



Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 09:48 PM JST

PDB ID : 8ZY1 / pdb_00008zy1
EMDB ID : EMD-60552
Title : Sarbecovirus BM48-31 Spike Trimer in a Locked Conformation
Authors : Wang, J.; Xiong, X.
Deposited on : 2024-06-16
Resolution : 3.10 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 : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

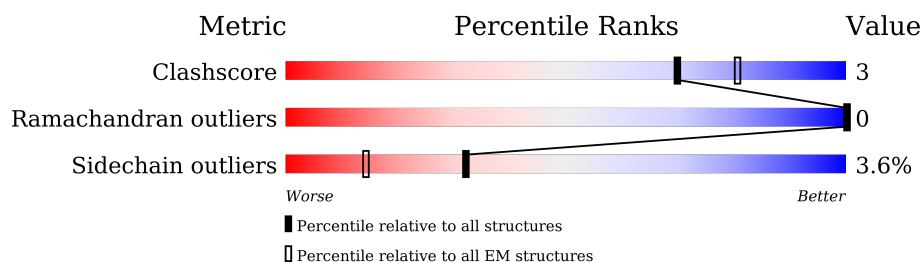
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	1273	75% 9% 15%
1	B	1273	75% 9% 15%
1	C	1273	75% 9% 15%
2	D	2	50% 50%
2	F	2	100%
2	G	2	50% 50%
2	I	2	100%
2	J	2	100%
2	L	2	100%

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Mol	Chain	Length	Quality of chain
3	E	4	 50% 50%
3	H	4	 50% 50%
3	K	4	 25% 75%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26025 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1076	Total	C	N	O	S	0	0
			8367	5331	1393	1597	46		
1	B	1076	Total	C	N	O	S	0	0
			8367	5331	1393	1597	46		
1	C	1076	Total	C	N	O	S	0	0
			8367	5331	1393	1597	46		

There are 237 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1195	GLY	-	expression tag	UNP E0XIZ3
A	1196	SER	-	expression tag	UNP E0XIZ3
A	1197	GLY	-	expression tag	UNP E0XIZ3
A	1198	TYR	-	expression tag	UNP E0XIZ3
A	1199	ILE	-	expression tag	UNP E0XIZ3
A	1200	PRO	-	expression tag	UNP E0XIZ3
A	1201	GLU	-	expression tag	UNP E0XIZ3
A	1202	ALA	-	expression tag	UNP E0XIZ3
A	1203	PRO	-	expression tag	UNP E0XIZ3
A	1204	ARG	-	expression tag	UNP E0XIZ3
A	1205	ASP	-	expression tag	UNP E0XIZ3
A	1206	GLY	-	expression tag	UNP E0XIZ3
A	1207	GLN	-	expression tag	UNP E0XIZ3
A	1208	ALA	-	expression tag	UNP E0XIZ3
A	1209	TYR	-	expression tag	UNP E0XIZ3
A	1210	VAL	-	expression tag	UNP E0XIZ3
A	1211	ARG	-	expression tag	UNP E0XIZ3
A	1212	LYS	-	expression tag	UNP E0XIZ3
A	1213	ASP	-	expression tag	UNP E0XIZ3
A	1214	GLY	-	expression tag	UNP E0XIZ3
A	1215	GLU	-	expression tag	UNP E0XIZ3
A	1216	TRP	-	expression tag	UNP E0XIZ3
A	1217	VAL	-	expression tag	UNP E0XIZ3
A	1218	LEU	-	expression tag	UNP E0XIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1219	LEU	-	expression tag	UNP E0XIZ3
A	1220	SER	-	expression tag	UNP E0XIZ3
A	1221	THR	-	expression tag	UNP E0XIZ3
A	1222	PHE	-	expression tag	UNP E0XIZ3
A	1223	LEU	-	expression tag	UNP E0XIZ3
A	1224	LEU	-	expression tag	UNP E0XIZ3
A	1225	GLU	-	expression tag	UNP E0XIZ3
A	1226	VAL	-	expression tag	UNP E0XIZ3
A	1227	LEU	-	expression tag	UNP E0XIZ3
A	1228	PHE	-	expression tag	UNP E0XIZ3
A	1229	GLN	-	expression tag	UNP E0XIZ3
A	1230	GLY	-	expression tag	UNP E0XIZ3
A	1231	PRO	-	expression tag	UNP E0XIZ3
A	1232	GLY	-	expression tag	UNP E0XIZ3
A	1233	HIS	-	expression tag	UNP E0XIZ3
A	1234	HIS	-	expression tag	UNP E0XIZ3
A	1235	HIS	-	expression tag	UNP E0XIZ3
A	1236	HIS	-	expression tag	UNP E0XIZ3
A	1237	HIS	-	expression tag	UNP E0XIZ3
A	1238	HIS	-	expression tag	UNP E0XIZ3
A	1239	HIS	-	expression tag	UNP E0XIZ3
A	1240	HIS	-	expression tag	UNP E0XIZ3
A	1241	SER	-	expression tag	UNP E0XIZ3
A	1242	ALA	-	expression tag	UNP E0XIZ3
A	1243	TRP	-	expression tag	UNP E0XIZ3
A	1244	SER	-	expression tag	UNP E0XIZ3
A	1245	HIS	-	expression tag	UNP E0XIZ3
A	1246	PRO	-	expression tag	UNP E0XIZ3
A	1247	GLN	-	expression tag	UNP E0XIZ3
A	1248	PHE	-	expression tag	UNP E0XIZ3
A	1249	GLU	-	expression tag	UNP E0XIZ3
A	1250	LYS	-	expression tag	UNP E0XIZ3
A	1251	GLY	-	expression tag	UNP E0XIZ3
A	1252	GLY	-	expression tag	UNP E0XIZ3
A	1253	GLY	-	expression tag	UNP E0XIZ3
A	1254	SER	-	expression tag	UNP E0XIZ3
A	1255	GLY	-	expression tag	UNP E0XIZ3
A	1256	GLY	-	expression tag	UNP E0XIZ3
A	1257	GLY	-	expression tag	UNP E0XIZ3
A	1258	GLY	-	expression tag	UNP E0XIZ3
A	1259	SER	-	expression tag	UNP E0XIZ3
A	1260	GLY	-	expression tag	UNP E0XIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1261	GLY	-	expression tag	UNP E0XIZ3
A	1262	SER	-	expression tag	UNP E0XIZ3
A	1263	ALA	-	expression tag	UNP E0XIZ3
A	1264	TRP	-	expression tag	UNP E0XIZ3
A	1265	SER	-	expression tag	UNP E0XIZ3
A	1266	HIS	-	expression tag	UNP E0XIZ3
A	1267	PRO	-	expression tag	UNP E0XIZ3
A	1268	GLN	-	expression tag	UNP E0XIZ3
A	1269	PHE	-	expression tag	UNP E0XIZ3
A	1270	GLU	-	expression tag	UNP E0XIZ3
A	1271	LYS	-	expression tag	UNP E0XIZ3
A	1272	SER	-	expression tag	UNP E0XIZ3
A	1273	ALA	-	expression tag	UNP E0XIZ3
B	1195	GLY	-	expression tag	UNP E0XIZ3
B	1196	SER	-	expression tag	UNP E0XIZ3
B	1197	GLY	-	expression tag	UNP E0XIZ3
B	1198	TYR	-	expression tag	UNP E0XIZ3
B	1199	ILE	-	expression tag	UNP E0XIZ3
B	1200	PRO	-	expression tag	UNP E0XIZ3
B	1201	GLU	-	expression tag	UNP E0XIZ3
B	1202	ALA	-	expression tag	UNP E0XIZ3
B	1203	PRO	-	expression tag	UNP E0XIZ3
B	1204	ARG	-	expression tag	UNP E0XIZ3
B	1205	ASP	-	expression tag	UNP E0XIZ3
B	1206	GLY	-	expression tag	UNP E0XIZ3
B	1207	GLN	-	expression tag	UNP E0XIZ3
B	1208	ALA	-	expression tag	UNP E0XIZ3
B	1209	TYR	-	expression tag	UNP E0XIZ3
B	1210	VAL	-	expression tag	UNP E0XIZ3
B	1211	ARG	-	expression tag	UNP E0XIZ3
B	1212	LYS	-	expression tag	UNP E0XIZ3
B	1213	ASP	-	expression tag	UNP E0XIZ3
B	1214	GLY	-	expression tag	UNP E0XIZ3
B	1215	GLU	-	expression tag	UNP E0XIZ3
B	1216	TRP	-	expression tag	UNP E0XIZ3
B	1217	VAL	-	expression tag	UNP E0XIZ3
B	1218	LEU	-	expression tag	UNP E0XIZ3
B	1219	LEU	-	expression tag	UNP E0XIZ3
B	1220	SER	-	expression tag	UNP E0XIZ3
B	1221	THR	-	expression tag	UNP E0XIZ3
B	1222	PHE	-	expression tag	UNP E0XIZ3
B	1223	LEU	-	expression tag	UNP E0XIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	LEU	-	expression tag	UNP E0XIZ3
B	1225	GLU	-	expression tag	UNP E0XIZ3
B	1226	VAL	-	expression tag	UNP E0XIZ3
B	1227	LEU	-	expression tag	UNP E0XIZ3
B	1228	PHE	-	expression tag	UNP E0XIZ3
B	1229	GLN	-	expression tag	UNP E0XIZ3
B	1230	GLY	-	expression tag	UNP E0XIZ3
B	1231	PRO	-	expression tag	UNP E0XIZ3
B	1232	GLY	-	expression tag	UNP E0XIZ3
B	1233	HIS	-	expression tag	UNP E0XIZ3
B	1234	HIS	-	expression tag	UNP E0XIZ3
B	1235	HIS	-	expression tag	UNP E0XIZ3
B	1236	HIS	-	expression tag	UNP E0XIZ3
B	1237	HIS	-	expression tag	UNP E0XIZ3
B	1238	HIS	-	expression tag	UNP E0XIZ3
B	1239	HIS	-	expression tag	UNP E0XIZ3
B	1240	HIS	-	expression tag	UNP E0XIZ3
B	1241	SER	-	expression tag	UNP E0XIZ3
B	1242	ALA	-	expression tag	UNP E0XIZ3
B	1243	TRP	-	expression tag	UNP E0XIZ3
B	1244	SER	-	expression tag	UNP E0XIZ3
B	1245	HIS	-	expression tag	UNP E0XIZ3
B	1246	PRO	-	expression tag	UNP E0XIZ3
B	1247	GLN	-	expression tag	UNP E0XIZ3
B	1248	PHE	-	expression tag	UNP E0XIZ3
B	1249	GLU	-	expression tag	UNP E0XIZ3
B	1250	LYS	-	expression tag	UNP E0XIZ3
B	1251	GLY	-	expression tag	UNP E0XIZ3
B	1252	GLY	-	expression tag	UNP E0XIZ3
B	1253	GLY	-	expression tag	UNP E0XIZ3
B	1254	SER	-	expression tag	UNP E0XIZ3
B	1255	GLY	-	expression tag	UNP E0XIZ3
B	1256	GLY	-	expression tag	UNP E0XIZ3
B	1257	GLY	-	expression tag	UNP E0XIZ3
B	1258	GLY	-	expression tag	UNP E0XIZ3
B	1259	SER	-	expression tag	UNP E0XIZ3
B	1260	GLY	-	expression tag	UNP E0XIZ3
B	1261	GLY	-	expression tag	UNP E0XIZ3
B	1262	SER	-	expression tag	UNP E0XIZ3
B	1263	ALA	-	expression tag	UNP E0XIZ3
B	1264	TRP	-	expression tag	UNP E0XIZ3
B	1265	SER	-	expression tag	UNP E0XIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	HIS	-	expression tag	UNP E0XIZ3
B	1267	PRO	-	expression tag	UNP E0XIZ3
B	1268	GLN	-	expression tag	UNP E0XIZ3
B	1269	PHE	-	expression tag	UNP E0XIZ3
B	1270	GLU	-	expression tag	UNP E0XIZ3
B	1271	LYS	-	expression tag	UNP E0XIZ3
B	1272	SER	-	expression tag	UNP E0XIZ3
B	1273	ALA	-	expression tag	UNP E0XIZ3
C	1195	GLY	-	expression tag	UNP E0XIZ3
C	1196	SER	-	expression tag	UNP E0XIZ3
C	1197	GLY	-	expression tag	UNP E0XIZ3
C	1198	TYR	-	expression tag	UNP E0XIZ3
C	1199	ILE	-	expression tag	UNP E0XIZ3
C	1200	PRO	-	expression tag	UNP E0XIZ3
C	1201	GLU	-	expression tag	UNP E0XIZ3
C	1202	ALA	-	expression tag	UNP E0XIZ3
C	1203	PRO	-	expression tag	UNP E0XIZ3
C	1204	ARG	-	expression tag	UNP E0XIZ3
C	1205	ASP	-	expression tag	UNP E0XIZ3
C	1206	GLY	-	expression tag	UNP E0XIZ3
C	1207	GLN	-	expression tag	UNP E0XIZ3
C	1208	ALA	-	expression tag	UNP E0XIZ3
C	1209	TYR	-	expression tag	UNP E0XIZ3
C	1210	VAL	-	expression tag	UNP E0XIZ3
C	1211	ARG	-	expression tag	UNP E0XIZ3
C	1212	LYS	-	expression tag	UNP E0XIZ3
C	1213	ASP	-	expression tag	UNP E0XIZ3
C	1214	GLY	-	expression tag	UNP E0XIZ3
C	1215	GLU	-	expression tag	UNP E0XIZ3
C	1216	TRP	-	expression tag	UNP E0XIZ3
C	1217	VAL	-	expression tag	UNP E0XIZ3
C	1218	LEU	-	expression tag	UNP E0XIZ3
C	1219	LEU	-	expression tag	UNP E0XIZ3
C	1220	SER	-	expression tag	UNP E0XIZ3
C	1221	THR	-	expression tag	UNP E0XIZ3
C	1222	PHE	-	expression tag	UNP E0XIZ3
C	1223	LEU	-	expression tag	UNP E0XIZ3
C	1224	LEU	-	expression tag	UNP E0XIZ3
C	1225	GLU	-	expression tag	UNP E0XIZ3
C	1226	VAL	-	expression tag	UNP E0XIZ3
C	1227	LEU	-	expression tag	UNP E0XIZ3
C	1228	PHE	-	expression tag	UNP E0XIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	GLN	-	expression tag	UNP E0XIZ3
C	1230	GLY	-	expression tag	UNP E0XIZ3
C	1231	PRO	-	expression tag	UNP E0XIZ3
C	1232	GLY	-	expression tag	UNP E0XIZ3
C	1233	HIS	-	expression tag	UNP E0XIZ3
C	1234	HIS	-	expression tag	UNP E0XIZ3
C	1235	HIS	-	expression tag	UNP E0XIZ3
C	1236	HIS	-	expression tag	UNP E0XIZ3
C	1237	HIS	-	expression tag	UNP E0XIZ3
C	1238	HIS	-	expression tag	UNP E0XIZ3
C	1239	HIS	-	expression tag	UNP E0XIZ3
C	1240	HIS	-	expression tag	UNP E0XIZ3
C	1241	SER	-	expression tag	UNP E0XIZ3
C	1242	ALA	-	expression tag	UNP E0XIZ3
C	1243	TRP	-	expression tag	UNP E0XIZ3
C	1244	SER	-	expression tag	UNP E0XIZ3
C	1245	HIS	-	expression tag	UNP E0XIZ3
C	1246	PRO	-	expression tag	UNP E0XIZ3
C	1247	GLN	-	expression tag	UNP E0XIZ3
C	1248	PHE	-	expression tag	UNP E0XIZ3
C	1249	GLU	-	expression tag	UNP E0XIZ3
C	1250	LYS	-	expression tag	UNP E0XIZ3
C	1251	GLY	-	expression tag	UNP E0XIZ3
C	1252	GLY	-	expression tag	UNP E0XIZ3
C	1253	GLY	-	expression tag	UNP E0XIZ3
C	1254	SER	-	expression tag	UNP E0XIZ3
C	1255	GLY	-	expression tag	UNP E0XIZ3
C	1256	GLY	-	expression tag	UNP E0XIZ3
C	1257	GLY	-	expression tag	UNP E0XIZ3
C	1258	GLY	-	expression tag	UNP E0XIZ3
C	1259	SER	-	expression tag	UNP E0XIZ3
C	1260	GLY	-	expression tag	UNP E0XIZ3
C	1261	GLY	-	expression tag	UNP E0XIZ3
C	1262	SER	-	expression tag	UNP E0XIZ3
C	1263	ALA	-	expression tag	UNP E0XIZ3
C	1264	TRP	-	expression tag	UNP E0XIZ3
C	1265	SER	-	expression tag	UNP E0XIZ3
C	1266	HIS	-	expression tag	UNP E0XIZ3
C	1267	PRO	-	expression tag	UNP E0XIZ3
C	1268	GLN	-	expression tag	UNP E0XIZ3
C	1269	PHE	-	expression tag	UNP E0XIZ3
C	1270	GLU	-	expression tag	UNP E0XIZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1271	LYS	-	expression tag	UNP E0XIZ3
C	1272	SER	-	expression tag	UNP E0XIZ3
C	1273	ALA	-	expression tag	UNP E0XIZ3

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		

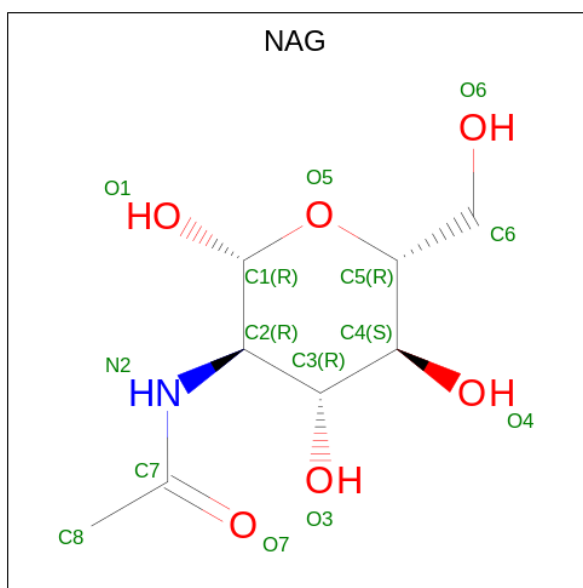
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	4	Total	C	N	O	0	0
			50	28	2	20		
3	H	4	Total	C	N	O	0	0
			50	28	2	20		
3	K	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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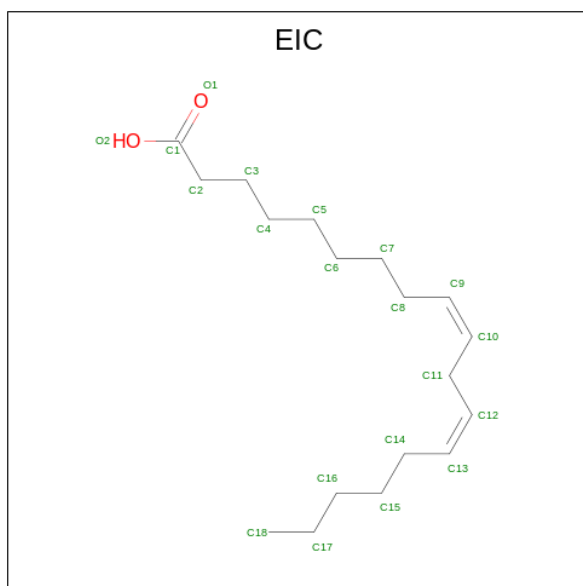
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4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

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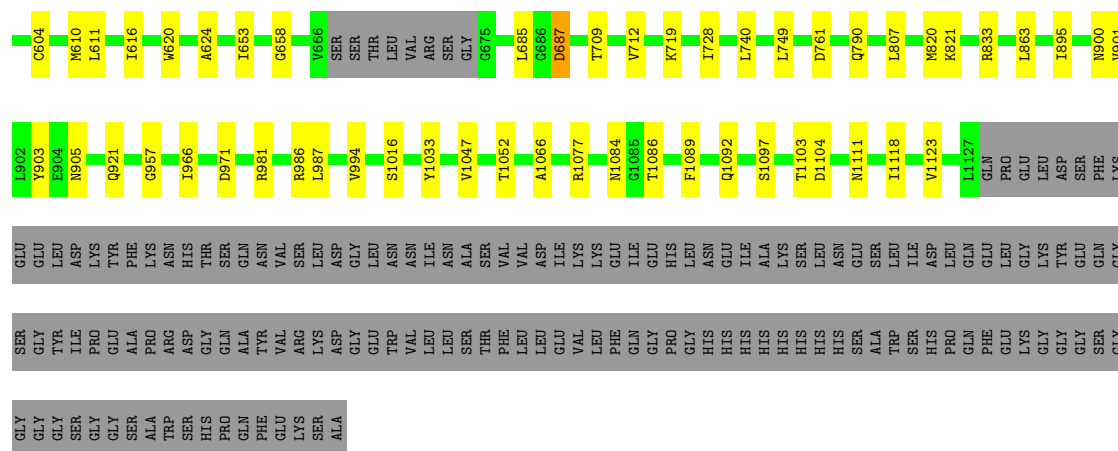
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$).

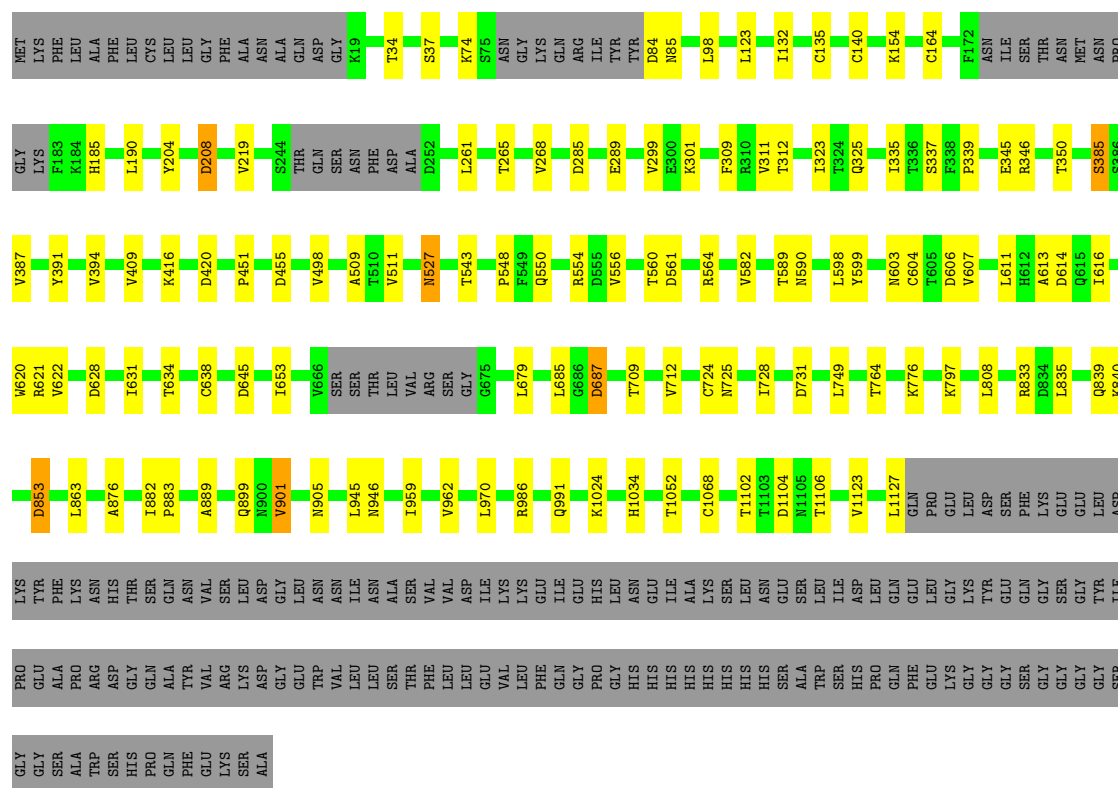


Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			20	18	2	
5	C	1	Total	C	O	0
			20	18	2	
5	C	1	Total	C	O	0
			20	18	2	



• Molecule 1: Spike glycoprotein

Chain C: 75% 9% 15%



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

Chain D: 50% 50%



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

Chain F:  100%

MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2
BMA3
MAN4

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

Chain H:  50% 50%



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

Chain K:  25% 75%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79256	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	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: MAN, BMA, NAG, EIC

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	0.14	0/8564	0.35	0/11650
1	B	0.14	0/8564	0.35	0/11650
1	C	0.13	0/8564	0.36	0/11650
All	All	0.14	0/25692	0.36	0/34950

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	8367	0	8101	60	0
1	B	8367	0	8100	64	0
1	C	8367	0	8100	57	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
3	E	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	50	0	43	0	0
3	K	50	0	43	0	0
4	A	182	0	169	2	0
4	B	182	0	169	1	0
4	C	182	0	169	0	0
5	B	20	0	31	0	0
5	C	40	0	62	1	0
All	All	26025	0	25180	173	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 3.

All (173) 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:613:ALA:HB1	1:C:621:ARG:HG2	1.77	0.65
1:A:208:ASP:OD1	1:A:208:ASP:N	2.34	0.60
1:B:616:ILE:HD12	1:B:620:TRP:HB3	1.84	0.60
1:A:318:VAL:H	1:A:518:THR:HB	1.68	0.58
1:B:790:GLN:NE2	1:B:921:GLN:OE1	2.36	0.58
1:B:1084:ASN:HB2	1:B:1089:PHE:HE2	1.69	0.57
1:B:712:VAL:HG22	1:B:1047:VAL:HG22	1.87	0.57
1:A:694:SER:O	1:A:695:ASN:ND2	2.38	0.57
1:B:895:ILE:HD12	1:B:1033:TYR:HB3	1.86	0.56
1:A:887:GLN:OE1	1:A:891:ARG:NH1	2.38	0.56
1:C:853:ASP:N	1:C:853:ASP:OD1	2.38	0.56
1:C:1102:THR:OG1	1:C:1104:ASP:OD1	2.21	0.56
1:A:290:LEU:HD11	1:A:304:TYR:HB2	1.86	0.56
1:C:606:ASP:N	1:C:606:ASP:OD1	2.39	0.56
1:A:1102:THR:OG1	1:A:1104:ASP:OD1	2.23	0.55
1:C:687:ASP:N	1:C:687:ASP:OD1	2.39	0.55
1:C:901:VAL:O	1:C:905:ASN:ND2	2.40	0.55
1:A:1084:ASN:HB2	1:A:1089:PHE:HE2	1.71	0.55
1:B:833:ARG:NH2	1:C:561:ASP:OD2	2.39	0.55
1:B:355:ASP:HB3	1:B:514:PRO:HG3	1.87	0.55
1:B:198:LEU:HD23	1:B:226:LEU:HD12	1.87	0.54
1:B:901:VAL:O	1:B:905:ASN:ND2	2.40	0.54
1:B:349:ILE:HB	1:B:387:VAL:HB	1.91	0.53
1:A:790:GLN:NE2	1:A:921:GLN:OE1	2.41	0.53
1:B:344:TRP:O	1:B:454:ARG:NH1	2.38	0.53
1:C:554:ARG:HH12	1:C:560:THR:HG22	1.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD11	1:A:261:LEU:HD21	1.90	0.53
1:C:550:GLN:O	1:C:564:ARG:NH2	2.42	0.53
1:A:749:LEU:HD22	1:A:994:VAL:HG21	1.92	0.52
1:B:322:ASN:ND2	4:B:1302:NAG:O6	2.42	0.52
1:A:385:SER:HA	1:A:509:ALA:HA	1.90	0.52
1:C:190:LEU:HD11	1:C:261:LEU:HD21	1.92	0.52
1:C:339:PRO:HG3	1:C:345:GLU:HG2	1.92	0.51
1:A:92:ASP:OD1	1:A:92:ASP:N	2.41	0.51
1:B:129:HIS:ND1	1:B:170:HIS:O	2.37	0.51
1:A:561:ASP:OD2	1:C:833:ARG:NH2	2.44	0.51
1:B:971:ASP:OD1	1:B:971:ASP:N	2.40	0.51
1:C:645:ASP:HB2	1:C:679:LEU:HD11	1.91	0.51
1:C:455:ASP:OD1	1:C:455:ASP:N	2.42	0.51
1:A:355:ASP:OD1	1:A:355:ASP:N	2.41	0.51
1:A:957:GLY:O	1:A:981:ARG:NH1	2.43	0.51
1:C:135:CYS:HA	1:C:164:CYS:HB3	1.92	0.51
1:A:378:LYS:NZ	1:C:970:LEU:O	2.44	0.50
1:A:889:ALA:HB1	1:A:899:GLN:HB2	1.93	0.50
1:C:1034:HIS:HA	1:C:1052:THR:HG22	1.93	0.50
1:A:67:LEU:HD13	1:A:257:PHE:HB3	1.94	0.50
1:A:704:PHE:HE2	1:A:909:ILE:HD11	1.75	0.50
1:B:957:GLY:O	1:B:981:ARG:NH1	2.45	0.50
1:C:391:TYR:HB3	1:C:498:VAL:HG12	1.94	0.50
1:C:85:ASN:OD1	1:C:85:ASN:N	2.43	0.50
1:A:554:ARG:NH2	1:A:560:THR:OG1	2.45	0.49
1:A:816:ASP:OD1	1:A:816:ASP:N	2.42	0.49
1:A:712:VAL:HG22	1:A:1047:VAL:HG22	1.92	0.49
1:B:326:LEU:HD21	1:B:358:VAL:HG11	1.94	0.49
1:C:590:ASN:OD1	1:C:590:ASN:N	2.46	0.49
1:A:852:THR:OG1	1:A:853:ASP:N	2.45	0.49
1:B:46:ASP:OD1	1:B:46:ASP:N	2.43	0.49
1:A:763:ASN:OD1	1:A:1005:ARG:NH1	2.41	0.48
1:C:84:ASP:N	1:C:84:ASP:OD1	2.45	0.48
1:B:85:ASN:N	1:B:85:ASN:OD1	2.47	0.48
1:A:932:GLY:O	1:A:936:ASP:HB2	2.14	0.48
1:A:616:ILE:HD12	1:A:620:TRP:HB3	1.96	0.48
1:A:971:ASP:OD1	1:A:971:ASP:N	2.44	0.48
1:A:561:ASP:HA	1:A:574:ILE:HB	1.96	0.48
1:A:603:ASN:ND2	4:A:1302:NAG:O7	2.43	0.47
1:A:550:GLN:O	1:A:564:ARG:NH2	2.47	0.47
1:B:355:ASP:OD1	1:B:355:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASP:OD1	1:C:208:ASP:N	2.38	0.47
1:A:850:LEU:O	1:B:658:GLY:N	2.45	0.47
1:B:687:ASP:OD1	1:B:687:ASP:N	2.47	0.47
1:C:185:HIS:HB3	1:C:204:TYR:HE1	1.80	0.47
1:C:1104:ASP:OD1	1:C:1104:ASP:N	2.38	0.47
1:A:1032:GLY:HA2	1:C:876:ALA:HB1	1.97	0.47
1:B:542:SER:OG	1:B:543:THR:N	2.47	0.47
1:A:592:SER:OG	1:A:593:SER:N	2.48	0.46
1:C:604:CYS:HB2	1:C:638:CYS:HB2	1.63	0.46
1:C:749:LEU:HD11	1:C:991:GLN:HG3	1.96	0.46
1:A:74:LYS:HD3	1:A:74:LYS:HA	1.81	0.46
1:B:318:VAL:H	1:B:518:THR:HG1	1.63	0.46
1:C:420:ASP:OD1	1:C:420:ASP:N	2.37	0.46
1:A:606:ASP:N	1:A:606:ASP:OD1	2.48	0.46
1:C:385:SER:HA	1:C:509:ALA:HA	1.98	0.46
1:B:252:ASP:HB3	1:B:253:ALA:H	1.59	0.46
1:C:882:ILE:HD12	1:C:883:PRO:HD2	1.97	0.46
1:A:542:SER:OG	1:A:543:THR:N	2.49	0.46
1:B:1077:ARG:NH1	1:B:1104:ASP:OD1	2.48	0.46
1:B:88:ILE:HG21	1:B:258:VAL:HG21	1.97	0.45
1:B:820:MET:HE2	1:B:820:MET:HB2	1.86	0.45
1:A:88:ILE:HG21	1:A:258:VAL:HG21	1.98	0.45
1:B:561:ASP:OD1	1:B:561:ASP:N	2.45	0.45
1:B:586:THR:HG22	1:B:595:VAL:HG12	1.98	0.45
1:A:100:GLU:OE2	1:A:187:ARG:NH1	2.44	0.45
1:A:536:THR:HB	1:C:731:ASP:HB3	1.99	0.45
1:C:614:ASP:OD1	1:C:614:ASP:N	2.49	0.45
1:B:109:ILE:HG12	1:B:122:VAL:HG12	1.98	0.45
1:C:548:PRO:HA	1:C:564:ARG:HH22	1.81	0.45
1:A:723:ASP:OD1	1:A:723:ASP:N	2.43	0.45
1:A:349:ILE:HB	1:A:387:VAL:HB	1.99	0.45
1:B:563:VAL:HG12	1:B:574:ILE:HD11	1.99	0.44
1:B:579:TYR:HB3	1:B:610:MET:HE2	1.99	0.44
1:A:355:ASP:HB3	1:A:514:PRO:HG3	1.99	0.44
1:B:135:CYS:HB3	1:B:164:CYS:HB2	1.60	0.44
1:B:900:ASN:O	1:B:903:TYR:N	2.51	0.44
1:C:728:ILE:HA	1:C:986:ARG:HD3	1.99	0.44
1:A:132:ILE:HD13	1:A:226:LEU:HD21	1.98	0.44
1:B:322:ASN:OD1	1:B:322:ASN:N	2.50	0.44
1:A:840:LYS:NZ	1:B:601:ASP:OD2	2.37	0.44
1:B:1066:ALA:HB3	1:B:1118:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1024:LYS:HA	1:C:1024:LYS:HD2	1.77	0.44
1:A:129:HIS:ND1	1:A:170:HIS:O	2.37	0.43
1:B:385:SER:HA	1:B:509:ALA:HA	2.00	0.43
1:C:154:LYS:HA	1:C:154:LYS:HD3	1.77	0.43
1:A:604:CYS:HB2	1:A:638:CYS:HB2	1.32	0.43
1:C:889:ALA:HB1	1:C:899:GLN:HG3	2.00	0.43
1:B:749:LEU:HD22	1:B:994:VAL:HG21	1.99	0.43
1:B:1092:GLN:H	1:B:1092:GLN:HG3	1.65	0.43
1:A:46:ASP:N	1:A:46:ASP:OD1	2.52	0.43
1:A:135:CYS:HA	1:A:164:CYS:HA	2.00	0.43
1:A:820:MET:HE2	1:A:820:MET:HB2	1.87	0.43
1:B:84:ASP:OD1	1:B:84:ASP:N	2.51	0.43
1:B:262:LYS:HG3	1:B:263:PRO:HD2	1.99	0.43
1:B:449:ILE:HD13	1:B:449:ILE:HA	1.89	0.43
1:B:728:ILE:HA	1:B:986:ARG:HD3	2.01	0.43
1:C:123:LEU:HG	1:C:132:ILE:HG12	2.00	0.43
1:B:592:SER:OG	1:B:593:SER:N	2.51	0.43
1:B:1097:SER:O	1:B:1097:SER:OG	2.32	0.43
1:B:74:LYS:HA	1:B:74:LYS:HD3	1.77	0.43
1:B:611:LEU:HD23	1:B:624:ALA:HB2	2.00	0.43
1:C:725:ASN:OD1	1:C:725:ASN:N	2.52	0.42
1:C:301:LYS:HG2	1:C:653:ILE:HD11	2.02	0.42
1:A:185:HIS:HB3	1:A:204:TYR:HE1	1.84	0.42
1:A:198:LEU:HD23	1:A:226:LEU:HD13	2.01	0.42
1:C:797:LYS:H	1:C:797:LYS:HG2	1.60	0.42
1:C:840:LYS:HB2	1:C:840:LYS:HE2	1.85	0.42
1:B:807:LEU:HD12	1:B:807:LEU:HA	1.88	0.42
1:C:74:LYS:HD3	1:C:74:LYS:HA	1.82	0.42
1:C:603:ASN:HD22	1:C:603:ASN:HA	1.69	0.42
1:A:1014:LYS:HE2	1:A:1014:LYS:HB2	1.90	0.42
1:C:945:LEU:HD12	1:C:945:LEU:HA	1.95	0.42
1:B:42:TYR:OH	1:B:59:HIS:O	2.31	0.41
1:C:839:GLN:NE2	1:C:946:ASN:OD1	2.51	0.41
1:B:356:TYR:O	1:B:359:LEU:HB2	2.21	0.41
1:B:719:LYS:NZ	1:B:761:ASP:OD2	2.44	0.41
1:C:289:GLU:HG3	1:C:309:PHE:HD2	1.85	0.41
1:C:416:LYS:HB3	1:C:451:PRO:HA	2.01	0.41
1:B:821:LYS:HA	1:B:821:LYS:HD3	1.87	0.41
1:C:611:LEU:HD12	1:C:611:LEU:HA	1.91	0.41
1:A:908:GLN:HE21	1:A:912:GLN:HE21	1.67	0.41
1:B:290:LEU:O	1:B:294:THR:OG1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:LYS:HE3	1:B:295:LYS:HB3	1.81	0.41
1:B:489:GLY:O	1:B:493:GLN:NE2	2.54	0.41
1:C:37:SER:O	1:C:37:SER:OG	2.33	0.41
1:C:582:VAL:HG22	1:C:599:TYR:HD1	1.86	0.41
1:C:616:ILE:HD12	1:C:620:TRP:HB3	2.03	0.41
1:B:230:LEU:HD12	1:B:230:LEU:HA	1.95	0.41
1:C:299:VAL:O	1:C:589:THR:OG1	2.36	0.41
1:C:335:ILE:HG23	1:C:337:SER:H	1.86	0.41
1:C:387:VAL:HG11	5:C:1302:EIC:H131	2.02	0.41
1:C:776:LYS:HB3	1:C:776:LYS:HE3	1.89	0.41
1:B:301:LYS:HE2	1:B:653:ILE:HD11	2.02	0.41
1:A:252:ASP:HB3	1:A:253:ALA:H	1.68	0.40
1:A:855:MET:HB3	1:B:685:LEU:HD21	2.03	0.40
1:B:23:LEU:H	1:B:23:LEU:HG	1.73	0.40
1:A:945:LEU:HD23	1:A:945:LEU:HA	1.96	0.40
1:B:336:THR:HA	1:B:496:ARG:HH22	1.86	0.40
1:B:987:LEU:HD12	1:B:987:LEU:HA	1.92	0.40
1:C:527:ASN:OD1	1:C:527:ASN:N	2.40	0.40
1:B:420:ASP:OD1	1:B:420:ASP:N	2.38	0.40
1:A:335:ILE:HG23	1:A:337:SER:H	1.87	0.40
1:A:626:ARG:HD3	1:A:626:ARG:HA	1.69	0.40
1:A:920:ILE:HD13	1:A:920:ILE:HA	1.97	0.40
1:B:363:SER:O	1:B:363:SER:OG	2.36	0.40
1:A:363:SER:HB2	4:A:1310:NAG:H62	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1066/1273 (84%)	1029 (96%)	37 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1066/1273 (84%)	1028 (96%)	38 (4%)	0	100	100
1	C	1066/1273 (84%)	1035 (97%)	31 (3%)	0	100	100
All	All	3198/3819 (84%)	3092 (97%)	106 (3%)	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	931/1095 (85%)	903 (97%)	28 (3%)	36	64
1	B	931/1095 (85%)	902 (97%)	29 (3%)	35	63
1	C	931/1095 (85%)	887 (95%)	44 (5%)	22	52
All	All	2793/3285 (85%)	2692 (96%)	101 (4%)	32	60

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	46	ASP
1	A	47	ILE
1	A	52	ILE
1	A	67	LEU
1	A	73	LEU
1	A	98	LEU
1	A	123	LEU
1	A	133	ASP
1	A	147	VAL
1	A	155	THR
1	A	208	ASP
1	A	258	VAL
1	A	312	THR
1	A	314	THR
1	A	326	LEU

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Mol	Chain	Res	Type
1	A	527	ASN
1	A	568	THR
1	A	678	ILE
1	A	695	ASN
1	A	722	VAL
1	A	735	CYS
1	A	802	SER
1	A	808	LEU
1	A	863	LEU
1	A	1080	VAL
1	A	1103	THR
1	A	1116	ILE
1	B	23	LEU
1	B	46	ASP
1	B	89	ASN
1	B	98	LEU
1	B	104	VAL
1	B	132	ILE
1	B	144	MET
1	B	172	PHE
1	B	185	HIS
1	B	208	ASP
1	B	224	LEU
1	B	258	VAL
1	B	271	ASP
1	B	294	THR
1	B	327	CYS
1	B	374	VAL
1	B	568	THR
1	B	604	CYS
1	B	687	ASP
1	B	709	THR
1	B	740	LEU
1	B	863	LEU
1	B	966	ILE
1	B	1016	SER
1	B	1052	THR
1	B	1086	THR
1	B	1103	THR
1	B	1111	ASN
1	B	1123	VAL
1	C	34	THR

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Mol	Chain	Res	Type
1	C	98	LEU
1	C	140	CYS
1	C	208	ASP
1	C	219	VAL
1	C	265	THR
1	C	268	VAL
1	C	285	ASP
1	C	311	VAL
1	C	312	THR
1	C	323	ILE
1	C	325	GLN
1	C	346	ARG
1	C	350	THR
1	C	385	SER
1	C	394	VAL
1	C	409	VAL
1	C	511	VAL
1	C	527	ASN
1	C	543	THR
1	C	556	VAL
1	C	598	LEU
1	C	607	VAL
1	C	622	VAL
1	C	628	ASP
1	C	631	ILE
1	C	634	THR
1	C	685	LEU
1	C	687	ASP
1	C	709	THR
1	C	712	VAL
1	C	724	CYS
1	C	764	THR
1	C	808	LEU
1	C	835	LEU
1	C	853	ASP
1	C	863	LEU
1	C	901	VAL
1	C	959	ILE
1	C	962	VAL
1	C	1068	CYS
1	C	1106	THR
1	C	1123	VAL

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Mol	Chain	Res	Type
1	C	1127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	148	ASN
1	A	189	HIS
1	A	284	GLN
1	A	305	GLN
1	A	330	ASN
1	A	429	ASN
1	A	615	GLN
1	A	676	HIS
1	A	760	GLN
1	A	842	ASN
1	A	905	ASN
1	A	912	GLN
1	A	940	GLN
1	A	1087	HIS
1	B	66	ASN
1	B	87	ASN
1	B	136	ASN
1	B	148	ASN
1	B	406	GLN
1	B	431	ASN
1	B	437	ASN
1	B	446	HIS
1	B	462	ASN
1	B	688	ASN
1	B	839	GLN
1	B	1092	GLN
1	B	1121	ASN
1	C	203	ASN
1	C	308	ASN
1	C	474	ASN
1	C	486	GLN
1	C	529	ASN
1	C	695	ASN
1	C	696	ASN
1	C	842	ASN
1	C	908	GLN

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Mol	Chain	Res	Type
1	C	912	GLN
1	C	1057	GLN
1	C	1060	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 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	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.73	0	17,19,21	1.17	2 (11%)
2	NAG	D	2	2	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	E	1	1,3	14,14,15	0.74	0	17,19,21	1.00	0
3	NAG	E	2	3	14,14,15	0.72	0	17,19,21	0.99	0
3	BMA	E	3	3	11,11,12	0.89	0	15,15,17	2.36	3 (20%)
3	MAN	E	4	3	11,11,12	0.69	0	15,15,17	1.31	1 (6%)
2	NAG	F	1	2,1	14,14,15	0.69	0	17,19,21	1.51	2 (11%)
2	NAG	F	2	2	14,14,15	0.72	0	17,19,21	1.46	3 (17%)
2	NAG	G	1	2,1	14,14,15	0.73	0	17,19,21	1.27	1 (5%)
2	NAG	G	2	2	14,14,15	0.70	0	17,19,21	0.89	0
3	NAG	H	1	1,3	14,14,15	0.76	0	17,19,21	0.98	0
3	NAG	H	2	3	14,14,15	0.72	0	17,19,21	0.90	0
3	BMA	H	3	3	11,11,12	0.90	1 (9%)	15,15,17	2.45	4 (26%)
3	MAN	H	4	3	11,11,12	0.71	0	15,15,17	1.28	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	1	2,1	14,14,15	0.71	0	17,19,21	1.50	2 (11%)
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	1.45	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.72	0	17,19,21	1.31	2 (11%)
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
3	NAG	K	1	1,3	14,14,15	0.76	0	17,19,21	1.01	1 (5%)
3	NAG	K	2	3	14,14,15	0.72	0	17,19,21	0.94	0
3	BMA	K	3	3	11,11,12	0.92	1 (9%)	15,15,17	2.43	5 (33%)
3	MAN	K	4	3	11,11,12	0.73	0	15,15,17	1.35	1 (6%)
2	NAG	L	1	2,1	14,14,15	0.68	0	17,19,21	1.49	1 (5%)
2	NAG	L	2	2	14,14,15	0.71	0	17,19,21	1.47	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	1/2/19/22	1/1/1/1
2	NAG	I	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
3	MAN	K	4	3	-	1/2/19/22	1/1/1/1
2	NAG	L	1	2,1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	3	BMA	C2-C3	2.05	1.55	1.52
3	K	3	BMA	C2-C3	2.05	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	7.44	122.27	112.19
3	K	3	BMA	C1-O5-C5	7.18	121.91	112.19
3	E	3	BMA	C1-O5-C5	7.09	121.80	112.19
2	I	1	NAG	C2-N2-C7	4.32	129.05	122.90
2	F	1	NAG	C2-N2-C7	4.31	129.04	122.90
3	K	4	MAN	C1-O5-C5	4.30	118.02	112.19
2	L	1	NAG	C2-N2-C7	4.23	128.92	122.90
2	L	2	NAG	C2-N2-C7	4.23	128.92	122.90
2	I	2	NAG	C2-N2-C7	4.23	128.92	122.90
2	F	2	NAG	C2-N2-C7	4.19	128.86	122.90
2	J	1	NAG	C1-O5-C5	4.17	117.84	112.19
3	E	4	MAN	C1-O5-C5	3.98	117.58	112.19
3	H	4	MAN	C1-O5-C5	3.93	117.51	112.19
2	G	1	NAG	C1-O5-C5	3.84	117.39	112.19
2	D	1	NAG	C1-O5-C5	3.38	116.78	112.19
3	K	3	BMA	C2-C3-C4	3.03	116.14	110.89
3	H	3	BMA	C2-C3-C4	3.01	116.10	110.89
3	E	3	BMA	C2-C3-C4	2.93	115.97	110.89
3	K	3	BMA	C3-C4-C5	2.86	115.34	110.24
3	H	3	BMA	C3-C4-C5	2.65	114.97	110.24
3	E	3	BMA	C3-C4-C5	2.46	114.62	110.24
2	J	1	NAG	O4-C4-C5	2.27	114.92	109.30
3	K	1	NAG	C1-O5-C5	2.22	115.20	112.19
2	J	2	NAG	O5-C1-C2	-2.22	107.78	111.29
3	K	3	BMA	O4-C4-C3	-2.21	105.23	110.35
3	H	3	BMA	O4-C4-C3	-2.15	105.37	110.35
3	K	3	BMA	O3-C3-C2	-2.11	105.96	109.99
2	I	1	NAG	O5-C1-C2	-2.07	108.02	111.29
2	F	2	NAG	O7-C7-N2	2.05	125.72	121.95
2	D	1	NAG	O4-C4-C5	2.03	114.34	109.30
2	L	2	NAG	O7-C7-N2	2.02	125.66	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-O5-C5	2.01	114.91	112.19
2	F	1	NAG	O5-C1-C2	-2.01	108.12	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

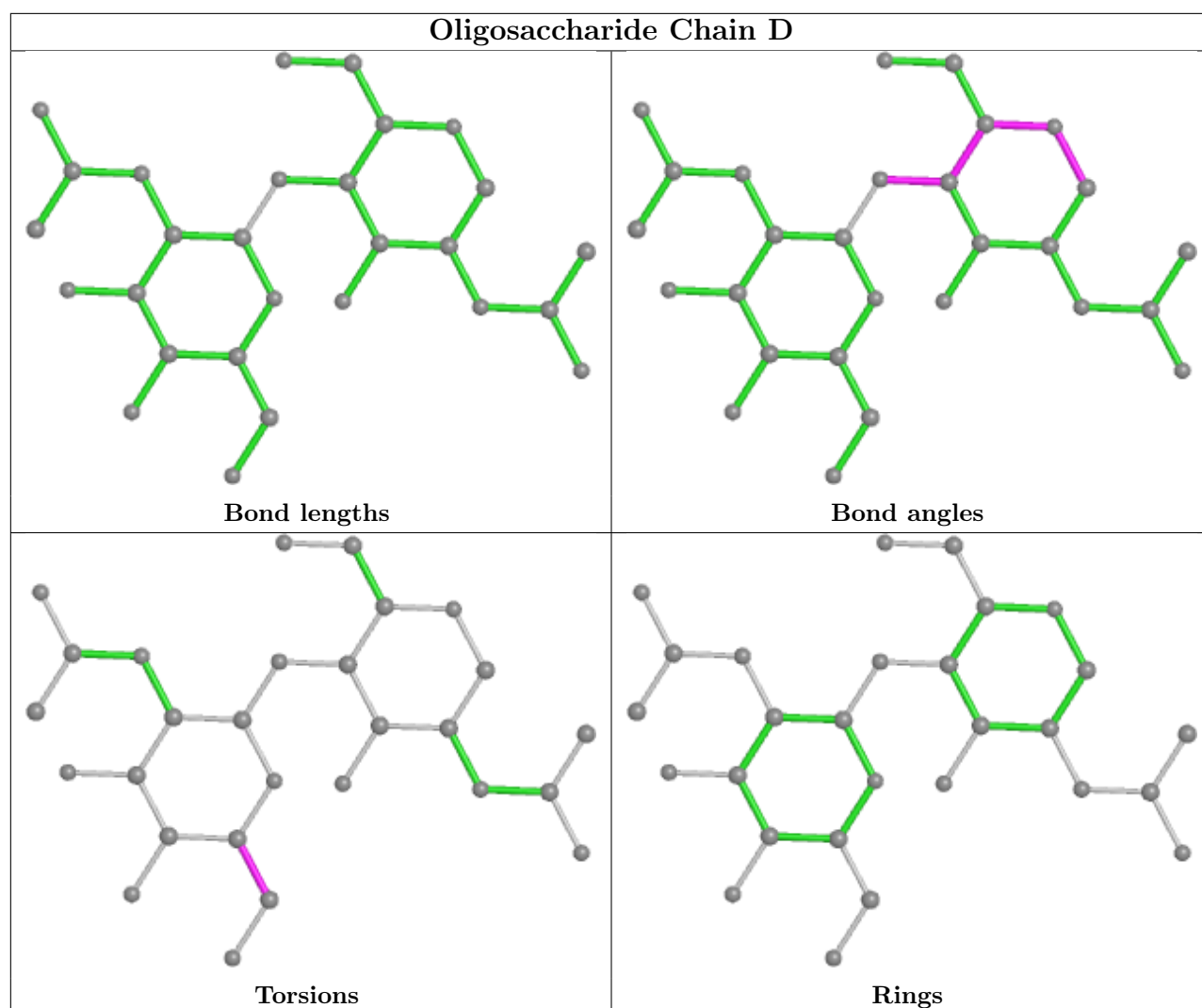
Mol	Chain	Res	Type	Atoms
3	E	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
3	K	4	MAN	C4-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	I	1	NAG	C3-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	F	1	NAG	C1-C2-N2-C7

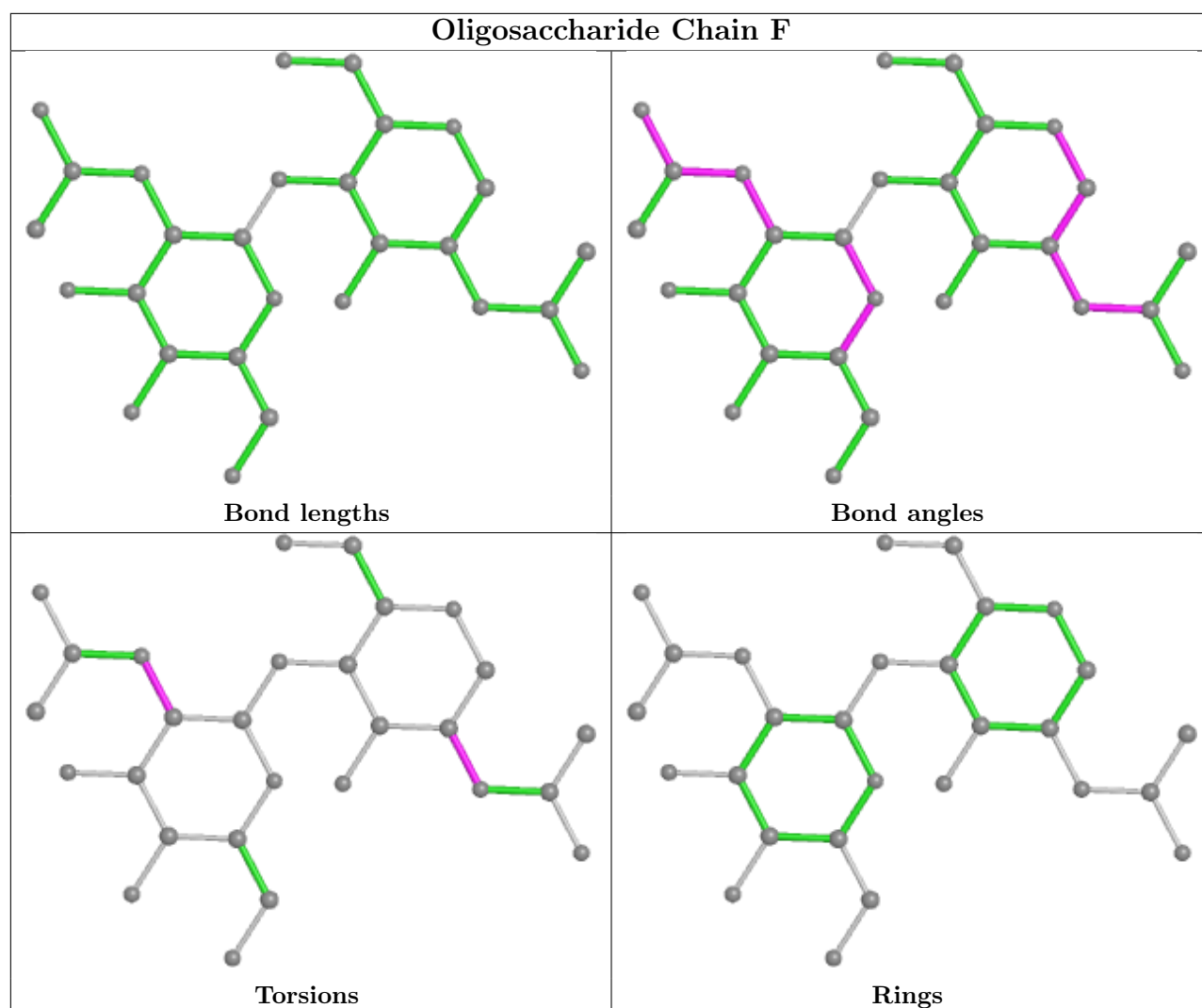
All (2) ring outliers are listed below:

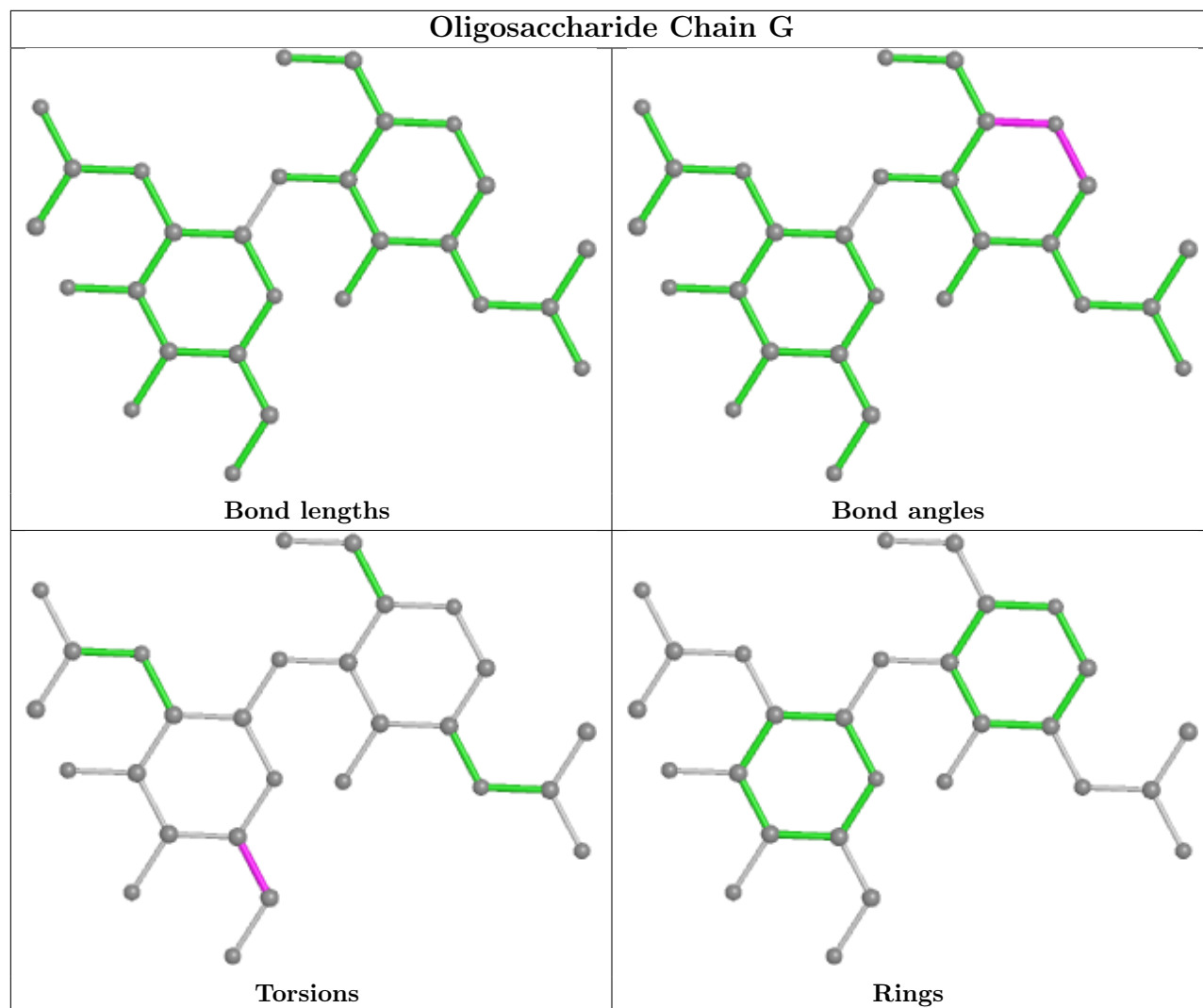
Mol	Chain	Res	Type	Atoms
3	H	4	MAN	C1-C2-C3-C4-C5-O5
3	K	4	MAN	C1-C2-C3-C4-C5-O5

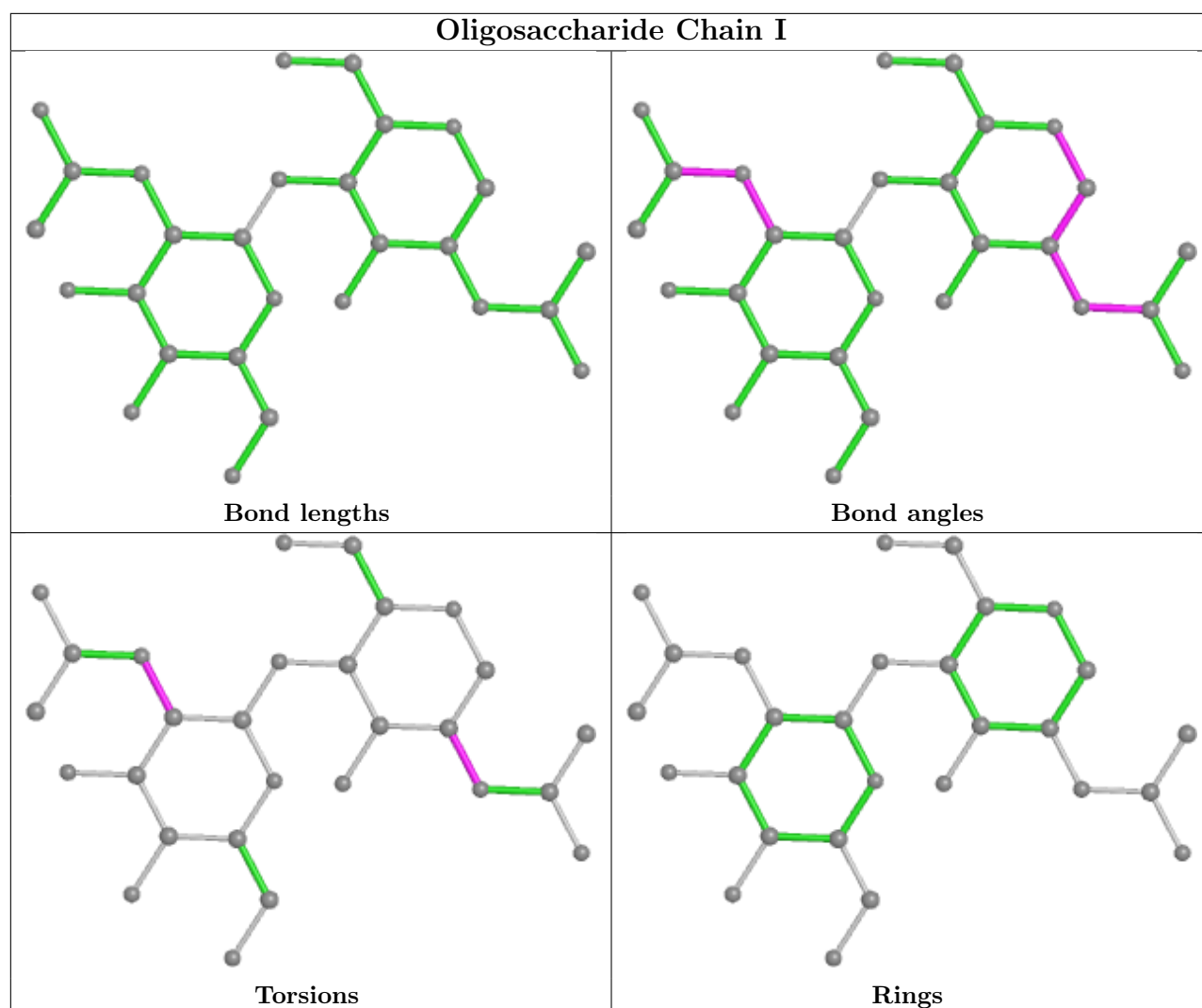
No monomer is involved in short contacts.

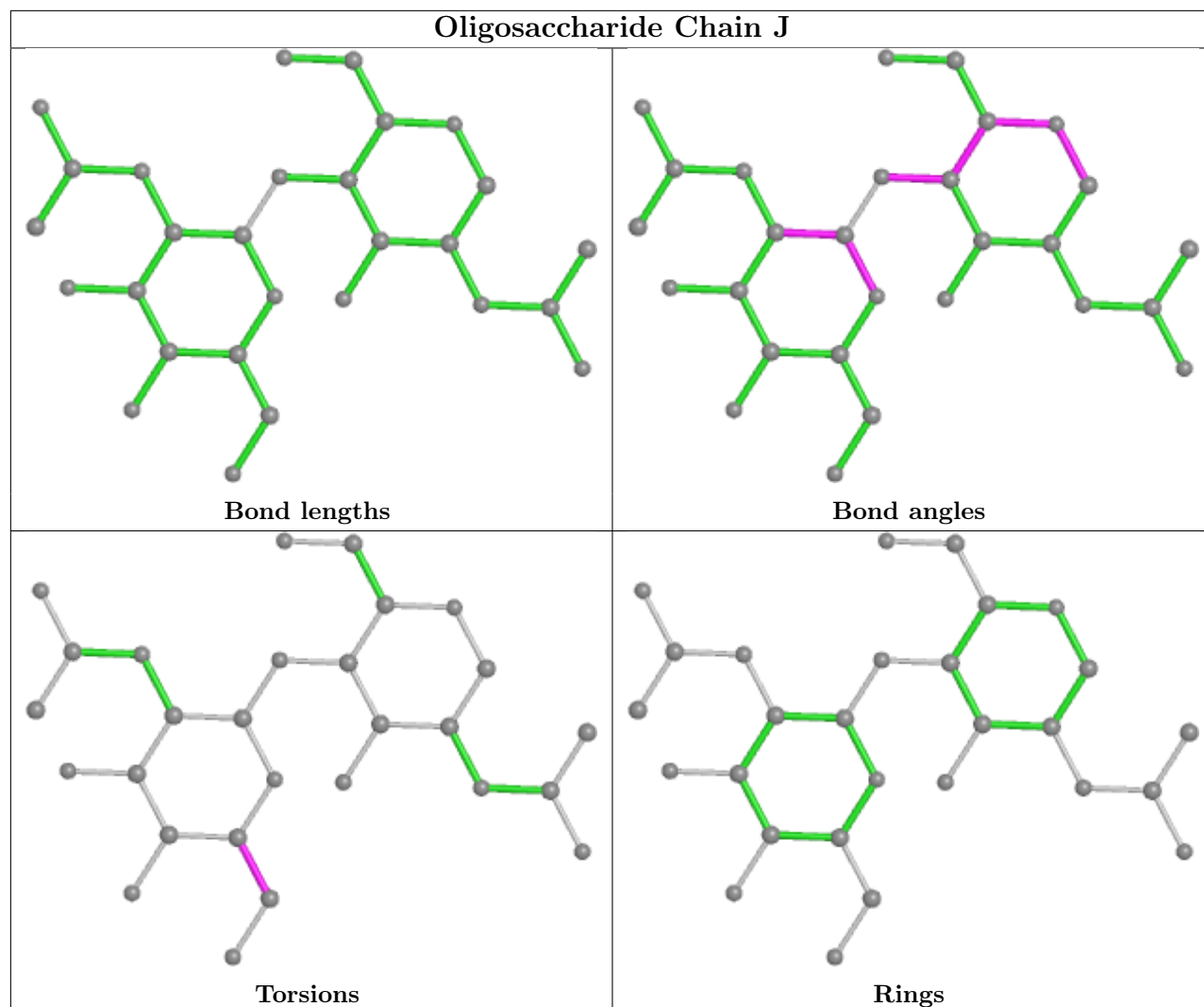
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

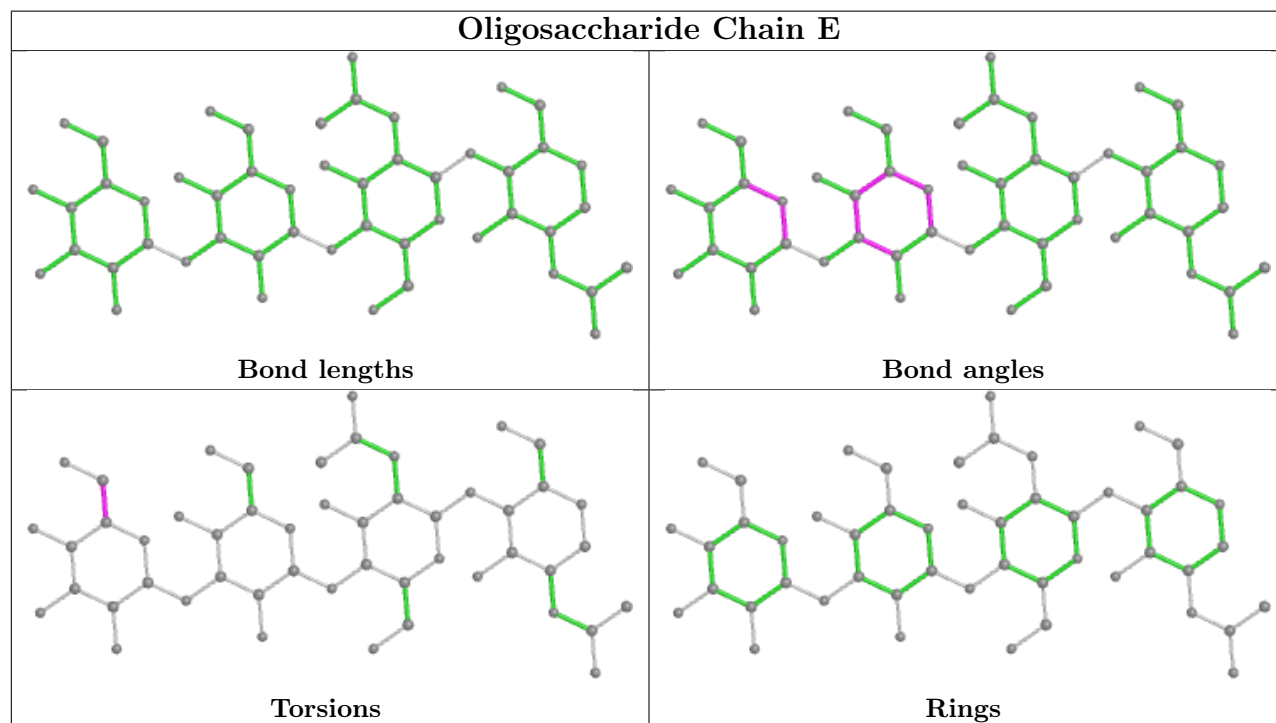
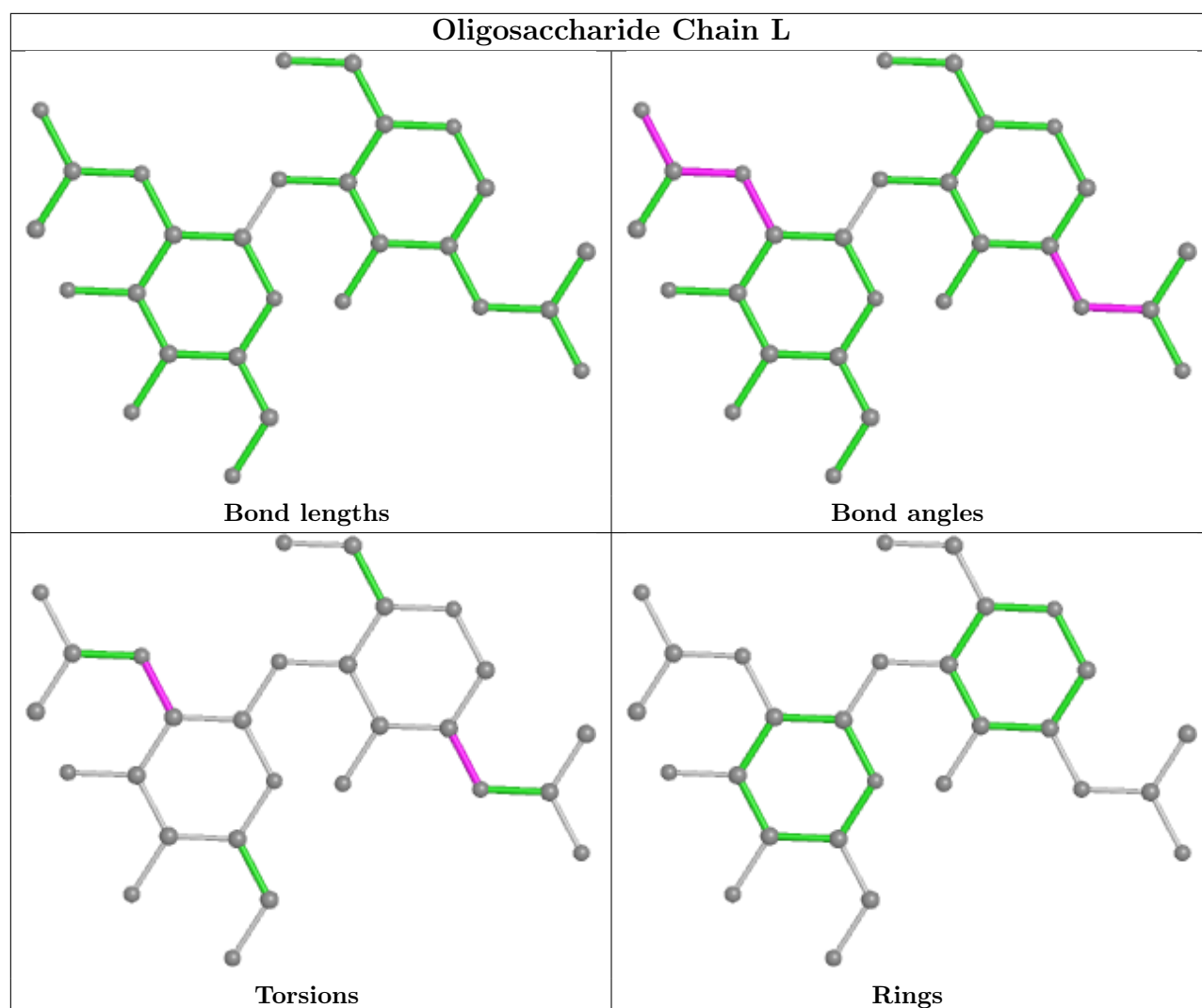


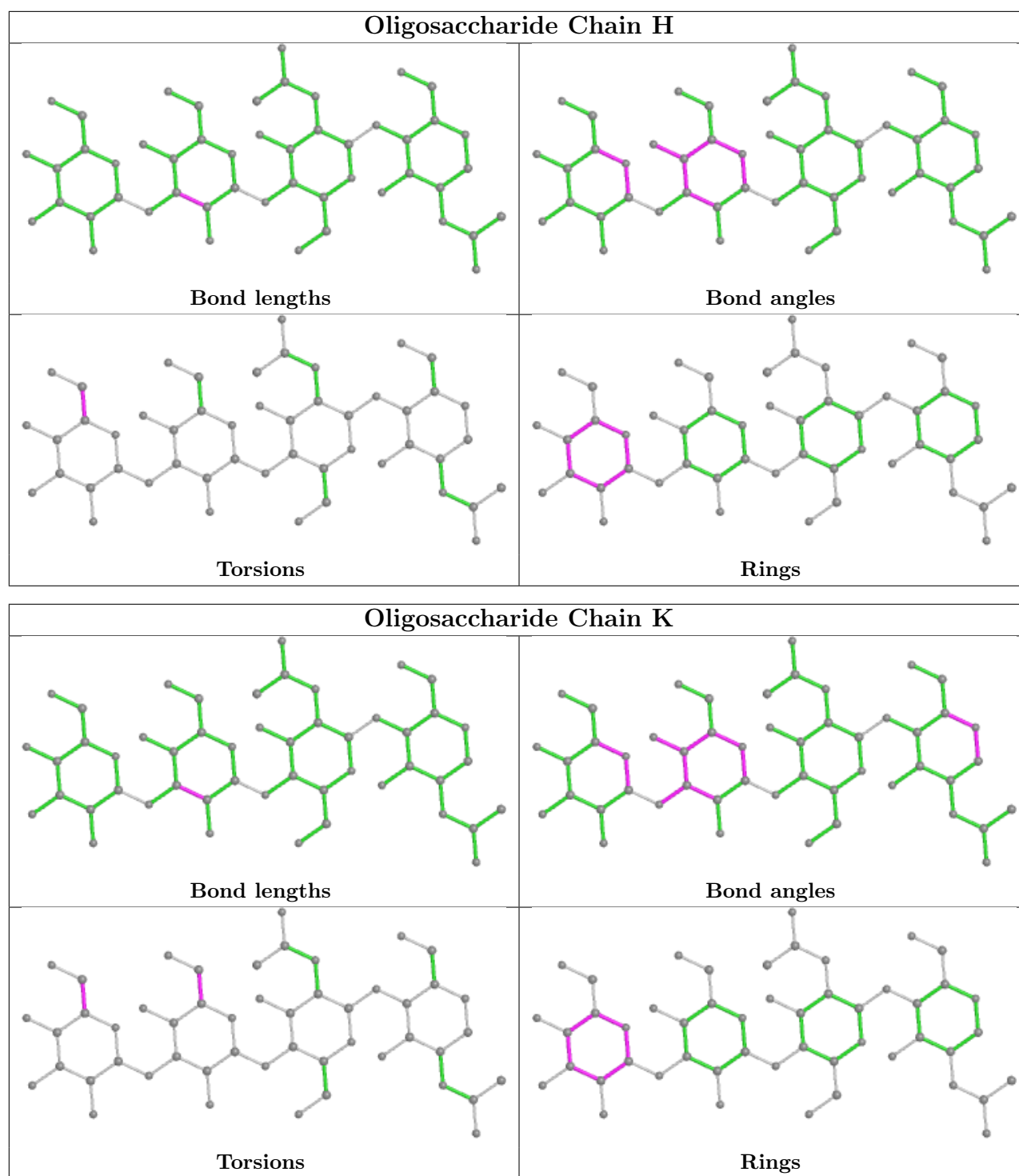












5.6 Ligand geometry [i](#)

42 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	$\# Z > 2$
4	NAG	C	1308	-	14,14,15	0.73	0	17,19,21	0.82	0
4	NAG	A	1309	1	14,14,15	0.72	0	17,19,21	1.59	2 (11%)
4	NAG	A	1307	-	14,14,15	0.69	0	17,19,21	1.12	2 (11%)
4	NAG	C	1313	1	14,14,15	0.69	0	17,19,21	1.50	2 (11%)
5	EIC	C	1301	-	19,19,19	0.58	0	19,19,19	0.55	0
4	NAG	B	1310	1	14,14,15	0.73	0	17,19,21	1.48	3 (17%)
4	NAG	A	1312	1	14,14,15	0.73	0	17,19,21	0.85	0
4	NAG	C	1304	-	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	C	1305	1	14,14,15	0.70	0	17,19,21	0.84	0
4	NAG	C	1310	1	14,14,15	0.69	0	17,19,21	0.97	1 (5%)
4	NAG	B	1308	-	14,14,15	0.71	0	17,19,21	0.87	0
4	NAG	C	1312	1	14,14,15	0.72	0	17,19,21	0.91	0
5	EIC	B	1301	-	19,19,19	0.60	0	19,19,19	0.56	0
4	NAG	B	1306	1	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
4	NAG	B	1309	1	14,14,15	0.69	0	17,19,21	0.88	0
4	NAG	C	1306	-	14,14,15	0.69	0	17,19,21	0.82	0
4	NAG	A	1308	1	14,14,15	0.69	0	17,19,21	0.87	0
4	NAG	A	1304	-	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	C	1314	1	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
4	NAG	A	1301	-	14,14,15	0.73	0	17,19,21	0.83	0
5	EIC	C	1302	-	19,19,19	0.59	0	19,19,19	0.58	0
4	NAG	B	1305	-	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	A	1306	-	14,14,15	0.72	0	17,19,21	0.86	0
4	NAG	B	1312	1	14,14,15	0.69	0	17,19,21	1.46	1 (5%)
4	NAG	B	1314	1	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
4	NAG	B	1303	-	14,14,15	0.71	0	17,19,21	0.82	0
4	NAG	B	1302	-	14,14,15	0.71	0	17,19,21	0.86	0
4	NAG	B	1313	1	14,14,15	0.71	0	17,19,21	0.91	0
4	NAG	C	1307	1	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
4	NAG	A	1303	1	14,14,15	0.72	0	17,19,21	0.87	0
4	NAG	C	1315	1	14,14,15	0.73	0	17,19,21	0.83	0
4	NAG	A	1302	-	14,14,15	0.70	0	17,19,21	0.82	0
4	NAG	A	1313	-	14,14,15	0.71	0	17,19,21	0.80	0
4	NAG	A	1305	1	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
4	NAG	C	1311	1	14,14,15	0.73	0	17,19,21	1.54	2 (11%)
4	NAG	B	1311	1	14,14,15	0.72	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1309	-	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
4	NAG	B	1304	1	14,14,15	0.73	0	17,19,21	0.89	0
4	NAG	A	1311	1	14,14,15	0.70	0	17,19,21	1.45	1 (5%)
4	NAG	C	1303	-	14,14,15	0.72	0	17,19,21	0.85	0
4	NAG	B	1307	-	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	A	1310	1	14,14,15	0.73	0	17,19,21	0.84	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
4	NAG	C	1308	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1307	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	1/6/23/26	0/1/1/1
5	EIC	C	1301	-	-	2/17/17/17	-
4	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
5	EIC	B	1301	-	-	6/17/17/17	-
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	1/6/23/26	0/1/1/1
5	EIC	C	1302	-	-	3/17/17/17	-
4	NAG	B	1305	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1314	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1313	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1309	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1313	NAG	C2-N2-C7	4.30	129.02	122.90
4	B	1312	NAG	C2-N2-C7	4.30	129.02	122.90
4	A	1309	NAG	C2-N2-C7	4.28	128.99	122.90
4	A	1311	NAG	C2-N2-C7	4.27	128.99	122.90
4	C	1311	NAG	C2-N2-C7	4.14	128.80	122.90
4	B	1310	NAG	C2-N2-C7	4.06	128.69	122.90
4	A	1309	NAG	C1-O5-C5	3.44	116.85	112.19
4	C	1311	NAG	C1-O5-C5	2.85	116.05	112.19
4	A	1307	NAG	C1-O5-C5	2.61	115.72	112.19
4	C	1310	NAG	O5-C1-C2	-2.40	107.51	111.29
4	B	1310	NAG	C1-O5-C5	2.38	115.41	112.19
4	C	1314	NAG	O5-C1-C2	-2.24	107.75	111.29
4	B	1306	NAG	C1-O5-C5	2.20	115.18	112.19
4	A	1307	NAG	O5-C1-C2	-2.18	107.85	111.29
4	C	1313	NAG	C1-O5-C5	2.12	115.07	112.19
4	C	1307	NAG	C1-O5-C5	2.11	115.05	112.19
4	C	1309	NAG	C1-O5-C5	2.10	115.04	112.19
4	A	1305	NAG	C1-O5-C5	2.09	115.02	112.19
4	B	1314	NAG	C1-O5-C5	2.06	114.98	112.19
4	B	1310	NAG	O7-C7-N2	2.02	125.66	121.95

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1301	EIC	C9-C10-C11-C12
4	A	1312	NAG	O5-C5-C6-O6
5	C	1302	EIC	C2-C3-C4-C5
5	C	1301	EIC	C6-C7-C8-C9
5	B	1301	EIC	C1-C2-C3-C4
5	B	1301	EIC	C4-C5-C6-C7
4	A	1310	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
5	C	1302	EIC	C3-C4-C5-C6
5	B	1301	EIC	C13-C14-C15-C16
4	A	1301	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
5	B	1301	EIC	C2-C3-C4-C5
4	A	1309	NAG	C3-C2-N2-C7
4	B	1310	NAG	C3-C2-N2-C7
4	C	1311	NAG	C3-C2-N2-C7
5	B	1301	EIC	O2-C1-C2-C3
5	B	1301	EIC	O1-C1-C2-C3
5	C	1302	EIC	C15-C16-C17-C18
4	A	1311	NAG	C3-C2-N2-C7
4	B	1312	NAG	C3-C2-N2-C7
4	C	1313	NAG	C3-C2-N2-C7
4	A	1312	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	A	1310	NAG	C4-C5-C6-O6

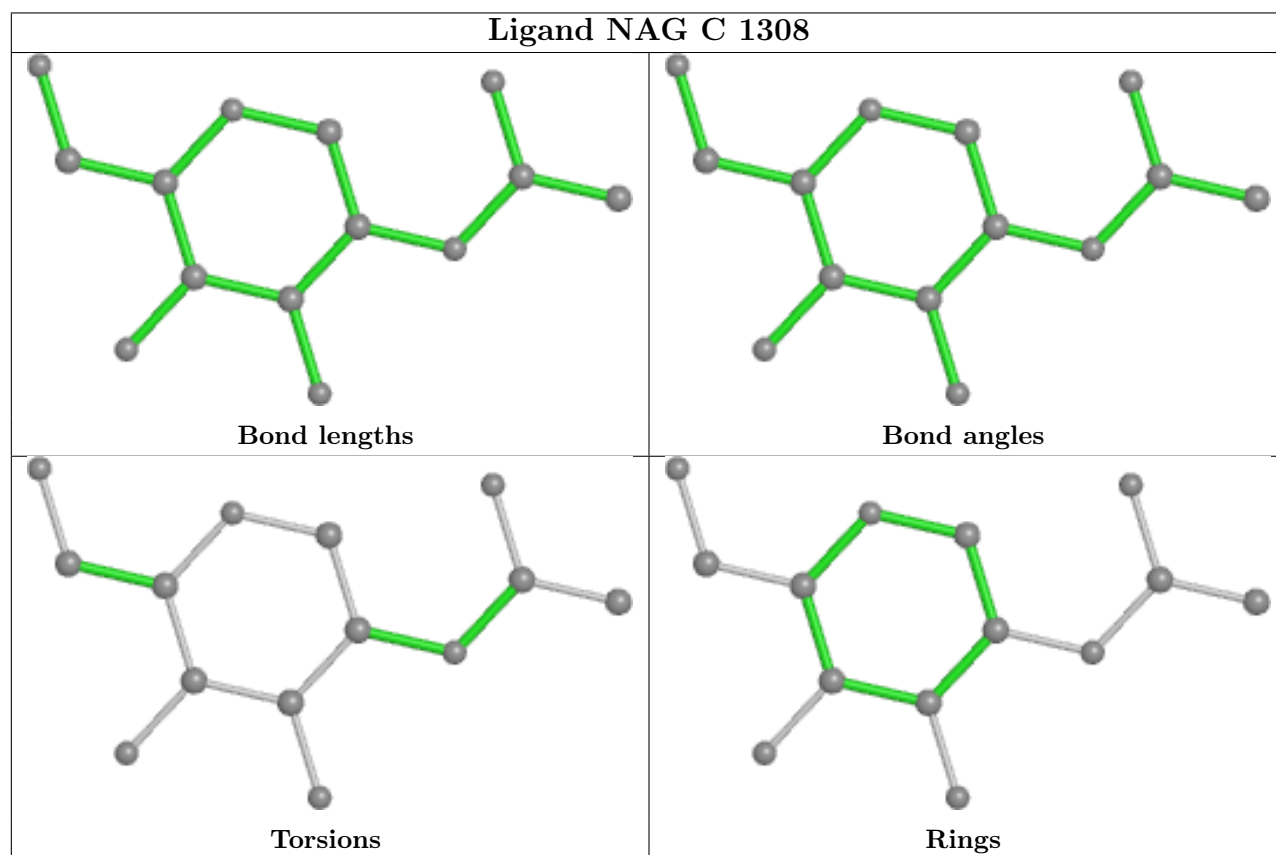
There are no ring outliers.

4 monomers are involved in 4 short contacts:

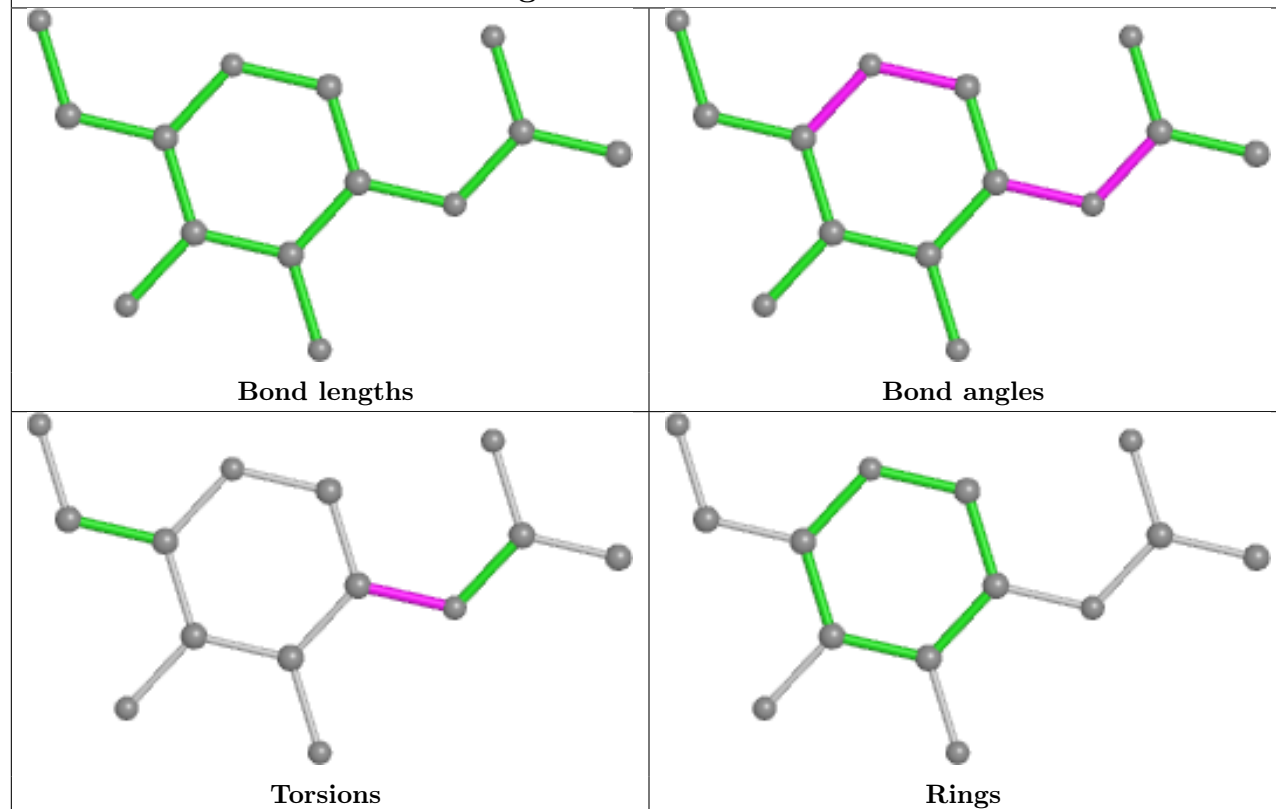
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1302	EIC	1	0
4	B	1302	NAG	1	0
4	A	1302	NAG	1	0
4	A	1310	NAG	1	0

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

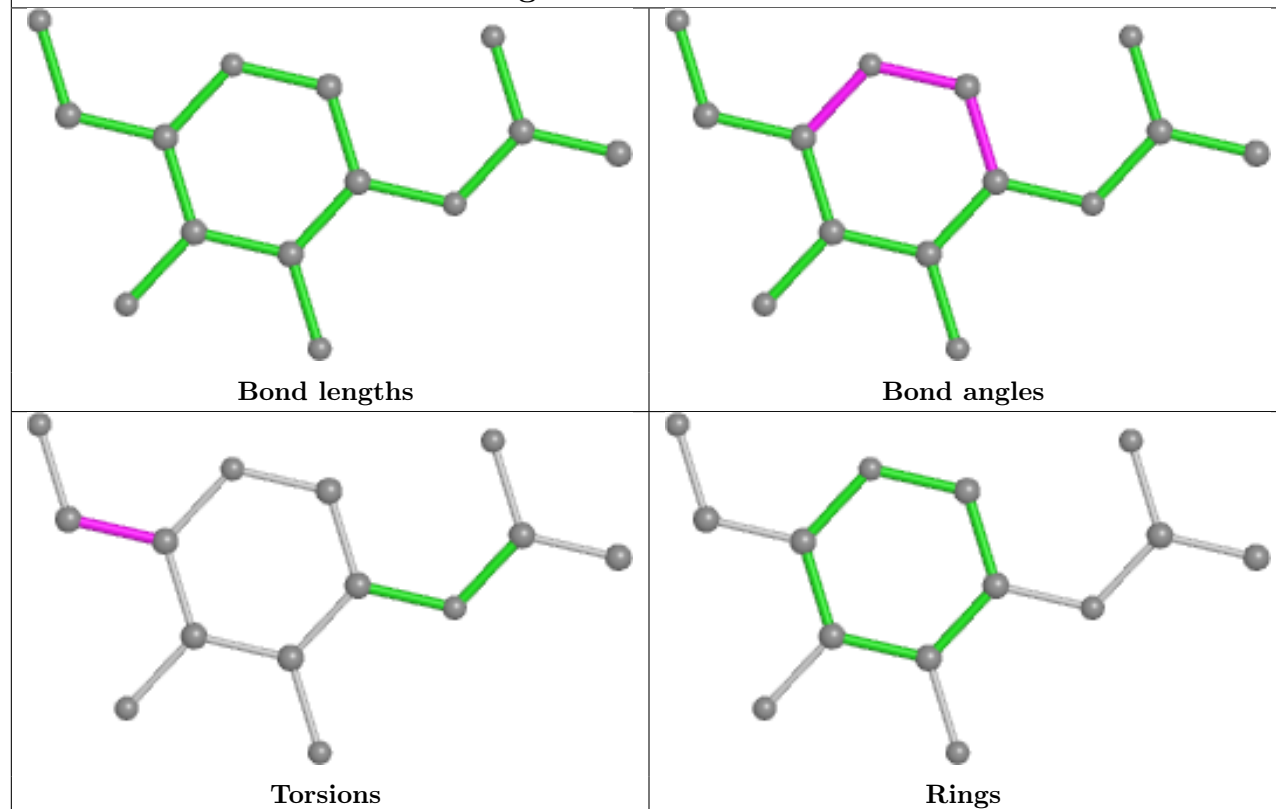
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

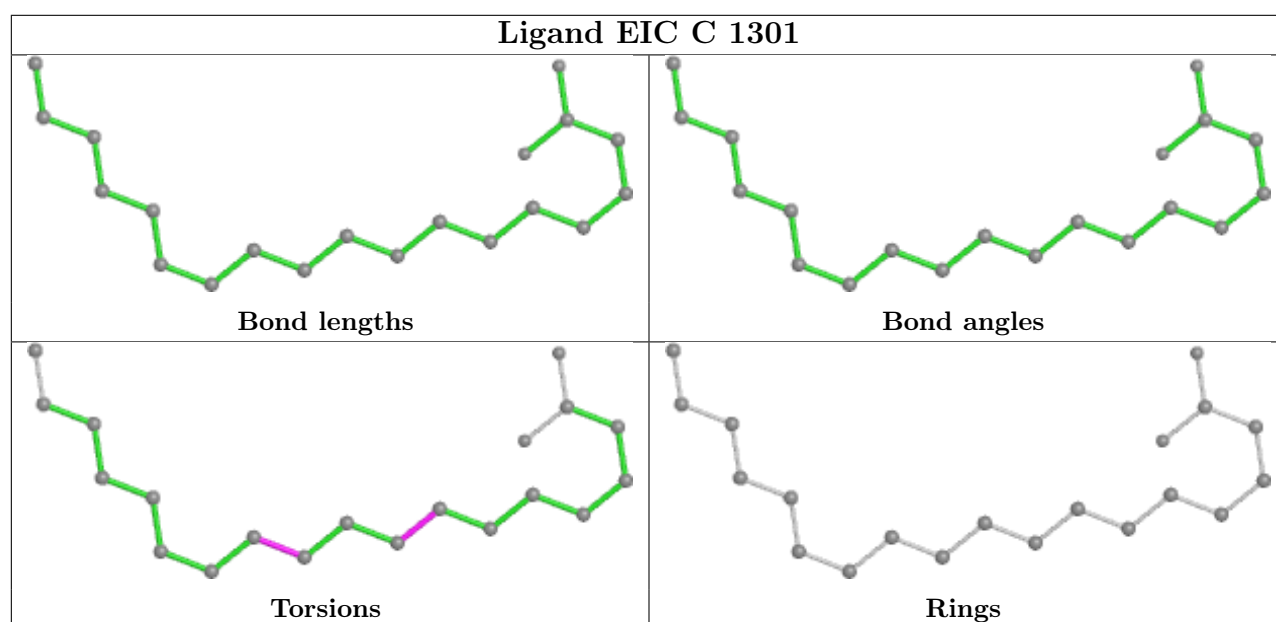
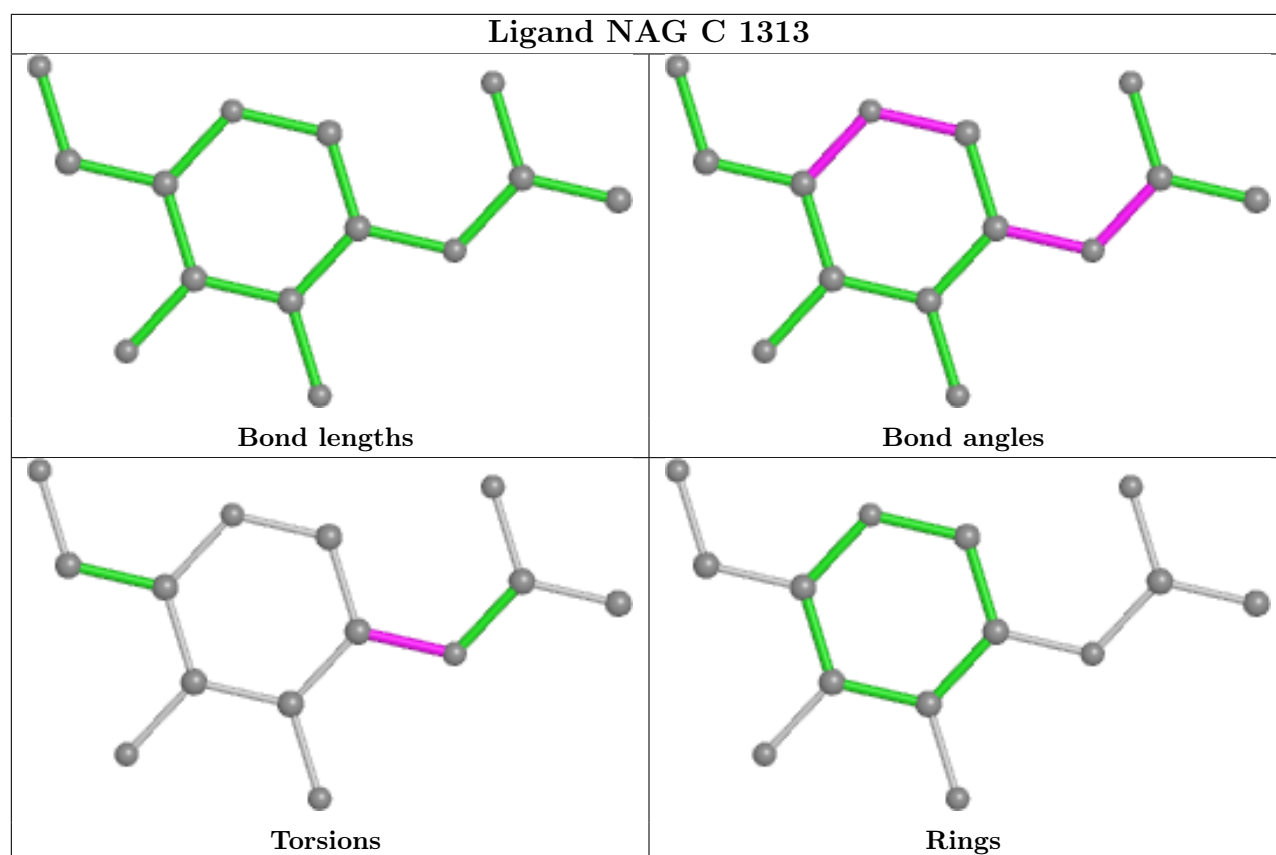


Ligand NAG A 1309

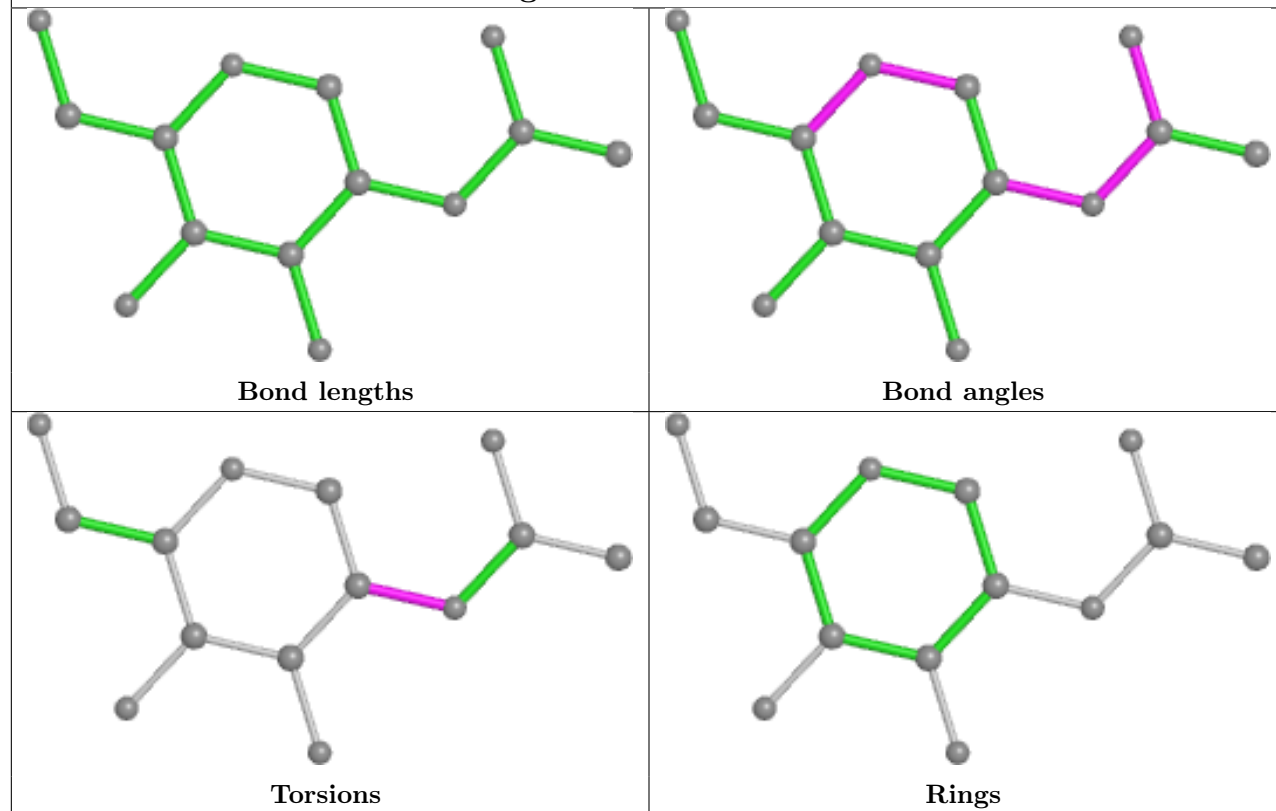


Ligand NAG A 1307

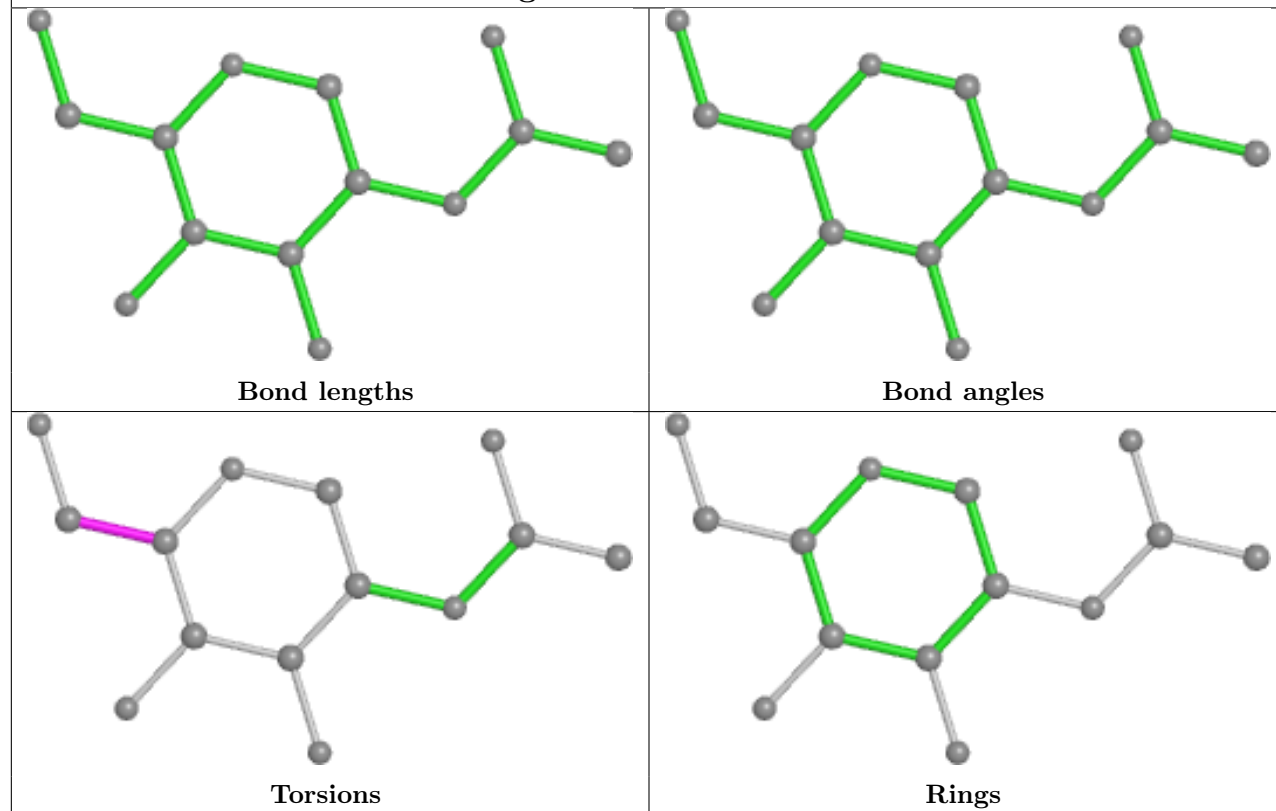


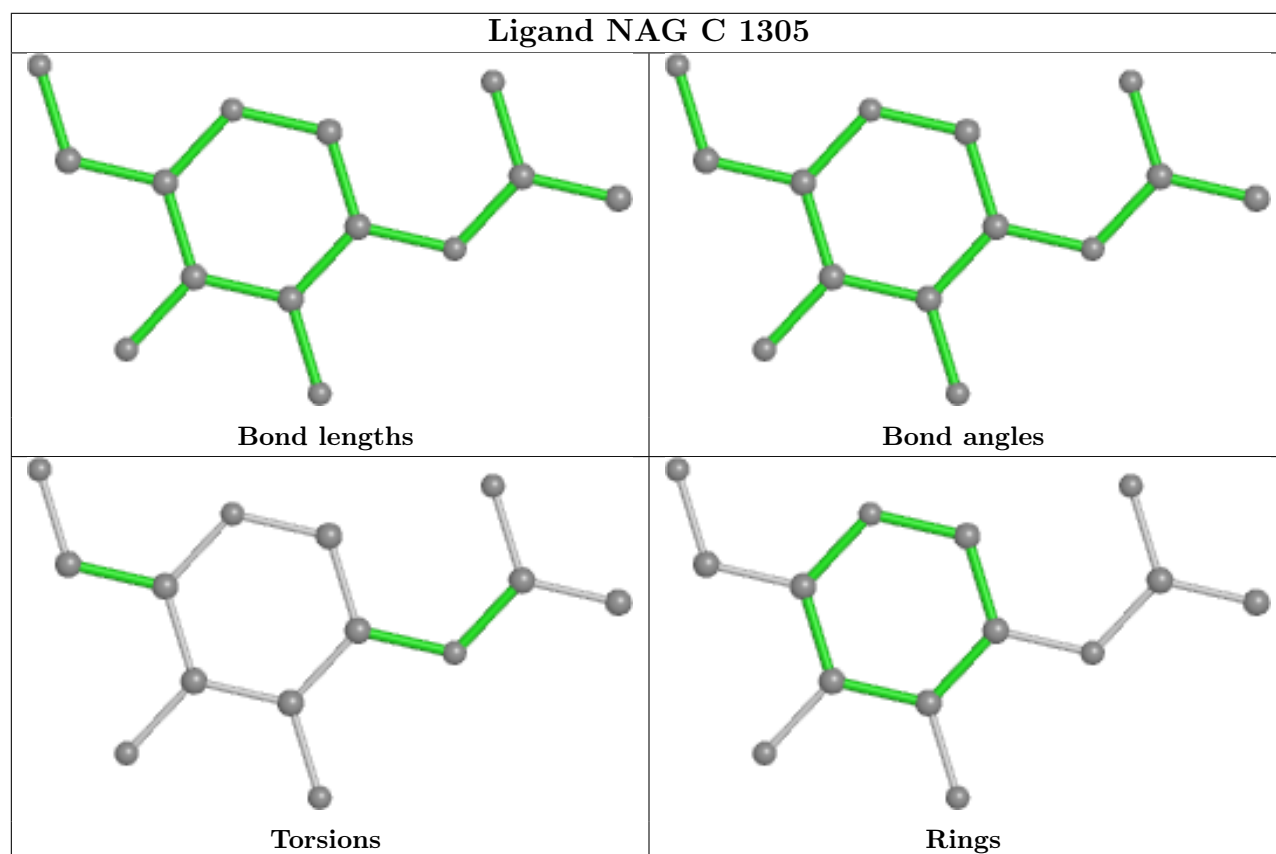
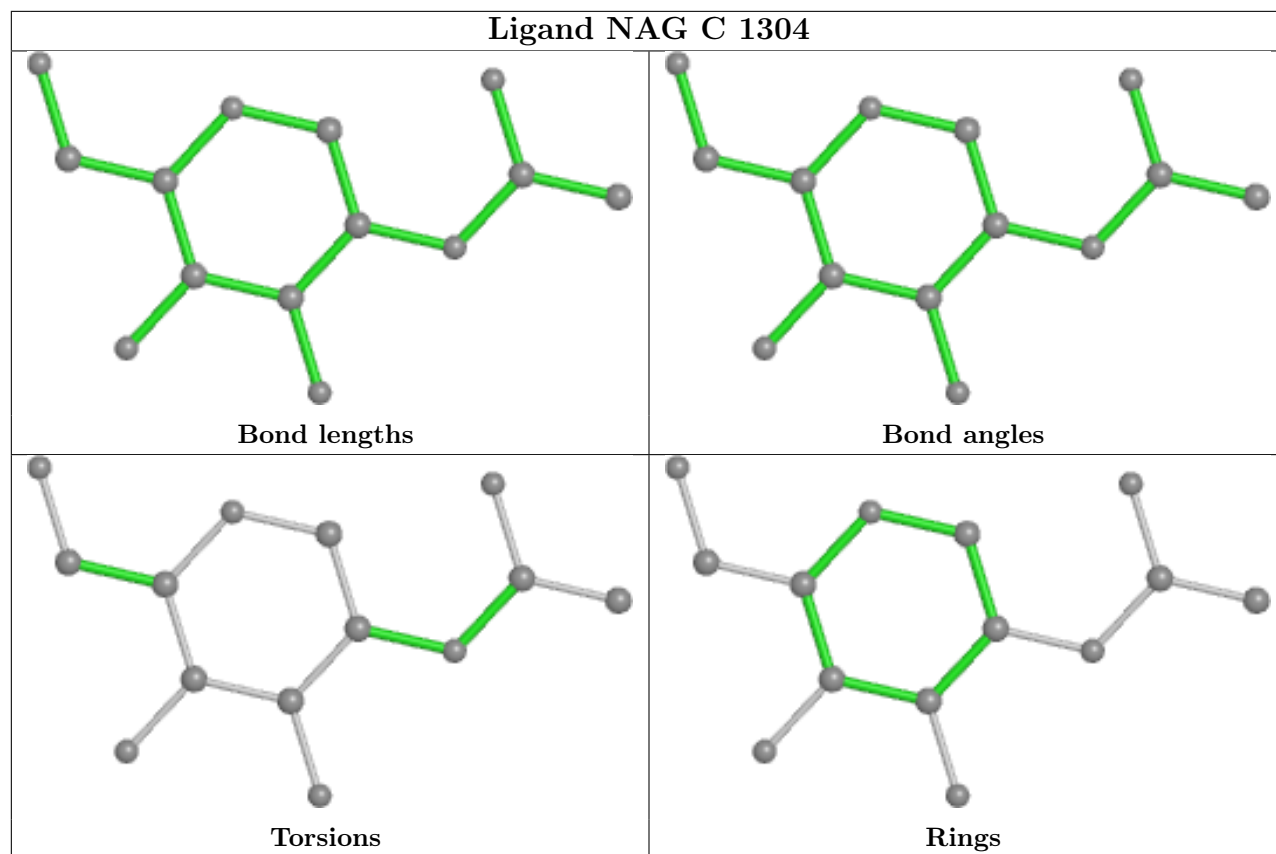


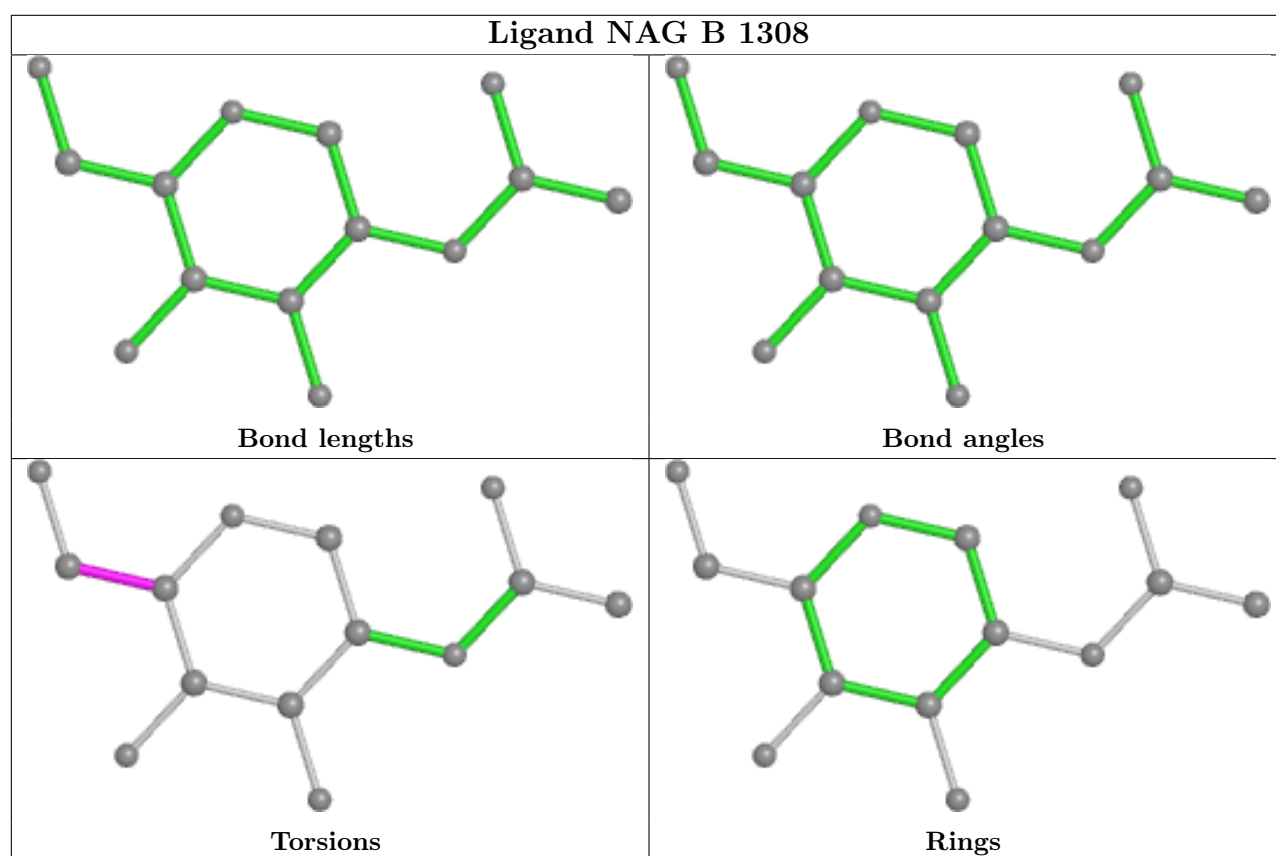
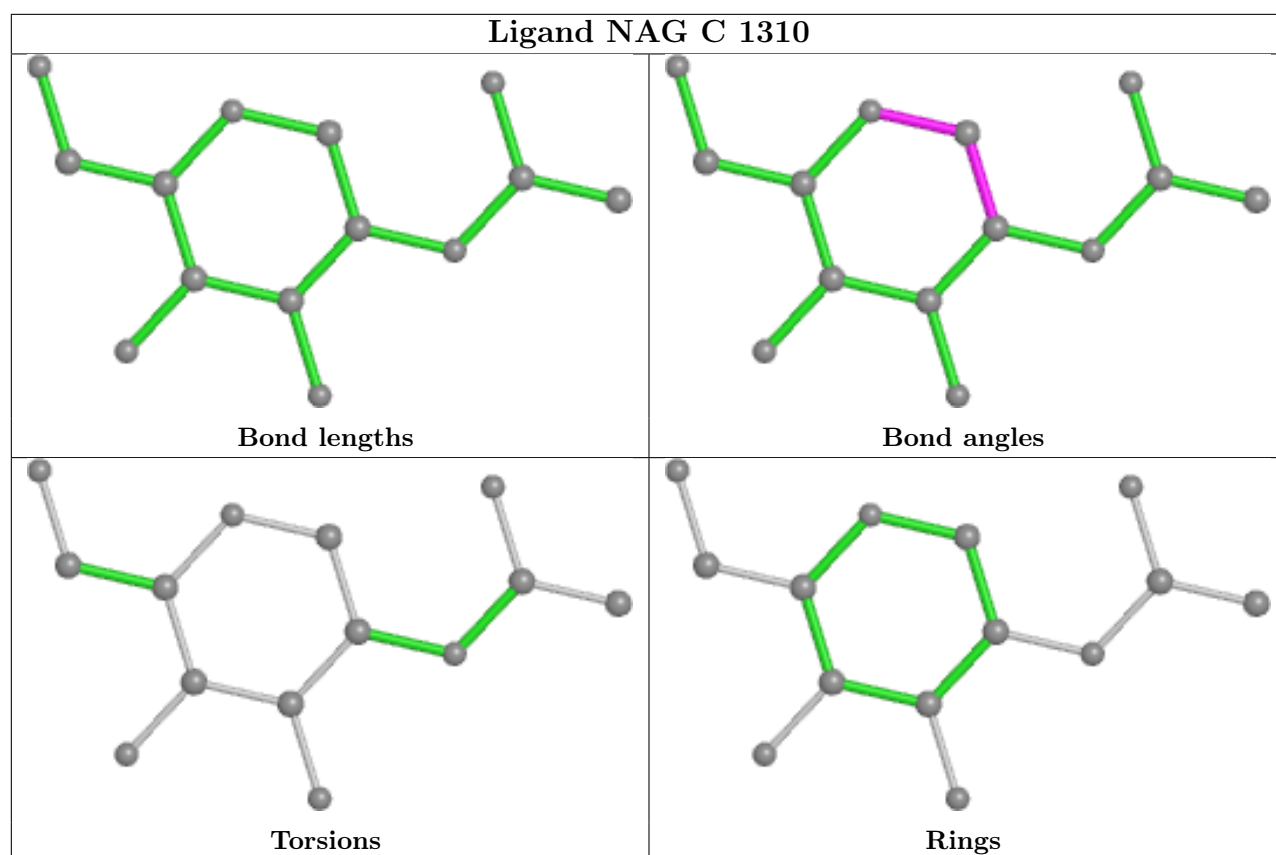
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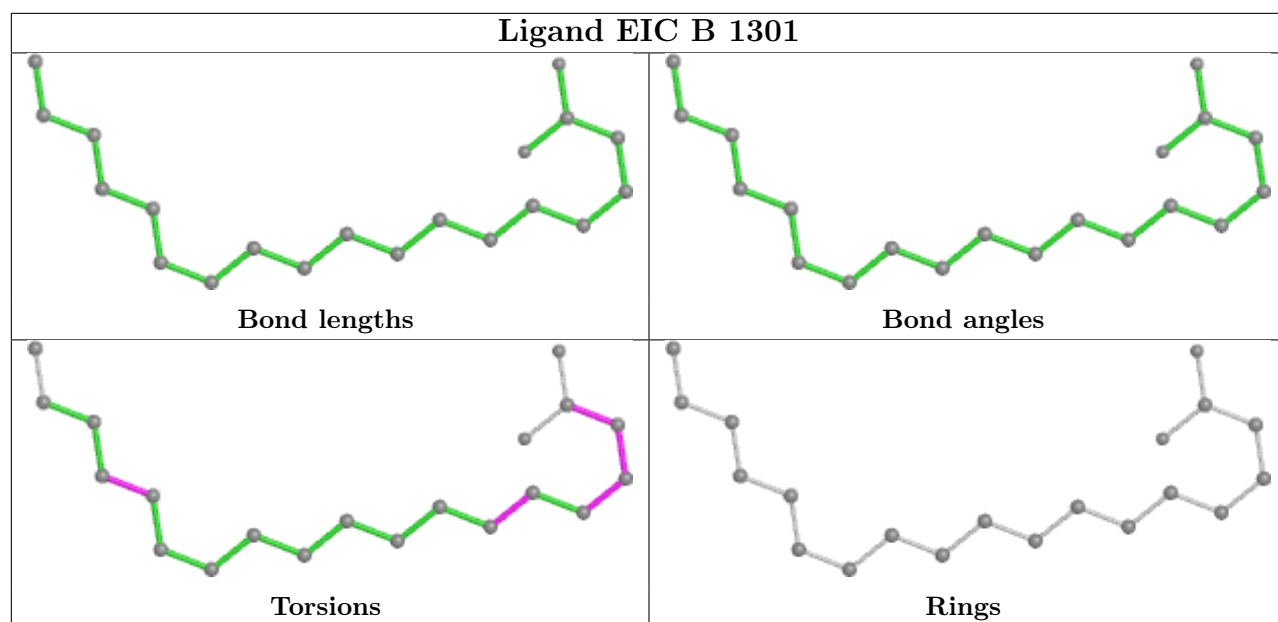
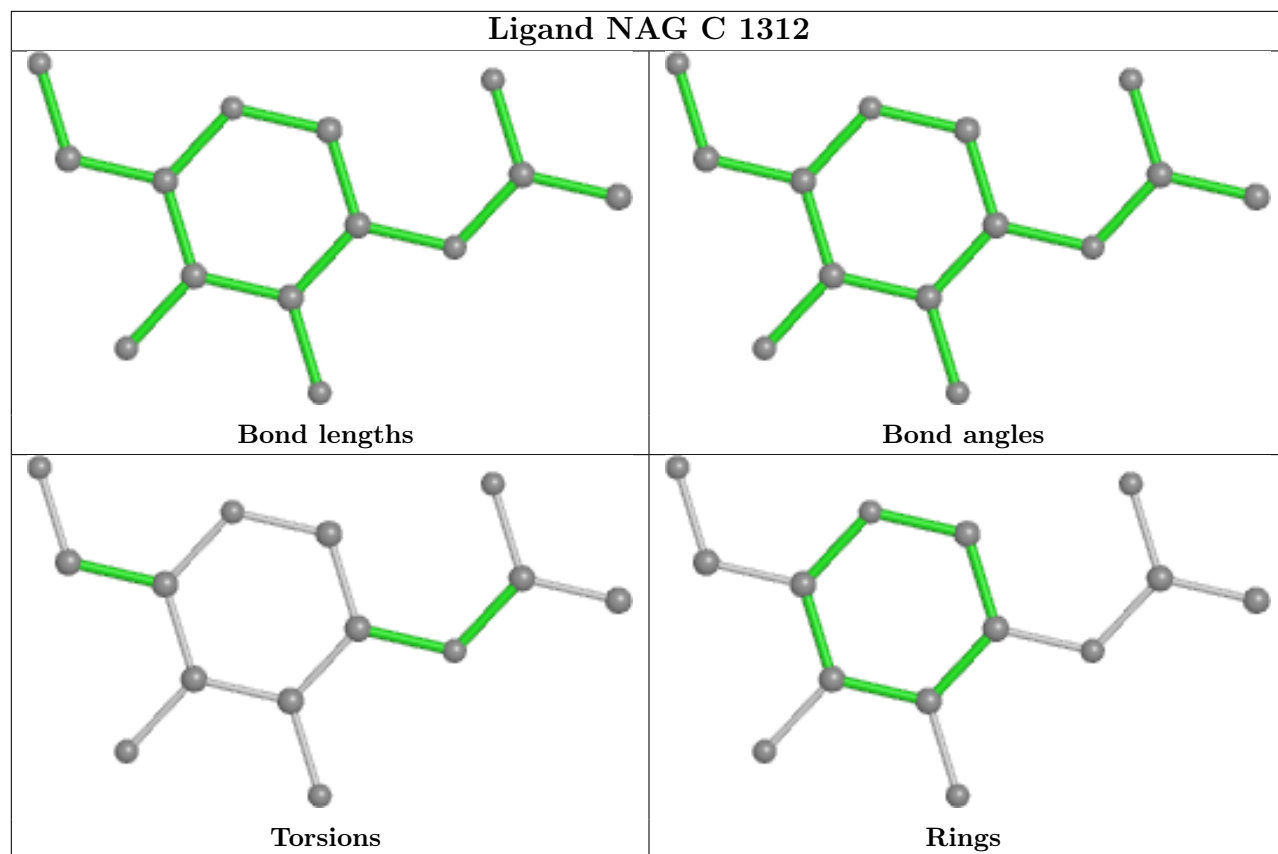


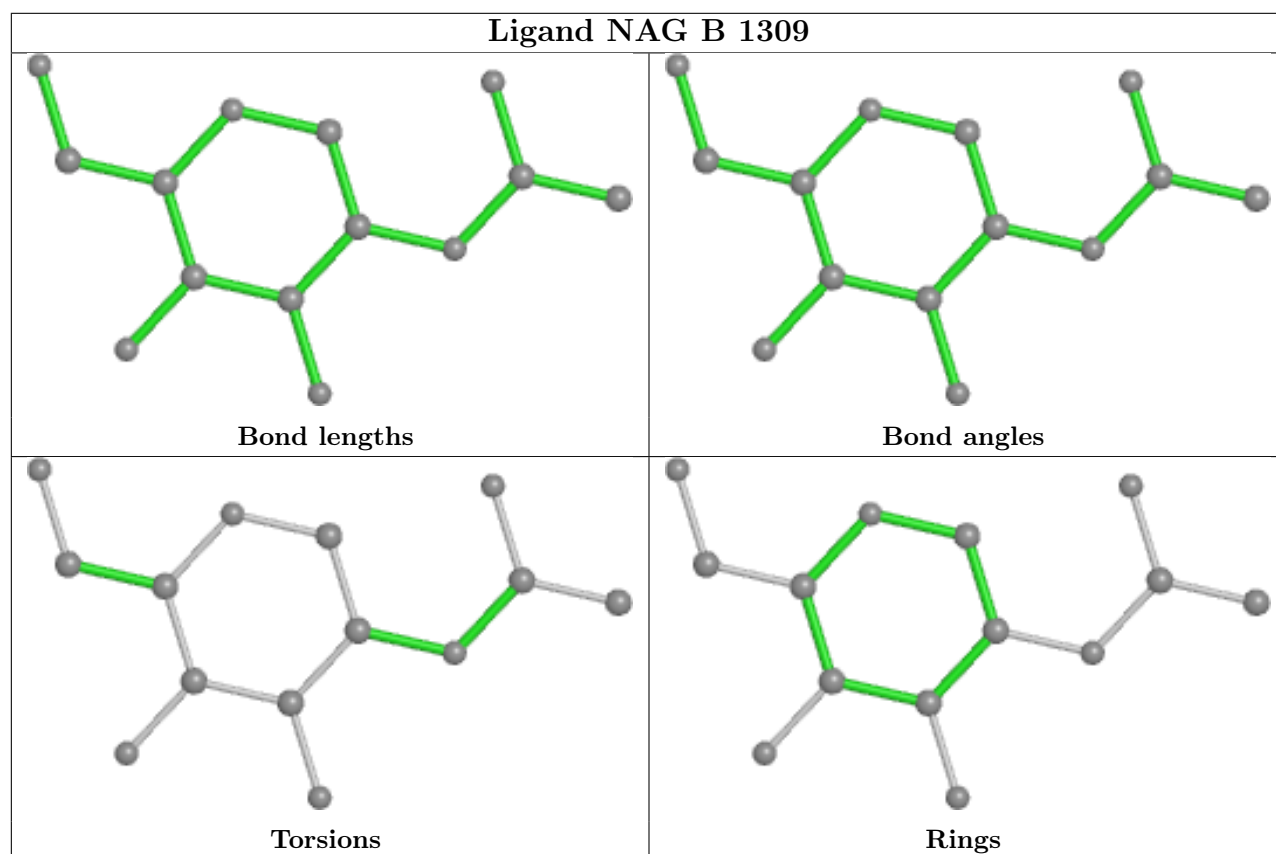
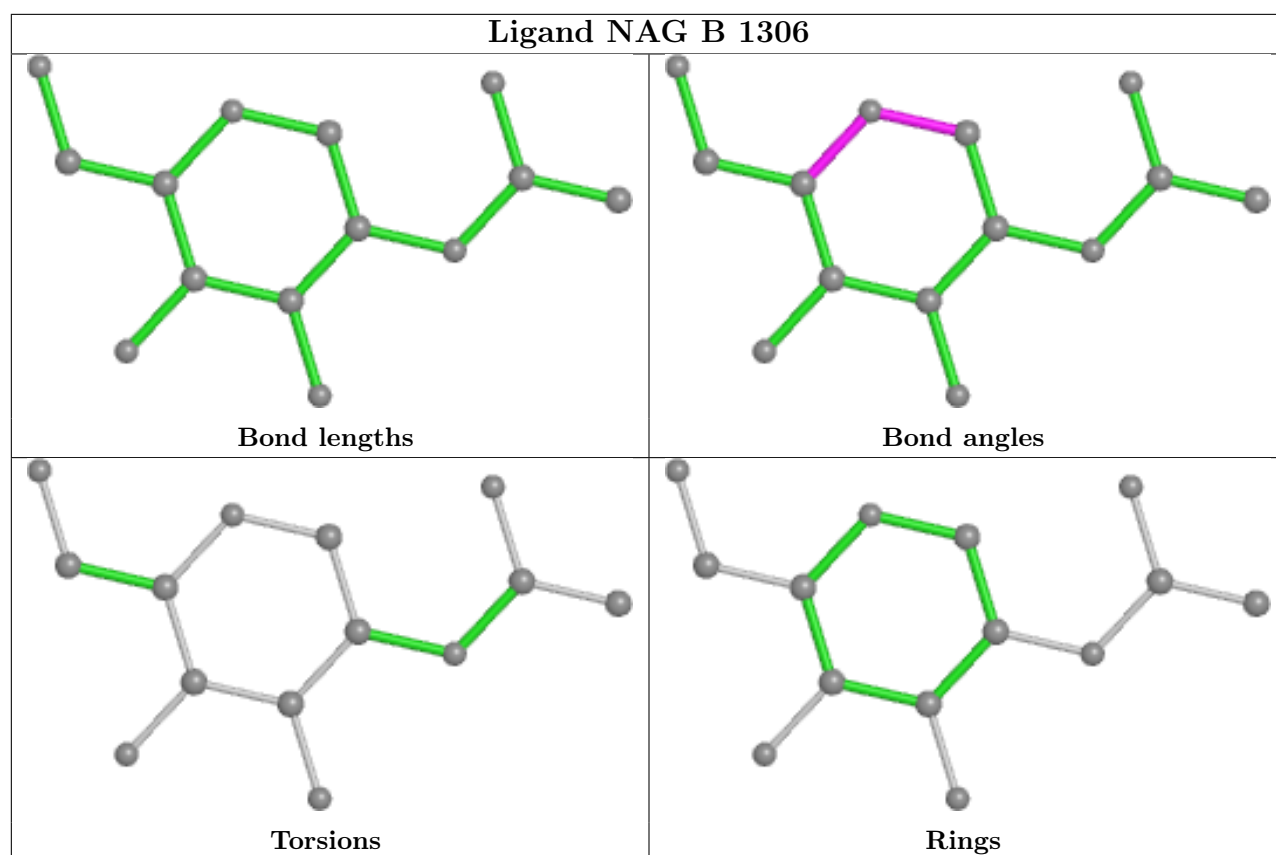
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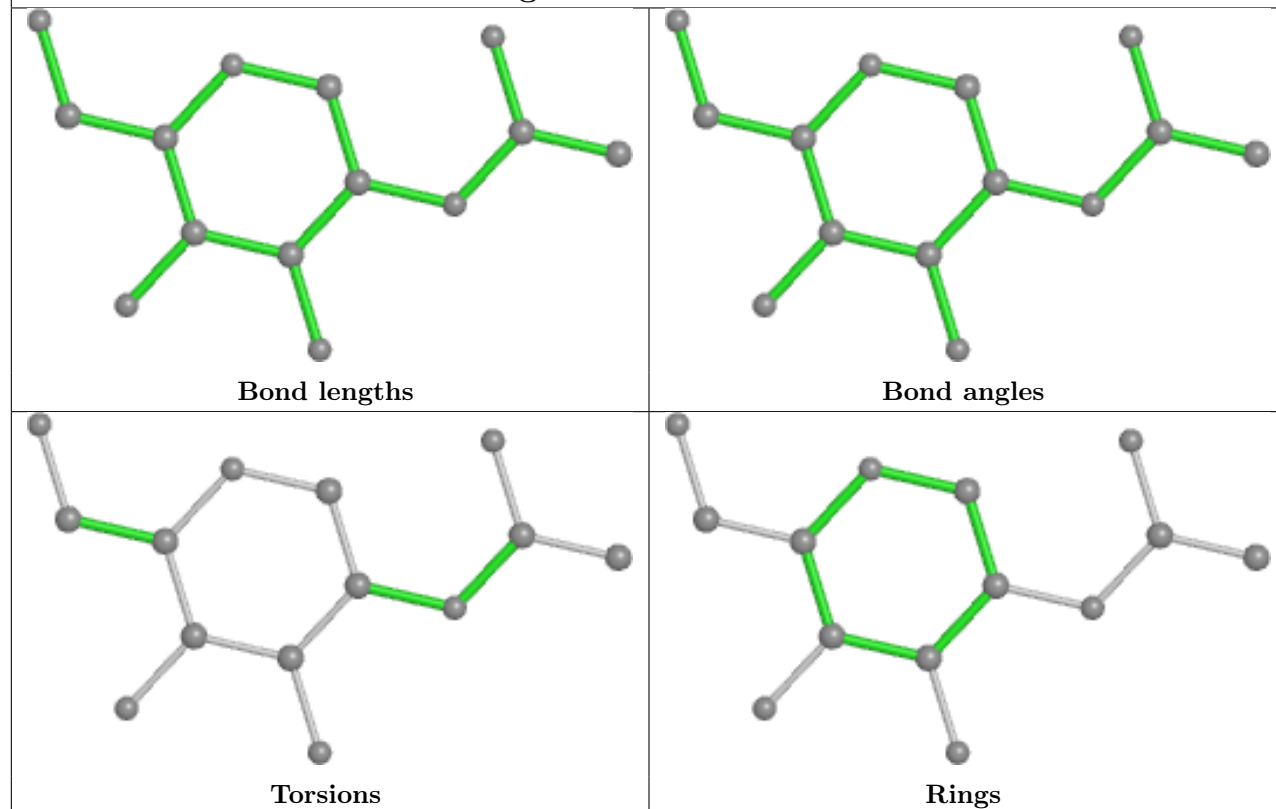




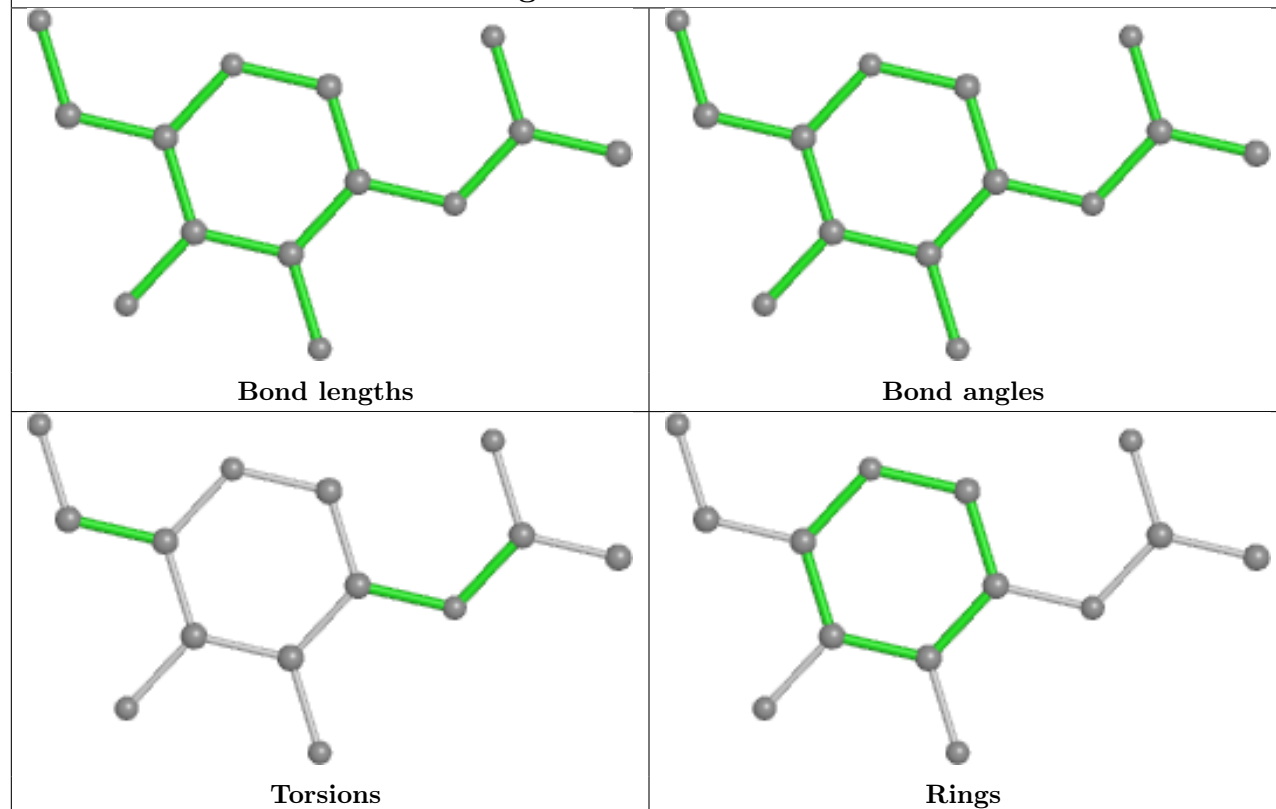




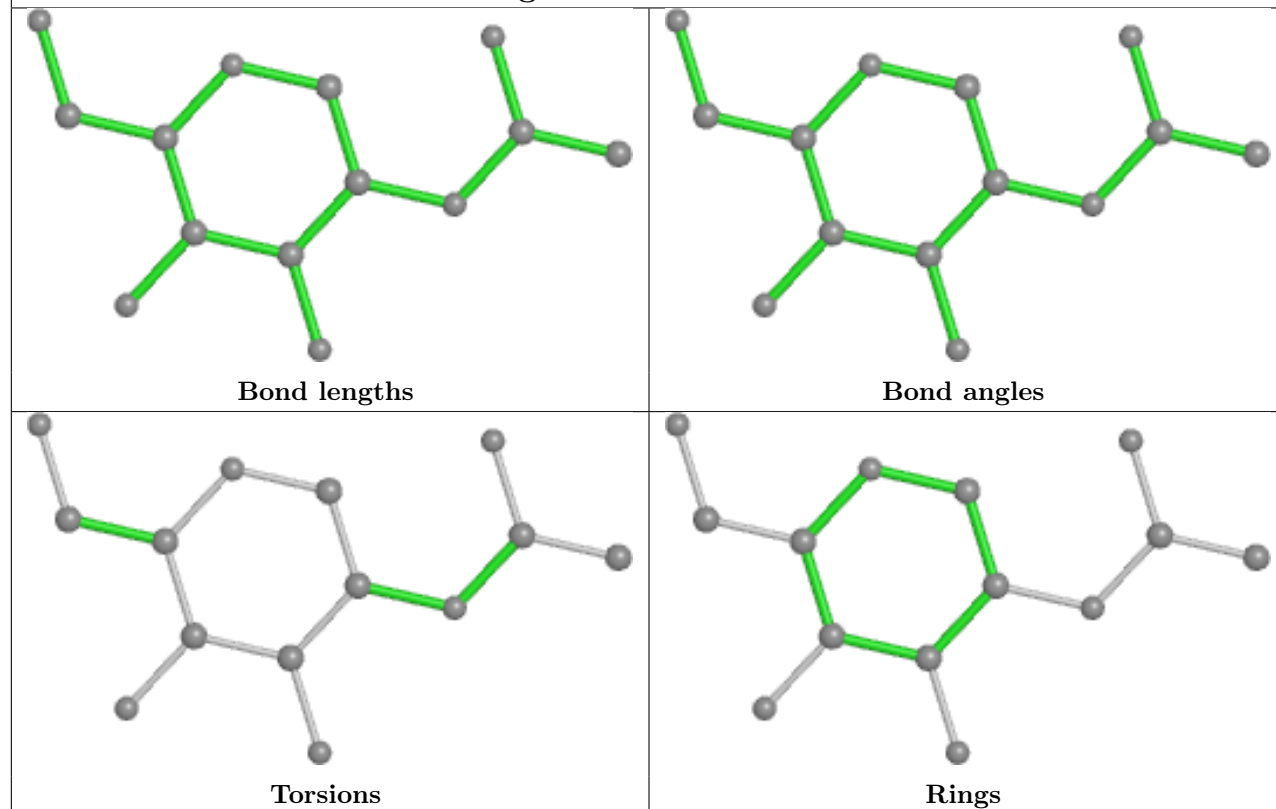
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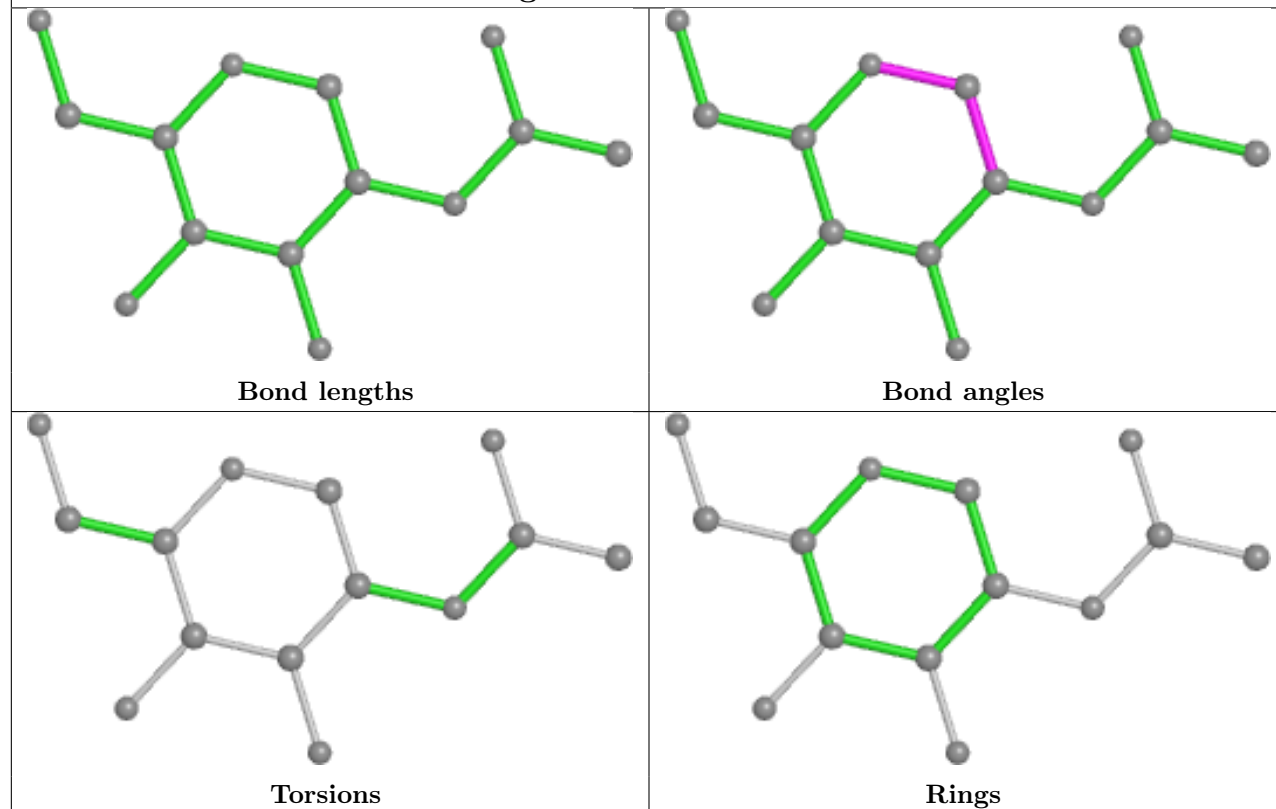
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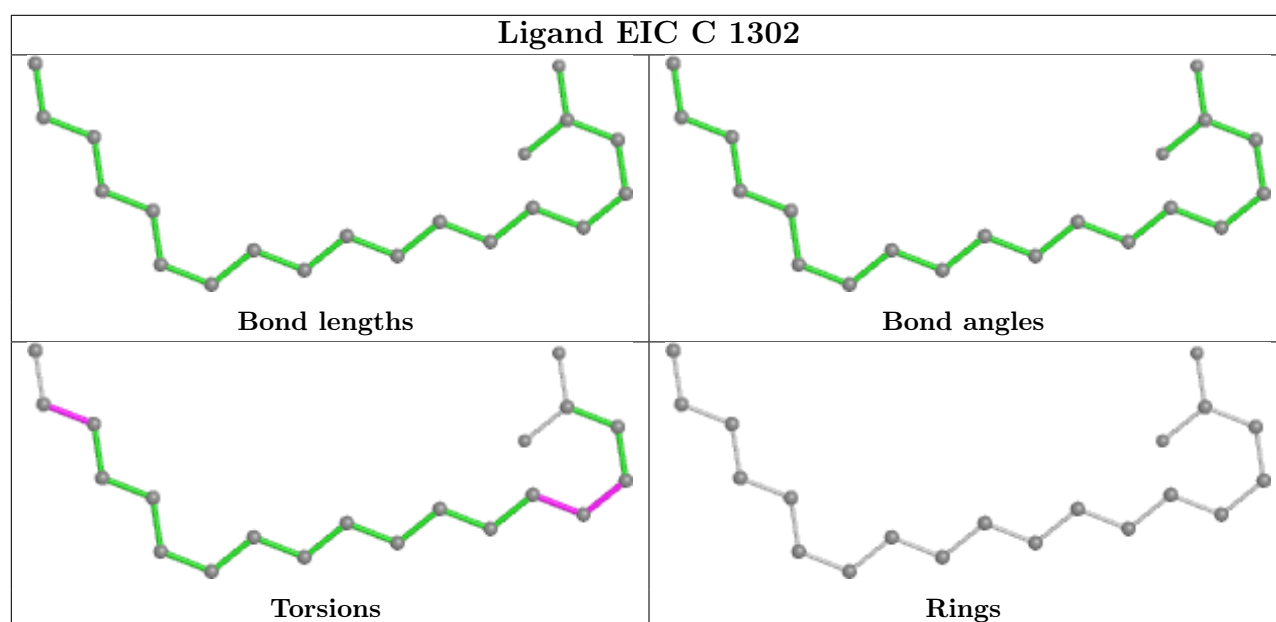
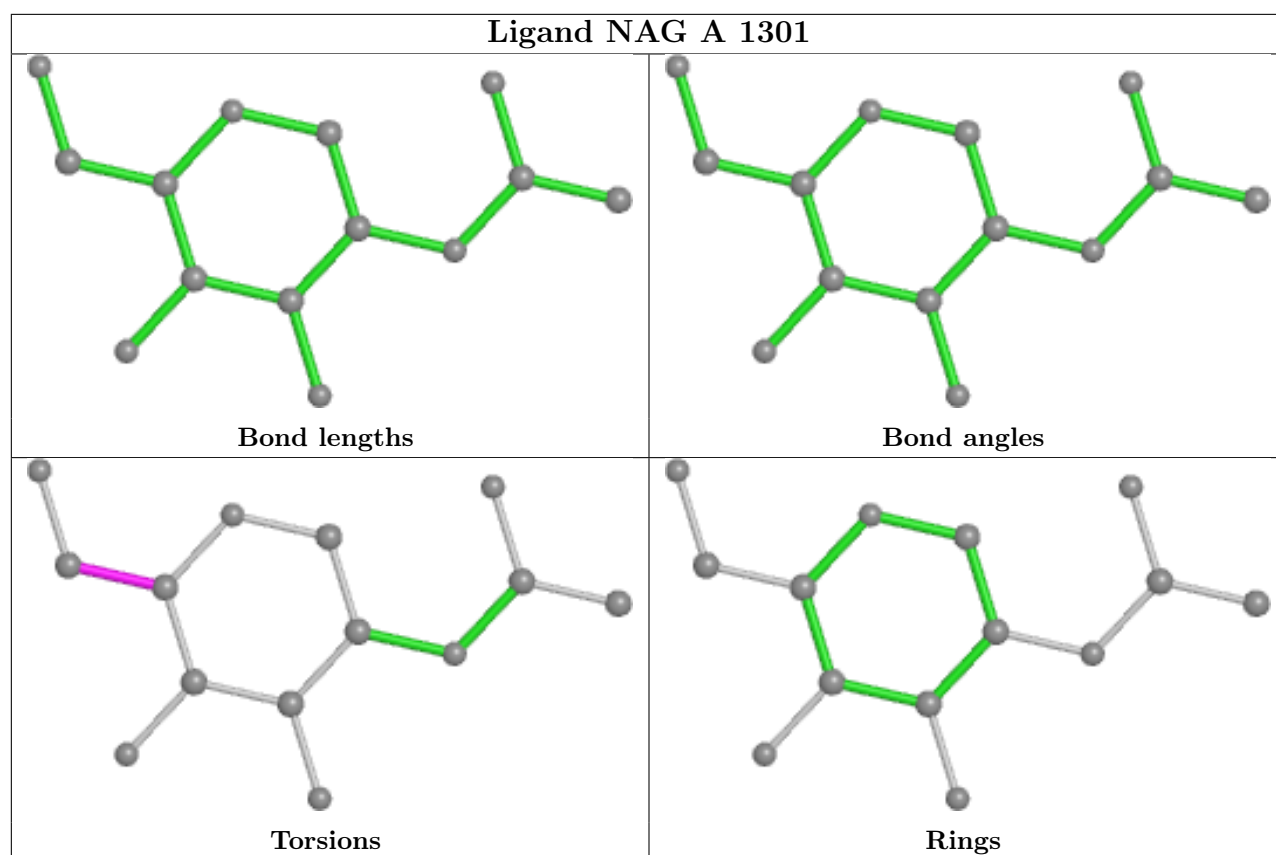


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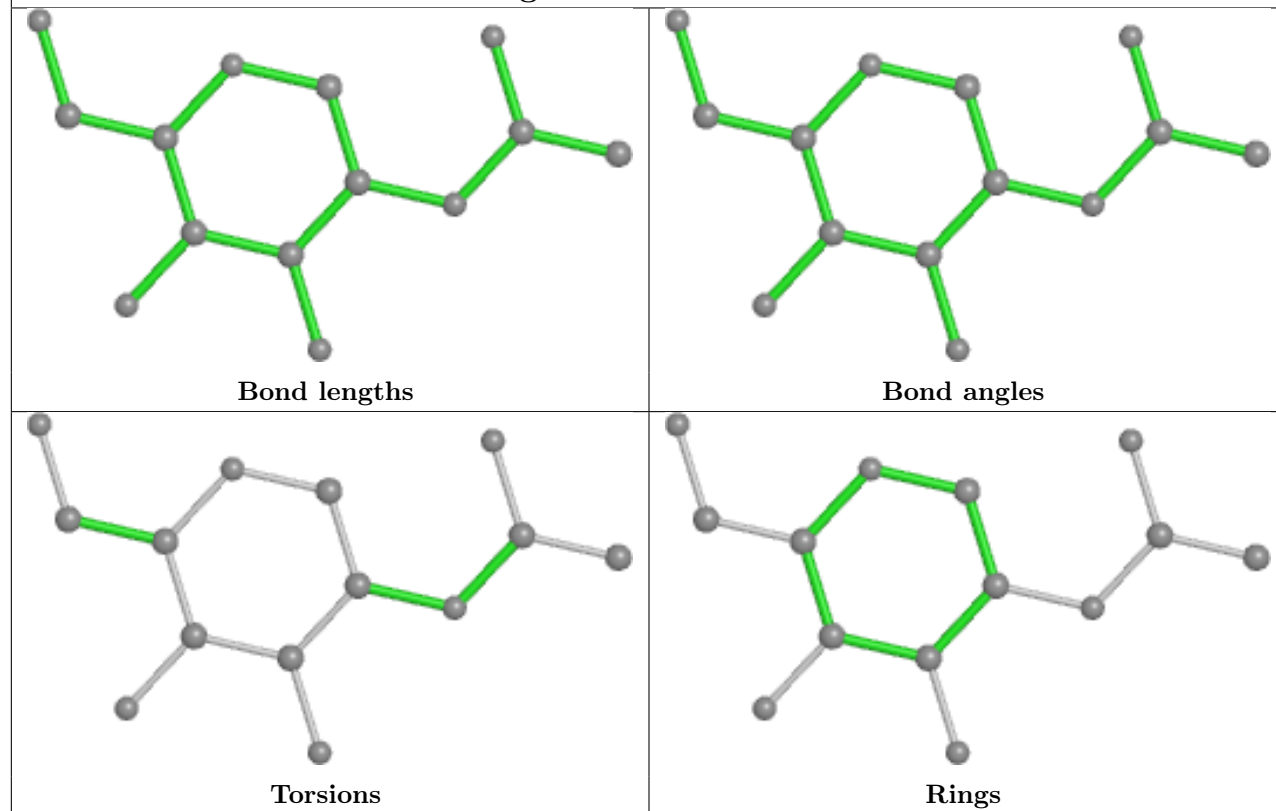


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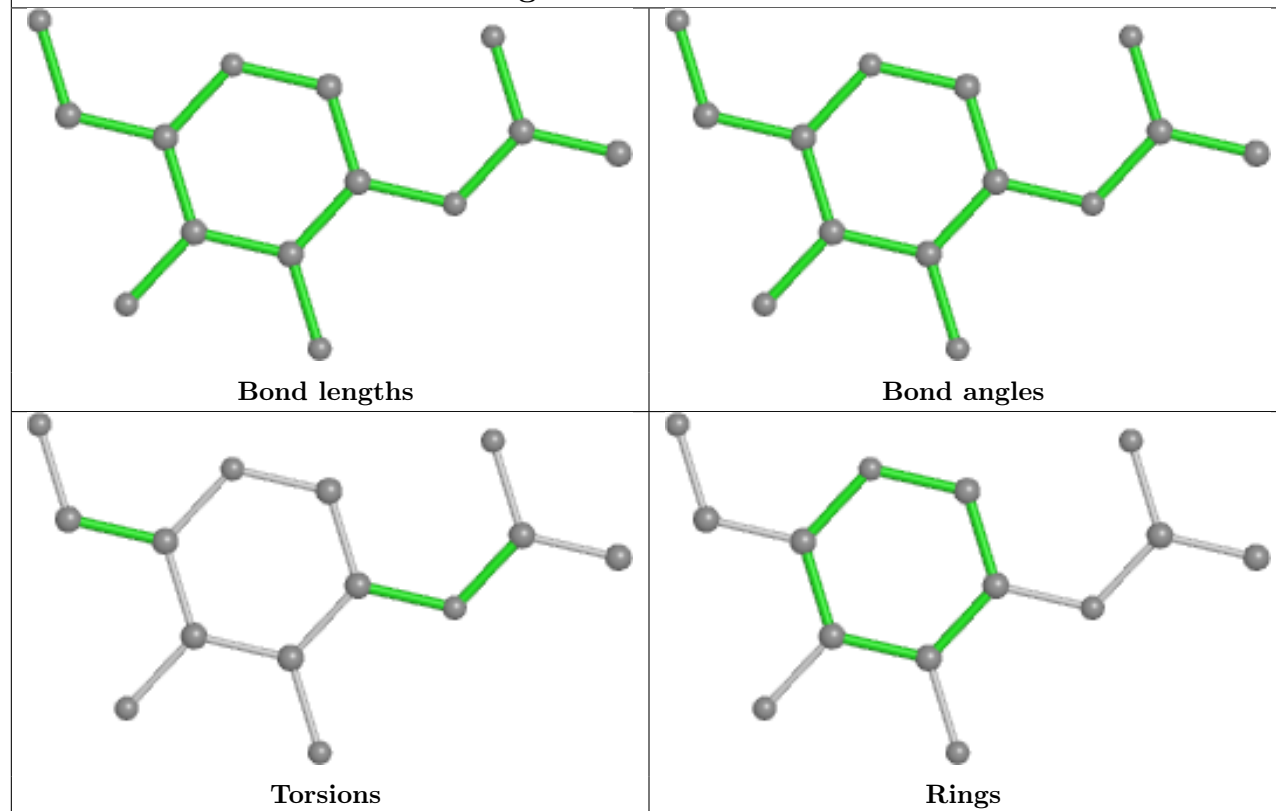




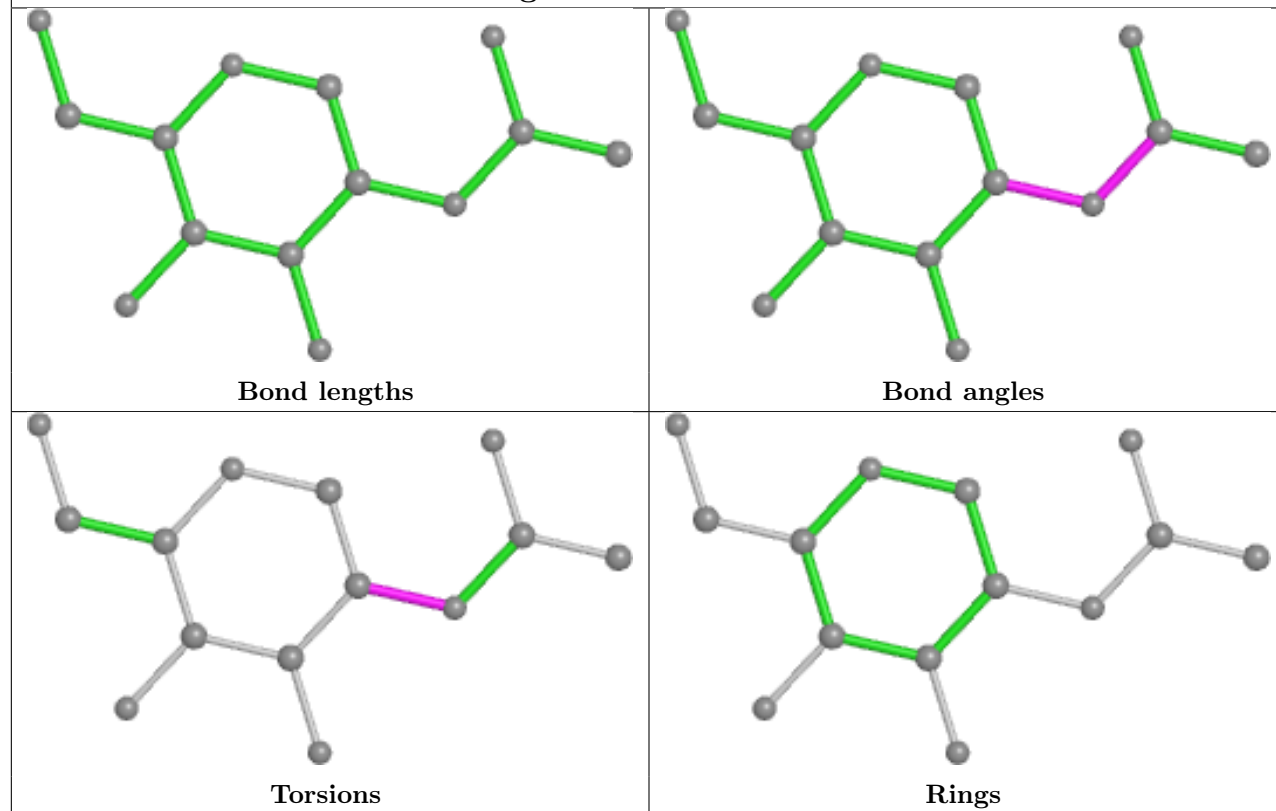
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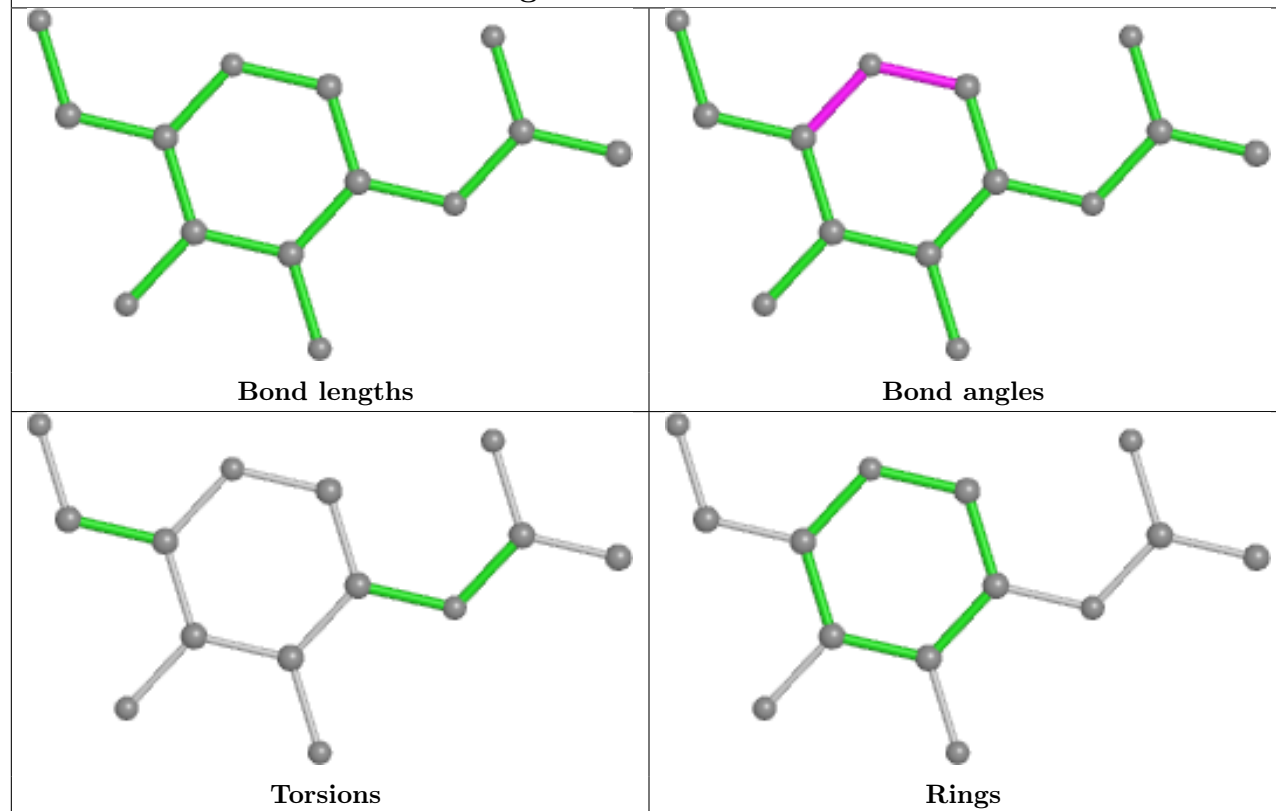
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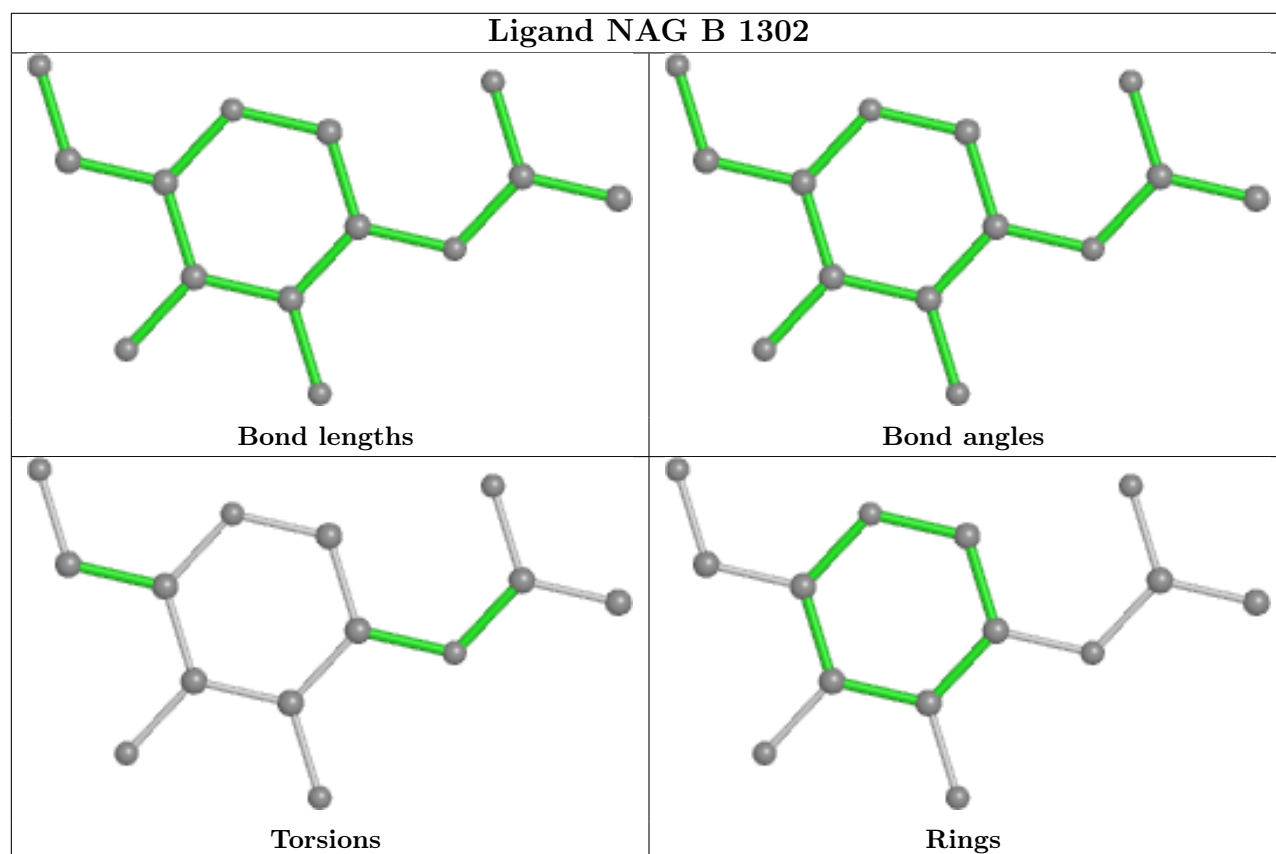
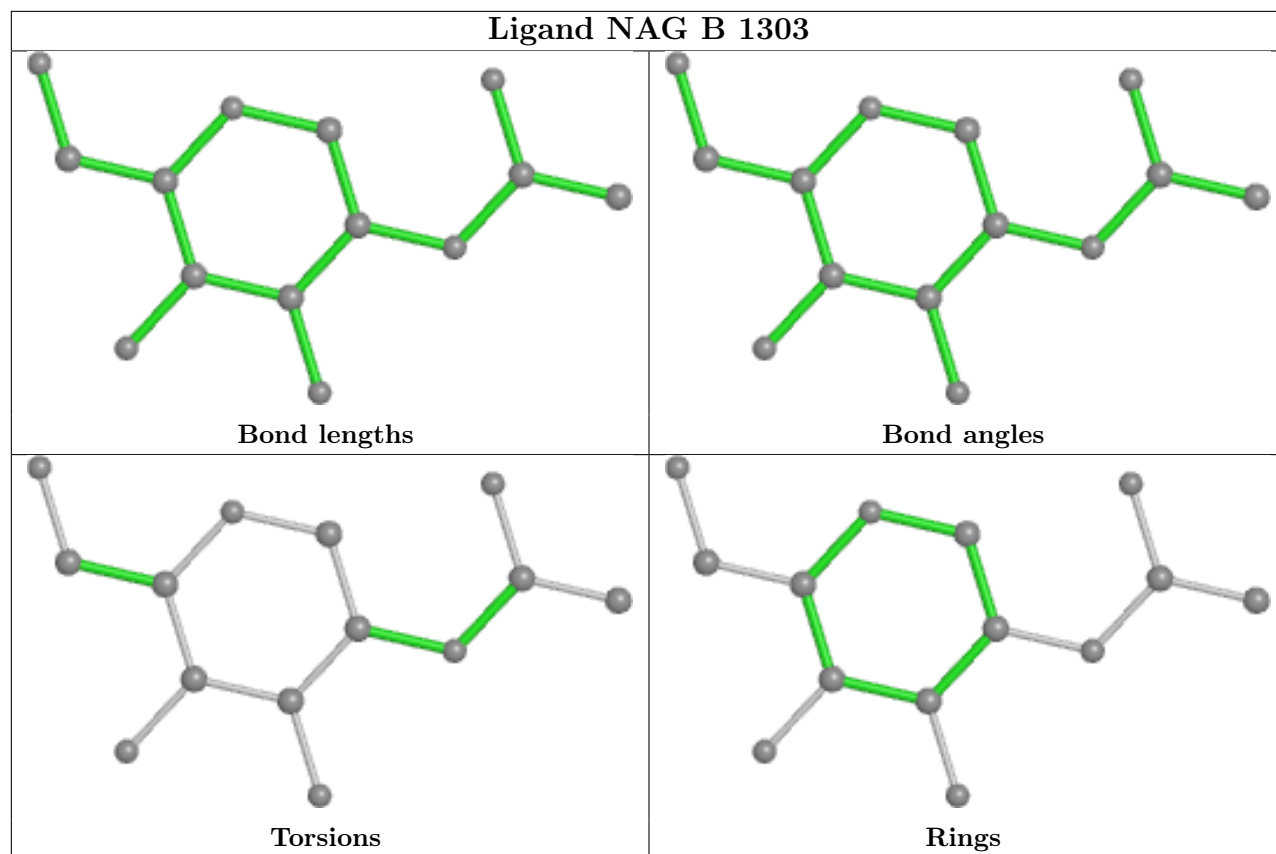


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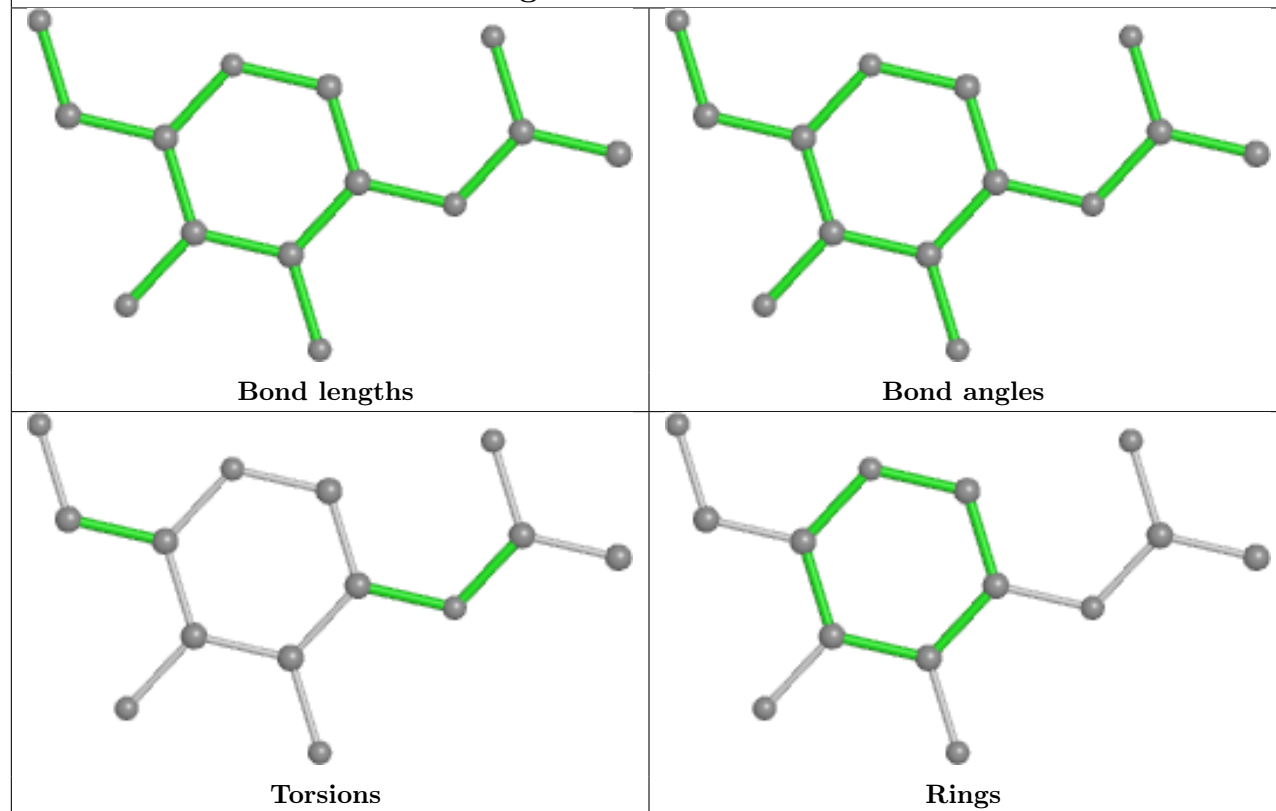


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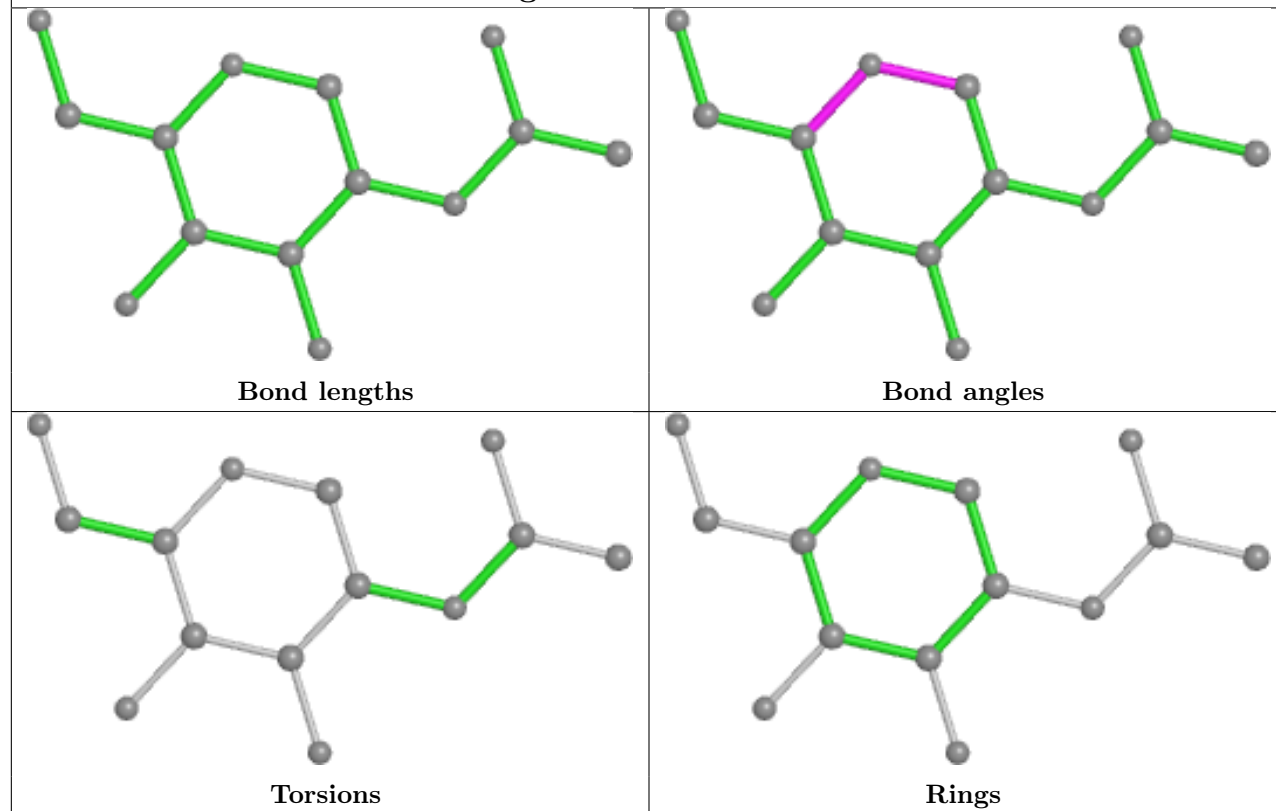




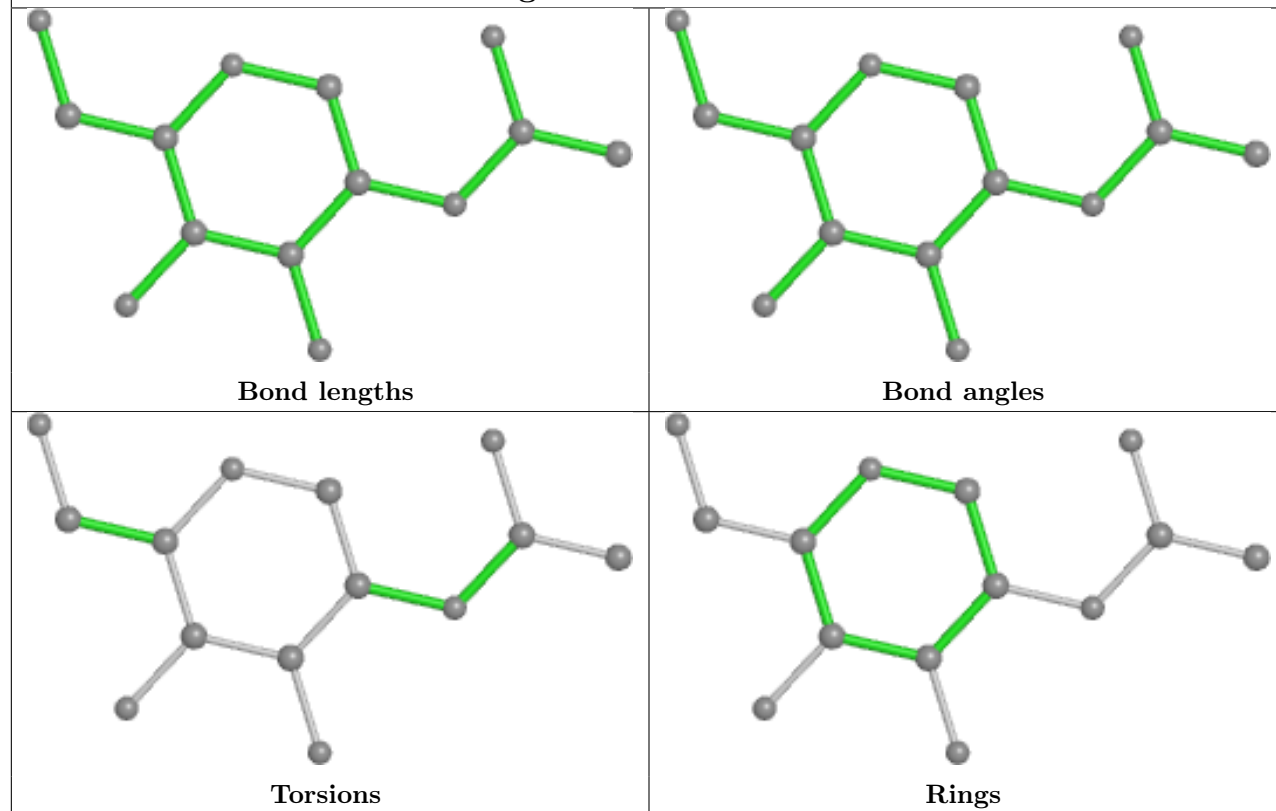
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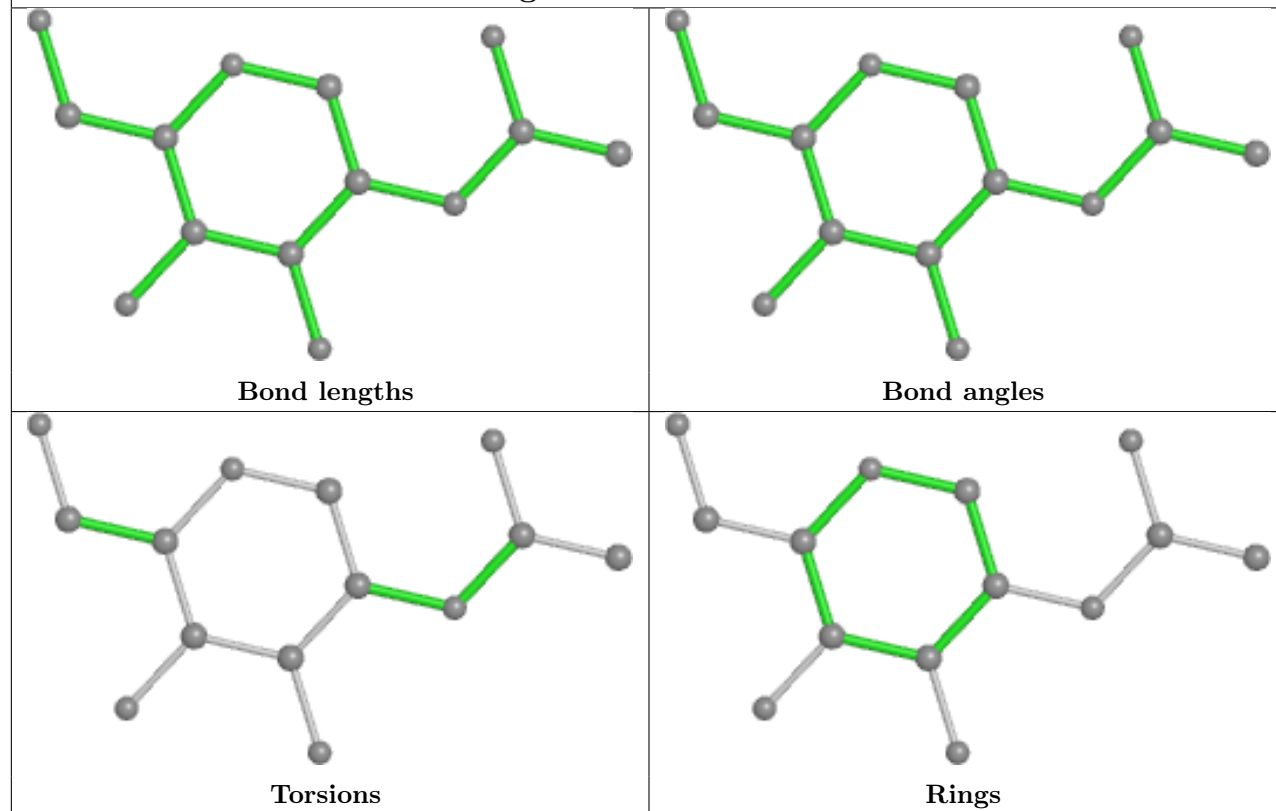
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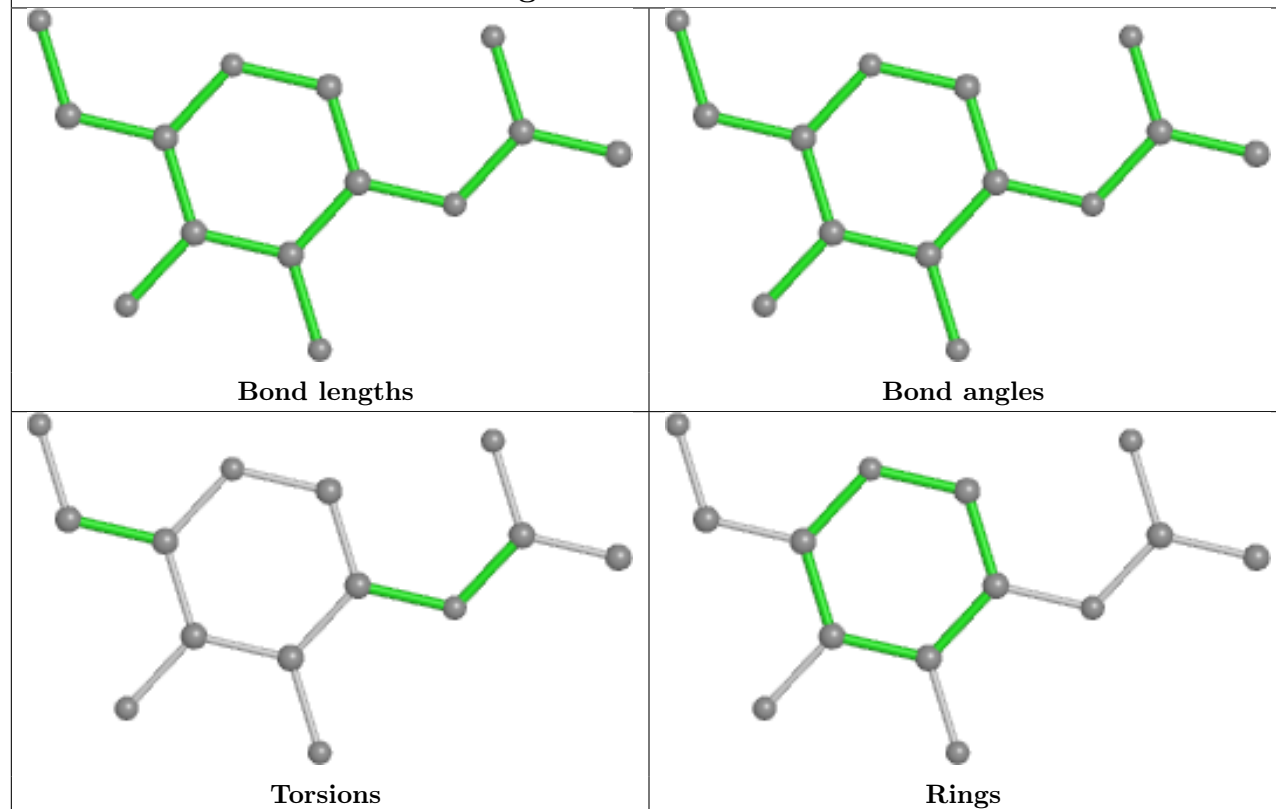
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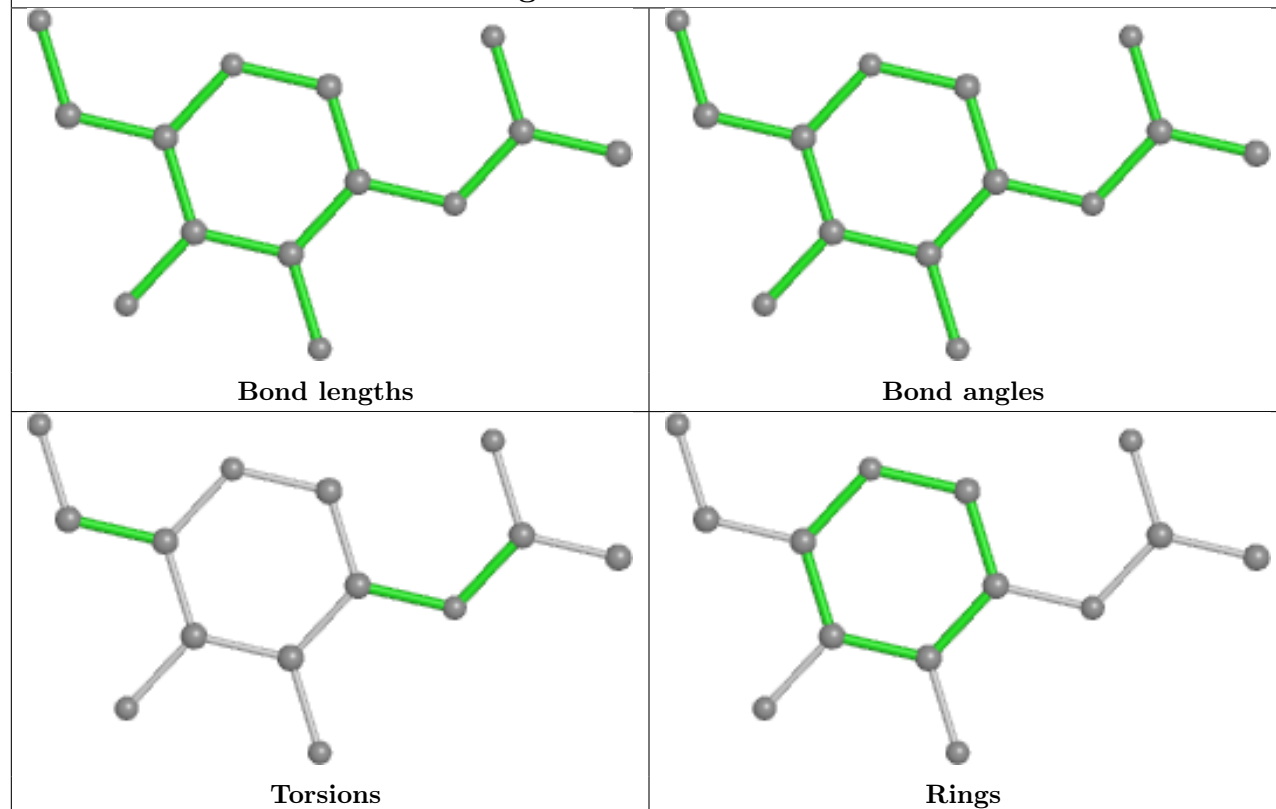
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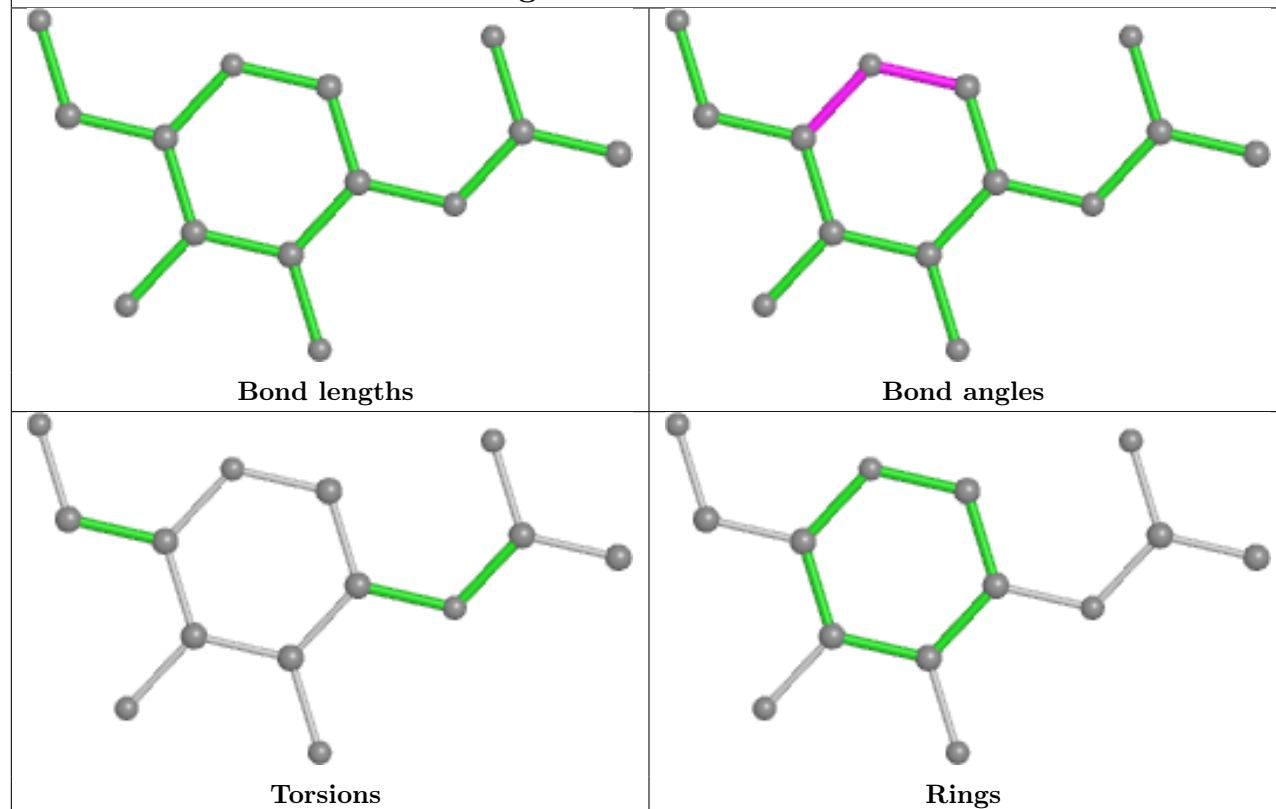
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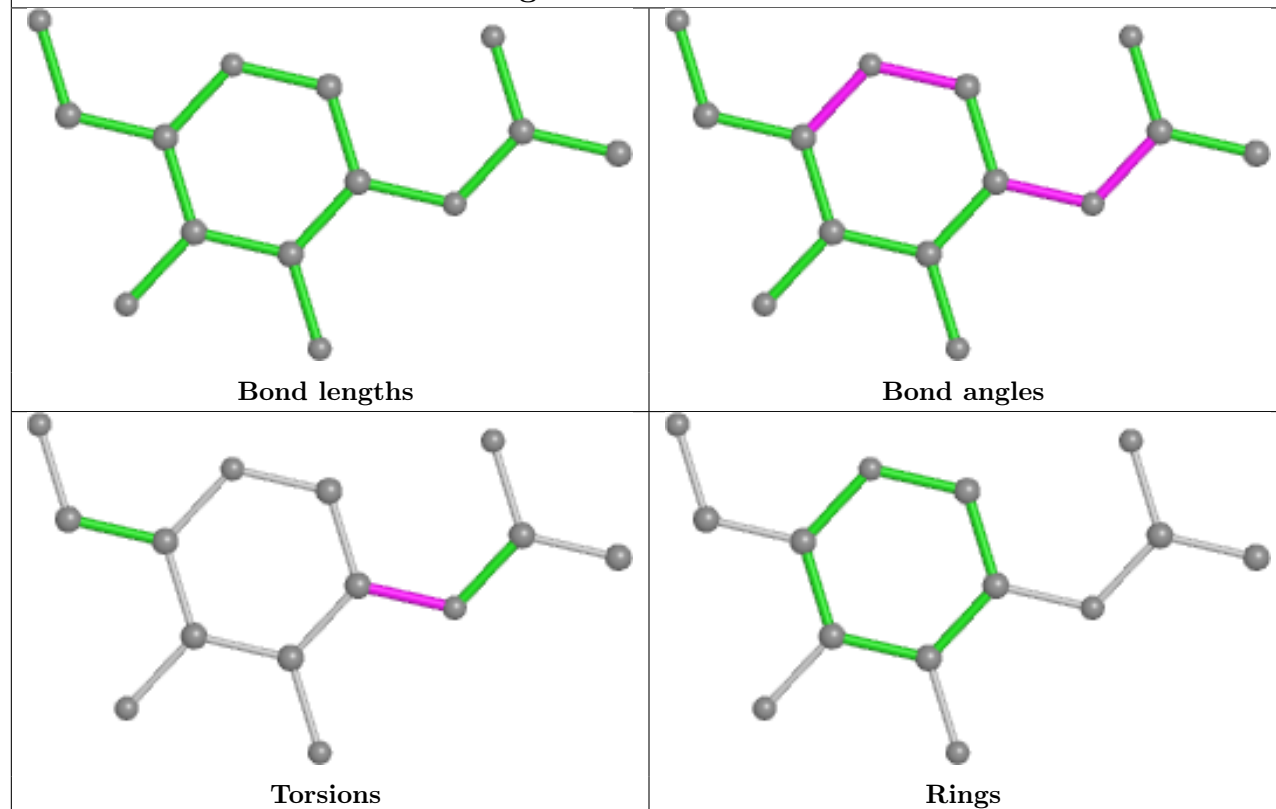
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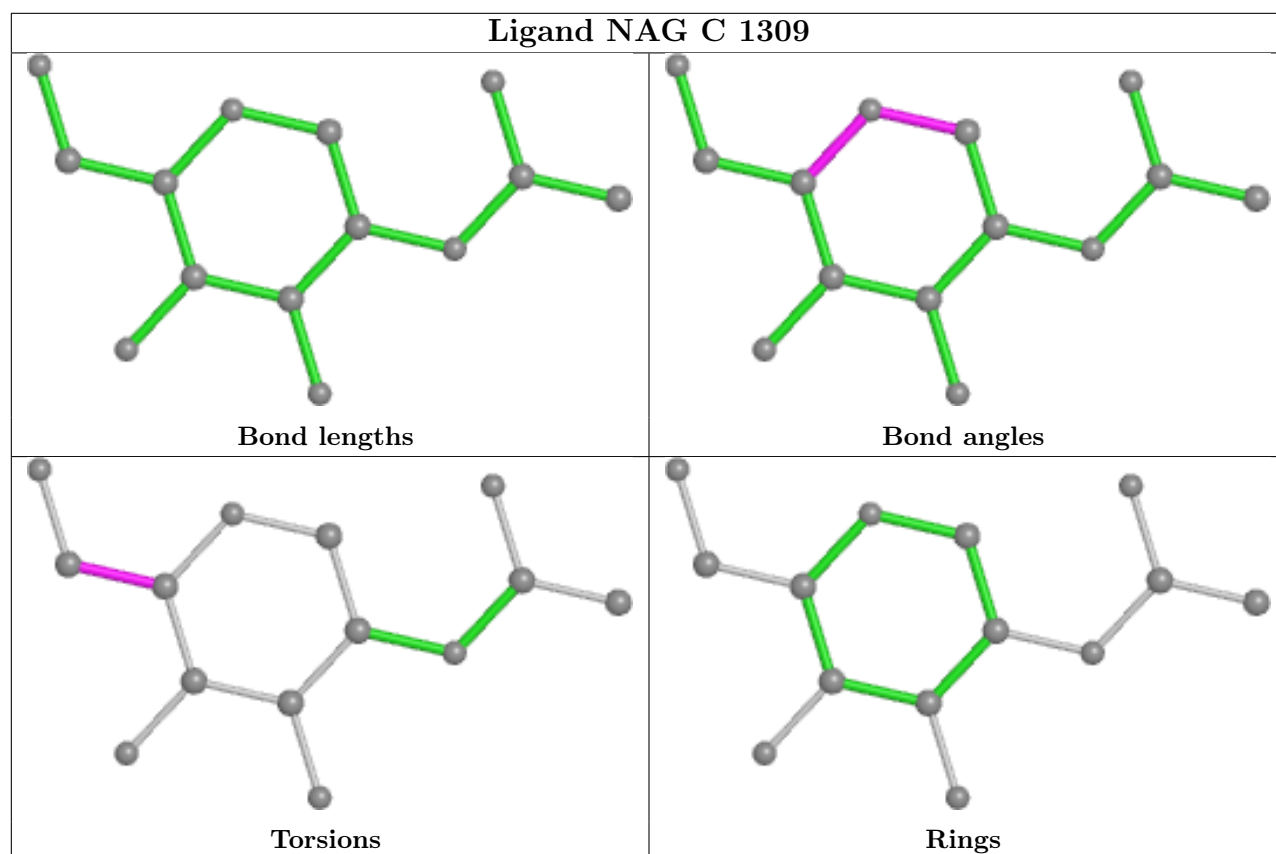
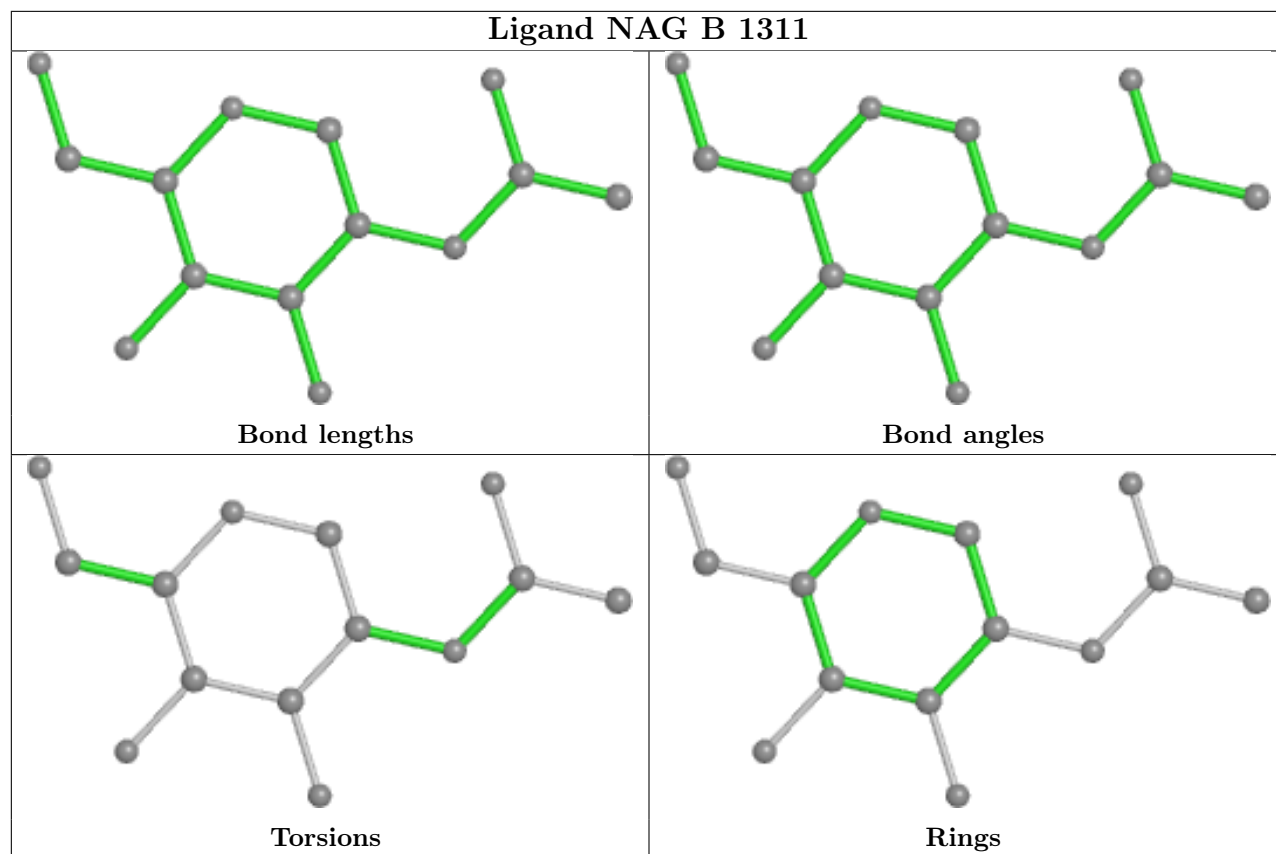


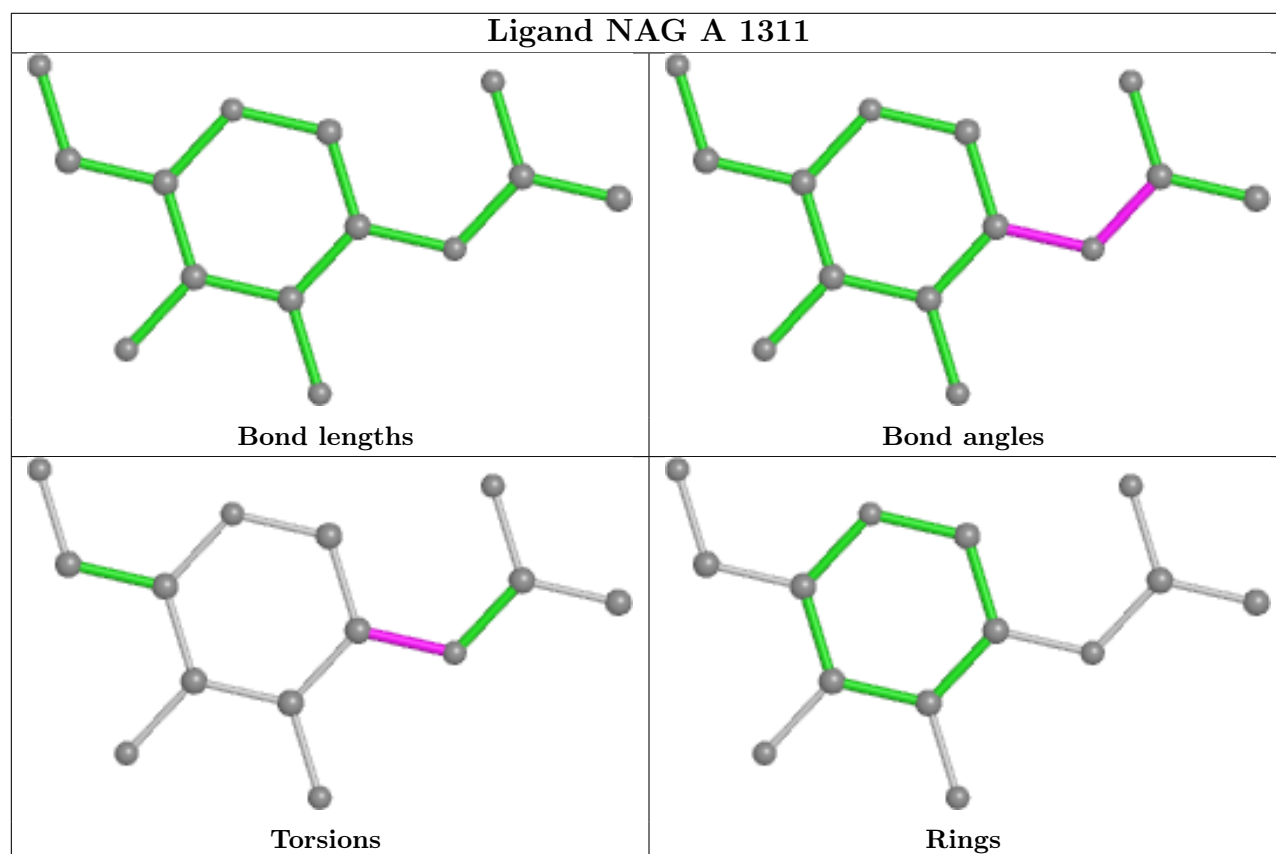
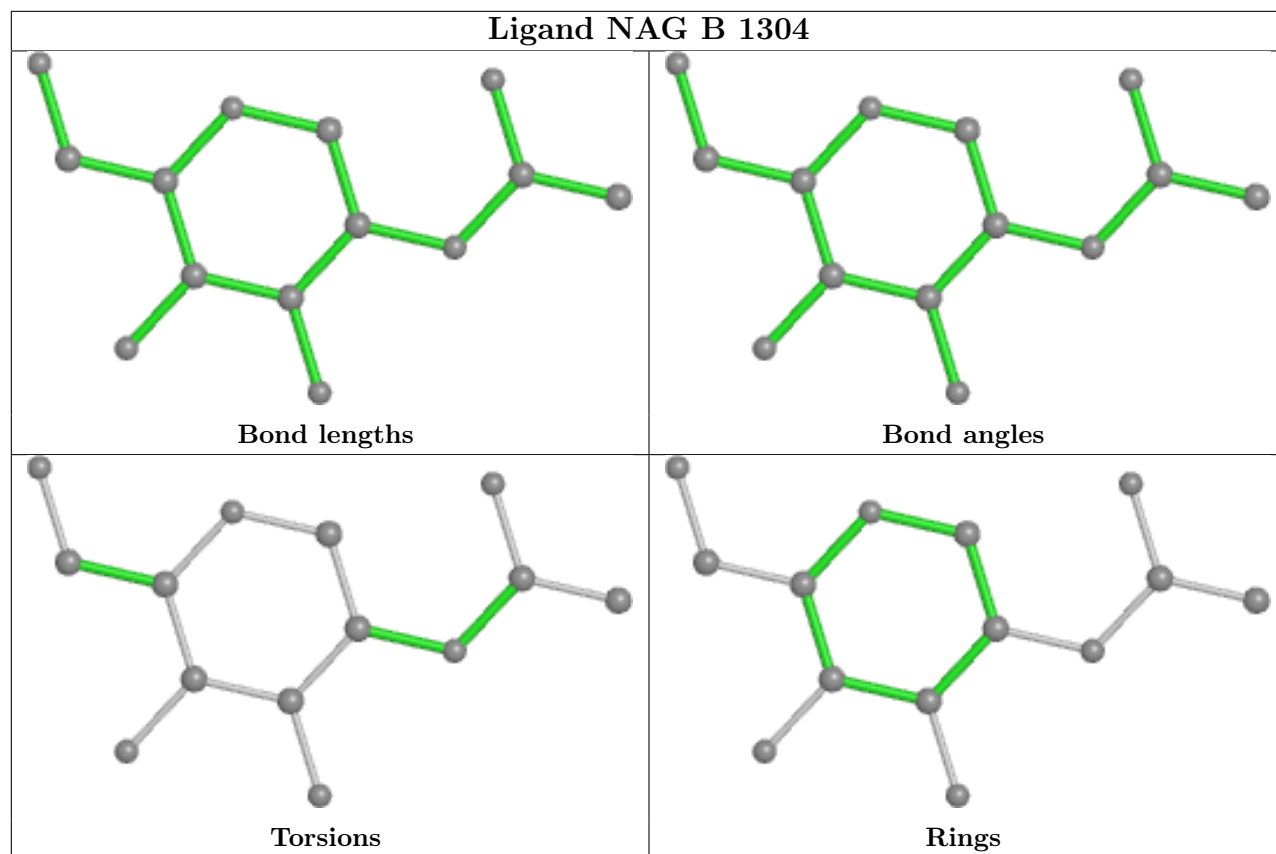
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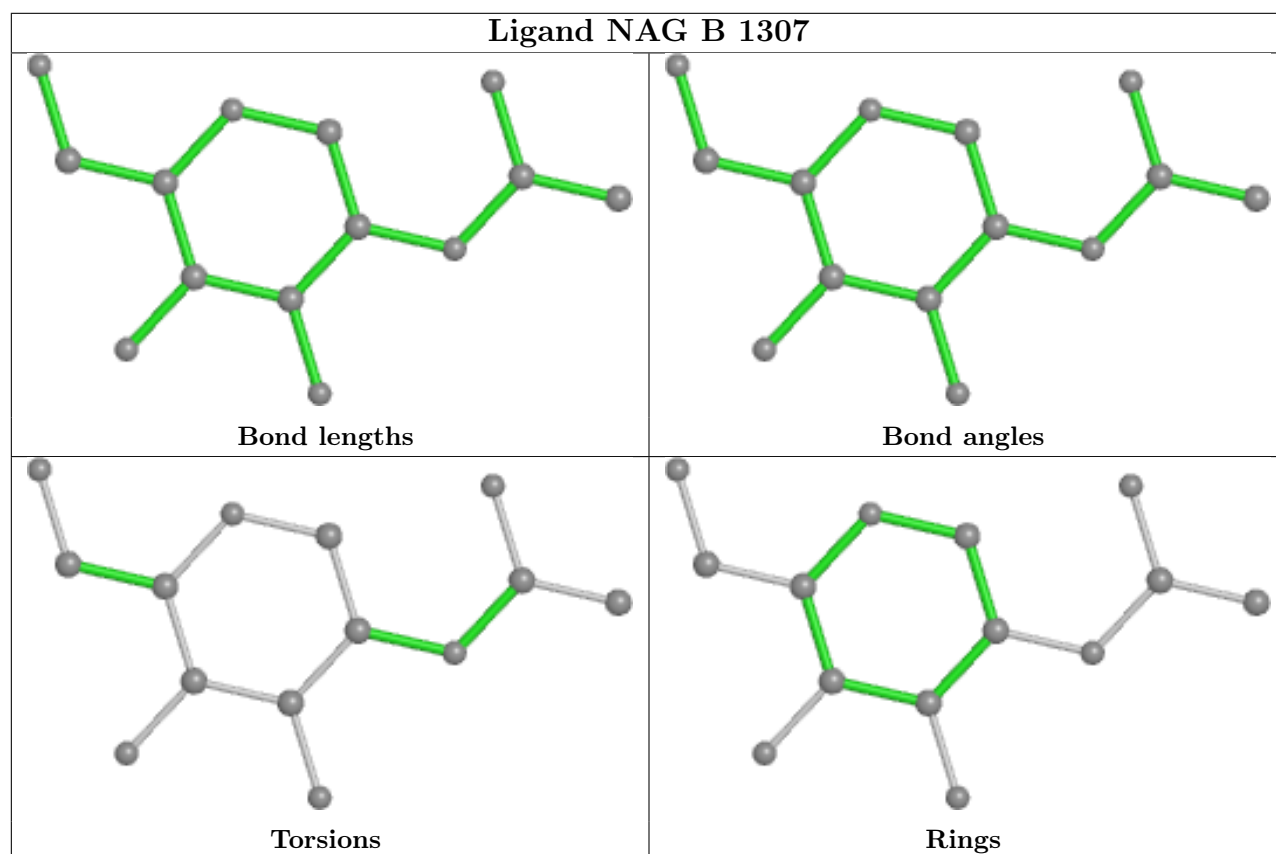
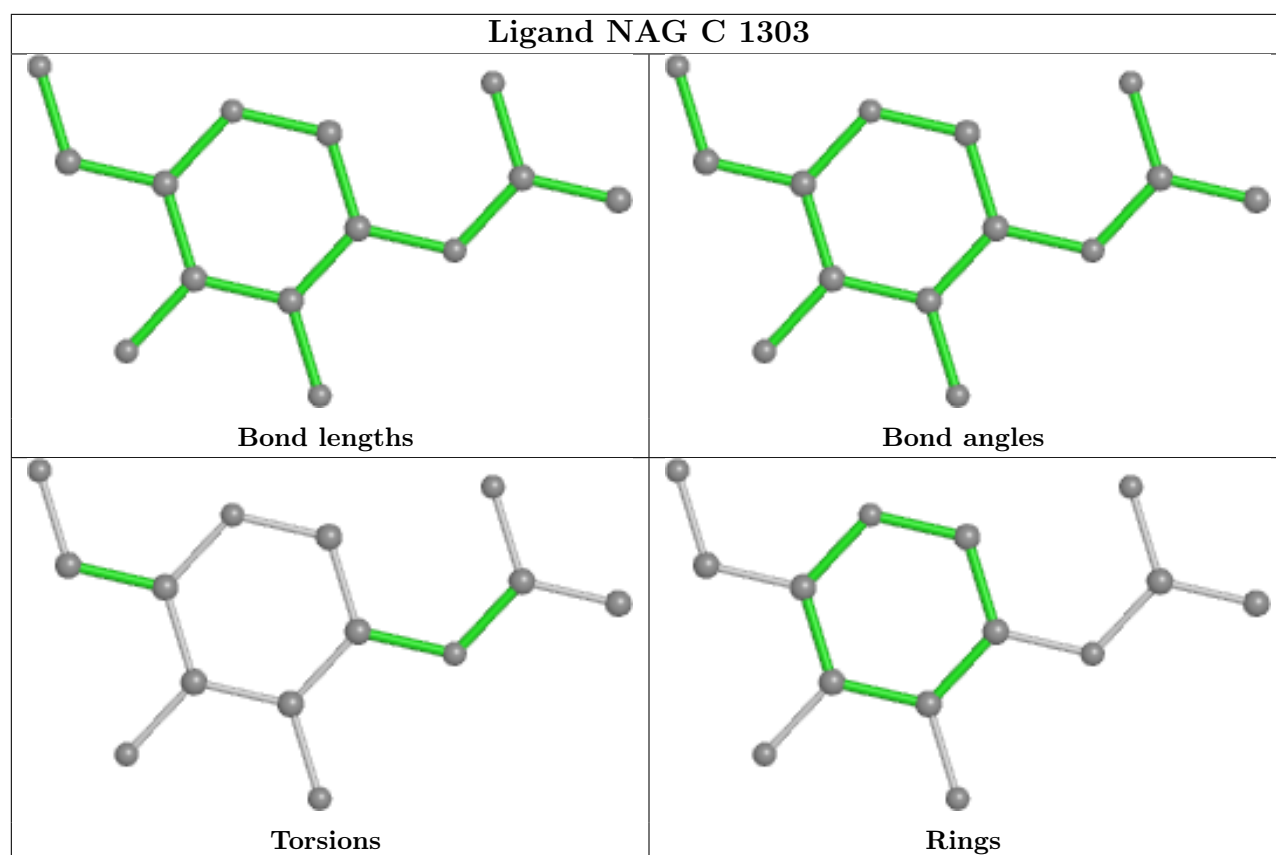


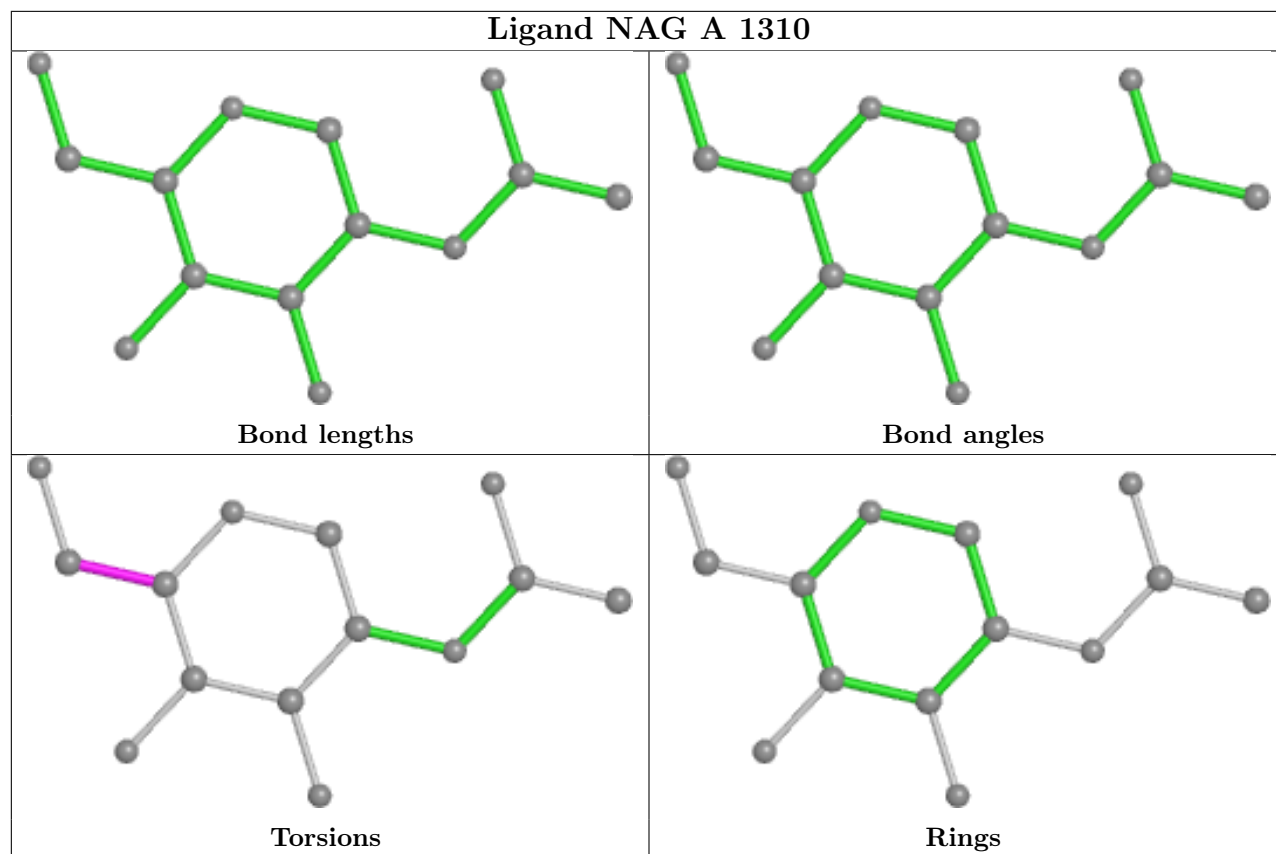
Ligand NAG C 1311











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.