



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:43 PM JST

PDB ID : 8HFX
EMDB ID : EMD-34727
Title : Cryo-EM structure of SARS-CoV-2 Omicron BA.1 spike protein in complex with white-tailed deer ACE2
Authors : Han, P.; Meng, Y.M.; Qi, J.X.
Deposited on : 2022-11-13
Resolution : 2.98 Å(reported)

This is a Full wwPDB EM Validation 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

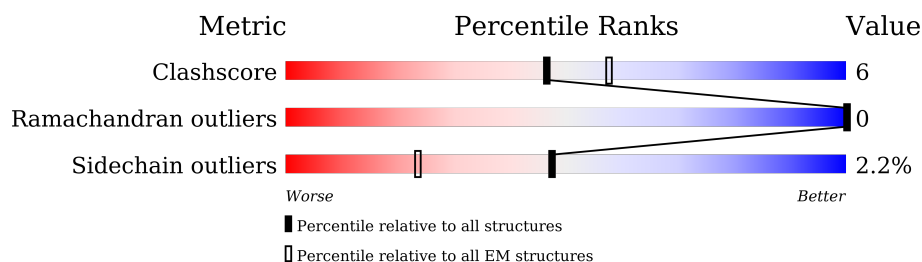
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1253	71% 13% 15%
1	B	1253	73% 11% 16%
1	C	1253	73% 11% 15%
2	E	613	70% 25% ..
3	D	2	50% 50%
3	G	2	100%
3	H	2	100%
3	I	2	100%
3	J	2	100%

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Mol	Chain	Length	Quality of chain
3	K	2	 100%
3	L	2	 100%
3	M	2	 50% 50%
3	N	2	 50% 50%
3	O	2	 100%
3	P	2	 50% 50%
3	Q	2	 100%
3	R	2	 100%
3	S	2	 50% 50%
3	T	2	 50% 50%
3	U	2	 50% 50%
3	V	2	 100%
4	F	3	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30807 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 Spike glycoprotein,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			8329	5334	1388	1569	38		
1	B	1058	Total	C	N	O	S	0	0
			8306	5319	1384	1565	38		
1	C	1062	Total	C	N	O	S	0	0
			8336	5339	1389	1570	38		

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	140	ASP	TYR	variant	UNP P0DTC2
A	206	ILE	LEU	variant	UNP P0DTC2
A	209	GLU	-	insertion	UNP P0DTC2
A	210	PRO	-	insertion	UNP P0DTC2
A	211	GLU	-	insertion	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2
A	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	814	PRO	PHE	conflict	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	889	PRO	ALA	conflict	UNP P0DTC2
A	896	PRO	ALA	conflict	UNP P0DTC2
A	939	PRO	ALA	conflict	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2
A	1206	GLY	-	linker	UNP P0DTC2
A	1207	SER	-	linker	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP M1E1E4
A	1238	TRP	-	expression tag	UNP M1E1E4
A	1239	SER	-	expression tag	UNP M1E1E4
A	1240	HIS	-	expression tag	UNP M1E1E4
A	1241	PRO	-	expression tag	UNP M1E1E4
A	1242	GLN	-	expression tag	UNP M1E1E4
A	1243	PHE	-	expression tag	UNP M1E1E4
A	1244	GLU	-	expression tag	UNP M1E1E4
A	1245	LYS	-	expression tag	UNP M1E1E4
A	1246	HIS	-	expression tag	UNP M1E1E4
A	1247	HIS	-	expression tag	UNP M1E1E4
A	1248	HIS	-	expression tag	UNP M1E1E4
A	1249	HIS	-	expression tag	UNP M1E1E4
A	1250	HIS	-	expression tag	UNP M1E1E4
A	1251	HIS	-	expression tag	UNP M1E1E4
A	1252	HIS	-	expression tag	UNP M1E1E4
A	1253	HIS	-	expression tag	UNP M1E1E4
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	93	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	140	ASP	TYR	variant	UNP P0DTC2
B	206	ILE	LEU	variant	UNP P0DTC2
B	209	GLU	-	insertion	UNP P0DTC2
B	210	PRO	-	insertion	UNP P0DTC2
B	211	GLU	-	insertion	UNP P0DTC2
B	336	ASP	GLY	variant	UNP P0DTC2
B	368	LEU	SER	variant	UNP P0DTC2
B	370	PRO	SER	variant	UNP P0DTC2
B	372	PHE	SER	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	437	LYS	ASN	variant	UNP P0DTC2
B	443	SER	GLY	variant	UNP P0DTC2
B	474	ASN	SER	variant	UNP P0DTC2
B	475	LYS	THR	variant	UNP P0DTC2
B	481	ALA	GLU	variant	UNP P0DTC2
B	490	ARG	GLN	variant	UNP P0DTC2
B	493	SER	GLY	variant	UNP P0DTC2
B	495	ARG	GLN	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	502	HIS	TYR	variant	UNP P0DTC2
B	544	LYS	THR	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	652	TYR	HIS	variant	UNP P0DTC2
B	676	LYS	ASN	variant	UNP P0DTC2
B	678	HIS	PRO	variant	UNP P0DTC2
B	761	LYS	ASN	variant	UNP P0DTC2
B	793	TYR	ASP	variant	UNP P0DTC2
B	814	PRO	PHE	conflict	UNP P0DTC2
B	853	LYS	ASN	variant	UNP P0DTC2
B	889	PRO	ALA	conflict	UNP P0DTC2
B	896	PRO	ALA	conflict	UNP P0DTC2
B	939	PRO	ALA	conflict	UNP P0DTC2
B	951	HIS	GLN	variant	UNP P0DTC2
B	966	LYS	ASN	variant	UNP P0DTC2
B	978	PHE	LEU	variant	UNP P0DTC2
B	983	PRO	LYS	engineered mutation	UNP P0DTC2
B	984	PRO	VAL	engineered mutation	UNP P0DTC2
B	1206	GLY	-	linker	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1207	SER	-	linker	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP M1E1E4
B	1238	TRP	-	expression tag	UNP M1E1E4
B	1239	SER	-	expression tag	UNP M1E1E4
B	1240	HIS	-	expression tag	UNP M1E1E4
B	1241	PRO	-	expression tag	UNP M1E1E4
B	1242	GLN	-	expression tag	UNP M1E1E4
B	1243	PHE	-	expression tag	UNP M1E1E4
B	1244	GLU	-	expression tag	UNP M1E1E4
B	1245	LYS	-	expression tag	UNP M1E1E4
B	1246	HIS	-	expression tag	UNP M1E1E4
B	1247	HIS	-	expression tag	UNP M1E1E4
B	1248	HIS	-	expression tag	UNP M1E1E4
B	1249	HIS	-	expression tag	UNP M1E1E4
B	1250	HIS	-	expression tag	UNP M1E1E4
B	1251	HIS	-	expression tag	UNP M1E1E4
B	1252	HIS	-	expression tag	UNP M1E1E4
B	1253	HIS	-	expression tag	UNP M1E1E4
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	93	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	140	ASP	TYR	variant	UNP P0DTC2
C	206	ILE	LEU	variant	UNP P0DTC2
C	209	GLU	-	insertion	UNP P0DTC2
C	210	PRO	-	insertion	UNP P0DTC2
C	211	GLU	-	insertion	UNP P0DTC2
C	336	ASP	GLY	variant	UNP P0DTC2
C	368	LEU	SER	variant	UNP P0DTC2
C	370	PRO	SER	variant	UNP P0DTC2
C	372	PHE	SER	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	437	LYS	ASN	variant	UNP P0DTC2
C	443	SER	GLY	variant	UNP P0DTC2
C	474	ASN	SER	variant	UNP P0DTC2
C	475	LYS	THR	variant	UNP P0DTC2
C	481	ALA	GLU	variant	UNP P0DTC2
C	490	ARG	GLN	variant	UNP P0DTC2
C	493	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	495	ARG	GLN	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	502	HIS	TYR	variant	UNP P0DTC2
C	544	LYS	THR	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	652	TYR	HIS	variant	UNP P0DTC2
C	676	LYS	ASN	variant	UNP P0DTC2
C	678	HIS	PRO	variant	UNP P0DTC2
C	761	LYS	ASN	variant	UNP P0DTC2
C	793	TYR	ASP	variant	UNP P0DTC2
C	814	PRO	PHE	conflict	UNP P0DTC2
C	853	LYS	ASN	variant	UNP P0DTC2
C	889	PRO	ALA	conflict	UNP P0DTC2
C	896	PRO	ALA	conflict	UNP P0DTC2
C	939	PRO	ALA	conflict	UNP P0DTC2
C	951	HIS	GLN	variant	UNP P0DTC2
C	966	LYS	ASN	variant	UNP P0DTC2
C	978	PHE	LEU	variant	UNP P0DTC2
C	983	PRO	LYS	engineered mutation	UNP P0DTC2
C	984	PRO	VAL	engineered mutation	UNP P0DTC2
C	1206	GLY	-	linker	UNP P0DTC2
C	1207	SER	-	linker	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP M1E1E4
C	1238	TRP	-	expression tag	UNP M1E1E4
C	1239	SER	-	expression tag	UNP M1E1E4
C	1240	HIS	-	expression tag	UNP M1E1E4
C	1241	PRO	-	expression tag	UNP M1E1E4
C	1242	GLN	-	expression tag	UNP M1E1E4
C	1243	PHE	-	expression tag	UNP M1E1E4
C	1244	GLU	-	expression tag	UNP M1E1E4
C	1245	LYS	-	expression tag	UNP M1E1E4
C	1246	HIS	-	expression tag	UNP M1E1E4
C	1247	HIS	-	expression tag	UNP M1E1E4
C	1248	HIS	-	expression tag	UNP M1E1E4
C	1249	HIS	-	expression tag	UNP M1E1E4
C	1250	HIS	-	expression tag	UNP M1E1E4
C	1251	HIS	-	expression tag	UNP M1E1E4
C	1252	HIS	-	expression tag	UNP M1E1E4
C	1253	HIS	-	expression tag	UNP M1E1E4

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	595	Total	C	N	O	S	0	0
			4886	3121	804	931	30		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



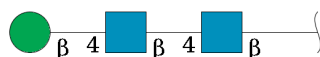
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	2	Total	C	N	O		0	0
			28	16	2	10			
3	G	2	Total	C	N	O		0	0
			28	16	2	10			
3	H	2	Total	C	N	O		0	0
			28	16	2	10			
3	I	2	Total	C	N	O		0	0
			28	16	2	10			
3	J	2	Total	C	N	O		0	0
			28	16	2	10			
3	K	2	Total	C	N	O		0	0
			28	16	2	10			
3	L	2	Total	C	N	O		0	0
			28	16	2	10			
3	M	2	Total	C	N	O		0	0
			28	16	2	10			
3	N	2	Total	C	N	O		0	0
			28	16	2	10			
3	O	2	Total	C	N	O		0	0
			28	16	2	10			
3	P	2	Total	C	N	O		0	0
			28	16	2	10			
3	Q	2	Total	C	N	O		0	0
			28	16	2	10			
3	R	2	Total	C	N	O		0	0
			28	16	2	10			
3	S	2	Total	C	N	O		0	0
			28	16	2	10			
3	T	2	Total	C	N	O		0	0
			28	16	2	10			
3	U	2	Total	C	N	O		0	0
			28	16	2	10			

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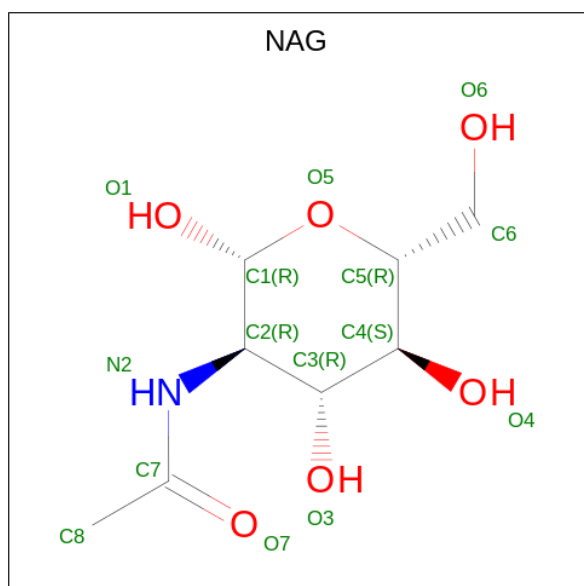
Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0

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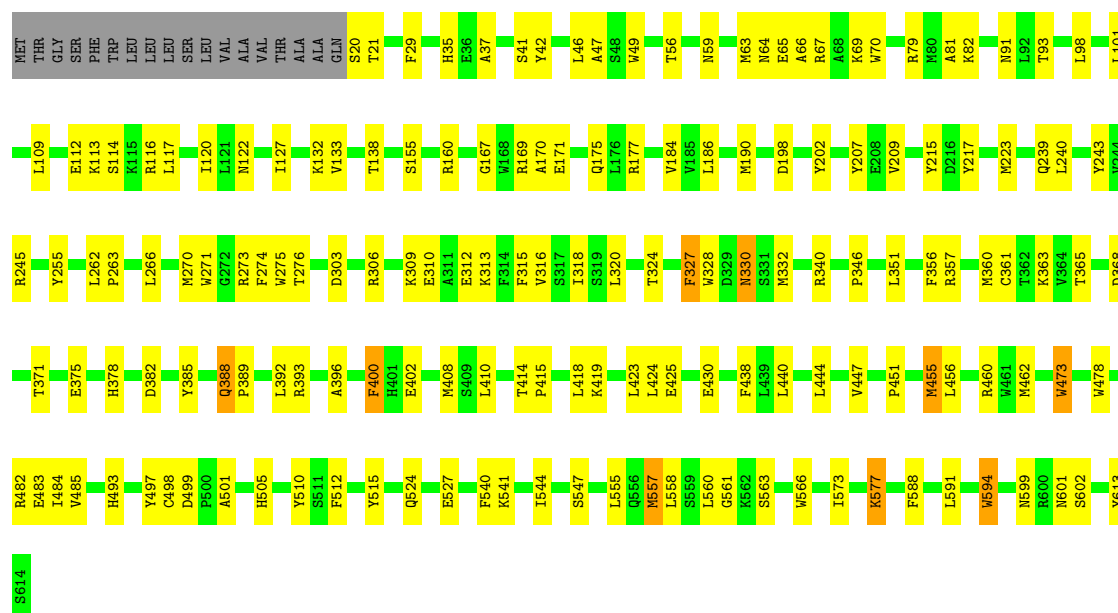
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	E	1	Total	Zn	0
			1	1	

Chain E:  70% 25% ..



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

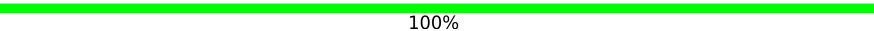


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

HA01
HA02
EM03

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	172986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, ZN

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	A	0.30	0/8526	0.54	0/11602
1	B	0.31	0/8503	0.53	0/11572
1	C	0.29	0/8535	0.53	0/11617
2	E	0.30	0/5021	0.53	0/6806
All	All	0.30	0/30585	0.53	0/41597

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8329	0	8150	97	0
1	B	8306	0	8128	88	0
1	C	8336	0	8155	88	0
2	E	4886	0	4644	94	0
3	D	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	28	0	25	1	0
3	L	28	0	25	0	0
3	M	28	0	25	1	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	1	0
3	T	28	0	25	1	0
3	U	28	0	25	1	0
3	V	28	0	25	2	0
4	F	39	0	34	0	0
5	A	126	0	117	1	0
5	B	154	0	143	4	0
5	C	112	0	104	2	0
5	E	42	0	39	0	0
6	E	1	0	0	0	0
All	All	30807	0	29939	360	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.

All (360) 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:C:53:ASP:OD1	1:C:54:LEU:N	2.14	0.80
1:B:228:ILE:HD12	1:B:230:ILE:H	1.46	0.79
1:B:388:CYS:HA	1:B:522:CYS:HB3	1.64	0.77
1:A:201:LYS:HE3	1:A:218:SER:HB3	1.69	0.74
2:E:47:ALA:HB1	2:E:63:MET:HA	1.70	0.72
2:E:109:LEU:HD21	2:E:114:SER:HB3	1.71	0.72
1:B:67:VAL:HG23	1:B:77:PHE:HB3	1.71	0.72
1:C:21:ARG:HH22	1:C:79:ASN:HB2	1.55	0.71
1:B:415:ILE:HG23	1:B:419:ASN:HB2	1.71	0.71
2:E:81:ALA:HB1	2:E:101:LEU:HD13	1.73	0.70
1:A:459:LYS:HD2	1:A:460:PRO:HD2	1.74	0.70
1:B:639:VAL:HG22	1:B:648:ILE:HG12	1.73	0.70
1:A:454:ARG:NH1	1:A:456:SER:O	2.25	0.69
1:A:801:GLN:NE2	1:A:932:GLN:OE1	2.26	0.68
1:B:97:ASN:O	1:B:100:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:557:MET:CE	2:E:573:ILE:HD12	2.25	0.67
1:B:14:GLN:O	1:B:153:ARG:NH1	2.28	0.67
1:B:315:PHE:HZ	1:B:612:VAL:HG21	1.60	0.67
2:E:67:ARG:HA	2:E:67:ARG:NH1	2.09	0.67
1:A:398:VAL:HG22	1:A:506:ARG:HG2	1.77	0.66
1:C:574:ARG:HH21	1:C:581:ILE:HD11	1.62	0.65
2:E:419:LYS:NZ	2:E:425:GLU:O	2.29	0.65
2:E:557:MET:HE1	2:E:573:ILE:HD12	1.78	0.65
1:A:1131:ASN:OD1	3:K:1:NAG:N2	2.30	0.65
1:B:357:ASN:H	1:B:520:THR:HB	1.61	0.64
1:C:1071:ASN:OD1	3:T:1:NAG:N2	2.31	0.64
1:C:612:VAL:HG12	1:C:614:CYS:H	1.62	0.64
2:E:245:ARG:HD3	2:E:262:LEU:HD21	1.80	0.64
1:A:97:ASN:OD1	1:A:100:ARG:NH2	2.26	0.63
1:C:1100:PHE:HZ	3:U:1:NAG:H62	1.63	0.63
1:A:449:LEU:HD22	1:A:489:LEU:HB3	1.80	0.63
2:E:169:ARG:HH12	2:E:270:MET:HB2	1.62	0.63
1:A:116:LEU:HD11	1:A:118:VAL:HG13	1.80	0.62
1:B:967:PHE:O	1:B:992:ARG:NH2	2.32	0.62
1:A:307:LYS:HG3	1:A:597:PRO:HA	1.80	0.62
1:B:1071:ASN:HD22	5:B:1308:NAG:H61	1.65	0.61
1:A:453:PHE:HB2	1:A:488:PRO:HB3	1.81	0.61
1:B:68:ILE:N	1:B:76:ARG:O	2.32	0.61
2:E:396:ALA:HB1	2:E:566:TRP:HB3	1.82	0.61
1:C:498:TYR:HB3	1:C:502:HIS:HB2	1.82	0.61
1:C:124:VAL:HG23	1:C:169:PRO:HA	1.82	0.61
1:B:807:SER:OG	1:B:808:LYS:NZ	2.31	0.61
1:B:122:THR:OG1	1:B:123:ASN:OD1	2.18	0.60
1:B:798:ASN:OD1	3:M:1:NAG:N2	2.33	0.60
2:E:98:LEU:HD23	2:E:101:LEU:HD21	1.83	0.60
2:E:392:LEU:HD13	2:E:563:SER:HA	1.83	0.60
1:B:454:ARG:NH1	1:B:456:SER:O	2.35	0.60
2:E:365:THR:HB	2:E:368:ASP:HB2	1.82	0.60
2:E:378:HIS:HE1	2:E:402:GLU:HA	1.67	0.60
1:A:129:CYS:HB3	1:A:161:CYS:HA	1.84	0.59
2:E:483:GLU:HG2	2:E:484:ILE:HG23	1.83	0.59
2:E:588:PHE:HB3	2:E:591:LEU:HB3	1.85	0.59
1:A:343:ARG:HG2	1:A:398:VAL:HG23	1.84	0.59
1:A:354:ARG:NH1	1:A:356:SER:OG	2.35	0.59
1:C:93:ILE:HG22	1:C:181:PHE:HB2	1.85	0.59
1:A:388:CYS:HB3	1:A:519:ALA:HB1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ASN:HB3	1:C:447:ASN:HD22	1.66	0.59
2:E:271:TRP:HB3	2:E:273:ARG:HD3	1.84	0.58
2:E:67:ARG:HH12	2:E:70:TRP:HD1	1.50	0.58
1:B:1025:LYS:NZ	1:B:1039:PHE:O	2.36	0.58
1:B:970:ILE:HD12	1:B:970:ILE:H	1.68	0.58
1:C:104:PHE:HB2	1:C:115:LEU:HB2	1.86	0.58
2:E:456:LEU:HB3	2:E:460:ARG:HH12	1.69	0.58
1:A:472:ALA:HB3	1:A:484:ASN:HB3	1.86	0.58
2:E:324:THR:O	2:E:328:TRP:HD1	1.87	0.57
2:E:56:THR:OG1	2:E:59:ASN:OD1	2.22	0.57
1:A:64:TRP:HE1	1:A:261:ALA:HB1	1.69	0.57
1:B:123:ASN:HD21	5:B:1311:NAG:H5	1.69	0.57
1:C:700:ASN:OD1	1:C:701:SER:N	2.37	0.57
2:E:207:TYR:HB3	2:E:566:TRP:HZ2	1.70	0.57
1:B:132:GLN:HB3	1:B:156:SER:HB3	1.87	0.57
1:B:855:LEU:HD13	1:B:956:LEU:HD22	1.87	0.57
1:A:151:GLU:OE2	1:A:153:ARG:NH2	2.37	0.57
2:E:577:LYS:HD2	2:E:577:LYS:O	2.04	0.57
1:A:98:ILE:HG23	1:A:99:ILE:HG12	1.87	0.56
1:A:346:SER:HB3	1:A:350:TRP:HA	1.86	0.56
2:E:544:ILE:O	2:E:547:SER:OG	2.22	0.56
2:E:451:PRO:HB2	2:E:485:VAL:HG22	1.86	0.56
2:E:155:SER:OG	2:E:160:ARG:NE	2.38	0.56
1:A:338:VAL:HG12	1:A:396:SER:HB3	1.87	0.56
2:E:540:PHE:CD1	2:E:541:LYS:HG2	2.40	0.56
1:C:17:ASN:OD1	1:C:135:ASN:ND2	2.39	0.56
1:C:318:GLN:HE21	1:C:626:LEU:HB2	1.70	0.56
1:C:16:VAL:O	1:C:153:ARG:NH2	2.39	0.55
2:E:455:MET:HB3	2:E:484:ILE:HD11	1.88	0.55
2:E:478:TRP:HB3	2:E:482:ARG:HE	1.71	0.55
1:C:134:CYS:HB2	1:C:153:ARG:NH1	2.20	0.55
1:C:231:ASN:OD1	5:C:1305:NAG:N2	2.39	0.55
1:B:451:ARG:NH2	1:B:464:ASP:O	2.39	0.55
1:B:575:ASP:HB3	1:B:578:THR:O	2.06	0.55
1:B:719:VAL:HG22	1:B:1062:VAL:HG22	1.89	0.55
1:C:596:THR:HG22	1:C:605:VAL:HG12	1.88	0.55
1:C:115:LEU:HD21	1:C:228:ILE:HG12	1.89	0.55
1:A:428:GLY:HA2	1:A:512:PHE:CE2	2.43	0.54
1:B:140:ASP:OD1	1:B:140:ASP:N	2.39	0.54
2:E:440:LEU:HD22	2:E:594:TRP:CH2	2.43	0.54
1:B:555:LYS:H	1:B:555:LYS:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LYS:HD2	1:C:131:PHE:HE2	1.73	0.54
1:C:354:ARG:NH2	1:C:393:TYR:OH	2.40	0.54
1:C:739:ILE:O	1:C:997:ARG:NH1	2.39	0.54
2:E:388:GLN:HG3	2:E:389:PRO:HD2	1.88	0.54
1:A:430:VAL:HG12	1:A:509:VAL:HG22	1.90	0.54
1:A:499:GLY:O	1:A:503:GLN:HG3	2.08	0.54
2:E:327:PHE:HB3	2:E:356:PHE:HB3	1.88	0.54
2:E:418:LEU:HB3	2:E:424:LEU:HB2	1.89	0.54
1:B:403:GLU:HB3	1:B:415:ILE:HD12	1.90	0.53
1:C:113:GLN:HA	1:C:130:GLU:HG3	1.90	0.53
2:E:493:HIS:ND1	2:E:499:ASP:OD2	2.39	0.53
2:E:418:LEU:HG	2:E:423:LEU:HB2	1.90	0.53
1:B:164:GLU:OE1	1:B:165:TYR:N	2.42	0.53
1:C:767:ILE:HD11	1:C:1009:LEU:HD23	1.91	0.53
1:A:357:ASN:H	1:A:520:THR:HG23	1.73	0.53
1:B:37:TYR:OH	1:B:54:LEU:O	2.23	0.53
1:B:853:LYS:HD3	1:B:963:LEU:HD12	1.91	0.53
1:C:89:TYR:OH	1:C:186:GLU:OE1	2.19	0.53
1:B:326:PHE:O	1:B:577:GLN:NE2	2.41	0.52
2:E:388:GLN:O	2:E:393:ARG:NH1	2.36	0.52
1:A:113:GLN:HE21	1:A:128:VAL:HG22	1.74	0.52
1:A:617:VAL:HG21	1:A:648:ILE:HD11	1.90	0.52
1:B:673:THR:HA	1:B:687:GLN:HG2	1.90	0.52
1:C:28:TYR:HB2	5:C:1302:NAG:H62	1.92	0.52
2:E:20:SER:OG	2:E:21:THR:N	2.43	0.52
2:E:484:ILE:HG13	2:E:485:VAL:HG23	1.92	0.52
1:A:487:PHE:CE2	1:A:489:LEU:HB2	2.46	0.51
1:C:131:PHE:CD1	1:C:155:TYR:HB2	2.46	0.51
2:E:133:VAL:HG22	2:E:167:GLY:HA3	1.92	0.51
1:A:230:ILE:HG13	1:A:231:ASN:H	1.76	0.51
1:C:656:SER:HB3	1:C:695:SER:HB3	1.92	0.51
2:E:318:ILE:HG13	2:E:320:LEU:HD23	1.92	0.51
1:A:633:TYR:O	1:A:637:SER:HB2	2.10	0.51
2:E:351:LEU:HD22	2:E:357:ARG:HE	1.76	0.51
1:A:320:THR:HG23	1:A:321:GLU:HG3	1.93	0.51
2:E:64:ASN:OD1	2:E:65:GLU:N	2.44	0.51
1:C:336:ASP:O	1:C:340:ASN:HB2	2.10	0.51
1:A:642:THR:OG1	1:A:645:GLY:O	2.22	0.50
1:B:984:PRO:HD3	1:C:410:GLY:HA3	1.93	0.50
1:B:1070:LYS:HB3	1:B:1072:PHE:CE2	2.46	0.50
1:A:243:ARG:CZ	1:A:255:TRP:HD1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:TYR:HE1	1:C:696:LEU:HB3	1.76	0.50
1:C:39:PRO:HG3	1:C:51:THR:HG21	1.93	0.50
1:C:183:ASN:OD1	1:C:202:HIS:NE2	2.44	0.50
2:E:330:ASN:H	2:E:330:ASN:ND2	2.10	0.50
1:A:1099:TRP:HB2	1:A:1132:ASN:HD21	1.76	0.50
1:C:1025:LYS:NZ	1:C:1039:PHE:O	2.45	0.50
2:E:91:ASN:OD1	2:E:93:THR:OG1	2.20	0.50
1:C:117:ILE:HG13	1:C:126:ILE:HG23	1.94	0.49
1:B:705:SER:HB3	1:B:708:SER:HB3	1.95	0.49
1:B:315:PHE:CZ	1:B:612:VAL:HG21	2.45	0.49
1:B:618:PRO:O	1:B:625:GLN:NE2	2.46	0.49
1:A:84:PHE:N	1:A:233:THR:O	2.39	0.49
1:A:803:LEU:HD23	1:A:875:LEU:HD23	1.95	0.49
1:C:659:CYS:HB2	1:C:694:MET:HE3	1.95	0.49
2:E:116:ARG:CZ	2:E:186:LEU:HD21	2.43	0.49
1:B:390:THR:HB	1:B:513:GLU:HB3	1.95	0.49
1:A:1025:LYS:NZ	1:A:1039:PHE:O	2.46	0.48
1:C:415:ILE:HD13	1:C:419:ASN:HD22	1.78	0.48
2:E:117:LEU:HD12	2:E:120:ILE:HD12	1.94	0.48
1:B:117:ILE:HG12	1:B:126:ILE:HG12	1.95	0.48
2:E:67:ARG:HA	2:E:67:ARG:HH11	1.75	0.48
1:A:21:ARG:HH21	1:A:77:PHE:HE2	1.60	0.48
1:B:331:ASN:O	1:B:359:VAL:HG22	2.13	0.48
2:E:309:LYS:HB3	2:E:313:LYS:HE2	1.95	0.48
1:A:68:ILE:N	1:A:76:ARG:O	2.40	0.48
2:E:360:MET:CE	2:E:361:CYS:H	2.27	0.48
2:E:351:LEU:HD22	2:E:357:ARG:NE	2.29	0.48
2:E:382:ASP:HA	2:E:385:TYR:CE2	2.49	0.48
2:E:400:PHE:HD1	2:E:400:PHE:O	1.97	0.48
1:A:66:HIS:HD1	1:A:67:VAL:H	1.61	0.48
1:A:469:ILE:N	1:A:469:ILE:HD12	2.29	0.48
2:E:170:ALA:HB1	2:E:497:TYR:CE1	2.48	0.48
2:E:555:LEU:HA	2:E:558:LEU:HB2	1.94	0.47
1:A:656:SER:HB3	1:A:695:SER:HB3	1.96	0.47
2:E:303:ASP:OD1	2:E:306:ARG:HB2	2.13	0.47
1:B:79:ASN:O	1:B:236:GLN:NE2	2.47	0.47
1:A:398:VAL:C	1:A:399:ILE:HD13	2.35	0.47
2:E:239:GLN:HE22	2:E:599:ASN:HB2	1.79	0.47
1:A:110:SER:HB3	1:A:132:GLN:HA	1.97	0.47
1:C:104:PHE:HD2	1:C:232:ILE:HG21	1.79	0.47
1:B:182:LYS:HA	1:B:205:ILE:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PHE:HZ	1:A:226:LEU:HD22	1.79	0.47
1:B:93:ILE:HG22	1:B:181:PHE:HB3	1.97	0.46
1:A:112:THR:O	1:A:130:GLU:HG3	2.15	0.46
1:B:559:PHE:HD1	1:C:41:LYS:HD2	1.81	0.46
2:E:49:TRP:CE2	2:E:357:ARG:HD3	2.50	0.46
2:E:79:ARG:HA	2:E:82:LYS:NZ	2.29	0.46
2:E:315:PHE:O	2:E:318:ILE:HG12	2.14	0.46
1:A:783:LYS:CD	1:A:783:LYS:H	2.28	0.46
1:B:323:ILE:N	1:B:537:ASN:O	2.47	0.46
2:E:306:ARG:O	2:E:310:GLU:HG2	2.15	0.46
2:E:430:GLU:N	2:E:430:GLU:OE1	2.48	0.46
1:A:97:ASN:HA	1:A:185:ARG:NH2	2.30	0.46
1:A:1071:ASN:OD1	5:A:1305:NAG:N2	2.48	0.46
1:C:82:LEU:HD13	1:C:264:VAL:HG21	1.96	0.46
1:C:347:VAL:HG22	1:C:419:ASN:HB3	1.97	0.46
2:E:66:ALA:HA	2:E:69:LYS:HG2	1.98	0.46
2:E:127:ILE:HD12	2:E:175:GLN:HB3	1.97	0.46
1:A:54:LEU:HD12	1:A:190:LYS:HD3	1.97	0.46
1:A:325:ARG:NE	1:A:575:ASP:OD1	2.42	0.46
1:A:723:ILE:HG12	1:A:1058:VAL:HG22	1.98	0.46
1:A:292:PRO:HG3	1:A:630:TRP:CE3	2.51	0.46
1:A:406:GLN:HE21	1:A:406:GLN:HB3	1.53	0.46
1:A:228:ILE:HG22	1:A:230:ILE:HB	1.98	0.46
2:E:184:VAL:HG11	2:E:473:TRP:CZ2	2.51	0.46
1:A:291:ASP:OD1	1:A:291:ASP:N	2.49	0.45
1:A:958:THR:HG21	1:B:759:GLN:HE21	1.80	0.45
1:B:78:ASP:OD1	1:B:78:ASP:N	2.49	0.45
2:E:505:HIS:HE1	2:E:512:PHE:HB2	1.81	0.45
1:B:899:MET:HB3	1:B:913:LEU:HD11	1.98	0.45
1:B:902:ARG:HD3	1:B:1046:LEU:O	2.16	0.45
1:A:630:TRP:HE3	1:A:630:TRP:O	2.00	0.45
1:A:1050:PRO:O	1:A:1051:GLN:NE2	2.45	0.45
1:B:64:TRP:CD1	1:B:263:TYR:HE1	2.35	0.45
1:B:98:ILE:HD13	1:B:260:ALA:HB2	1.98	0.45
1:C:18:LEU:HD13	1:C:77:PHE:HE1	1.81	0.45
1:C:135:ASN:OD1	1:C:135:ASN:N	2.49	0.45
2:E:440:LEU:HD22	2:E:594:TRP:HH2	1.81	0.45
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.90	0.45
1:B:358:CYS:O	1:B:521:VAL:HA	2.17	0.45
1:B:783:LYS:CD	1:B:783:LYS:H	2.29	0.45
2:E:371:THR:O	2:E:375:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ARG:HG3	1:A:344:PHE:N	2.32	0.45
1:C:353:LYS:HB3	1:C:394:ALA:HB3	1.98	0.45
1:B:151:GLU:OE2	1:B:153:ARG:NE	2.47	0.45
1:C:131:PHE:CG	1:C:158:ALA:HB2	2.52	0.45
1:C:925:ASN:HD22	3:S:1:NAG:C7	2.30	0.45
1:A:215:GLN:OE1	1:A:215:GLN:HA	2.16	0.45
1:C:341:ALA:HB3	1:C:344:PHE:HE1	1.81	0.45
1:C:350:TRP:O	1:C:463:ARG:NH2	2.37	0.45
2:E:388:GLN:OE1	2:E:561:GLY:HA3	2.17	0.45
1:B:66:HIS:H	1:B:76:ARG:NH1	2.15	0.45
1:B:974:LEU:HA	1:B:977:ILE:HD13	1.99	0.45
1:A:62:VAL:HB	1:A:264:VAL:O	2.16	0.44
1:A:452:LEU:HD11	2:E:35:HIS:CE1	2.52	0.44
1:A:784:GLN:OE1	1:C:700:ASN:ND2	2.44	0.44
1:B:67:VAL:HG23	1:B:77:PHE:CB	2.44	0.44
1:C:152:PHE:N	1:C:152:PHE:CD1	2.83	0.44
2:E:243:TYR:HE2	2:E:440:LEU:HD21	1.82	0.44
1:C:37:TYR:OH	1:C:54:LEU:O	2.20	0.44
1:A:321:GLU:OE1	1:A:531:VAL:HG11	2.17	0.44
1:A:526:LYS:HD3	1:A:526:LYS:HA	1.65	0.44
1:C:314:ASN:ND2	1:C:590:GLY:O	2.49	0.44
1:A:414:ASN:OD1	1:A:415:ILE:HG12	2.18	0.44
1:A:1001:LEU:HD23	1:A:1001:LEU:HA	1.82	0.44
1:C:111:LYS:HE2	1:C:111:LYS:HB3	1.83	0.44
1:C:134:CYS:HB2	1:C:153:ARG:HH12	1.82	0.44
1:A:433:TRP:HZ3	1:A:508:VAL:HG23	1.82	0.44
1:C:236:GLN:HG3	1:C:237:THR:N	2.32	0.44
1:C:355:ILE:HB	1:C:392:VAL:HB	1.98	0.44
2:E:274:PHE:CE2	2:E:276:THR:HB	2.52	0.44
2:E:444:LEU:HA	2:E:447:VAL:HG12	2.00	0.44
1:A:66:HIS:ND1	1:A:260:ALA:O	2.46	0.44
1:B:628:PRO:HD2	1:B:630:TRP:NE1	2.33	0.44
1:C:36:VAL:HG11	1:C:217:PHE:CZ	2.53	0.44
1:C:94:GLU:O	1:C:181:PHE:HB3	2.18	0.44
1:B:64:TRP:HD1	1:B:65:PHE:N	2.15	0.44
1:C:881:SER:OG	1:C:884:THR:OG1	2.34	0.44
1:A:348:TYR:HD1	1:A:349:ALA:N	2.16	0.44
1:B:1071:ASN:ND2	5:B:1308:NAG:H61	2.33	0.44
1:C:212:ASP:OD1	1:C:212:ASP:N	2.51	0.44
1:C:241:LEU:HD12	1:C:241:LEU:O	2.17	0.44
1:C:270:ARG:NH1	1:C:287:ASP:OD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:VAL:HA	1:C:1061:HIS:O	2.18	0.44
2:E:132:LYS:HG3	2:E:171:GLU:HB3	2.00	0.44
1:C:414:ASN:O	1:C:418:TYR:HB2	2.17	0.43
1:C:846:LEU:HD23	1:C:846:LEU:O	2.17	0.43
2:E:557:MET:HA	2:E:560:LEU:HB2	2.00	0.43
1:C:110:SER:HA	1:C:130:GLU:HB3	1.99	0.43
2:E:46:LEU:HA	2:E:351:LEU:HD21	2.01	0.43
2:E:498:CYS:SG	2:E:501:ALA:HB2	2.58	0.43
2:E:505:HIS:CE1	2:E:512:PHE:HB2	2.53	0.43
1:B:125:VAL:HG22	5:B:1311:NAG:H62	2.01	0.43
1:B:138:PHE:CD1	1:B:138:PHE:C	2.92	0.43
1:C:351:ASN:O	1:C:395:ASP:HA	2.18	0.43
2:E:460:ARG:CZ	2:E:505:HIS:HD2	2.30	0.43
2:E:263:PRO:HD2	2:E:266:LEU:HD12	2.00	0.43
1:A:185:ARG:HB3	1:A:187:PHE:CE1	2.53	0.43
1:B:68:ILE:HB	1:B:76:ARG:H	1.84	0.43
1:C:341:ALA:HB3	1:C:344:PHE:CE1	2.54	0.43
1:C:549:LEU:HA	1:C:583:ASP:O	2.17	0.43
1:C:1050:PRO:O	1:C:1051:GLN:NE2	2.52	0.43
1:A:575:ASP:HB3	1:A:578:THR:O	2.18	0.43
2:E:524:GLN:HA	2:E:527:GLU:HG2	2.01	0.43
1:A:41:LYS:H	1:C:516:HIS:CE1	2.37	0.43
1:A:1099:TRP:HB2	1:A:1132:ASN:ND2	2.34	0.43
1:B:291:ASP:OD1	1:B:291:ASP:N	2.52	0.43
1:C:705:SER:HB3	1:C:708:SER:HB3	2.00	0.42
1:C:318:GLN:NE2	1:C:626:LEU:HD13	2.34	0.42
1:C:719:VAL:HG22	1:C:1062:VAL:HG22	2.00	0.42
1:A:414:ASN:O	1:A:419:ASN:ND2	2.50	0.42
1:C:165:TYR:HD1	1:C:166:VAL:N	2.17	0.42
2:E:312:GLU:O	2:E:316:VAL:HG13	2.19	0.42
1:A:1139:GLN:HA	1:A:1139:GLN:OE1	2.19	0.42
2:E:177:ARG:HH21	2:E:498:CYS:HA	1.85	0.42
1:A:532:LYS:NZ	1:A:551:GLU:OE2	2.53	0.42
1:B:107:THR:OG1	1:B:112:THR:OG1	2.35	0.42
1:B:123:ASN:OD1	1:B:123:ASN:N	2.51	0.42
1:B:713:THR:OG1	1:B:1068:GLN:O	2.24	0.42
1:B:400:ARG:O	1:B:404:VAL:HG23	2.19	0.42
1:C:136:ASP:N	1:C:136:ASP:OD1	2.53	0.42
1:C:328:ASN:OD1	1:C:328:ASN:N	2.51	0.42
1:A:781:GLN:HG3	1:A:1026:MET:HG2	2.02	0.42
1:C:913:LEU:HD12	1:C:920:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:37:ALA:O	2:E:41:SER:N	2.50	0.42
3:V:1:NAG:H62	3:V:2:NAG:C7	2.49	0.42
1:B:336:ASP:OD1	1:B:336:ASP:N	2.49	0.41
1:B:631:ARG:O	1:B:631:ARG:HG3	2.20	0.41
1:C:624:ASP:OD1	1:C:624:ASP:N	2.53	0.41
1:B:95:LYS:HZ3	1:B:180:ASN:N	2.18	0.41
1:A:125:VAL:HG22	1:A:166:VAL:HG22	2.01	0.41
1:B:237:THR:O	1:B:238:LEU:HD23	2.21	0.41
1:B:325:ARG:NH1	1:B:575:ASP:OD2	2.52	0.41
1:A:403:GLU:HG3	1:A:415:ILE:HG13	2.01	0.41
1:B:851:LYS:HA	1:B:855:LEU:O	2.21	0.41
2:E:410:LEU:O	2:E:414:THR:HG23	2.20	0.41
1:A:1138:LEU:HD13	1:A:1142:LEU:HB2	2.03	0.41
1:A:325:ARG:CZ	1:A:530:LEU:HD23	2.51	0.41
1:B:352:ARG:HD2	1:B:393:TYR:HB3	2.02	0.41
1:B:863:THR:OG1	1:B:866:MET:HG3	2.21	0.41
2:E:169:ARG:HA	2:E:169:ARG:NE	2.36	0.41
2:E:209:VAL:HB	2:E:217:TYR:H	1.85	0.41
1:B:543:LEU:HD21	1:B:570:THR:HG21	2.03	0.41
1:C:126:ILE:HG21	1:C:226:LEU:HD21	2.02	0.41
1:A:97:ASN:HA	1:A:185:ARG:HH22	1.85	0.41
1:B:428:GLY:HA2	1:B:512:PHE:CD2	2.56	0.41
2:E:112:GLU:HG2	2:E:113:LYS:N	2.36	0.41
2:E:346:PRO:HG3	2:E:360:MET:SD	2.60	0.41
1:A:40:ASP:OD2	1:A:44:ARG:NH1	2.30	0.41
1:A:124:VAL:O	1:A:166:VAL:HA	2.21	0.41
1:A:891:LEU:HB3	1:C:710:ALA:HB3	2.02	0.41
1:B:25:PRO:HA	1:B:26:PRO:HD3	1.93	0.41
1:B:459:LYS:HE2	1:B:459:LYS:HB3	1.85	0.41
1:B:945:LEU:HD21	1:B:1056:GLY:HA3	2.02	0.41
2:E:98:LEU:O	2:E:101:LEU:HG	2.21	0.41
2:E:462:MET:SD	2:E:462:MET:N	2.94	0.41
2:E:601:ASN:OD1	2:E:602:SER:N	2.53	0.41
1:A:382:THR:O	1:A:383:LYS:HG2	2.21	0.41
1:A:631:ARG:HG3	1:A:634:SER:HB3	2.03	0.41
1:B:363:SER:HA	1:B:366:TYR:CD2	2.56	0.41
2:E:415:PRO:O	2:E:418:LEU:HB2	2.21	0.41
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.03	0.40
1:C:126:ILE:HB	1:C:165:TYR:HB3	2.03	0.40
1:C:593:SER:OG	1:C:610:GLN:OE1	2.36	0.40
1:A:67:VAL:O	1:A:260:ALA:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:HD22	1:B:159:ASN:HA	1.58	0.40
1:C:116:LEU:C	1:C:117:ILE:HD12	2.42	0.40
1:A:416:ALA:O	1:A:421:LYS:HB2	2.21	0.40
1:B:526:LYS:HD3	1:B:526:LYS:HA	1.89	0.40
1:C:103:ILE:HD11	1:C:108:LEU:HD23	2.04	0.40
1:C:368:LEU:H	1:C:368:LEU:HD23	1.86	0.40
1:C:373:THR:HB	1:C:432:ALA:HB3	2.03	0.40
1:A:554:LYS:HB2	1:A:581:ILE:HG21	2.03	0.40
1:B:44:ARG:O	1:B:280:GLY:HA2	2.21	0.40
1:B:630:TRP:HE3	1:B:630:TRP:O	2.03	0.40
2:E:324:THR:HA	2:E:328:TRP:CD1	2.56	0.40
1:A:58:PHE:HB3	1:A:59:PHE:CD2	2.56	0.40
1:A:436:ASN:HB2	1:A:503:GLN:HB3	2.02	0.40
1:A:855:LEU:HD13	1:A:956:LEU:HD22	2.03	0.40
1:B:439:ASP:OD2	1:B:506:ARG:NE	2.54	0.40
1:C:1131:ASN:OD1	3:V:1:NAG:N2	2.54	0.40
2:E:240:LEU:HD11	2:E:444:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

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 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	A	1043/1253 (83%)	1004 (96%)	39 (4%)	0	100	100
1	B	1042/1253 (83%)	1009 (97%)	33 (3%)	0	100	100
1	C	1046/1253 (84%)	1005 (96%)	41 (4%)	0	100	100
2	E	593/613 (97%)	571 (96%)	22 (4%)	0	100	100
All	All	3724/4372 (85%)	3589 (96%)	135 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	932/1097 (85%)	914 (98%)	18 (2%)	52	77
1	B	931/1097 (85%)	919 (99%)	12 (1%)	65	84
1	C	933/1097 (85%)	918 (98%)	15 (2%)	58	81
2	E	527/541 (97%)	499 (95%)	28 (5%)	19	49
All	All	3323/3832 (87%)	3250 (98%)	73 (2%)	47	74

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	148	MET
1	A	155	TYR
1	A	165	TYR
1	A	203	THR
1	A	333	CYS
1	A	336	ASP
1	A	338	VAL
1	A	342	THR
1	A	348	TYR
1	A	374	PHE
1	A	397	PHE
1	A	445	ASN
1	A	583	ASP
1	A	625	GLN
1	A	643	ARG
1	A	783	LYS
1	A	954	GLN
1	B	138	PHE
1	B	155	TYR
1	B	164	GLU
1	B	243	ARG
1	B	537	ASN
1	B	559	PHE

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Mol	Chain	Res	Type
1	B	562	PHE
1	B	673	THR
1	B	688	SER
1	B	783	LYS
1	B	899	MET
1	B	1026	MET
1	C	78	ASP
1	C	153	ARG
1	C	155	TYR
1	C	165	TYR
1	C	195	TYR
1	C	218	SER
1	C	241	LEU
1	C	279	ASN
1	C	354	ARG
1	C	371	PHE
1	C	405	ARG
1	C	417	ASP
1	C	424	ASP
1	C	899	MET
1	C	932	GLN
2	E	29	PHE
2	E	42	TYR
2	E	122	ASN
2	E	138	THR
2	E	190	MET
2	E	198	ASP
2	E	202	TYR
2	E	215	TYR
2	E	223	MET
2	E	255	TYR
2	E	275	TRP
2	E	327	PHE
2	E	330	ASN
2	E	332	MET
2	E	340	ARG
2	E	363	LYS
2	E	388	GLN
2	E	400	PHE
2	E	408	MET
2	E	438	PHE
2	E	455	MET

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Mol	Chain	Res	Type
2	E	473	TRP
2	E	510	TYR
2	E	515	TYR
2	E	557	MET
2	E	577	LYS
2	E	594	TRP
2	E	613	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	406	GLN
1	A	445	ASN
1	A	502	HIS
1	A	801	GLN
1	B	119	ASN
1	B	159	ASN
1	B	357	ASN
1	B	445	ASN
1	B	561	GLN
1	B	759	GLN
1	B	999	GLN
1	B	1002	GLN
1	C	318	GLN
1	C	447	ASN
1	C	925	ASN
2	E	330	ASN
2	E	505	HIS
2	E	524	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

37 monosaccharides 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	$\# Z > 2$
3	NAG	D	1	3,2	14,14,15	0.42	0	17,19,21	0.73	1 (5%)
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.55	0
4	NAG	F	1	2,4	14,14,15	0.34	0	17,19,21	0.44	0
4	NAG	F	2	4	14,14,15	0.41	0	17,19,21	0.57	0
4	BMA	F	3	4	11,11,12	0.94	0	15,15,17	0.82	0
3	NAG	G	1	3,1	14,14,15	0.51	0	17,19,21	0.57	0
3	NAG	G	2	3	14,14,15	0.52	0	17,19,21	0.54	0
3	NAG	H	1	3,1	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	H	2	3	14,14,15	0.40	0	17,19,21	0.72	0
3	NAG	I	1	3,1	14,14,15	0.36	0	17,19,21	0.49	0
3	NAG	I	2	3	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	J	1	3,1	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	J	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	K	1	3,1	14,14,15	0.45	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
3	NAG	L	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	L	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	NAG	M	1	3,1	14,14,15	0.43	0	17,19,21	0.77	1 (5%)
3	NAG	M	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	N	1	3,1	14,14,15	0.90	1 (7%)	17,19,21	0.69	0
3	NAG	N	2	3	14,14,15	0.16	0	17,19,21	0.41	0
3	NAG	O	1	3,1	14,14,15	0.32	0	17,19,21	0.49	0
3	NAG	O	2	3	14,14,15	0.44	0	17,19,21	0.60	0
3	NAG	P	1	3,1	14,14,15	0.36	0	17,19,21	1.12	1 (5%)
3	NAG	P	2	3	14,14,15	0.47	0	17,19,21	0.45	0
3	NAG	Q	1	3,1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	Q	2	3	14,14,15	0.45	0	17,19,21	0.53	0
3	NAG	R	1	3,1	14,14,15	0.21	0	17,19,21	0.67	1 (5%)
3	NAG	R	2	3	14,14,15	0.97	1 (7%)	17,19,21	0.65	0
3	NAG	S	1	3,1	14,14,15	0.45	0	17,19,21	0.66	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	S	2	3	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	T	1	3,1	14,14,15	0.36	0	17,19,21	0.54	0
3	NAG	T	2	3	14,14,15	0.22	0	17,19,21	0.34	0
3	NAG	U	1	3,1	14,14,15	0.41	0	17,19,21	0.55	0
3	NAG	U	2	3	14,14,15	0.36	0	17,19,21	0.53	0
3	NAG	V	1	3,1	14,14,15	0.28	0	17,19,21	0.45	0
3	NAG	V	2	3	14,14,15	0.57	0	17,19,21	0.68	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	NAG	D	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	3/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	2	NAG	O5-C1	-3.54	1.38	1.43
3	N	1	NAG	O5-C1	-3.21	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	NAG	C1-O5-C5	3.10	116.39	112.19
3	K	2	NAG	C1-O5-C5	2.61	115.73	112.19
3	M	1	NAG	C1-O5-C5	2.49	115.56	112.19
3	D	1	NAG	C1-O5-C5	2.20	115.17	112.19
3	S	1	NAG	C1-O5-C5	2.17	115.13	112.19
3	R	1	NAG	C1-O5-C5	2.07	114.99	112.19

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	U	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	F	3	BMA	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C1-C2-N2-C7
3	O	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6

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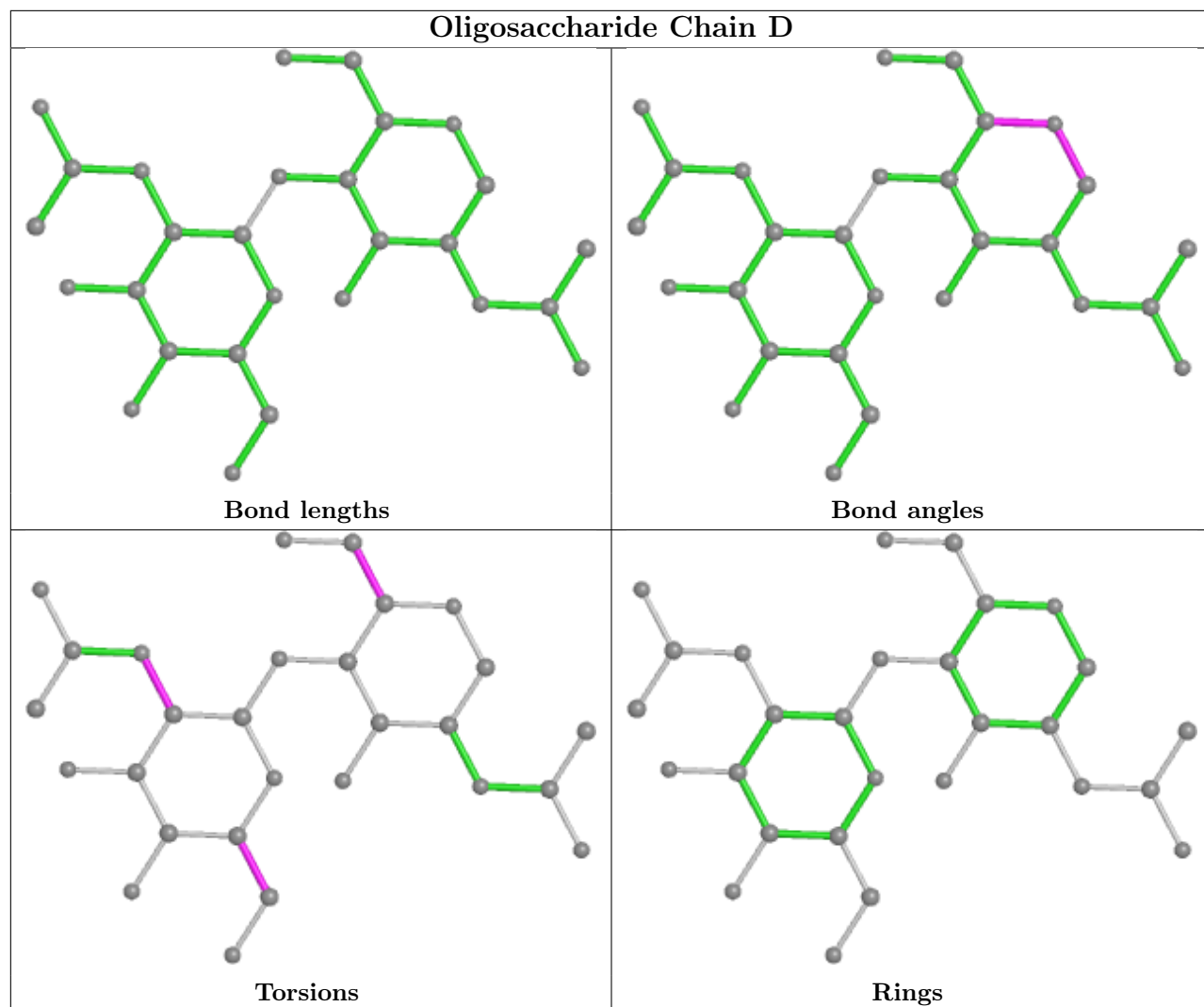
Mol	Chain	Res	Type	Atoms
3	S	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	S	1	NAG	C1-C2-N2-C7
3	K	1	NAG	C4-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
3	T	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	L	2	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	N	1	NAG	C3-C2-N2-C7
3	K	1	NAG	O5-C5-C6-O6
3	N	1	NAG	C1-C2-N2-C7
3	V	2	NAG	C1-C2-N2-C7
3	D	2	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
3	Q	2	NAG	C3-C2-N2-C7
3	V	2	NAG	C3-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7
3	Q	2	NAG	C1-C2-N2-C7

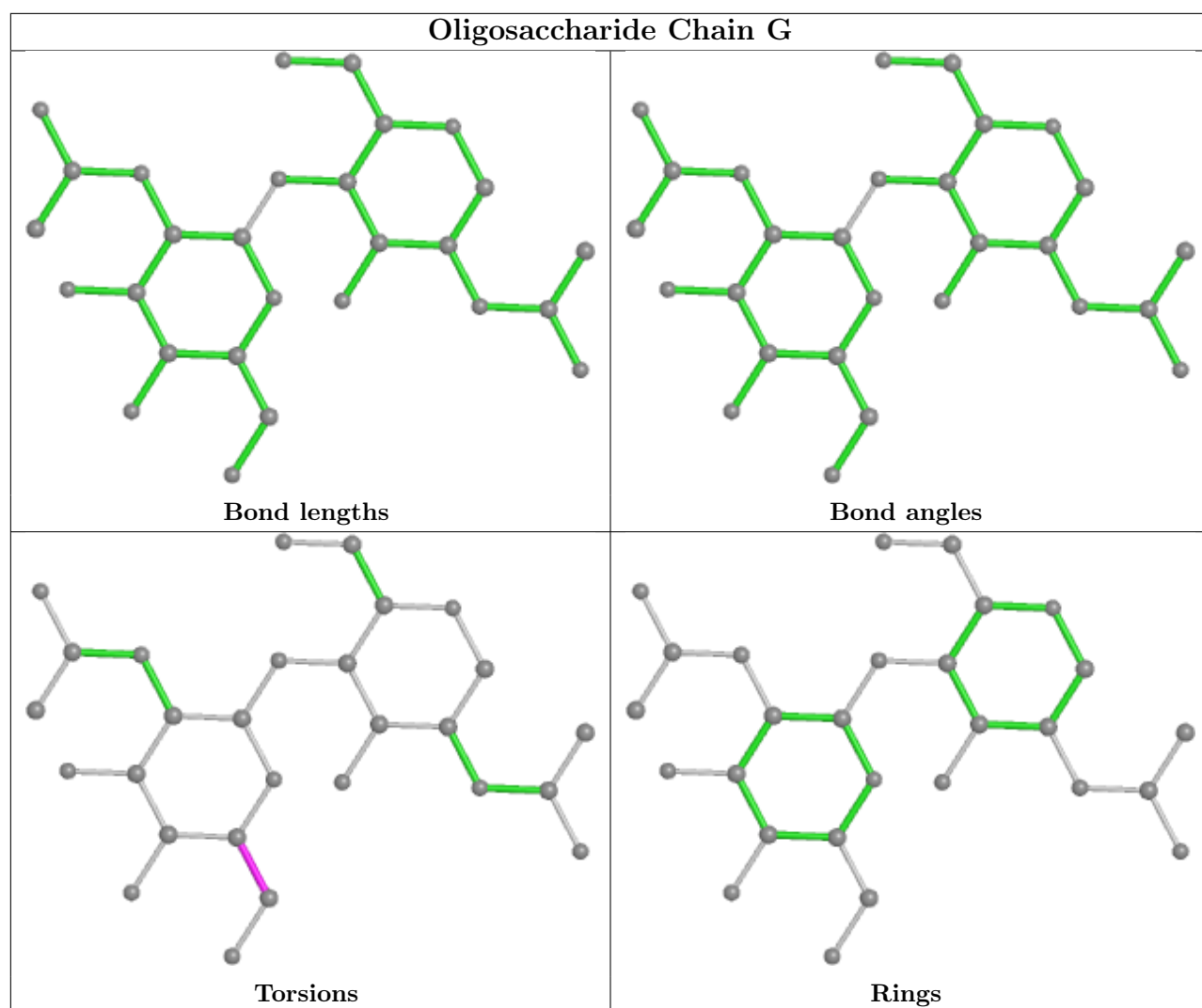
There are no ring outliers.

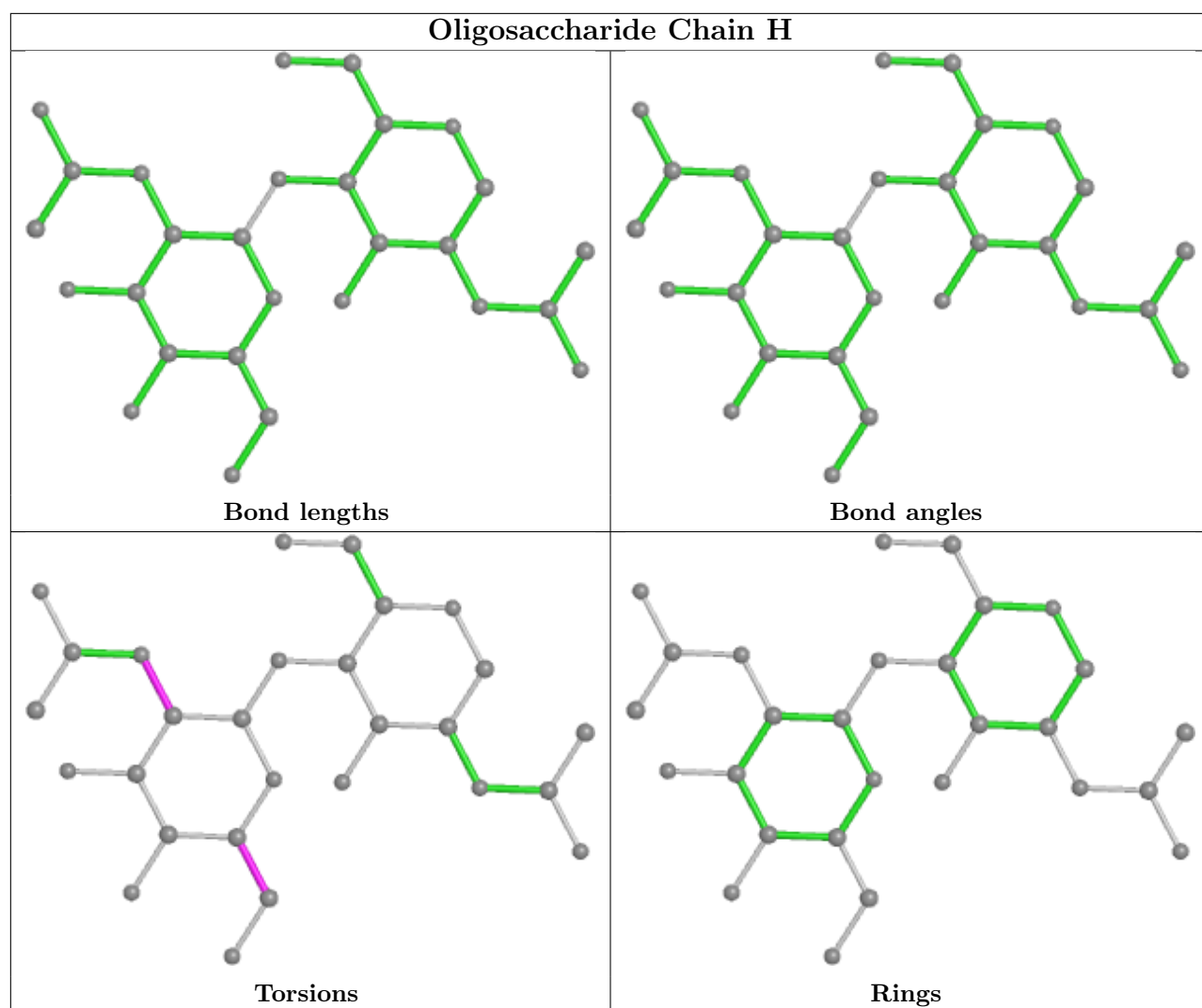
7 monomers are involved in 7 short contacts:

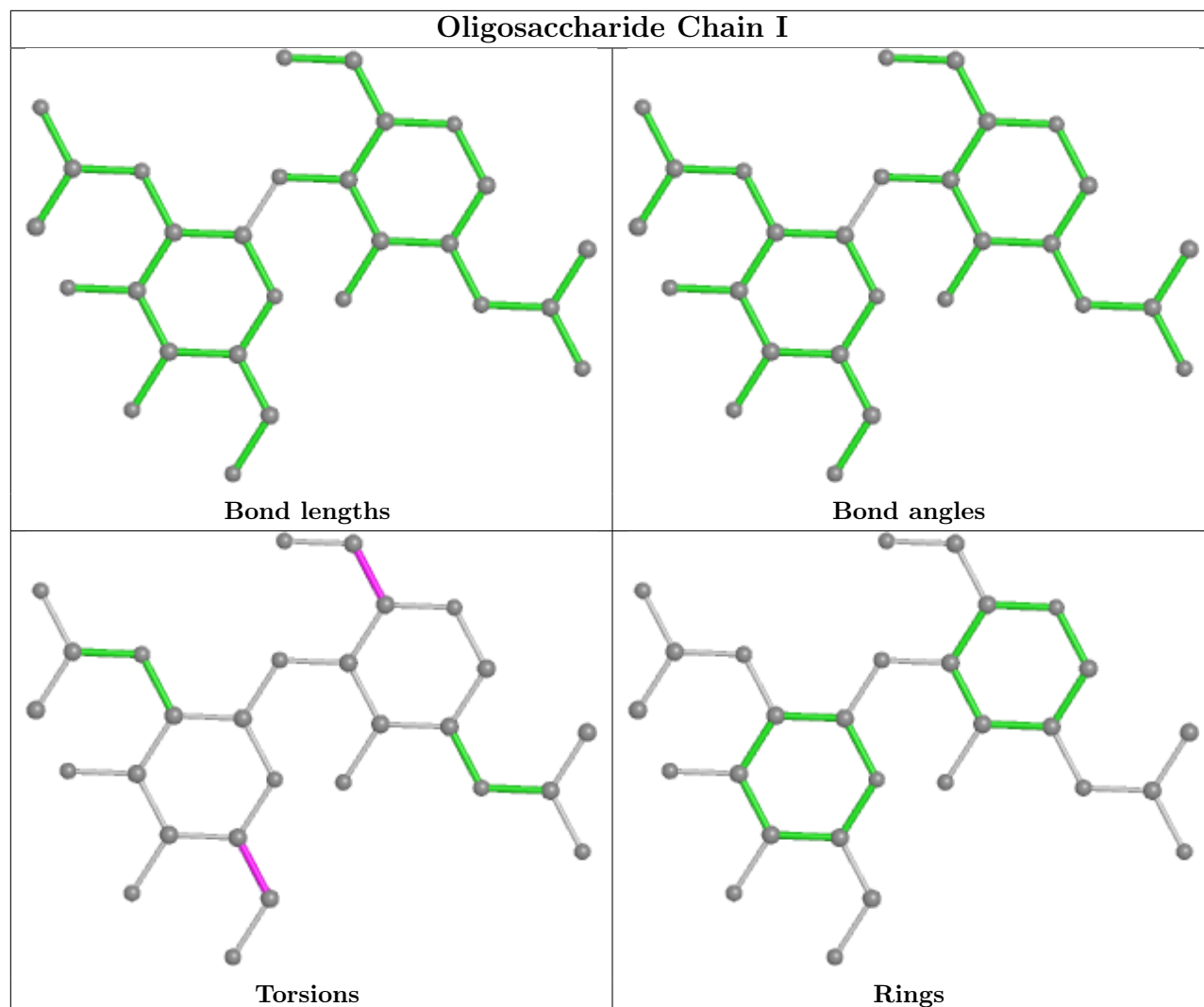
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	1	NAG	1	0
3	U	1	NAG	1	0
3	M	1	NAG	1	0
3	V	1	NAG	2	0
3	V	2	NAG	1	0
3	K	1	NAG	1	0
3	T	1	NAG	1	0

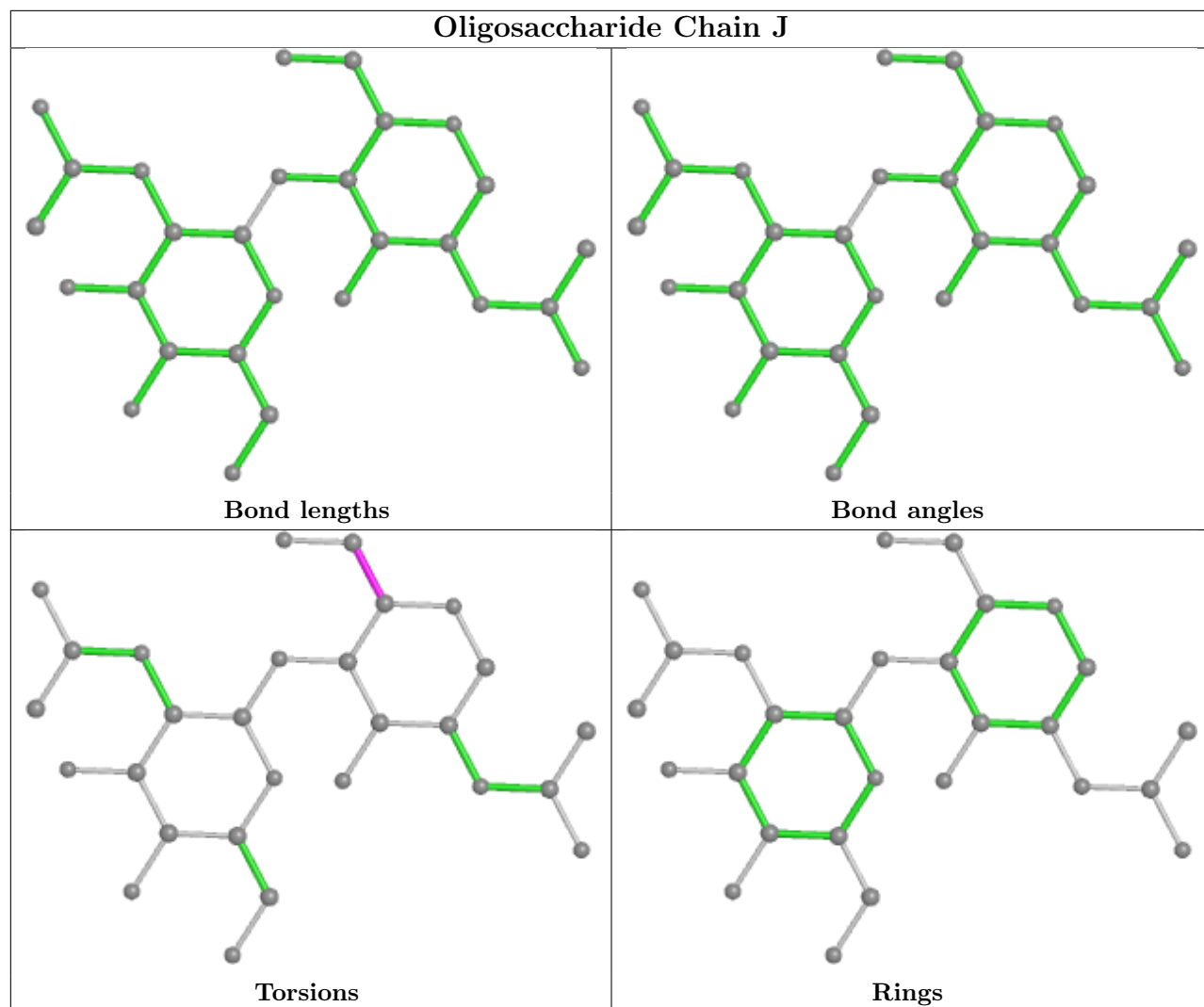
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

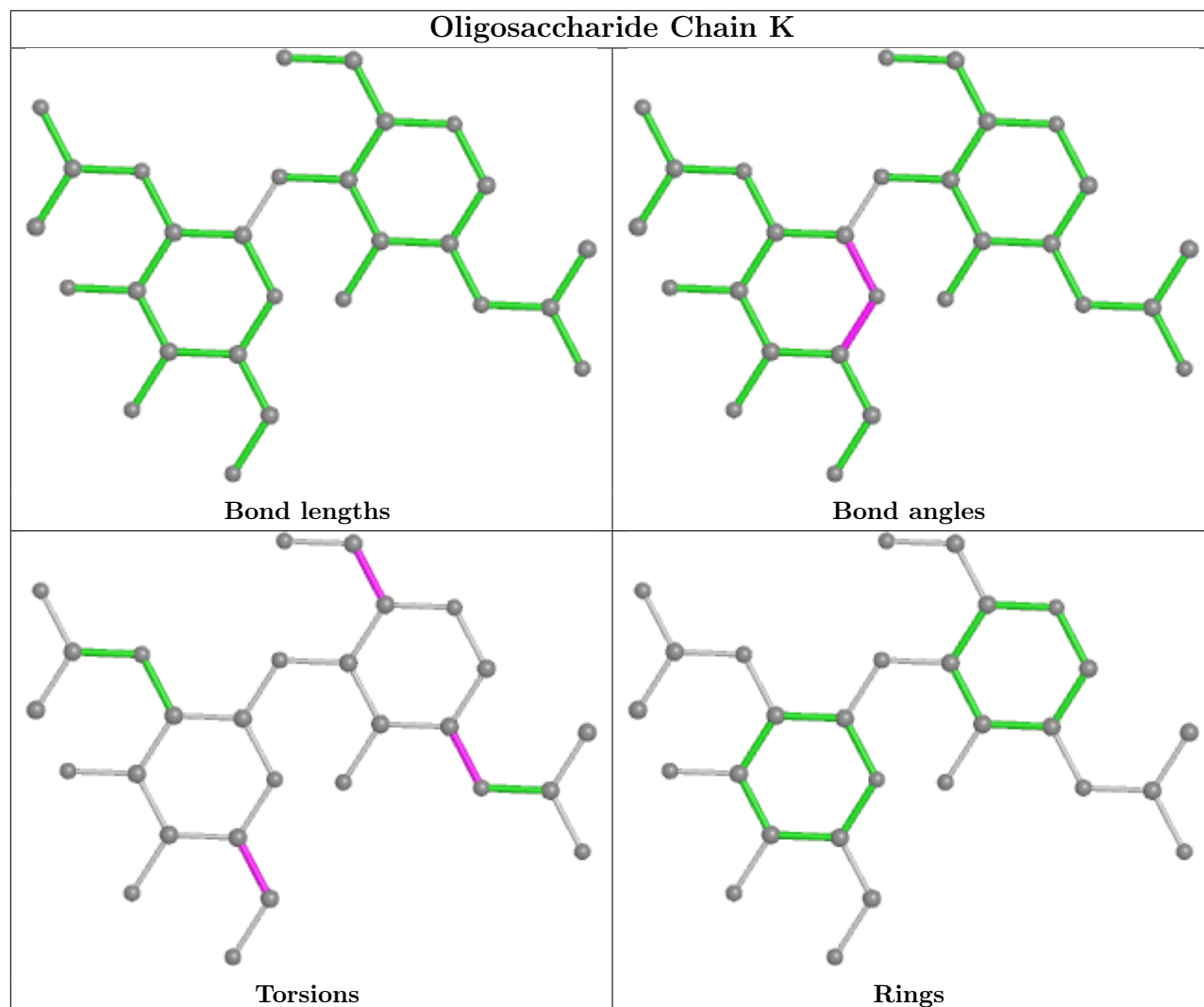


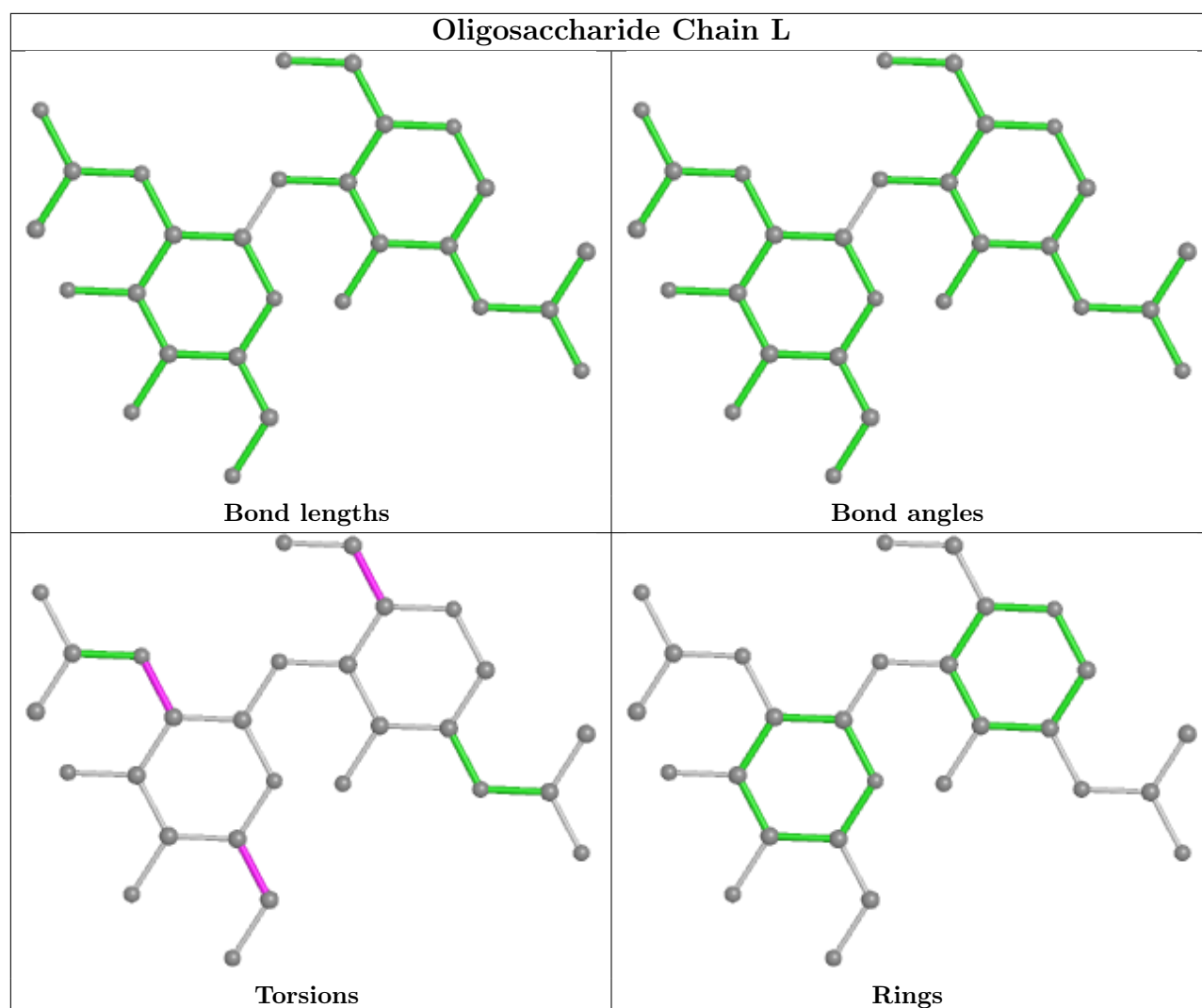


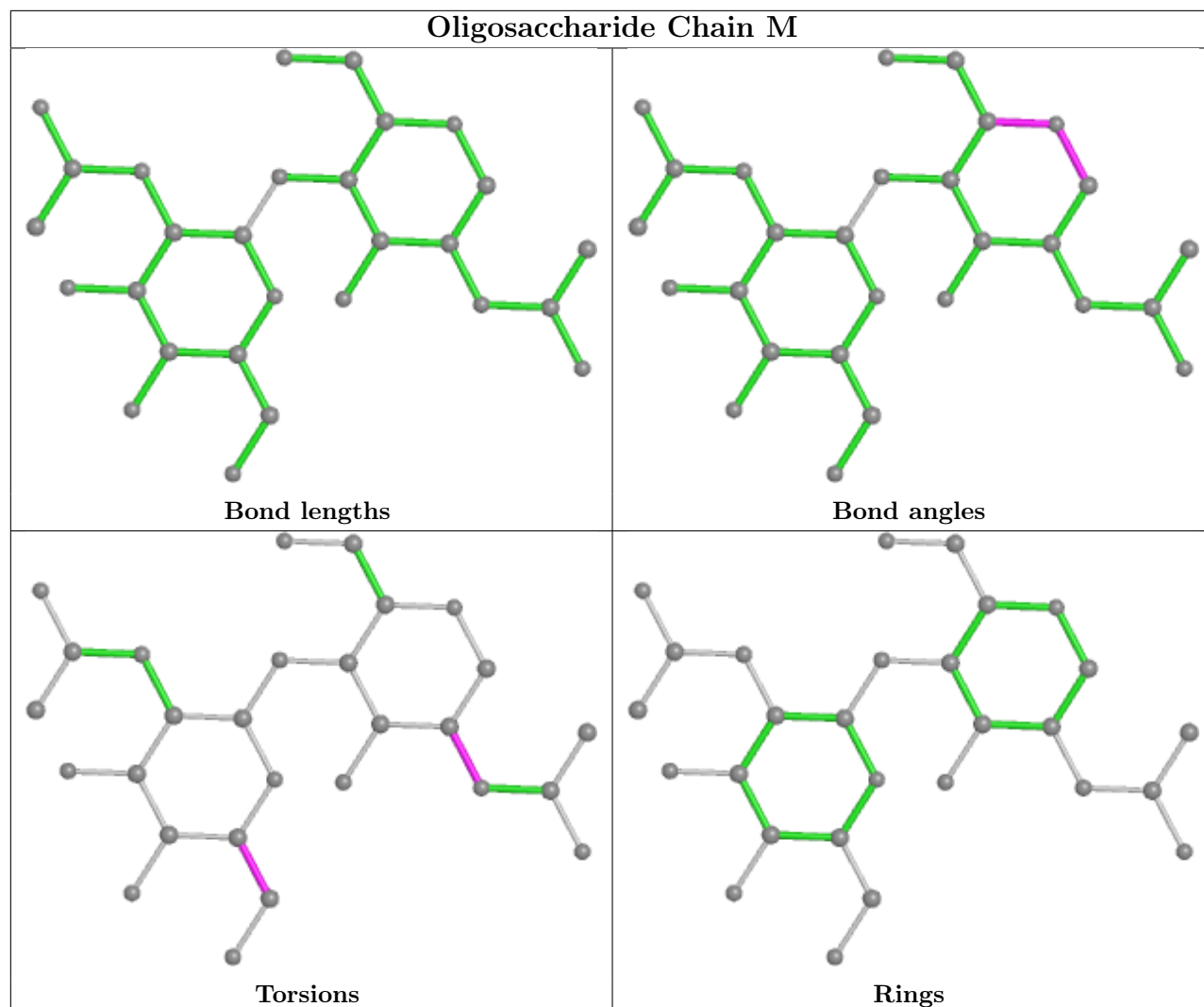


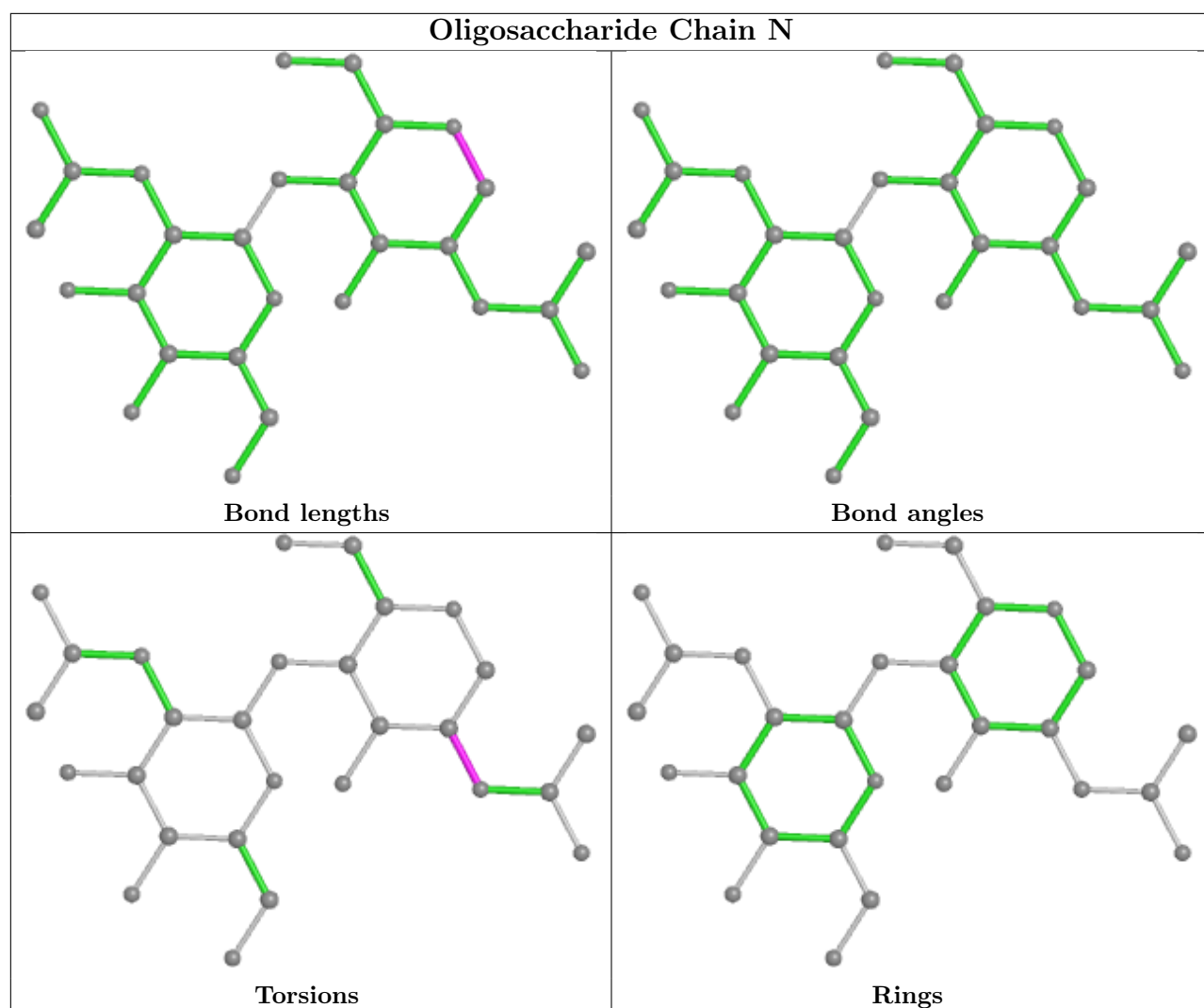


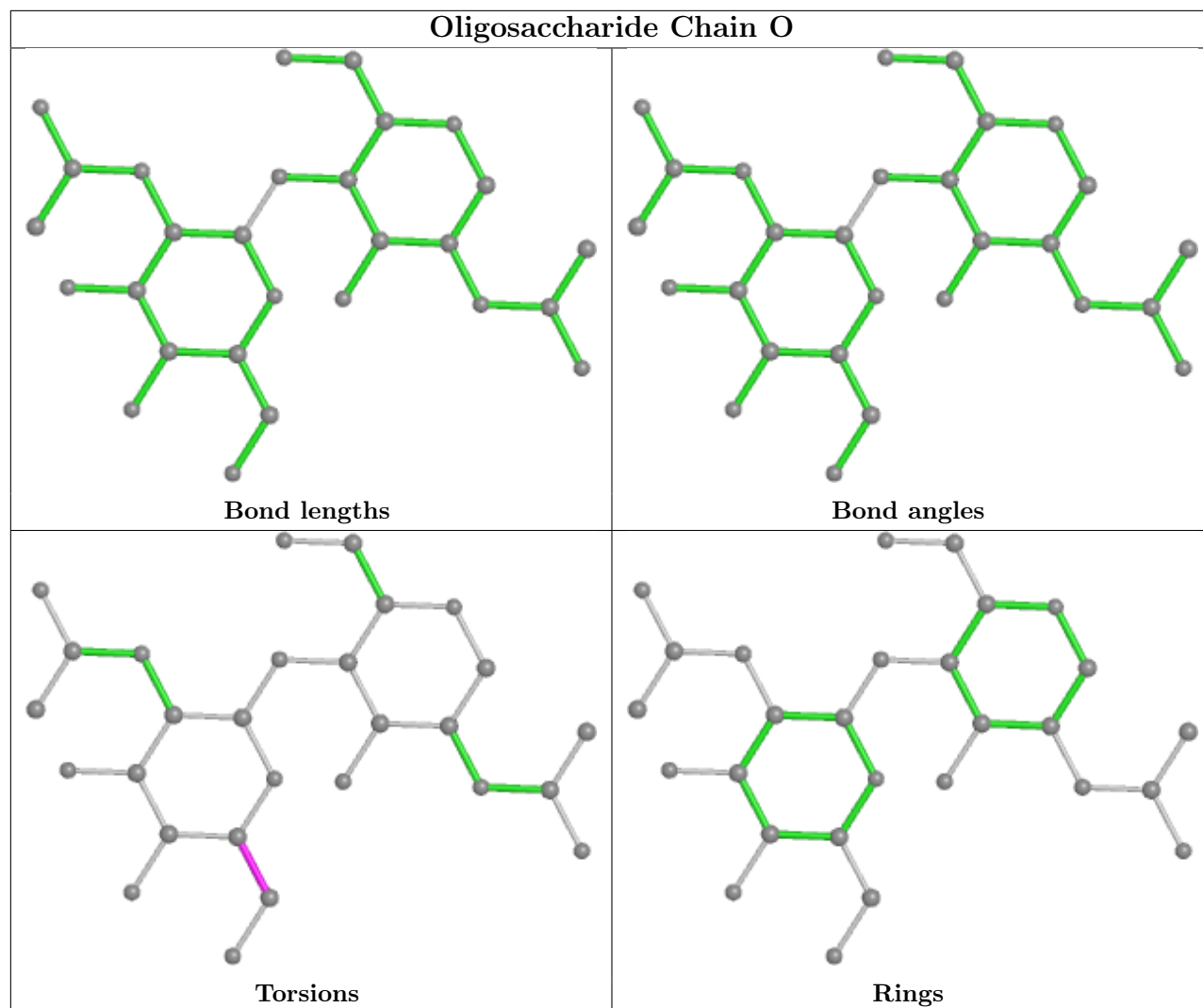


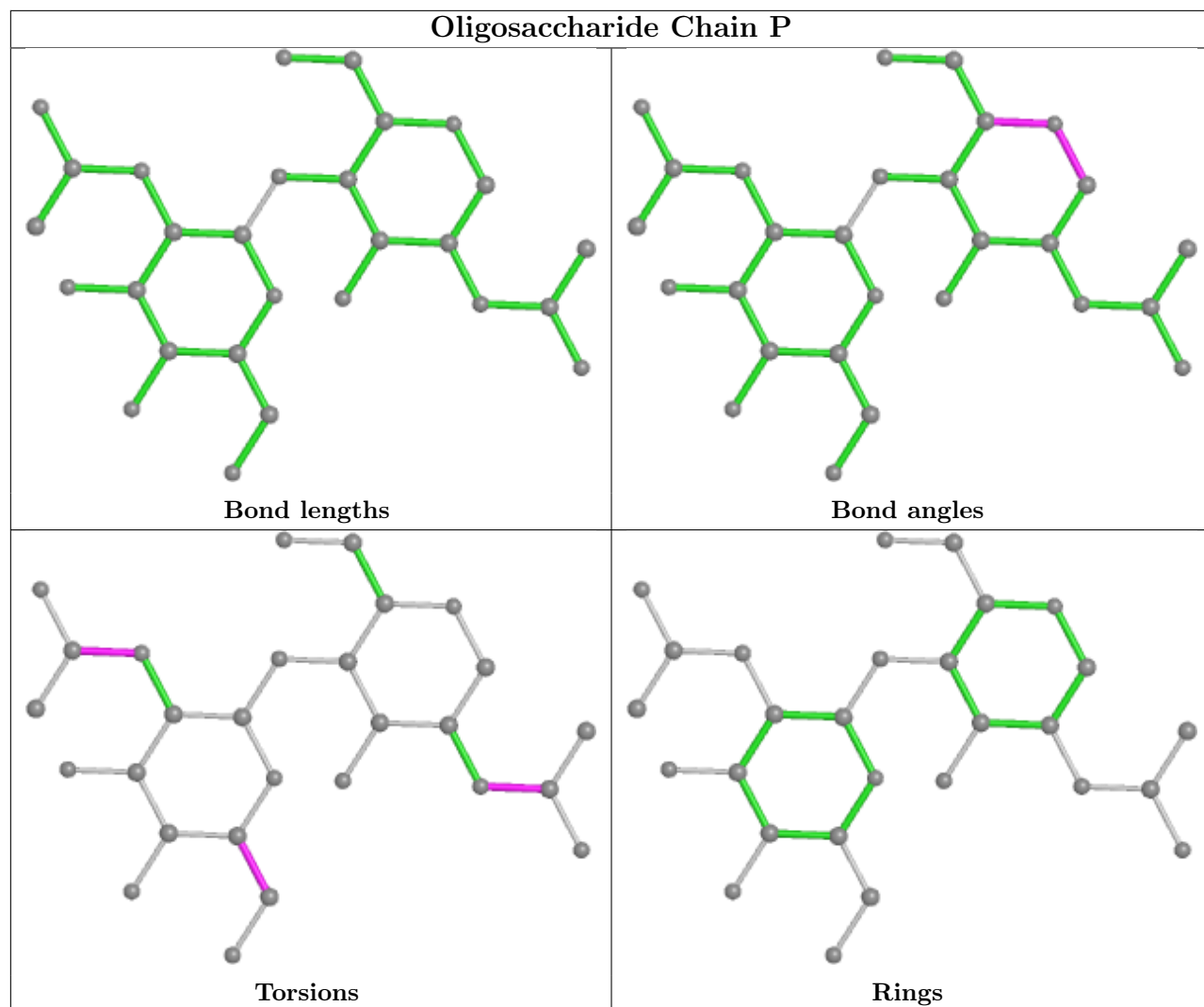


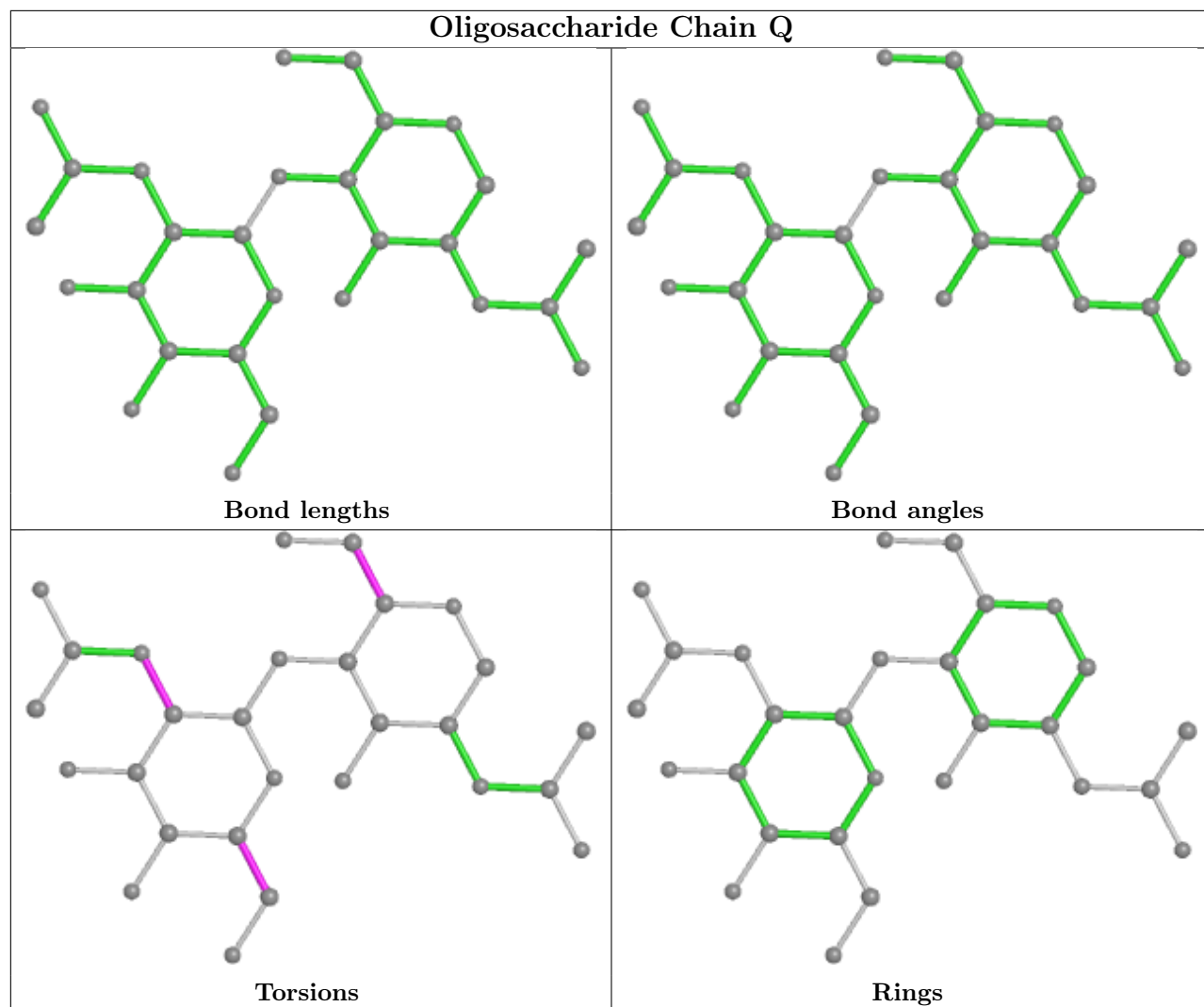


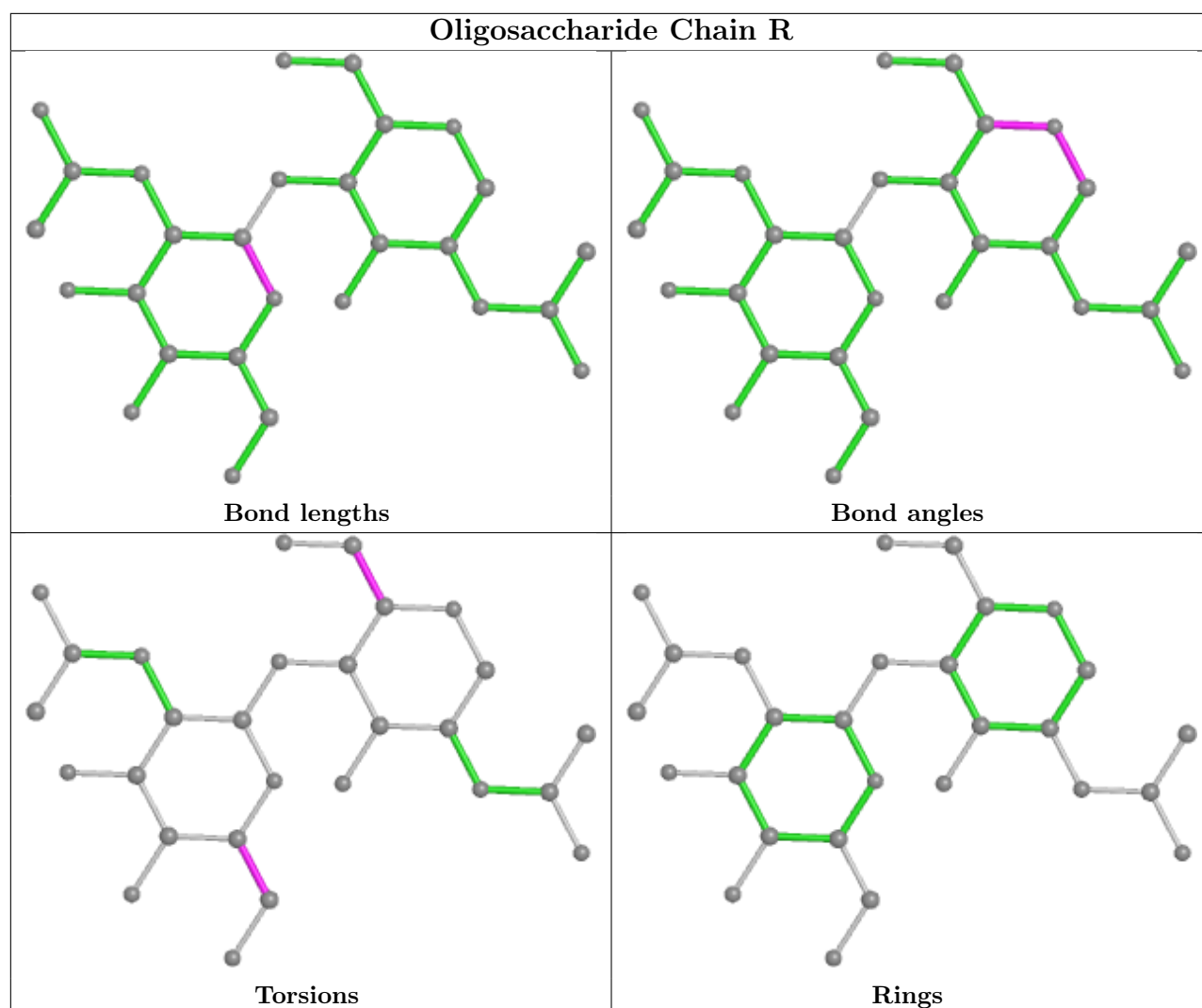


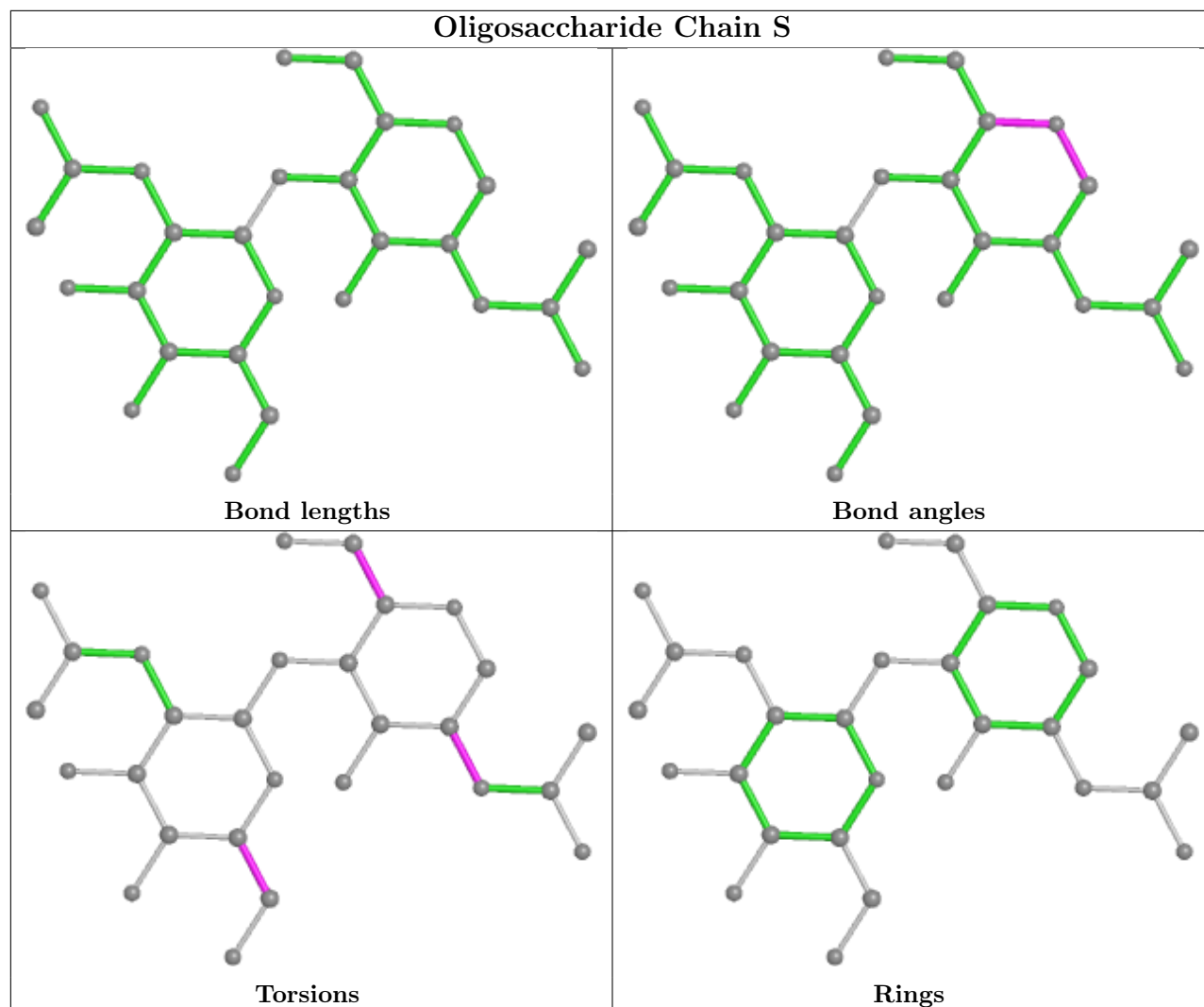


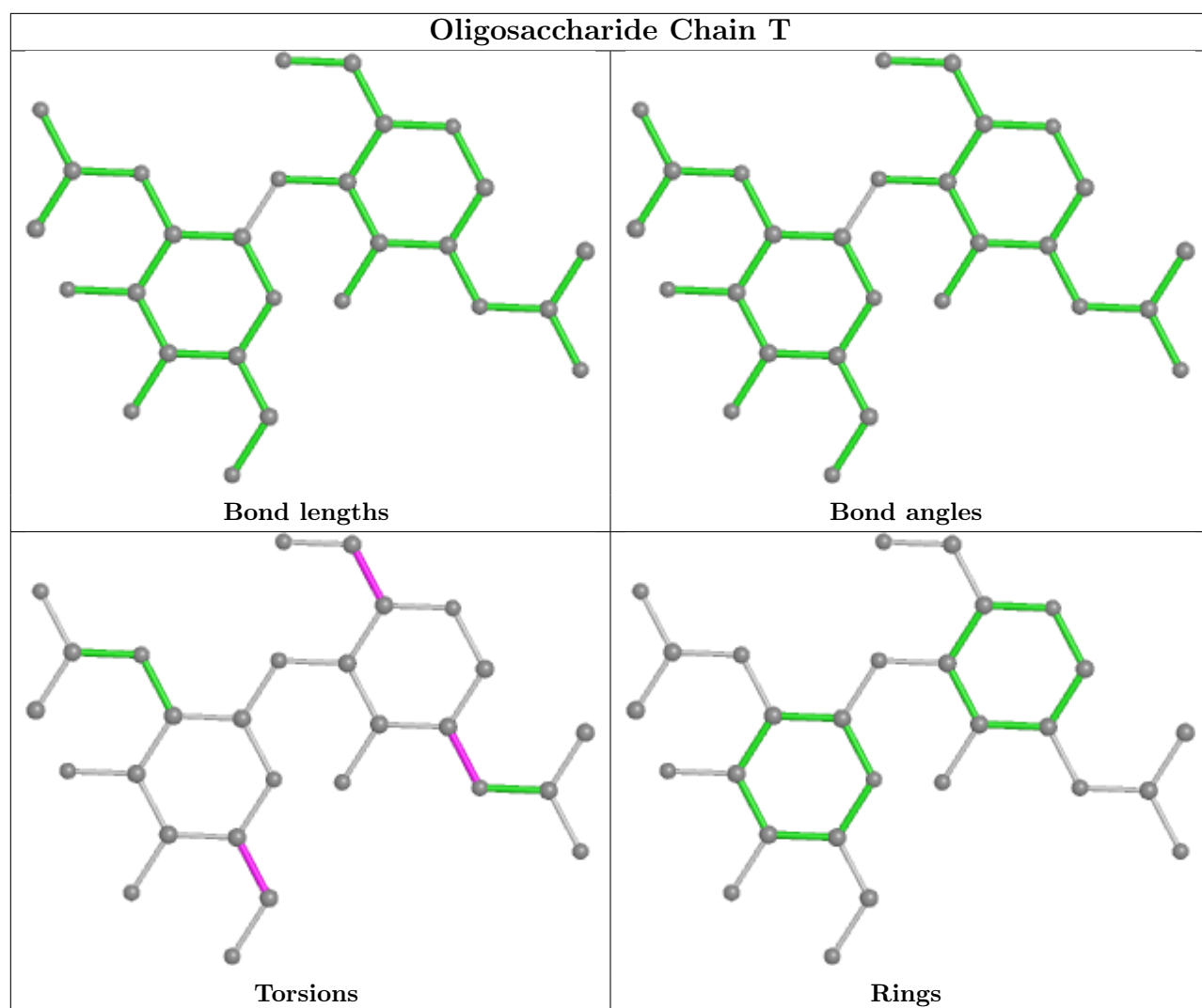


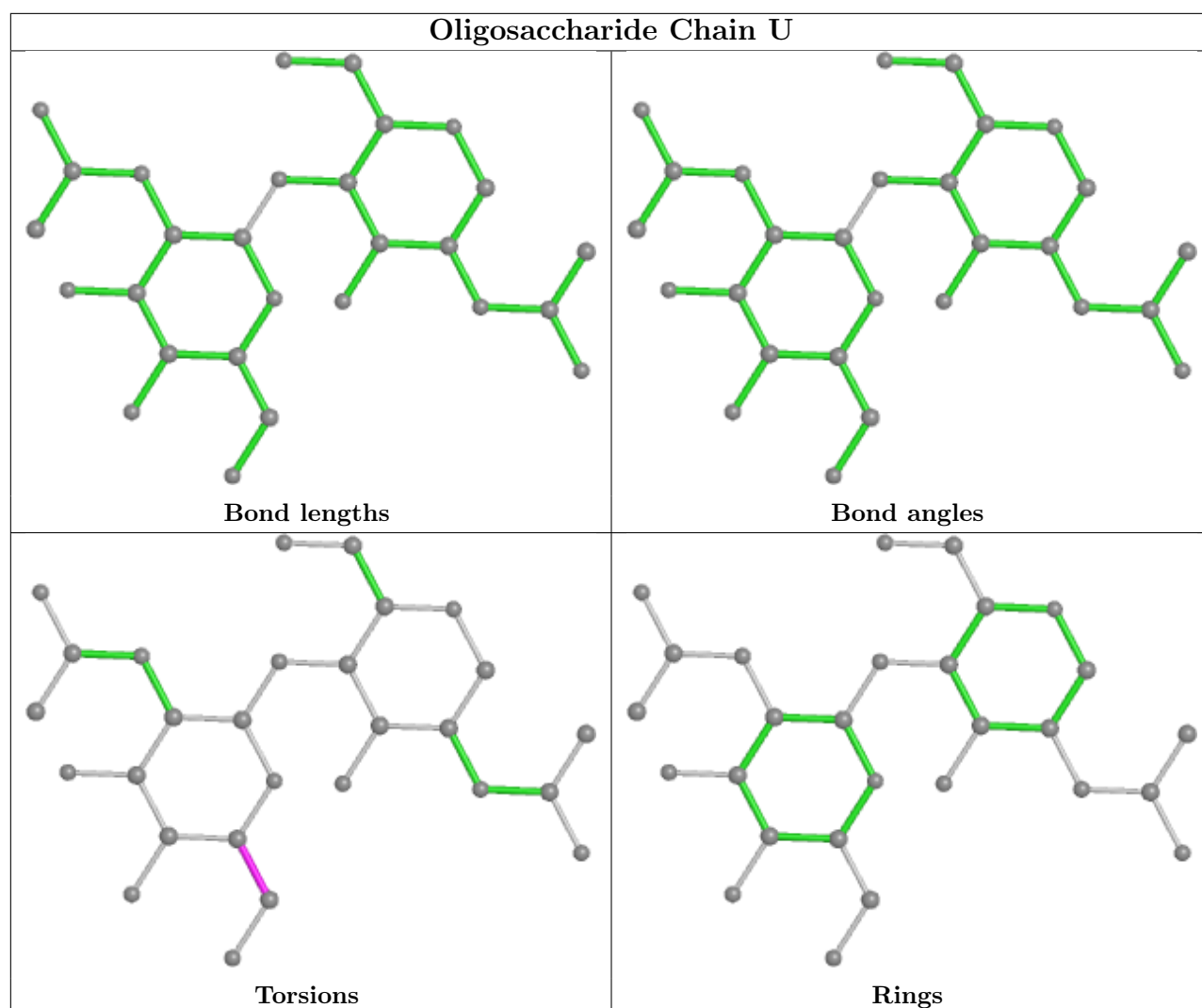


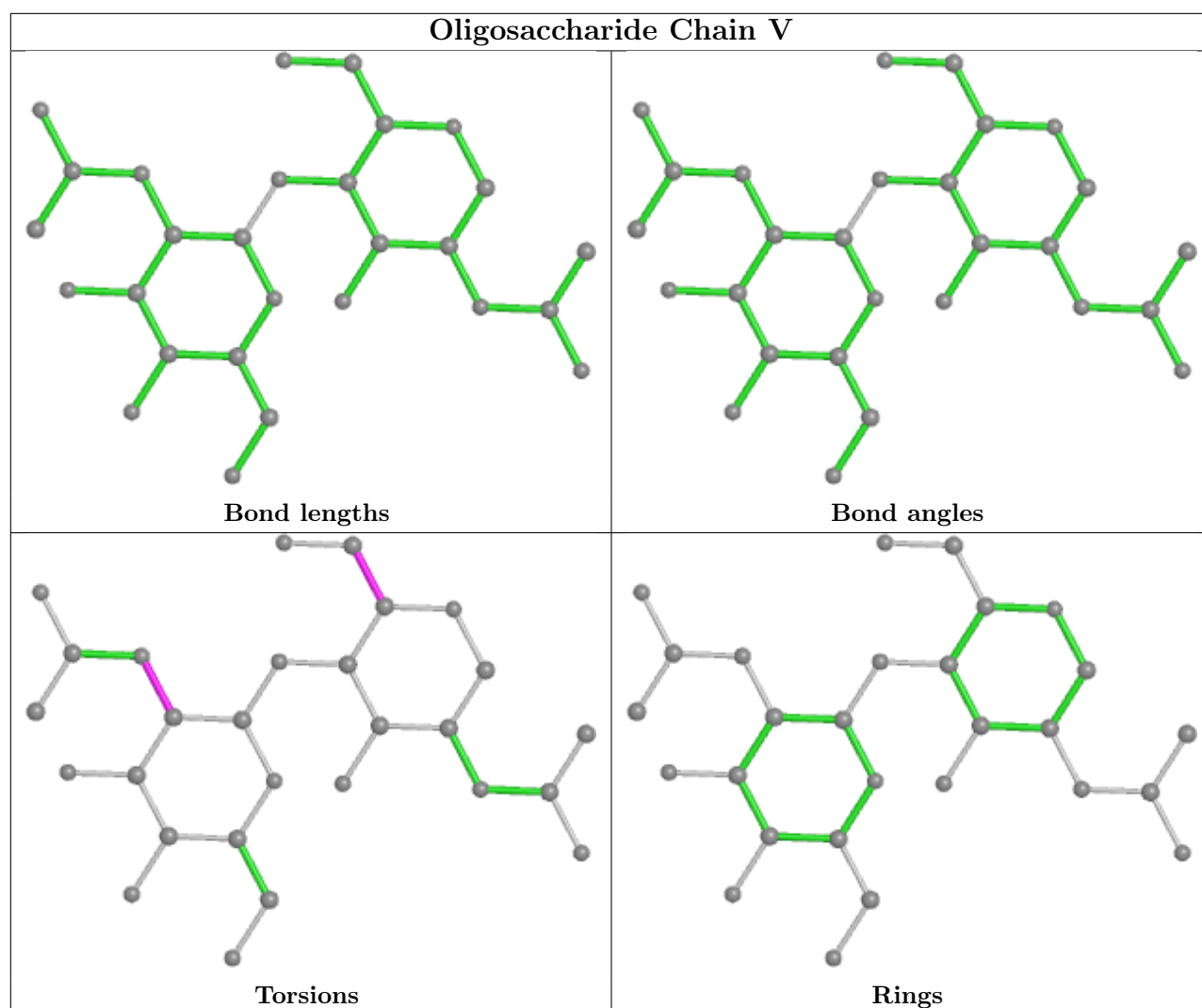


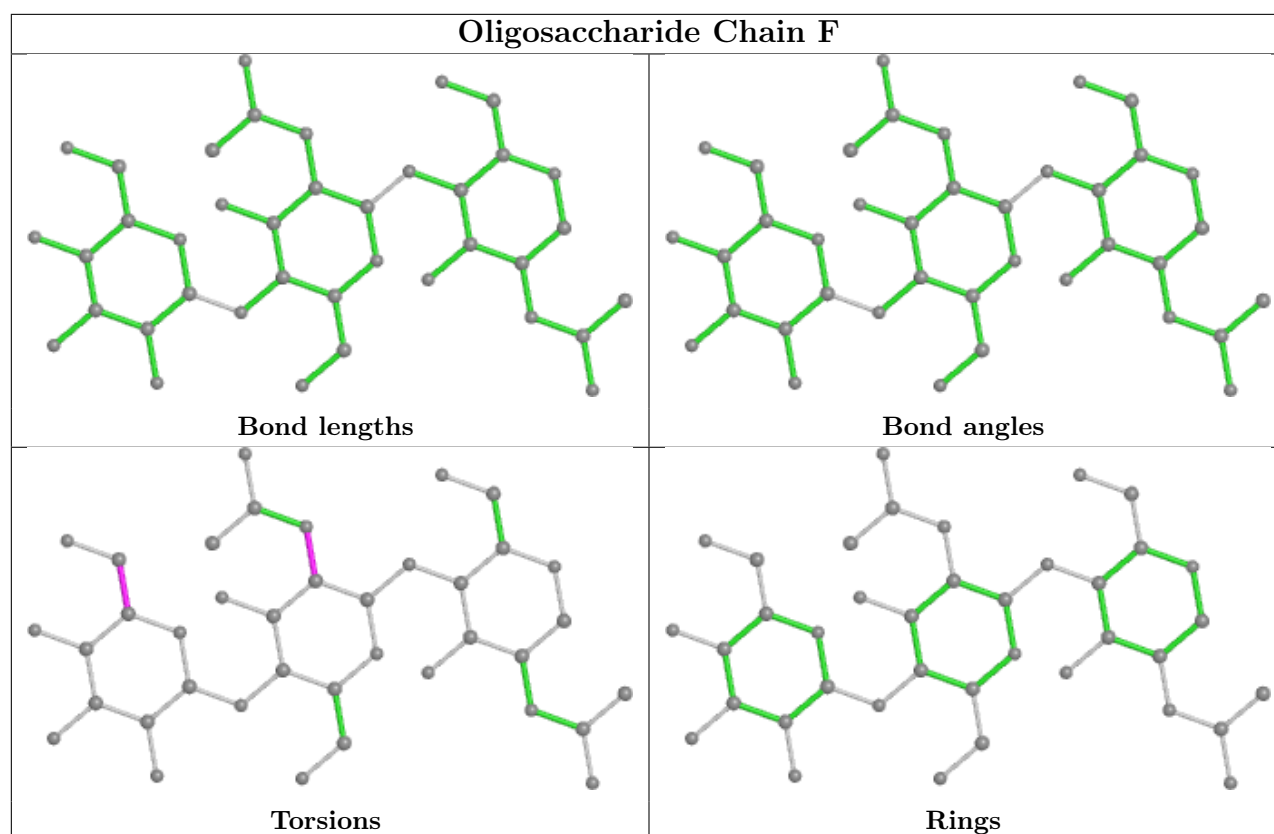












5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	A	1302	1	14,14,15	0.41	0	17,19,21	0.51	0
5	NAG	A	1307	1	14,14,15	0.24	0	17,19,21	0.50	0
5	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	E	701	2	14,14,15	0.61	1 (7%)	17,19,21	0.45	0
5	NAG	A	1303	1	14,14,15	0.27	0	17,19,21	0.53	0
5	NAG	B	1306	1	14,14,15	0.35	0	17,19,21	0.49	0
5	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1303	1	14,14,15	0.32	0	17,19,21	0.46	0
5	NAG	A	1304	1	14,14,15	0.46	0	17,19,21	0.71	1 (5%)
5	NAG	C	1307	1	14,14,15	0.48	0	17,19,21	0.39	0
5	NAG	B	1301	1	14,14,15	0.72	1 (7%)	17,19,21	0.51	0
5	NAG	A	1306	1	14,14,15	0.38	0	17,19,21	0.71	0
5	NAG	A	1308	1	14,14,15	1.00	2 (14%)	17,19,21	0.97	1 (5%)
5	NAG	B	1302	1	14,14,15	0.37	0	17,19,21	0.44	0
5	NAG	C	1306	1	14,14,15	0.49	0	17,19,21	0.54	0
5	NAG	A	1305	1	14,14,15	0.53	0	17,19,21	0.81	1 (5%)
5	NAG	B	1303	1	14,14,15	0.37	0	17,19,21	0.65	0
5	NAG	B	1309	1	14,14,15	0.60	1 (7%)	17,19,21	0.52	0
5	NAG	C	1305	1	14,14,15	0.35	0	17,19,21	0.58	0
5	NAG	C	1302	1	14,14,15	0.45	0	17,19,21	0.40	0
5	NAG	E	703	2	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1301	1	14,14,15	0.18	0	17,19,21	0.48	0
5	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.63	0
5	NAG	B	1304	1	14,14,15	0.45	0	17,19,21	0.53	0
5	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.57	0
5	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.40	0
5	NAG	E	702	2	14,14,15	0.71	1 (7%)	17,19,21	0.39	0
5	NAG	B	1308	1	14,14,15	0.81	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	C	1304	1	14,14,15	0.42	0	17,19,21	0.51	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
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	E	701	2	-	3/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1304	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
5	NAG	E	703	2	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	E	702	2	-	4/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	1/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1308	NAG	O5-C1	2.87	1.48	1.43
5	A	1308	NAG	O5-C1	2.78	1.48	1.43
5	E	702	NAG	O5-C1	-2.43	1.39	1.43
5	B	1301	NAG	O5-C1	-2.38	1.39	1.43
5	A	1308	NAG	C1-C2	2.30	1.55	1.52
5	E	701	NAG	O5-C1	-2.08	1.40	1.43
5	B	1309	NAG	O5-C1	2.04	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1308	NAG	C1-O5-C5	4.84	118.75	112.19
5	A	1308	NAG	C1-O5-C5	3.59	117.06	112.19
5	A	1305	NAG	C1-O5-C5	2.88	116.10	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1304	NAG	C1-O5-C5	2.23	115.21	112.19

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1305	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	E	702	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	E	703	NAG	O5-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	E	702	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	E	703	NAG	C4-C5-C6-O6
5	A	1303	NAG	C8-C7-N2-C2
5	A	1303	NAG	O7-C7-N2-C2
5	A	1304	NAG	C8-C7-N2-C2
5	A	1304	NAG	O7-C7-N2-C2
5	A	1309	NAG	C8-C7-N2-C2
5	A	1309	NAG	O7-C7-N2-C2
5	B	1301	NAG	C8-C7-N2-C2
5	B	1301	NAG	O7-C7-N2-C2
5	B	1306	NAG	C8-C7-N2-C2
5	B	1306	NAG	O7-C7-N2-C2
5	E	701	NAG	C8-C7-N2-C2
5	E	701	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	E	702	NAG	C8-C7-N2-C2
5	E	702	NAG	O7-C7-N2-C2
5	B	1303	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	E	701	NAG	O5-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	C	1301	NAG	C3-C2-N2-C7
5	C	1308	NAG	C3-C2-N2-C7
5	B	1307	NAG	O5-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	A	1306	NAG	C3-C2-N2-C7
5	B	1307	NAG	C3-C2-N2-C7
5	B	1310	NAG	C3-C2-N2-C7
5	A	1306	NAG	C1-C2-N2-C7
5	B	1307	NAG	C1-C2-N2-C7

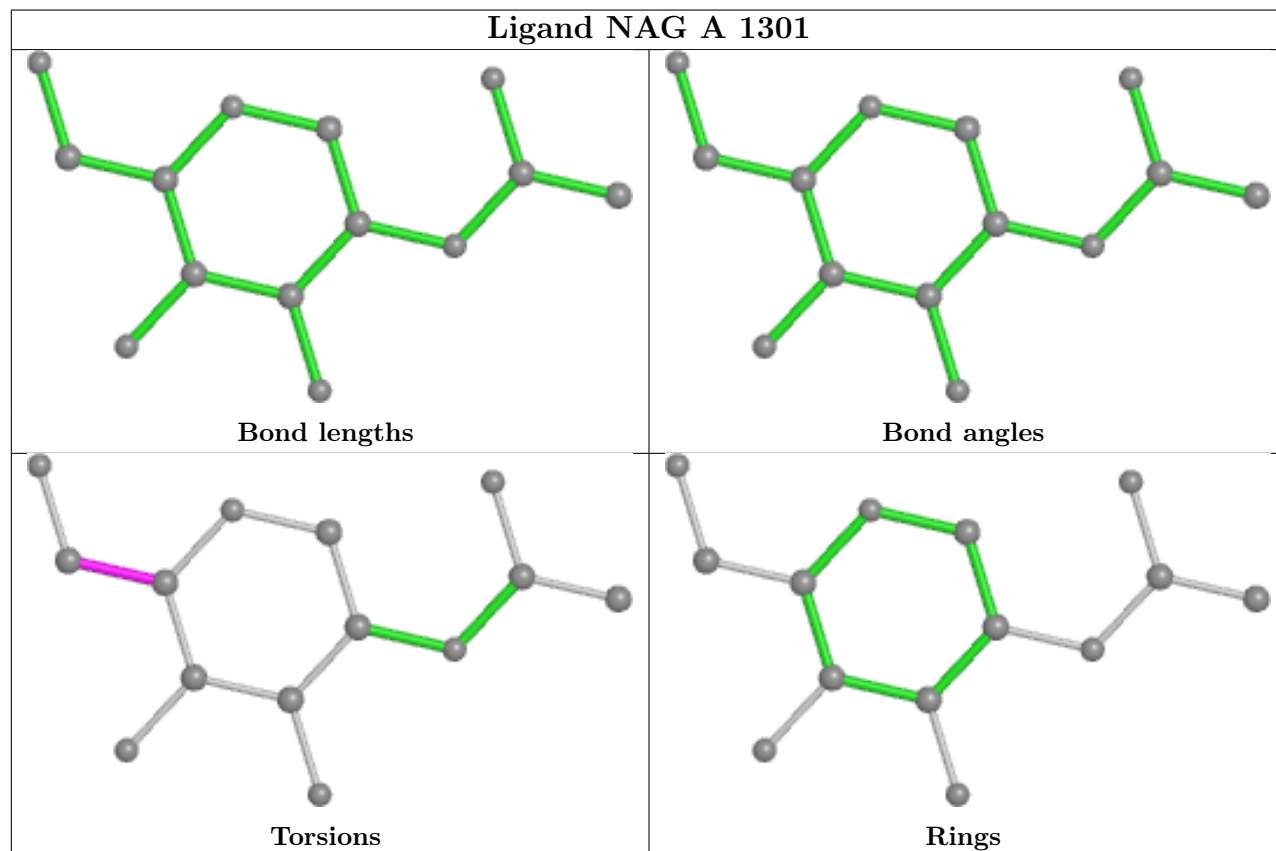
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1305	NAG	1	0
5	C	1305	NAG	1	0
5	C	1302	NAG	1	0
5	B	1311	NAG	2	0
5	B	1308	NAG	2	0

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

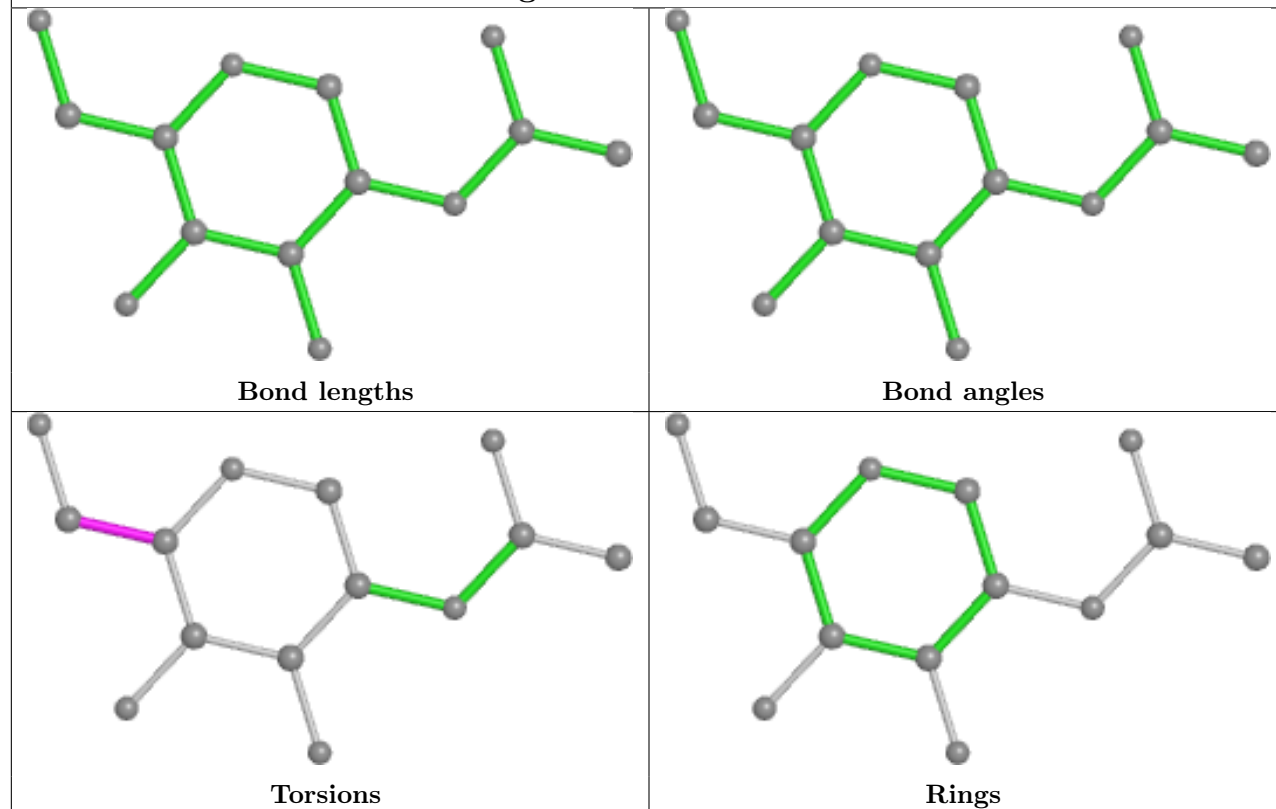
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

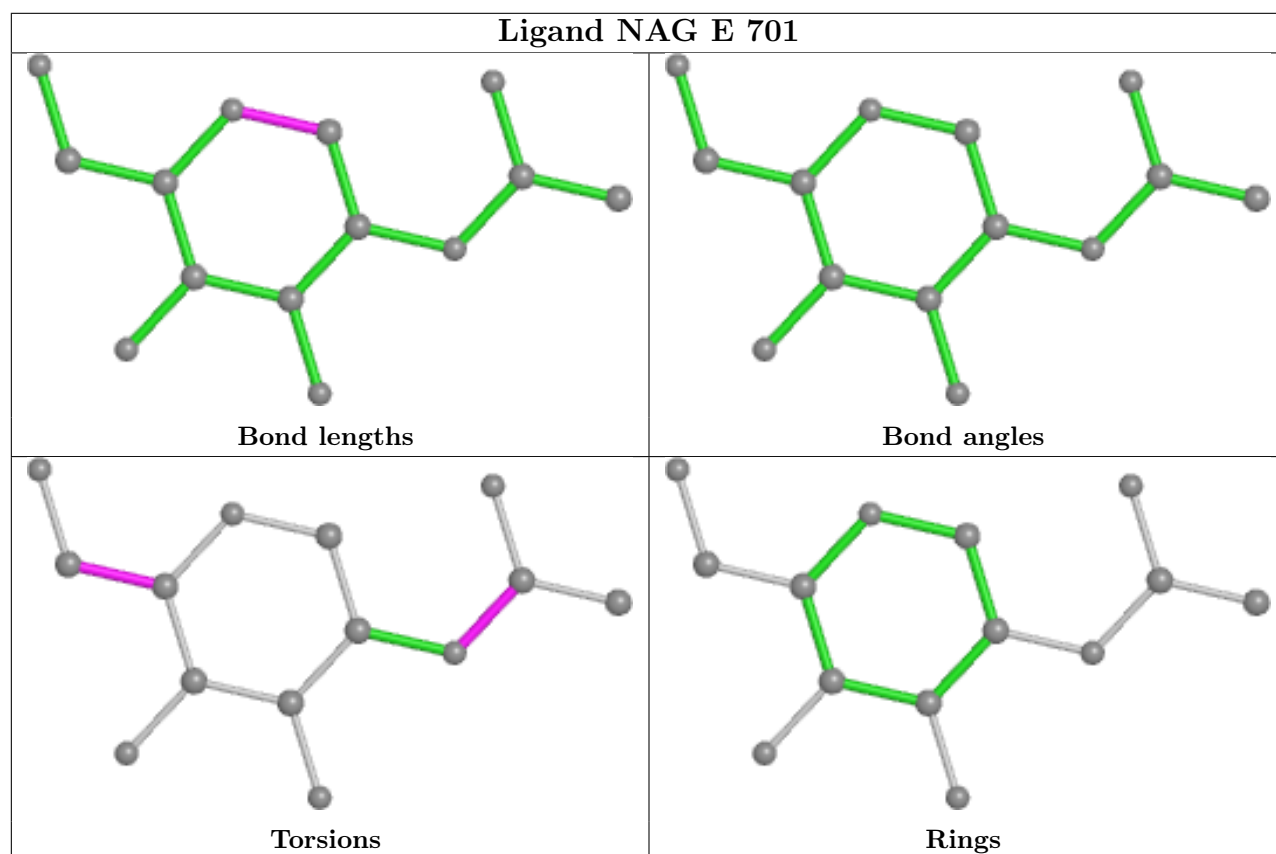
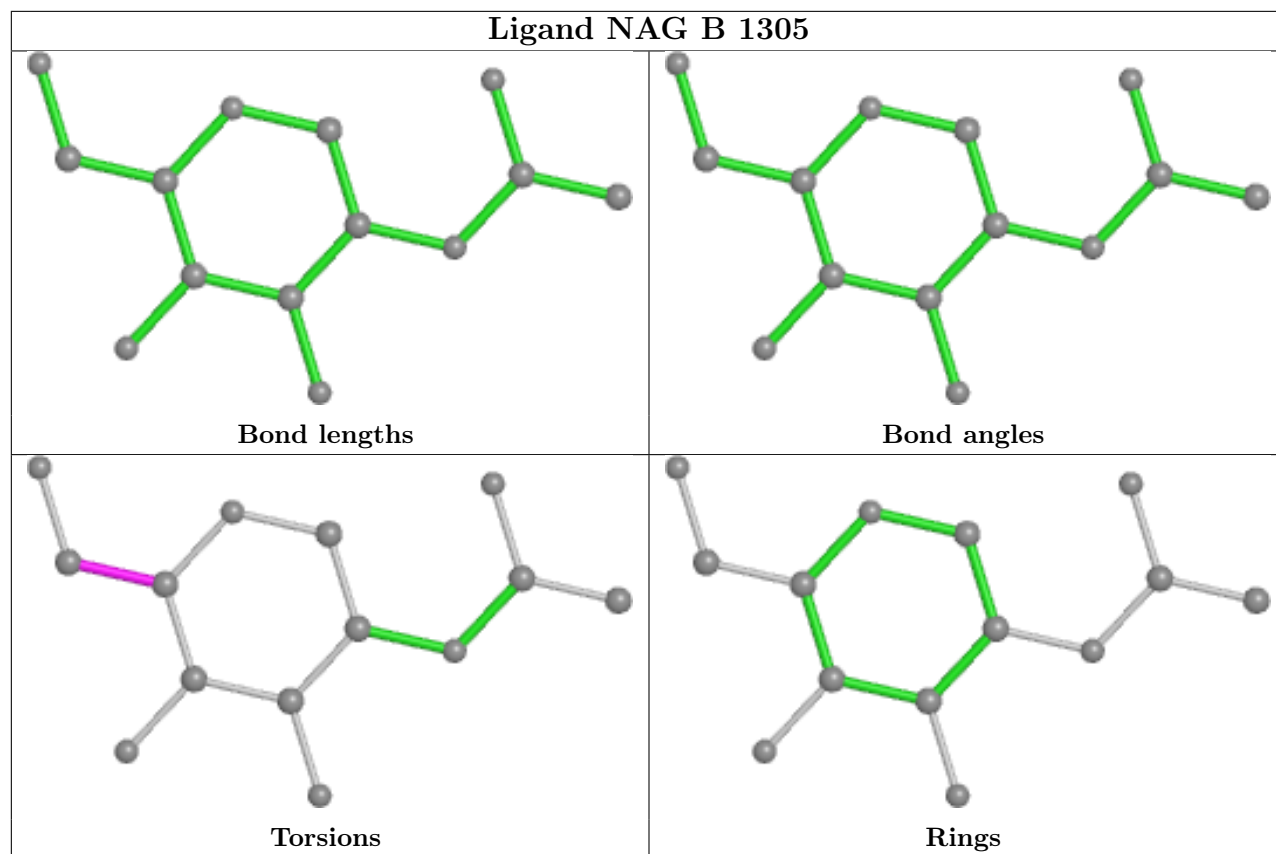


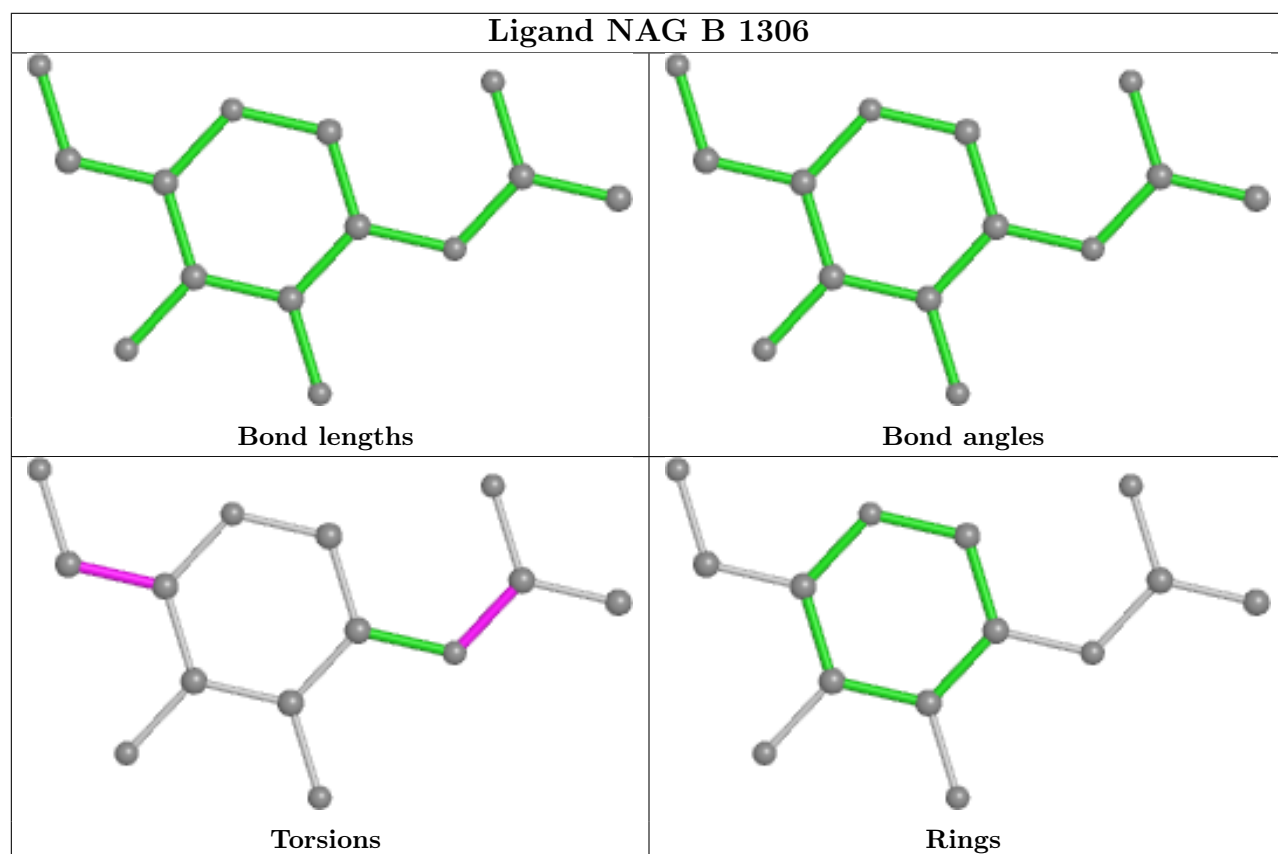
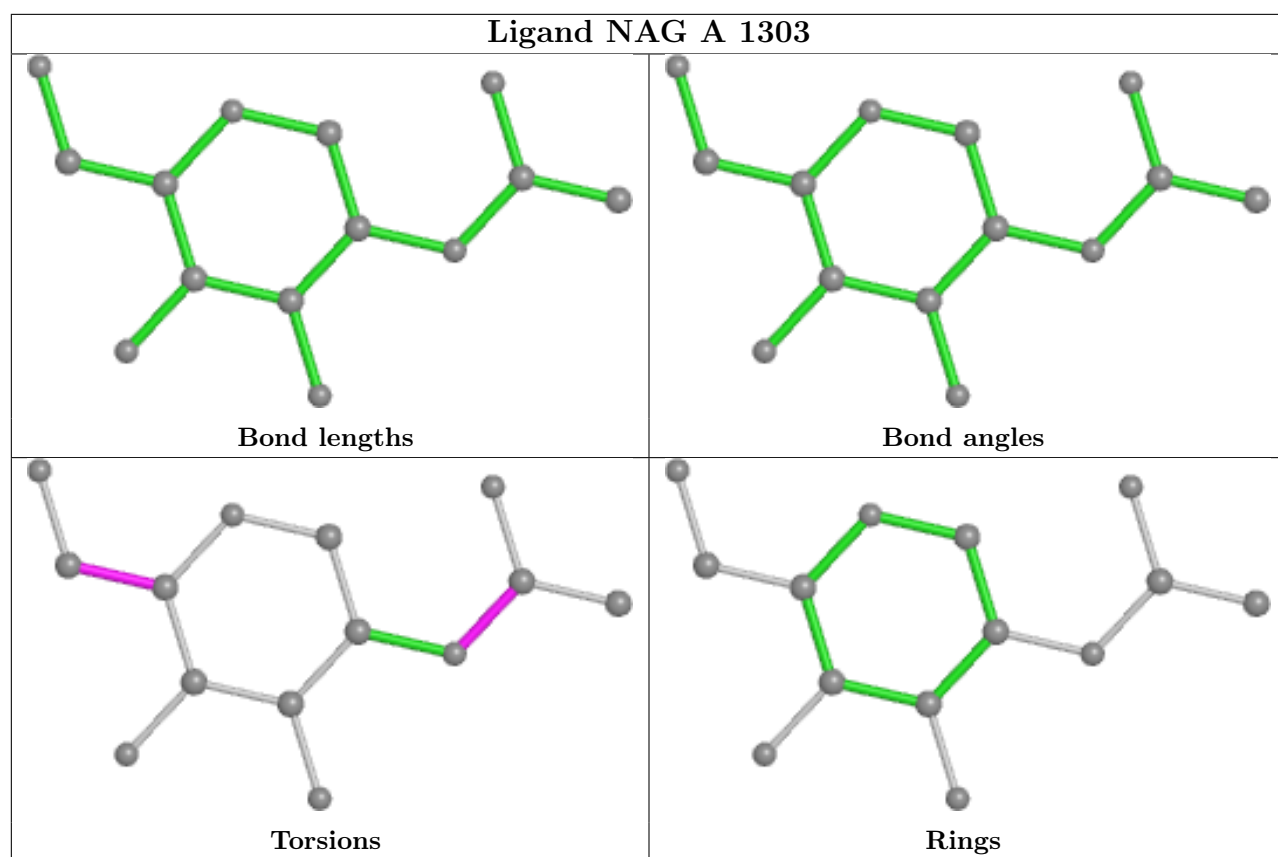
Ligand NAG A 1302

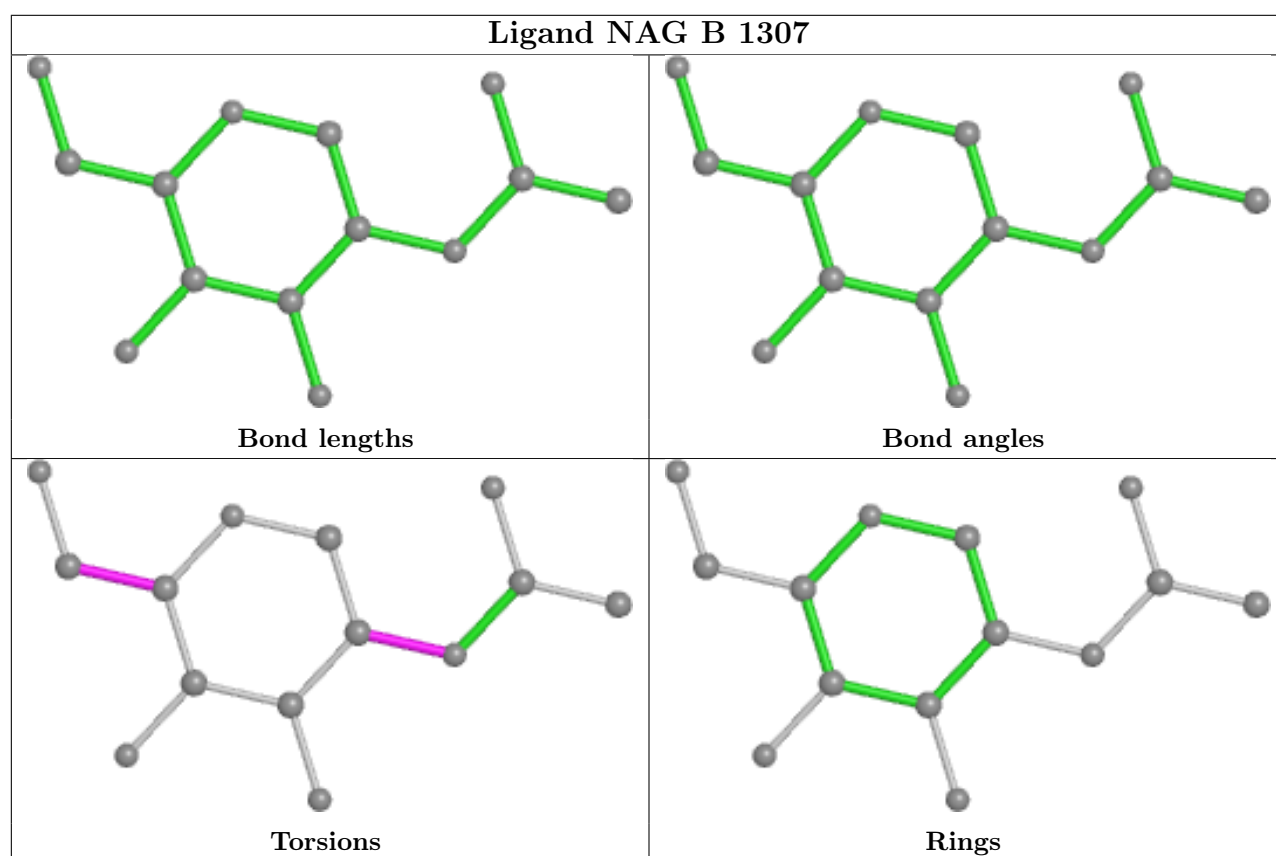
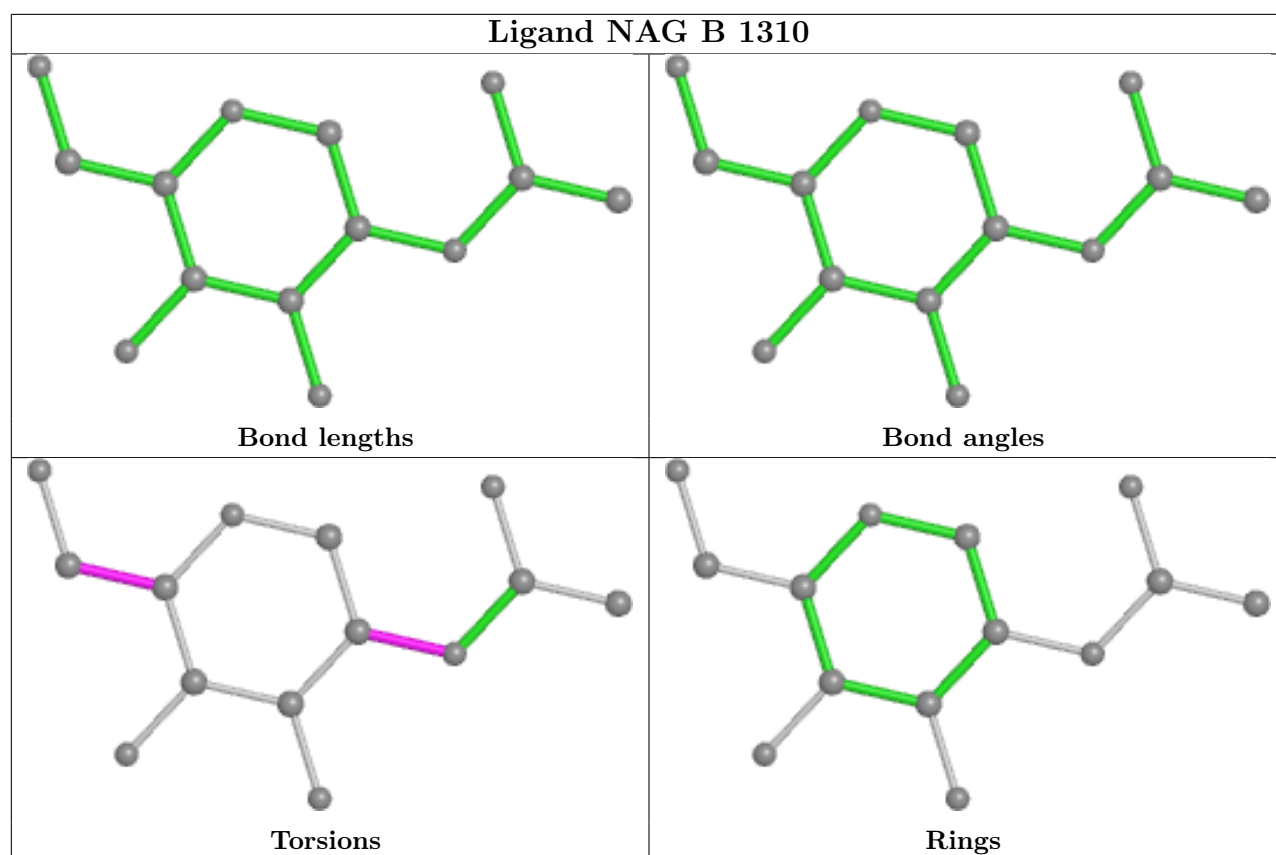


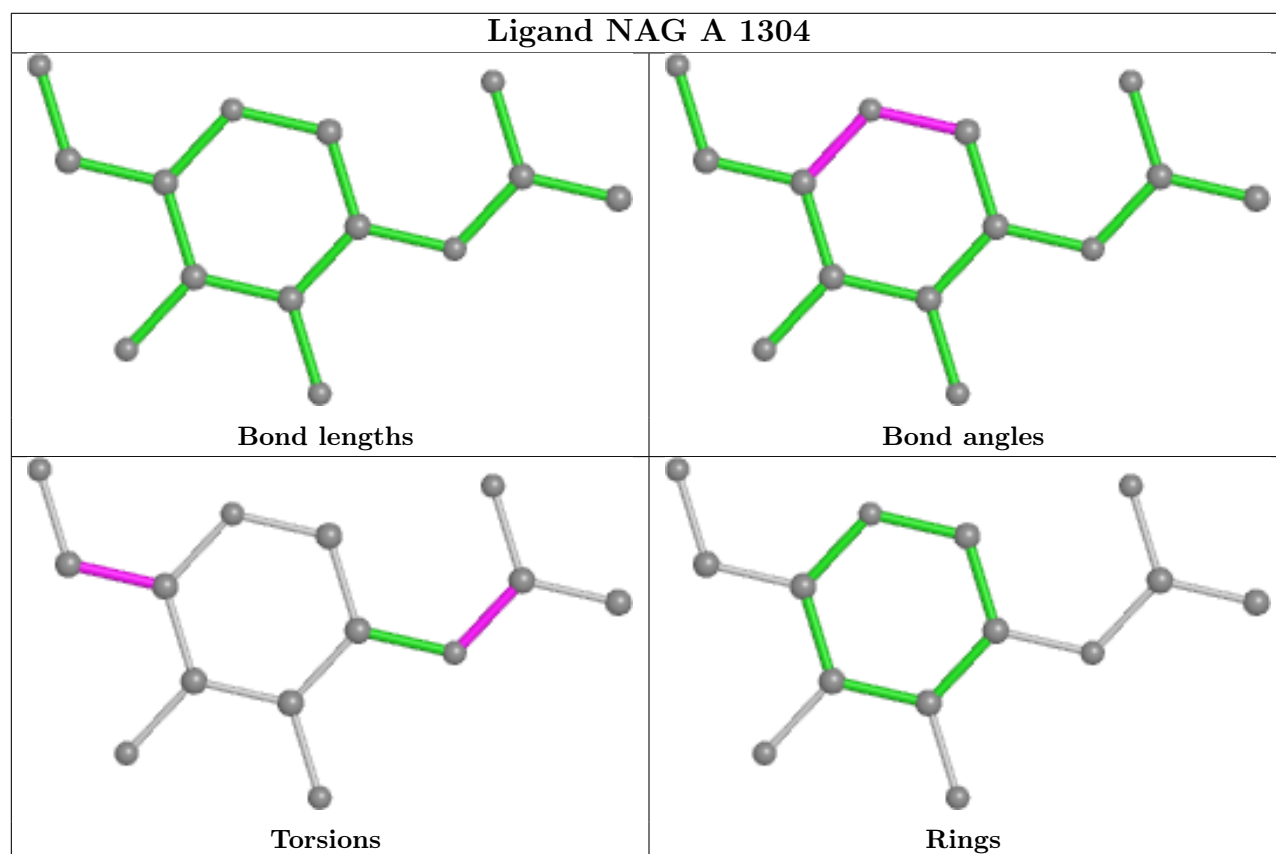
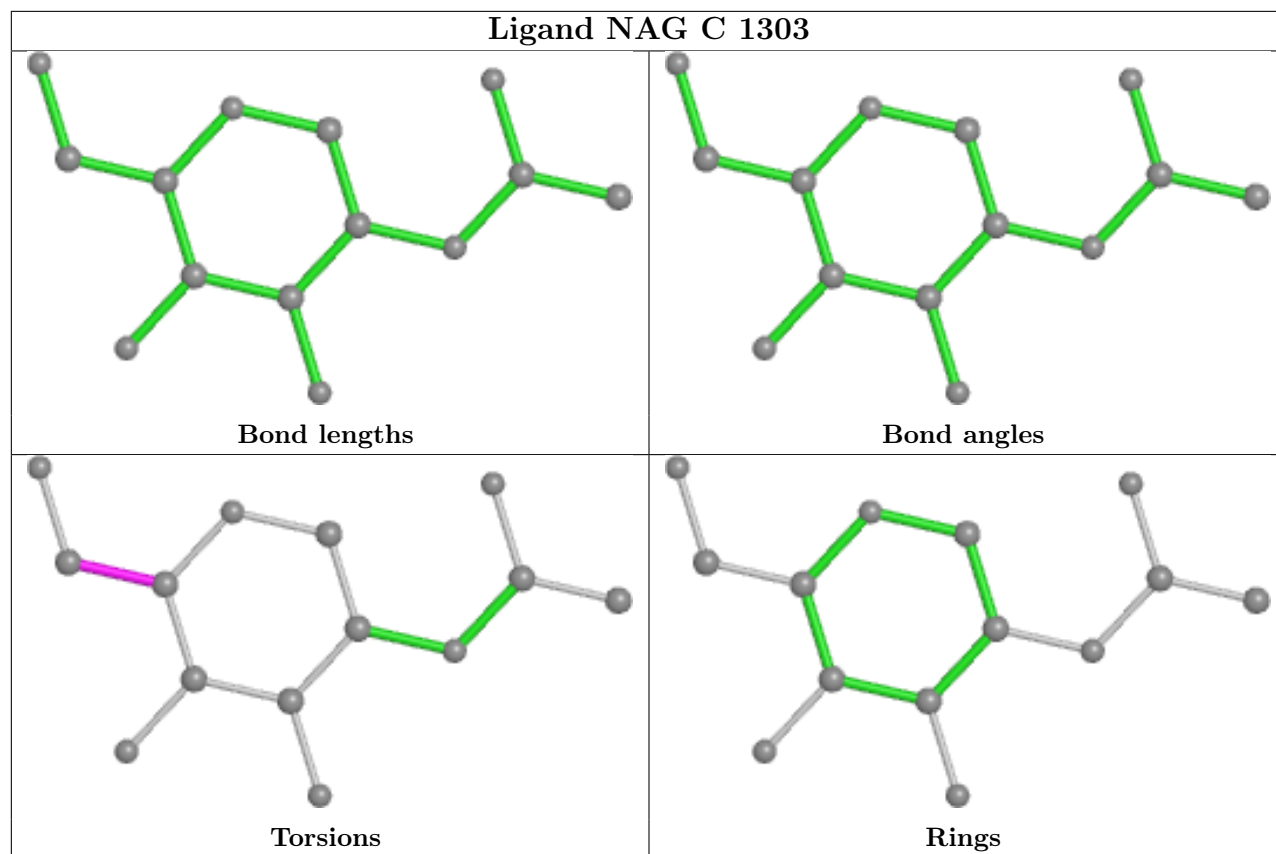
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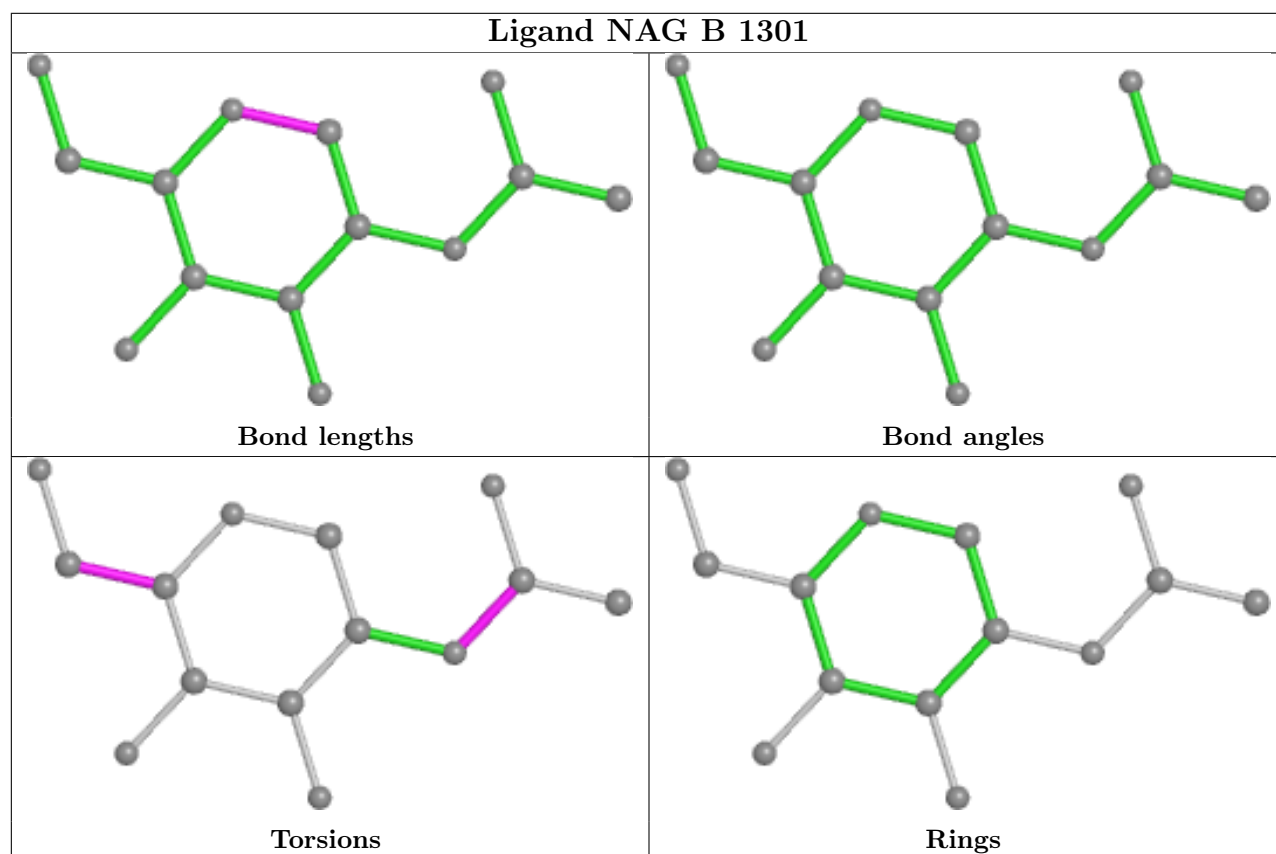
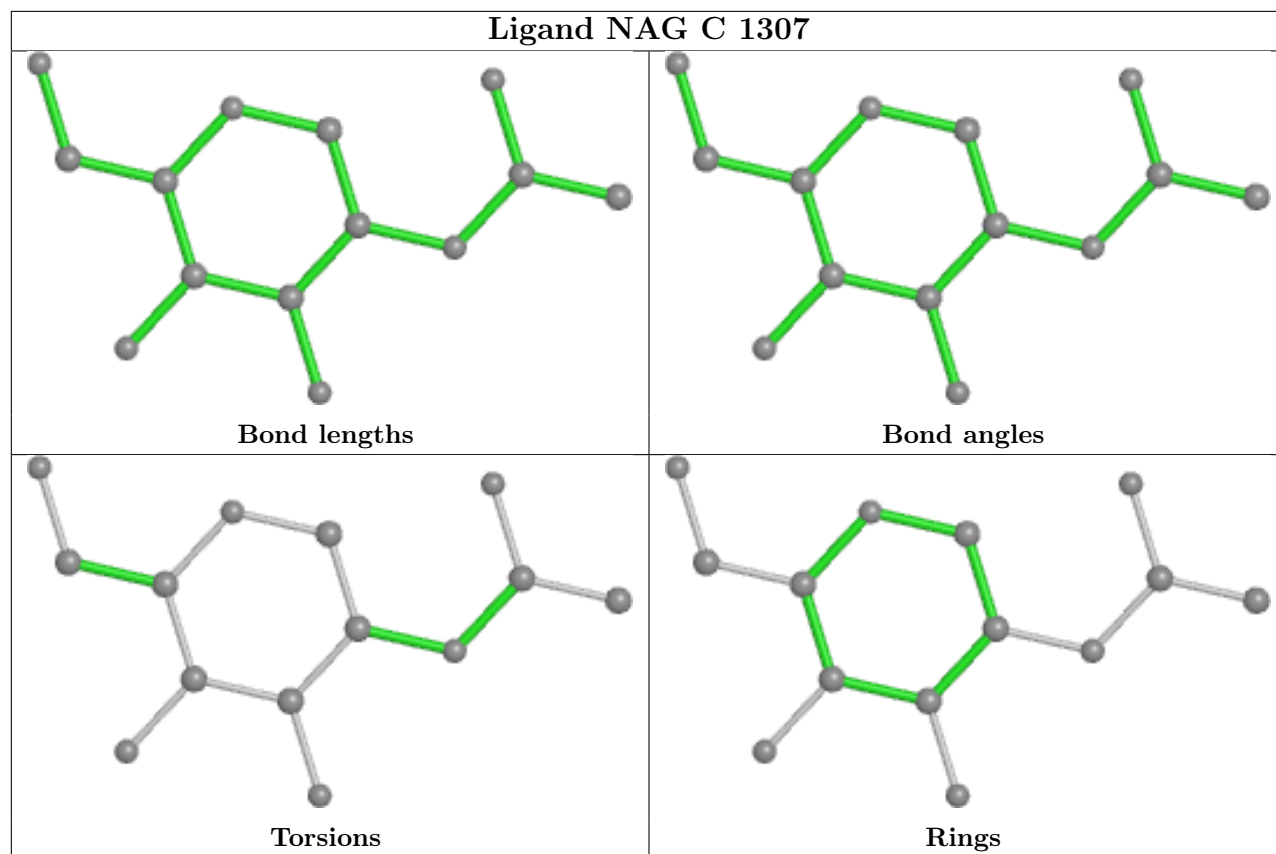




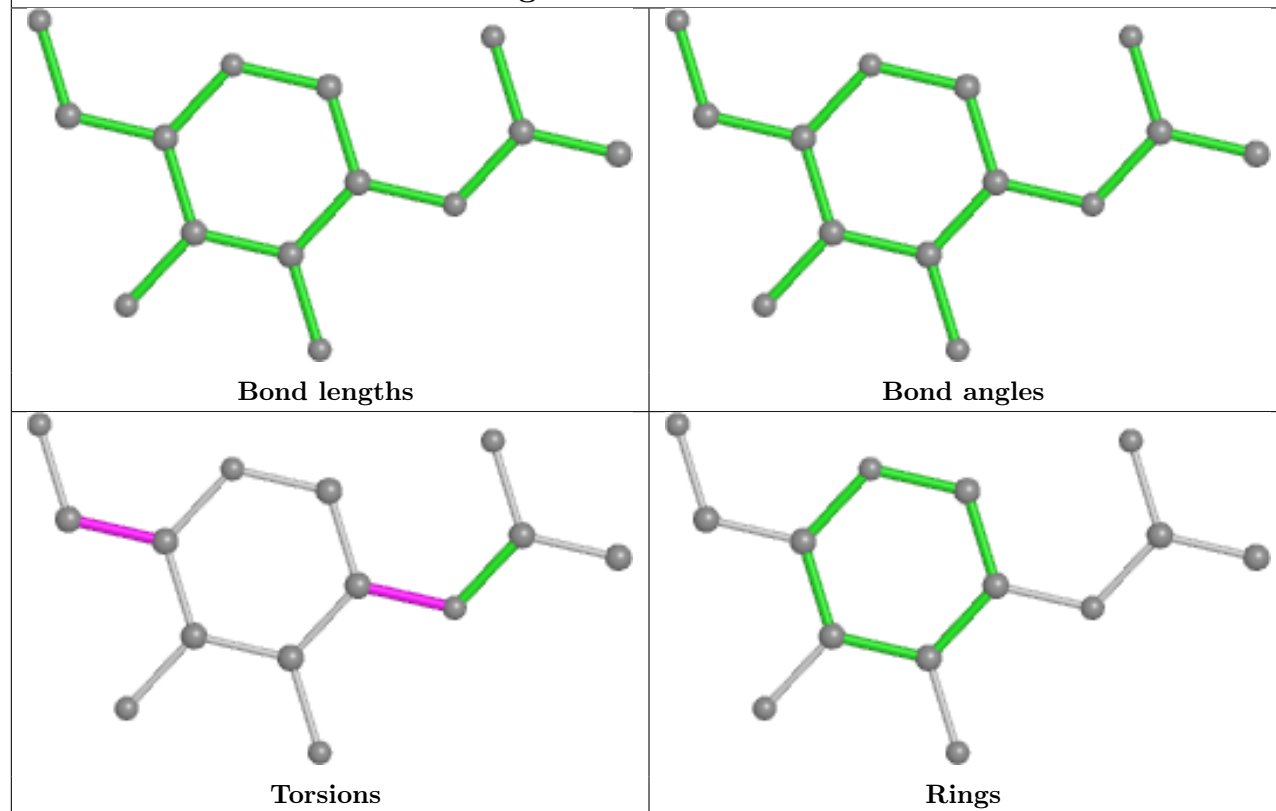




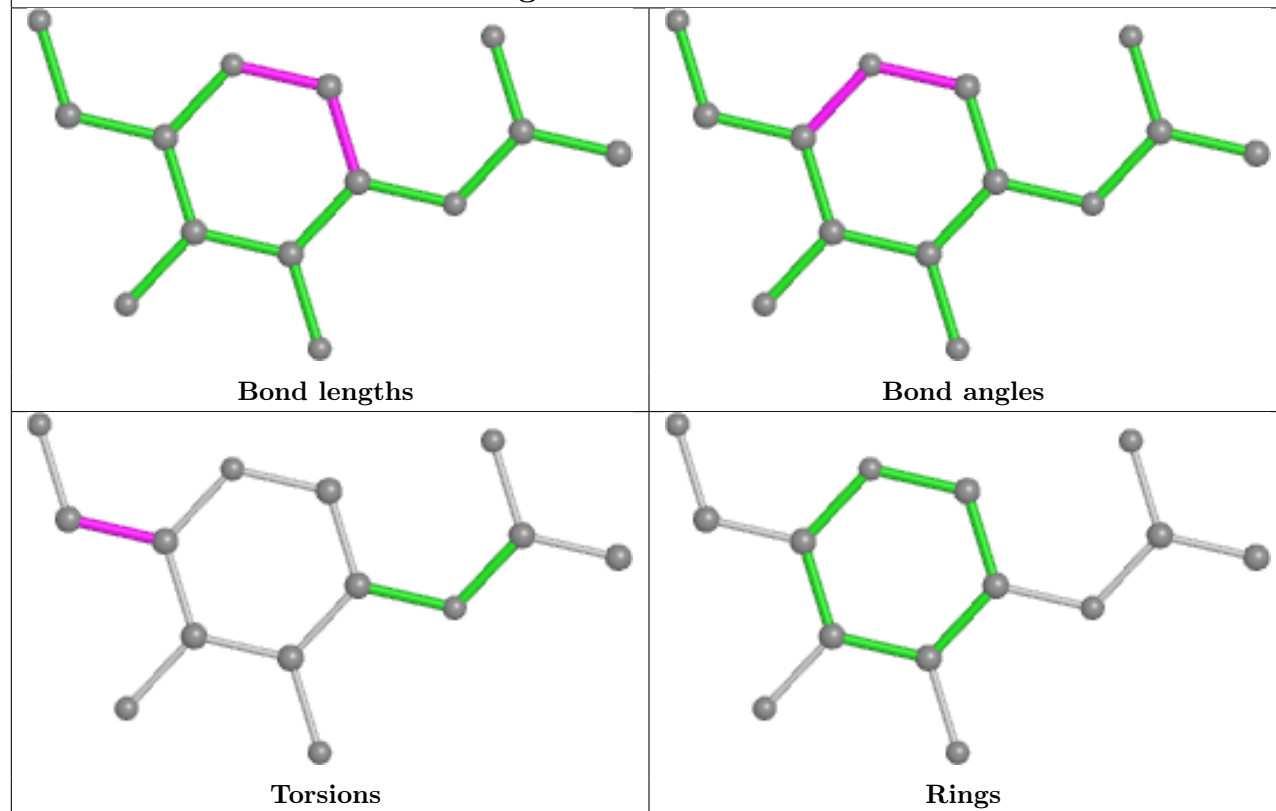


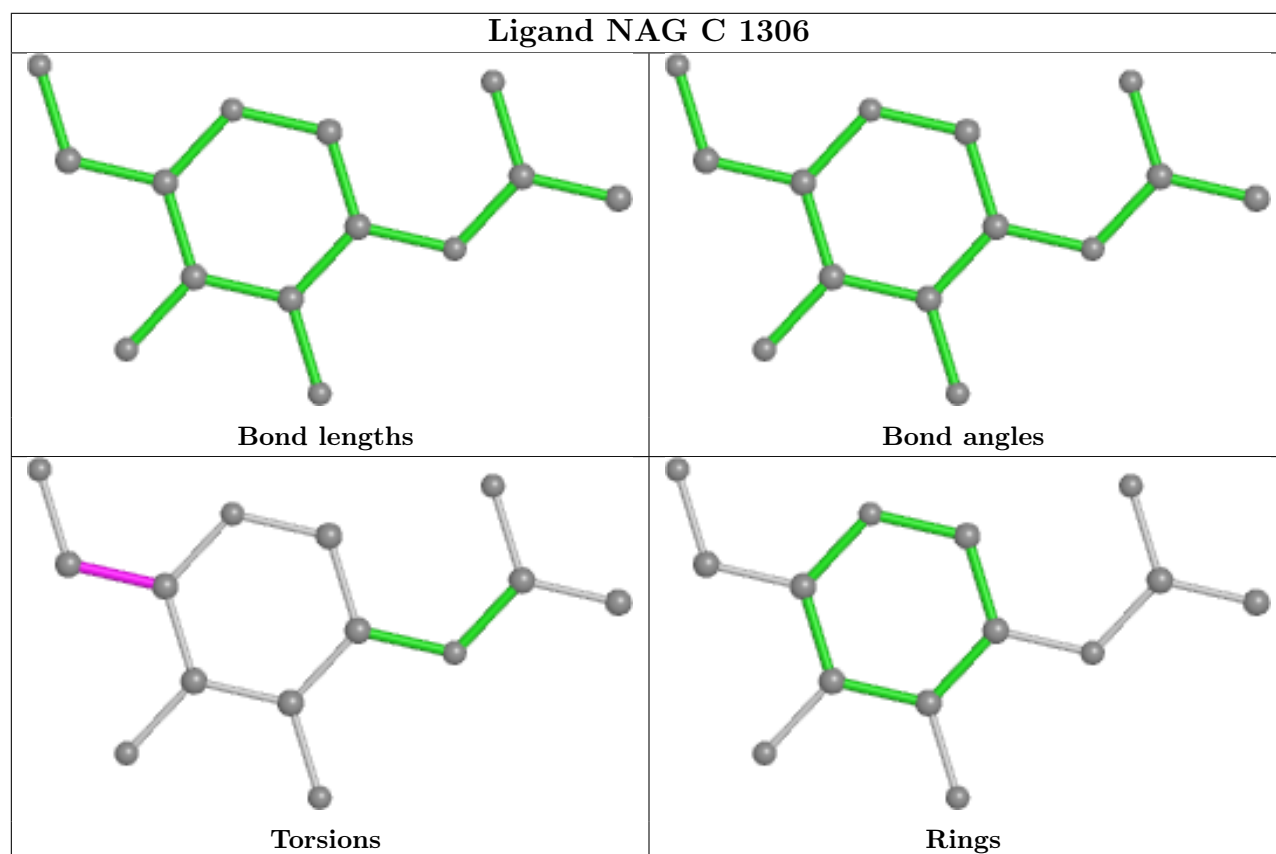
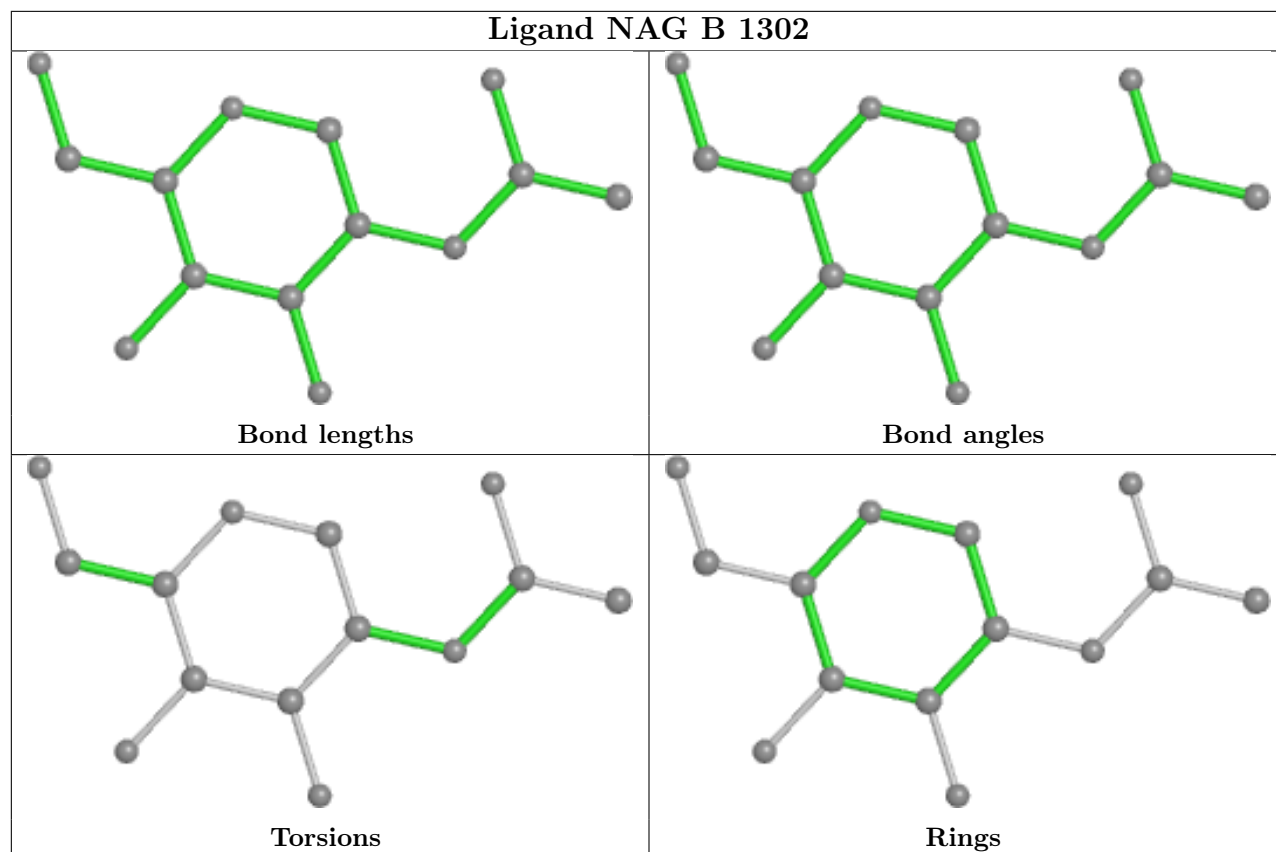


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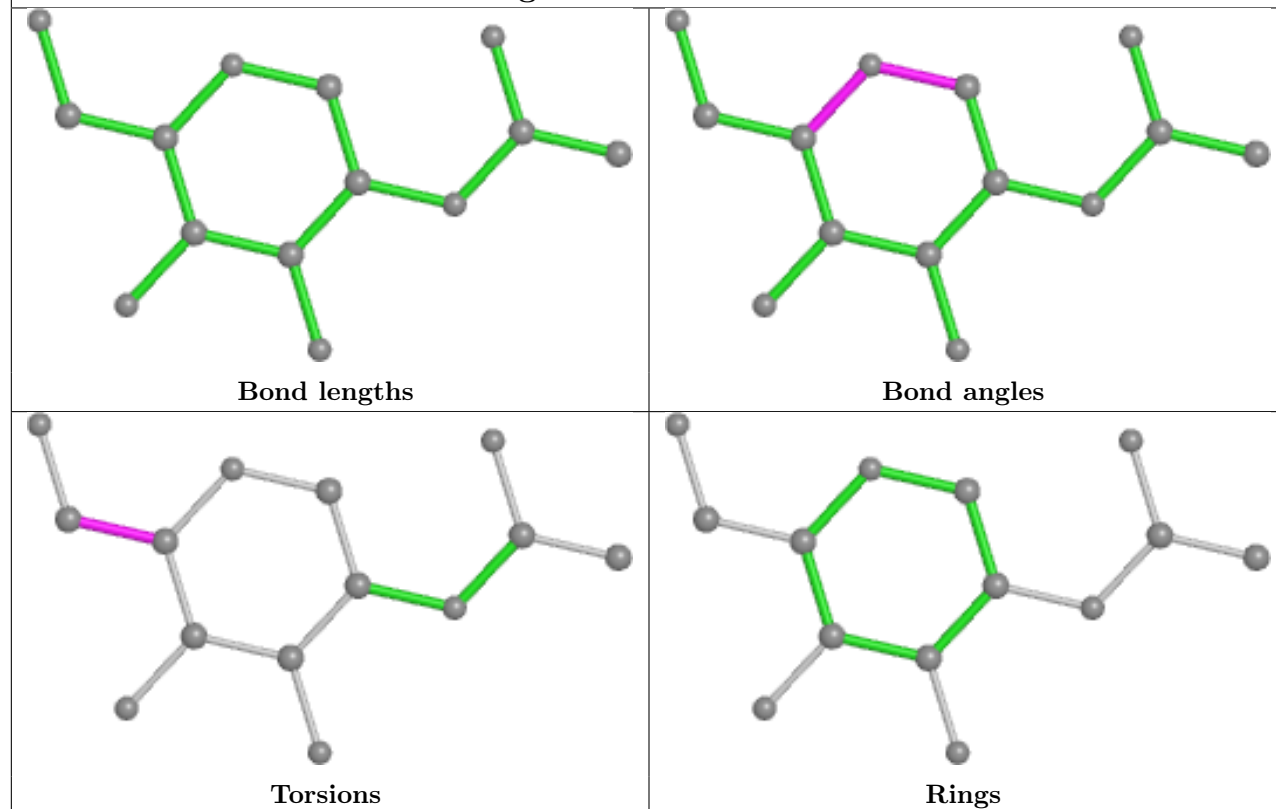


Ligand NAG A 1308

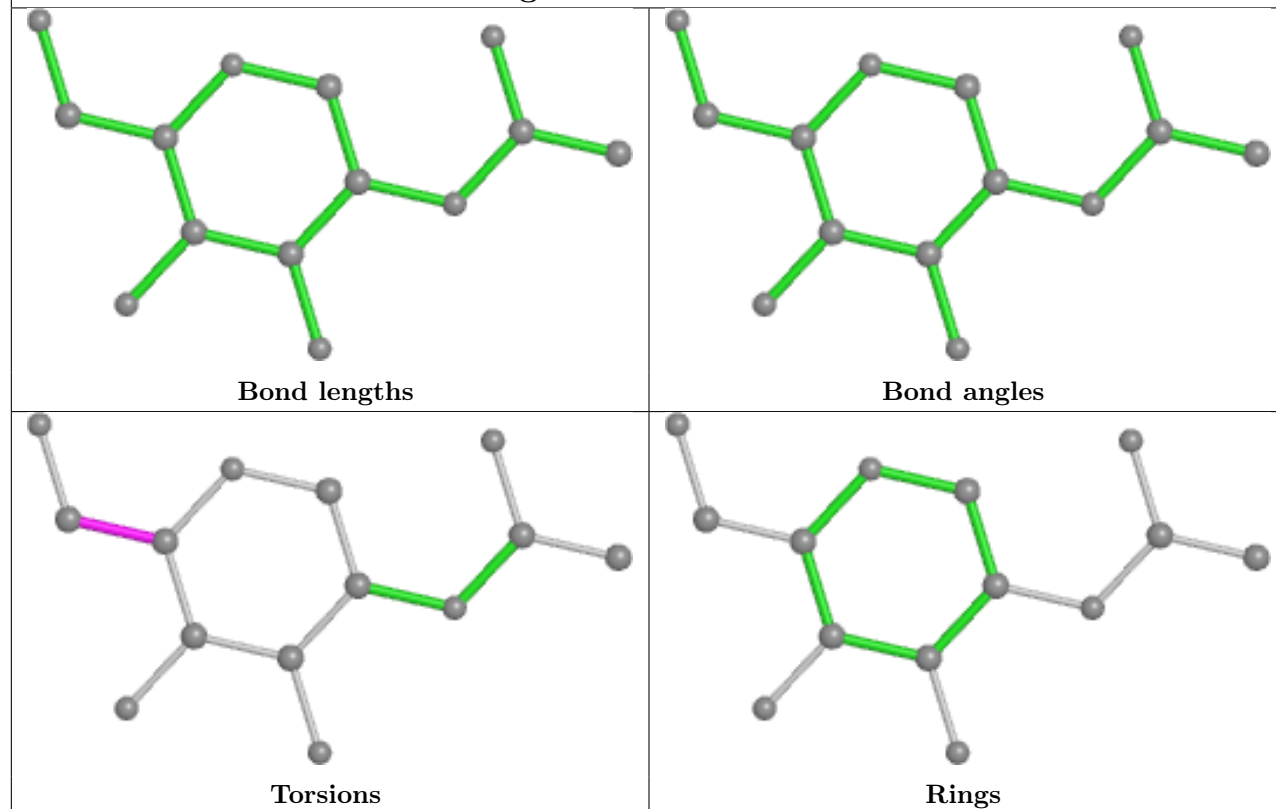


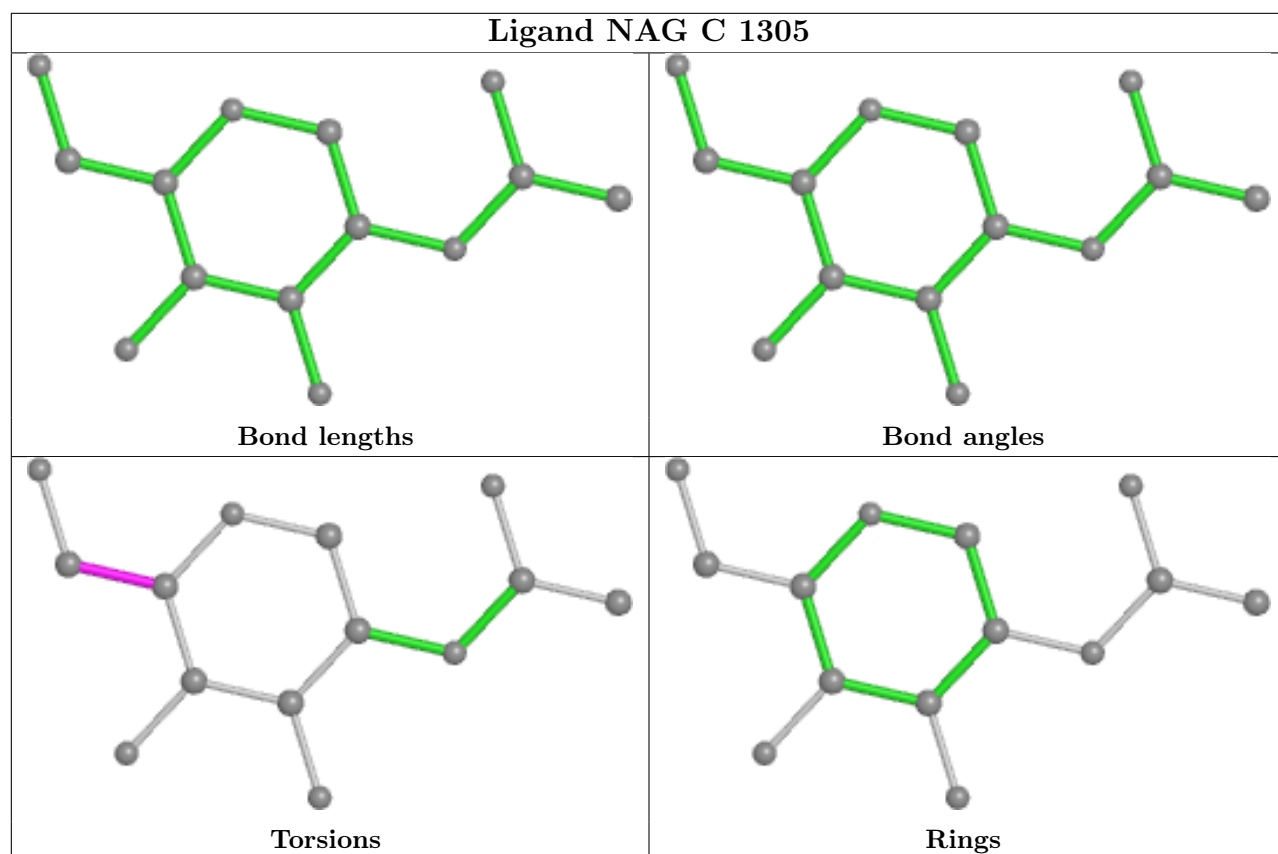
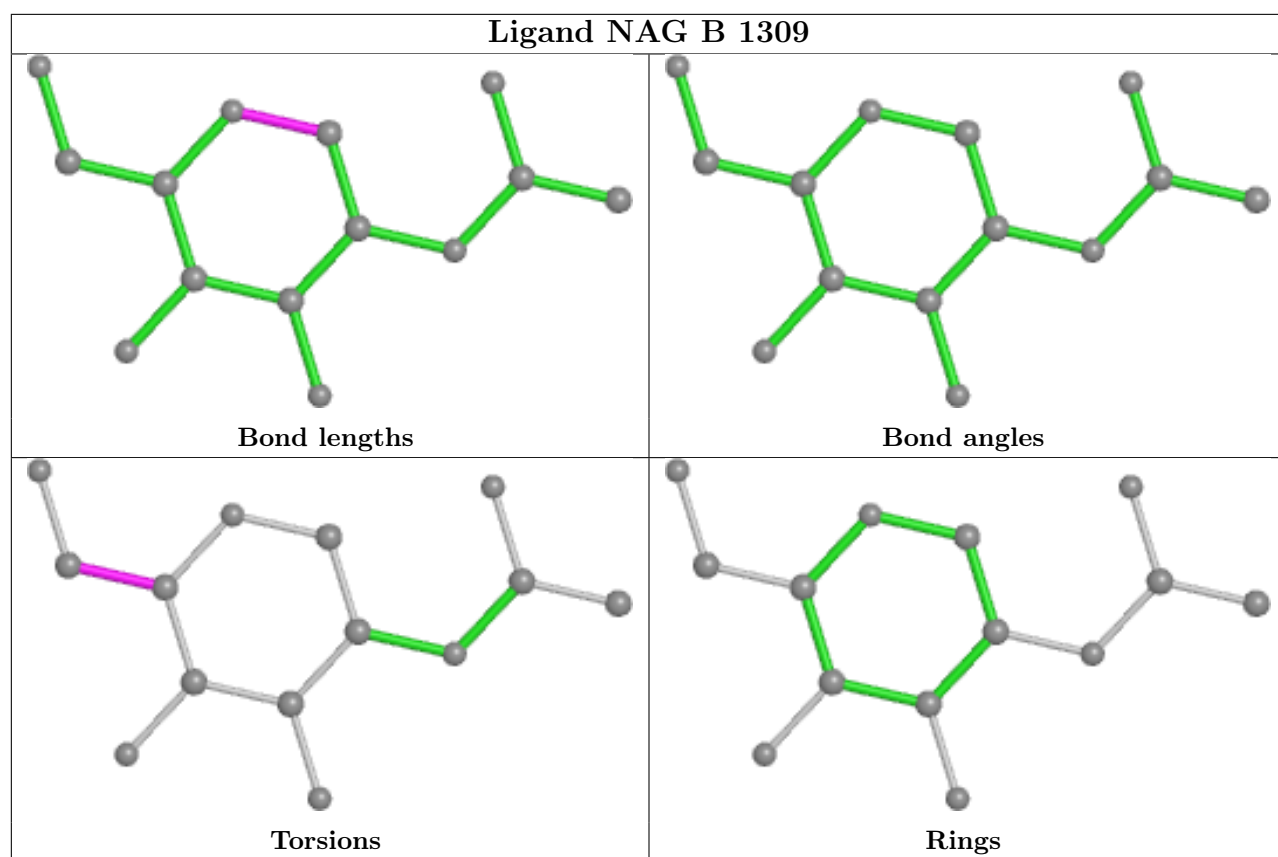


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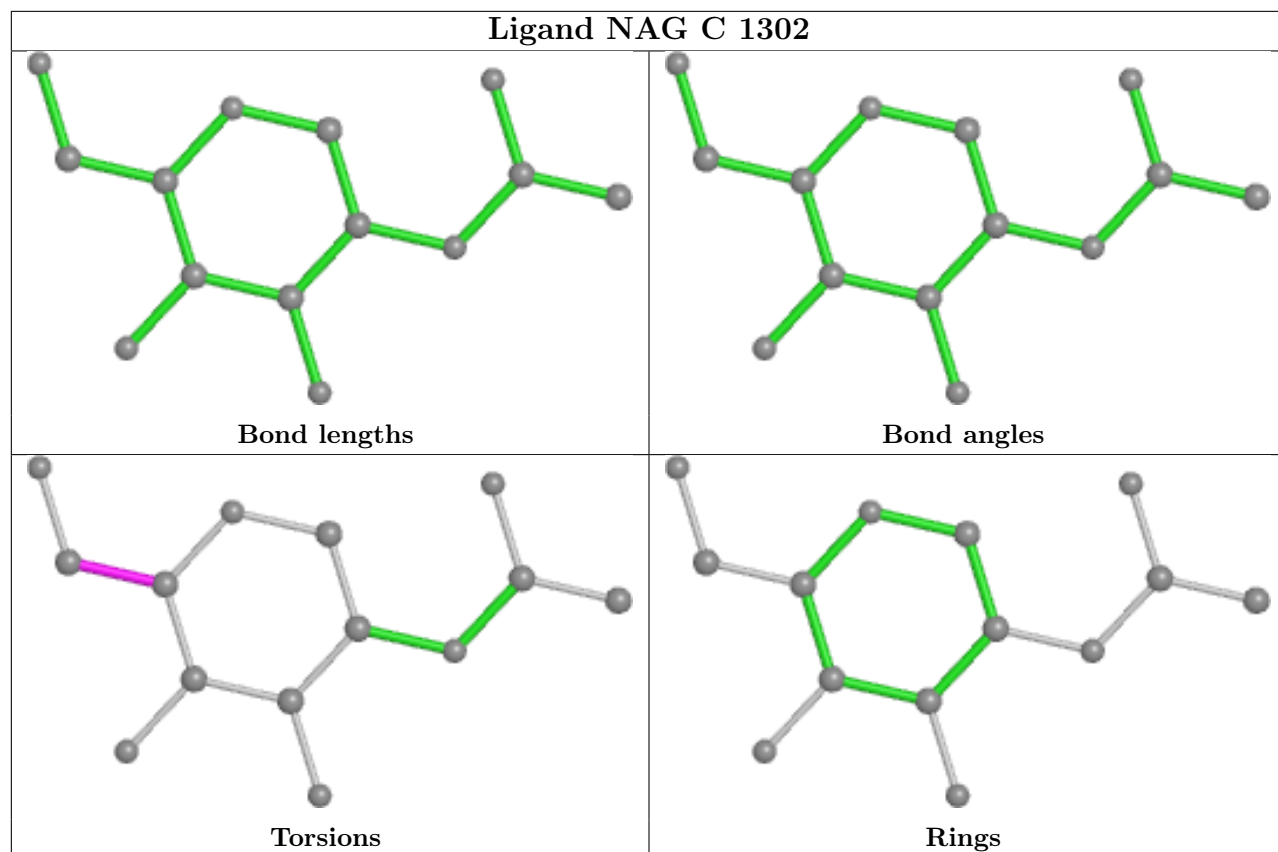


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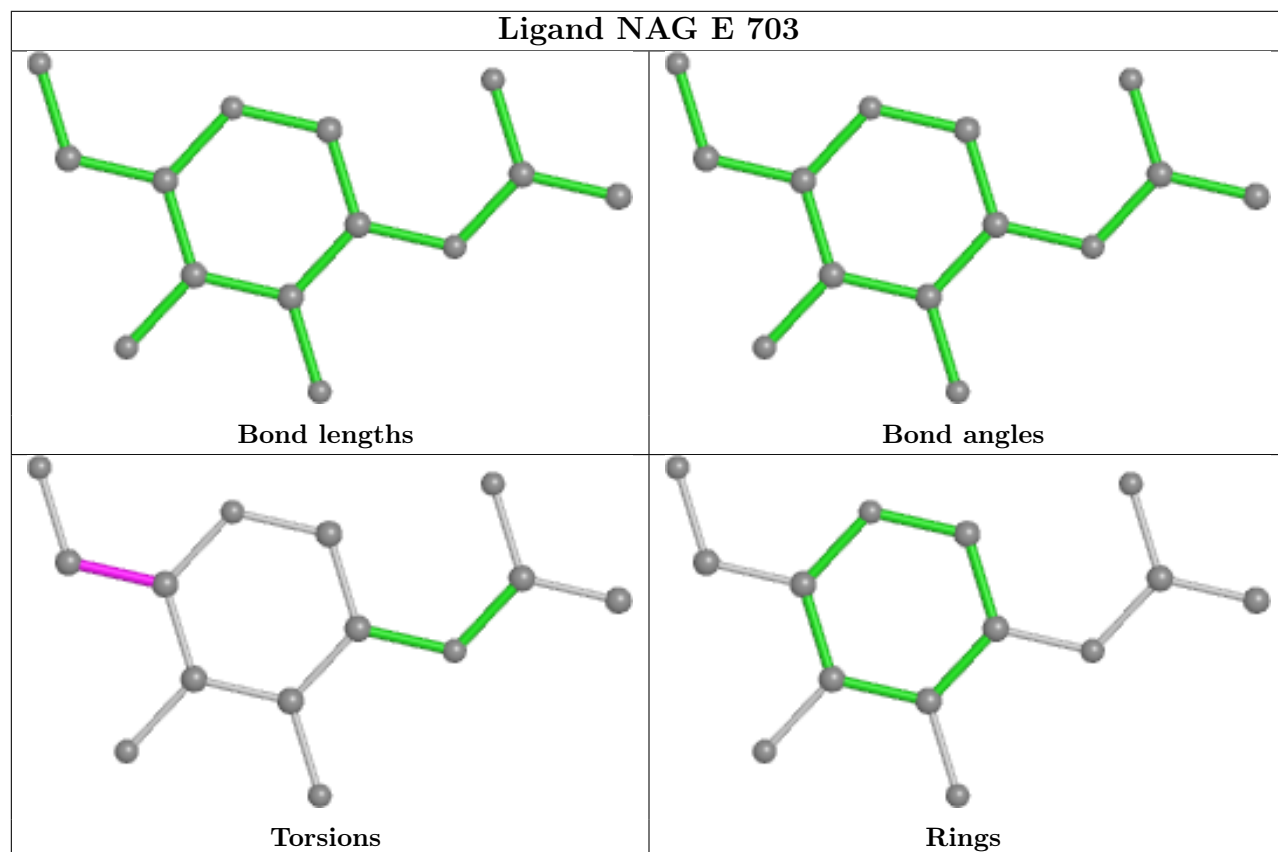




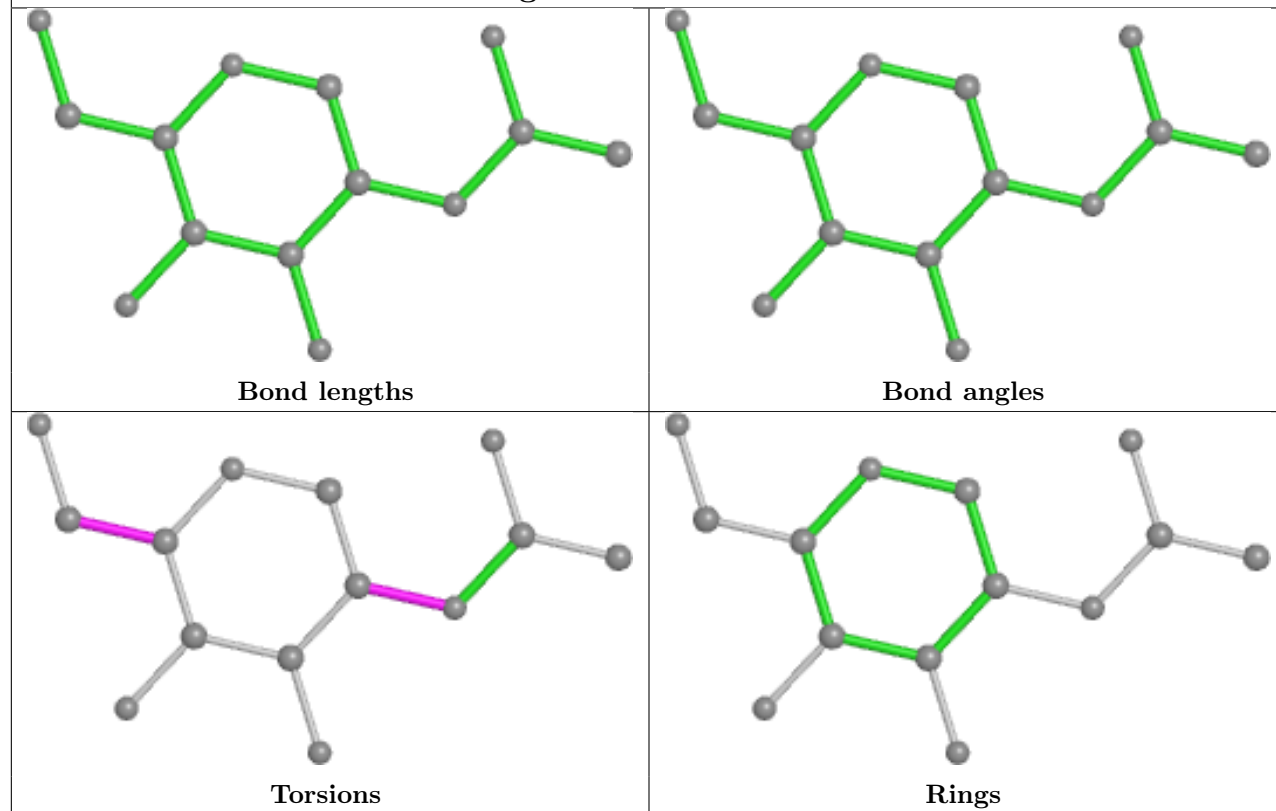
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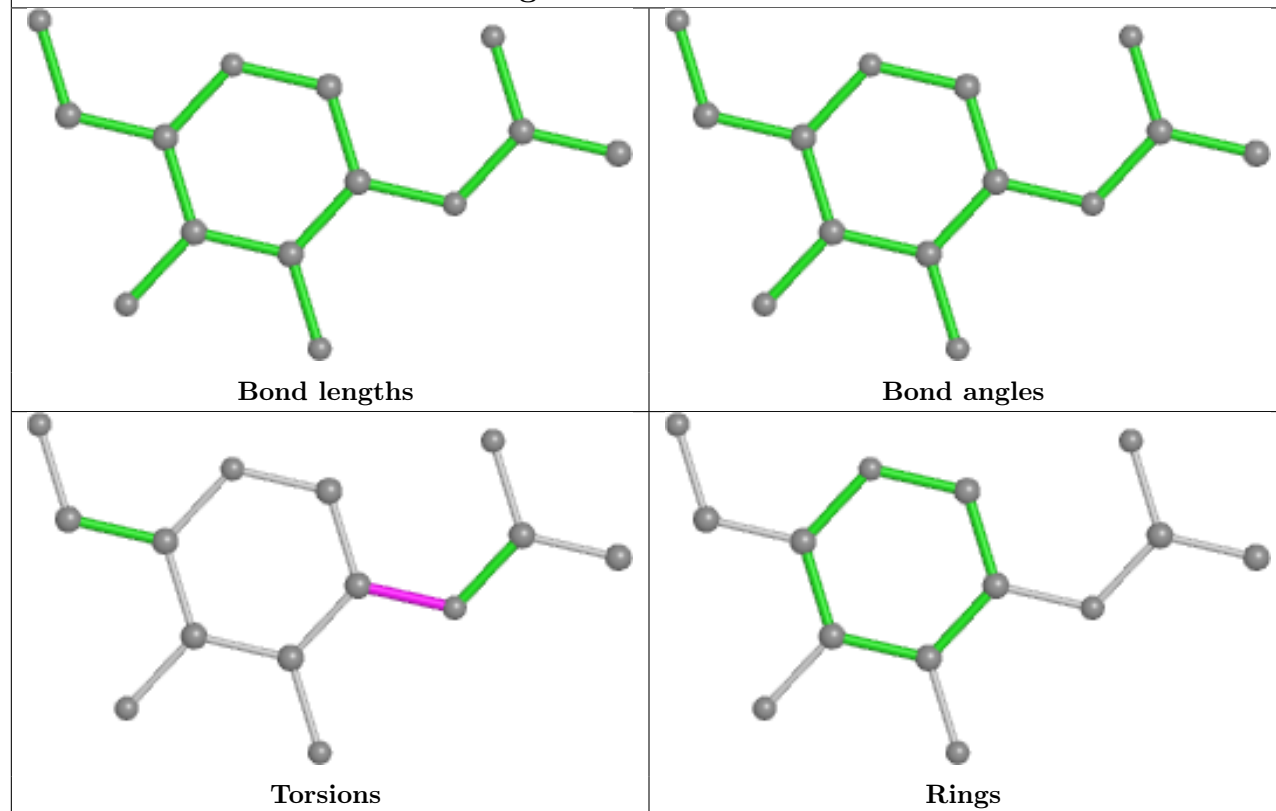
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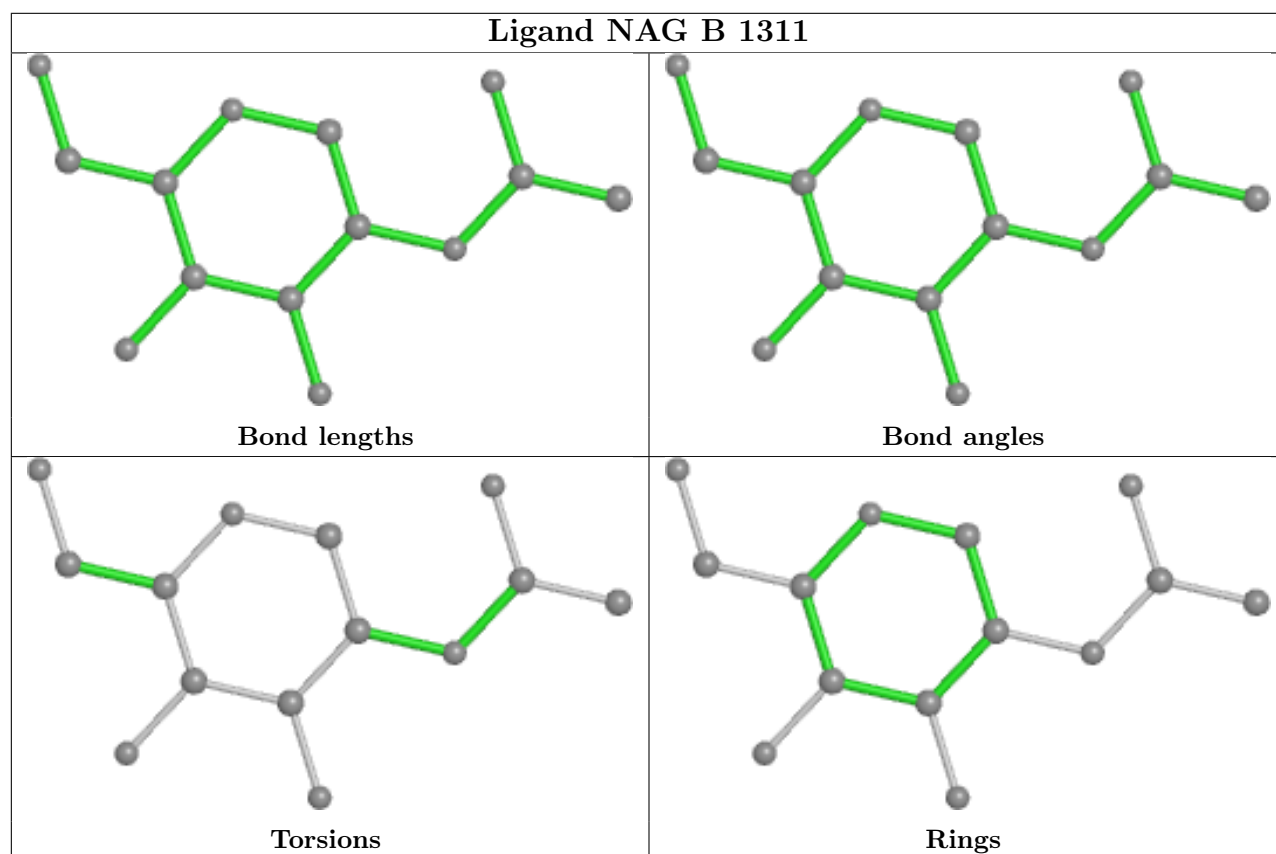
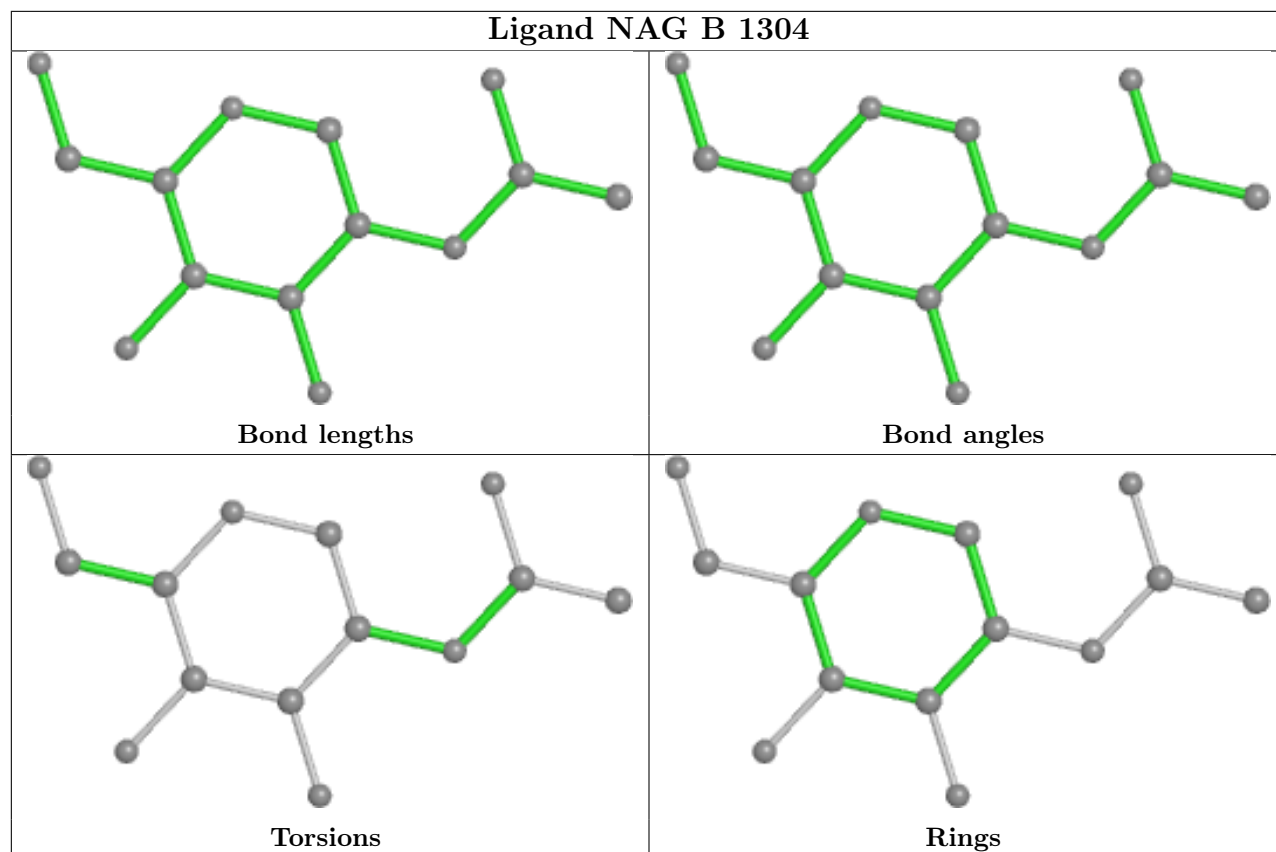


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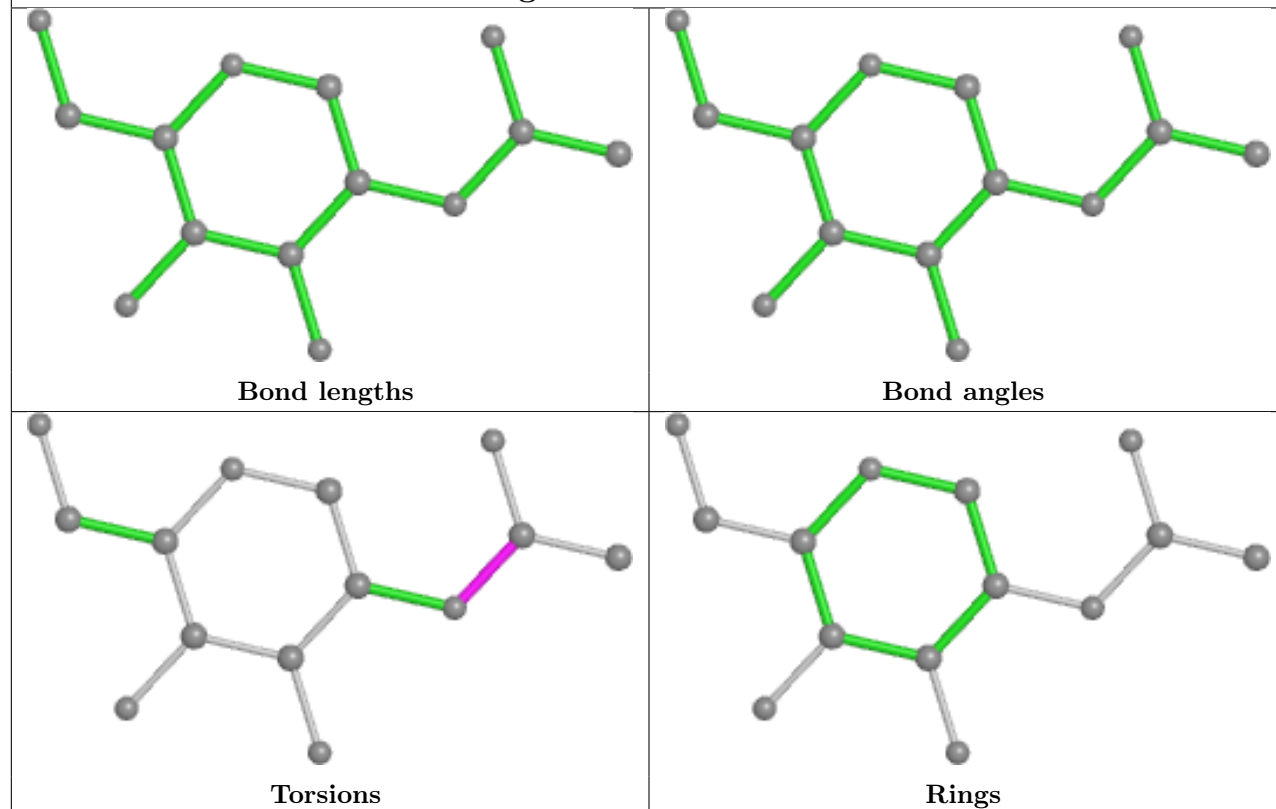


Ligand NAG C 1308

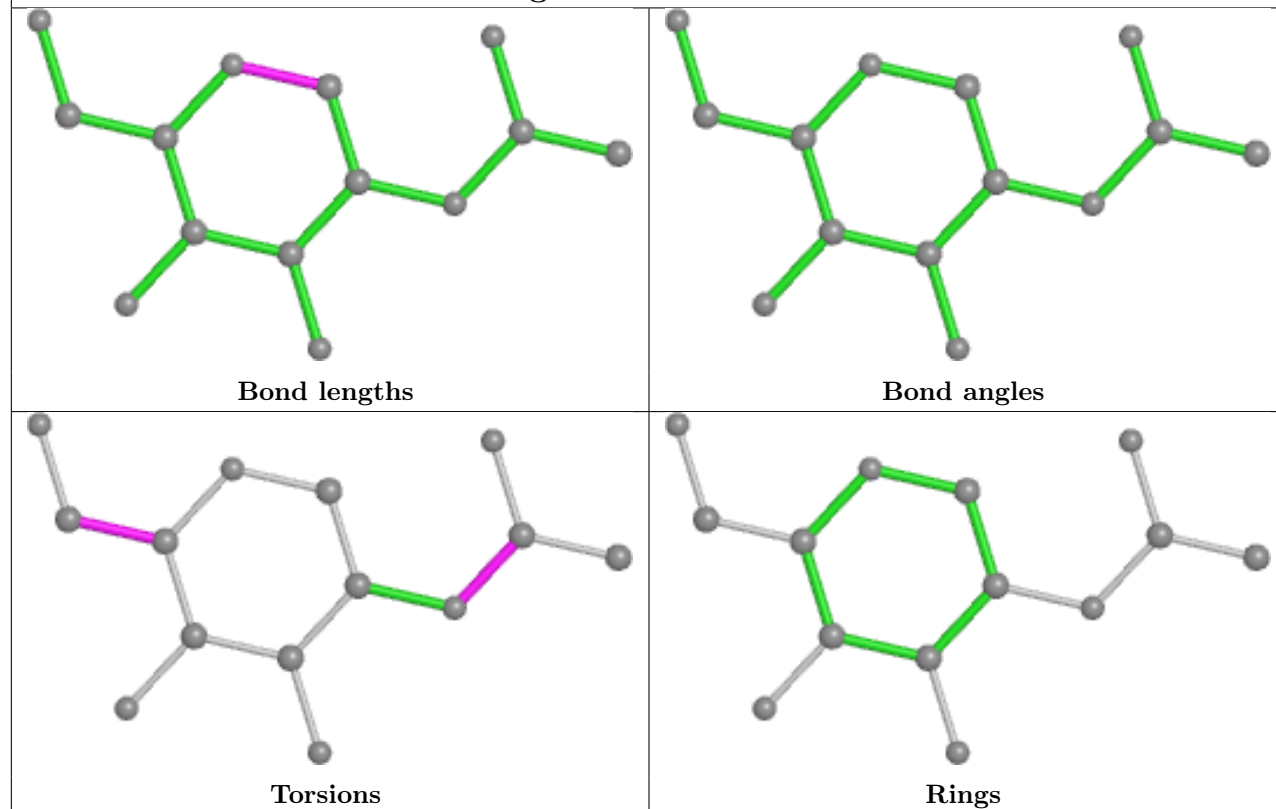




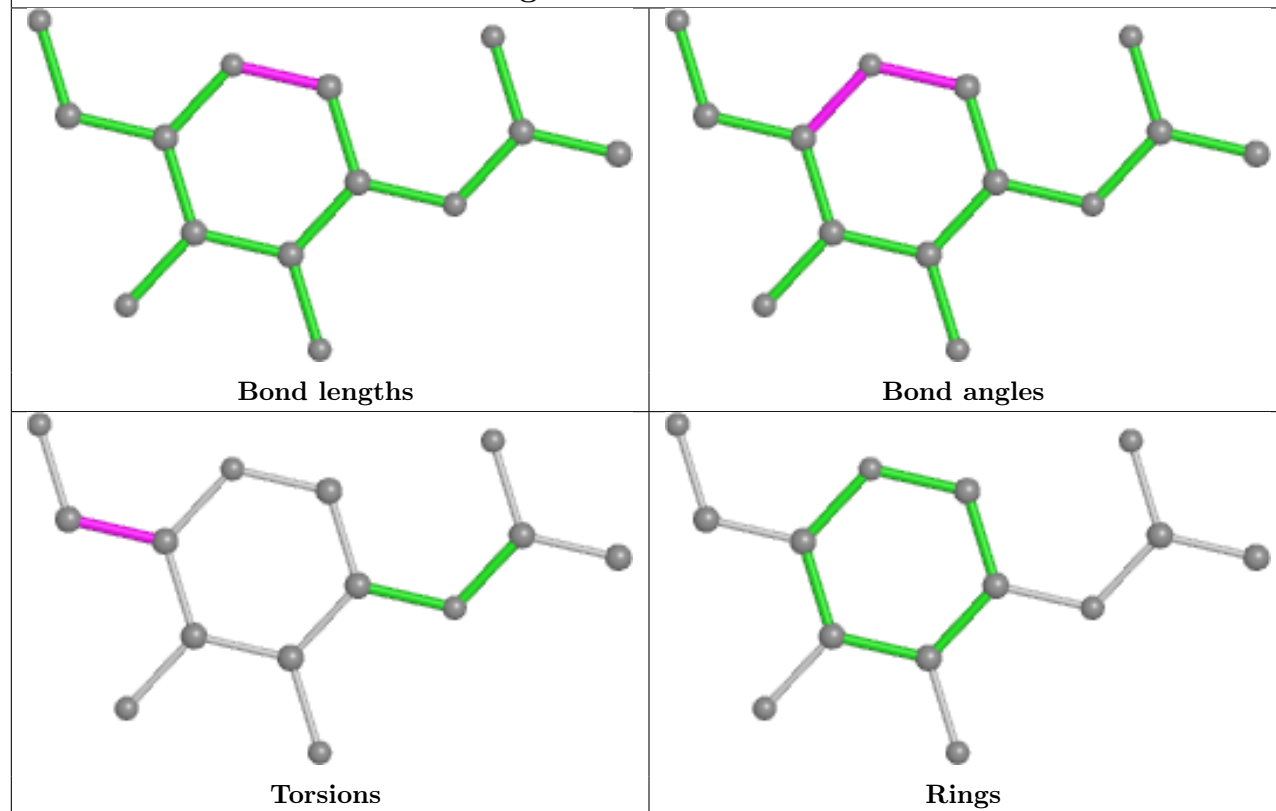
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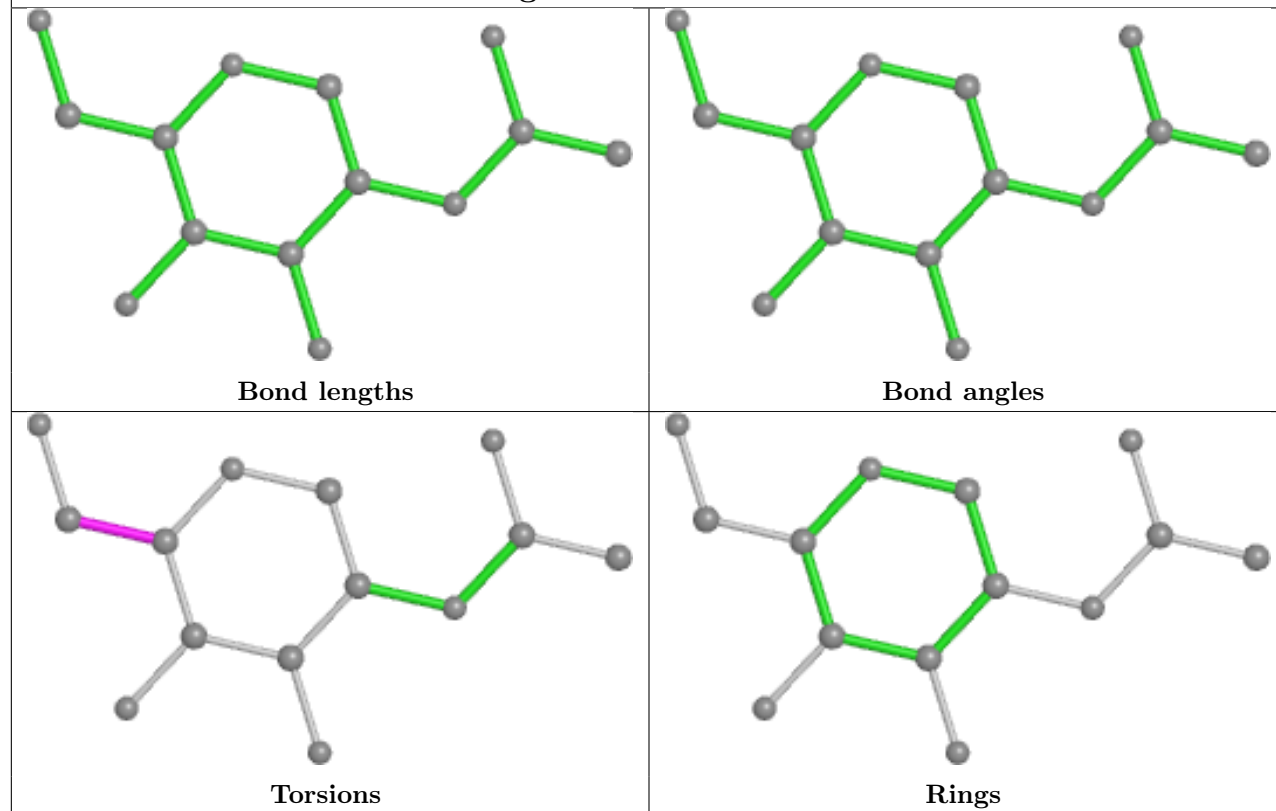
Ligand NAG E 702



Ligand NAG B 1308



Ligand NAG C 1304



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.