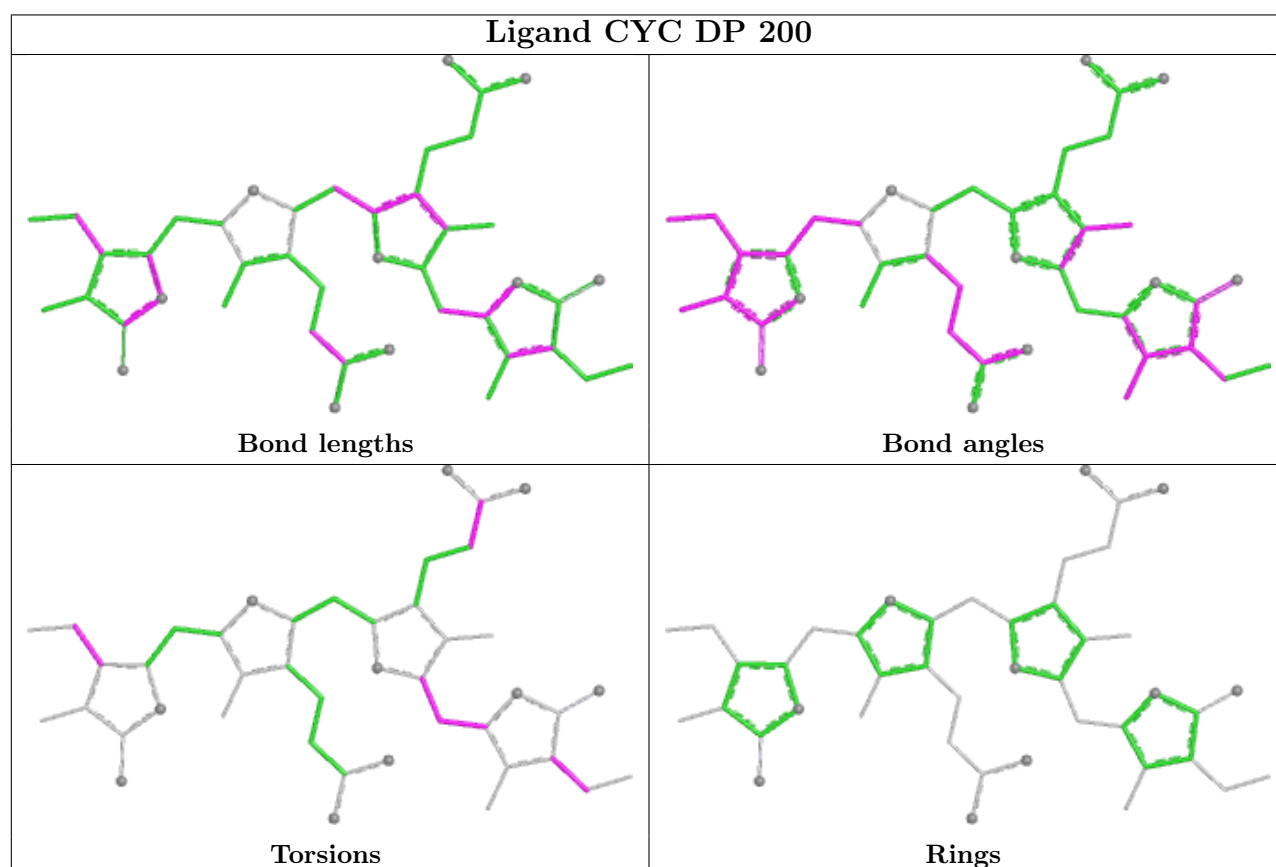
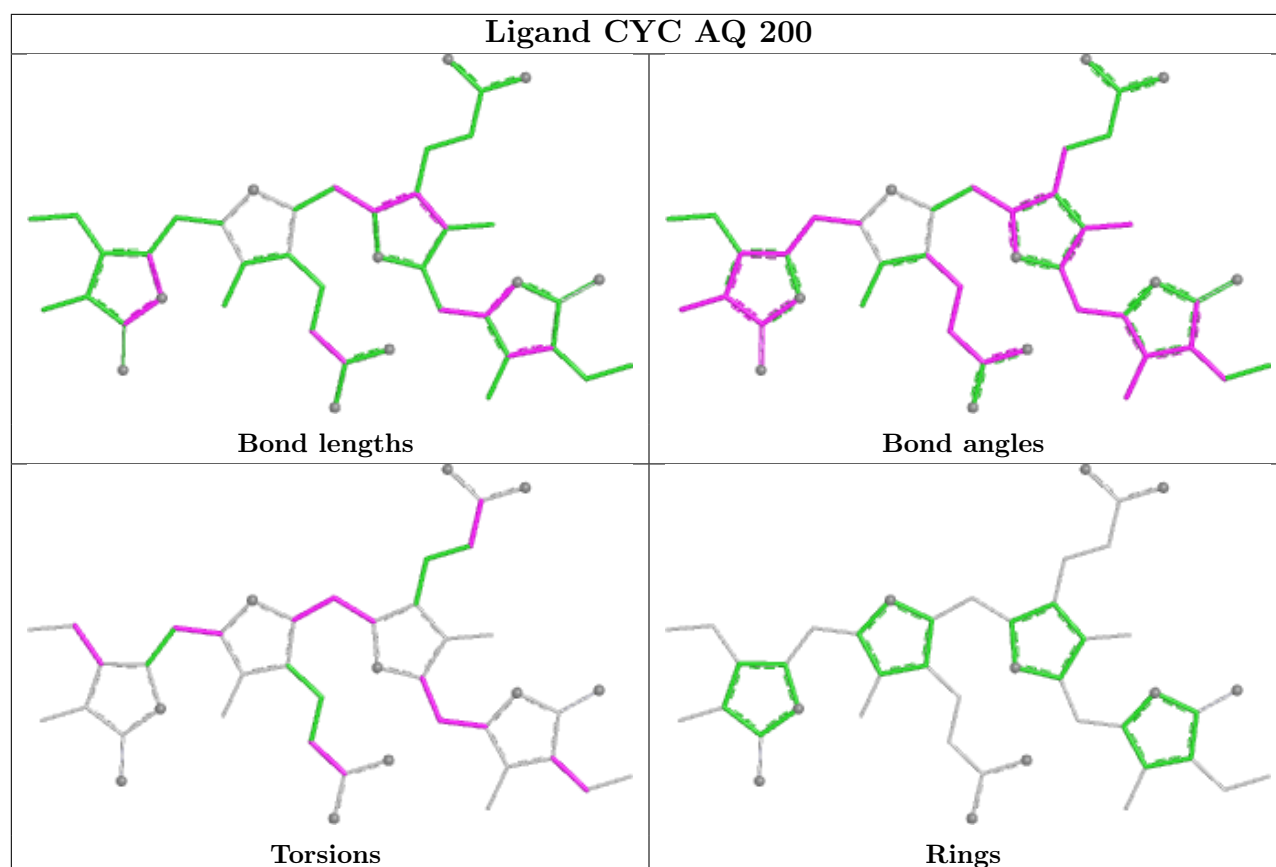


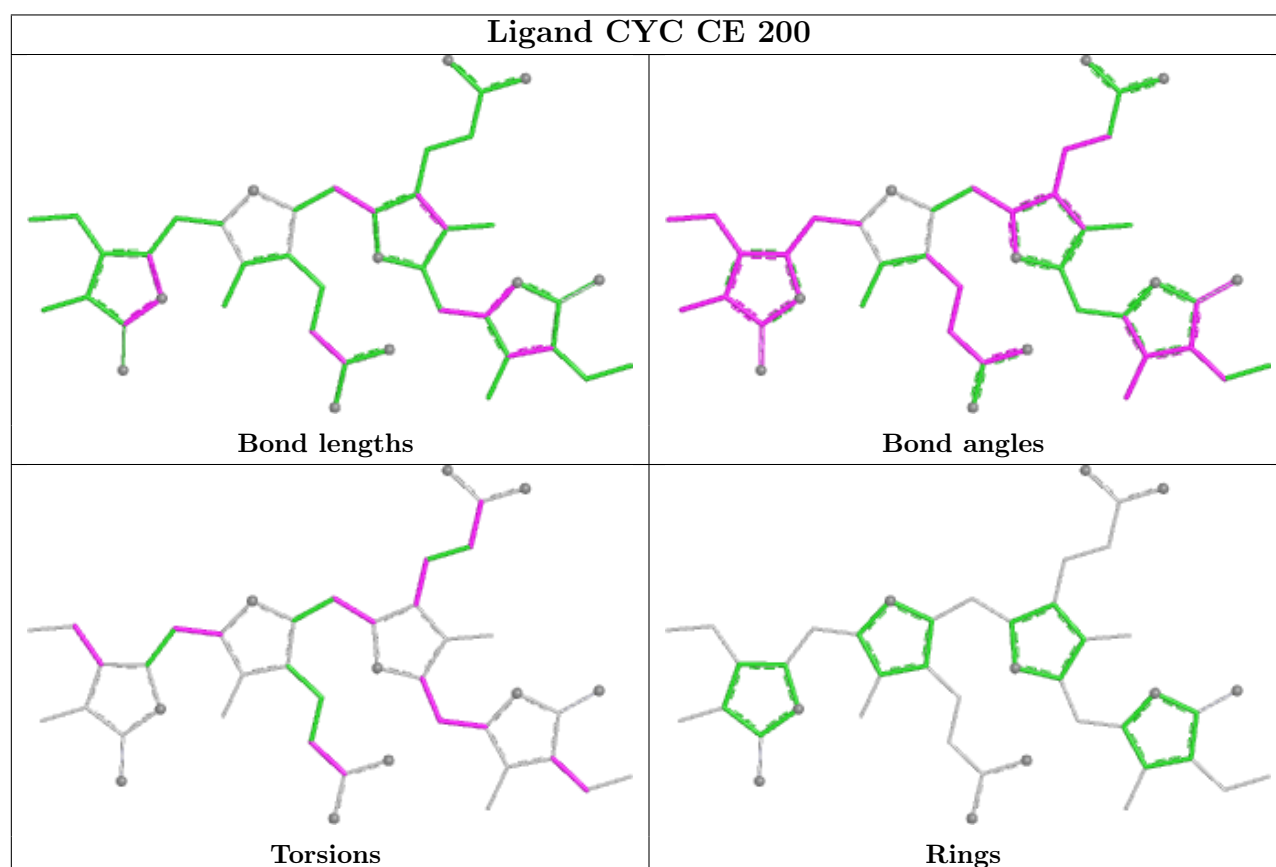
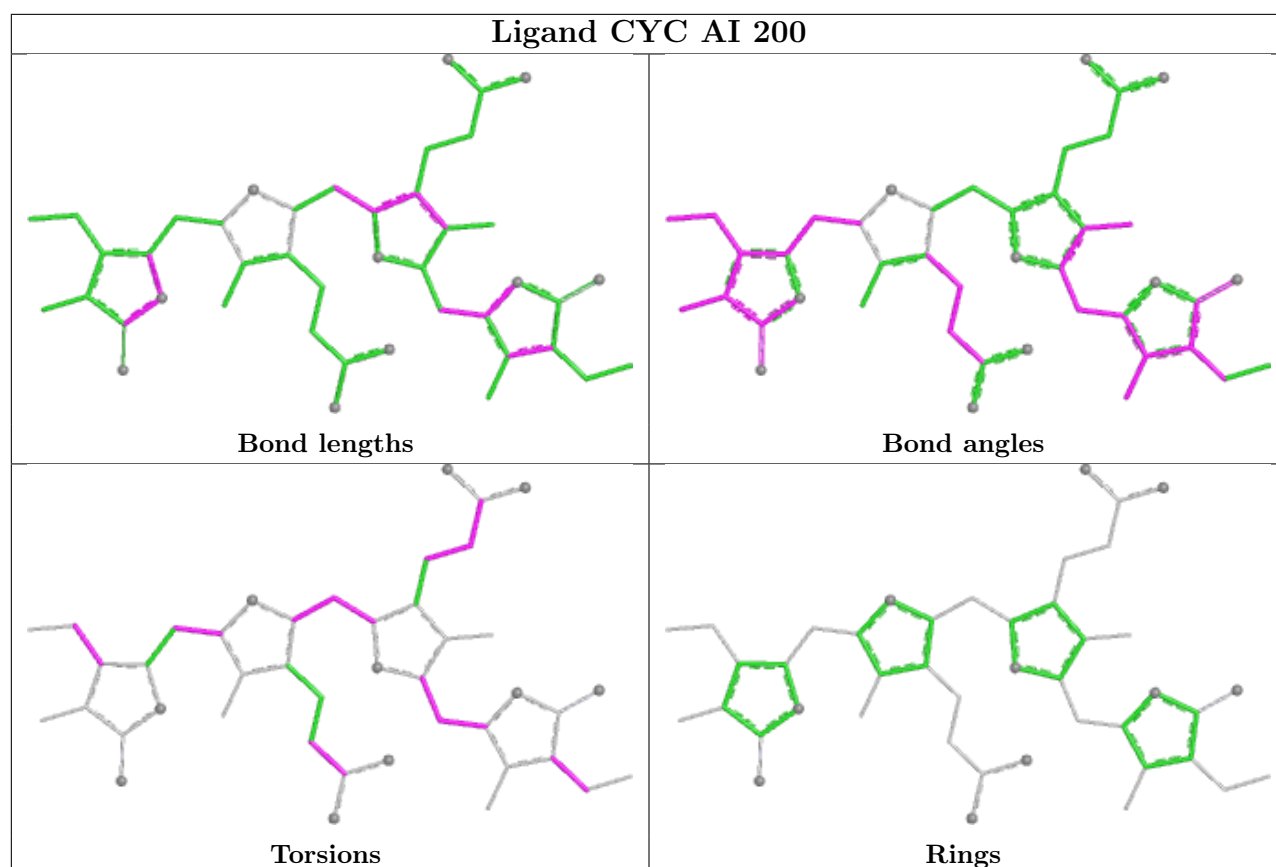
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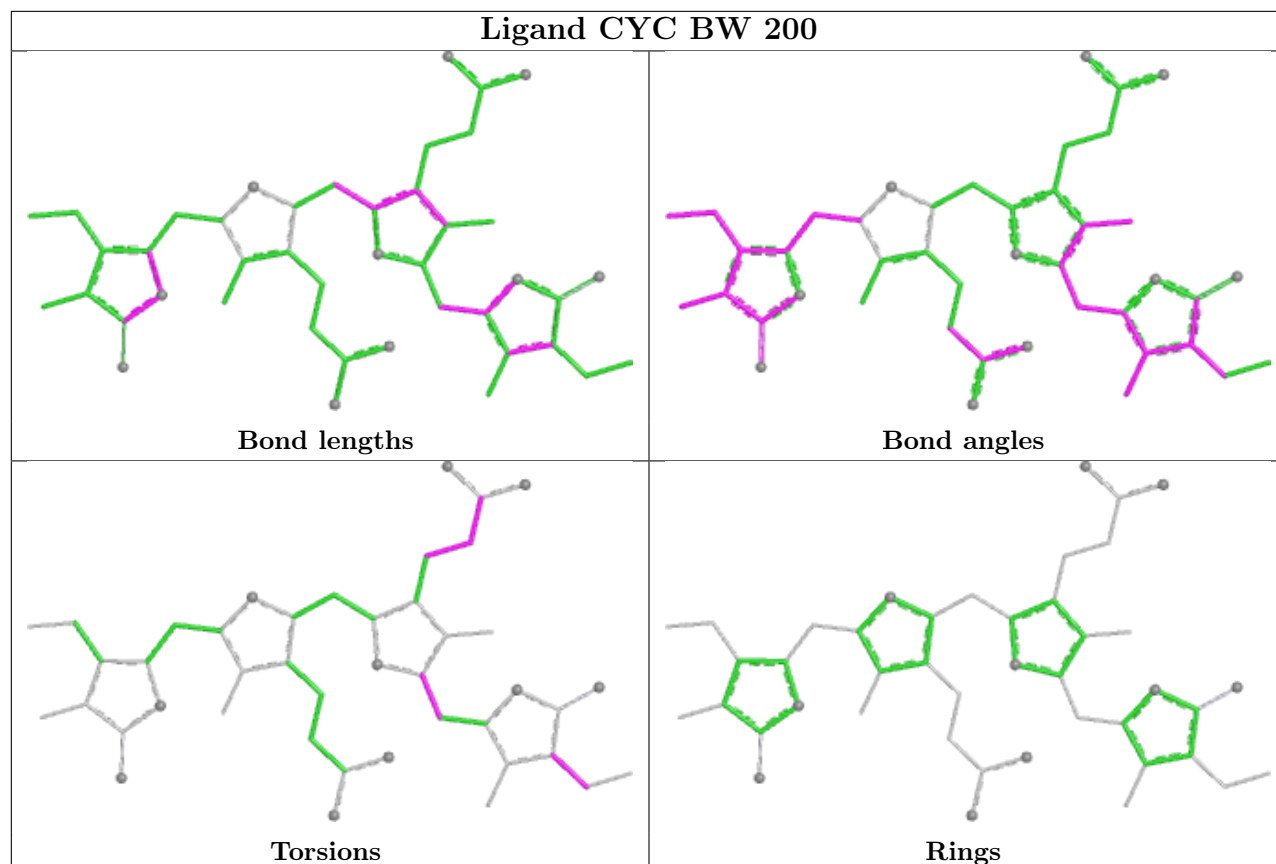
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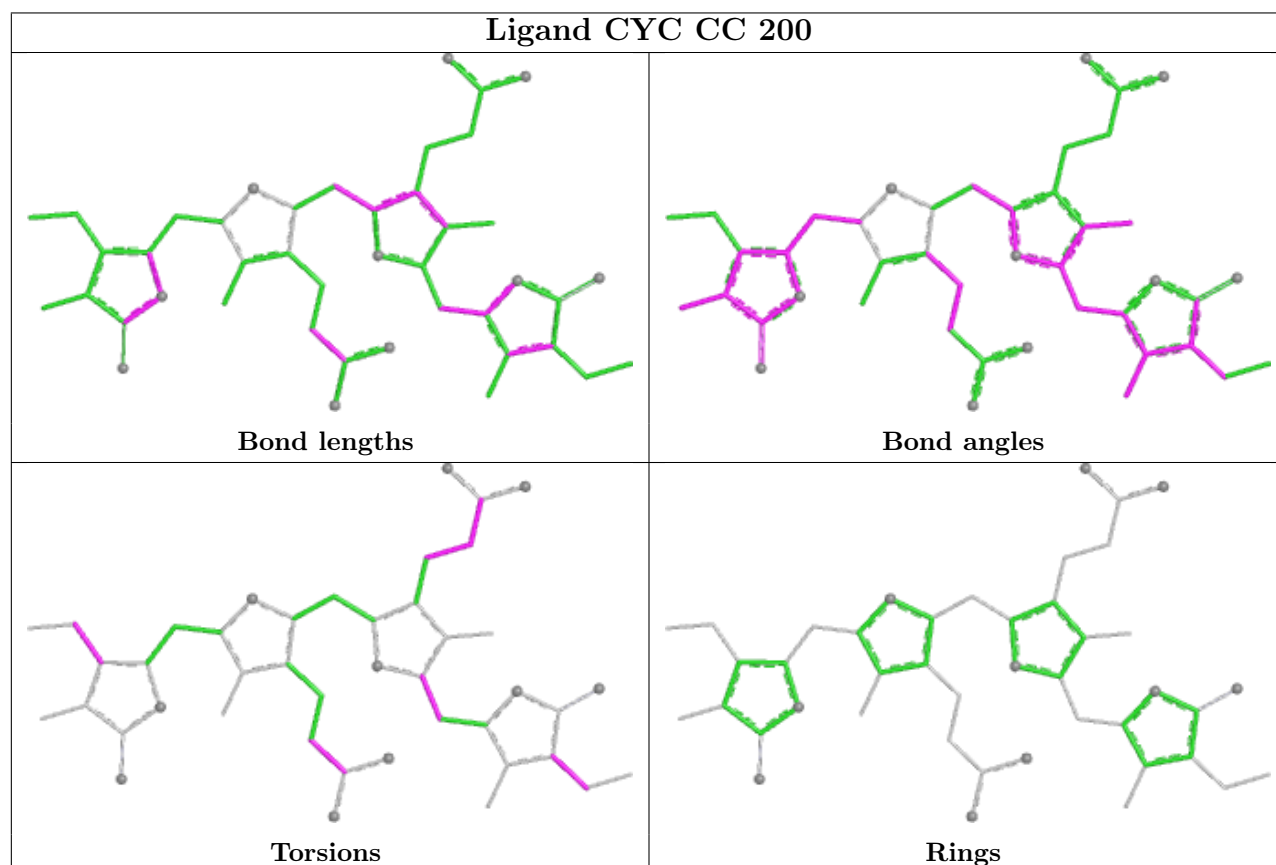


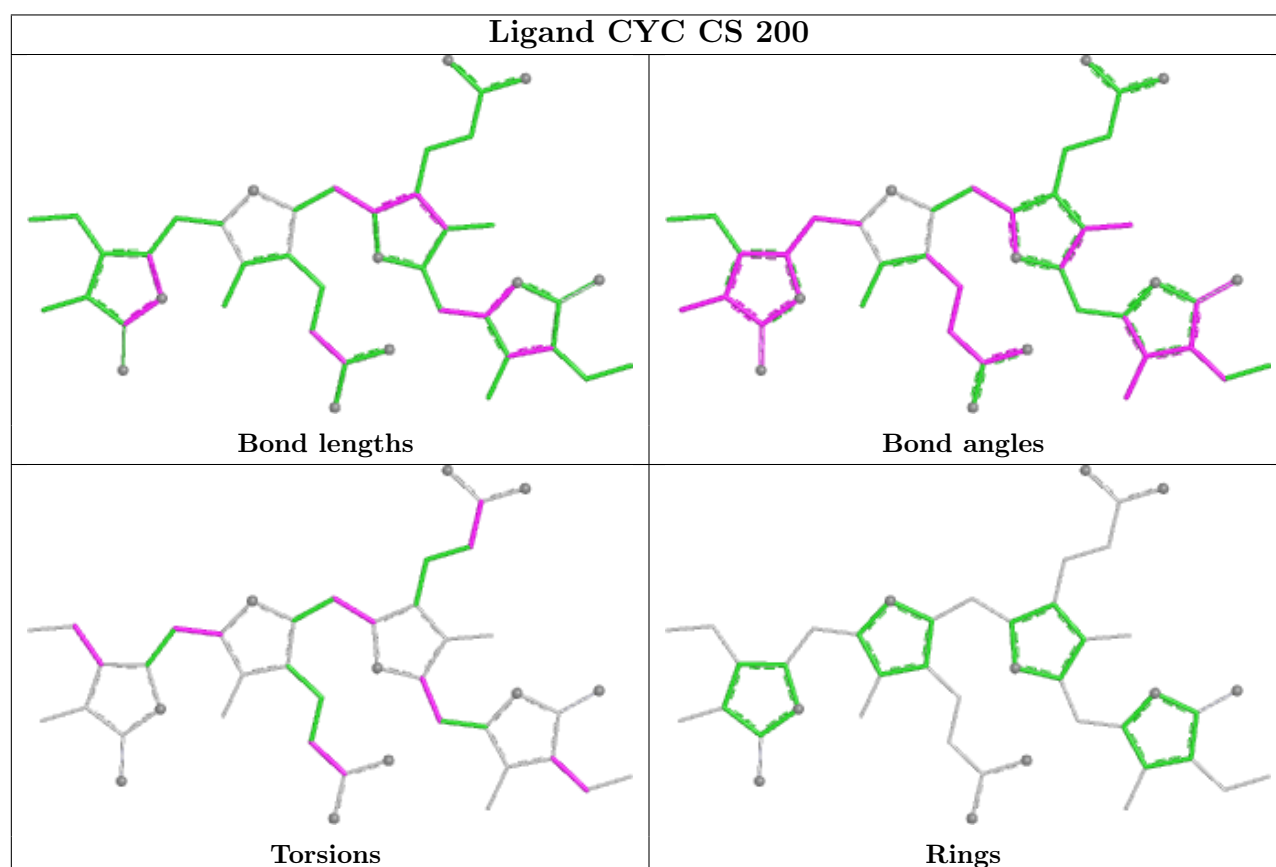
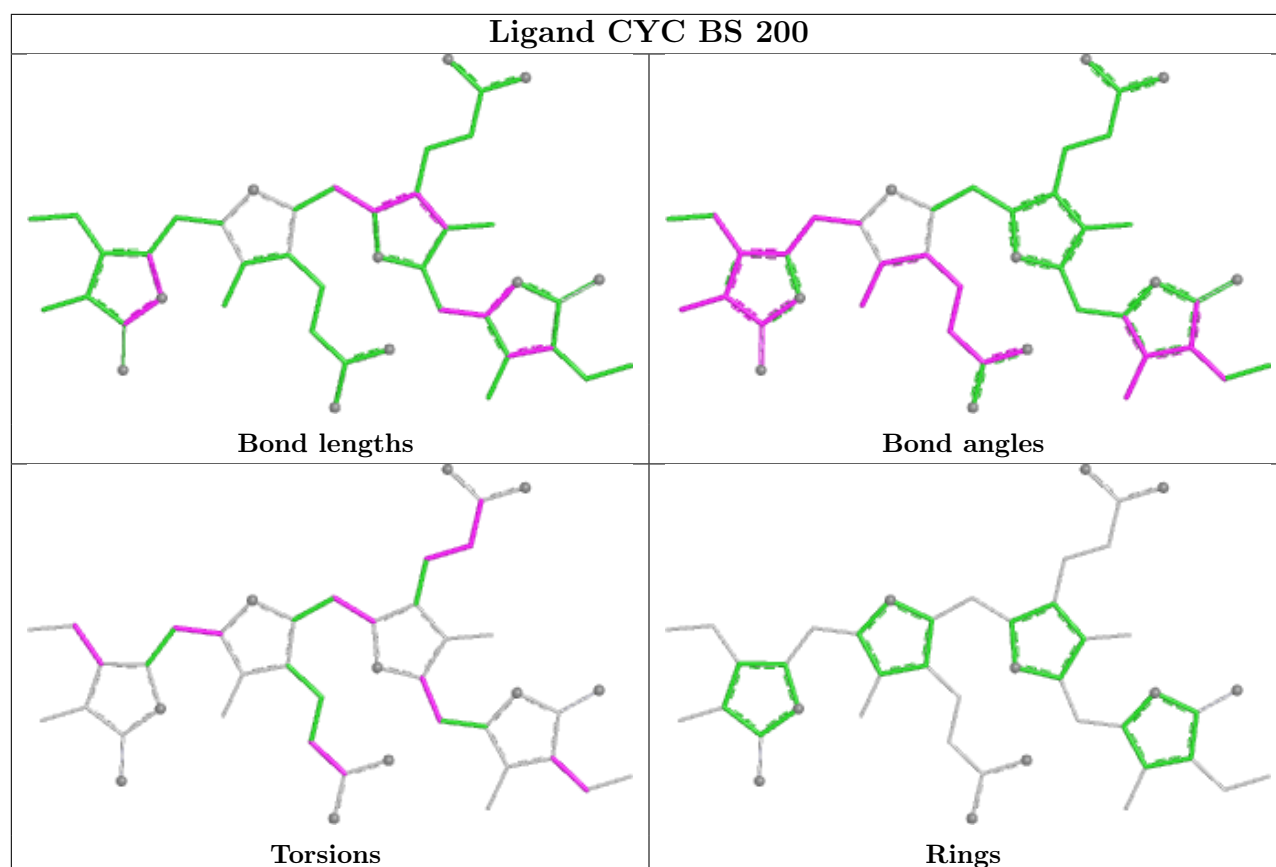


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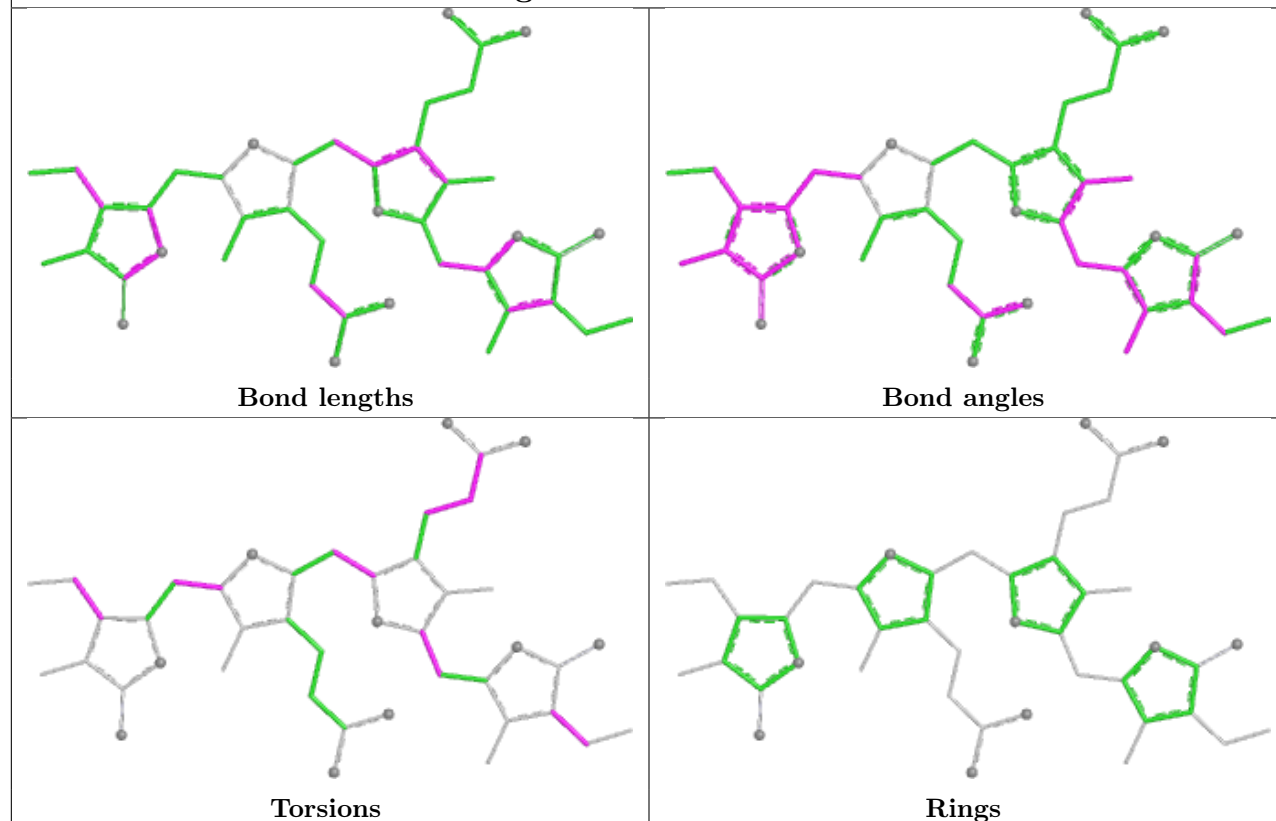


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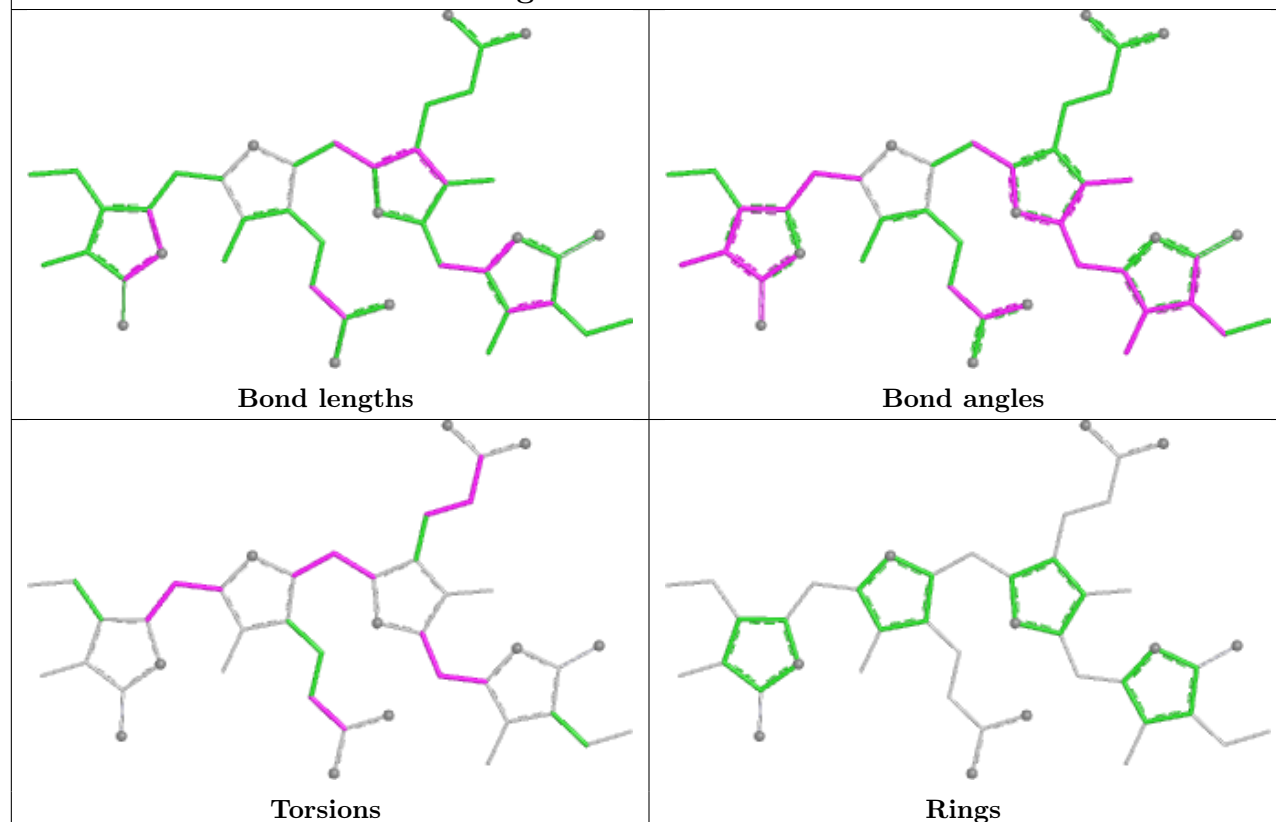




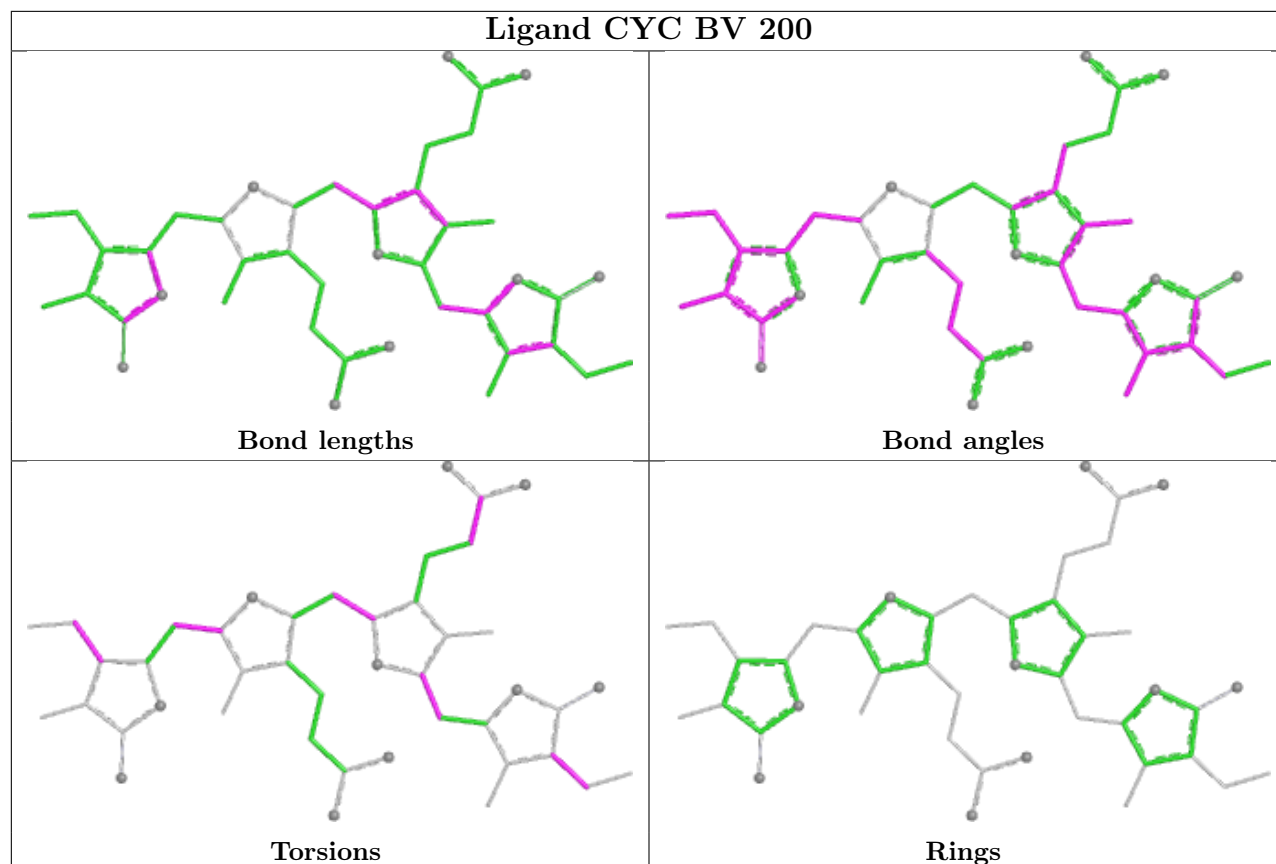
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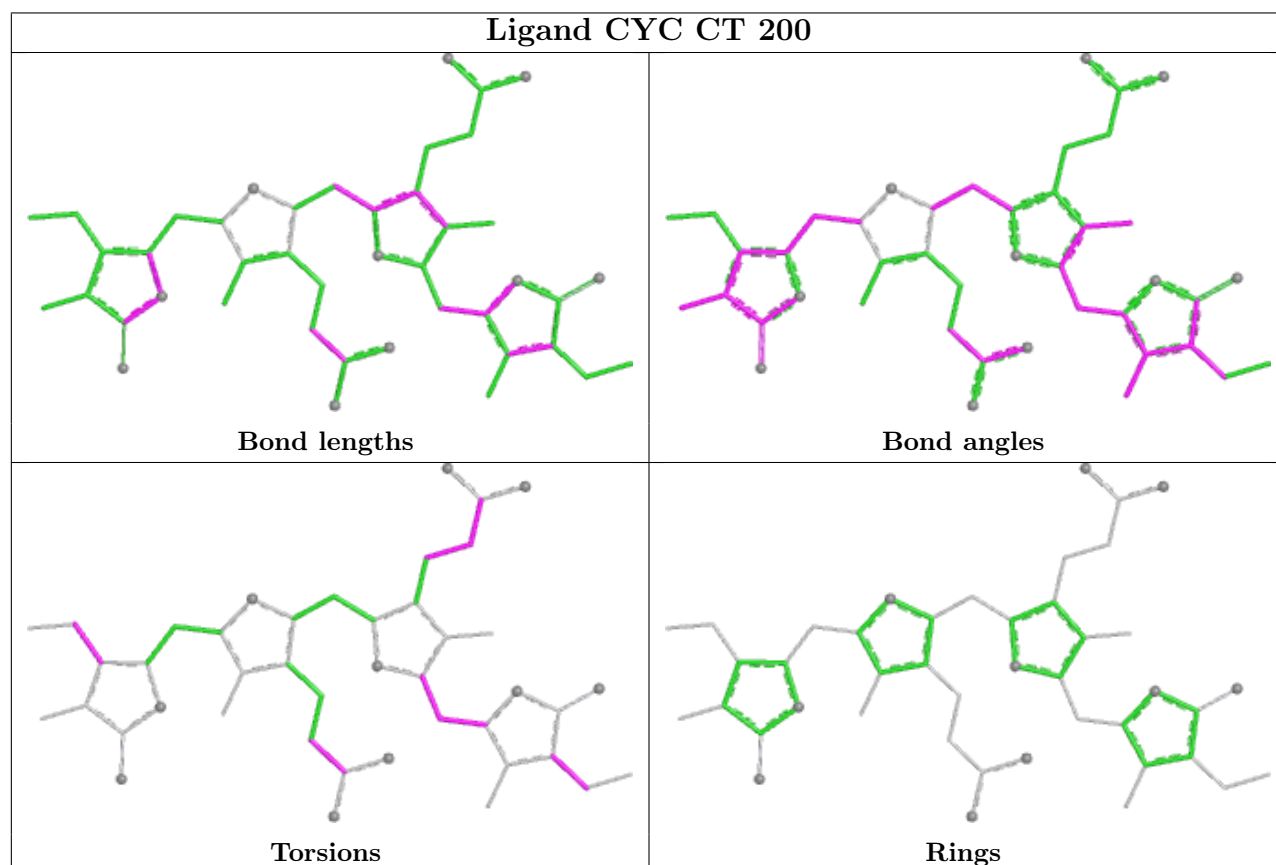
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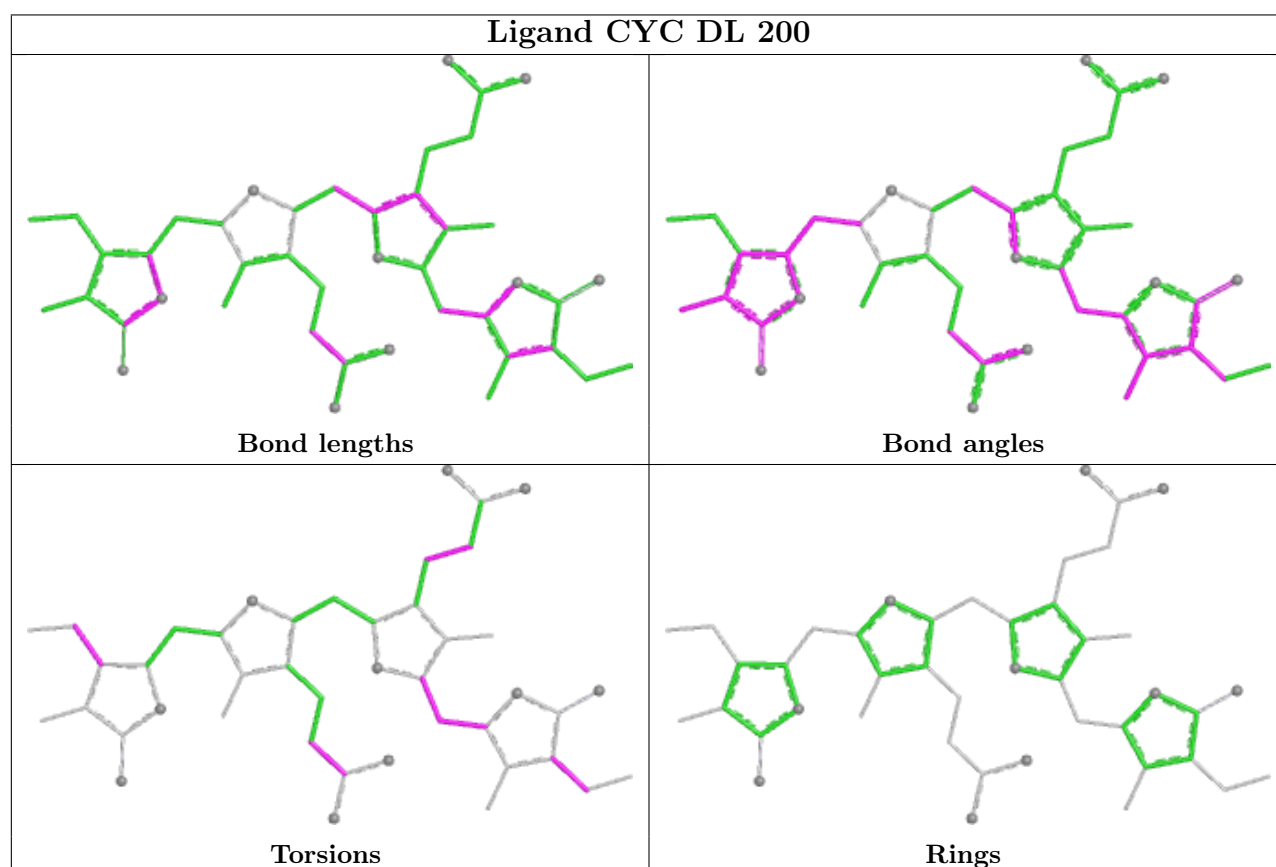
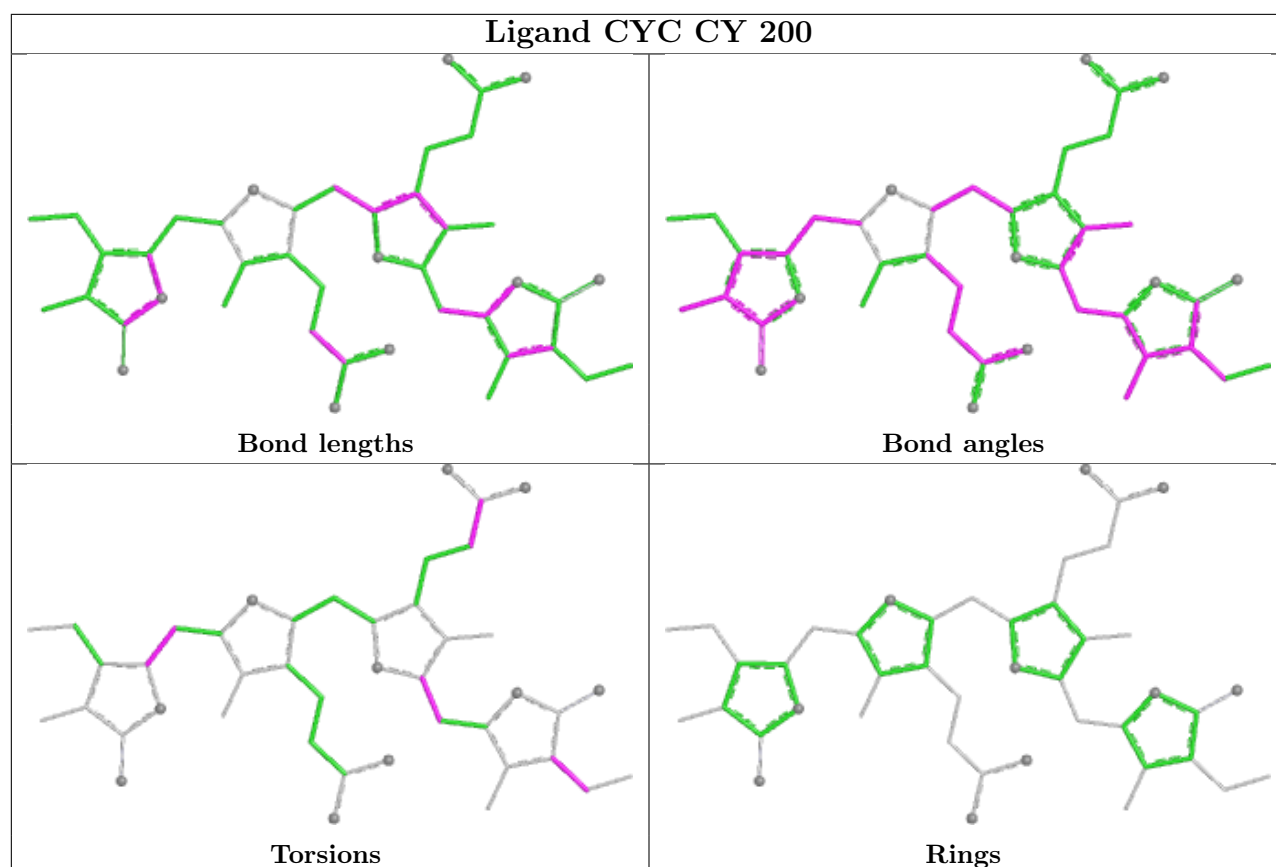


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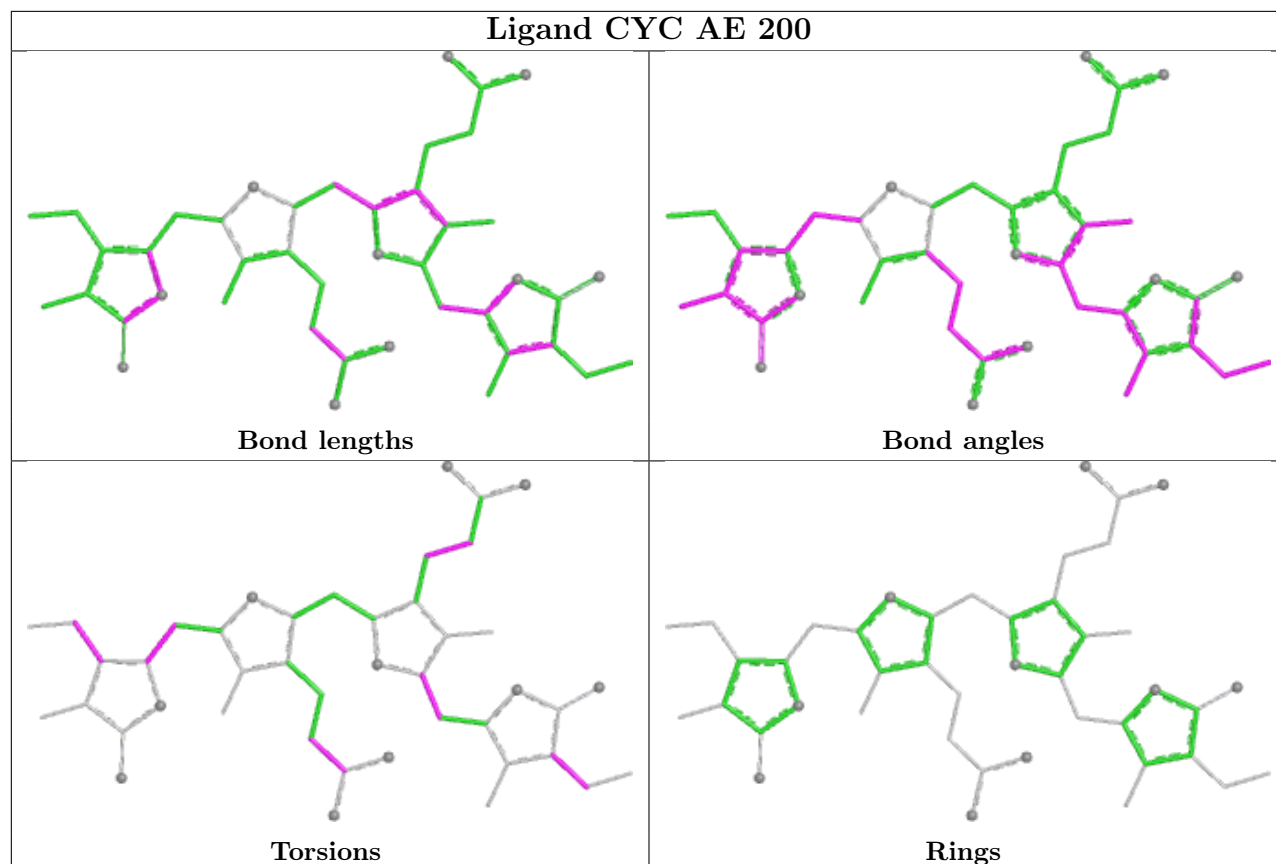


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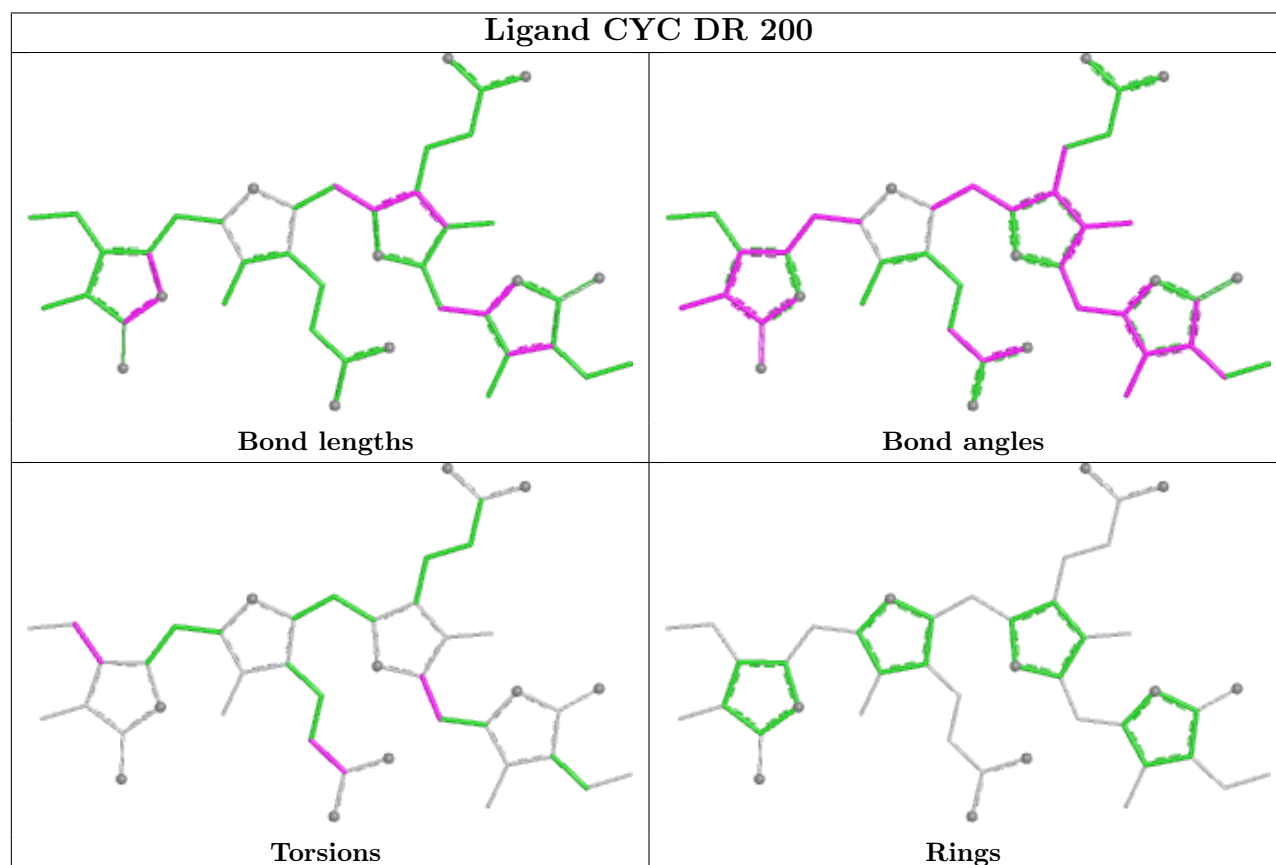




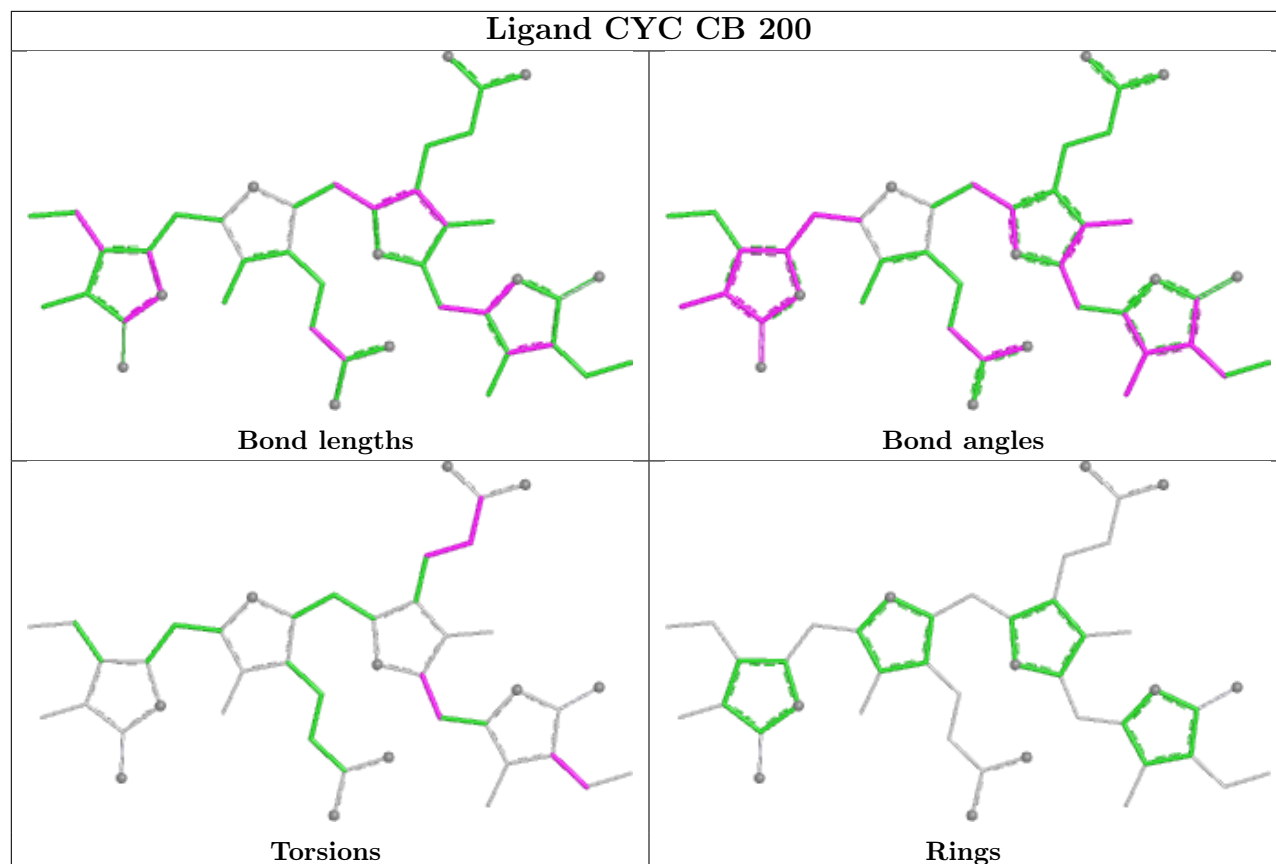
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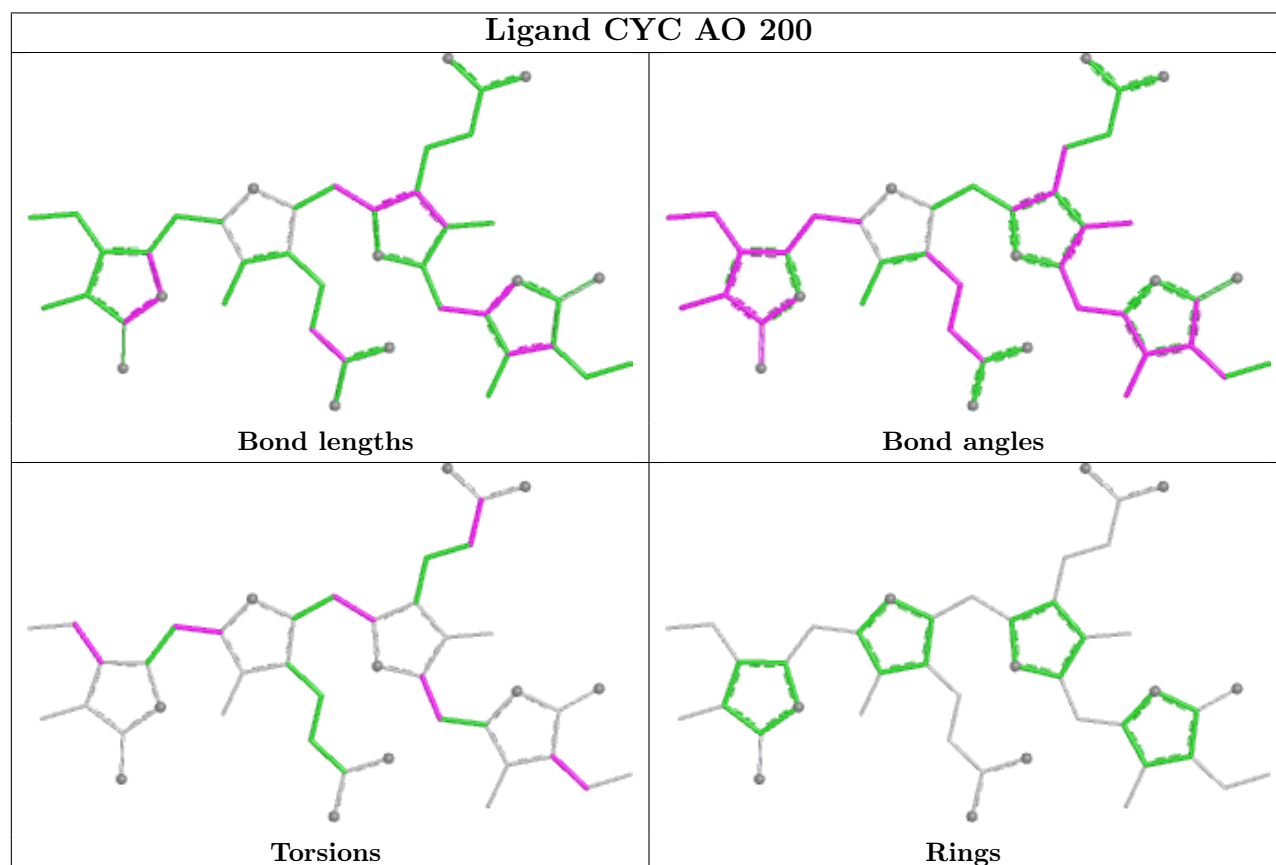
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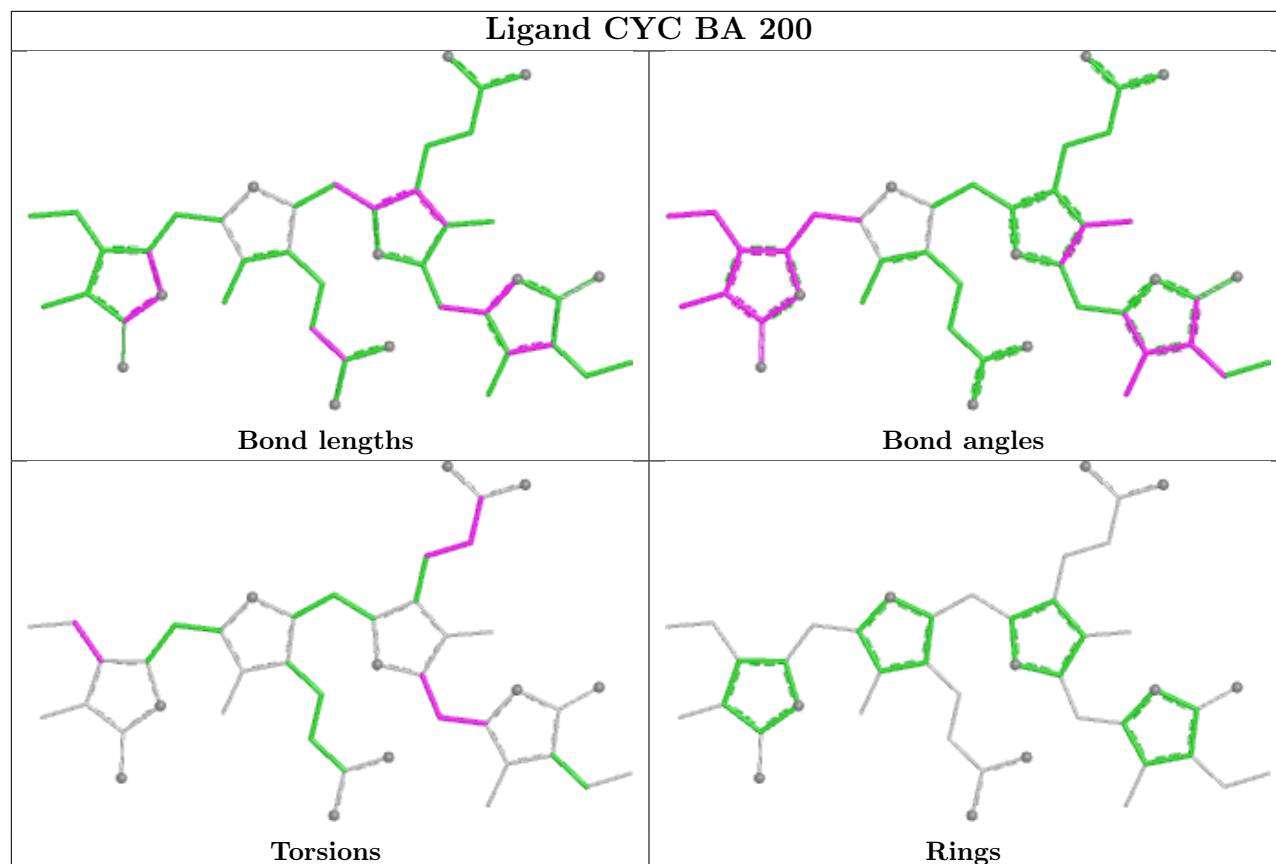
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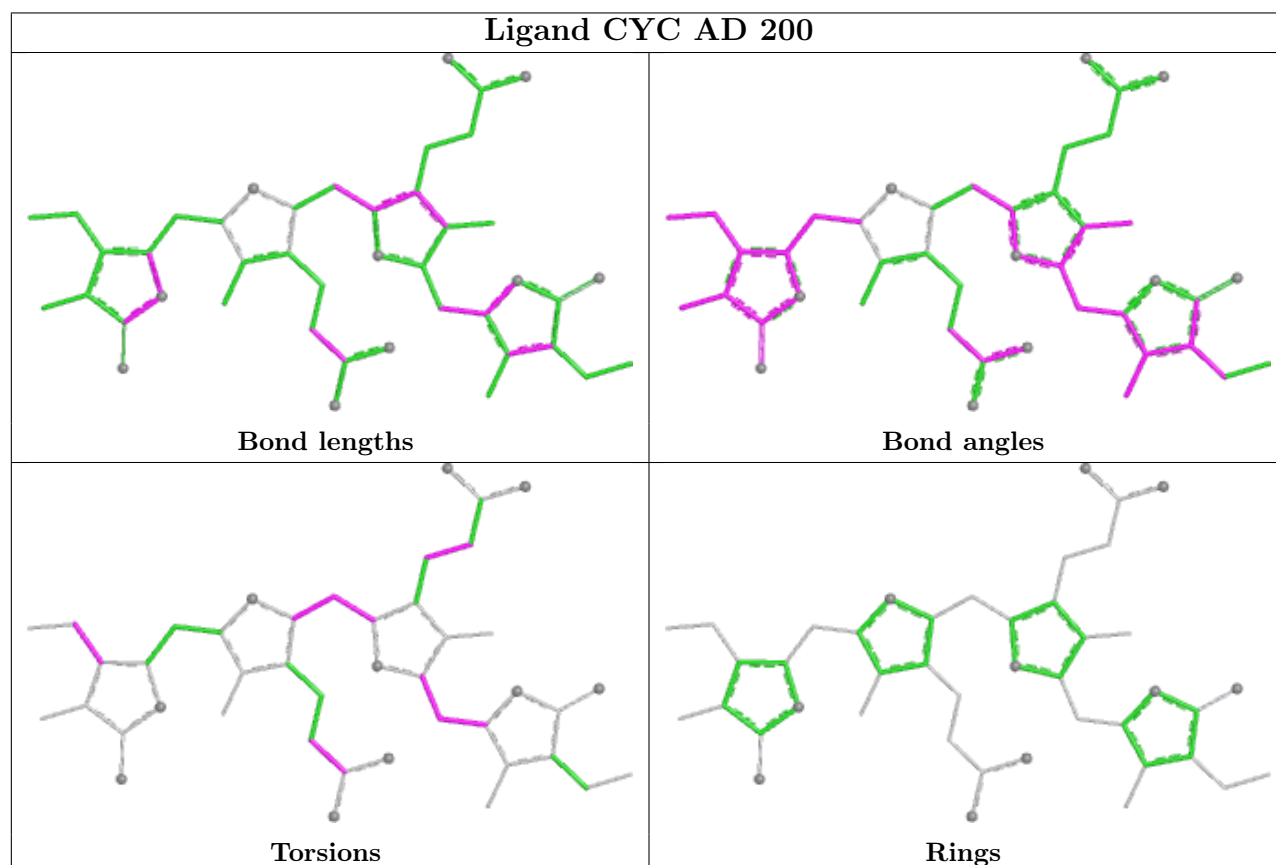
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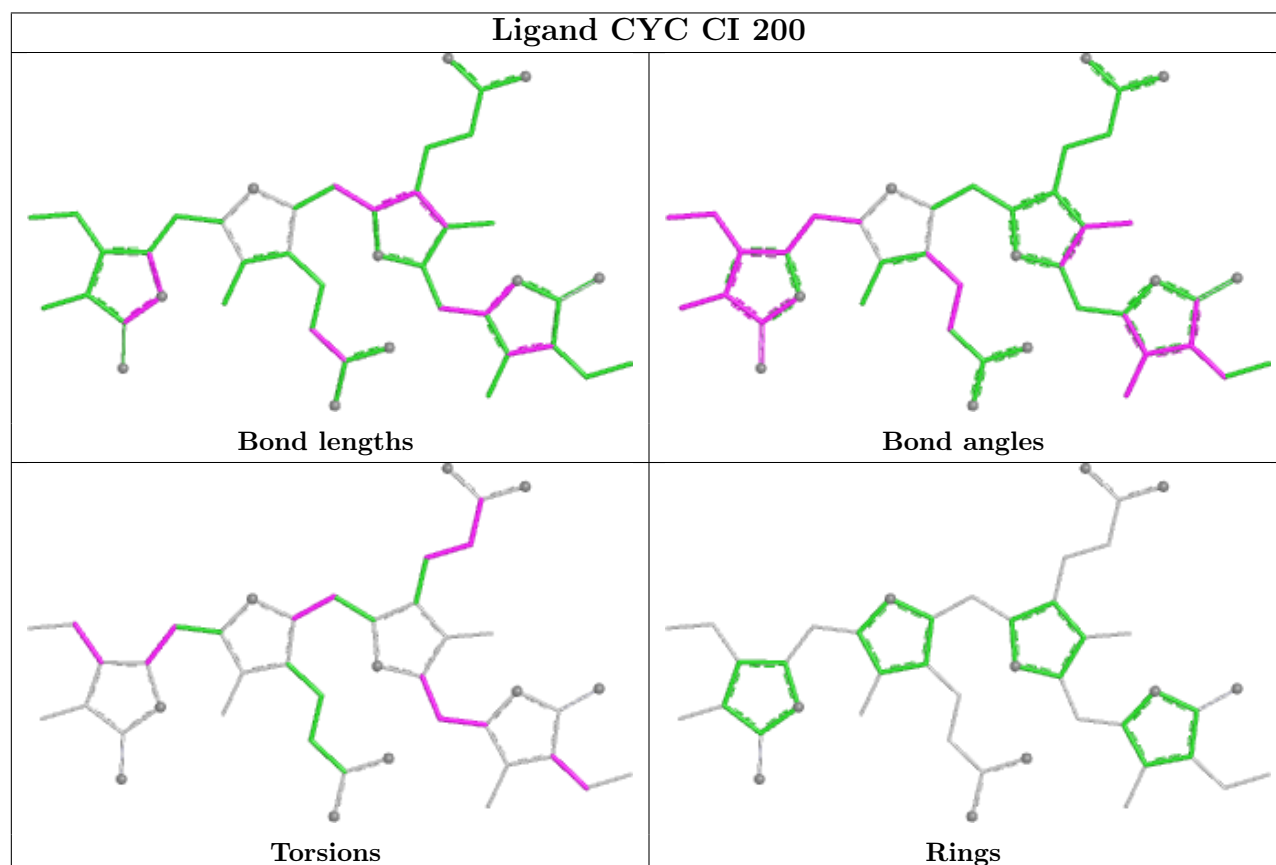
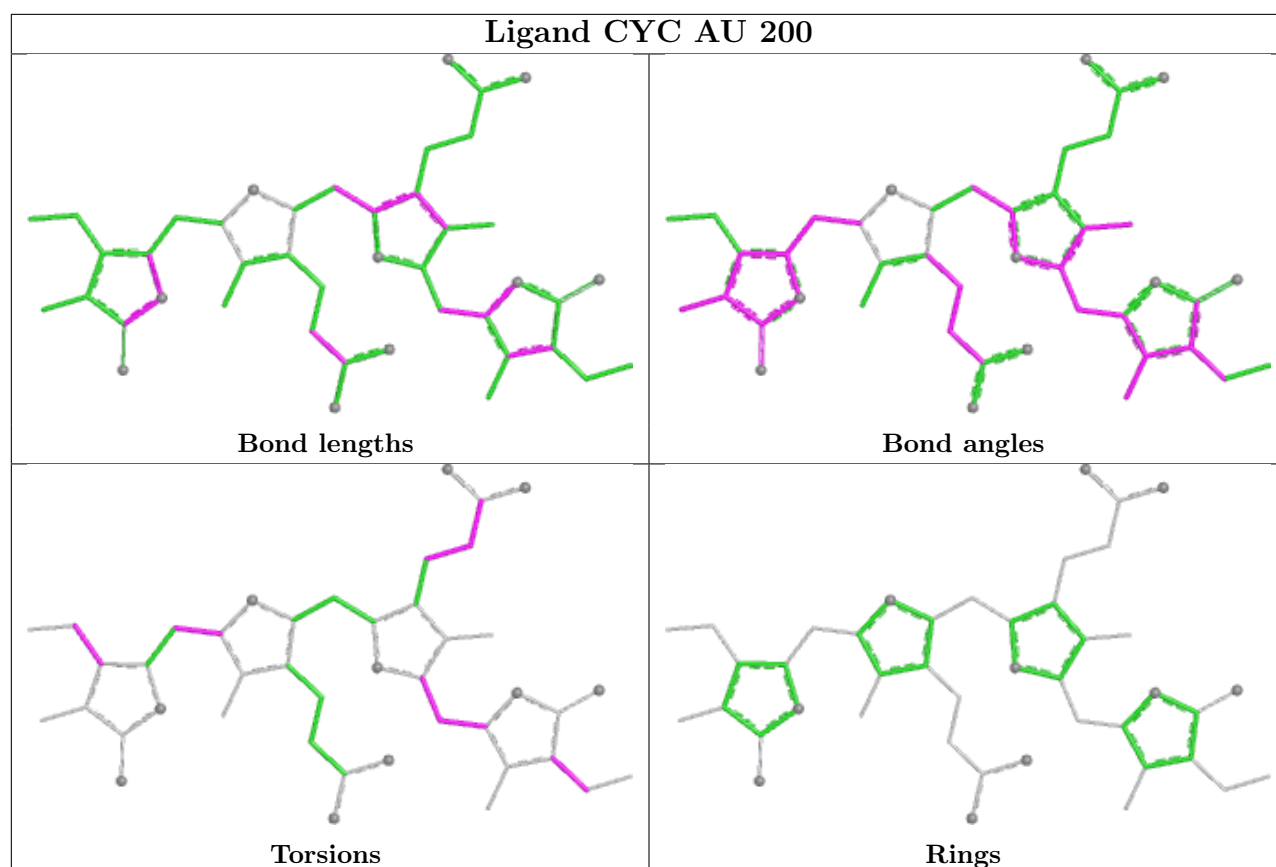


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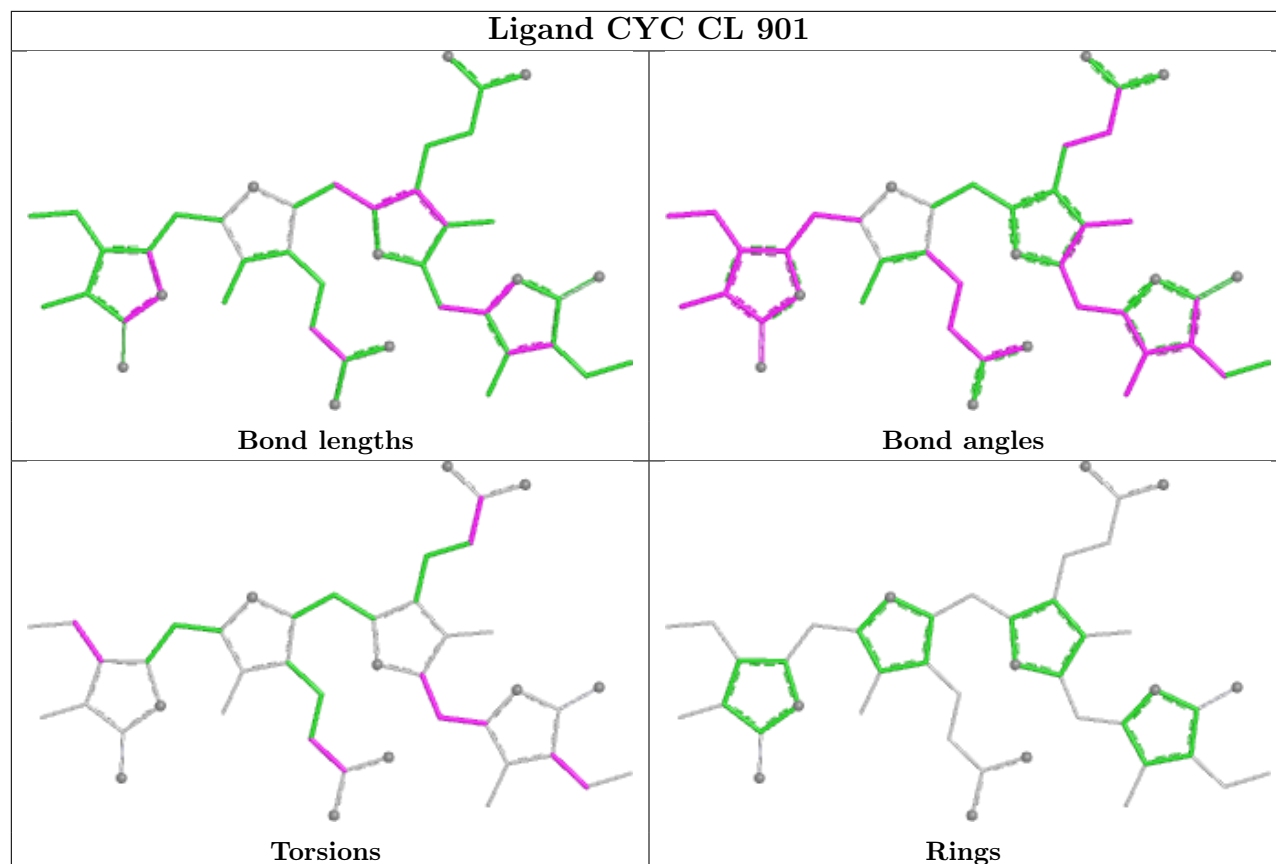


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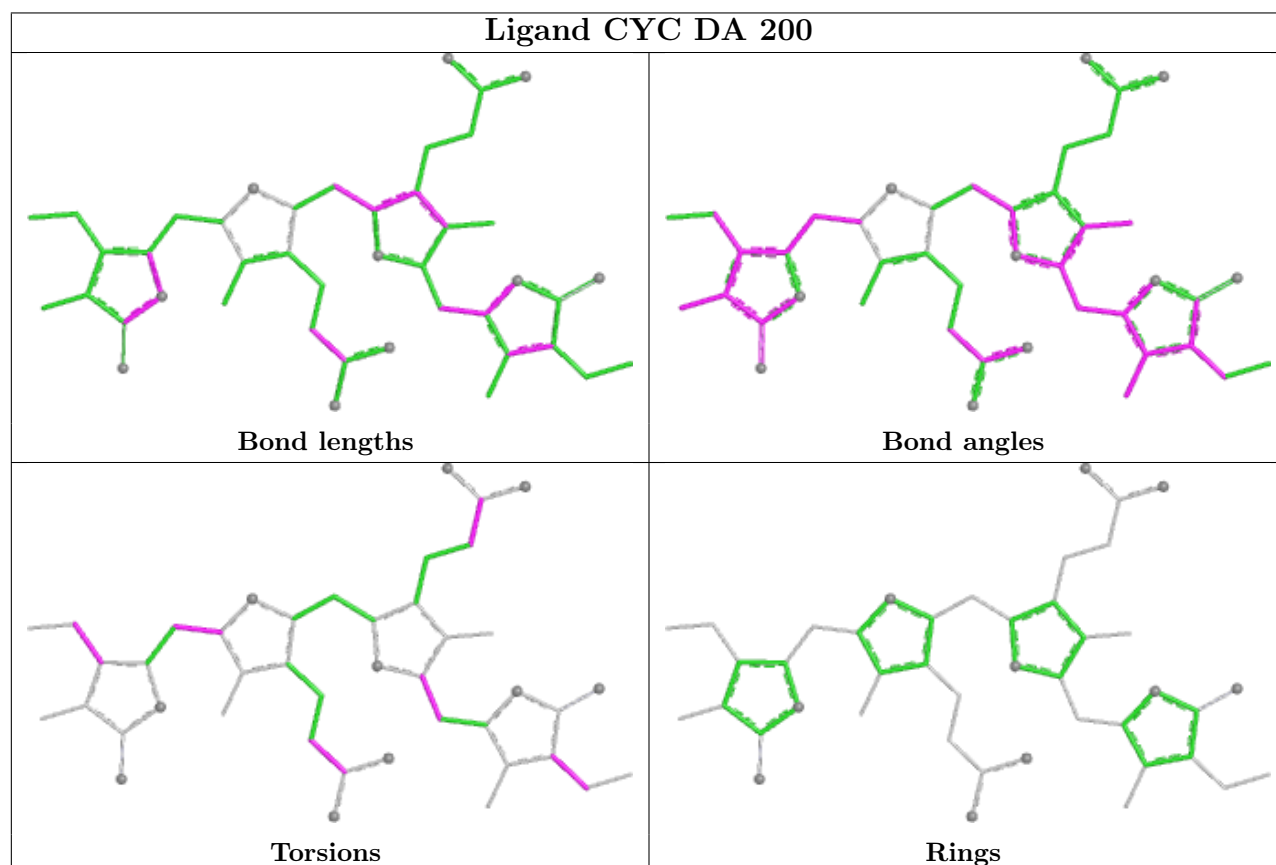




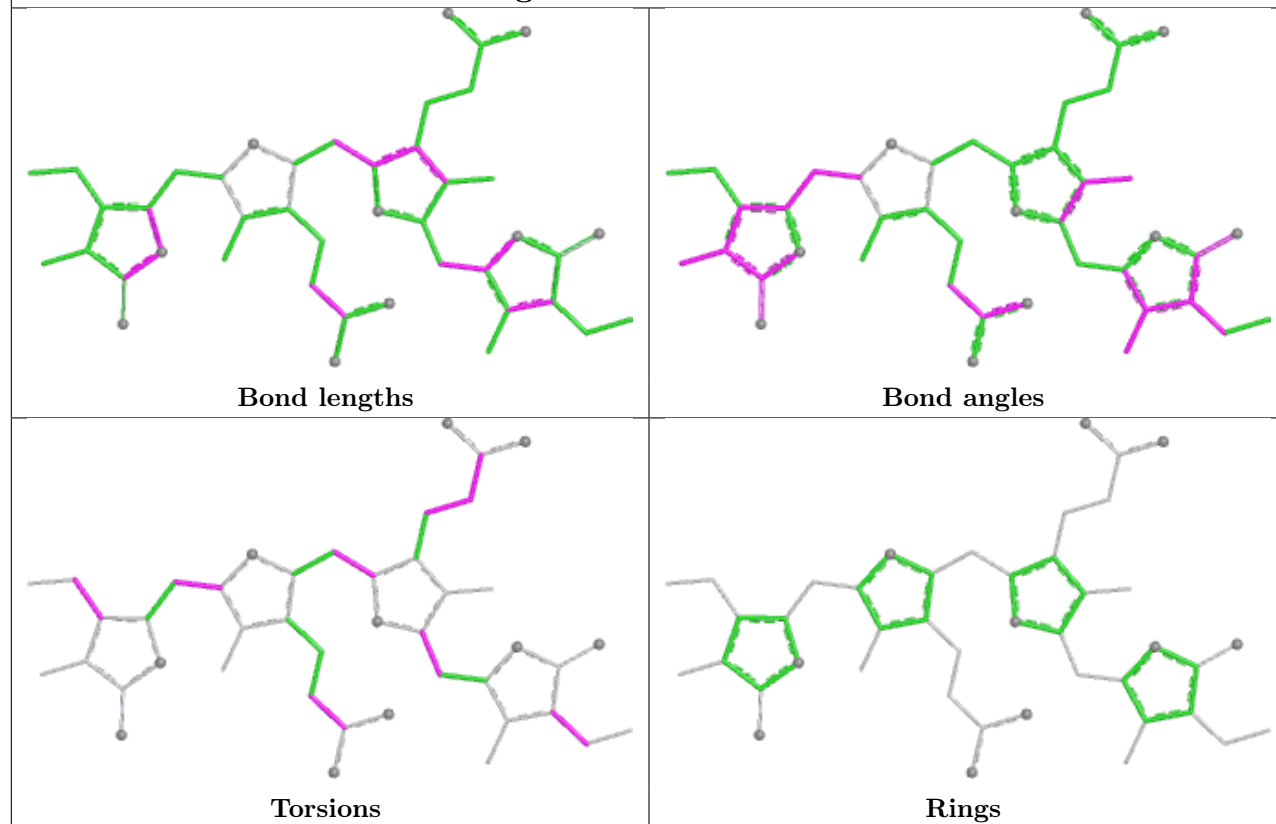
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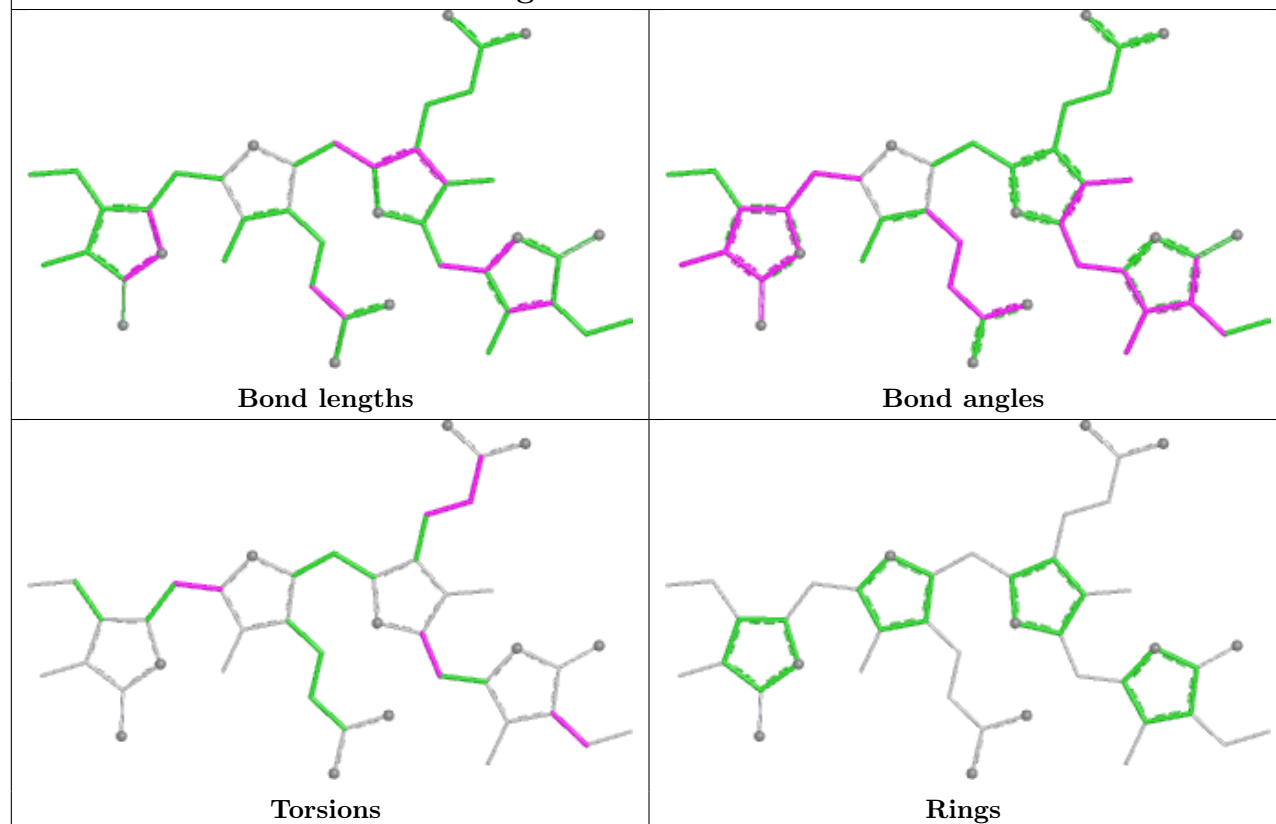
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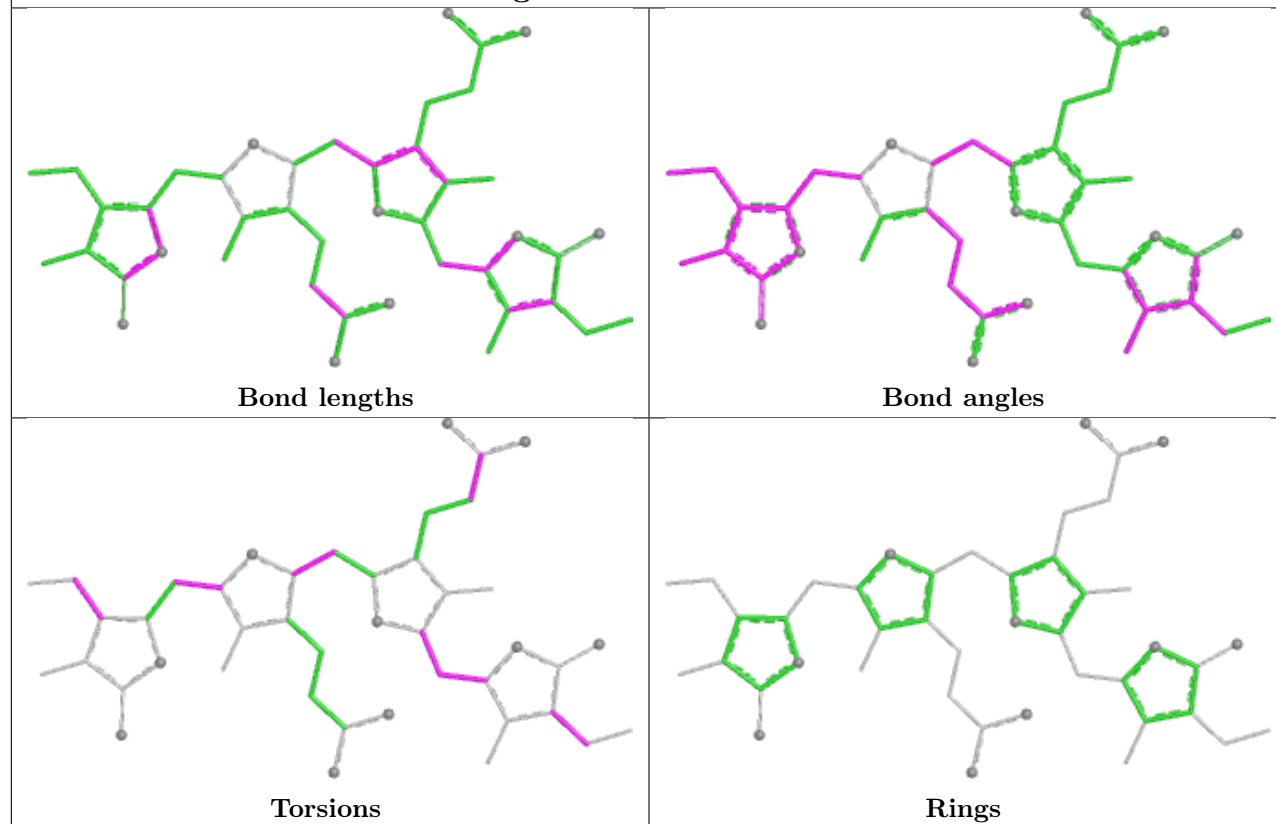
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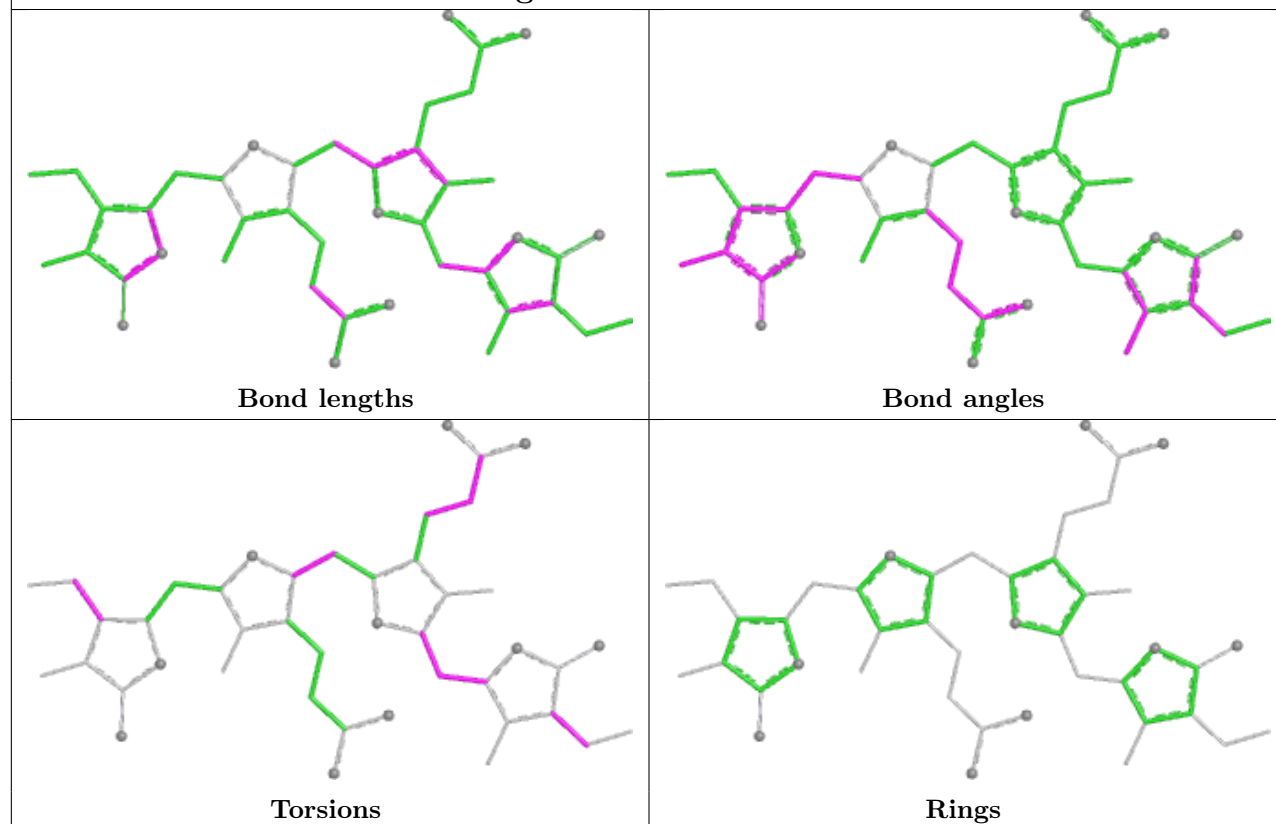
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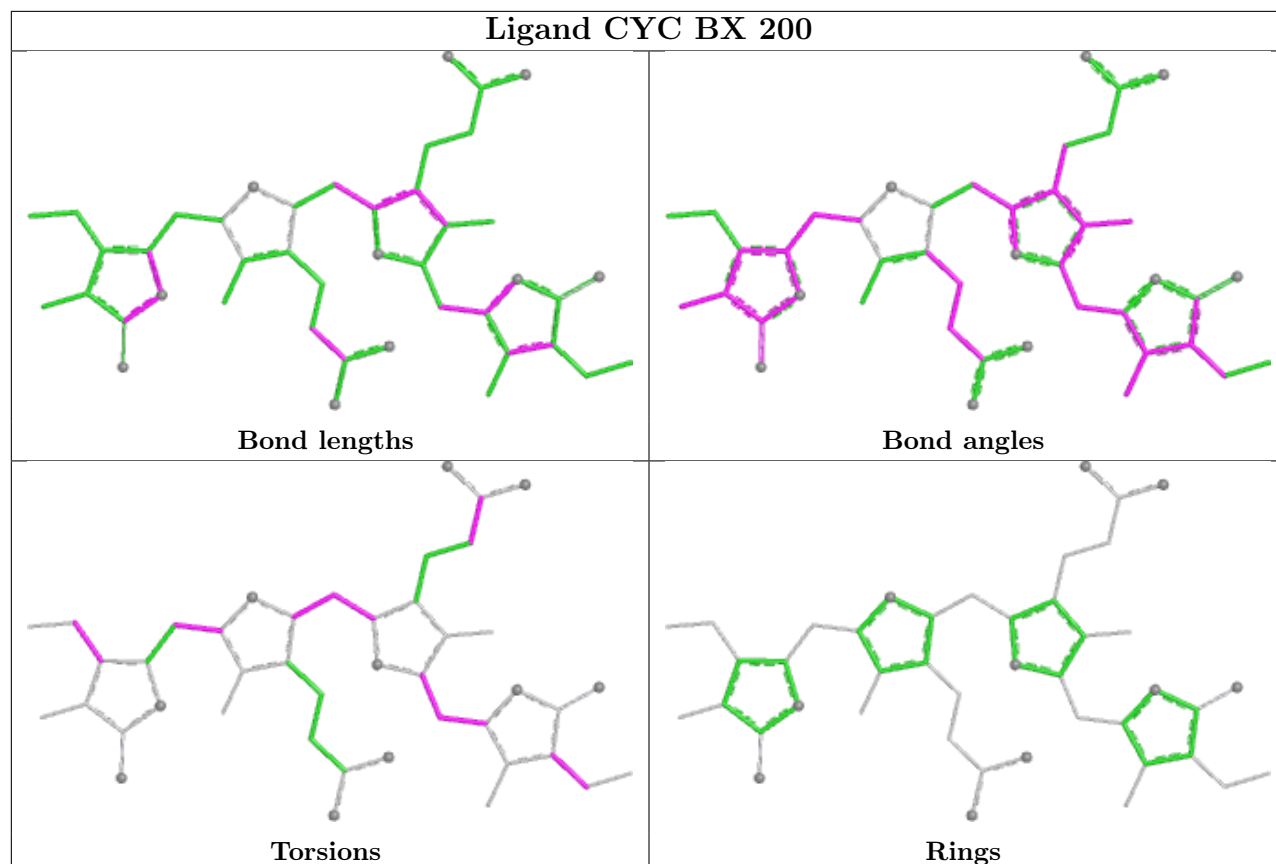
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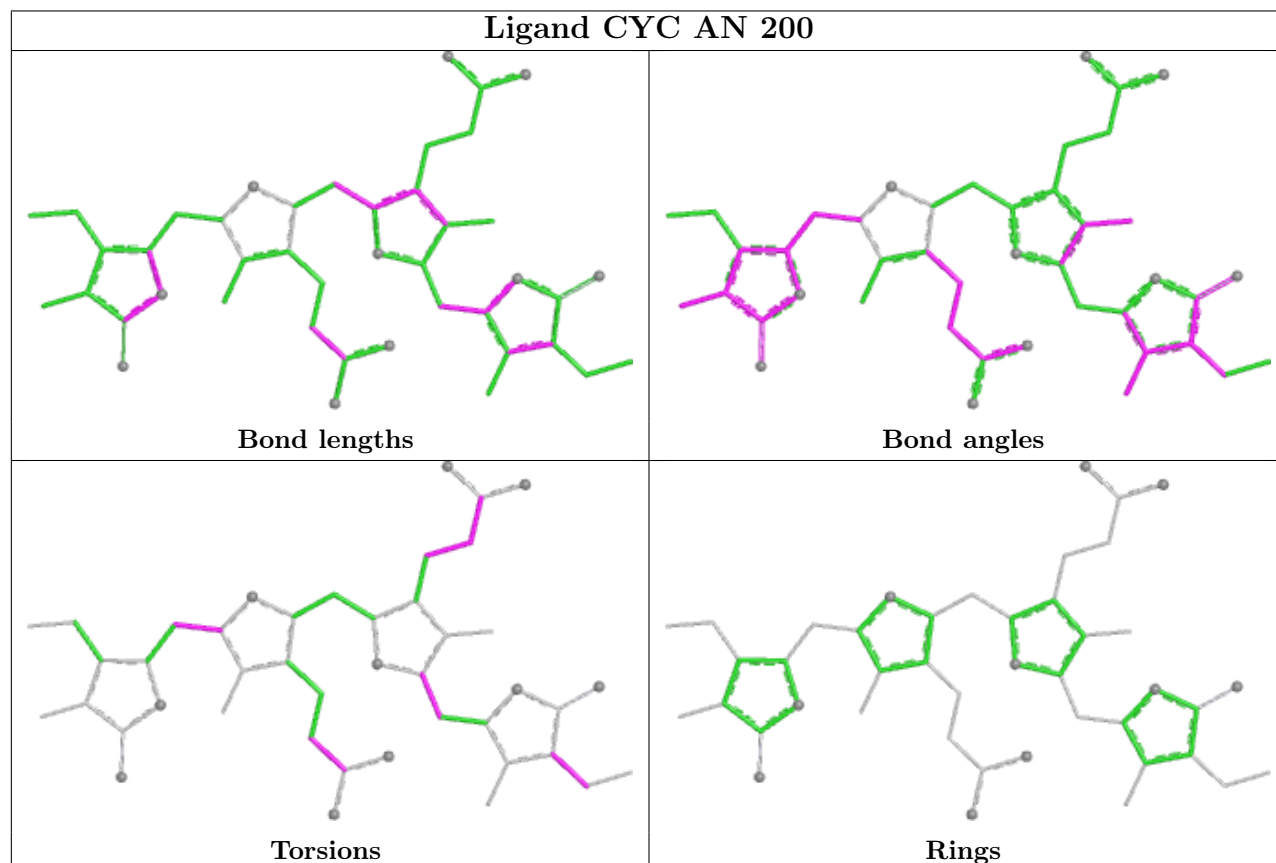
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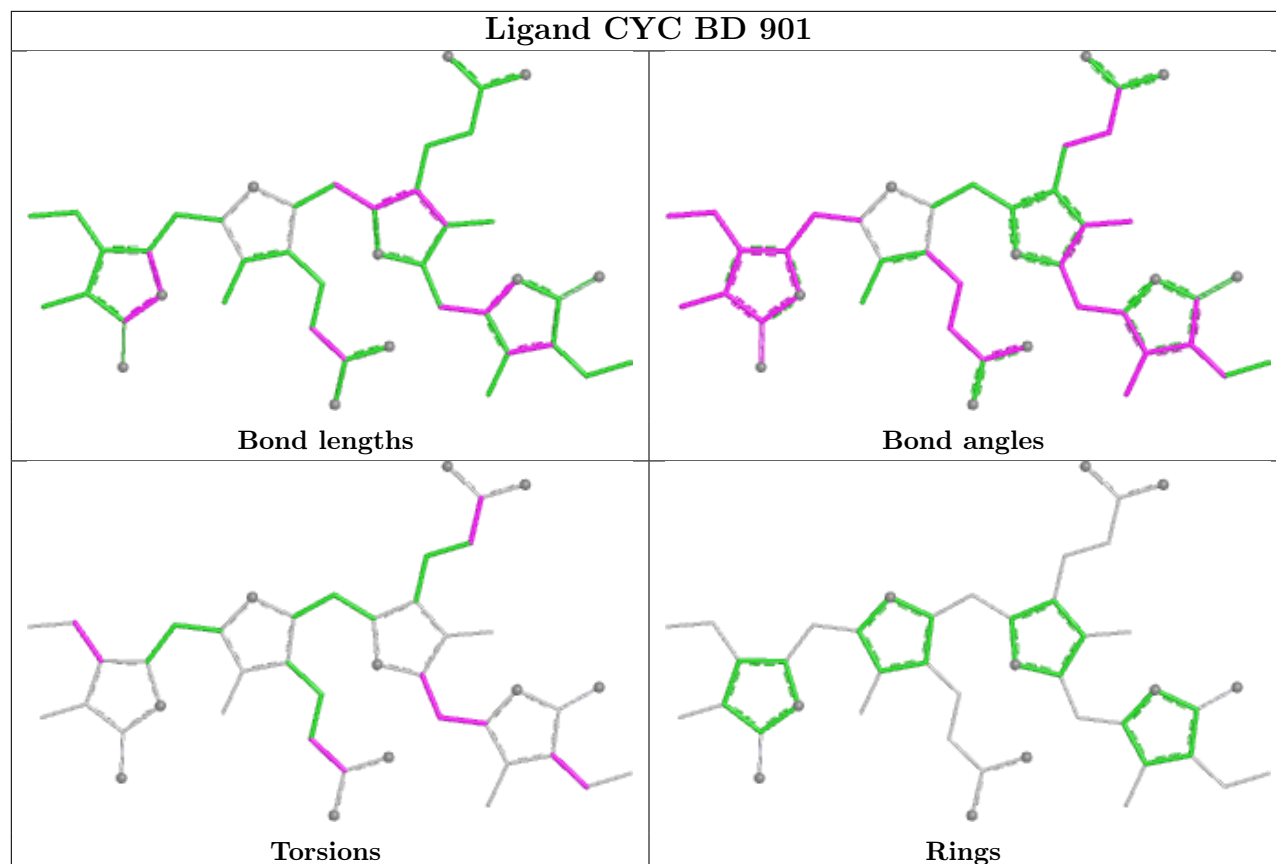
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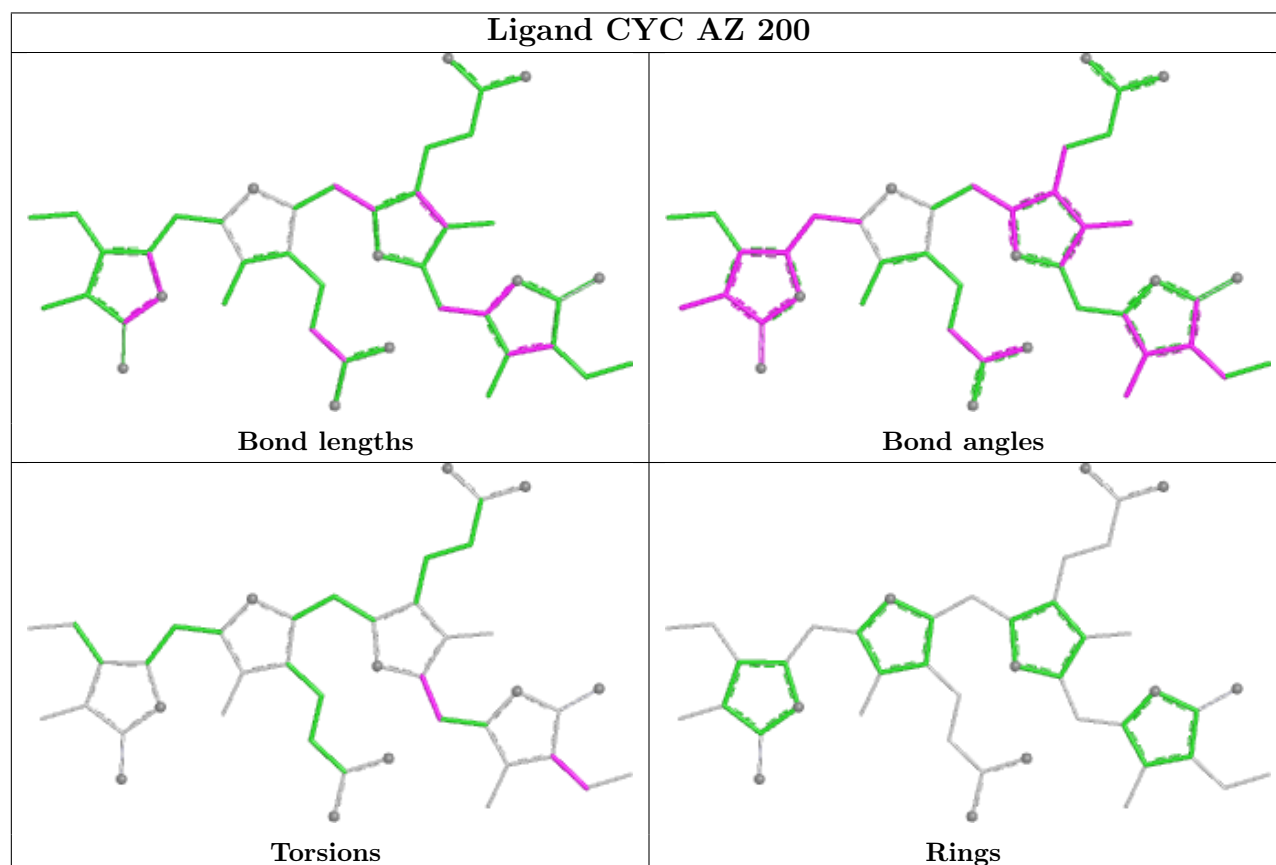
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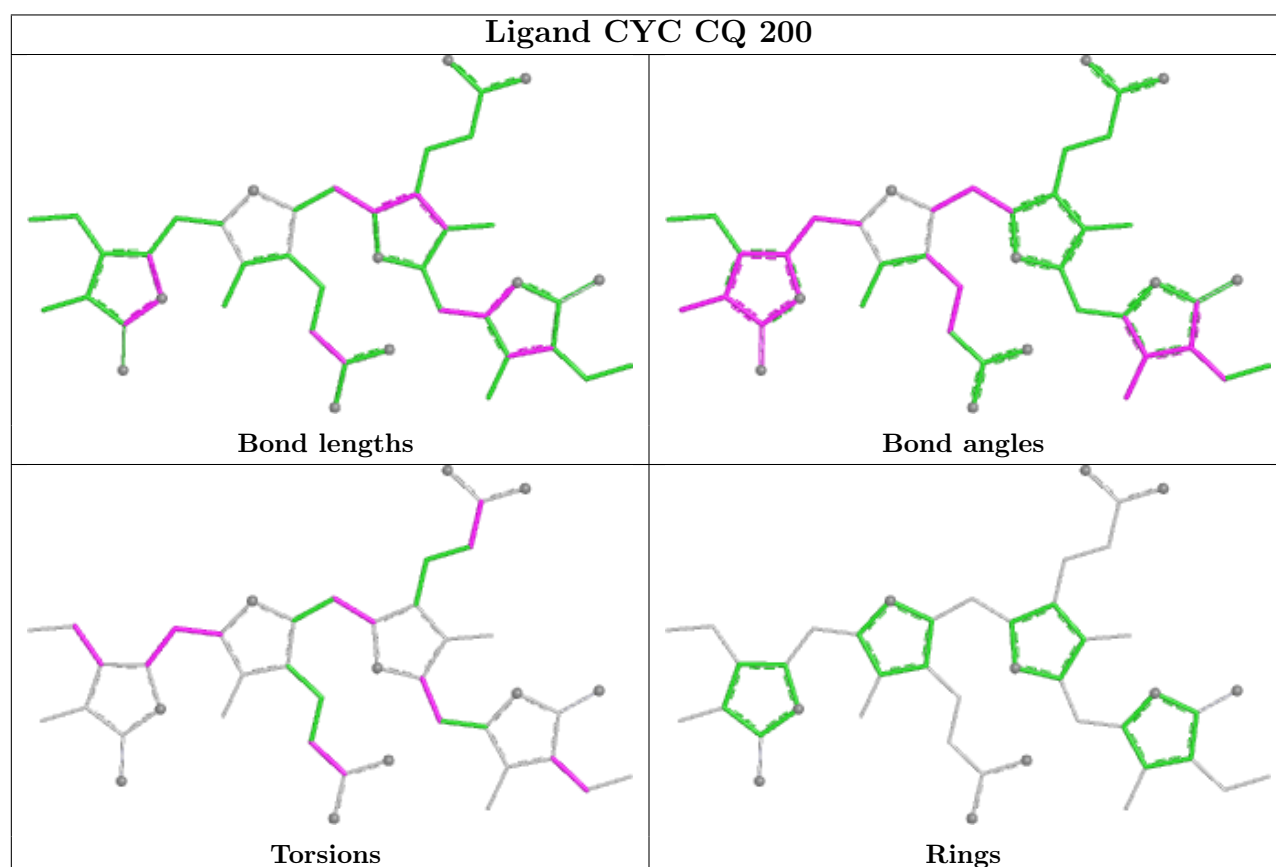
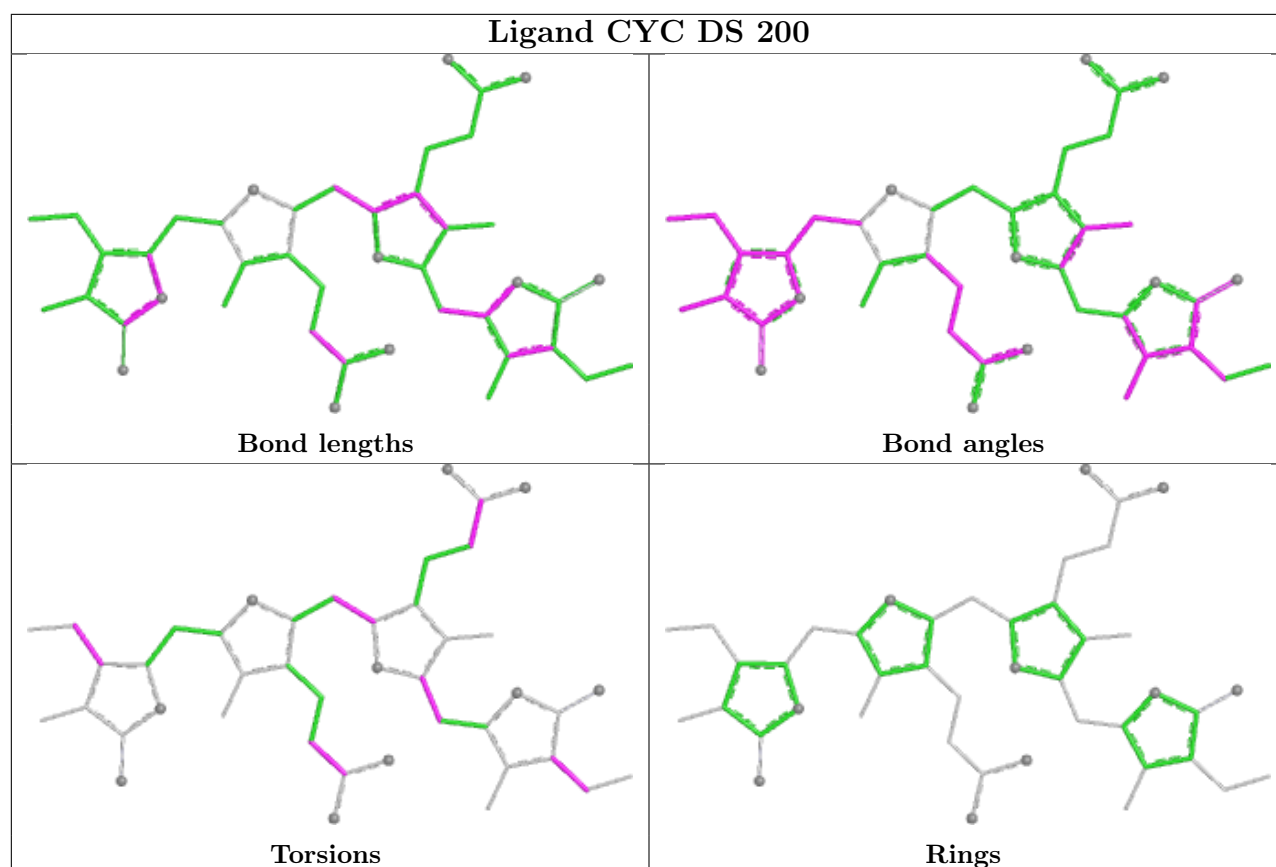


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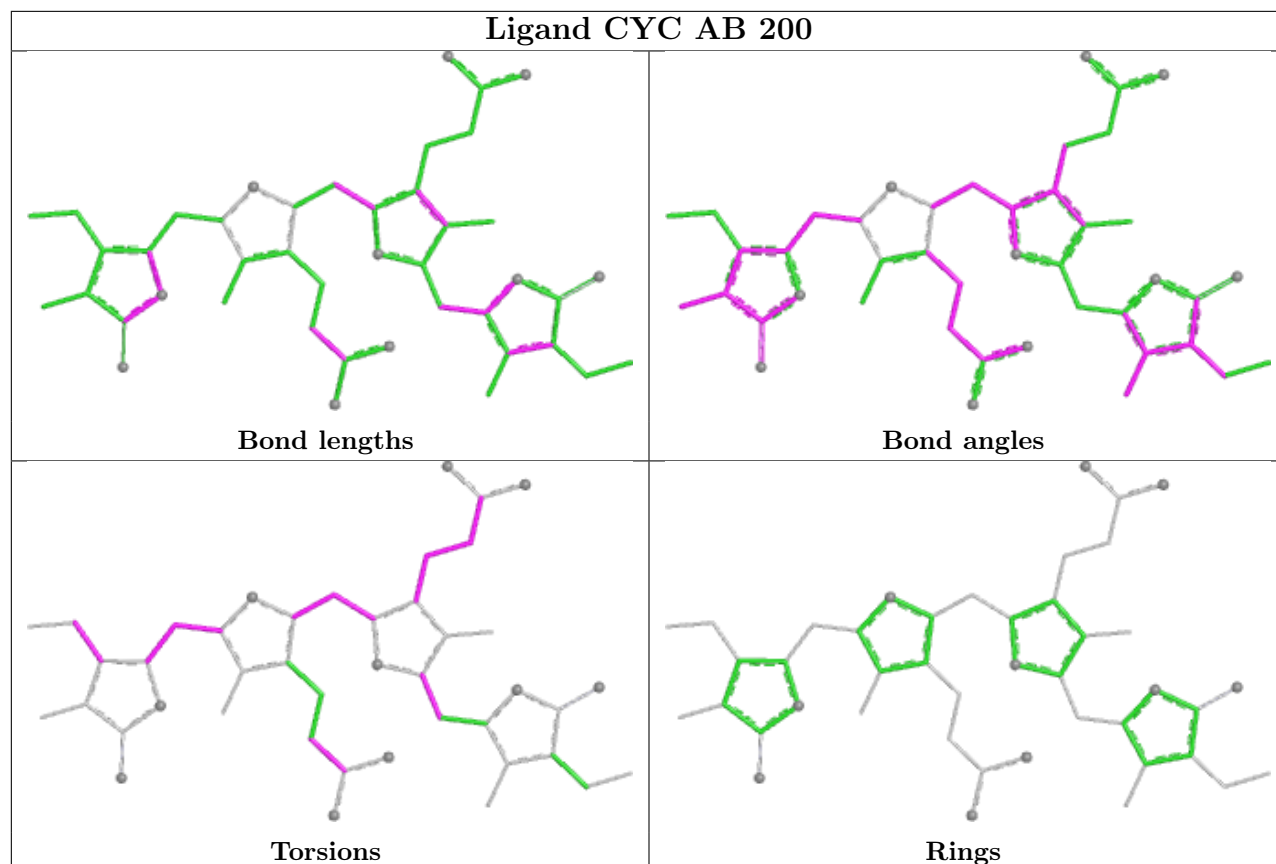


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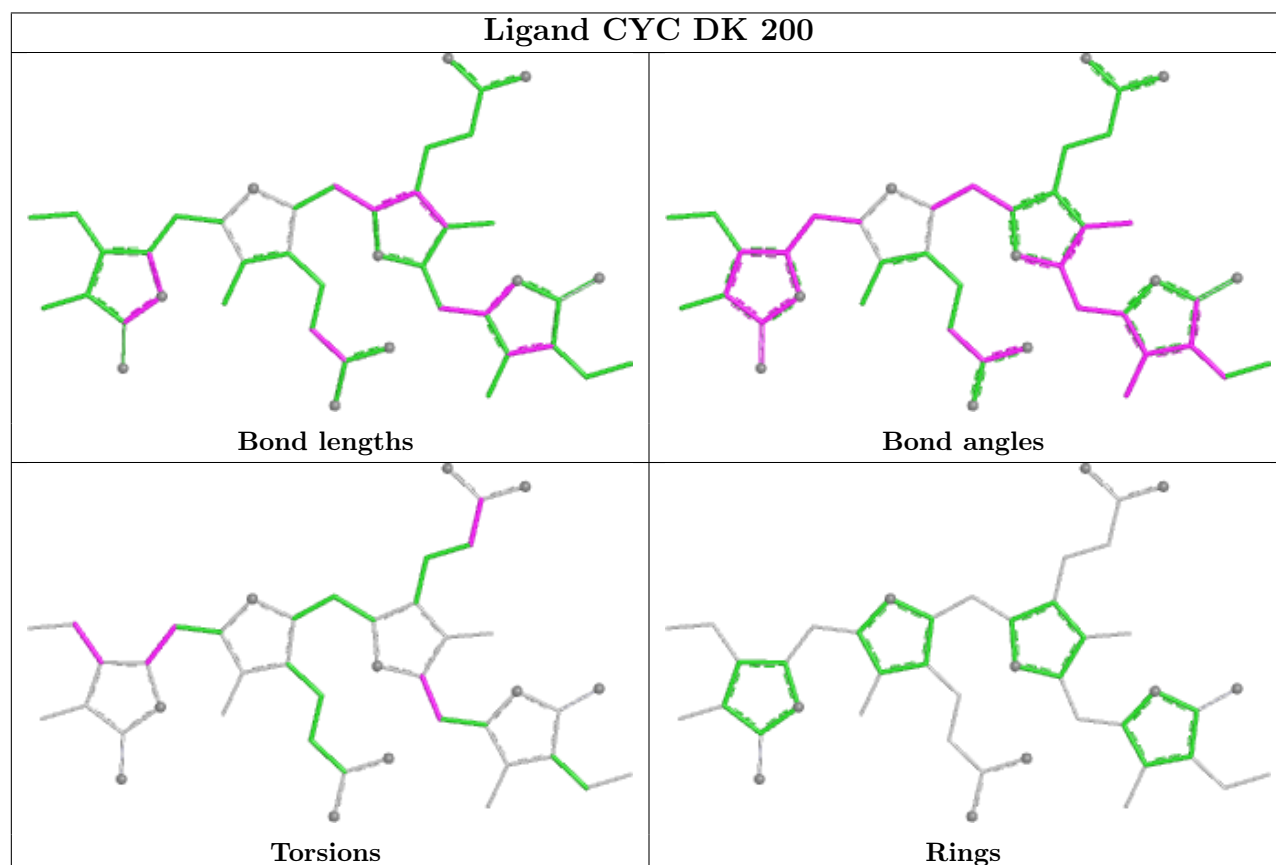


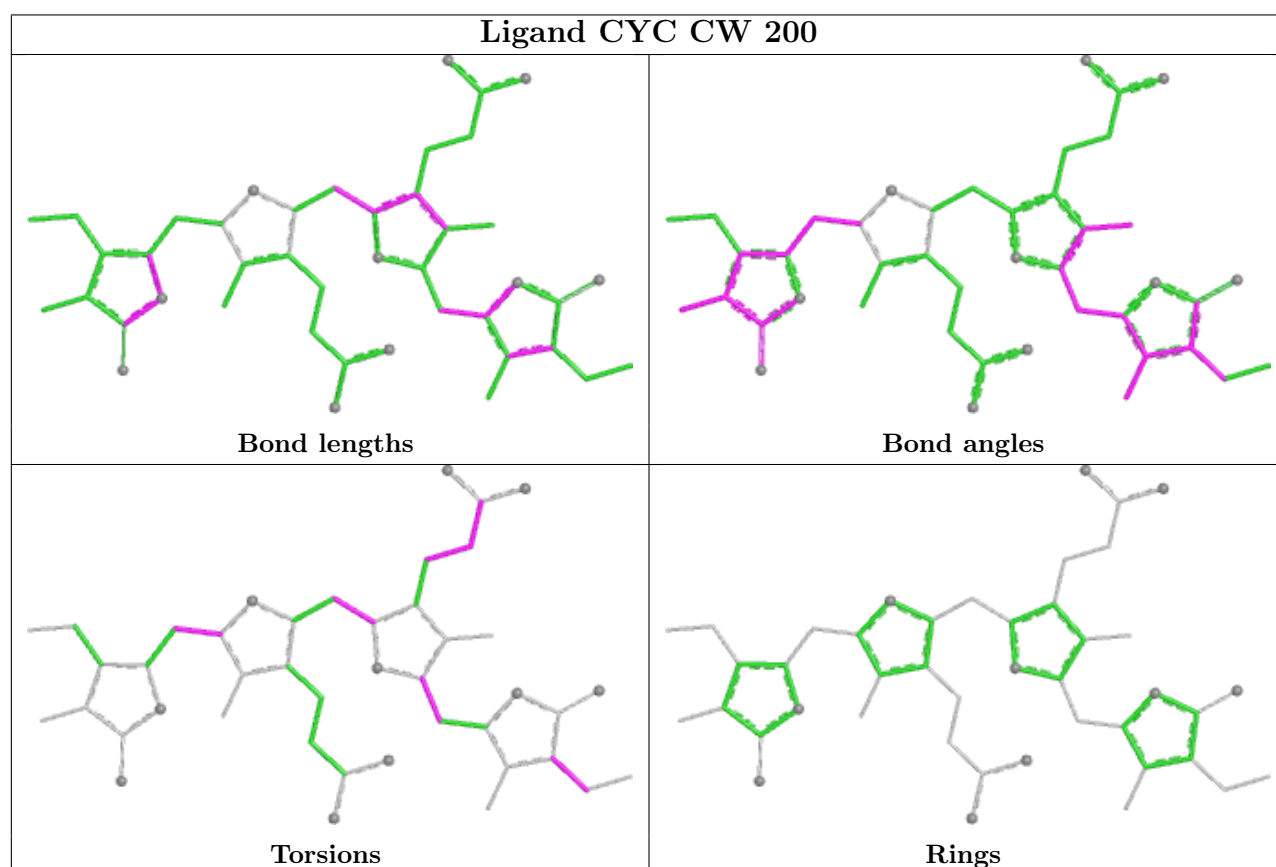
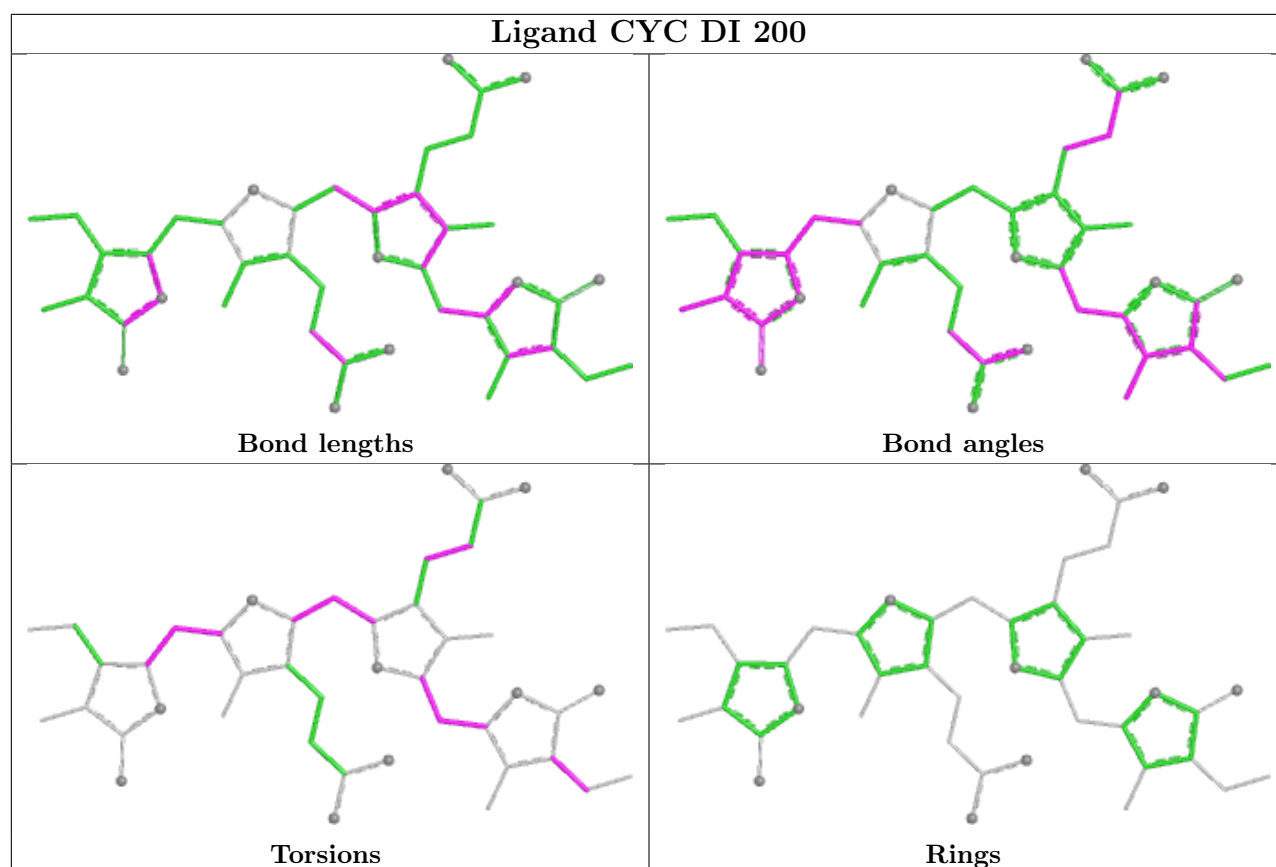


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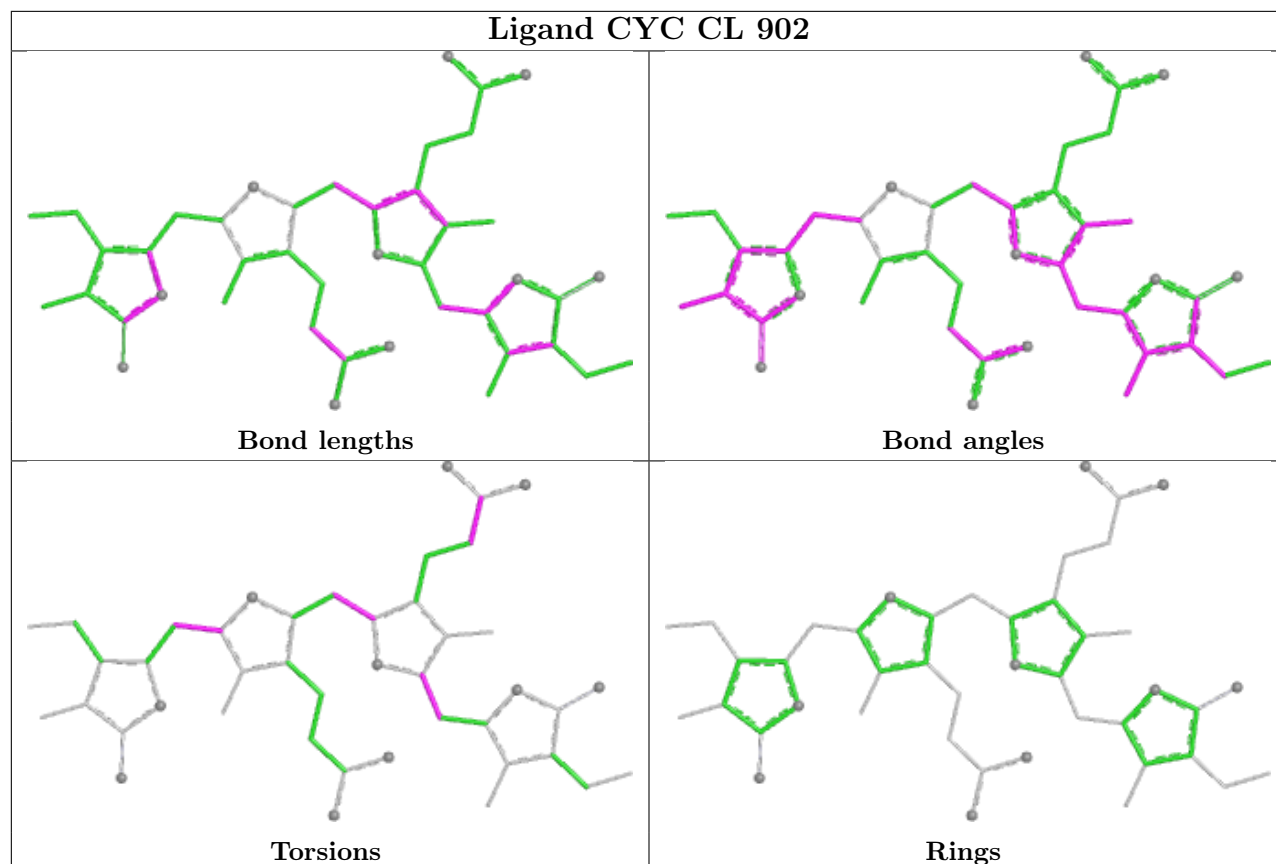


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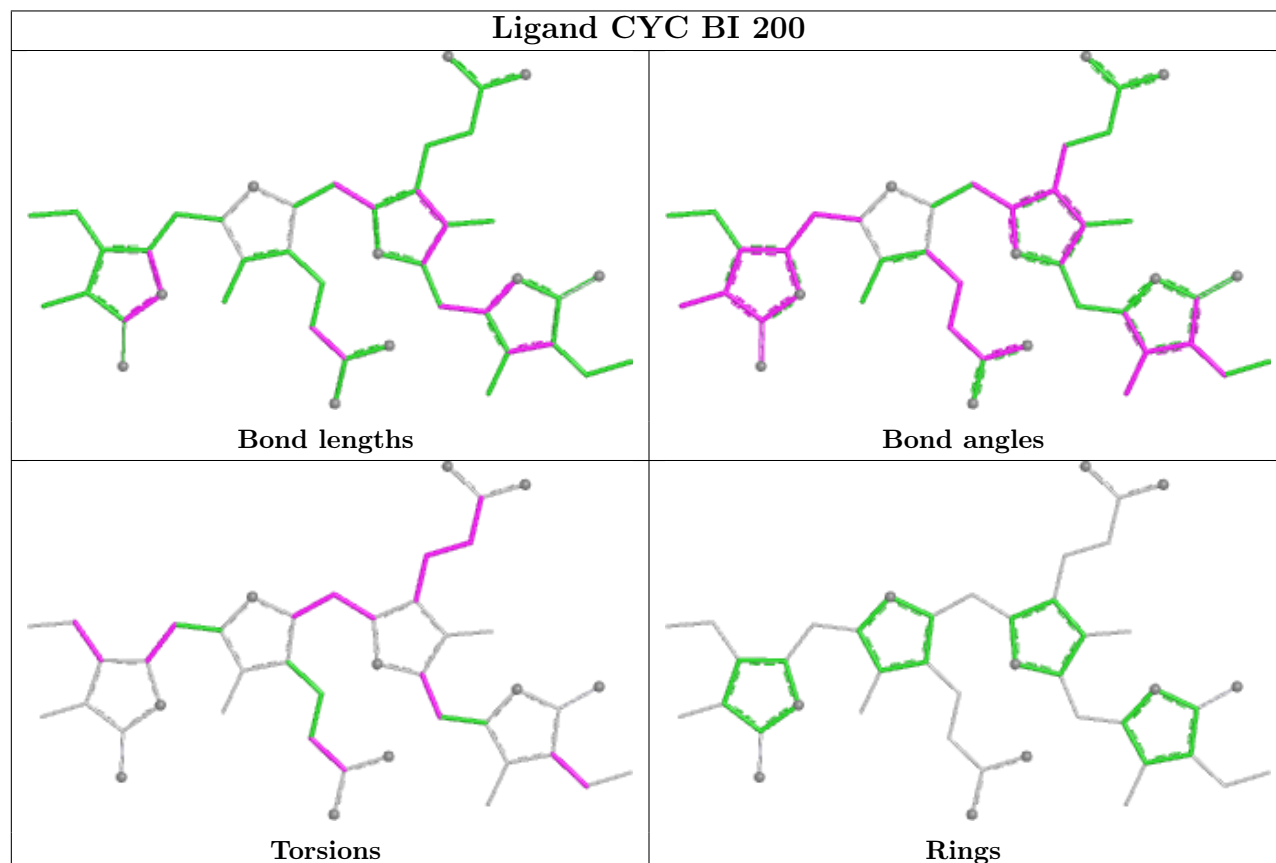




Ligand CYC CL 902



Ligand CYC BI 200



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

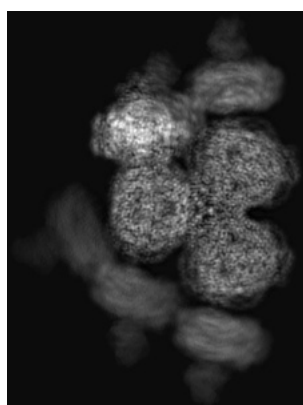
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25028. These allow visual inspection of the internal detail of the map and identification of artifacts.

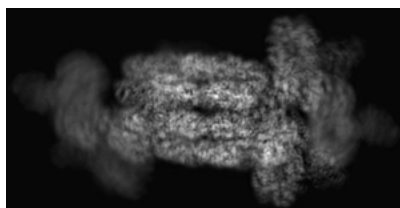
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

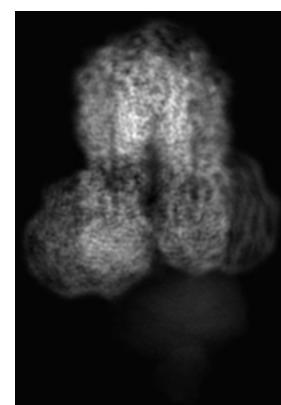
6.1.1 Primary map



X



Y

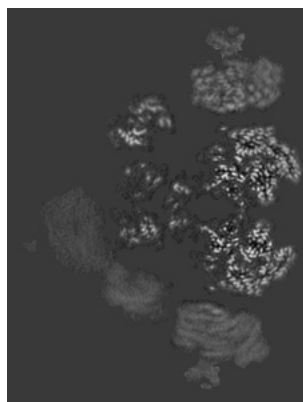


Z

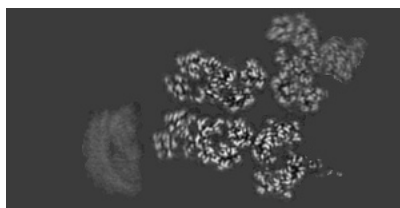
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

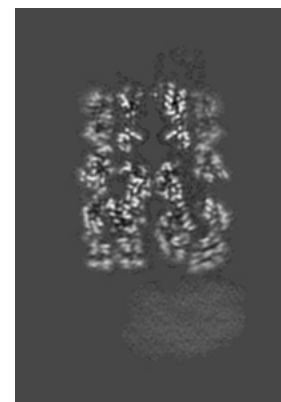
6.2.1 Primary map



X Index: 106



Y Index: 154

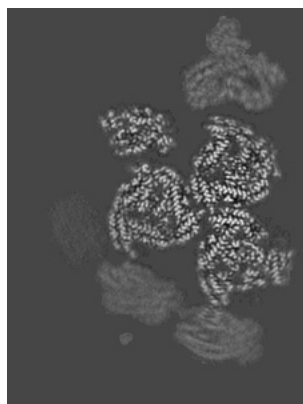


Z Index: 207

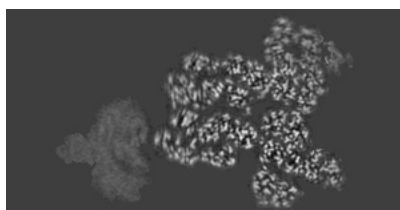
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

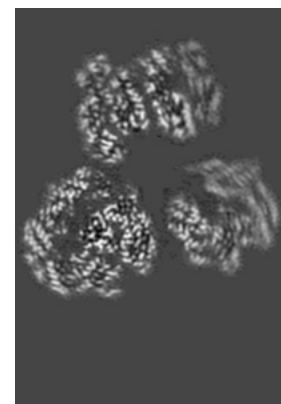
6.3.1 Primary map



X Index: 91



Y Index: 139

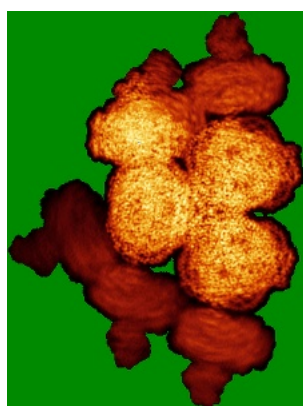


Z Index: 280

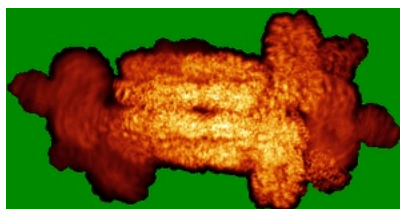
The images above show the largest variance slices of the map in three orthogonal directions.

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

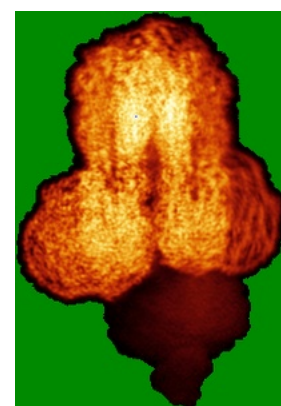
6.4.1 Primary map



X



Y

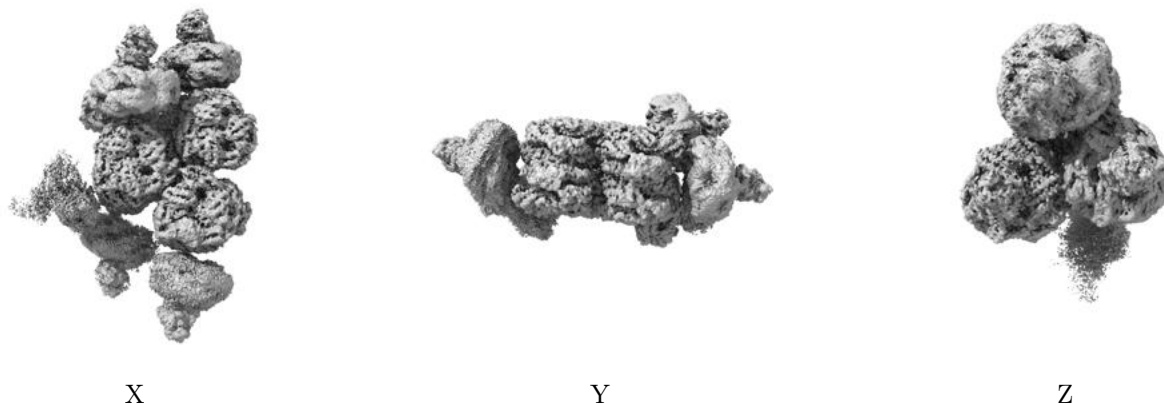


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

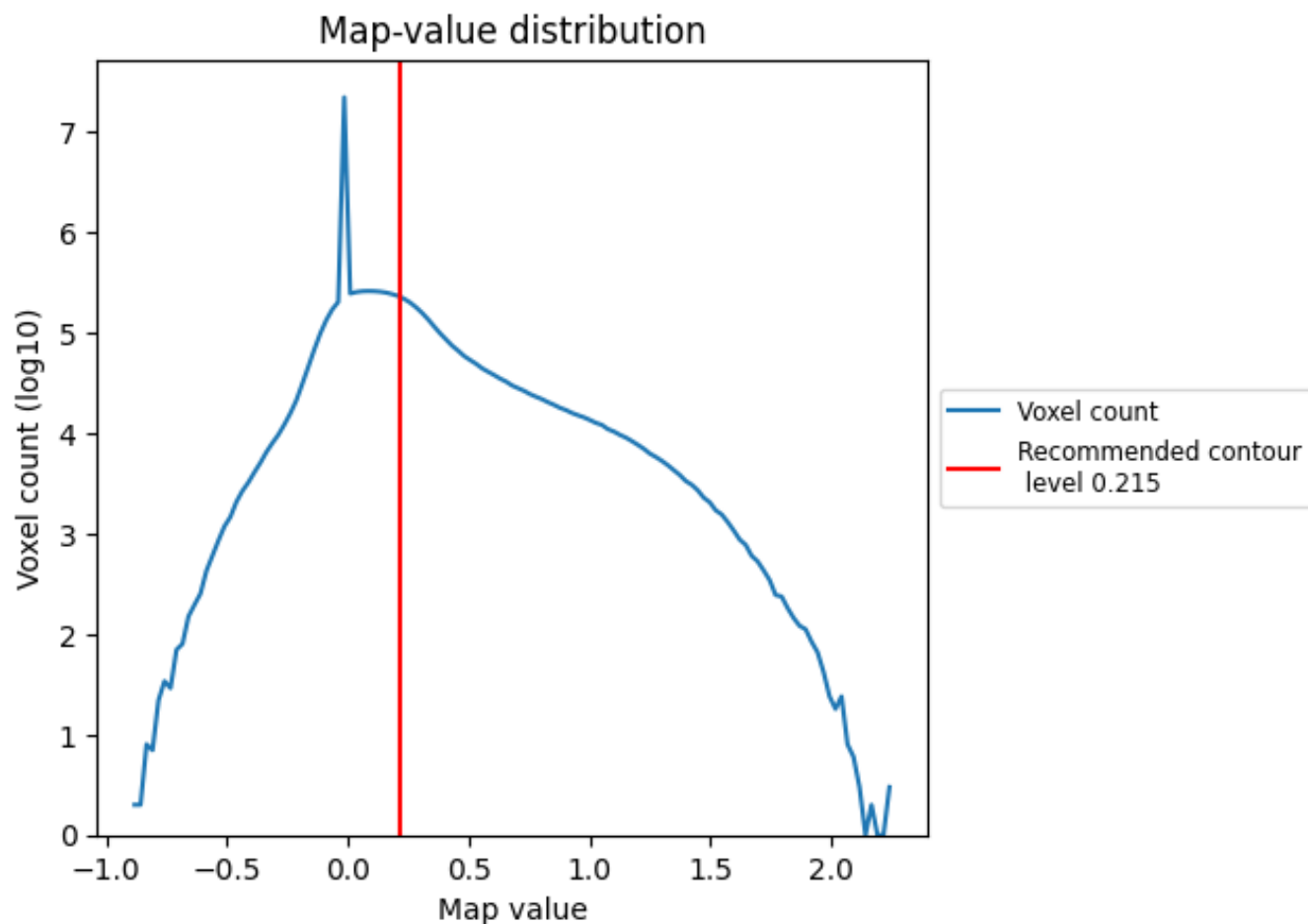
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

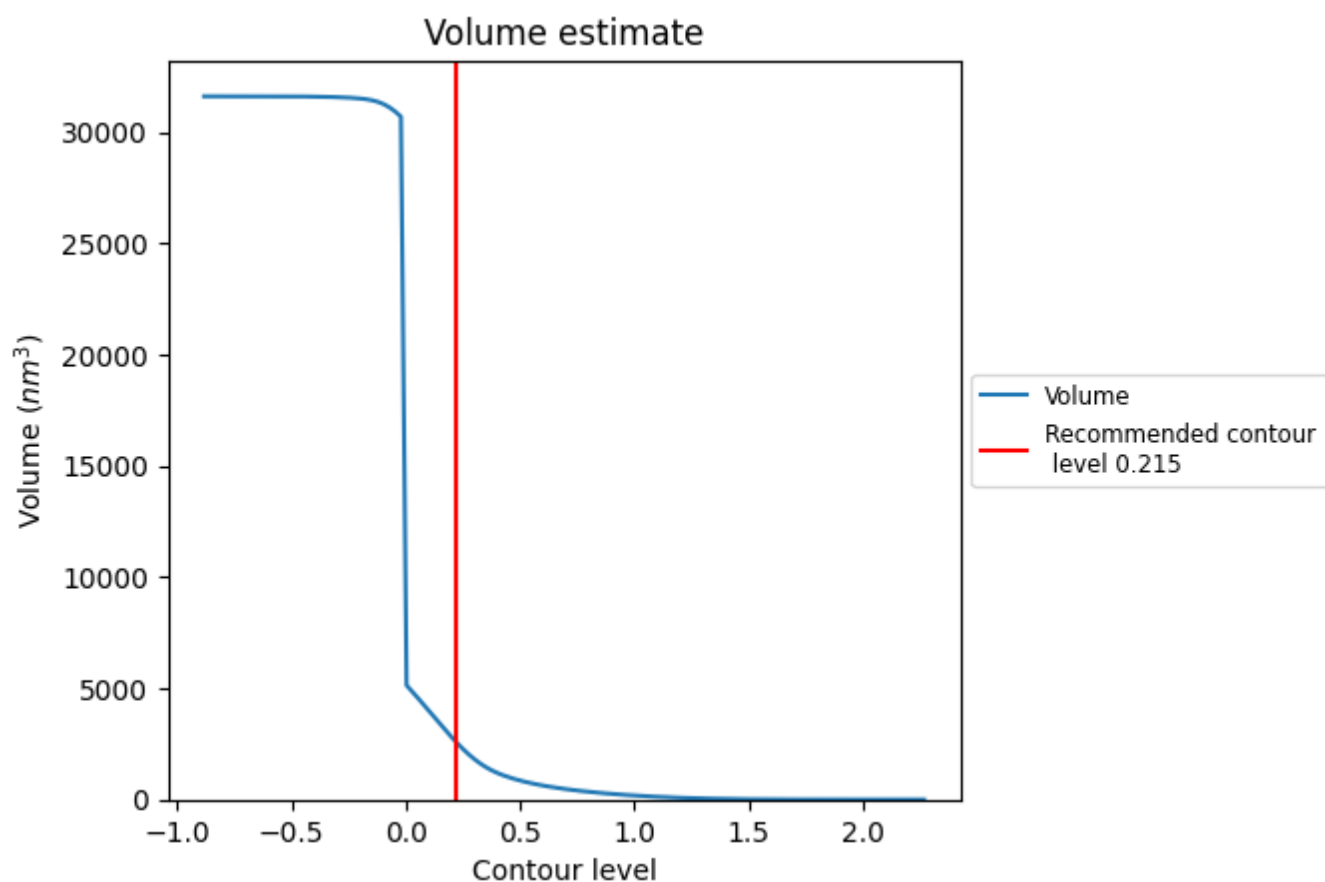
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2638 nm³; this corresponds to an approximate mass of 2383 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

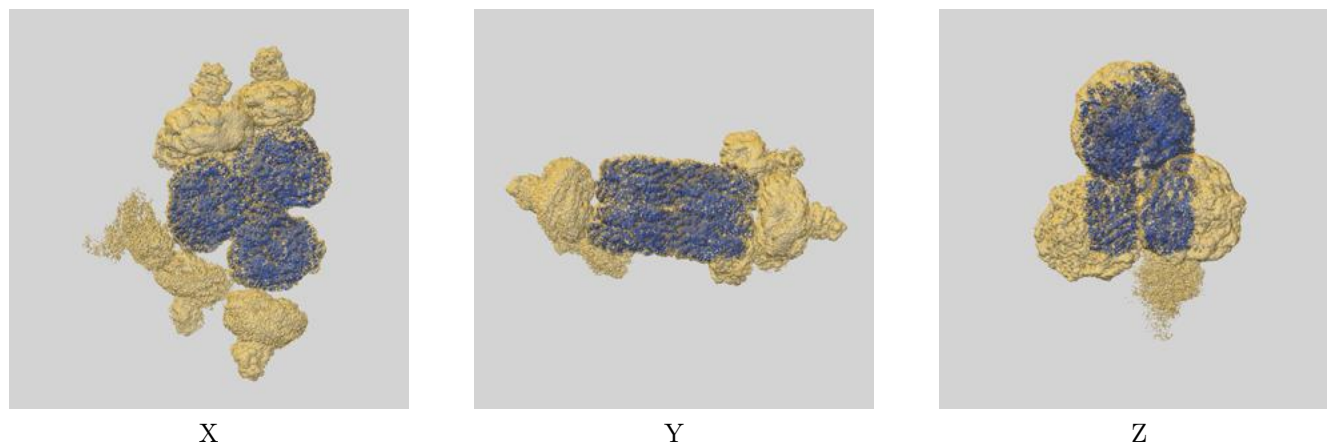
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

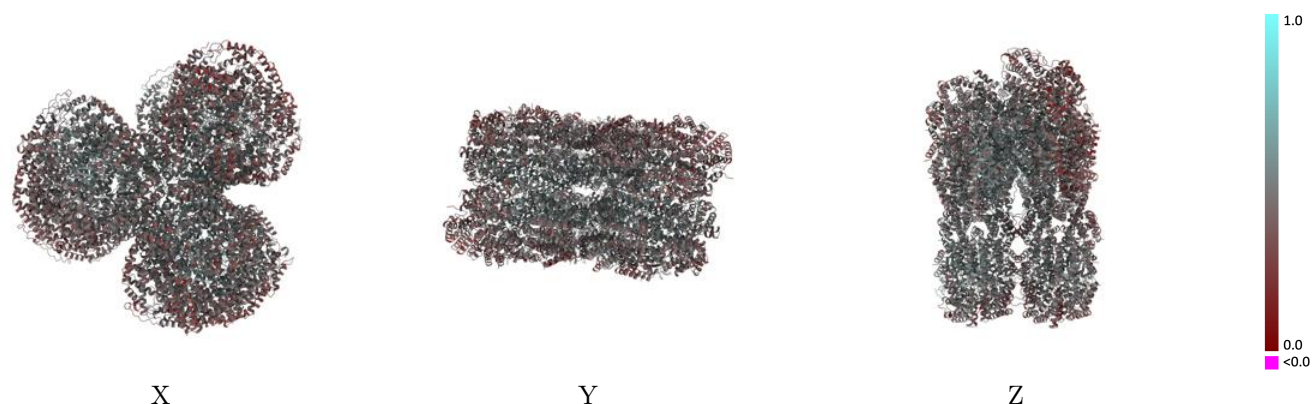
This section contains information regarding the fit between EMDB map EMD-25028 and PDB model 7SC7. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



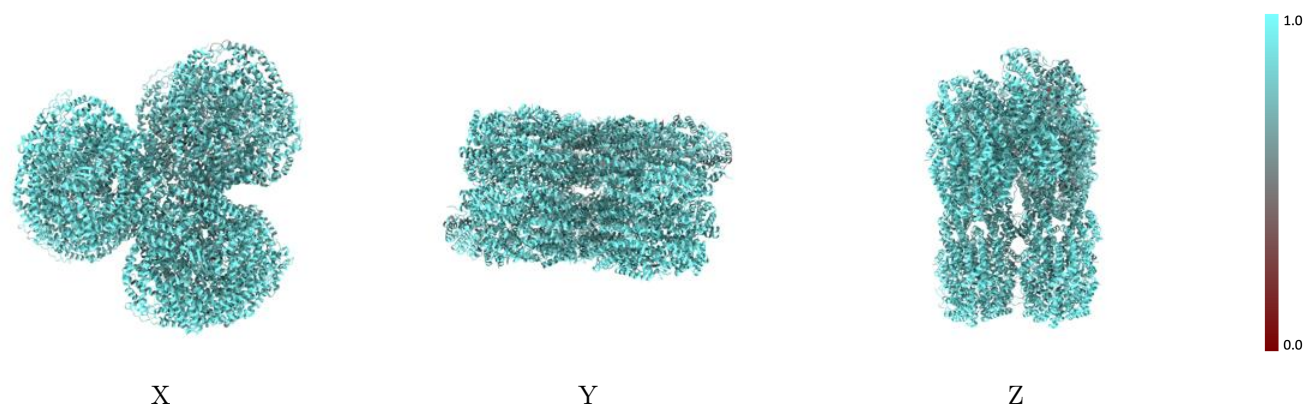
The images above show the 3D surface view of the map at the recommended contour level 0.215 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



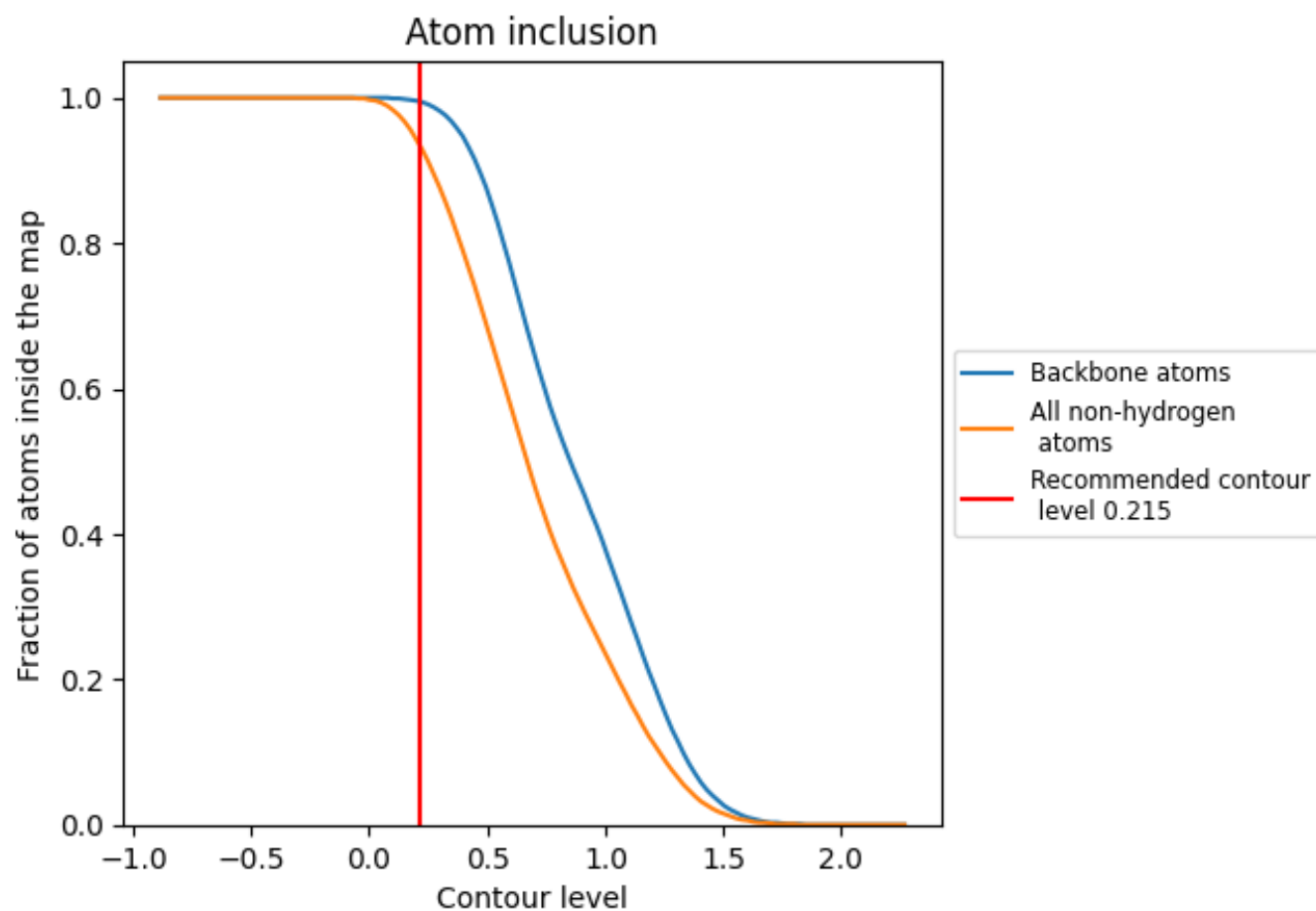
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.215).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 93% 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 (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.4540
AA	 0.8330	 0.3830
AB	 0.8930	 0.3760
AC	 0.8490	 0.3670
AD	 0.8990	 0.4060
AE	 0.8840	 0.4340
AF	 0.8680	 0.3910
AH	 0.9600	 0.4380
AI	 0.9700	 0.5240
AJ	 0.9620	 0.5270
AK	 0.9540	 0.5130
AL	 0.9610	 0.4740
AN	 0.9720	 0.4710
AO	 0.9700	 0.5390
AP	 0.9630	 0.5180
AQ	 0.9620	 0.5130
AR	 0.9560	 0.4550
AS	 0.9640	 0.4910
AU	 0.9180	 0.4000
AV	 0.9230	 0.4010
AW	 0.9420	 0.3550
AX	 0.9220	 0.4230
AY	 0.9410	 0.4160
AZ	 0.8470	 0.4390
BA	 0.9010	 0.4730
BB	 0.8080	 0.4640
BD	 0.9600	 0.4970
BF	 0.9500	 0.4100
BG	 0.9410	 0.4380
BH	 0.7710	 0.3660
BI	 0.8340	 0.3480
BJ	 0.7780	 0.3570
BK	 0.8250	 0.3860
BL	 0.8340	 0.4060
BM	 0.8120	 0.3760























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Chain	Atom inclusion	Q-score
BO	 0.9470	 0.4260
BP	 0.9660	 0.5140
BQ	 0.9580	 0.5150
BR	 0.9540	 0.5000
BS	 0.9610	 0.4590
BU	 0.9620	 0.4690
BV	 0.9700	 0.5350
BW	 0.9610	 0.5140
BX	 0.9690	 0.5150
BY	 0.9530	 0.4800
BZ	 0.9650	 0.4940
CB	 0.9340	 0.4440
CC	 0.9640	 0.4240
CD	 0.9560	 0.4380
CE	 0.9620	 0.4320
CF	 0.9460	 0.4680
CG	 0.9650	 0.4640
CI	 0.8290	 0.4270
CJ	 0.9130	 0.5000
CL	 0.9580	 0.4920
CN	 0.9460	 0.4400
CO	 0.9370	 0.4280
CP	 0.9660	 0.4590
CQ	 0.9590	 0.4210
CR	 0.9420	 0.3870
CS	 0.9700	 0.4690
CT	 0.9560	 0.4950
CU	 0.9700	 0.4930
CW	 0.9430	 0.4030
CX	 0.9560	 0.4590
CY	 0.9530	 0.5010
CZ	 0.9530	 0.4880
DA	 0.9660	 0.4990
DB	 0.9400	 0.4230
DD	 0.9770	 0.5200
DE	 0.8600	 0.3460
DF	 0.8720	 0.3620
DG	 0.9300	 0.3850
DH	 0.9590	 0.4430
DI	 0.9550	 0.4570
DJ	 0.9550	 0.4320
DK	 0.9430	 0.4370

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Chain	Atom inclusion	Q-score
DL	 0.9660	 0.4410
DN	 0.9470	 0.4330
DO	 0.9280	 0.4120
DP	 0.9270	 0.4120
DQ	 0.9450	 0.4780
DR	 0.9570	 0.4880
DS	 0.9580	 0.4710
DU	 0.9620	 0.5070
DV	 0.8580	 0.3450
DW	 0.9160	 0.4180