



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:26 AM UTC

PDB ID : 1RVV / pdb_00001rvv
Title : SYNTHASE/RIBOFLAVIN SYNTHASE COMPLEX OF BACILLUS SUB-
TILIS
Authors : Ritsert, K.; Huber, R.; Turk, D.; Ladenstein, R.; Schmidt-Baese, K.; Bacher,
A.
Deposited on : 1995-10-25
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

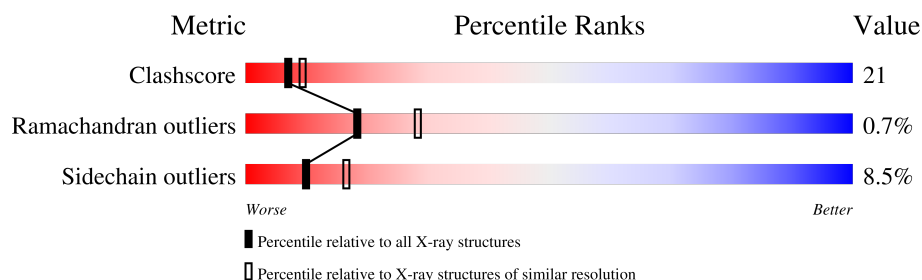
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

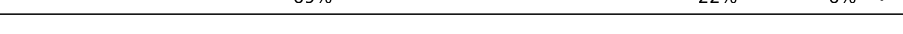
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	154	69% 23% 6% .
1	2	154	68% 23% 6% .
1	3	154	70% 21% 6% .
1	4	154	64% 27% 6% .
1	A	154	68% 23% 6% .
1	B	154	69% 23% 6% .
1	C	154	68% 24% 6% .
1	D	154	68% 23% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	154	 70% 21% 6% .
1	F	154	 67% 25% 6% .
1	G	154	 68% 23% 6% .
1	H	154	 71% 21% 6% .
1	I	154	 69% 23% 6% .
1	J	154	 67% 25% 5% .
1	K	154	 66% 25% 6% .
1	L	154	 69% 23% 6% .
1	M	154	 67% 25% 6% .
1	N	154	 68% 24% 6% .
1	O	154	 64% 28% 6% .
1	P	154	 67% 25% 6% .
1	Q	154	 68% 23% 6% .
1	R	154	 67% 25% 5% .
1	S	154	 69% 22% 6% .
1	T	154	 68% 24% 6% .
1	U	154	 68% 24% 6% .
1	V	154	 68% 23% 6% .
1	W	154	 69% 22% 6% .
1	X	154	 64% 28% 5% .
1	Y	154	 69% 23% 6% .
1	Z	154	 68% 24% 6% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	INI	1	200	-	X	-	-
3	INI	2	200	-	X	-	-
3	INI	3	200	-	X	-	-
3	INI	4	200	-	X	-	-
3	INI	A	200	-	X	-	-
3	INI	B	200	-	X	-	-
3	INI	C	200	-	X	-	-
3	INI	D	200	-	X	-	-
3	INI	E	200	-	X	-	-
3	INI	F	200	-	X	-	-
3	INI	G	200	-	X	-	-
3	INI	H	200	-	X	-	-
3	INI	I	200	-	X	-	-
3	INI	J	200	-	X	-	-
3	INI	K	200	-	X	-	-
3	INI	L	200	-	X	-	-
3	INI	M	200	-	X	-	-
3	INI	N	200	-	X	-	-
3	INI	O	200	-	X	-	-
3	INI	P	200	-	X	-	-
3	INI	Q	200	-	X	-	-
3	INI	R	200	-	X	-	-
3	INI	S	200	-	X	-	-
3	INI	T	200	-	X	-	-
3	INI	U	200	-	X	-	-
3	INI	V	200	-	X	-	-
3	INI	W	200	-	X	-	-
3	INI	X	200	-	X	-	-
3	INI	Y	200	-	X	-	-
3	INI	Z	200	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36150 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RIBOFLAVIN SYNTHASE.

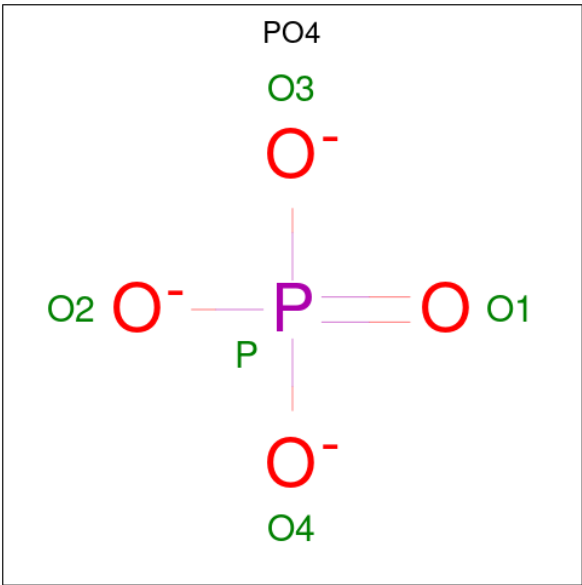
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	B	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	C	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	D	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	E	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	F	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	G	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	H	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	I	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	J	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	K	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	L	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	M	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	N	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	O	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			
1	P	154	Total	C	N	O	S	18	0	0
			1144	721	196	222	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	R	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	S	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	T	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	U	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	V	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	W	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	X	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	Y	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	Z	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	1	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	2	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	3	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0
1	4	154	Total 1144	C 721	N 196	O 222	S 5	18	0	0

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



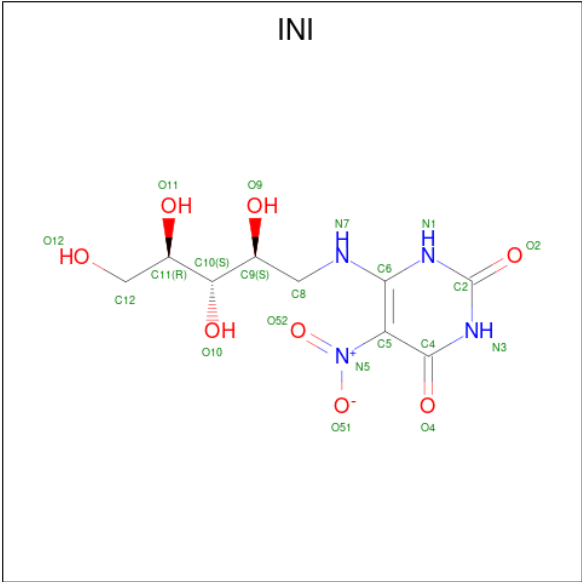
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	T	1	Total	O	P	0	0
			5	4	1		
2	U	1	Total	O	P	0	0
			5	4	1		
2	V	1	Total	O	P	0	0
			5	4	1		
2	W	1	Total	O	P	0	0
			5	4	1		
2	X	1	Total	O	P	0	0
			5	4	1		
2	Y	1	Total	O	P	0	0
			5	4	1		
2	Z	1	Total	O	P	0	0
			5	4	1		
2	1	1	Total	O	P	0	0
			5	4	1		
2	2	1	Total	O	P	0	0
			5	4	1		
2	3	1	Total	O	P	0	0
			5	4	1		
2	4	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 5-NITRO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (CCD ID: INI) (formula: C₉H₁₄N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	9	4	8		
3	B	1	Total	C	N	O	0	0
			21	9	4	8		
3	C	1	Total	C	N	O	0	0
			21	9	4	8		
3	D	1	Total	C	N	O	0	0
			21	9	4	8		
3	E	1	Total	C	N	O	0	0
			21	9	4	8		
3	F	1	Total	C	N	O	0	0
			21	9	4	8		
3	G	1	Total	C	N	O	0	0
			21	9	4	8		
3	H	1	Total	C	N	O	0	0
			21	9	4	8		
3	I	1	Total	C	N	O	0	0
			21	9	4	8		
3	J	1	Total	C	N	O	0	0
			21	9	4	8		
3	K	1	Total	C	N	O	0	0
			21	9	4	8		
3	L	1	Total	C	N	O	0	0
			21	9	4	8		
3	M	1	Total	C	N	O	0	0
			21	9	4	8		
3	N	1	Total	C	N	O	0	0
			21	9	4	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	1	Total	C	N	O	0	0
			21	9	4	8		
3	P	1	Total	C	N	O	0	0
			21	9	4	8		
3	Q	1	Total	C	N	O	0	0
			21	9	4	8		
3	R	1	Total	C	N	O	0	0
			21	9	4	8		
3	S	1	Total	C	N	O	0	0
			21	9	4	8		
3	T	1	Total	C	N	O	0	0
			21	9	4	8		
3	U	1	Total	C	N	O	0	0
			21	9	4	8		
3	V	1	Total	C	N	O	0	0
			21	9	4	8		
3	W	1	Total	C	N	O	0	0
			21	9	4	8		
3	X	1	Total	C	N	O	0	0
			21	9	4	8		
3	Y	1	Total	C	N	O	0	0
			21	9	4	8		
3	Z	1	Total	C	N	O	0	0
			21	9	4	8		
3	1	1	Total	C	N	O	0	0
			21	9	4	8		
3	2	1	Total	C	N	O	0	0
			21	9	4	8		
3	3	1	Total	C	N	O	0	0
			21	9	4	8		
3	4	1	Total	C	N	O	0	0
			21	9	4	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	38	Total	O	0	0
			38	38		
4	B	31	Total	O	0	0
			31	31		
4	C	36	Total	O	0	0
			36	36		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	35	Total 35	O 35	0	0
4	E	35	Total 35	O 35	0	0
4	F	35	Total 35	O 35	0	0
4	G	38	Total 38	O 38	0	0
4	H	35	Total 35	O 35	0	0
4	I	31	Total 31	O 31	0	0
4	J	34	Total 34	O 34	0	0
4	K	39	Total 39	O 39	0	0
4	L	35	Total 35	O 35	0	0
4	M	35	Total 35	O 35	0	0
4	N	32	Total 32	O 32	0	0
4	O	36	Total 36	O 36	0	0
4	P	38	Total 38	O 38	0	0
4	Q	32	Total 32	O 32	0	0
4	R	34	Total 34	O 34	0	0
4	S	32	Total 32	O 32	0	0
4	T	34	Total 34	O 34	0	0
4	U	36	Total 36	O 36	0	0
4	V	39	Total 39	O 39	0	0
4	W	35	Total 35	O 35	0	0
4	X	33	Total 33	O 33	0	0

Continued on next page...

Continued from previous page...

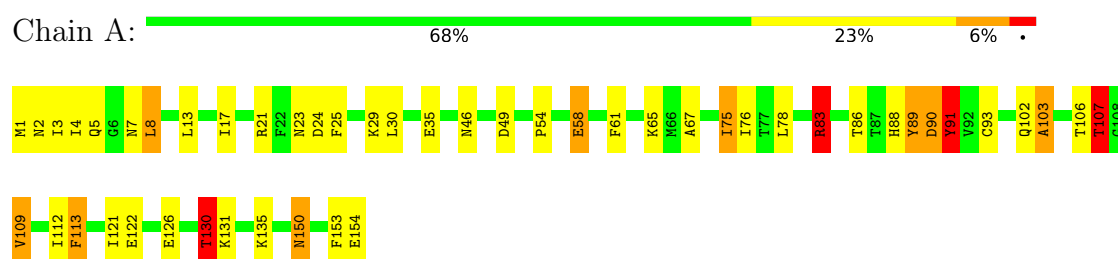
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Y	37	Total 37	O 37	0	0
4	Z	38	Total 38	O 38	0	0
4	1	35	Total 35	O 35	0	0
4	2	35	Total 35	O 35	0	0
4	3	32	Total 32	O 32	0	0
4	4	35	Total 35	O 35	0	0

3 Residue-property plots [i](#)

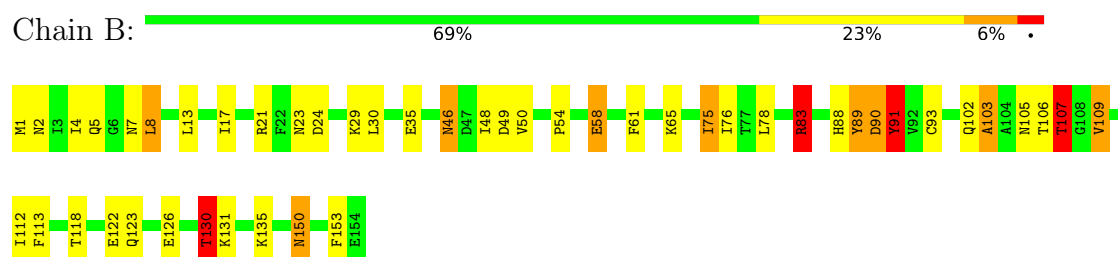
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

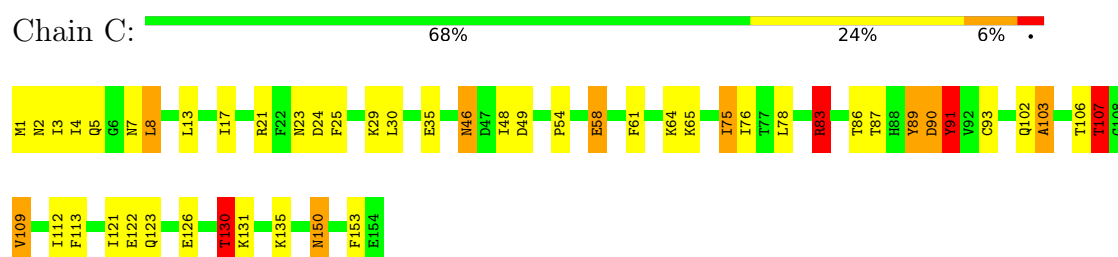
• Molecule 1: RIBOFLAVIN SYNTHASE



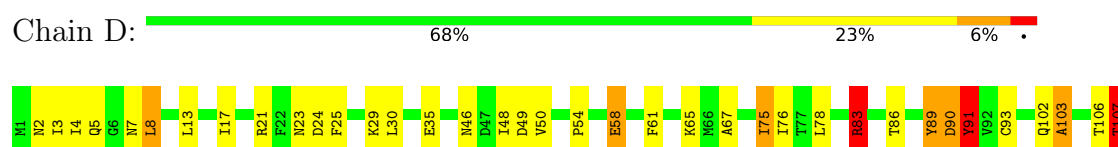
• Molecule 1: RIBOFLAVIN SYNTHASE



• Molecule 1: RIBOFLAVIN SYNTHASE



• Molecule 1: RIBOFLAVIN SYNTHASE





• Molecule 1: RIBOFLAVIN SYNTHASE

Chain E: 70% 21% 6% .



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain F: 67% 25% 6% .



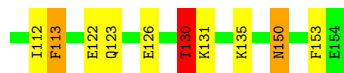
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain G: 68% 23% 6% .



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain H: 71% 21% 6% .



• Molecule 1: RIBOFLAVIN SYNTHASE

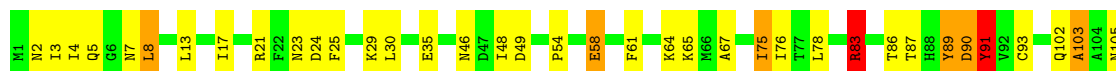
Chain I: 69% 23% 6% .





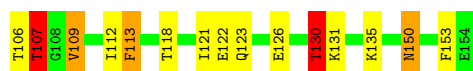
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain J: 67% 25% 5%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain K: 66% 25% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain L: 69% 23% 6%



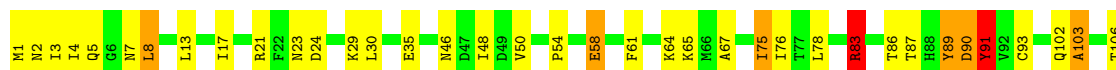
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain M: 67% 25% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

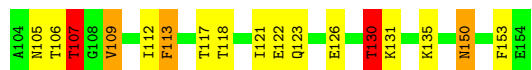
Chain N: 68% 24% 6%





• Molecule 1: RIBOFLAVIN SYNTHASE

Chain O: 64% 28% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain P: 67% 25% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain Q: 68% 23% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain R: 67% 25% 5%



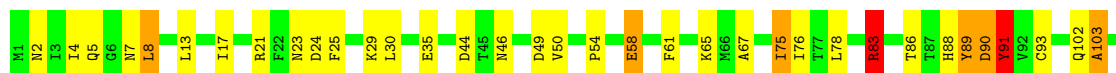
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain S: 69% 22% 6%





• Molecule 1: RIBOFLAVIN SYNTHASE



• Molecule 1: RIBOFLAVIN SYNTHASE



• Molecule 1: RIBOFLAVIN SYNTHASE



• Molecule 1: RIBOFLAVIN SYNTHASE



• Molecule 1: RIBOFLAVIN SYNTHASE





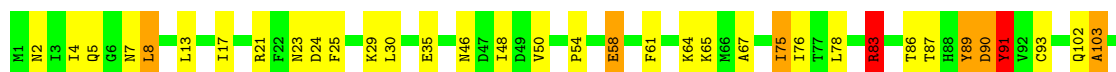
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain Y: 69% 23% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain Z: 68% 24% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

Chain 1: 69% 23% 6%



• Molecule 1: RIBOFLAVIN SYNTHASE

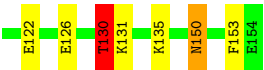
Chain 2: 68% 23% 6%



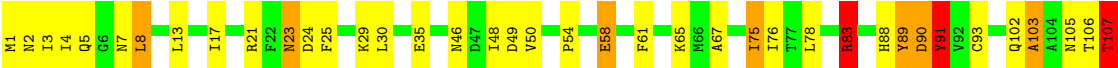
• Molecule 1: RIBOFLAVIN SYNTHASE

Chain 3: 70% 21% 6%





● Molecule 1: RIBOFLAVIN SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.90Å 192.60Å 168.60Å 90.00° 134.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.237 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36150	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, INI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.96	0/1159	1.77	19/1569 (1.2%)
1	2	0.96	0/1159	1.77	19/1569 (1.2%)
1	3	0.96	0/1159	1.77	19/1569 (1.2%)
1	4	0.96	0/1159	1.77	19/1569 (1.2%)
1	A	0.96	0/1159	1.77	19/1569 (1.2%)
1	B	0.96	0/1159	1.77	19/1569 (1.2%)
1	C	0.96	0/1159	1.77	19/1569 (1.2%)
1	D	0.96	0/1159	1.77	19/1569 (1.2%)
1	E	0.96	0/1159	1.77	19/1569 (1.2%)
1	F	0.96	0/1159	1.77	19/1569 (1.2%)
1	G	0.96	0/1159	1.77	19/1569 (1.2%)
1	H	0.96	0/1159	1.77	19/1569 (1.2%)
1	I	0.96	0/1159	1.77	19/1569 (1.2%)
1	J	0.96	0/1159	1.77	19/1569 (1.2%)
1	K	0.96	0/1159	1.77	19/1569 (1.2%)
1	L	0.96	0/1159	1.77	19/1569 (1.2%)
1	M	0.96	0/1159	1.77	19/1569 (1.2%)
1	N	0.96	0/1159	1.77	19/1569 (1.2%)
1	O	0.96	0/1159	1.77	19/1569 (1.2%)
1	P	0.96	0/1159	1.77	19/1569 (1.2%)
1	Q	0.96	0/1159	1.77	19/1569 (1.2%)
1	R	0.96	0/1159	1.77	19/1569 (1.2%)
1	S	0.96	0/1159	1.77	19/1569 (1.2%)
1	T	0.96	0/1159	1.77	19/1569 (1.2%)
1	U	0.96	0/1159	1.77	19/1569 (1.2%)
1	V	0.96	0/1159	1.77	19/1569 (1.2%)
1	W	0.96	0/1159	1.77	19/1569 (1.2%)
1	X	0.96	0/1159	1.77	19/1569 (1.2%)
1	Y	0.96	0/1159	1.77	19/1569 (1.2%)
1	Z	0.96	0/1159	1.77	19/1569 (1.2%)
All	All	0.96	0/34770	1.77	570/47070 (1.2%)

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	1	0	2
1	2	0	2
1	3	0	2
1	4	0	2
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
1	Z	0	2
All	All	0	60

There are no bond length outliers.

The worst 5 of 570 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	46	ASN	CA-CB-CG	-8.80	103.80	112.60
1	D	46	ASN	CA-CB-CG	-8.78	103.82	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	46	ASN	CA-CB-CG	-8.78	103.82	112.60
1	E	46	ASN	CA-CB-CG	-8.76	103.84	112.60
1	J	46	ASN	CA-CB-CG	-8.76	103.84	112.60

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	ARG	Sidechain
1	A	91	TYR	Sidechain
1	B	83	ARG	Sidechain
1	B	91	TYR	Sidechain
1	C	83	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1144	0	1157	68	0
1	2	1144	0	1157	75	0
1	3	1144	0	1157	67	0
1	4	1144	0	1157	93	0
1	A	1144	0	1157	65	1
1	B	1144	0	1157	69	0
1	C	1144	0	1157	84	0
1	D	1144	0	1157	80	0
1	E	1144	0	1157	76	0
1	F	1144	0	1157	88	0
1	G	1144	0	1157	85	1
1	H	1144	0	1157	61	0
1	I	1144	0	1157	69	0
1	J	1144	0	1157	80	0
1	K	1144	0	1157	84	0
1	L	1144	0	1157	63	0
1	M	1144	0	1157	69	0
1	N	1144	0	1157	71	1
1	O	1144	0	1157	91	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1144	0	1157	65	0
1	Q	1144	0	1157	72	0
1	R	1144	0	1156	79	0
1	S	1144	0	1155	70	0
1	T	1144	0	1157	79	1
1	U	1144	0	1156	72	0
1	V	1144	0	1156	73	0
1	W	1144	0	1157	68	0
1	X	1144	0	1157	85	0
1	Y	1144	0	1157	88	0
1	Z	1144	0	1157	81	1
2	1	5	0	0	0	0
2	2	5	0	0	0	0
2	3	5	0	0	0	0
2	4	5	0	0	0	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
2	U	5	0	0	0	0
2	V	5	0	0	0	0
2	W	5	0	0	0	0
2	X	5	0	0	0	0
2	Y	5	0	0	0	0
2	Z	5	0	0	0	0
3	1	21	0	14	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	21	0	14	1	0
3	3	21	0	14	5	0
3	4	21	0	14	1	0
3	A	21	0	14	3	0
3	B	21	0	14	1	0
3	C	21	0	14	1	0
3	D	21	0	14	1	0
3	E	21	0	14	3	0
3	F	21	0	14	1	0
3	G	21	0	14	3	0
3	H	21	0	14	4	0
3	I	21	0	14	2	0
3	J	21	0	14	1	0
3	K	21	0	14	2	0
3	L	21	0	14	3	0
3	M	21	0	14	1	0
3	N	21	0	14	2	0
3	O	21	0	14	3	0
3	P	21	0	14	1	0
3	Q	21	0	14	1	0
3	R	21	0	14	2	0
3	S	21	0	14	1	0
3	T	21	0	14	3	0
3	U	21	0	14	3	0
3	V	21	0	14	1	0
3	W	21	0	14	5	0
3	X	21	0	14	2	0
3	Y	21	0	14	1	0
3	Z	21	0	14	3	0
4	1	35	0	0	6	2
4	2	35	0	0	6	0
4	3	32	0	0	2	0
4	4	35	0	0	6	1
4	A	38	0	0	6	0
4	B	31	0	0	6	1
4	C	36	0	0	6	0
4	D	35	0	0	6	0
4	E	35	0	0	1	0
4	F	35	0	0	6	0
4	G	38	0	0	6	1
4	H	35	0	0	6	0
4	I	31	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	34	0	0	6	1
4	K	39	0	0	2	0
4	L	35	0	0	6	1
4	M	35	0	0	6	0
4	N	32	0	0	2	0
4	O	36	0	0	6	1
4	P	38	0	0	6	0
4	Q	32	0	0	5	0
4	R	34	0	0	11	0
4	S	32	0	0	5	0
4	T	34	0	0	6	1
4	U	36	0	0	6	0
4	V	39	0	0	6	0
4	W	35	0	0	6	0
4	X	33	0	0	6	0
4	Y	37	0	0	3	0
4	Z	38	0	0	3	1
All	All	36150	0	35125	1443	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 1443 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:5:GLN:HE21	1:W:21:ARG:NH2	1.05	1.47
1:X:5:GLN:HE21	1:Y:21:ARG:NH2	1.09	1.47
1:C:5:GLN:NE2	1:D:21:ARG:HH22	1.13	1.46
1:K:21:ARG:HH22	1:O:5:GLN:NE2	1.15	1.45
1:2:5:GLN:HE21	1:3:21:ARG:NH2	1.06	1.45

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:ASP:CA	4:1:930:HOH:O[3_555]	1.02	1.18
4:L:405:HOH:O	4:T:665:HOH:O[3_454]	1.30	0.90
1:A:154:GLU:OE2	4:4:1035:HOH:O[4_556]	1.65	0.55
1:O:44:ASP:N	4:1:930:HOH:O[3_555]	1.70	0.50
1:O:45:THR:CG2	4:Z:928:HOH:O[3_555]	1.80	0.40

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	2	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	3	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	4	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	A	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	B	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	C	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	D	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	18	28
1	E	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	F	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	G	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	H	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	I	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	J	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	K	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	L	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	M	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	N	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	O	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	P	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	Q	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	R	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	S	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	T	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	U	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	X	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	18	28
1	Y	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
1	Z	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
All	All	4560/4620 (99%)	4438 (97%)	92 (2%)	30 (1%)	18	28

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	TYR
1	B	89	TYR
1	C	89	TYR
1	D	89	TYR
1	E	89	TYR

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	2	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	3	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	4	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	A	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	B	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	C	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	D	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	E	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	F	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	G	118/118 (100%)	108 (92%)	10 (8%)	10	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	I	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	J	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	K	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	L	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	M	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	N	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	O	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	P	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	Q	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	R	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	S	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	T	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	U	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	V	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	W	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	X	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	Y	118/118 (100%)	108 (92%)	10 (8%)	10	16
1	Z	118/118 (100%)	108 (92%)	10 (8%)	10	16
All	All	3540/3540 (100%)	3240 (92%)	300 (8%)	10	16

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	13	LEU
1	3	107	THR
1	X	130	THR
1	1	8	LEU
1	J	122	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 199 such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	150	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	88	HIS
1	R	105	ASN
1	T	88	HIS
1	W	102	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	$\# Z > 2$
2	PO4	O	500	-	4,4,4	1.12	0	6,6,6	0.41	0
3	INI	4	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	K	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.75	11 (52%)
2	PO4	D	500	-	4,4,4	1.12	0	6,6,6	0.42	0
3	INI	C	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	Y	200	-	19,21,21	2.88	8 (42%)	21,29,29	3.75	11 (52%)
3	INI	P	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	Q	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	INI	B	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	3	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	G	500	-	4,4,4	1.12	0	6,6,6	0.42	0
2	PO4	P	500	-	4,4,4	1.13	0	6,6,6	0.42	0
2	PO4	E	500	-	4,4,4	1.11	0	6,6,6	0.42	0
2	PO4	3	500	-	4,4,4	1.13	0	6,6,6	0.42	0
3	INI	Z	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	E	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	Y	500	-	4,4,4	1.12	0	6,6,6	0.41	0
2	PO4	X	500	-	4,4,4	1.11	0	6,6,6	0.42	0
2	PO4	2	500	-	4,4,4	1.11	0	6,6,6	0.41	0
2	PO4	Q	500	-	4,4,4	1.11	0	6,6,6	0.42	0
3	INI	D	200	-	19,21,21	2.88	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	2	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.75	11 (52%)
2	PO4	B	500	-	4,4,4	1.12	0	6,6,6	0.41	0
3	INI	G	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	1	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.75	11 (52%)
2	PO4	U	500	-	4,4,4	1.13	0	6,6,6	0.42	0
3	INI	A	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	N	500	-	4,4,4	1.12	0	6,6,6	0.41	0
3	INI	M	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.75	11 (52%)
3	INI	O	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	W	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	R	500	-	4,4,4	1.13	0	6,6,6	0.42	0
2	PO4	W	500	-	4,4,4	1.11	0	6,6,6	0.41	0
3	INI	F	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	F	500	-	4,4,4	1.13	0	6,6,6	0.41	0
2	PO4	V	500	-	4,4,4	1.13	0	6,6,6	0.41	0
3	INI	S	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	V	200	-	19,21,21	2.88	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	L	500	-	4,4,4	1.12	0	6,6,6	0.42	0
2	PO4	S	500	-	4,4,4	1.12	0	6,6,6	0.41	0
3	INI	J	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.75	11 (52%)
2	PO4	K	500	-	4,4,4	1.12	0	6,6,6	0.41	0
2	PO4	C	500	-	4,4,4	1.13	0	6,6,6	0.41	0
3	INI	I	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.75	11 (52%)
2	PO4	4	500	-	4,4,4	1.11	0	6,6,6	0.41	0
3	INI	X	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	INI	R	200	-	19,21,21	2.90	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	H	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	H	500	-	4,4,4	1.12	0	6,6,6	0.42	0
2	PO4	J	500	-	4,4,4	1.12	0	6,6,6	0.41	0
3	INI	N	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
3	INI	U	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	I	500	-	4,4,4	1.12	0	6,6,6	0.41	0
3	INI	T	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	Z	500	-	4,4,4	1.12	0	6,6,6	0.41	0
2	PO4	T	500	-	4,4,4	1.12	0	6,6,6	0.41	0
2	PO4	A	500	-	4,4,4	1.12	0	6,6,6	0.41	0
2	PO4	M	500	-	4,4,4	1.12	0	6,6,6	0.41	0
3	INI	L	200	-	19,21,21	2.89	8 (42%)	21,29,29	3.74	11 (52%)
2	PO4	1	500	-	4,4,4	1.12	0	6,6,6	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	INI	4	200	-	-	10/17/19/19	0/1/1/1
3	INI	K	200	-	-	10/17/19/19	0/1/1/1
3	INI	C	200	-	-	10/17/19/19	0/1/1/1
3	INI	Y	200	-	-	10/17/19/19	0/1/1/1
3	INI	P	200	-	-	10/17/19/19	0/1/1/1
3	INI	Q	200	-	-	10/17/19/19	0/1/1/1
3	INI	B	200	-	-	10/17/19/19	0/1/1/1
3	INI	3	200	-	-	10/17/19/19	0/1/1/1
3	INI	Z	200	-	-	10/17/19/19	0/1/1/1
3	INI	E	200	-	-	10/17/19/19	0/1/1/1
3	INI	D	200	-	-	10/17/19/19	0/1/1/1
3	INI	2	200	-	-	10/17/19/19	0/1/1/1
3	INI	G	200	-	-	10/17/19/19	0/1/1/1
3	INI	1	200	-	-	10/17/19/19	0/1/1/1
3	INI	A	200	-	-	10/17/19/19	0/1/1/1
3	INI	O	200	-	-	10/17/19/19	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	INI	M	200	-	-	10/17/19/19	0/1/1/1
3	INI	W	200	-	-	10/17/19/19	0/1/1/1
3	INI	F	200	-	-	10/17/19/19	0/1/1/1
3	INI	S	200	-	-	10/17/19/19	0/1/1/1
3	INI	V	200	-	-	10/17/19/19	0/1/1/1
3	INI	J	200	-	-	10/17/19/19	0/1/1/1
3	INI	I	200	-	-	10/17/19/19	0/1/1/1
3	INI	X	200	-	-	10/17/19/19	0/1/1/1
3	INI	R	200	-	-	10/17/19/19	0/1/1/1
3	INI	H	200	-	-	10/17/19/19	0/1/1/1
3	INI	N	200	-	-	10/17/19/19	0/1/1/1
3	INI	U	200	-	-	10/17/19/19	0/1/1/1
3	INI	T	200	-	-	10/17/19/19	0/1/1/1
3	INI	L	200	-	-	10/17/19/19	0/1/1/1

The worst 5 of 240 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	200	INI	C11-C10	7.46	1.66	1.53
3	S	200	INI	C11-C10	7.46	1.66	1.53
3	4	200	INI	C11-C10	7.46	1.66	1.53
3	3	200	INI	C11-C10	7.45	1.66	1.53
3	X	200	INI	C11-C10	7.45	1.66	1.53

The worst 5 of 330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	200	INI	C12-C11-C10	8.62	129.73	112.17
3	Y	200	INI	C12-C11-C10	8.61	129.73	112.17
3	2	200	INI	C12-C11-C10	8.61	129.71	112.17
3	J	200	INI	C12-C11-C10	8.61	129.71	112.17
3	3	200	INI	C12-C11-C10	8.60	129.71	112.17

There are no chirality outliers.

5 of 300 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	200	INI	N1-C6-N7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	200	INI	C5-C6-N7-C8
3	A	200	INI	C9-C10-C11-O11
3	A	200	INI	C9-C10-C11-C12
3	A	200	INI	O10-C10-C11-O11

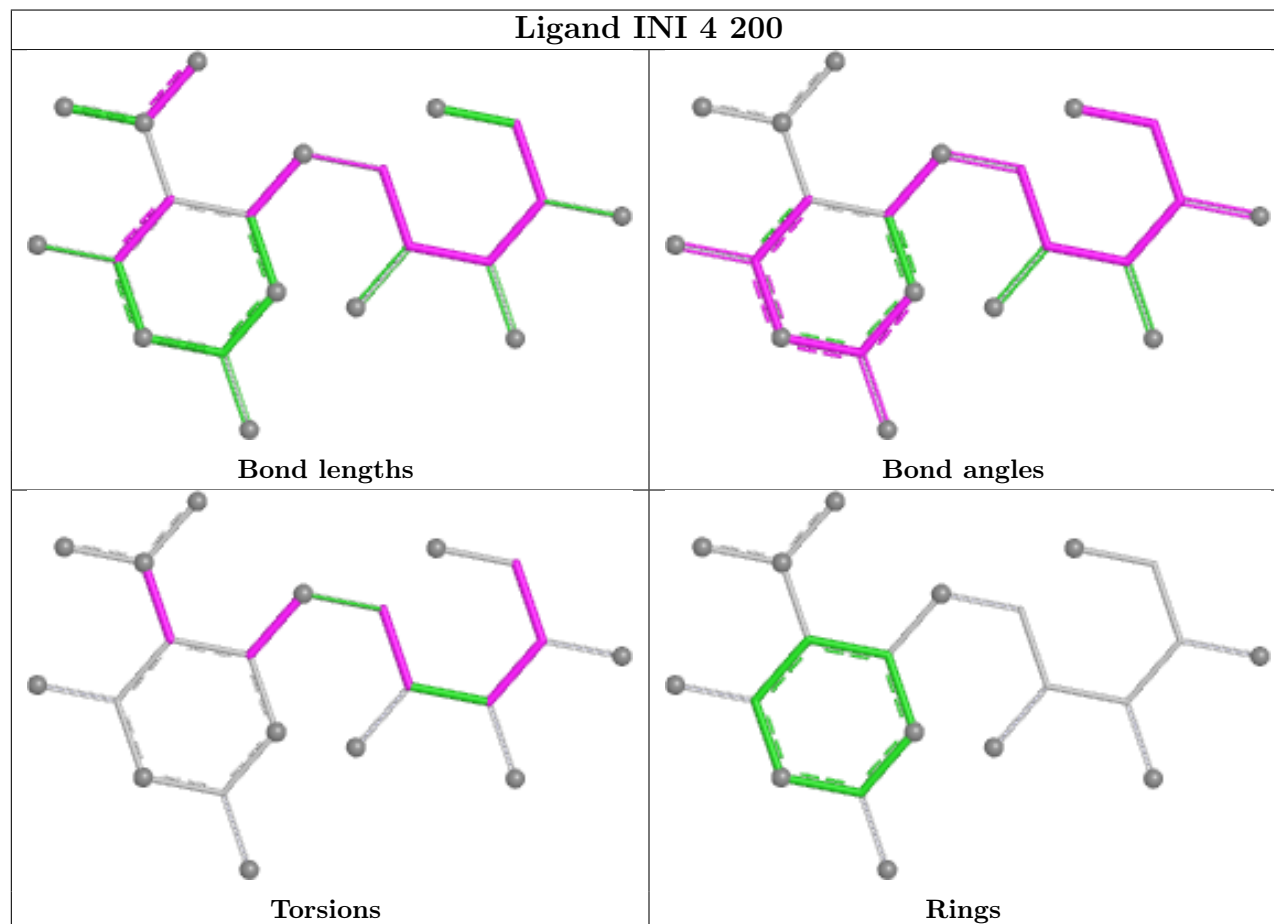
There are no ring outliers.

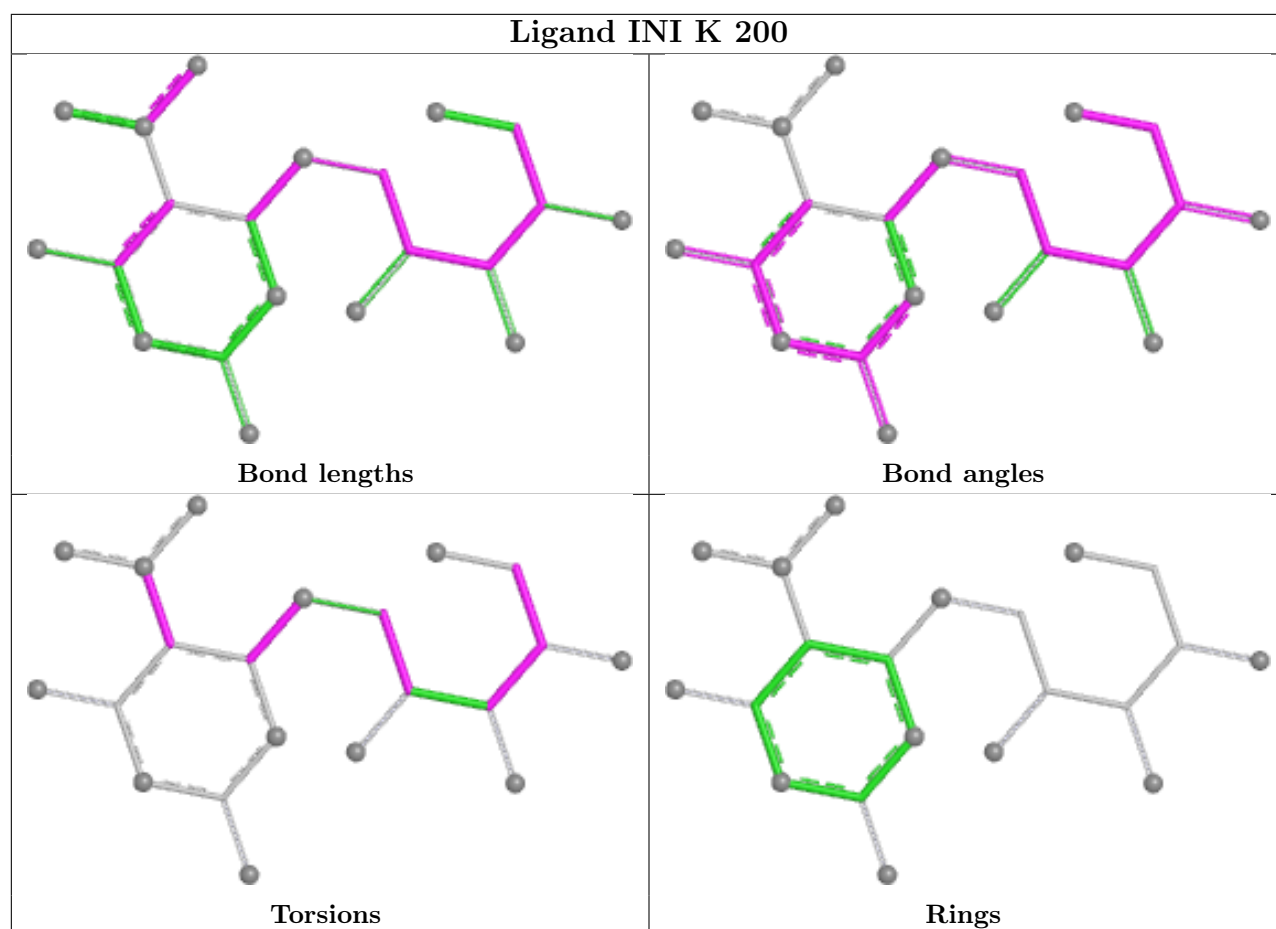
30 monomers are involved in 63 short contacts:

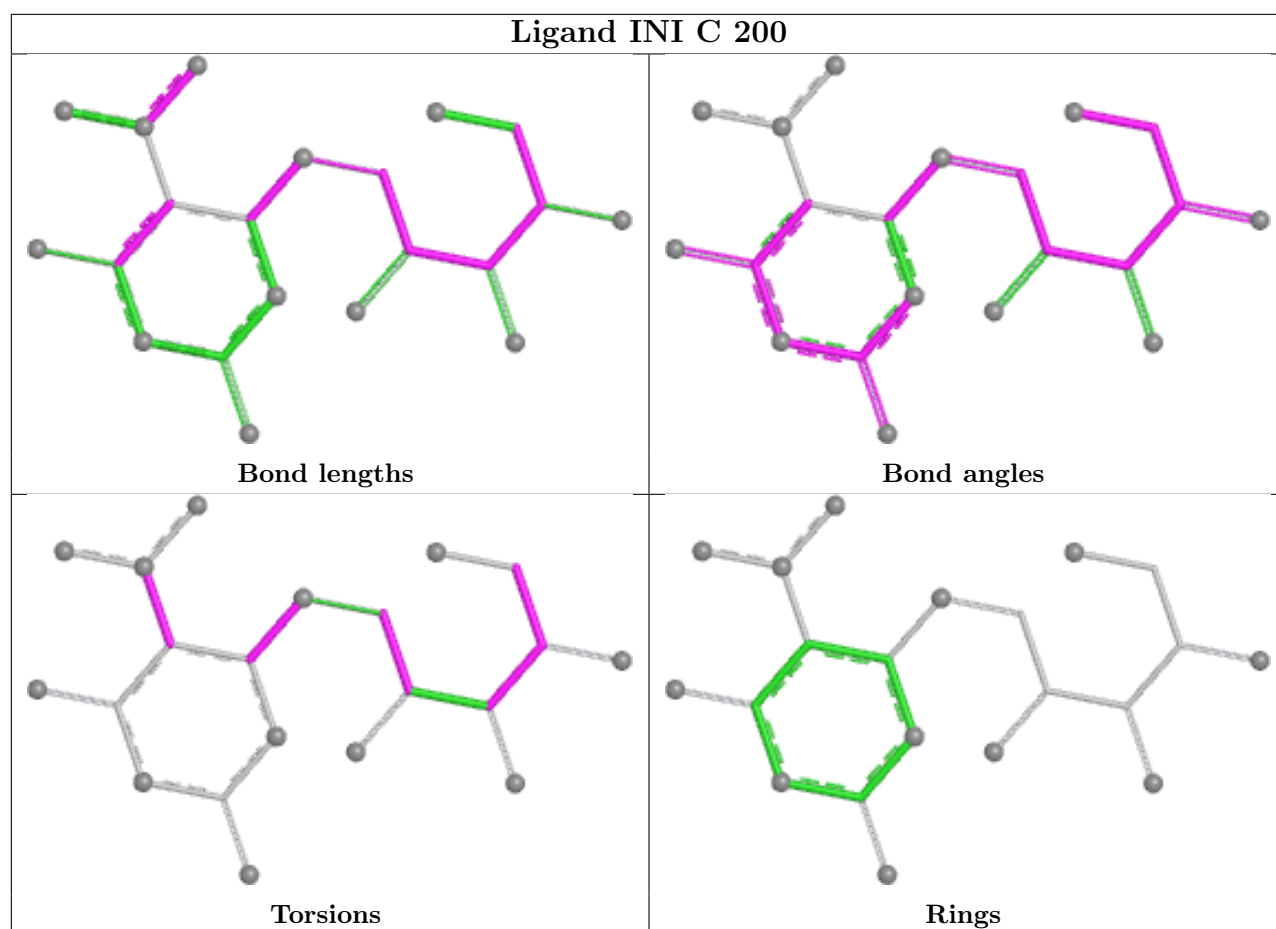
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	200	INI	1	0
3	K	200	INI	2	0
3	C	200	INI	1	0
3	Y	200	INI	1	0
3	P	200	INI	1	0
3	Q	200	INI	1	0
3	B	200	INI	1	0
3	3	200	INI	5	0
3	Z	200	INI	3	0
3	E	200	INI	3	0
3	D	200	INI	1	0
3	2	200	INI	1	0
3	G	200	INI	3	0
3	1	200	INI	2	0
3	A	200	INI	3	0
3	M	200	INI	1	0
3	O	200	INI	3	0
3	W	200	INI	5	0
3	F	200	INI	1	0
3	S	200	INI	1	0
3	V	200	INI	1	0
3	J	200	INI	1	0
3	I	200	INI	2	0
3	X	200	INI	2	0
3	R	200	INI	2	0
3	H	200	INI	4	0
3	N	200	INI	2	0
3	U	200	INI	3	0
3	T	200	INI	3	0
3	L	200	INI	3	0

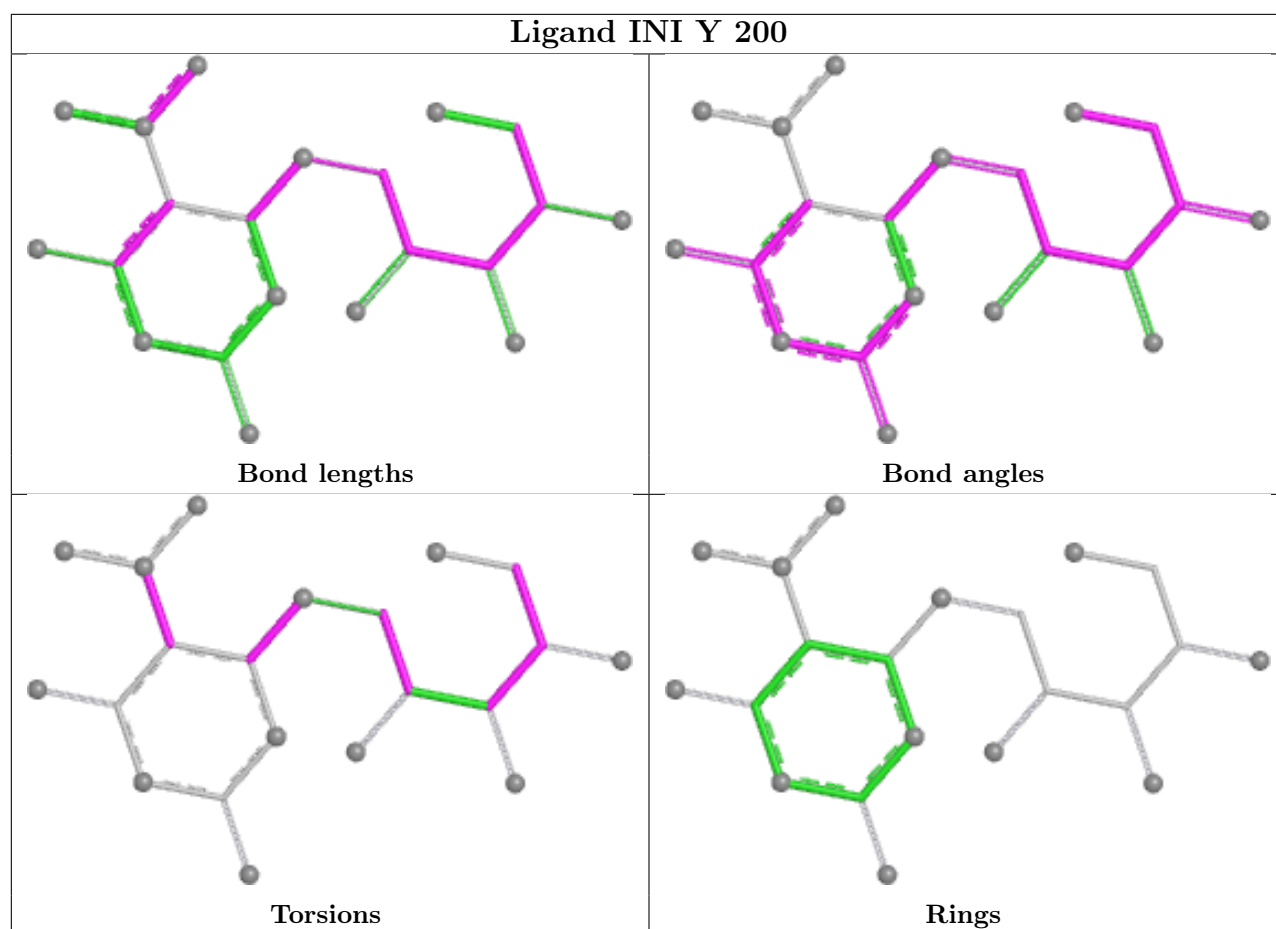
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

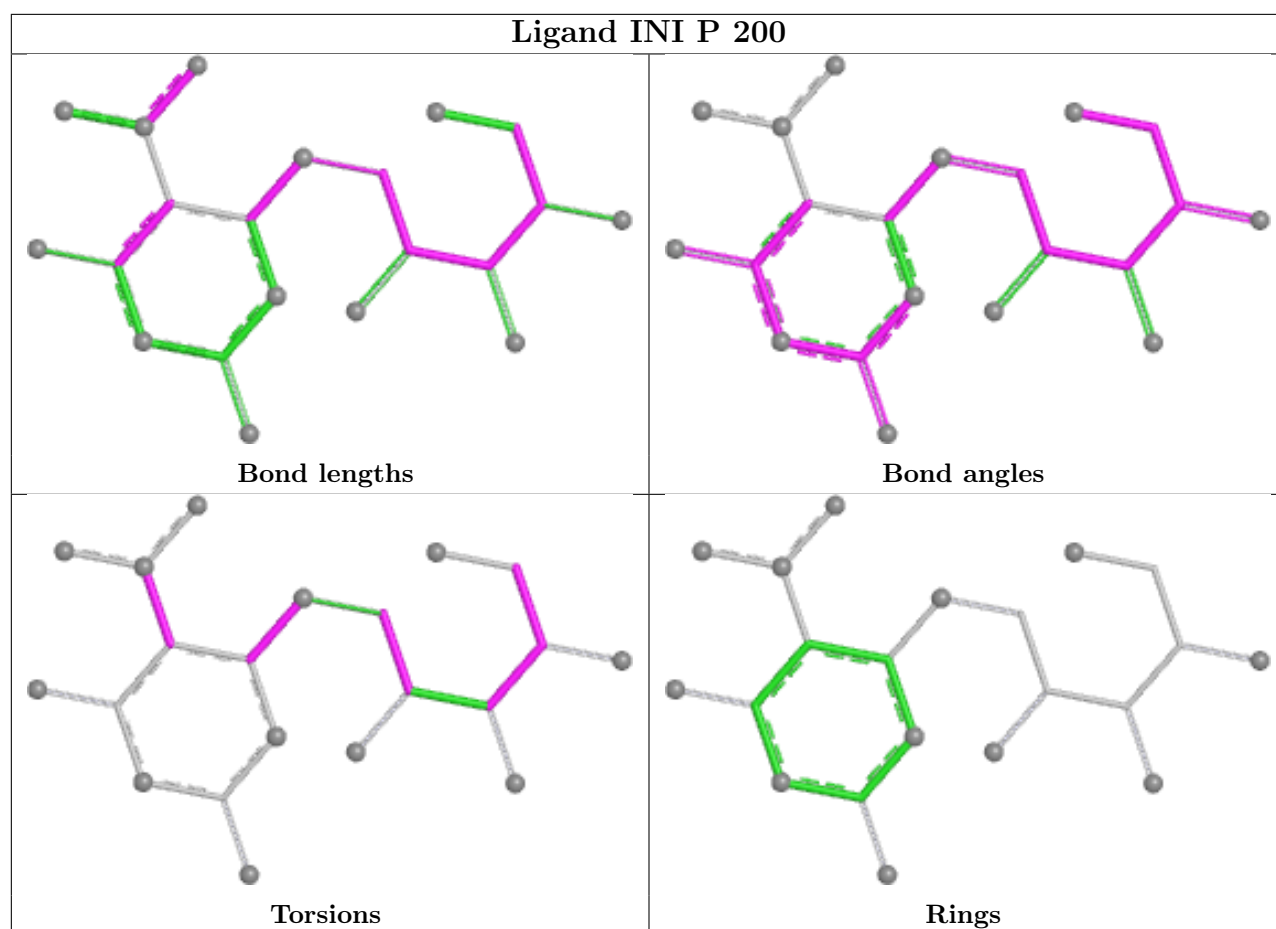
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

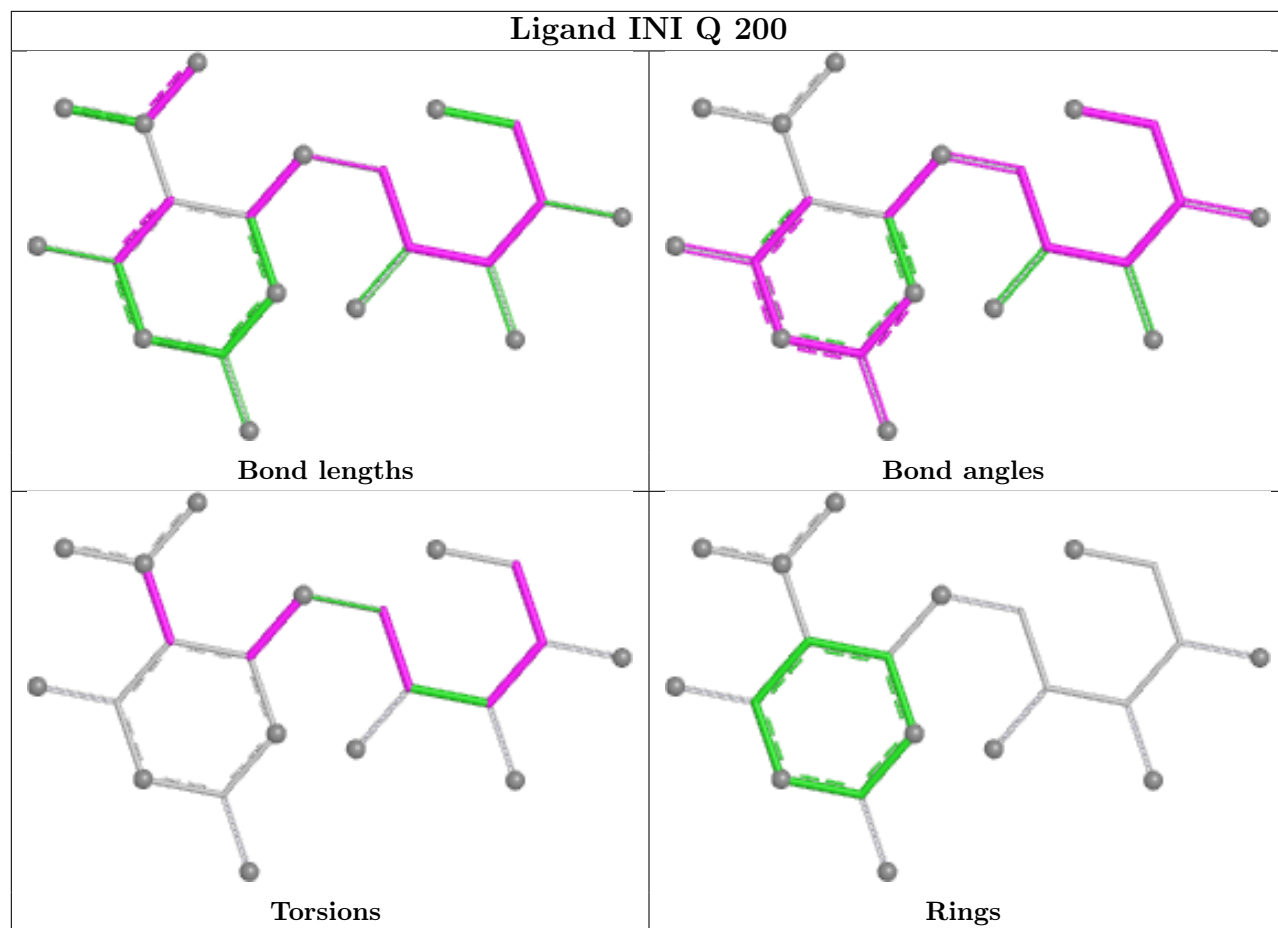


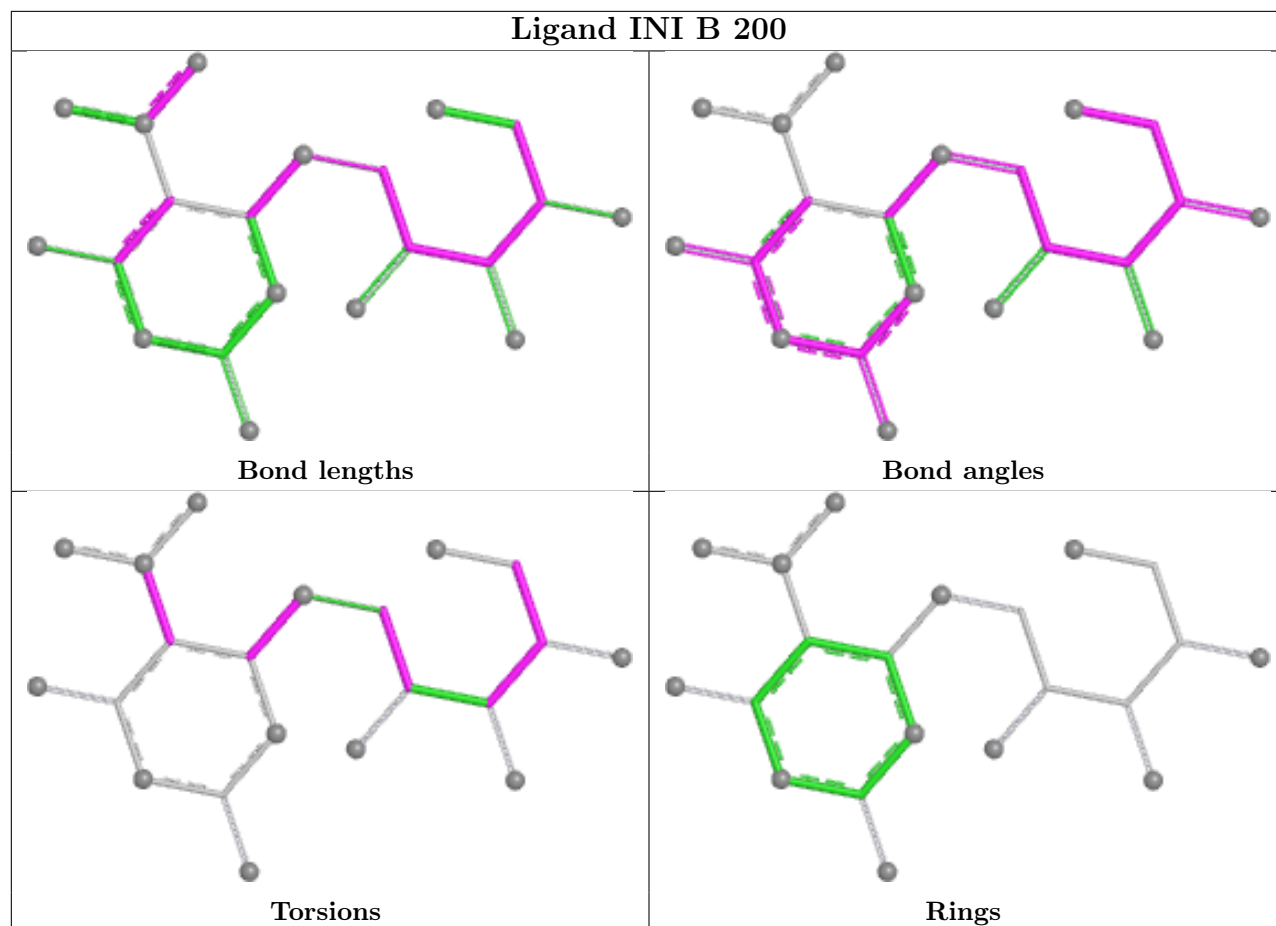


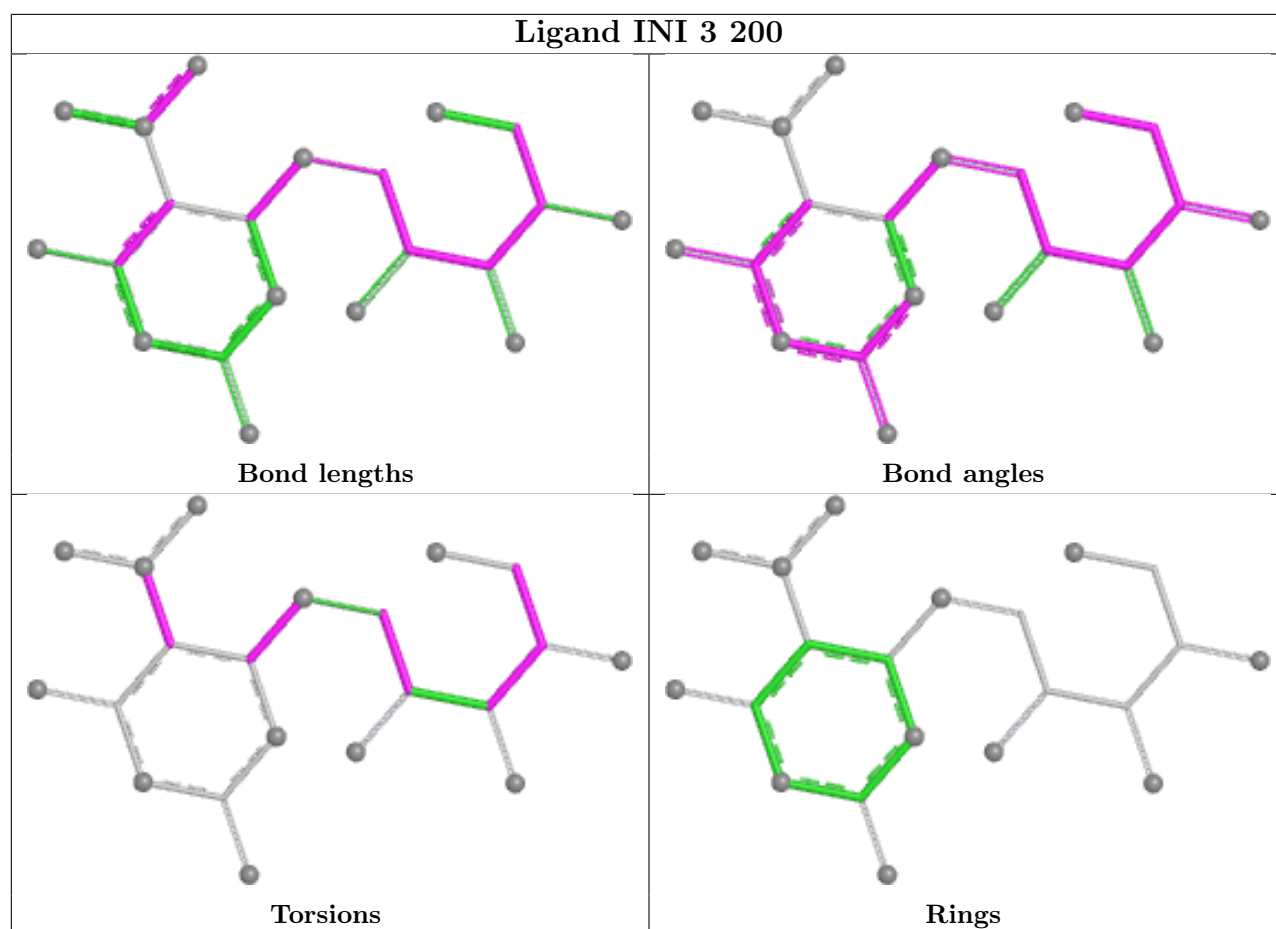


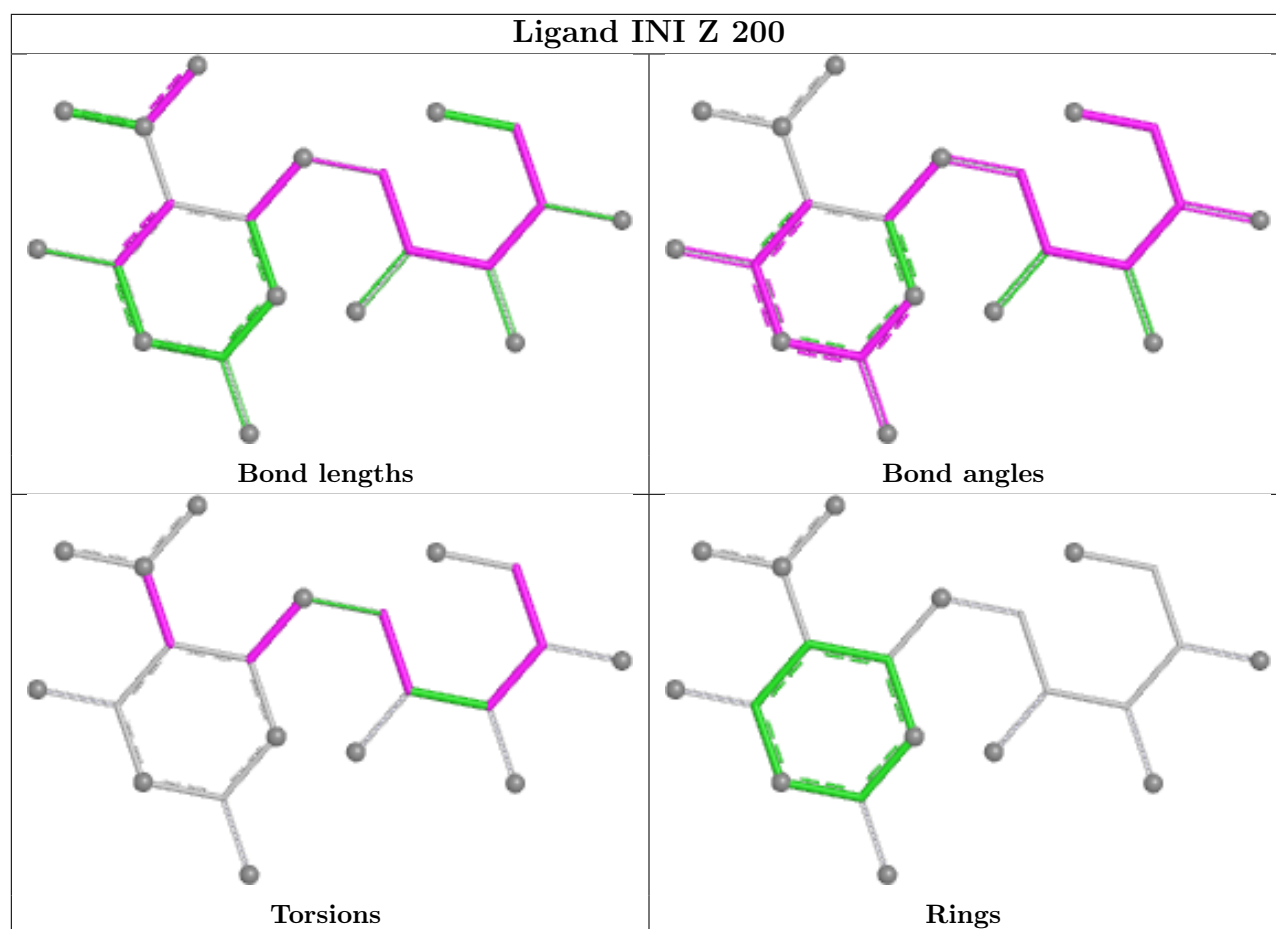


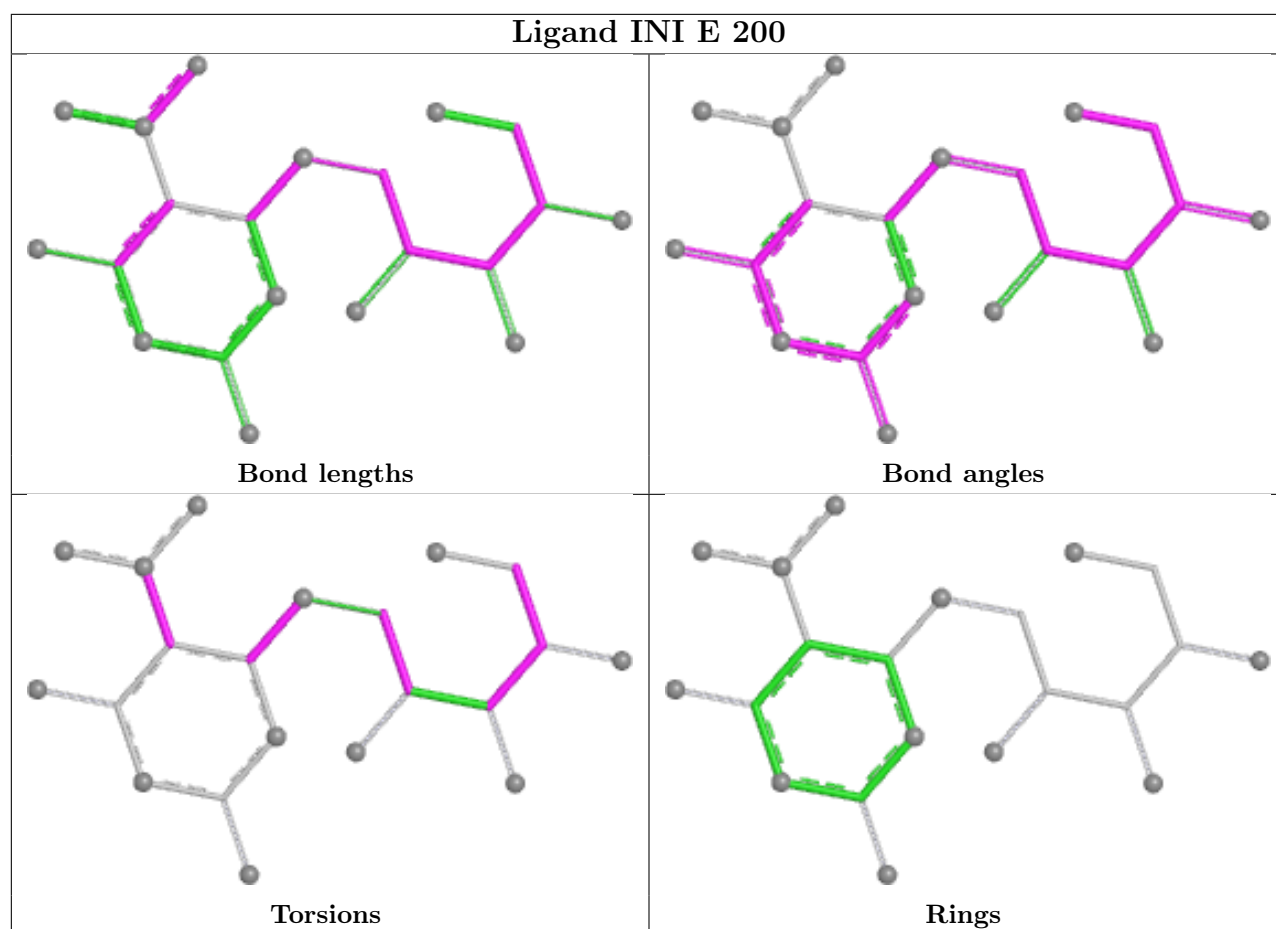


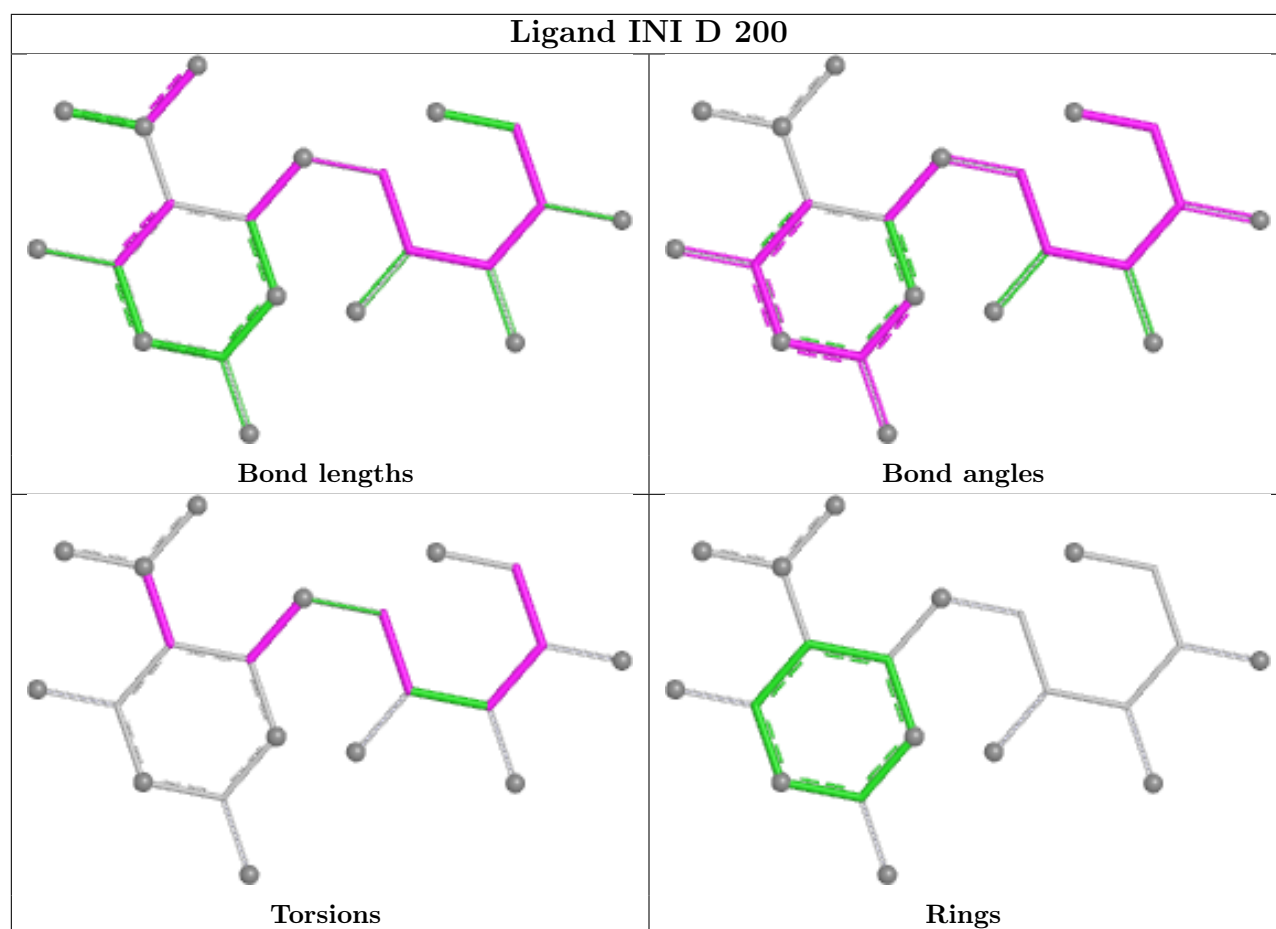


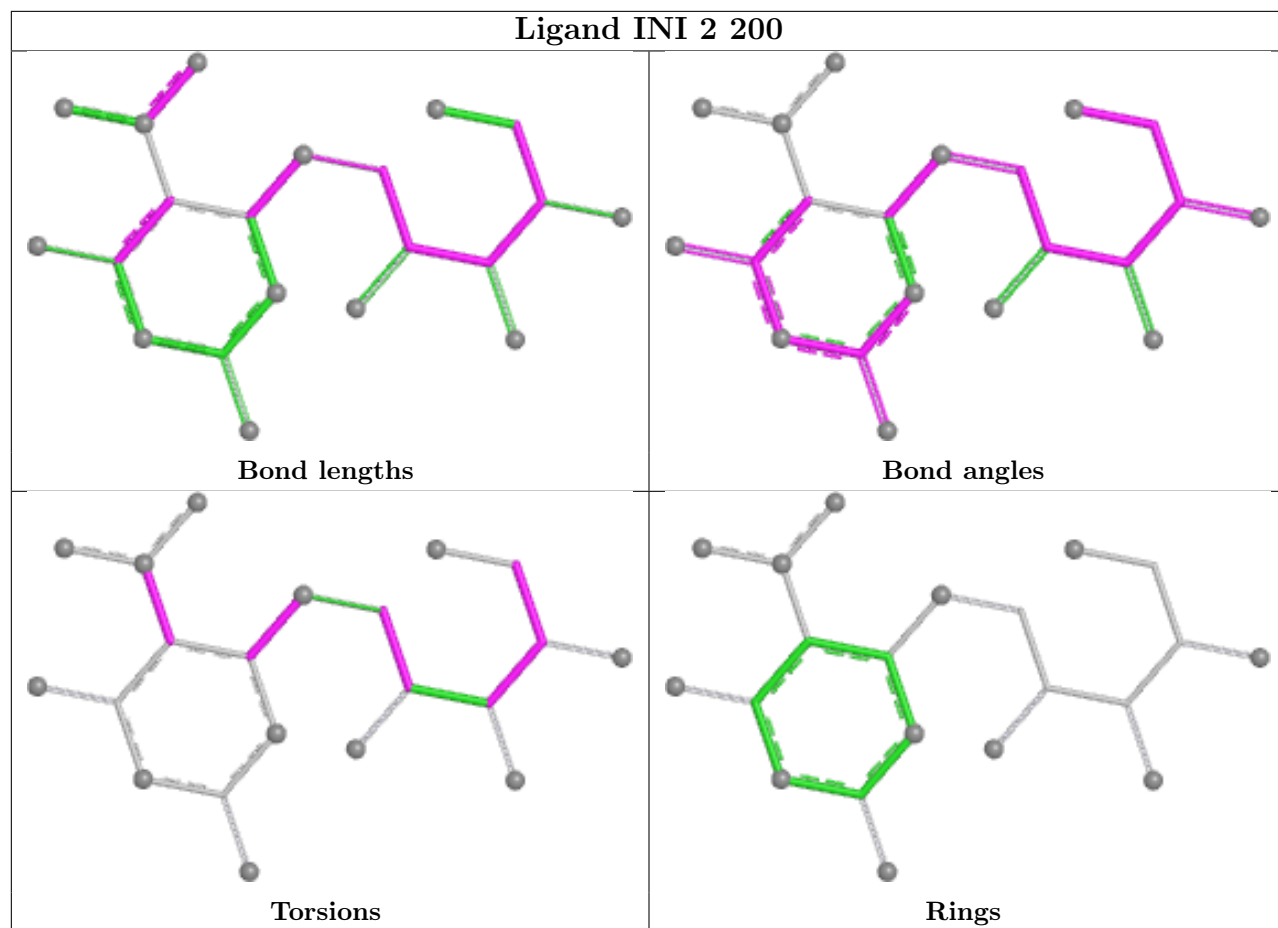


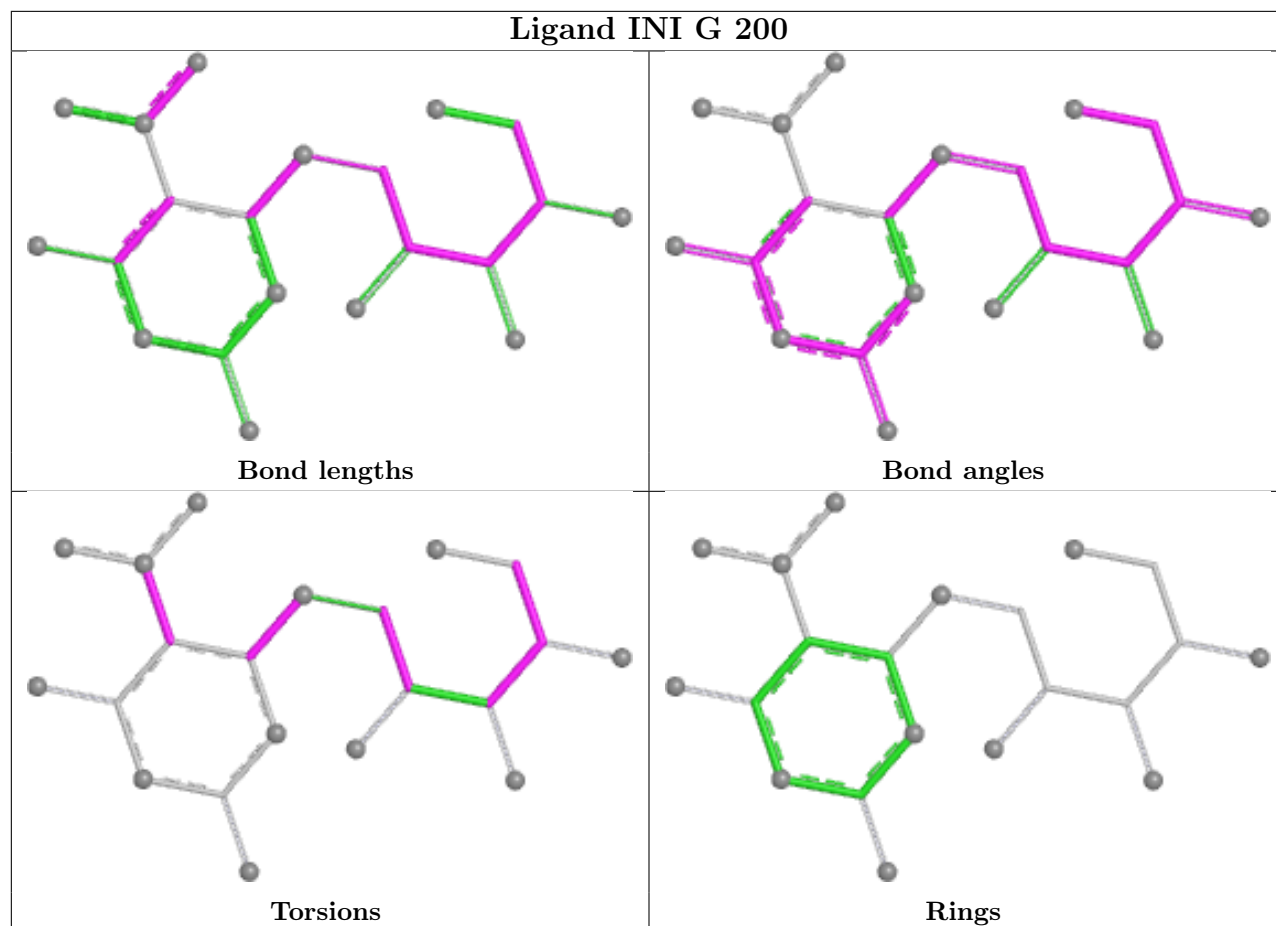


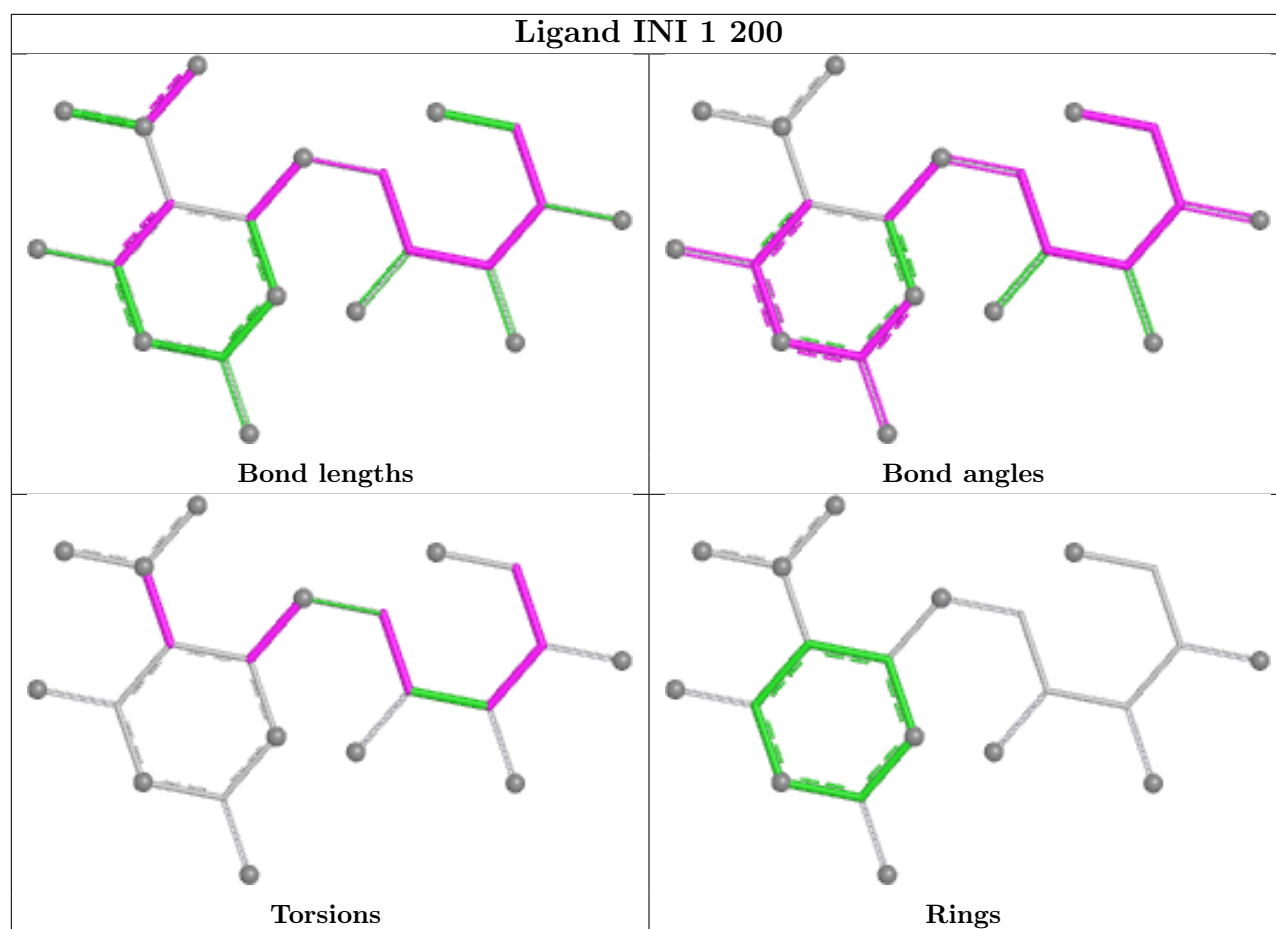


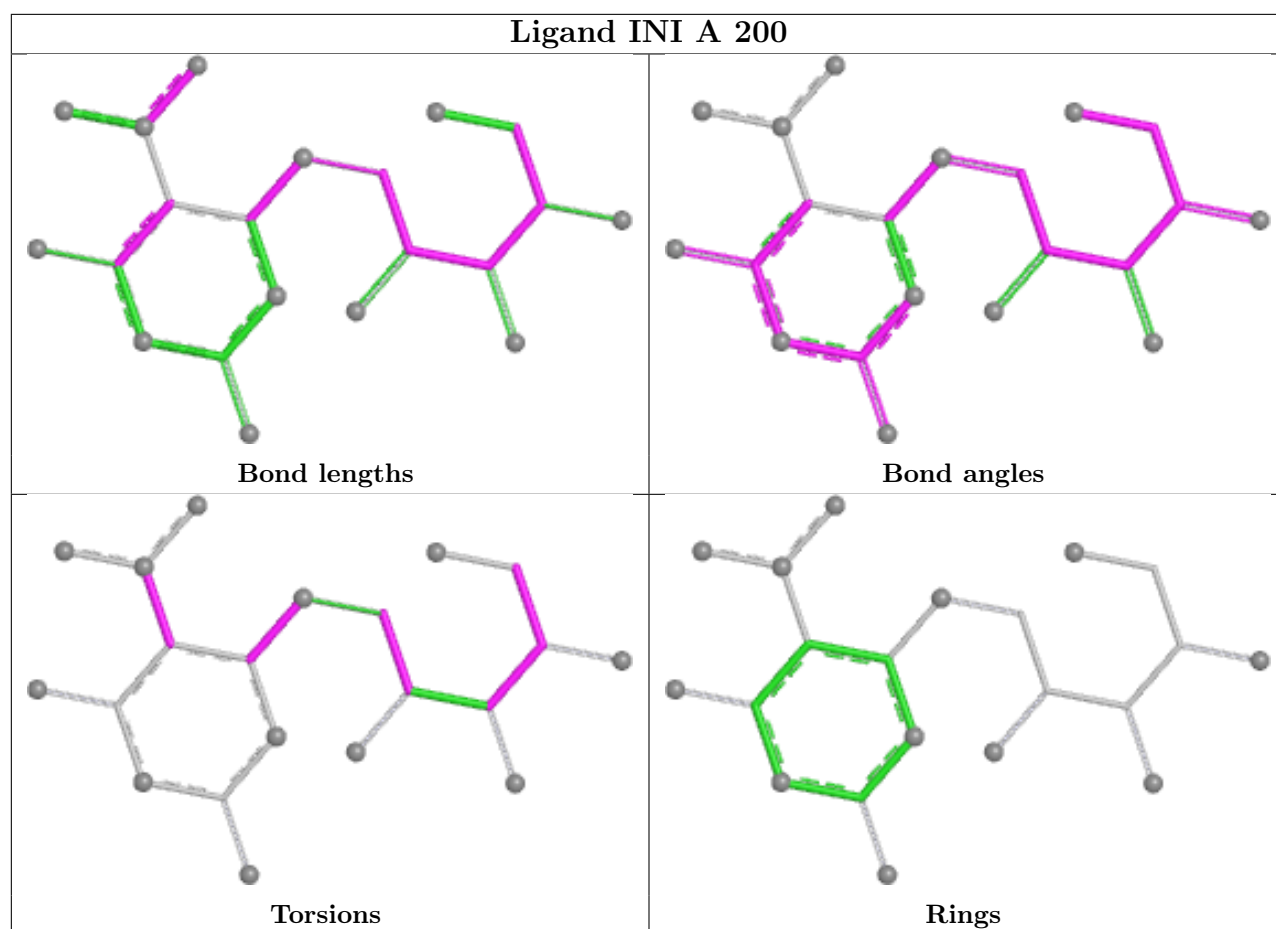


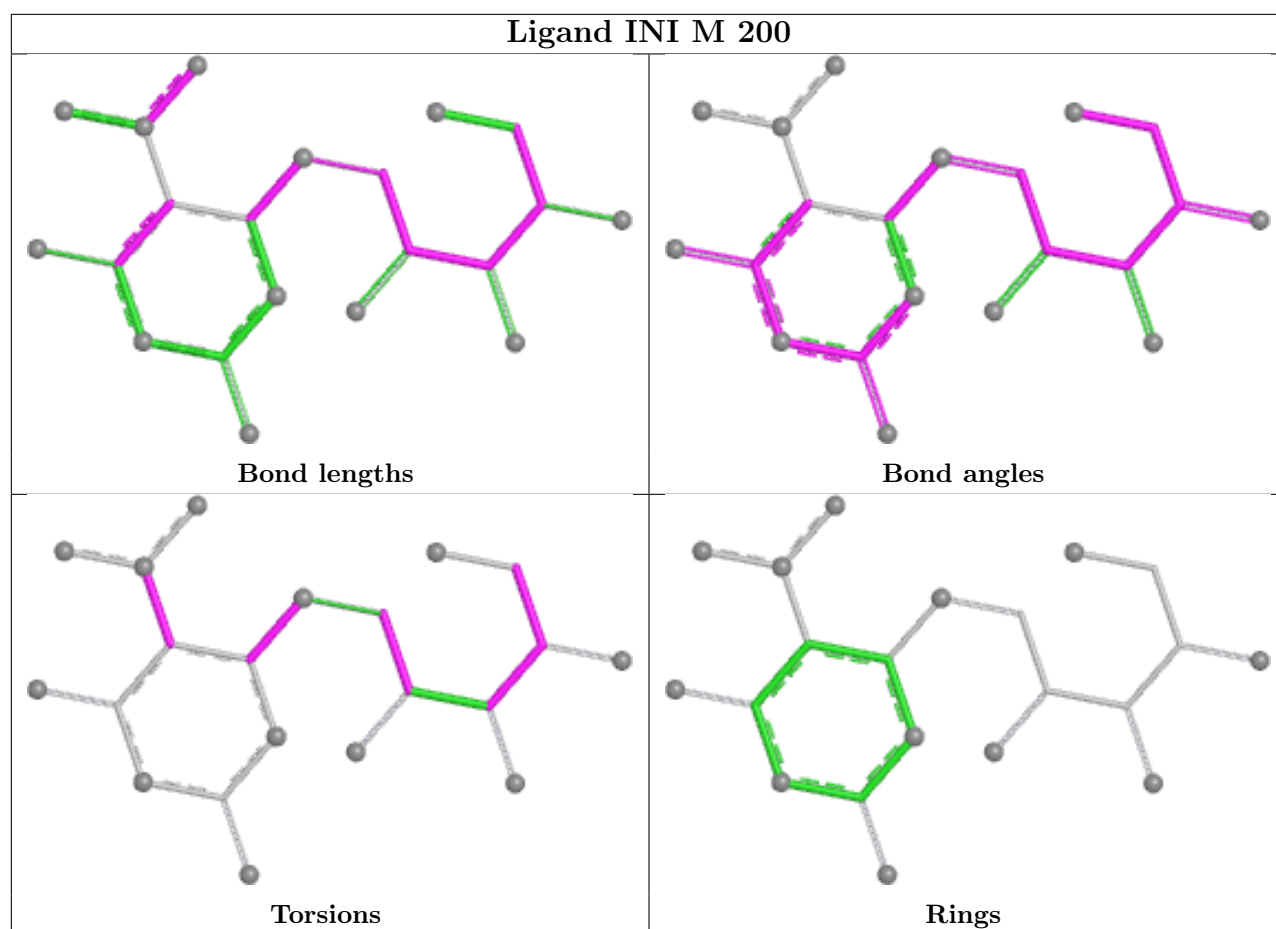


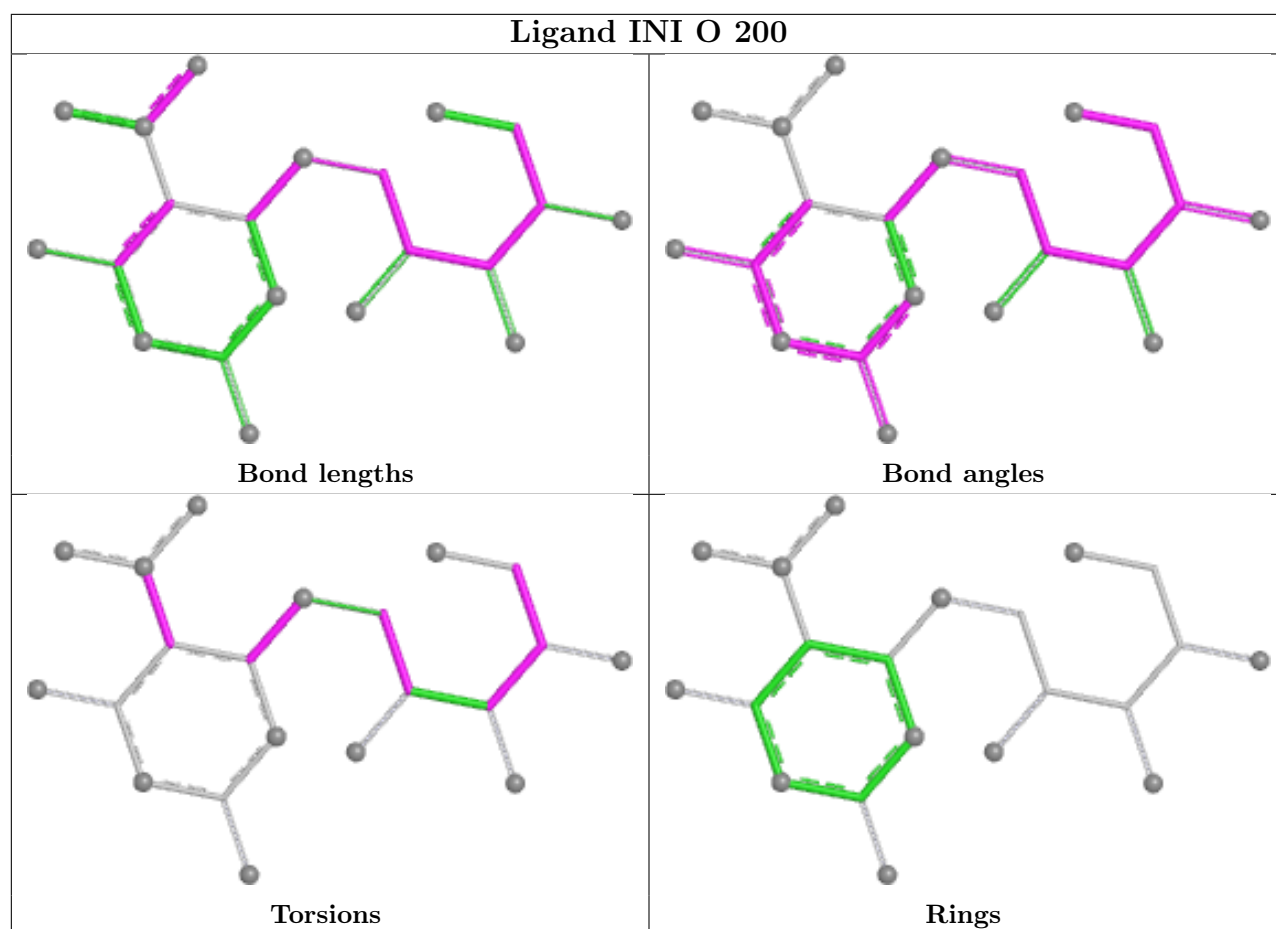


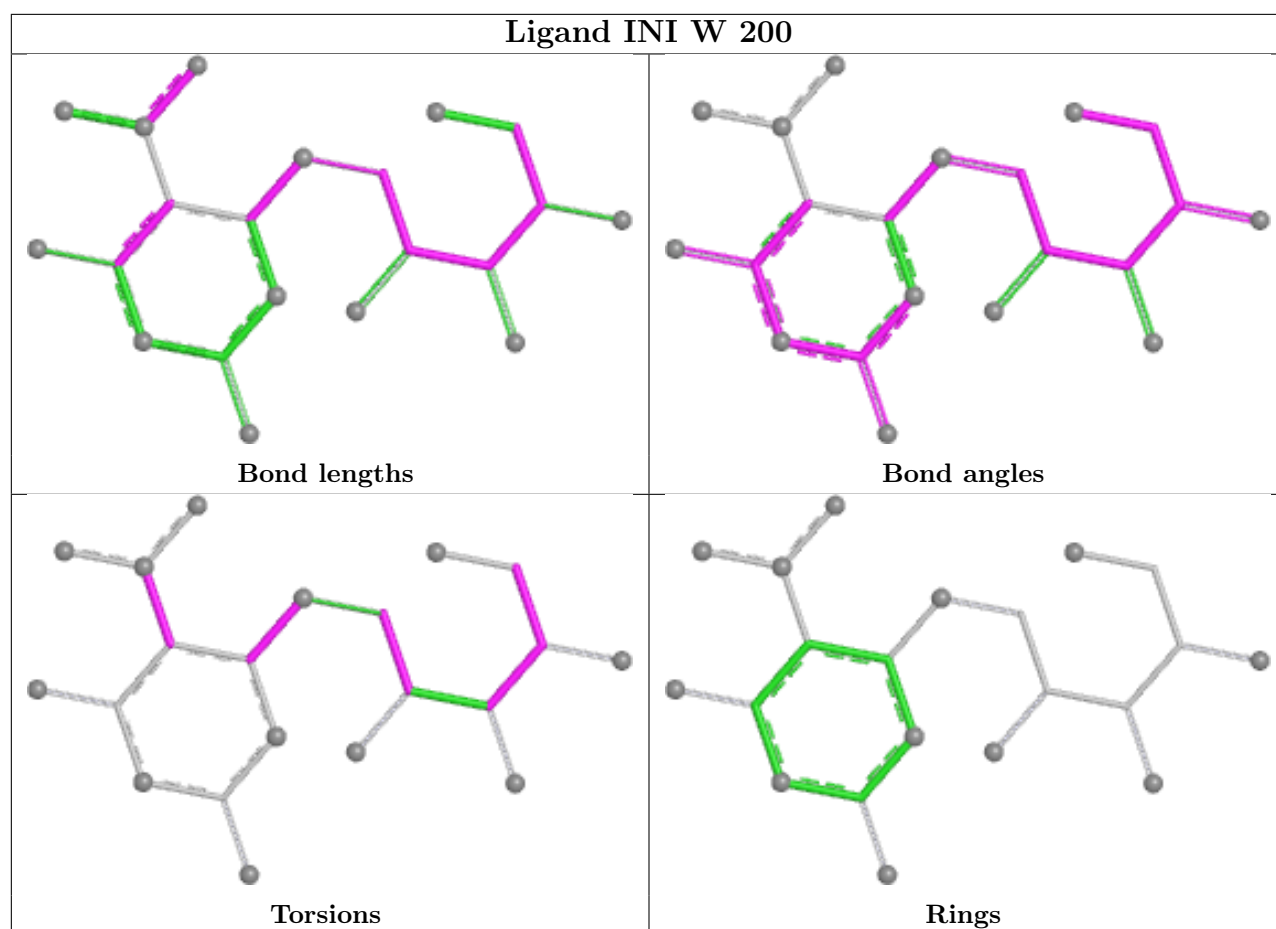


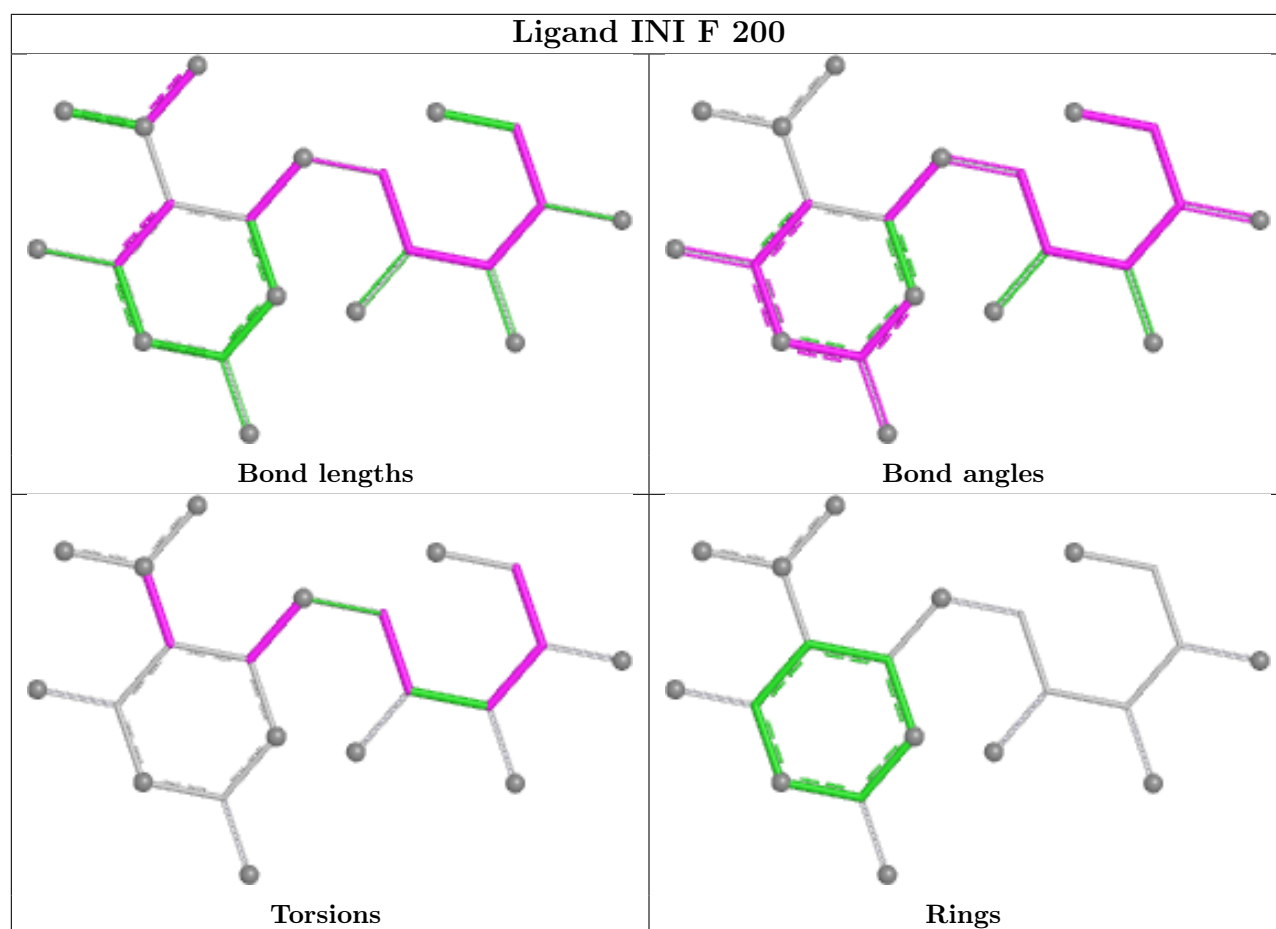


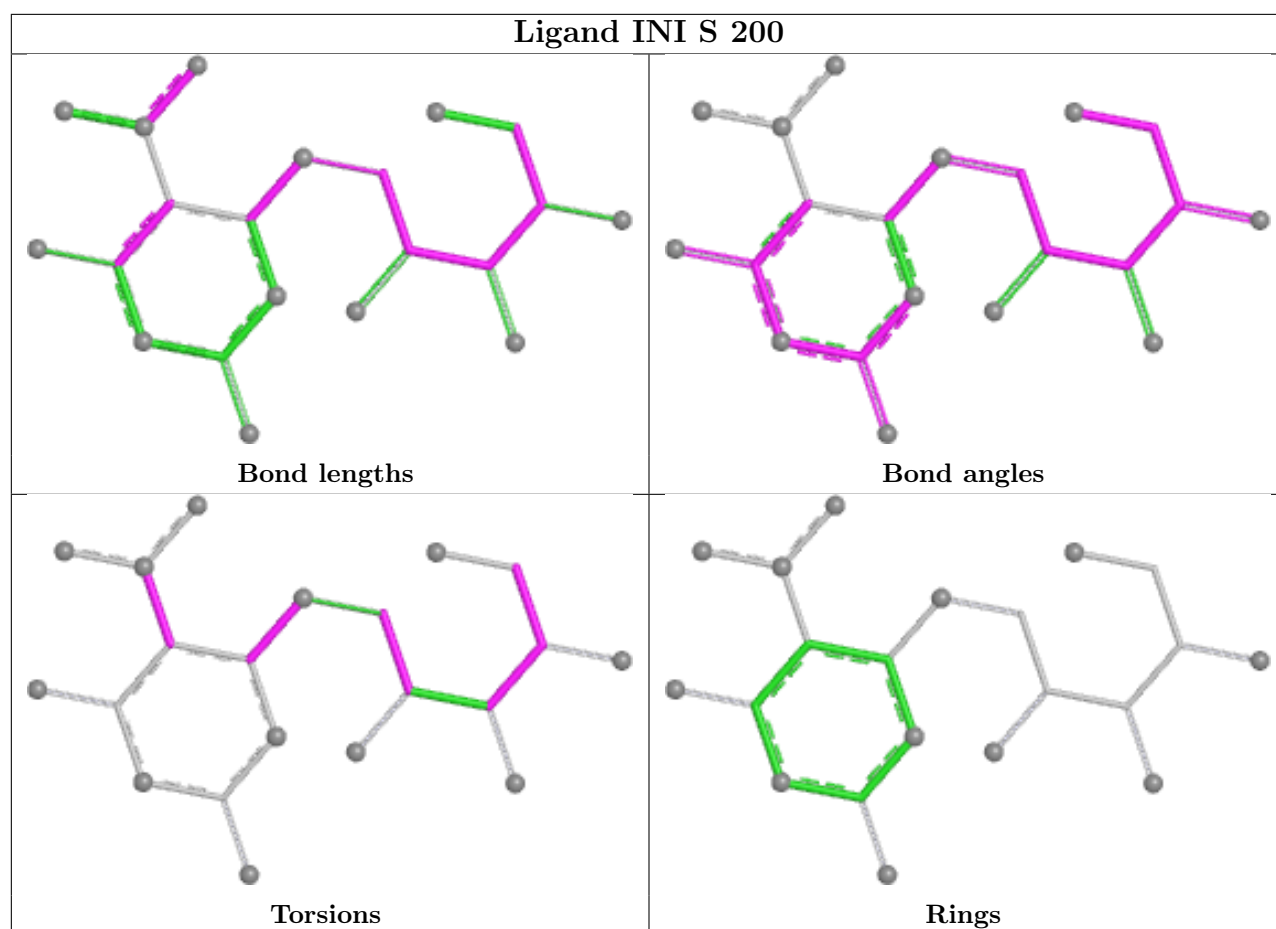


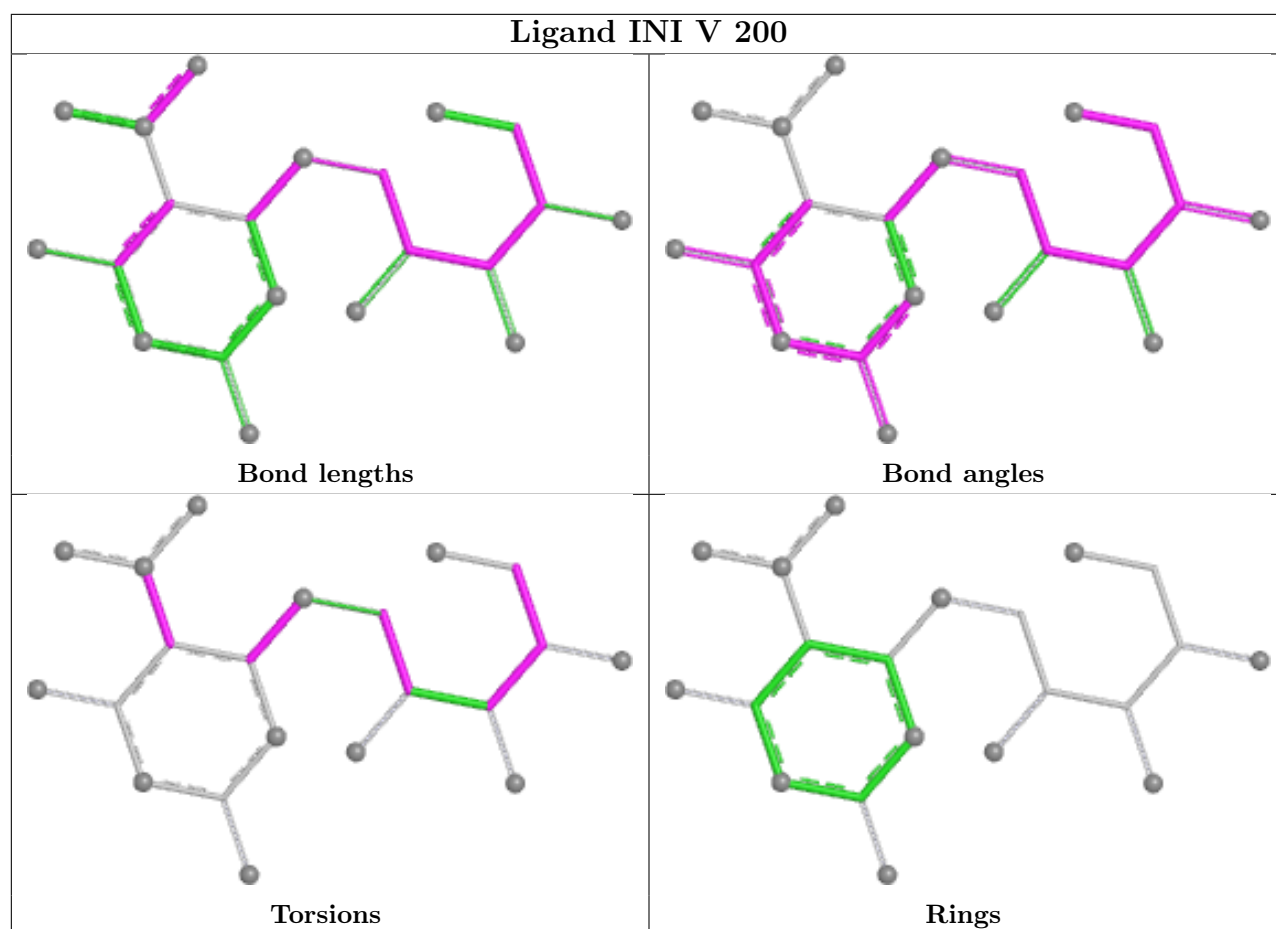


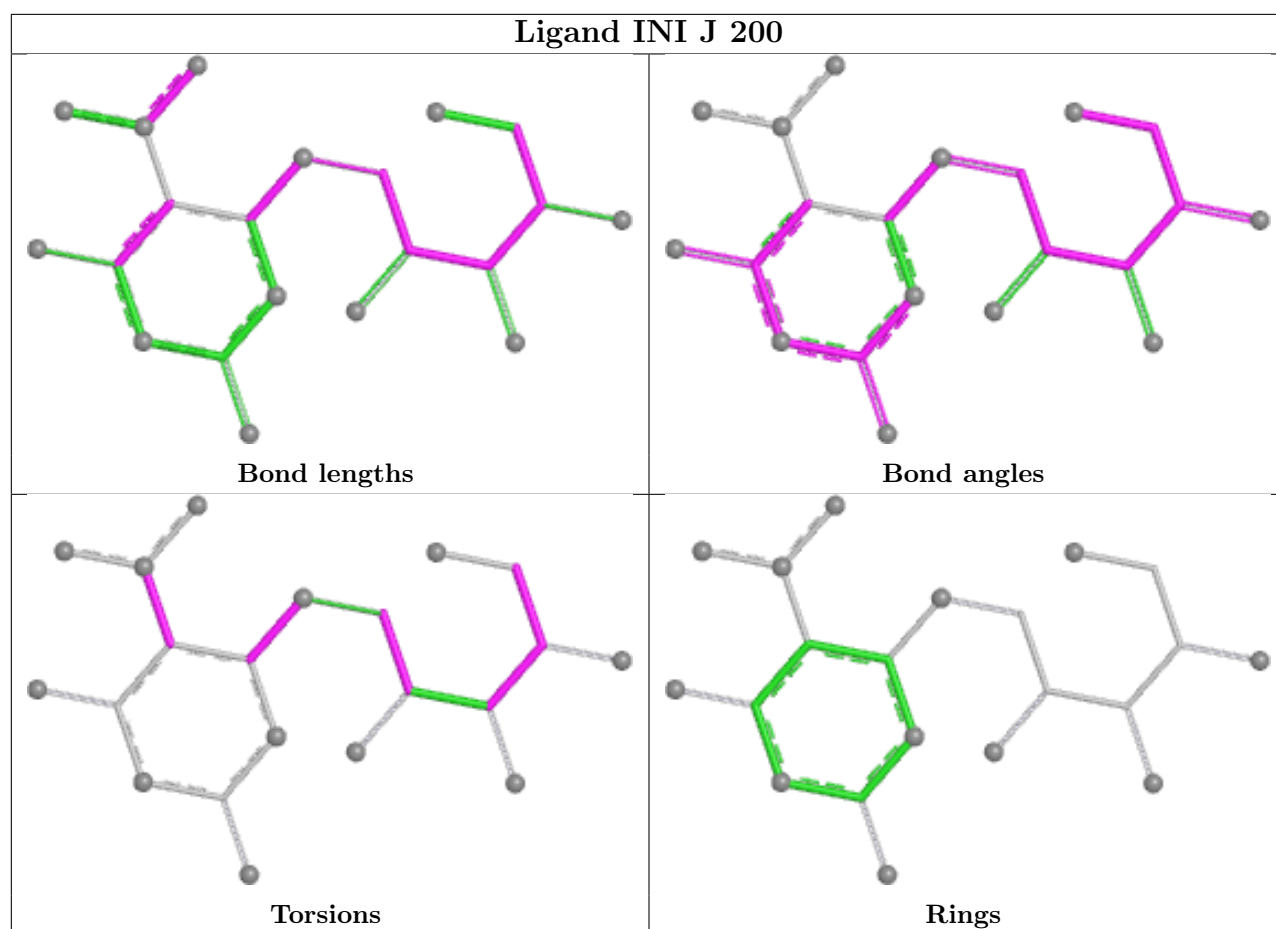


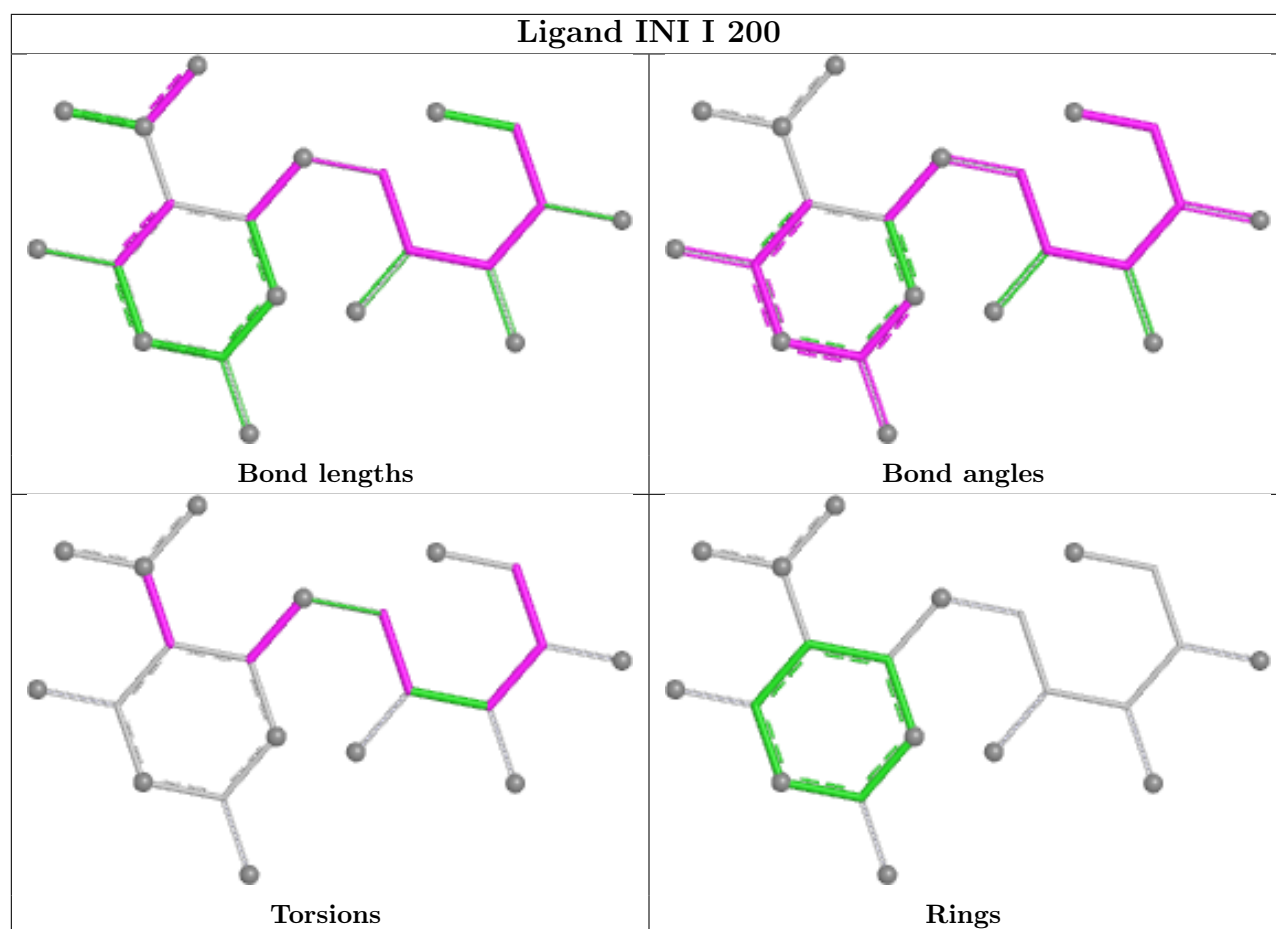


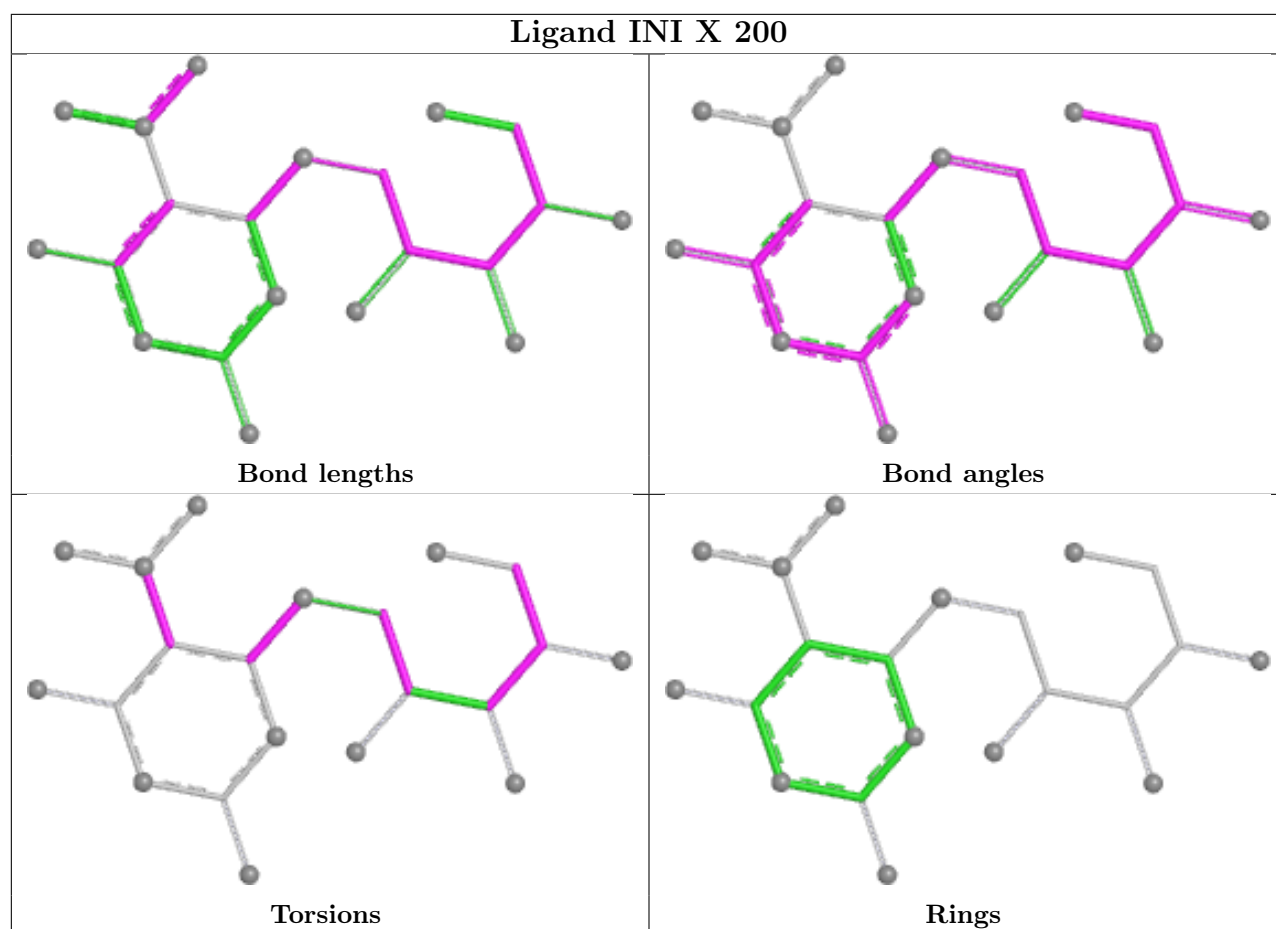


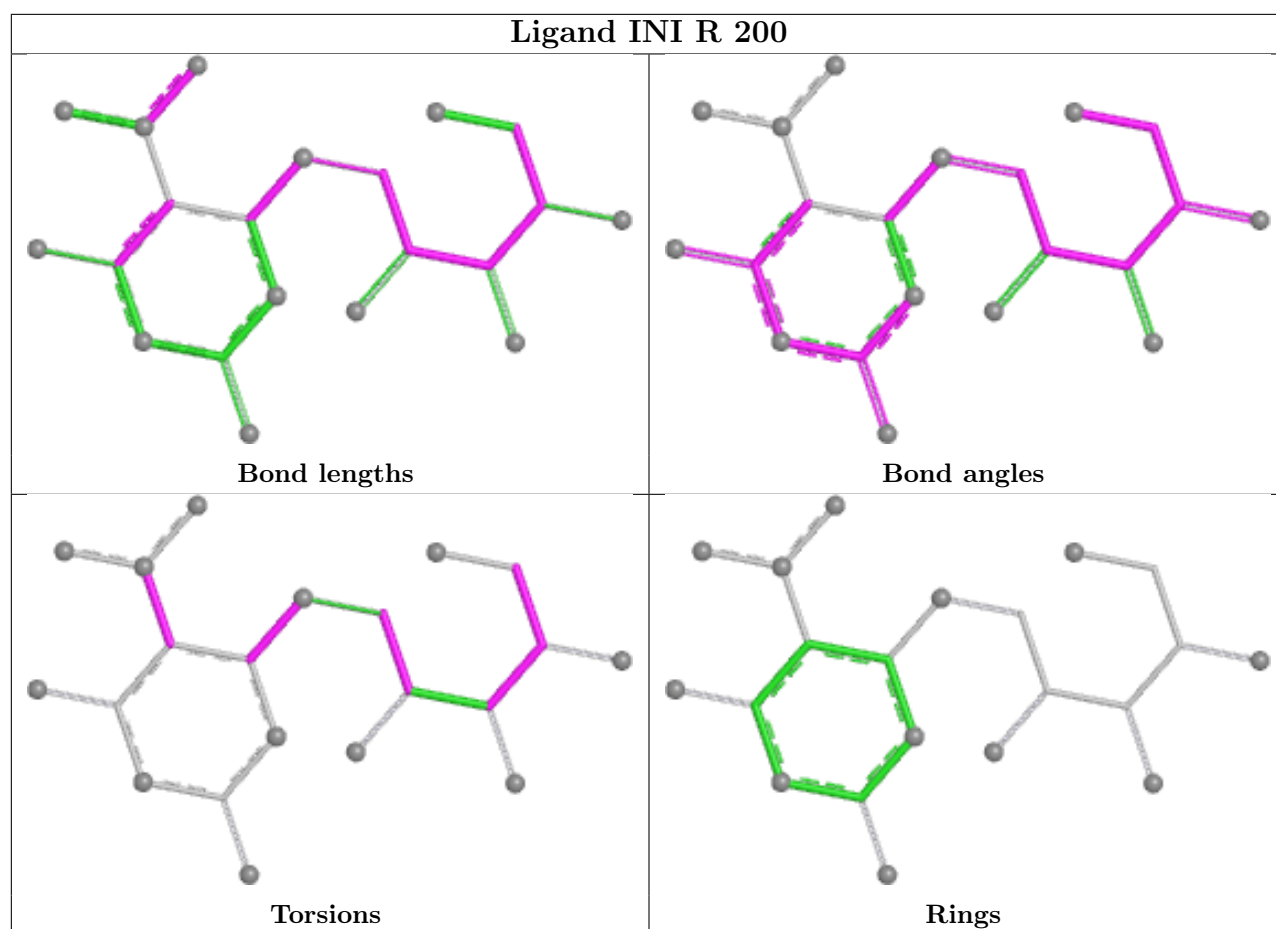


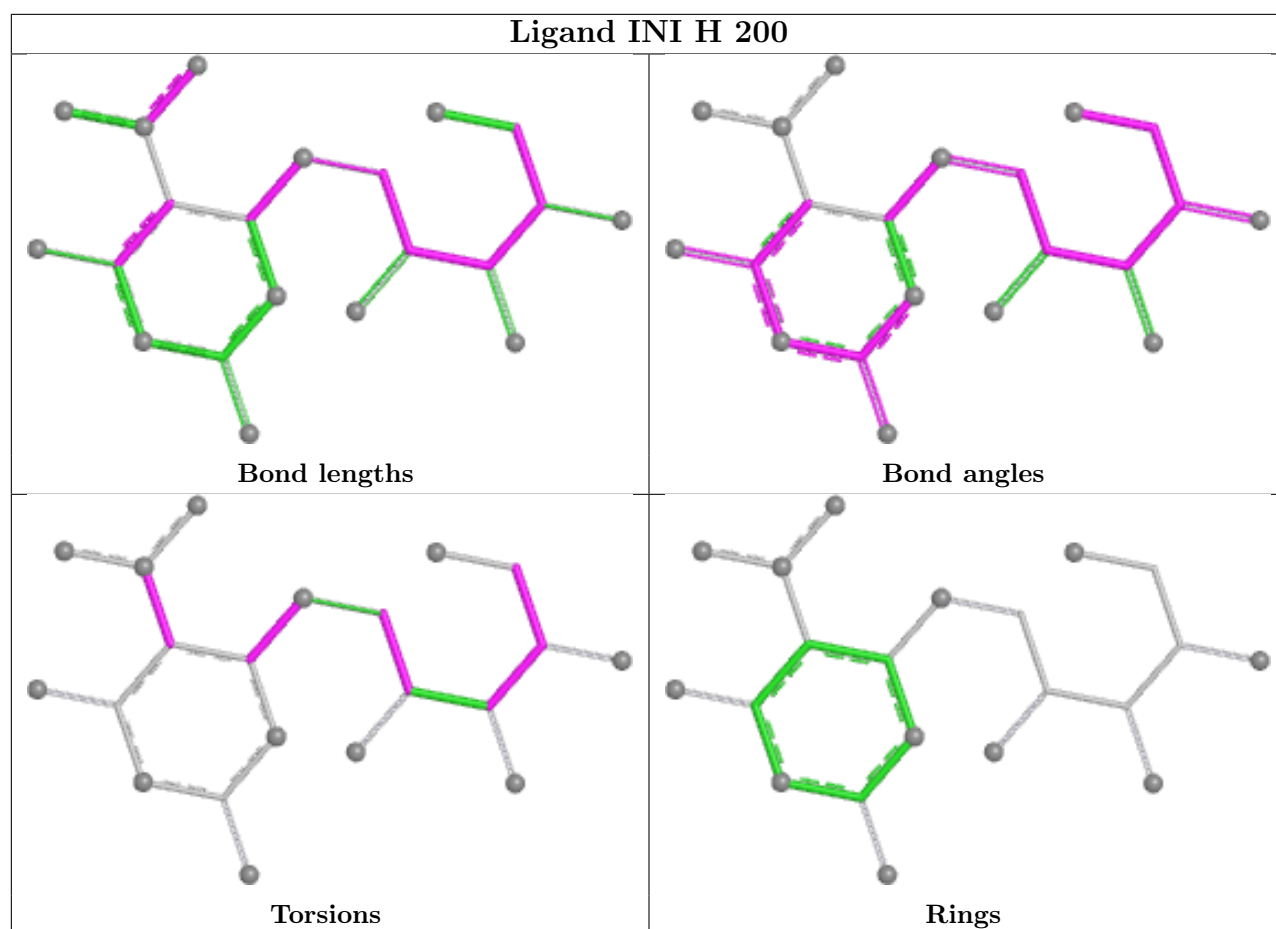


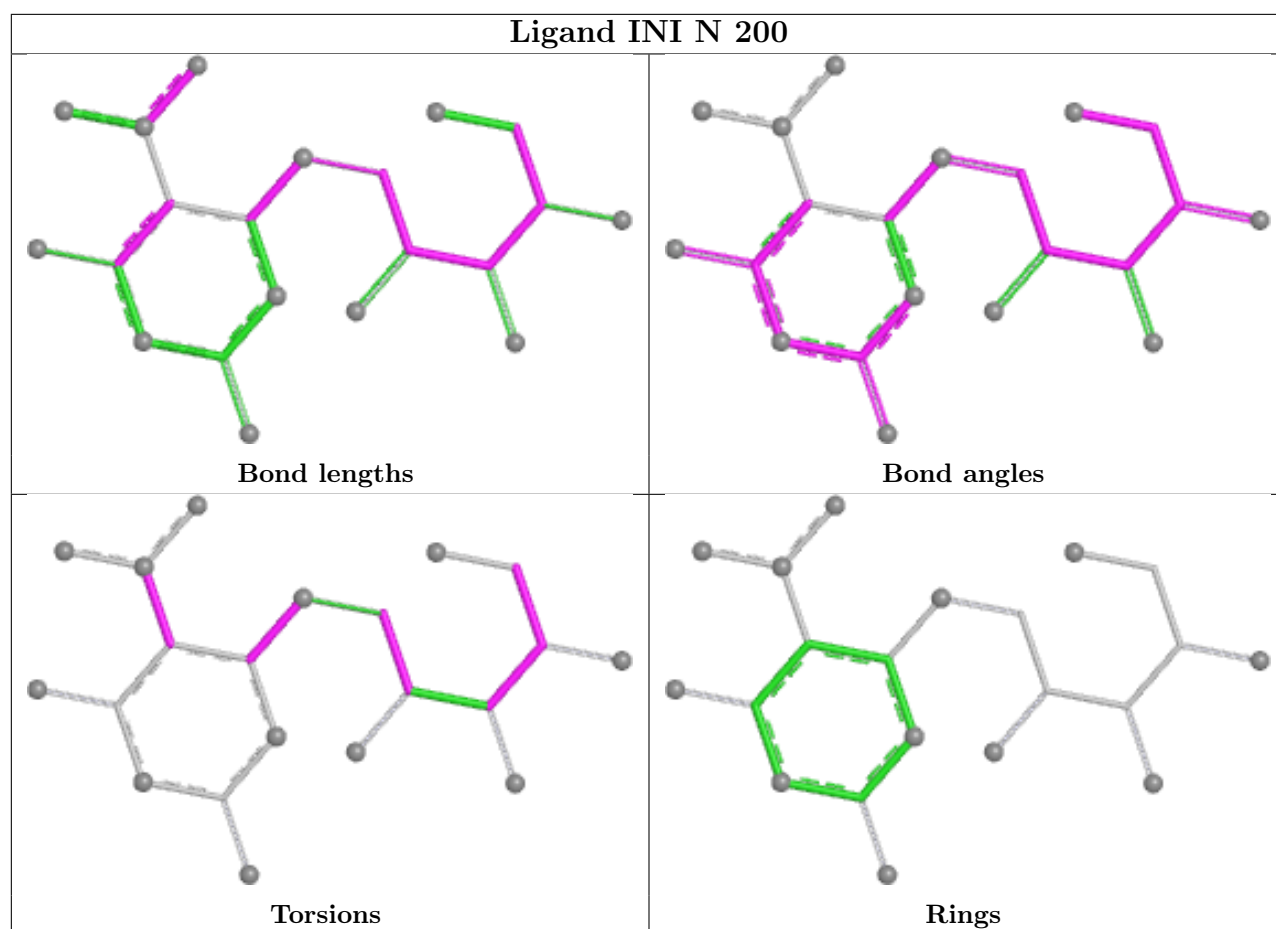


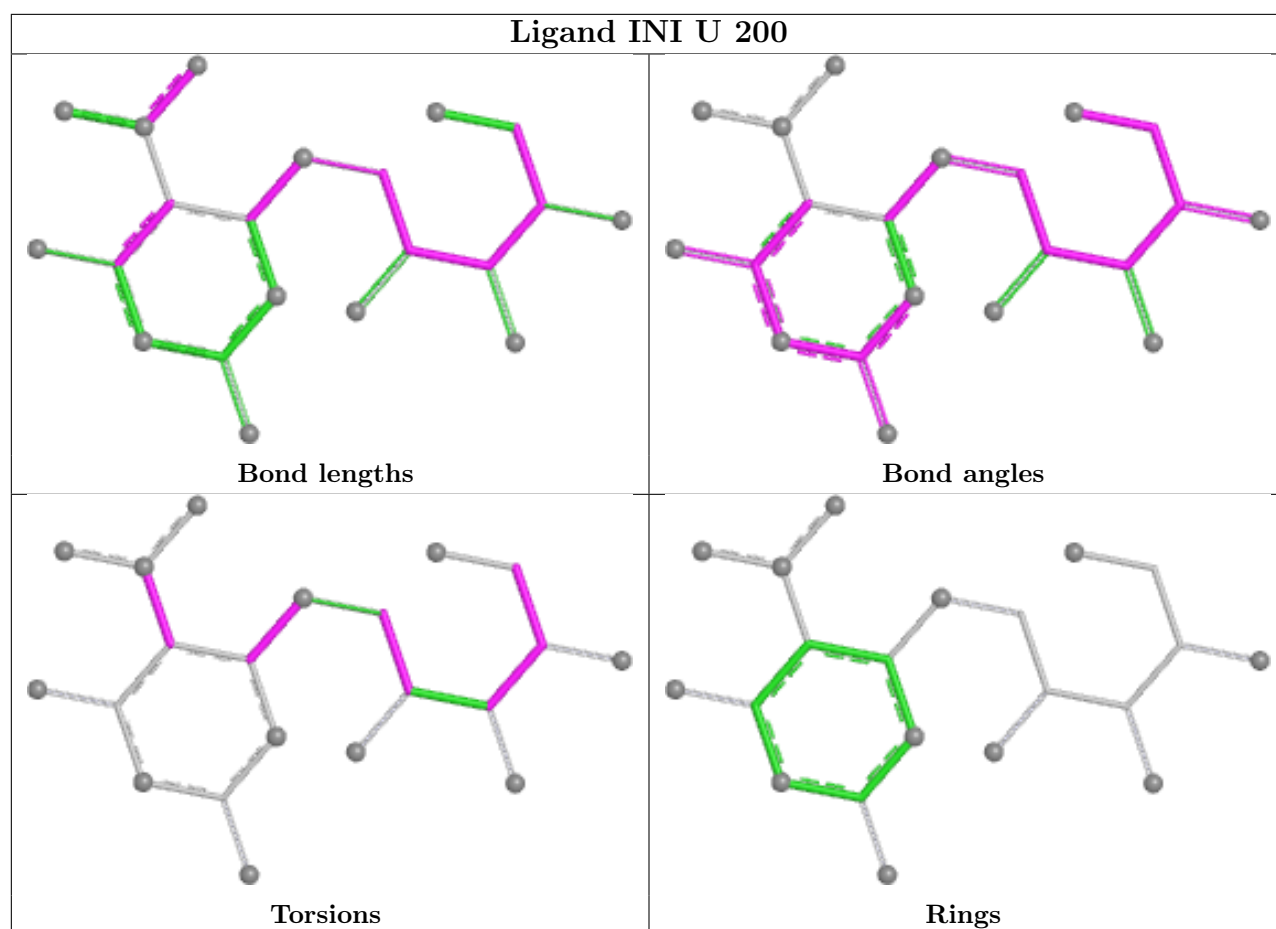


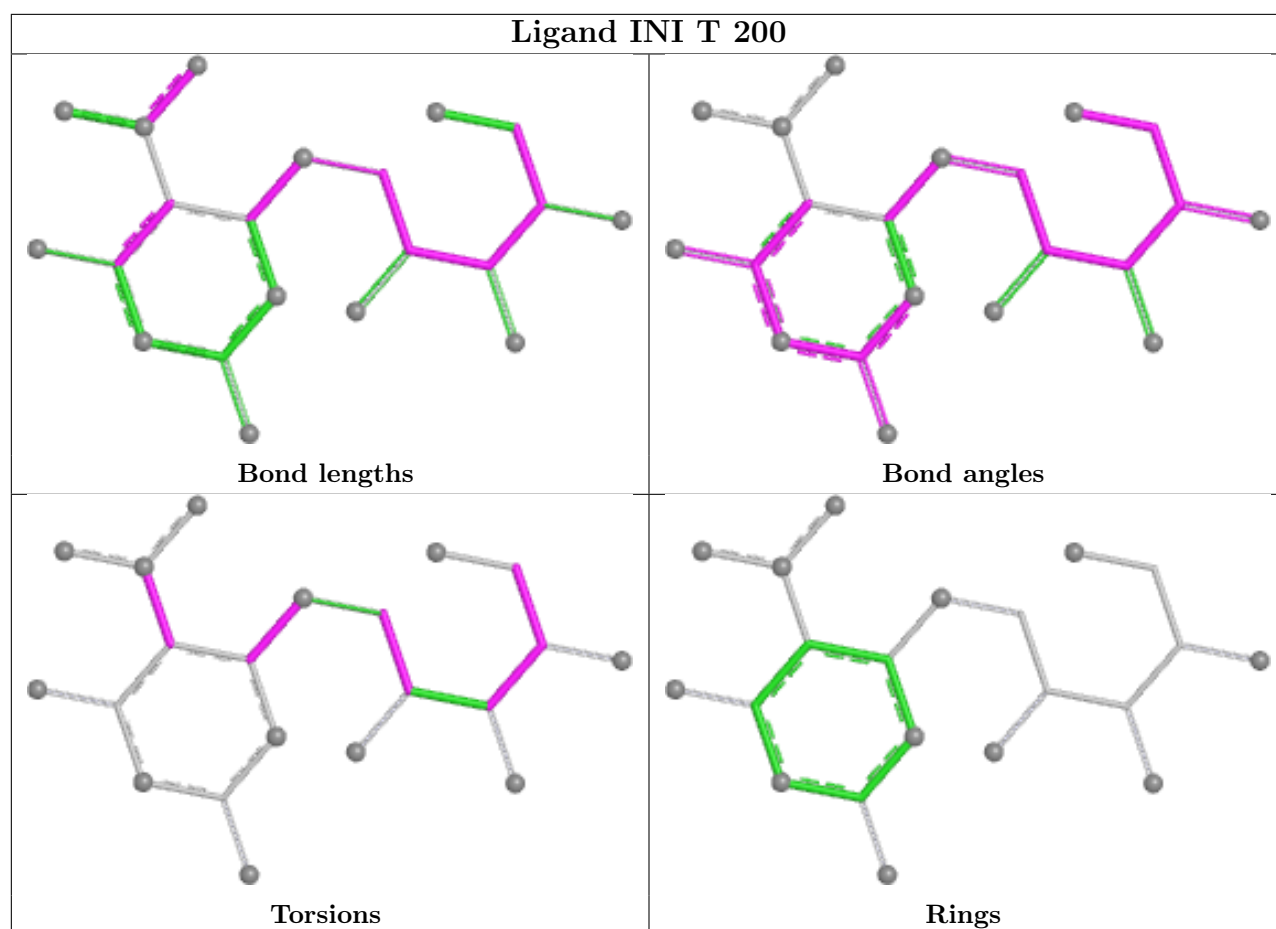


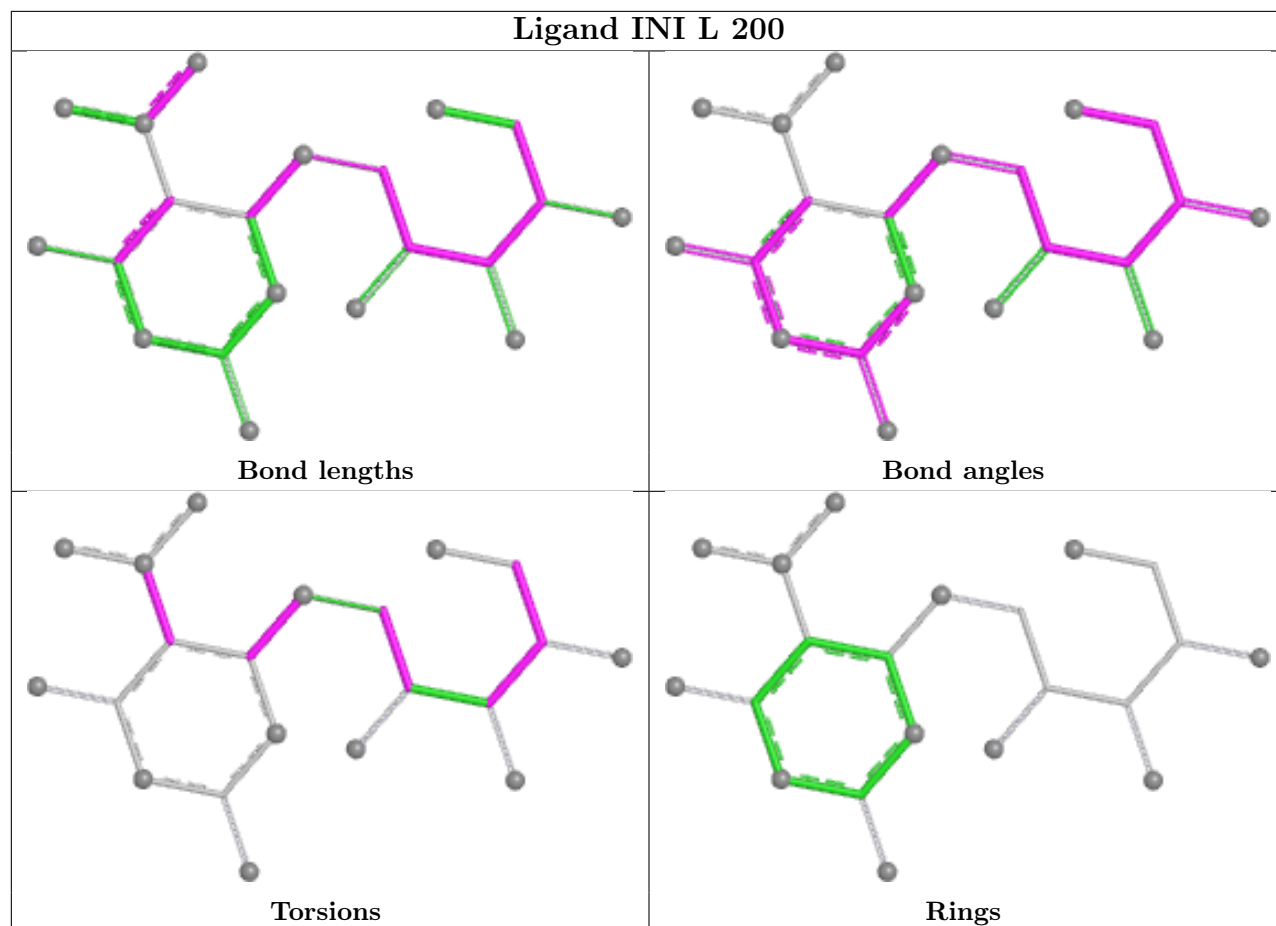












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.