



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 03:04 PM JST

PDB ID : 8ZC3
EMDB ID : EMD-39921
Title : SARS-CoV-2 Omicron BA.4 spike trimer (6P) in complex with 3 D1F6 Fabs
(1 RBD up)
Authors : Liu, B.; Gao, X.; Li, Z.; Chen, Q.; He, J.; Xiong, X.
Deposited on : 2024-04-28
Resolution : 4.69 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **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

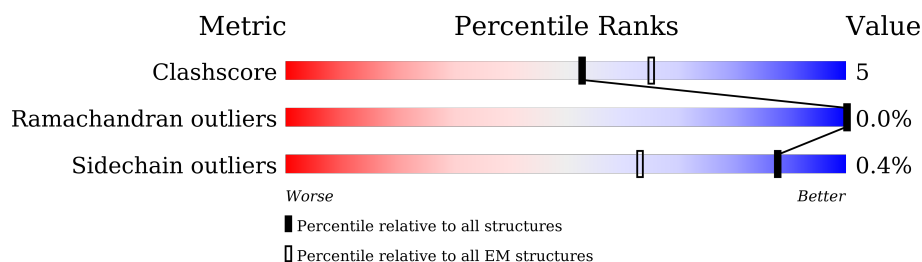
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.69 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	1238	71% 9% 20%
1	B	1238	69% 11% 20%
1	C	1238	71% 9% 20%
2	D	223	84% 11% .
2	M	223	83% 12% .
2	N	223	83% 13% .
3	E	230	77% 17% . .
3	Q	230	82% 13% .
3	R	230	83% 13% .

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Mol	Chain	Length	Quality of chain
4	F	2	 100%
4	G	2	 100%
4	H	2	 50%50%
4	I	2	 50%50%
4	J	2	 100%
4	K	2	 50%50%
4	L	2	 100%
4	O	2	 100%
4	P	2	 100%
4	S	2	 100%
4	T	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33856 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	993	Total	C	N	O	S	0	0
			7778	4988	1288	1468	34		
1	B	994	Total	C	N	O	S	0	0
			7790	4994	1293	1469	34		
1	C	993	Total	C	N	O	S	0	0
			7778	4988	1288	1468	34		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	683	LYS	ASN	variant	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	683	LYS	ASN	variant	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	683	LYS	ASN	variant	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Light chain of D1F6 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	M	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		
2	N	213	Total	C	N	O	S	0	0
			1591	1001	266	320	4		

- Molecule 3 is a protein called Heavy chain of D1F6 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	Q	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		
3	R	221	Total	C	N	O	S	0	0
			1679	1061	280	328	10		

- Molecule 4 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
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (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	
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	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
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

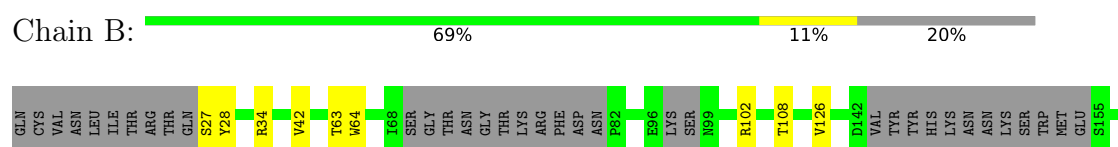
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Spike glycoprotein



• Molecule 1: Spike glycoprotein






PHE	F1143	L938	T747	S605	TRP	ASN	GLN
	L1144	N751	ALA	N606	THR	ASN	CYS
	L1145	N751	ALA	N616	ALA	LYS	VAL
	D1146	Q965	GLY	N616	GLY	ASN	VAL
	S1147	Q760	THR	A262	TRP	ASN	LEU
	LYS	S974	THR	A262	MET	ILE	THR
	GLU	L977	THR	R273	E154	ARG	THR
	GLU	L822	ALA	T274	Y160	GLN	THR
	LEU	R983	ILE	G283	TRP	GLN	S27
	ASP	R1000	THR	P322	ALA	SER	
PHE	L1003	ALA	ASP	ALA	ALA	ASN	R34
	L1004	ASP	GLN	GLN	ASN	ASN	G95
	ASN	GLY	ALA	THR	CYS	CYS	Y38
	R1019	PHE	THR	PRO	THR	THR	
	THR	ILE	ILE	THR	F168	F168	Q52
	SER	LYS	LYS	TRP	I402	L176	L56
	PRO	GLN	GLN	ARG	E406	MET	P57
	ASP	TYR	TYR	VAL	ASP	ASP	
	VAL	GLY	GLY	TYR	LEU	LEU	I68
	ASP	Q1036	ASP	ASP	N417	GLU	SER
ILE	S1037	CYS	THR	THR	I418	GLY	GLY
	K1038	LEU	GLY	GLY	Y421	LYS	THR
	ASP	GLY	GLY	GLY	N422	GLN	ASN
	ILE	ASP	ASP	N641	Y421	GLY	THR
	SER	ILE	ILE	Q644	D428	ASN	THR
	GLY	ALA	ALA	Q644	D428	PHE	LYS
	ILE	ARG	ARG	C649	V433	ARG	ARG
	ASN	L1083	ASP	C649	V433	R190	PHE
	ALA	Q1071	LEU	V656	D442	ASN	ASP
	VAL	C1082	CYS	N657	N448	N196	ASN
ASN	ASN	VAL	ALA	N658	N448	ASN	P82
	ILE	R1091	GLN	Q675	R457	I210	N87
	GLN	LYS	PHE	THR	GLN	ASN	D88
	LYS	W1102	GLN	GLN	V503	LEU	GLY
	ILE	V1104	THR	LYS	V512	ARG	T95
	ASP	T1105	SER	SER	V512	D215	GLU
	ARG	Q1106	ARG	ARG	P521	G219	LYS
	LEU	L864	LEU	SER	V539	L226	SER
	ASN	F1109	GLU	VAL	V539	V227	ASN
	VAL	I1115	THR	ALA	N542	L226	I100
LYS	T1117	LYS	GLN	S691	Q563	H245	T108
	D1118	ASN	ARG	T716	Q564	ARG	T109
	ASN	A879	THR	T716	Q564	THR	K129
	C1126	R852	ASN	T724	I569	LEU	V130
	GLU	L894	THR	T724	I569	THR	C131
	SER	N1135	LEU	V736	R577	PRO	E132
	LEU	Y1138	ILE	D737	D578	GLY	D142
	ASP	D1139	THR	C738	P579	ASP	VAL
	LEU	P1140	GLY	T742	Q580	SER	TYR
	GLN	C1142	THR	T742	T581	SER	TYR
PHE	L1143	T324	THR	I742	L582	CYS	HIS
	L1144	T324	THR	I742	L582	CYS	TYR
	L1145	T324	THR	I742	L582	CYS	TYR
	L1146	T324	THR	I742	L582	CYS	TYR
	L1147	T324	THR	I742	L582	CYS	TYR
	L1148	T324	THR	I742	L582	CYS	TYR
	L1149	T324	THR	I742	L582	CYS	TYR
	L1150	T324	THR	I742	L582	CYS	TYR
	L1151	T324	THR	I742	L582	CYS	TYR
	L1152	T324	THR	I742	L582	CYS	TYR


LEU GLY LYS TYR GLN TYR ILE LYS GLY ARG GLU ASN LEU TYR PHE GLN GLY GLY GLY SER GLY TYR ILE PRO GLU ALA PRO ARG ASP GLY GLN ALA TYR VAL ARG LYS ASP GLY GLY TER VAL LEU LEU SER THR PHE LEU GLY HIS HIS HIS HIS

• Molecule 2: Light chain of D1F6 Fab

Chain D:  84% 11% .


GLN P2 P8 S27 N32 Y35 L47 L48 I49 Y50 R55 F63 D86 A90 A91 A92 D93 T105 L110 GLY THR LYS LEU THR THR VAL LEU G118 Q119 P120 L136 L142 T147 I147 A158 K182 T192 Q195 V196 K197 Q205 V206
E221 CYS SER

• Molecule 2: Light chain of D1F6 Fab

Chain M:  83% 12% .


GLN P2 A10 P14 N28 Y35 Q39 L40 A43 K46 K51 Q54 R55 P60 F63 F64 A75 I76 D86 A90 V100 V107 L110 GLY THR LYS LEU THR THR VAL LEU G118 V126 T127 K140 T192 Q195 K215
E221 CYS SER

• Molecule 2: Light chain of D1F6 Fab

Chain N:  83% 13% .


GLN P2 Q6 C22 S25 M28 I29 V34 Q38 Q39 L40 P41 Q42 A43 K46 G44 L48 K51 Q54 R55 E61 R62 A72 S77 V85 A91 A103 L110 GLY THR LYS LEU THR THR VAL LEU G118 K140 P175 Q178 A185
P193 T207 T212 E221 CYS SER

• Molecule 3: Heavy chain of D1F6 Fab

Chain E:  77% 17% . .

GLU V2 A9 V11 K12 K13 K19 F29 Y32 R33 I34 R38 Q39 A40 Q43 G44 L45 I51 D57 R67 W70 D73 I76 T77 T78 V79 Y80 S85 L86 R87 D90 T91 A92 V93 R98 T116 L122 V123 T124 V125 S126 S127
A128 P133 L138 S141 SER LYS THR SER GLY T149 L155 V156 K157 D158 Y159 F160 P161 V177 G188 V196 S229 CYS

• Molecule 3: Heavy chain of D1F6 Fab

Chain Q:  82% 13% .

GLU V2 Q3 L4 V11 G15 H35 W36 V37 R38 L45 E46 W47 S52 S55 D56 D57 T71 R72 Y80 L86 Y94 Y102 N106 Q109 G118 T124 V125 S126 S127 A128 K131 V135 S141 SER LYS THR THR SER GLY T149



- Molecule 3: Heavy chain of D1F6 Fab

Chain R: 83% 13%



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

Chain F: 100%



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

Chain G: 100%



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

Chain H: 50% 50%



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

Chain I: 50% 50%



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

Chain J: 100%



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

Chain K:  50% 50%



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

Chain L:  100%



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

Chain O:  100%



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

Chain P:  100%



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

Chain S:  100%



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

Chain T:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	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

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	0.26	0/7960	0.52	0/10830
1	B	0.27	0/7972	0.52	0/10845
1	C	0.26	0/7960	0.51	0/10830
2	D	0.26	0/1633	0.51	0/2229
2	M	0.25	0/1633	0.49	0/2229
2	N	0.25	0/1633	0.53	0/2229
3	E	0.25	0/1722	0.52	0/2349
3	Q	0.26	0/1722	0.53	0/2349
3	R	0.26	0/1722	0.52	0/2349
All	All	0.26	0/33957	0.52	0/46239

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	7778	0	7601	73	0
1	B	7790	0	7616	93	0
1	C	7778	0	7601	68	0
2	D	1591	0	1539	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1591	0	1539	14	0
2	N	1591	0	1539	16	0
3	E	1679	0	1624	35	0
3	Q	1679	0	1624	28	0
3	R	1679	0	1624	21	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	1	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
5	A	140	0	130	0	0
5	B	126	0	117	0	0
5	C	126	0	117	0	0
All	All	33856	0	32946	340	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 5.

The worst 5 of 340 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)
3:Q:126:SER:HB2	3:Q:160:PHE:CZ	1.37	1.52
3:Q:126:SER:CB	3:Q:160:PHE:CE1	1.98	1.46
3:Q:126:SER:HB3	3:Q:160:PHE:CE1	1.60	1.24
3:Q:126:SER:CB	3:Q:160:PHE:HE1	1.40	1.23
3:Q:126:SER:HB2	3:Q:160:PHE:CE1	1.64	1.23

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	971/1238 (78%)	928 (96%)	43 (4%)	0	100	100
1	B	972/1238 (78%)	942 (97%)	30 (3%)	0	100	100
1	C	971/1238 (78%)	934 (96%)	36 (4%)	1 (0%)	48	83
2	D	209/223 (94%)	200 (96%)	9 (4%)	0	100	100
2	M	209/223 (94%)	203 (97%)	6 (3%)	0	100	100
2	N	209/223 (94%)	201 (96%)	8 (4%)	0	100	100
3	E	217/230 (94%)	209 (96%)	8 (4%)	0	100	100
3	Q	217/230 (94%)	205 (94%)	12 (6%)	0	100	100
3	R	217/230 (94%)	201 (93%)	15 (7%)	1 (0%)	25	64
All	All	4192/5073 (83%)	4023 (96%)	167 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1141	LEU
3	R	57	ASP

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	869/1075 (81%)	868 (100%)	1 (0%)	92	95
1	B	871/1075 (81%)	868 (100%)	3 (0%)	91	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	869/1075 (81%)	866 (100%)	3 (0%)	91	92
2	D	178/187 (95%)	177 (99%)	1 (1%)	84	88
2	M	178/187 (95%)	177 (99%)	1 (1%)	84	88
2	N	178/187 (95%)	178 (100%)	0	100	100
3	E	191/198 (96%)	186 (97%)	5 (3%)	41	61
3	Q	191/198 (96%)	189 (99%)	2 (1%)	73	82
3	R	191/198 (96%)	191 (100%)	0	100	100
All	All	3716/4380 (85%)	3700 (100%)	16 (0%)	88	91

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	3	GLN
2	M	140	LYS
3	E	13	LYS
3	E	124	THR
2	D	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1054	GLN
1	B	901	GLN
3	Q	3	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 ⓘ

22 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	$\# Z > 2$
4	NAG	F	1	1,4	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	G	1	1,4	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	H	1	1,4	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	H	2	4	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	I	1	1,4	14,14,15	0.65	0	17,19,21	2.01	2 (11%)
4	NAG	I	2	4	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	J	1	1,4	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	J	2	4	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	K	1	1,4	14,14,15	0.29	0	17,19,21	0.63	0
4	NAG	K	2	4	14,14,15	0.46	0	17,19,21	0.88	1 (5%)
4	NAG	L	1	1,4	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	L	2	4	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	O	1	1,4	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	O	2	4	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	P	1	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	P	2	4	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	S	1	1,4	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	S	2	4	14,14,15	0.25	0	17,19,21	0.51	0
4	NAG	T	1	1,4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	T	2	4	14,14,15	0.33	0	17,19,21	0.45	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	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	3/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C2-N2-C7	6.92	132.75	122.90
4	I	1	NAG	C1-C2-N2	3.37	116.25	110.49
4	K	2	NAG	C2-N2-C7	2.40	126.33	122.90

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

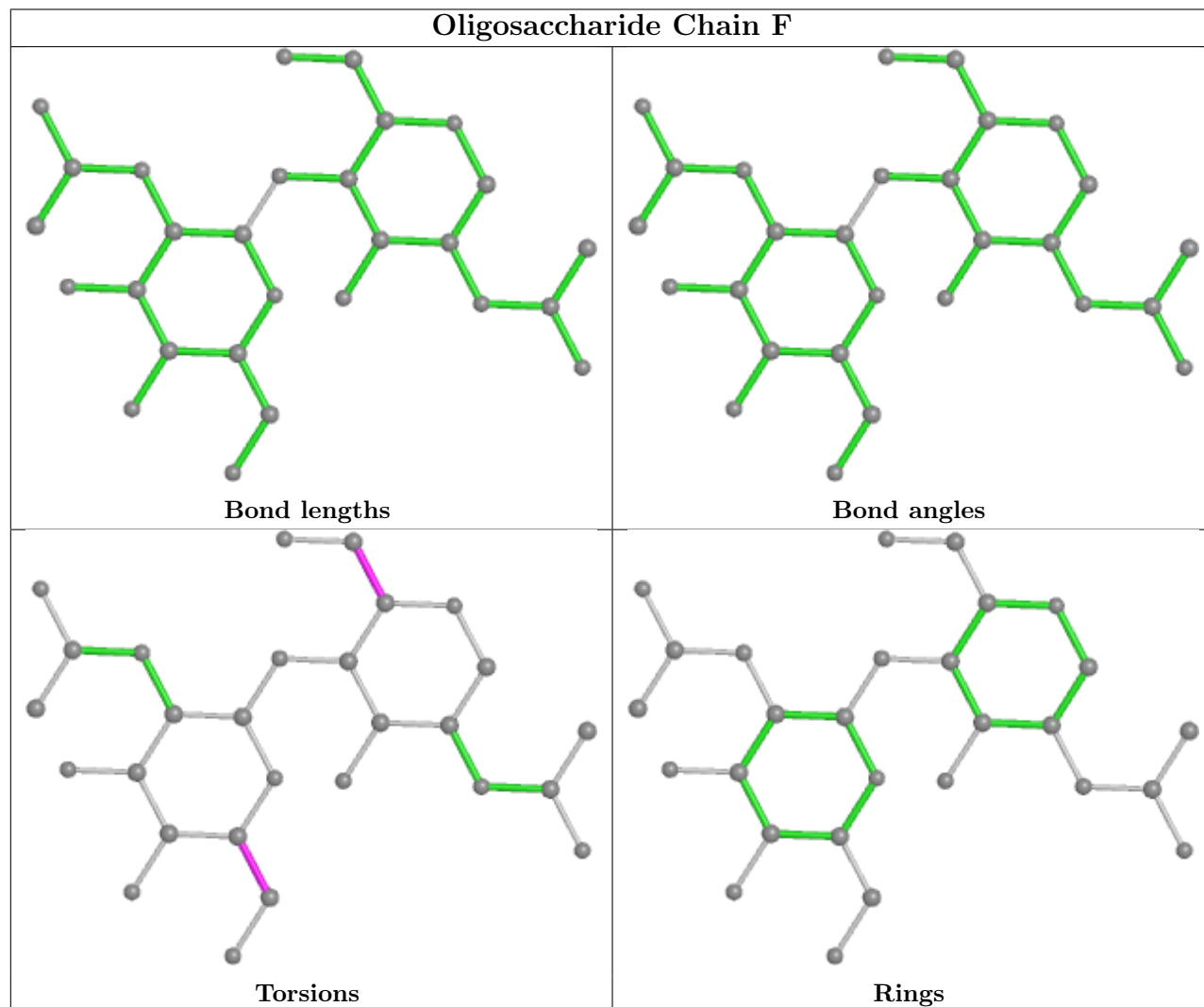
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6

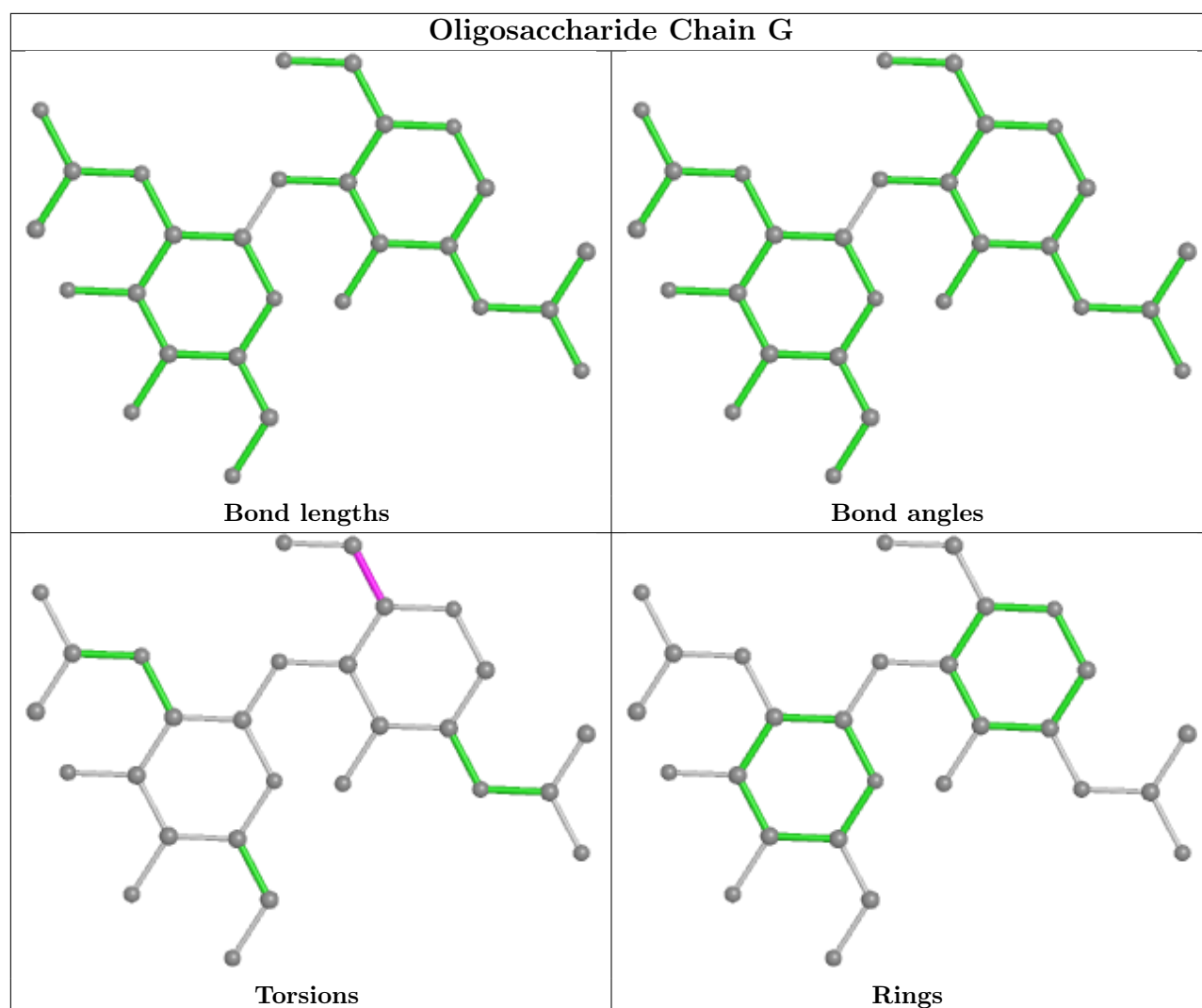
There are no ring outliers.

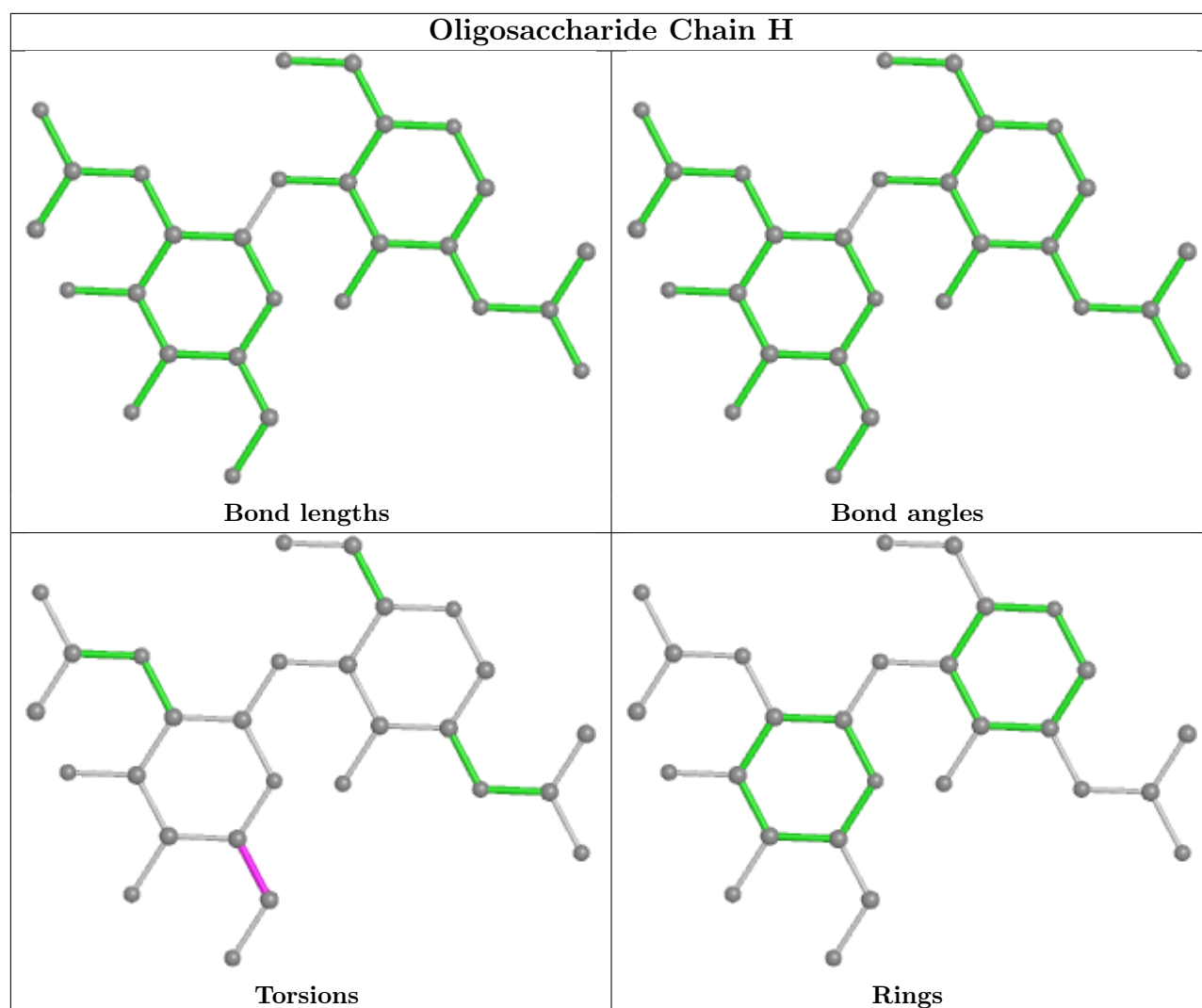
1 monomer is involved in 1 short contact:

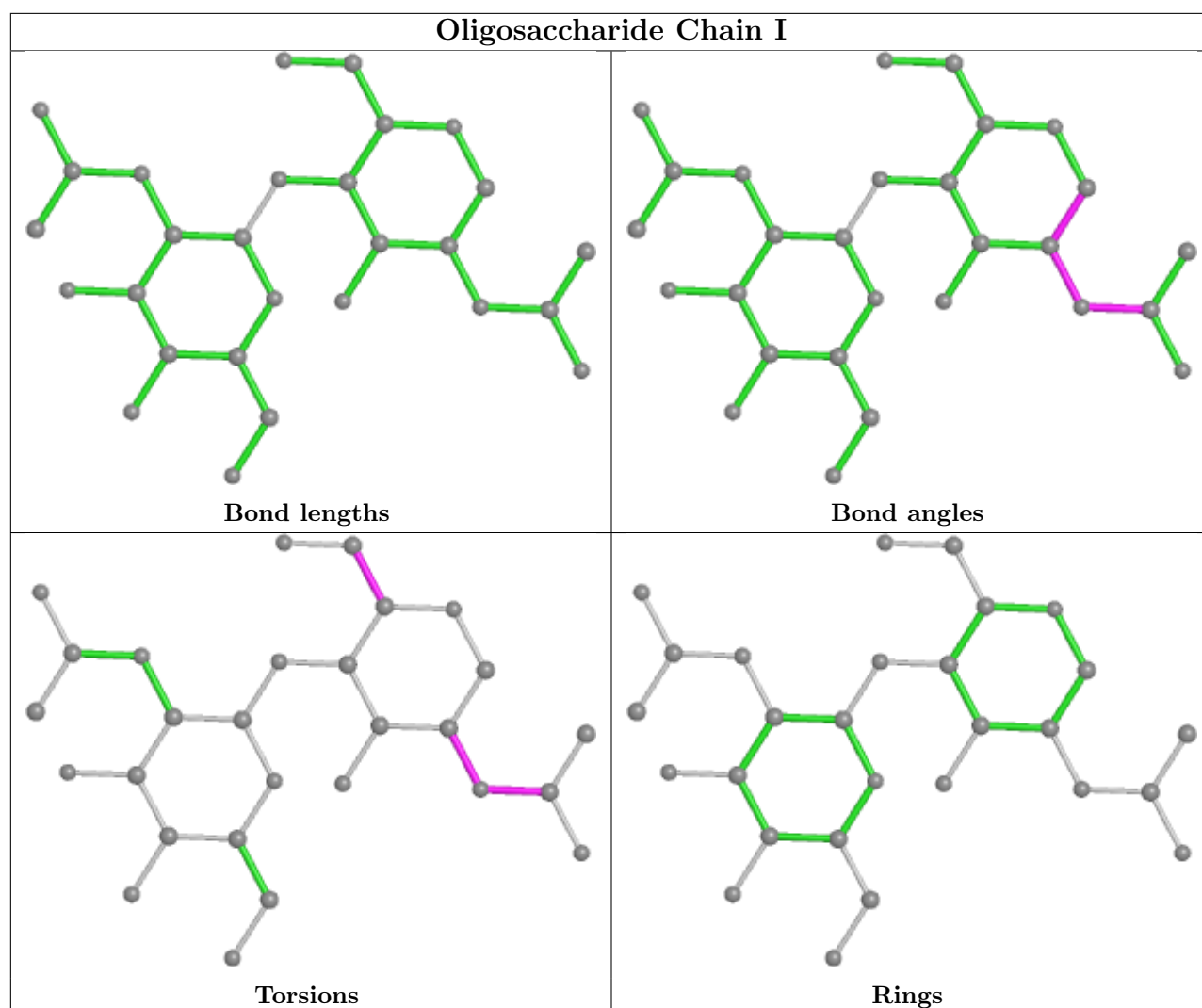
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	1	0

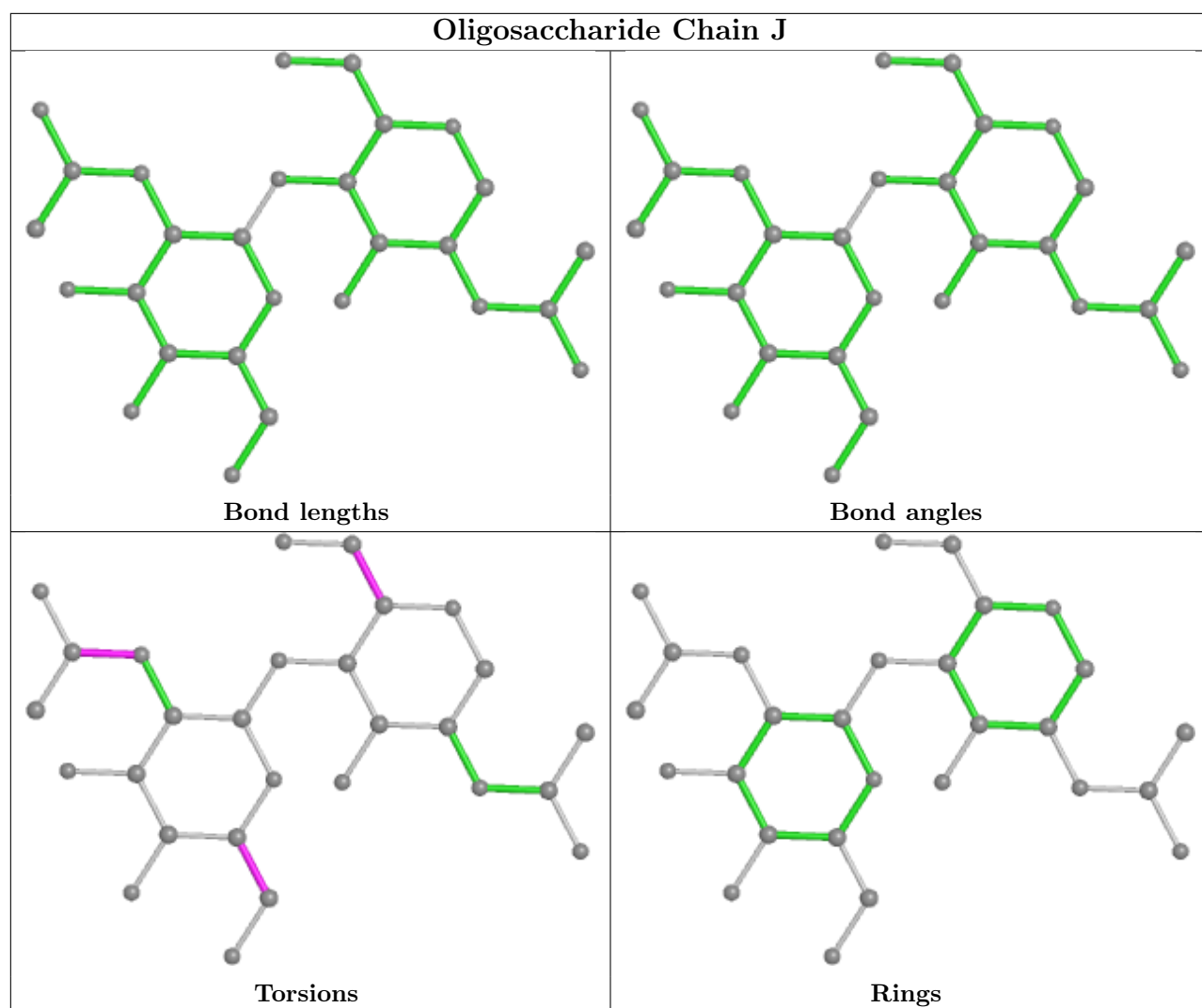
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

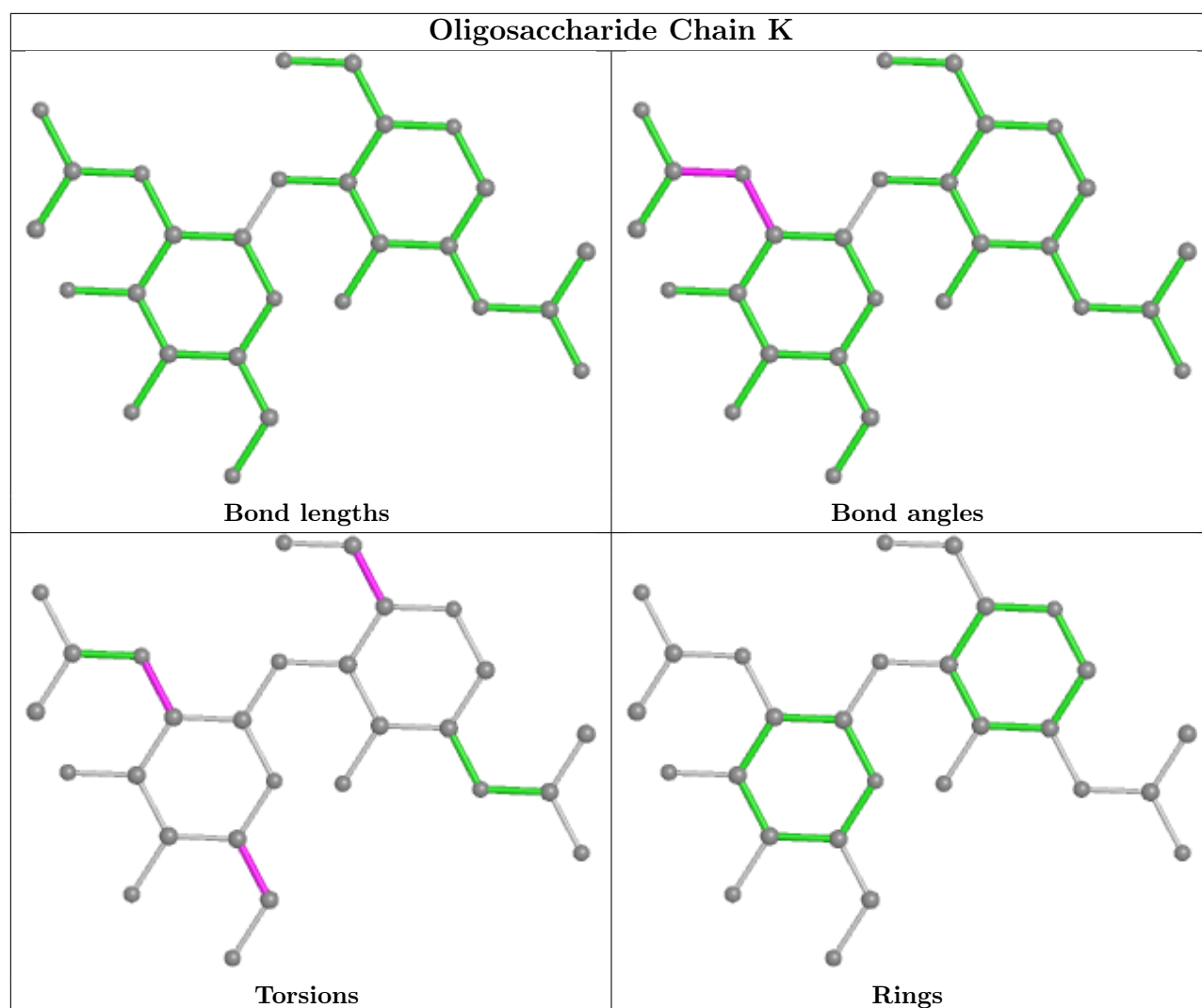


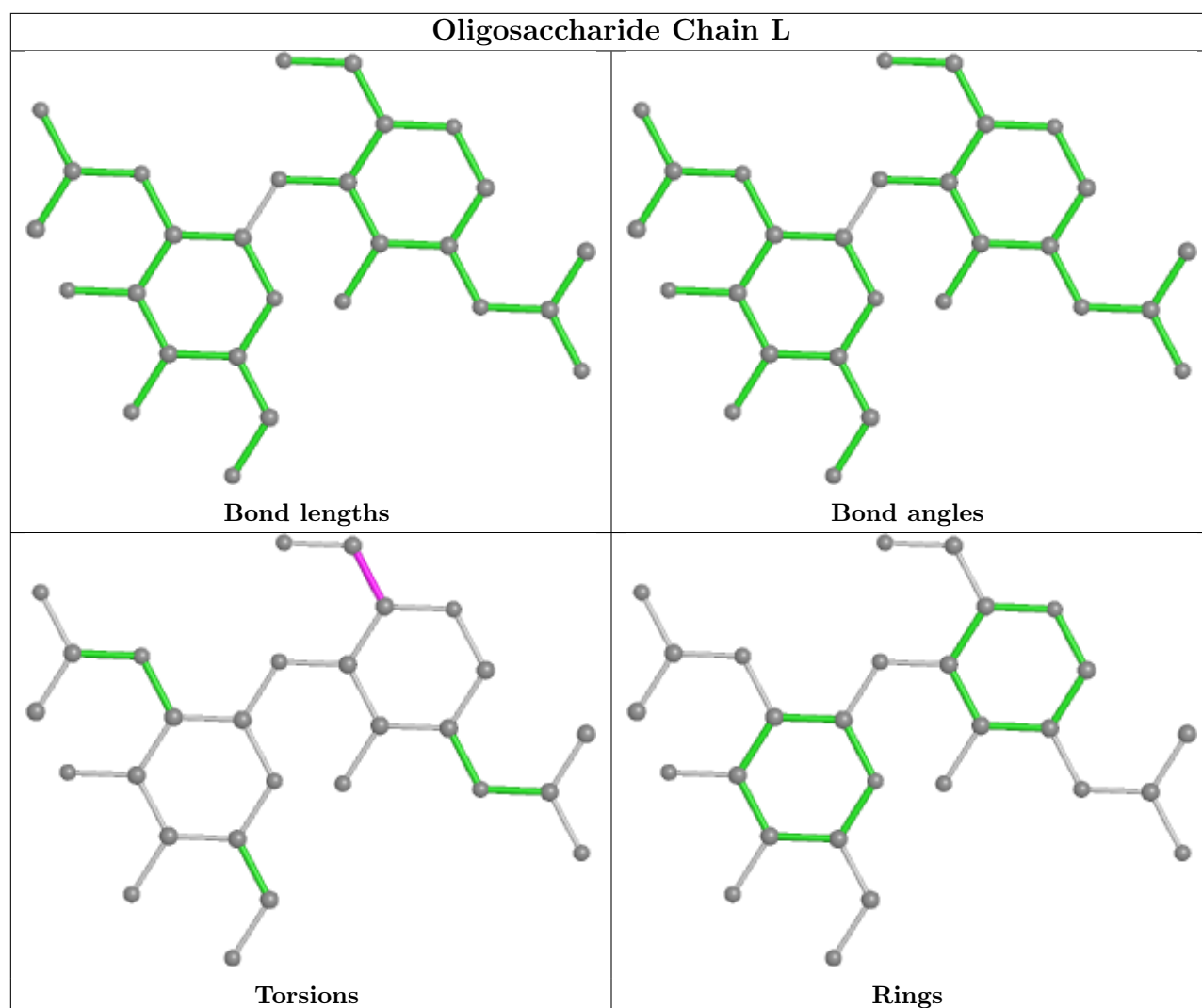


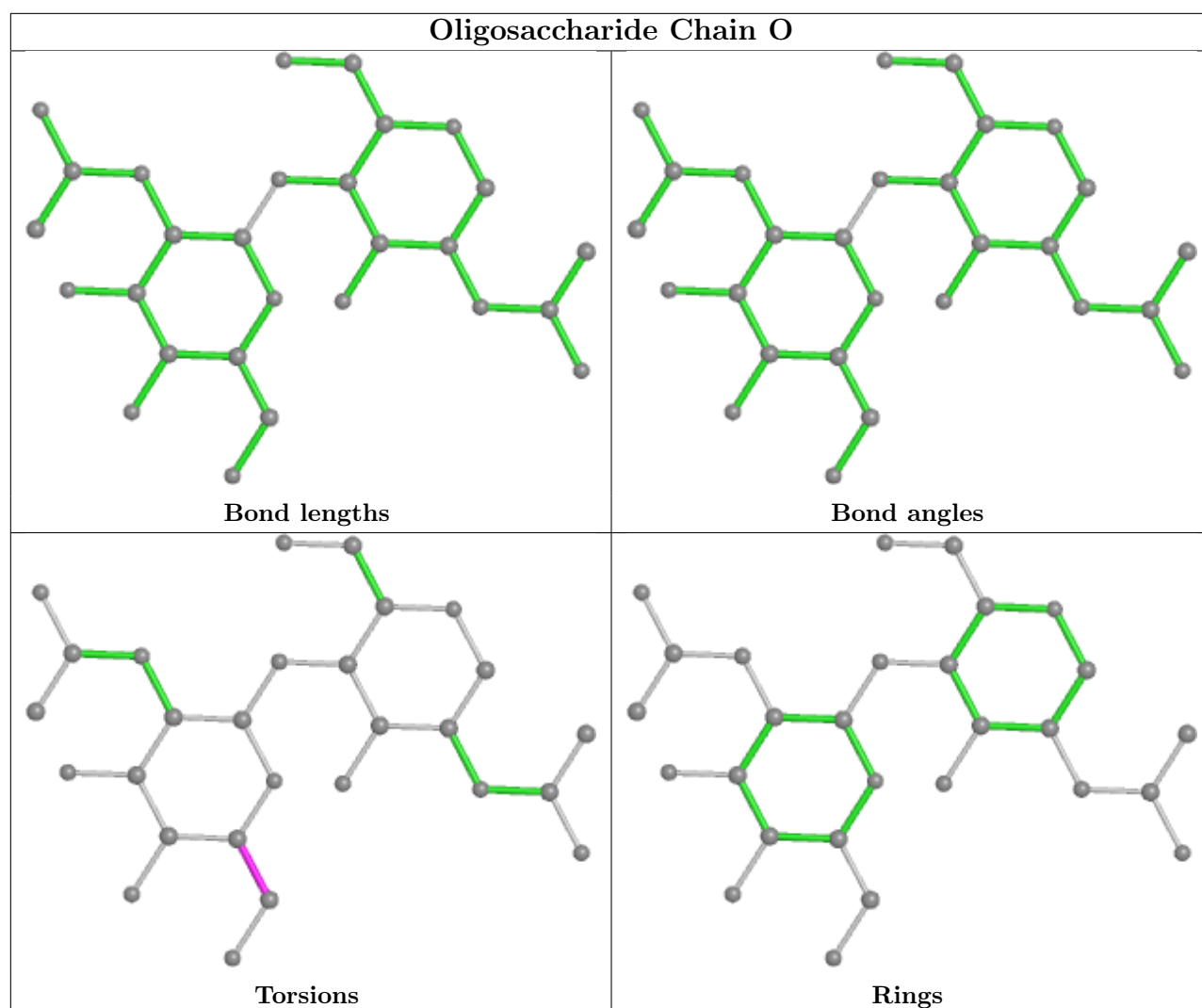


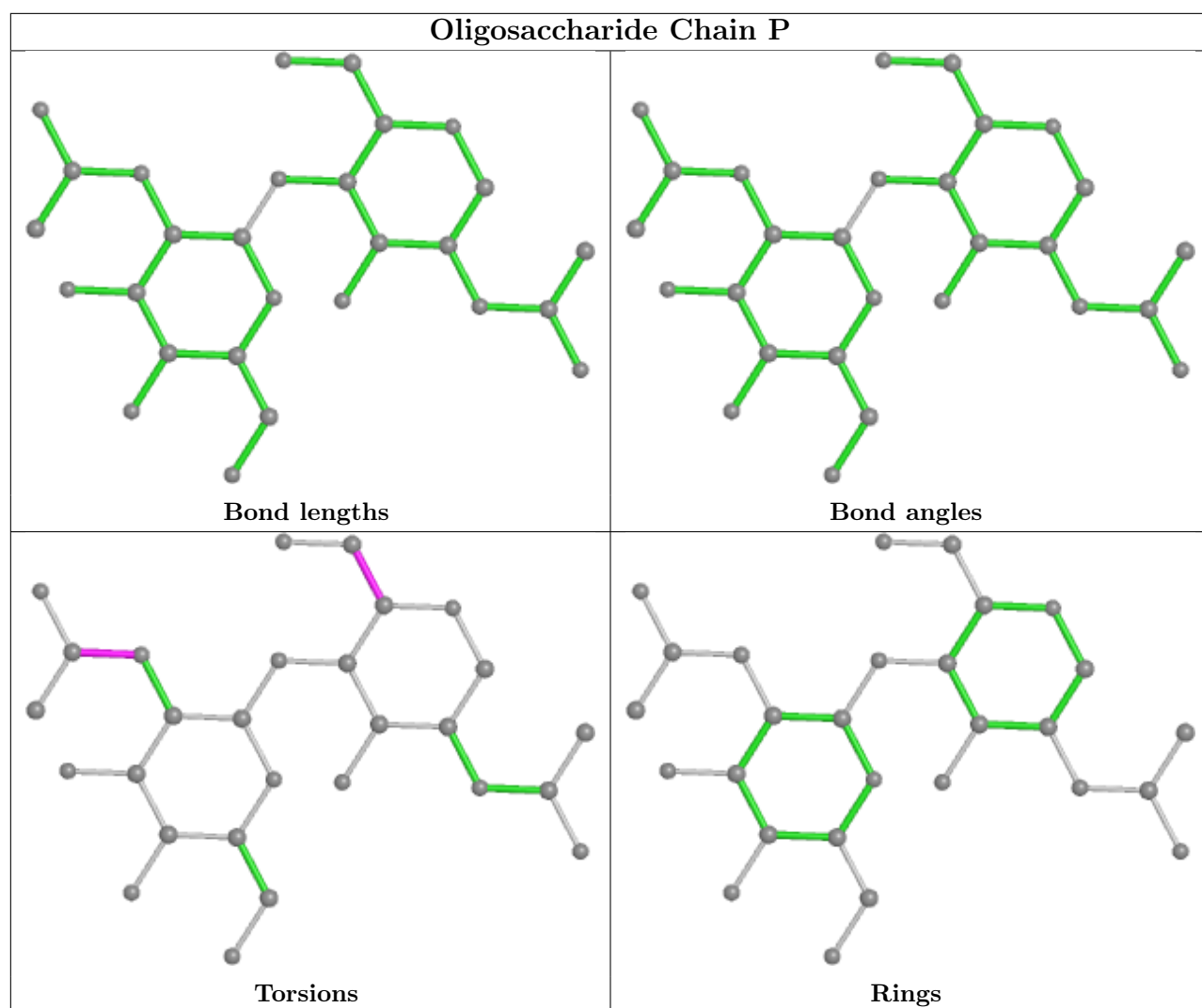


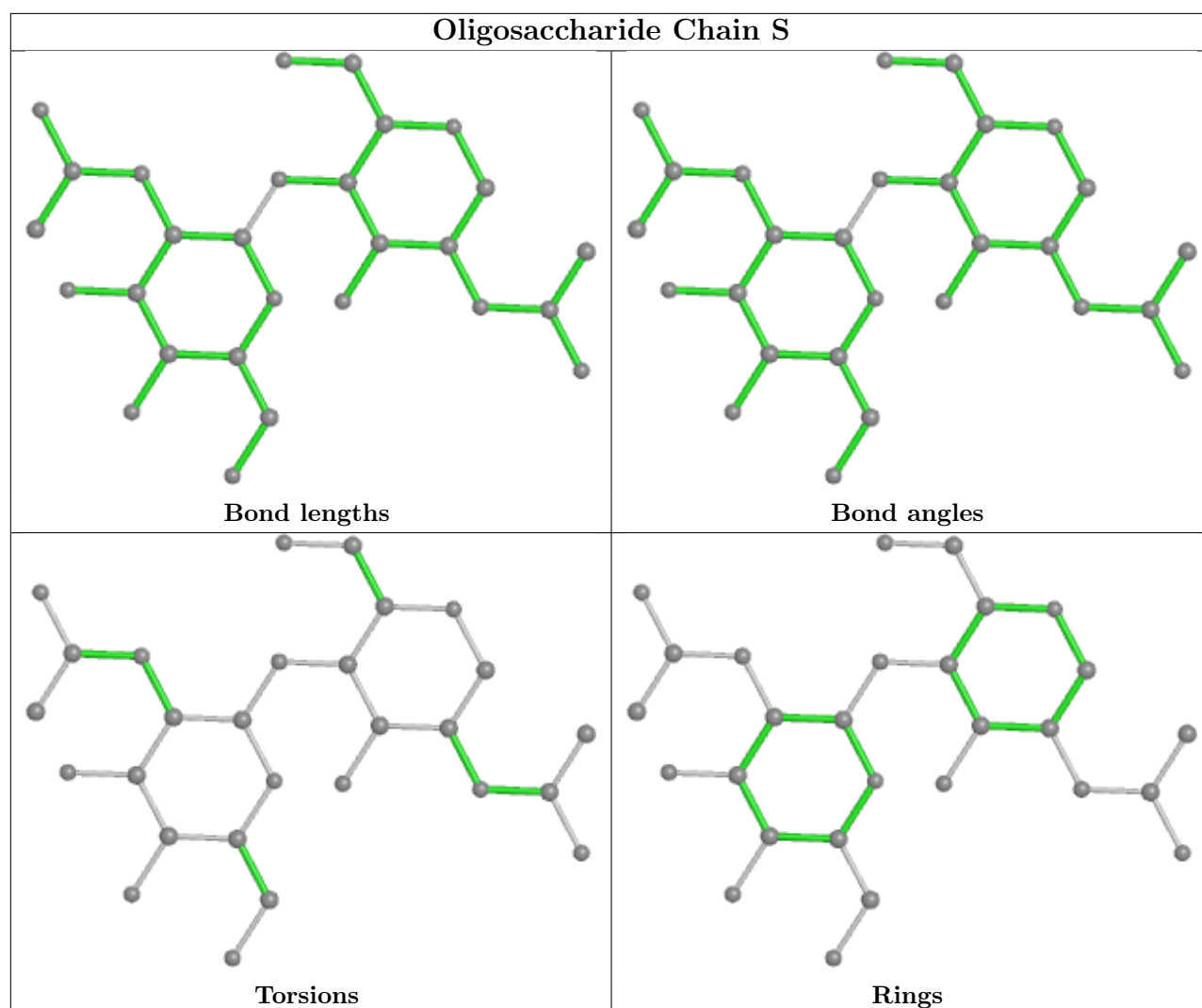


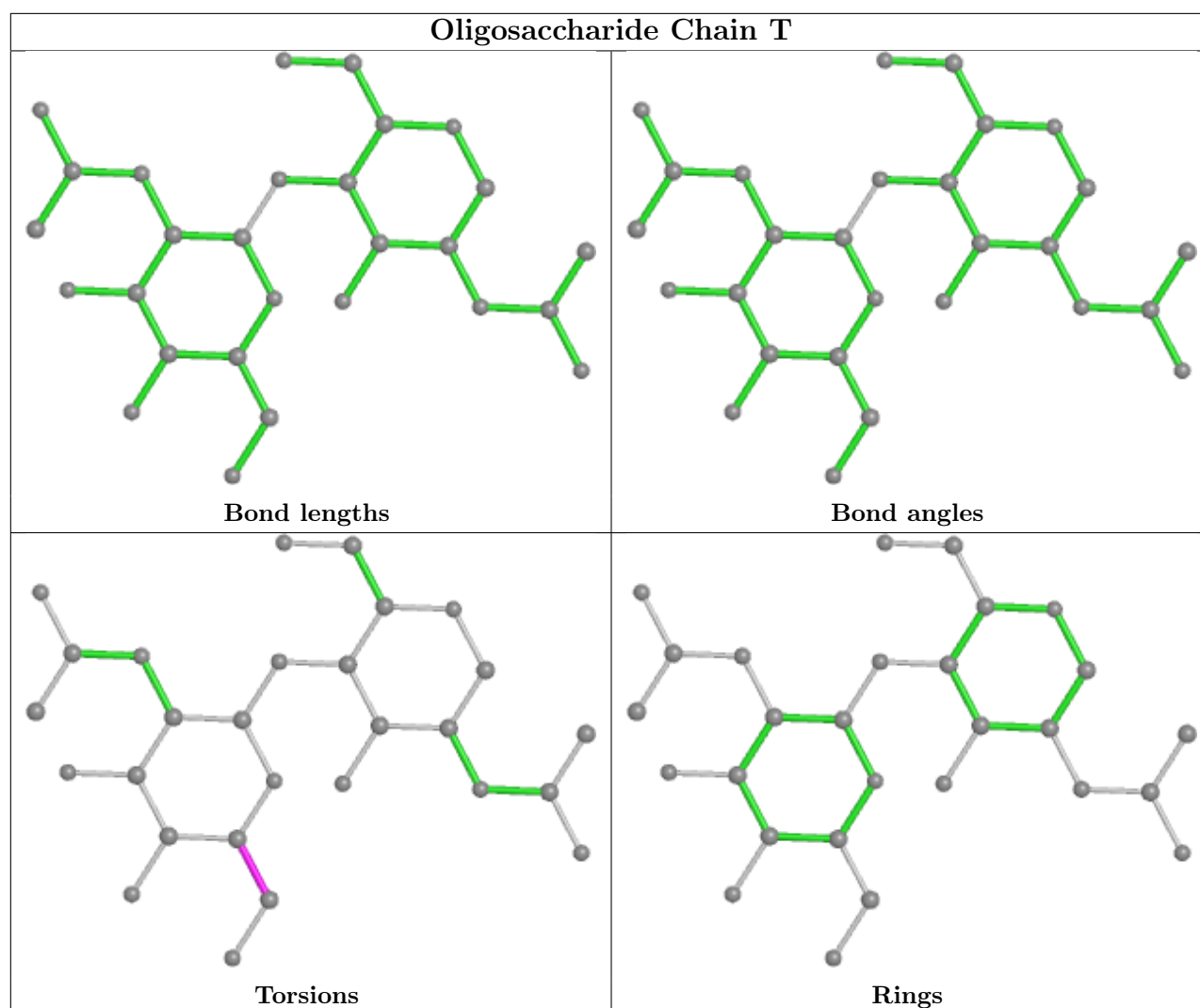












5.6 Ligand geometry [i](#)

28 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	$\# Z > 2$
5	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.42	0
5	NAG	C	1305	1	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	C	1308	1	14,14,15	0.31	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1302	1	14,14,15	0.35	0	17,19,21	0.43	0
5	NAG	C	1309	1	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
5	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.46	0
5	NAG	B	1306	1	14,14,15	0.81	1 (7%)	17,19,21	0.65	0
5	NAG	A	1308	1	14,14,15	0.35	0	17,19,21	0.46	0
5	NAG	A	1309	1	14,14,15	0.32	0	17,19,21	0.52	0
5	NAG	A	1307	1	14,14,15	0.29	0	17,19,21	0.45	0
5	NAG	B	1302	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	C	1304	1	14,14,15	0.78	1 (7%)	17,19,21	1.97	2 (11%)
5	NAG	B	1304	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.46	0
5	NAG	B	1301	1	14,14,15	0.34	0	17,19,21	0.50	0
5	NAG	A	1304	1	14,14,15	0.30	0	17,19,21	0.43	0
5	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	A	1301	1	14,14,15	0.30	0	17,19,21	0.45	0
5	NAG	C	1307	1	14,14,15	0.44	0	17,19,21	0.81	1 (5%)
5	NAG	B	1308	1	14,14,15	0.27	0	17,19,21	0.43	0
5	NAG	B	1309	1	14,14,15	0.60	0	17,19,21	1.98	2 (11%)
5	NAG	C	1301	1	14,14,15	0.30	0	17,19,21	0.44	0
5	NAG	A	1310	1	14,14,15	0.46	0	17,19,21	0.38	0
5	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.44	0
5	NAG	A	1302	1	14,14,15	0.32	0	17,19,21	0.48	0
5	NAG	A	1306	1	14,14,15	0.28	0	17,19,21	0.50	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	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	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)
5	B	1306	NAG	O5-C1	2.81	1.48	1.43
5	C	1304	NAG	C1-C2	2.37	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1309	NAG	C2-N2-C7	6.94	132.79	122.90
5	C	1304	NAG	C2-N2-C7	6.85	132.65	122.90
5	B	1309	NAG	C1-C2-N2	3.24	116.03	110.49
5	C	1304	NAG	C1-C2-N2	3.04	115.69	110.49
5	C	1309	NAG	C2-N2-C7	2.45	126.39	122.90

There are no chirality outliers.

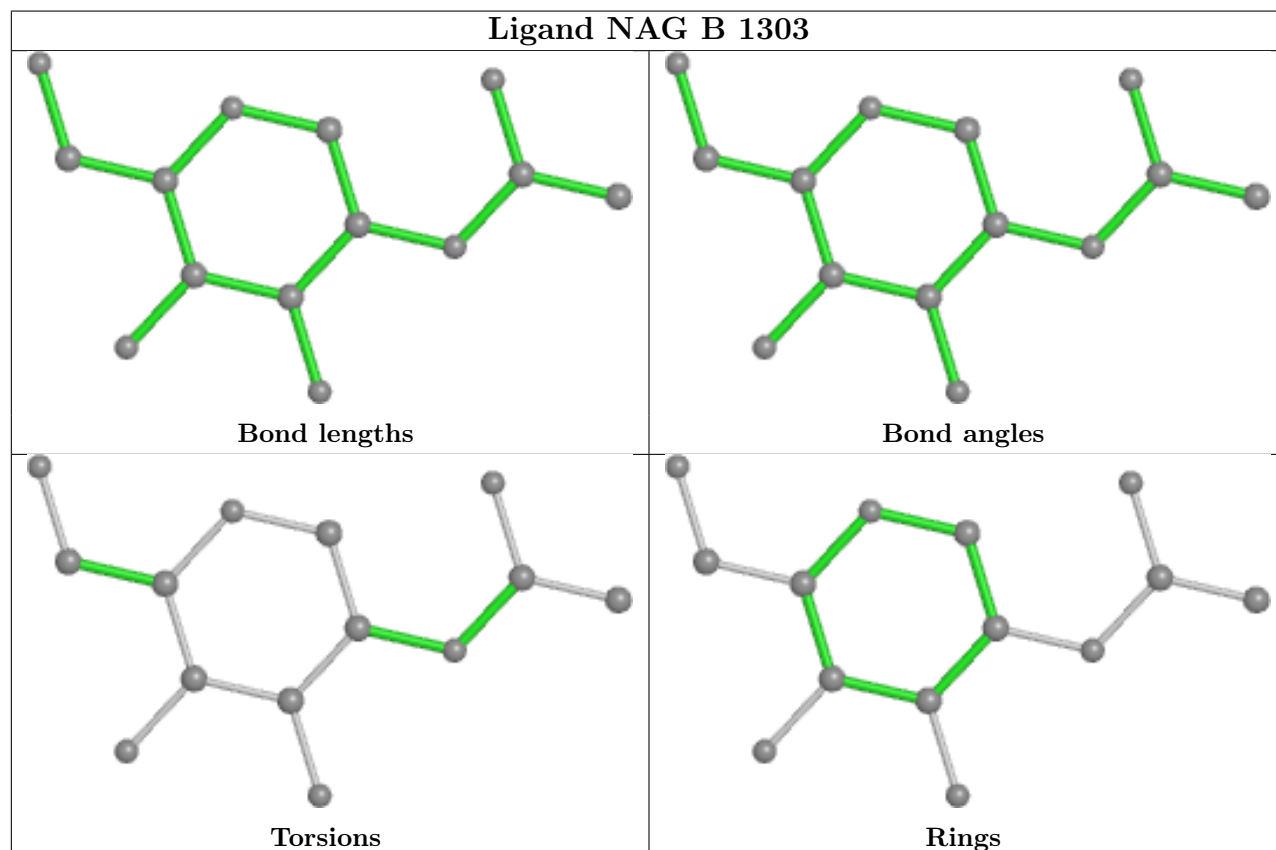
5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1301	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6

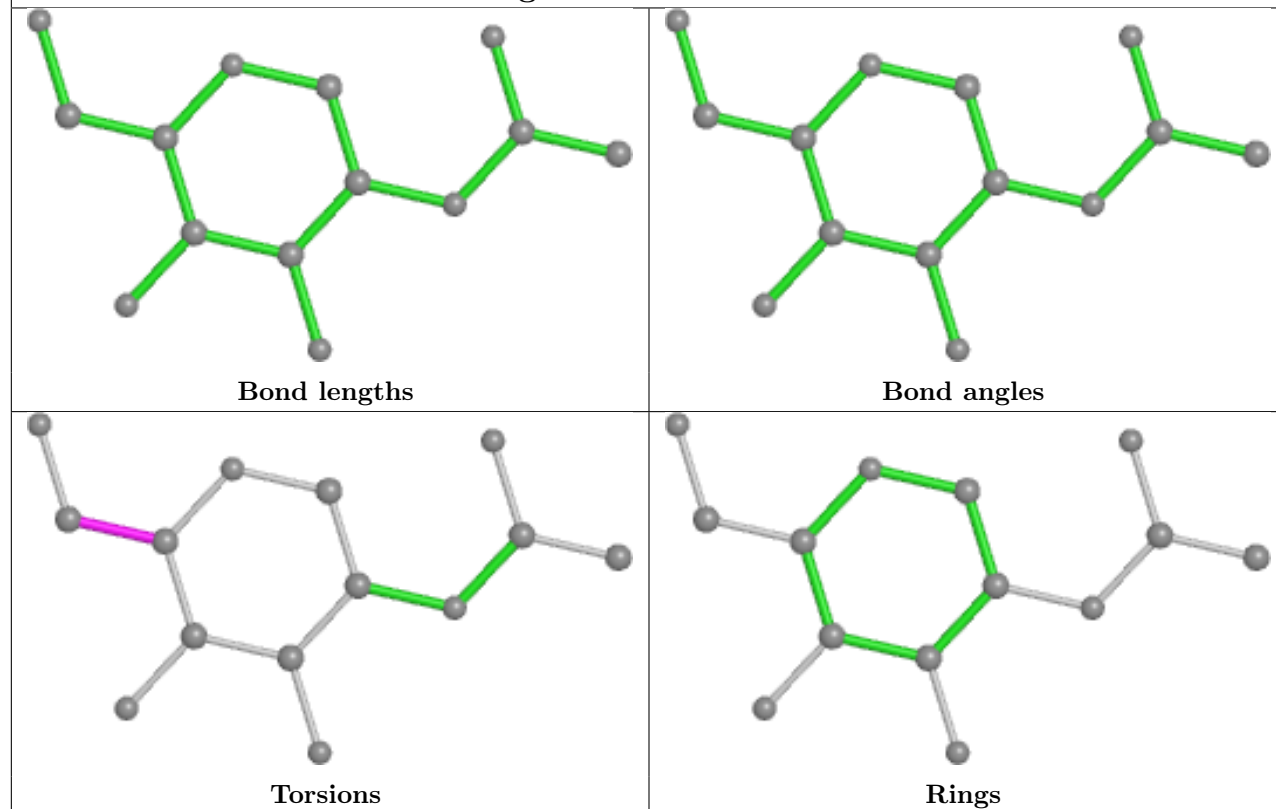
There are no ring outliers.

No monomer is involved in short contacts.

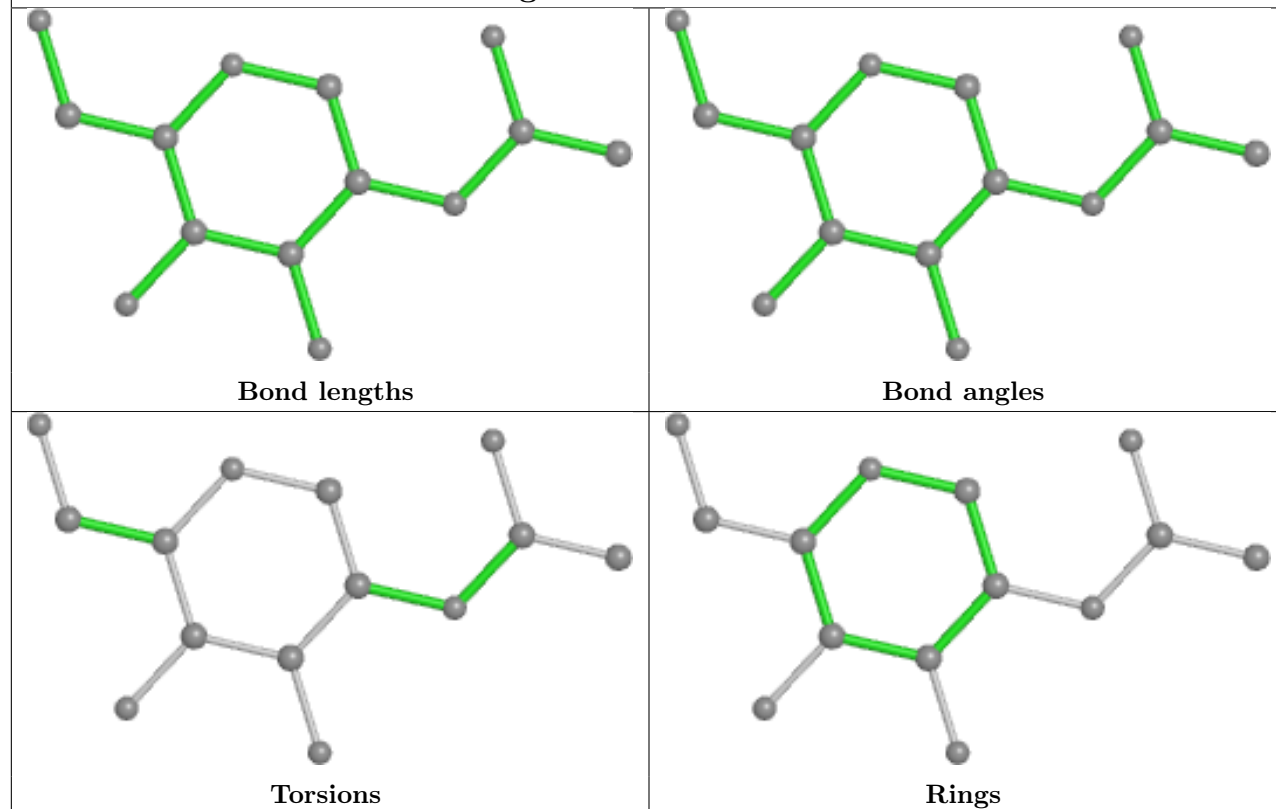
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

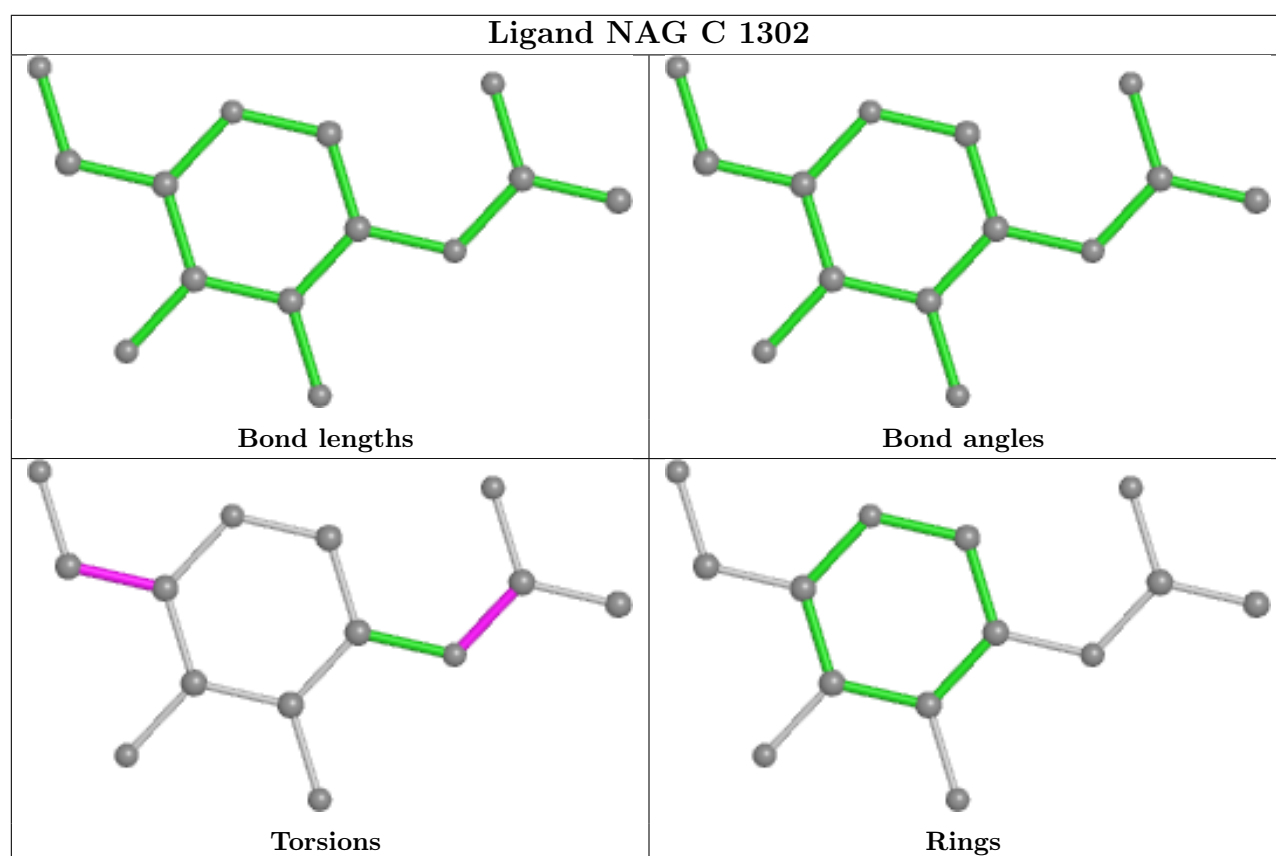
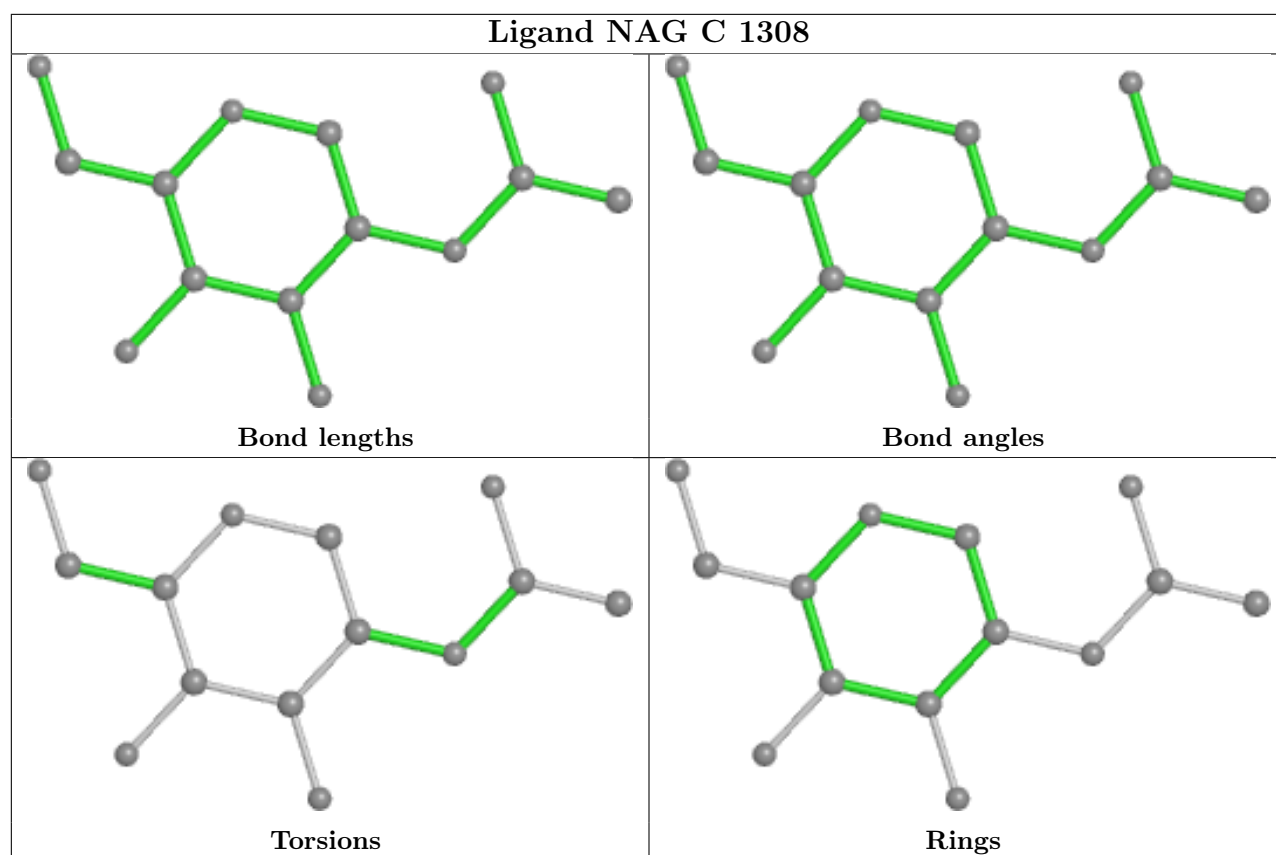


Ligand NAG A 1305

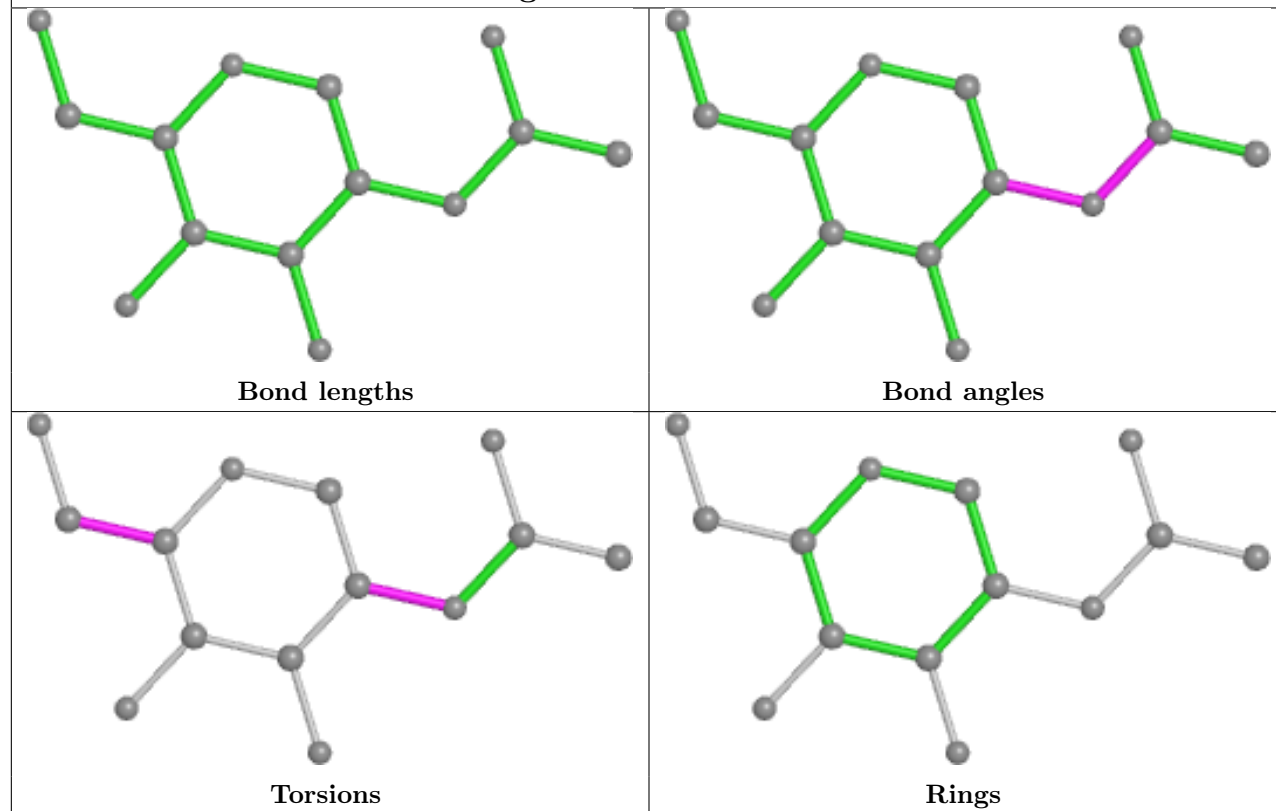


Ligand NAG C 1305

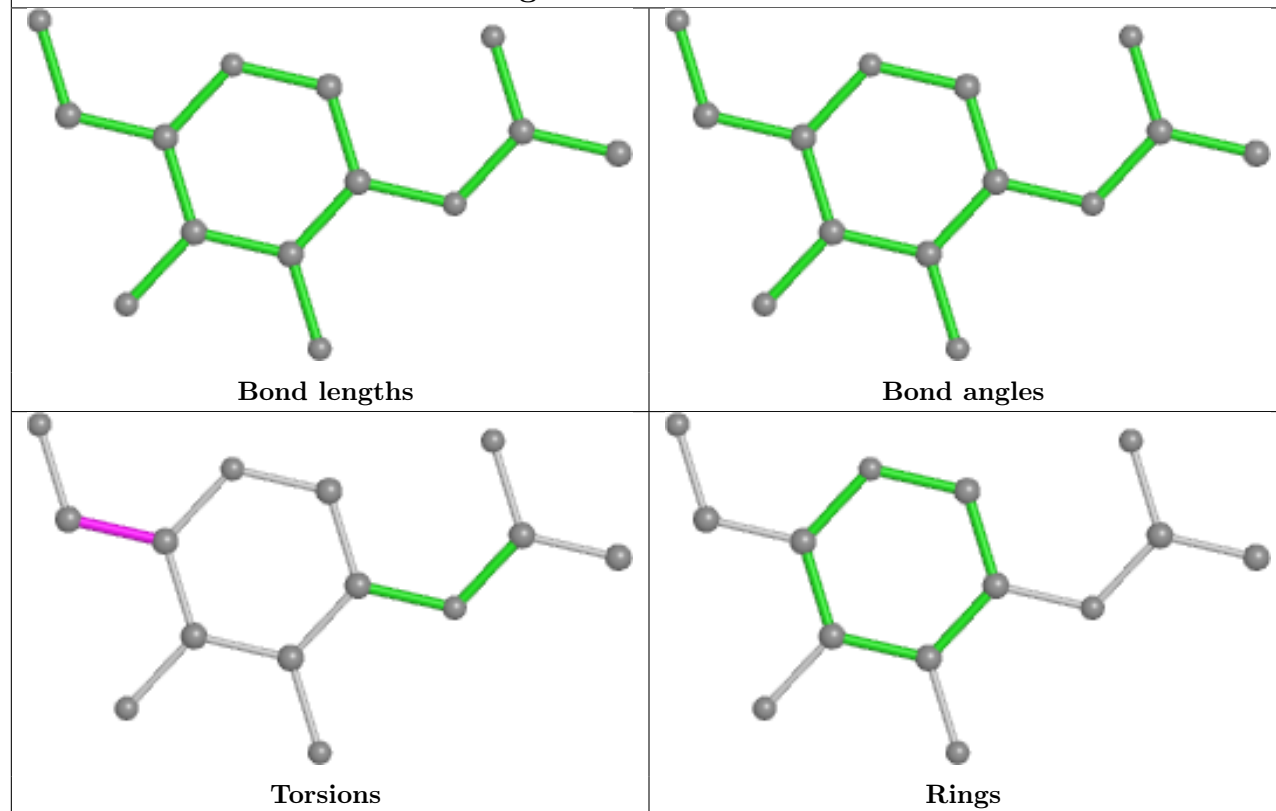


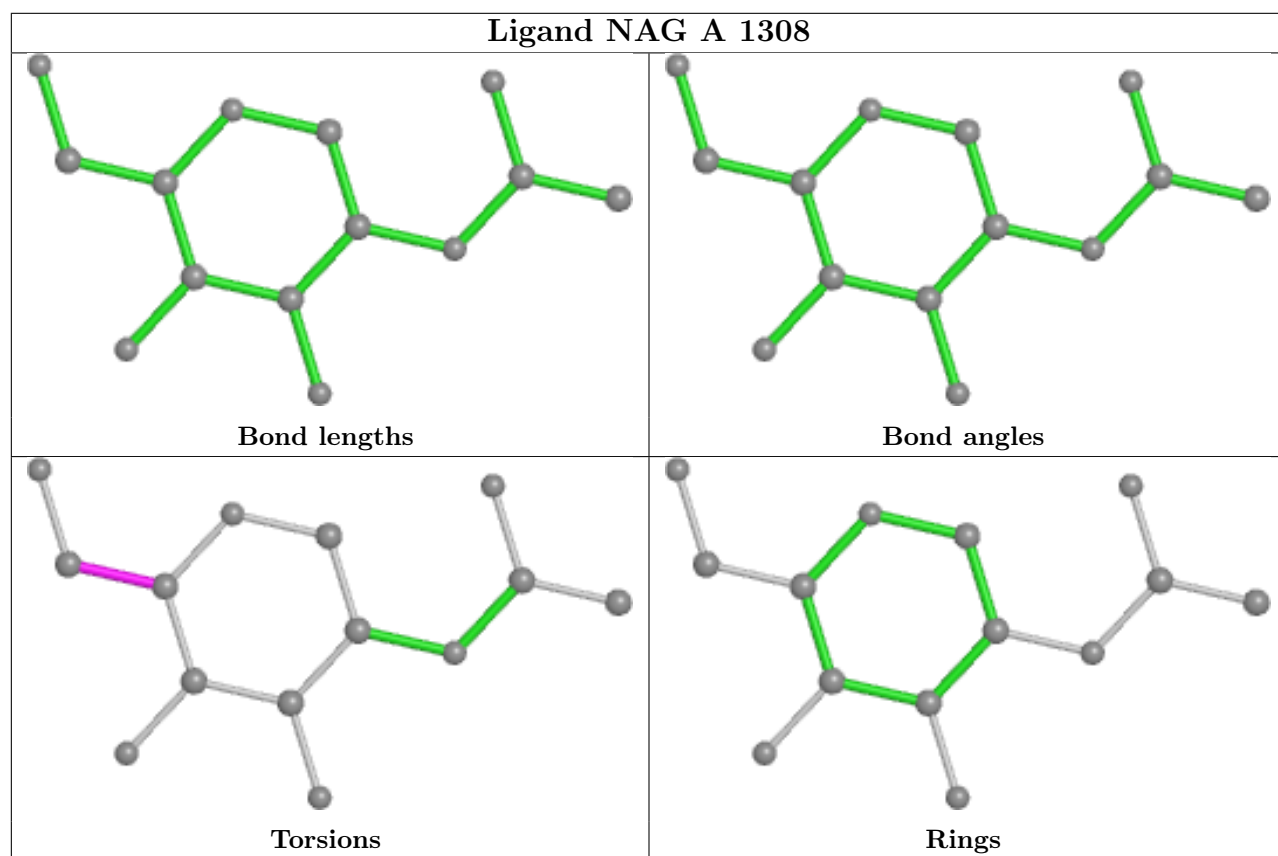
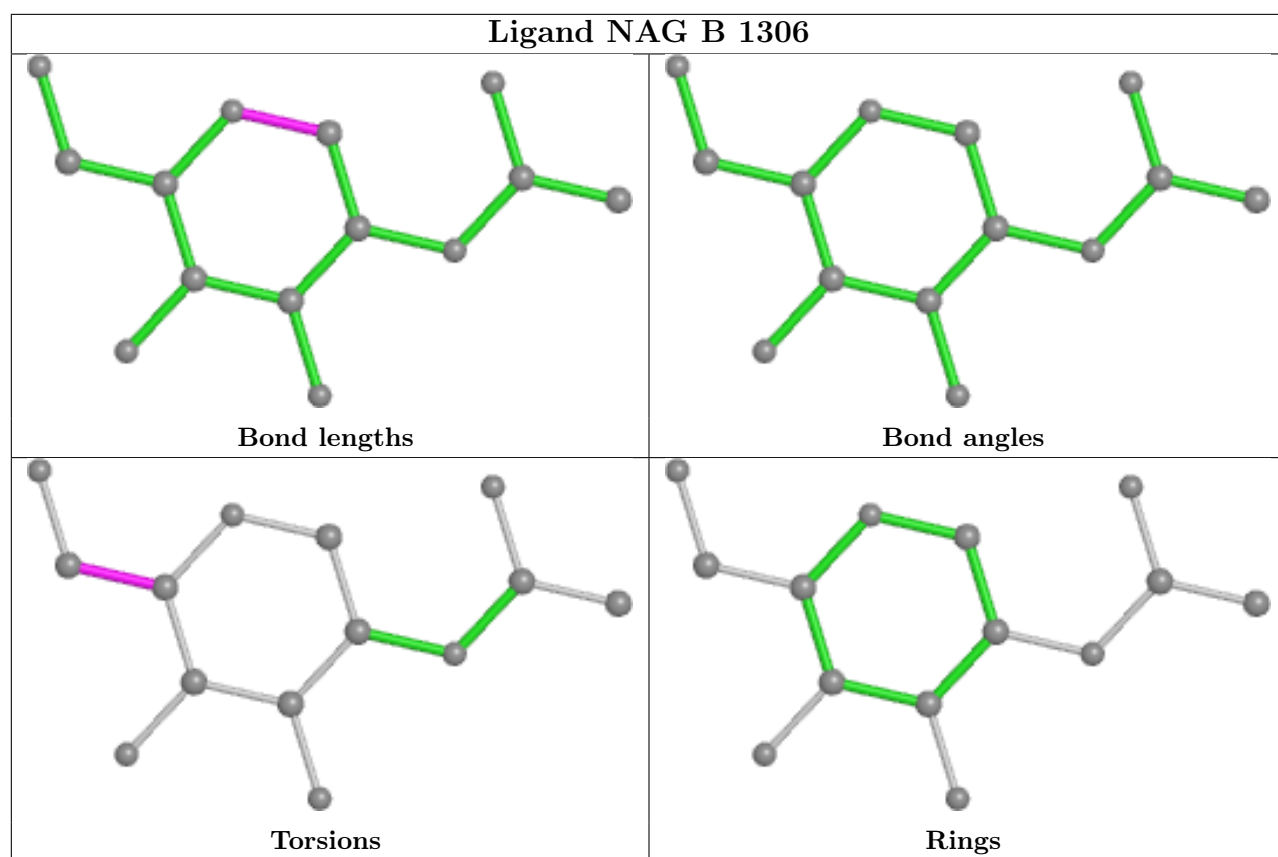


Ligand NAG C 1309

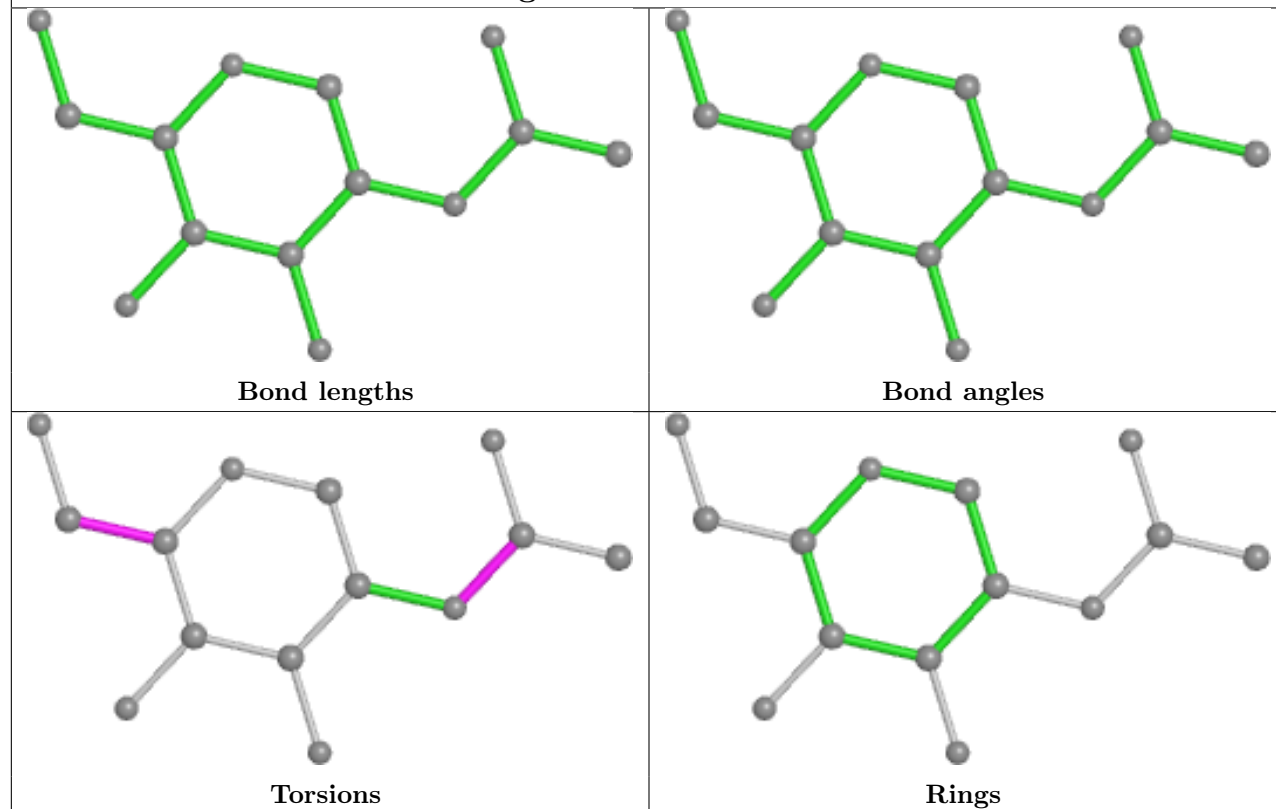


Ligand NAG C 1306

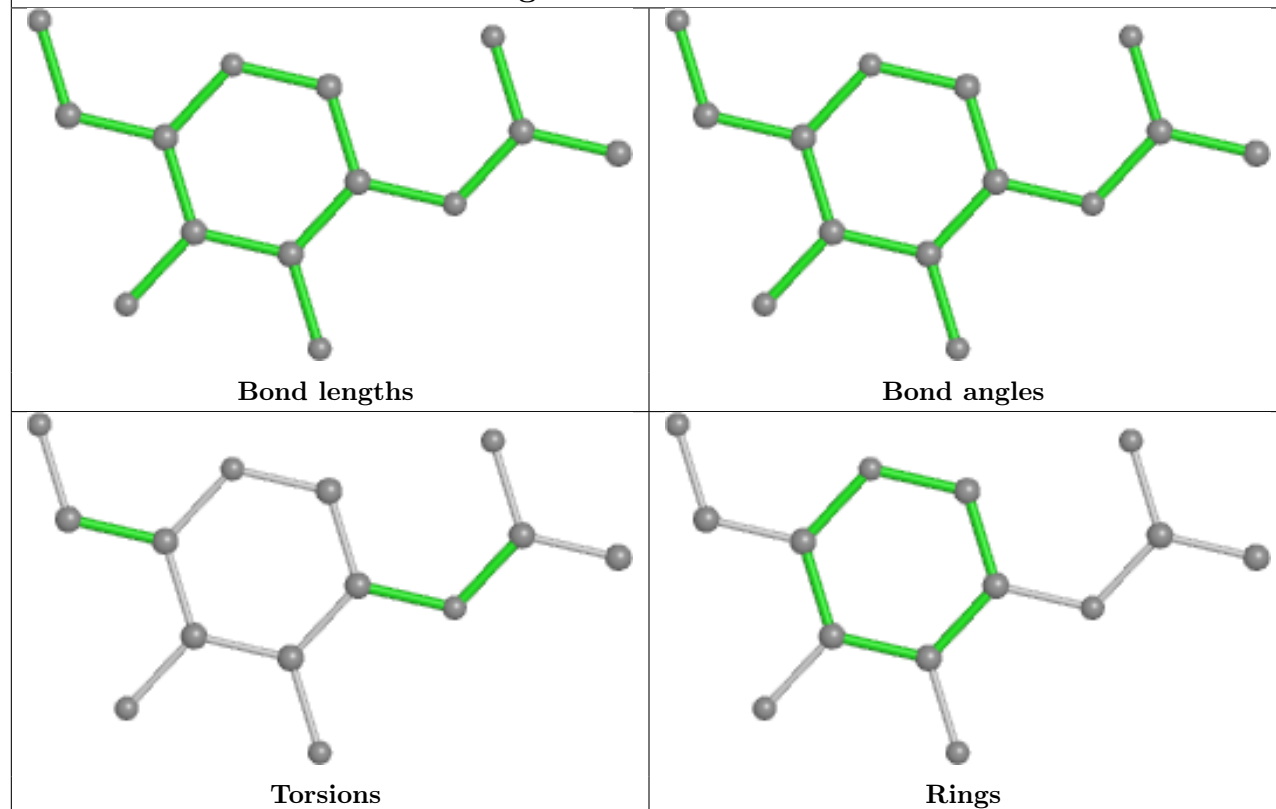




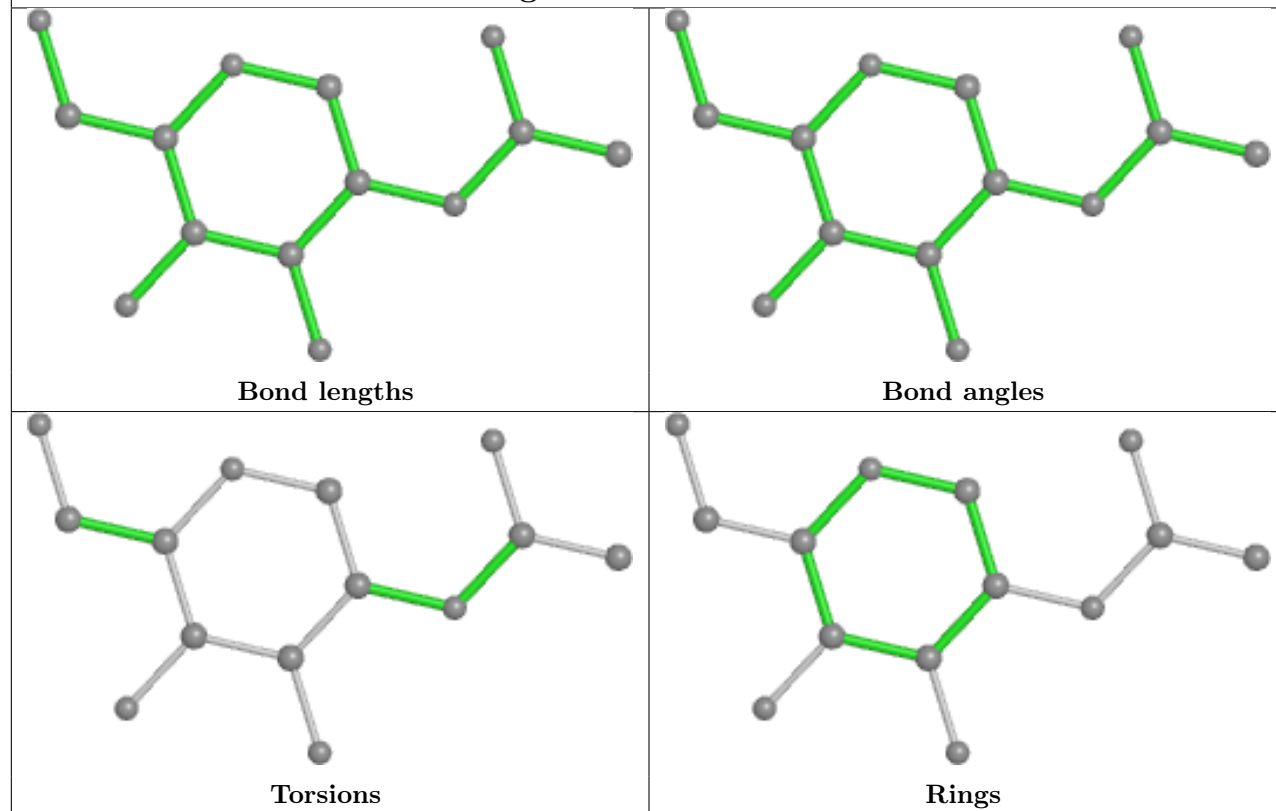
Ligand NAG A 1309



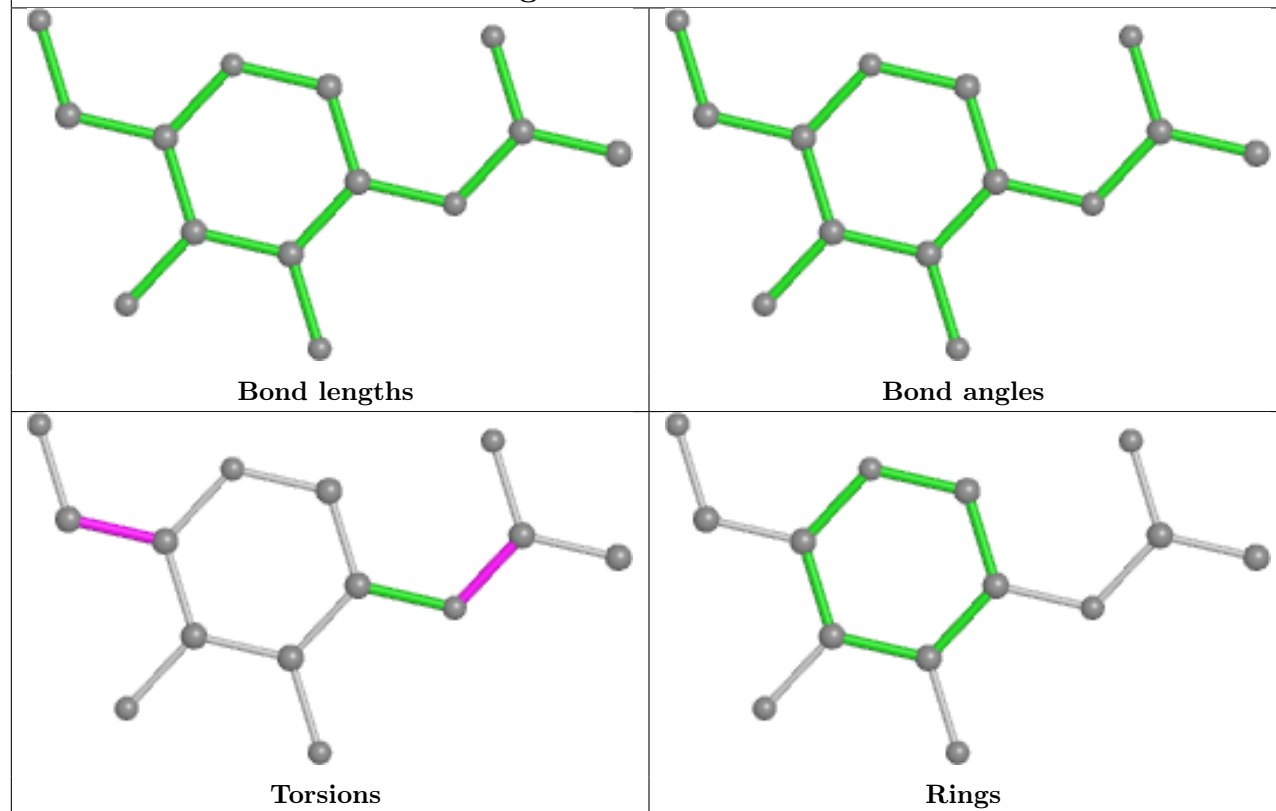
Ligand NAG A 1307



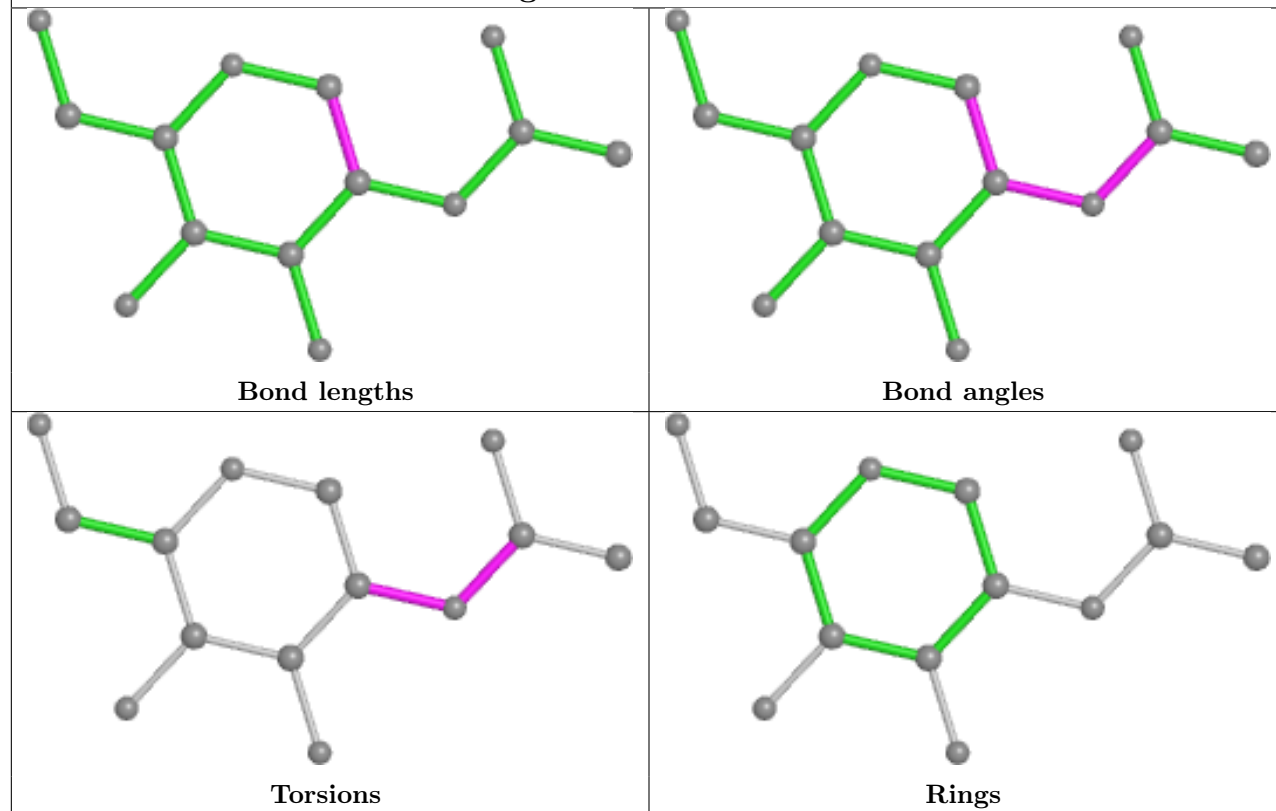
Ligand NAG B 1302



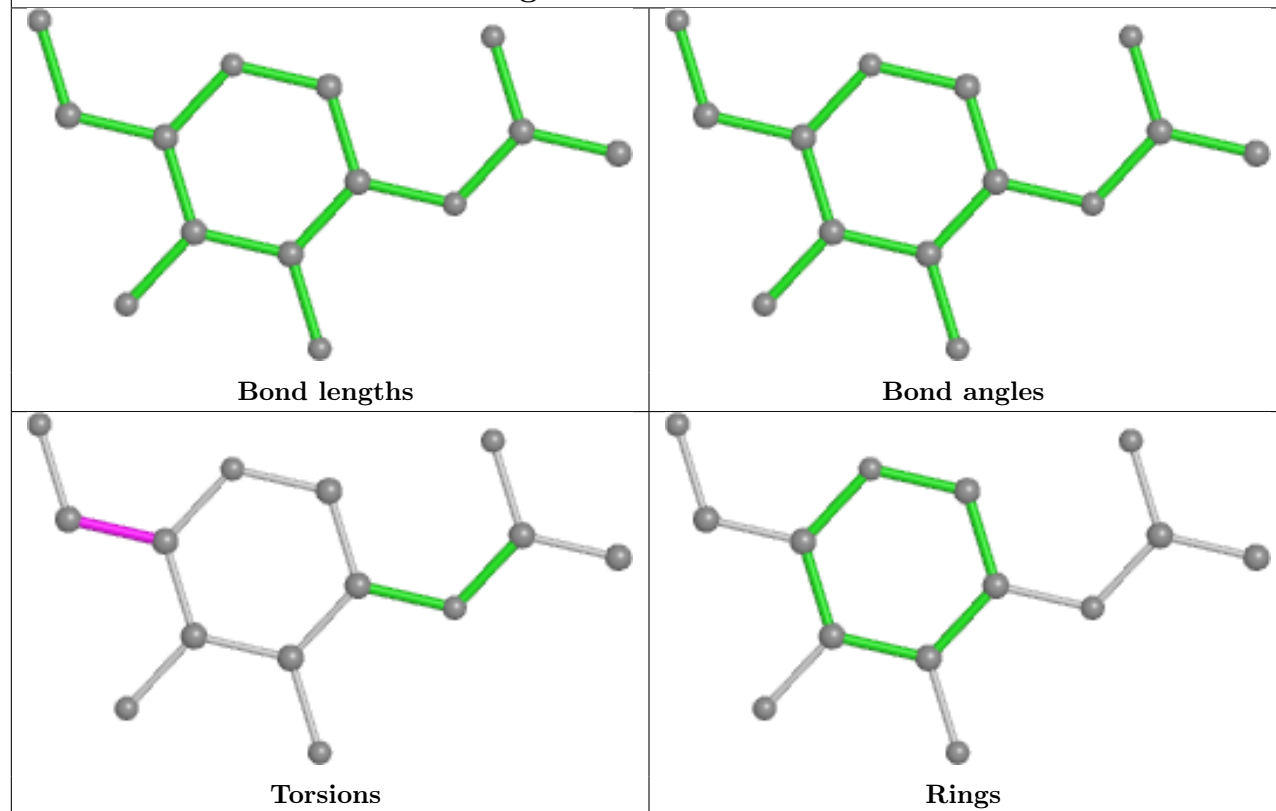
Ligand NAG B 1305

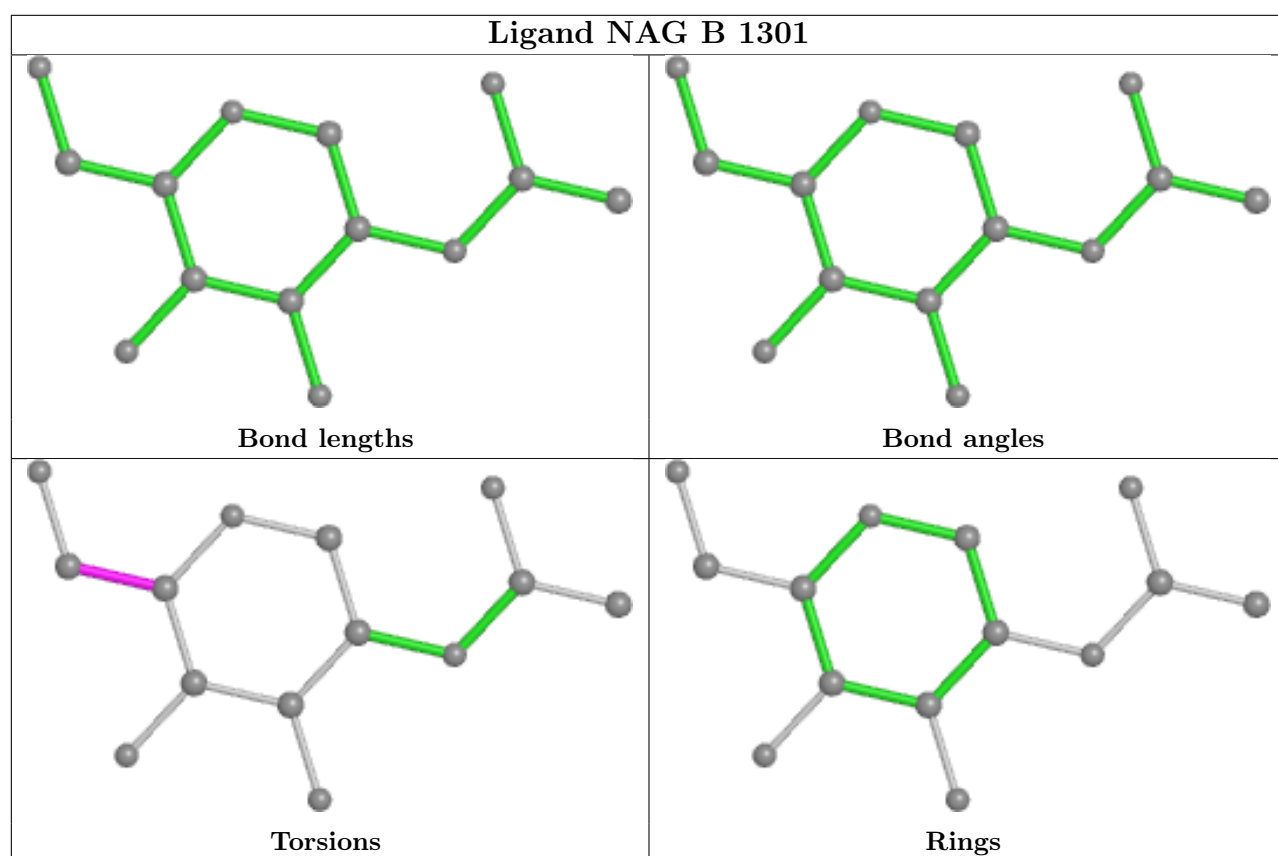
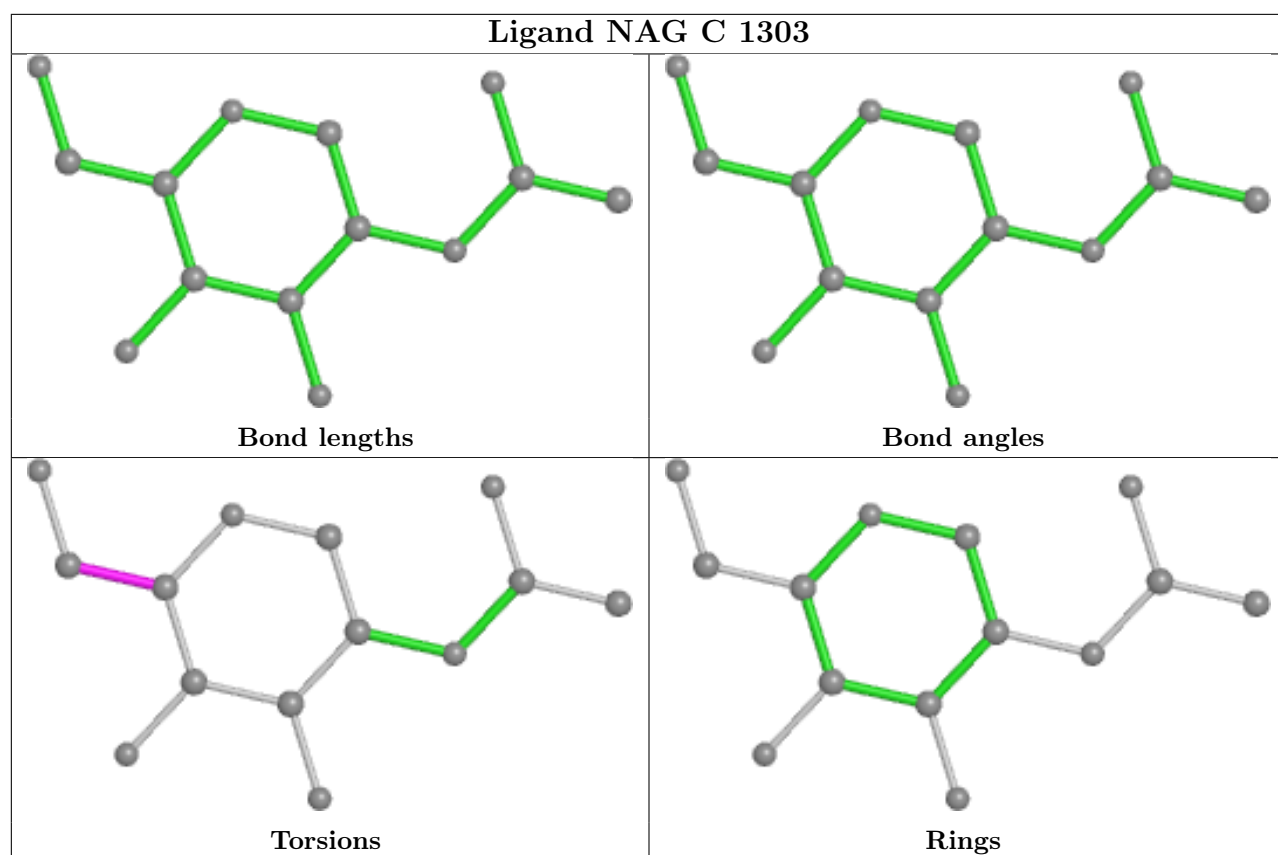


Ligand NAG C 1304

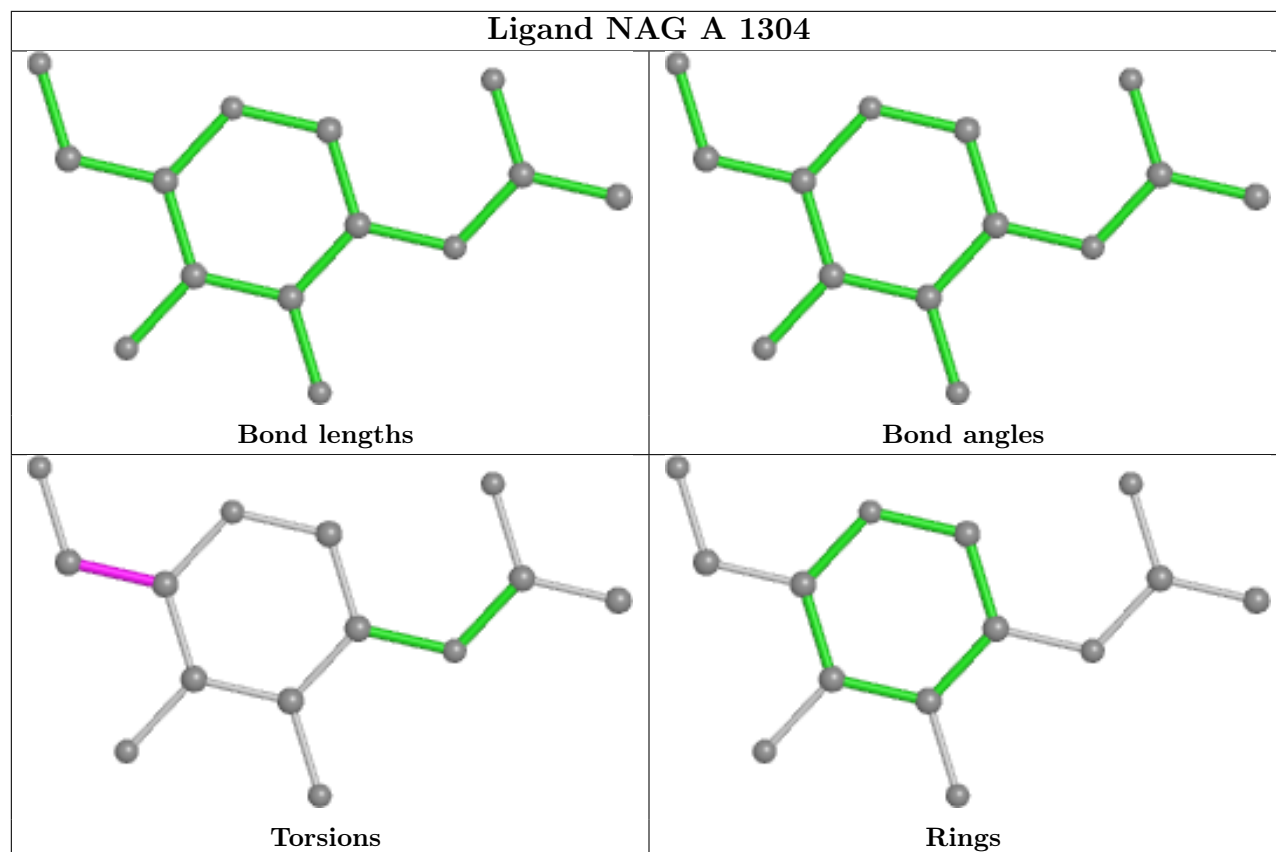


Ligand NAG B 1304

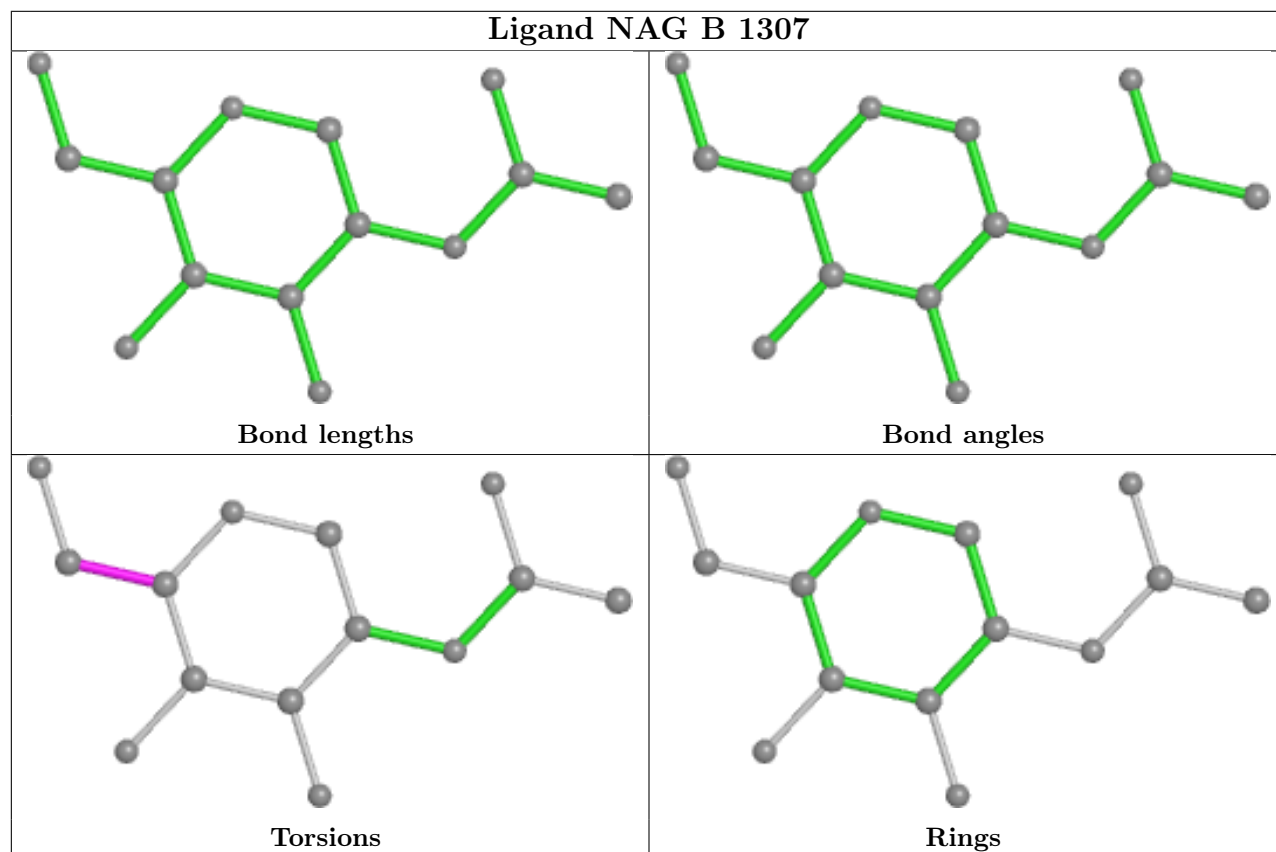


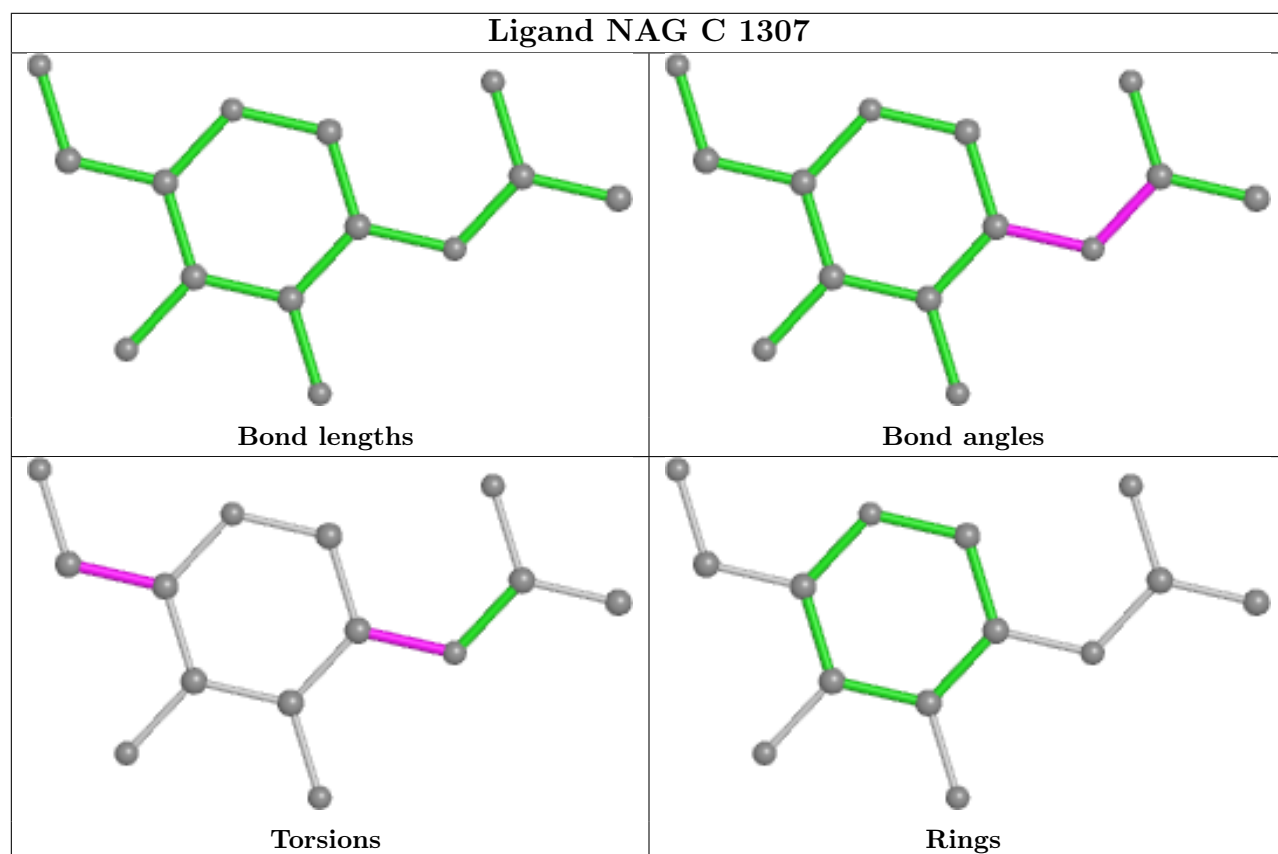
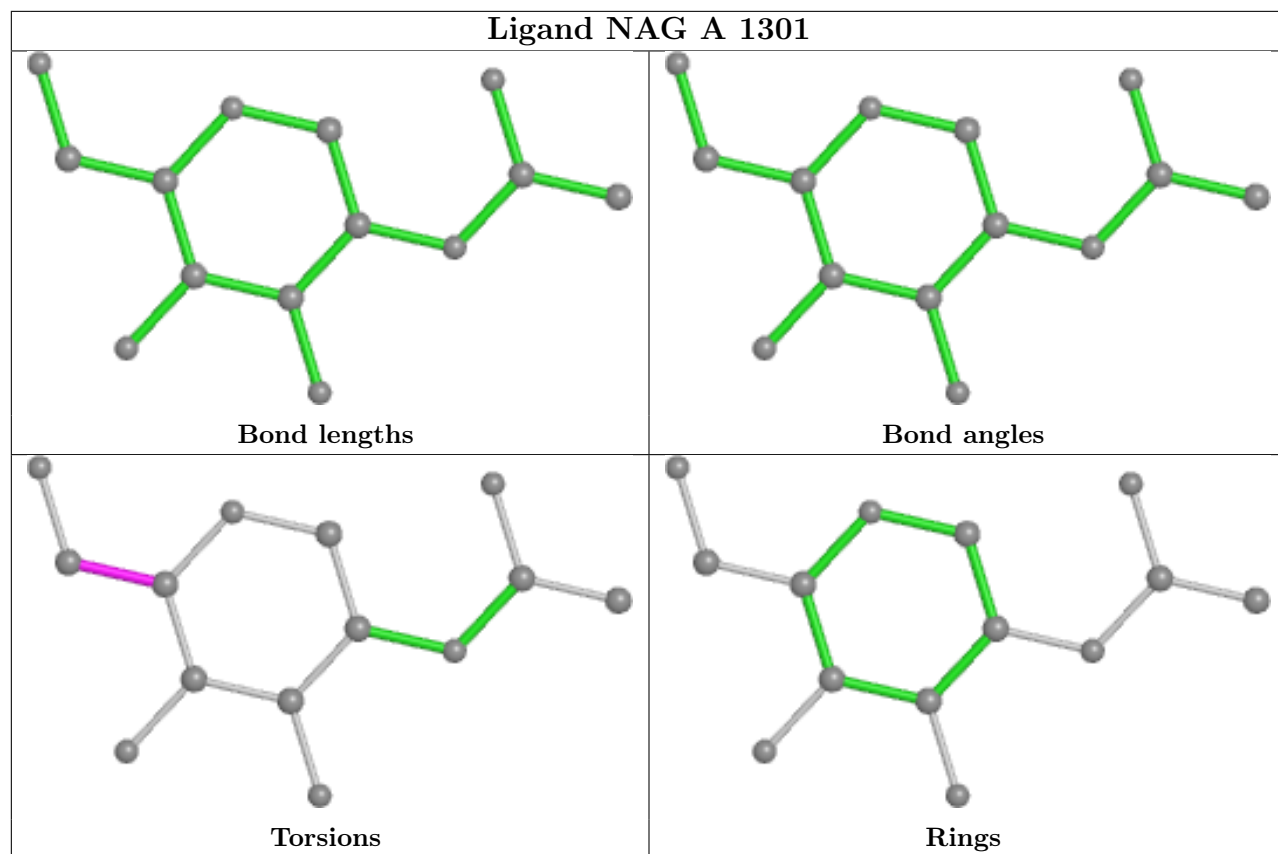


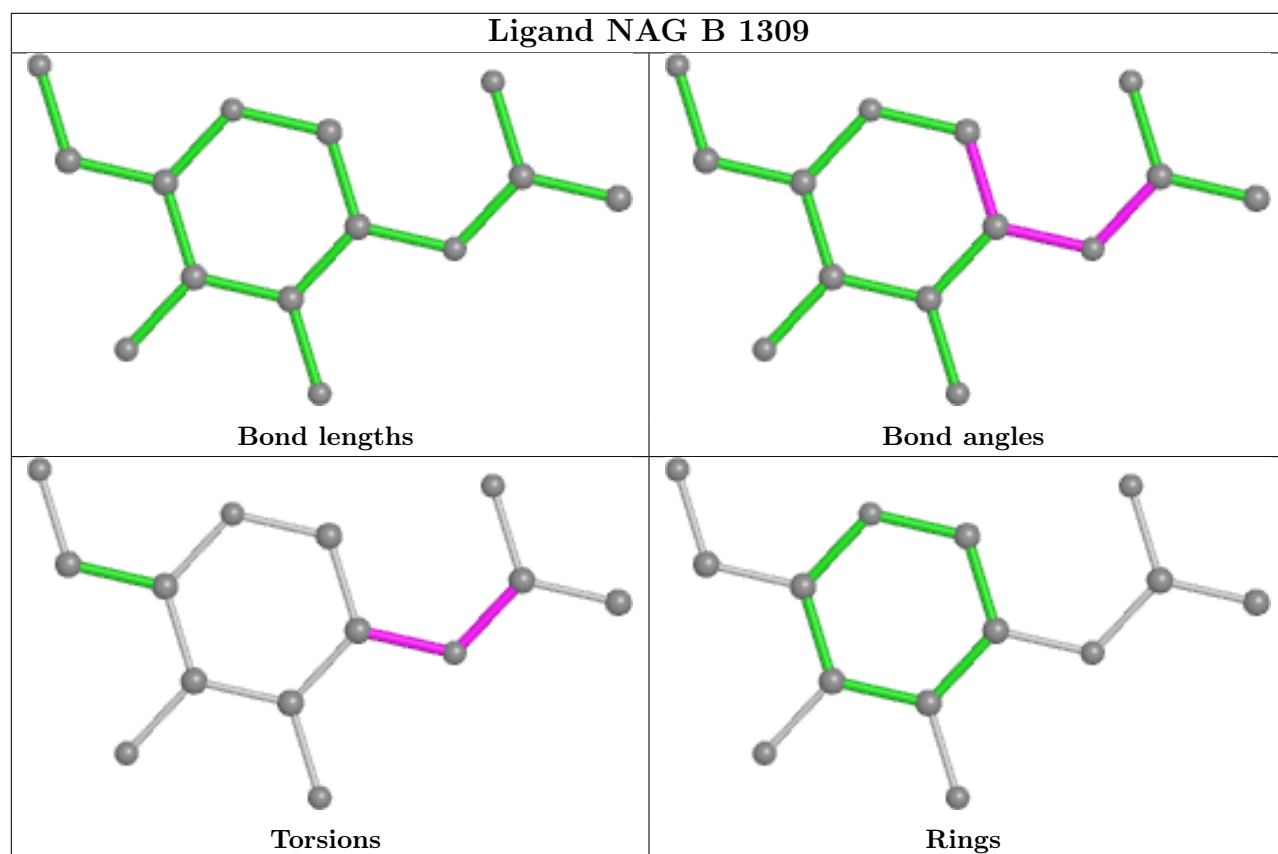
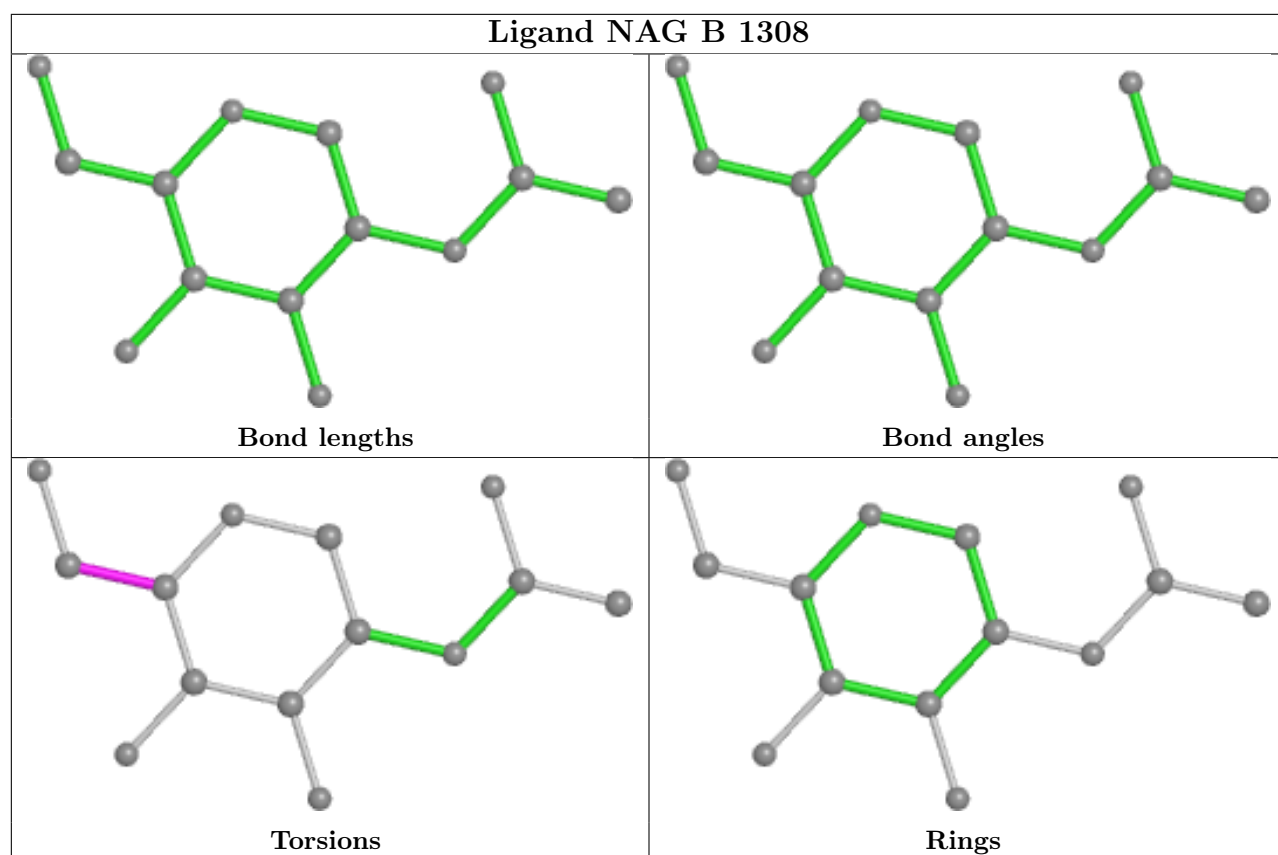
Ligand NAG A 1304

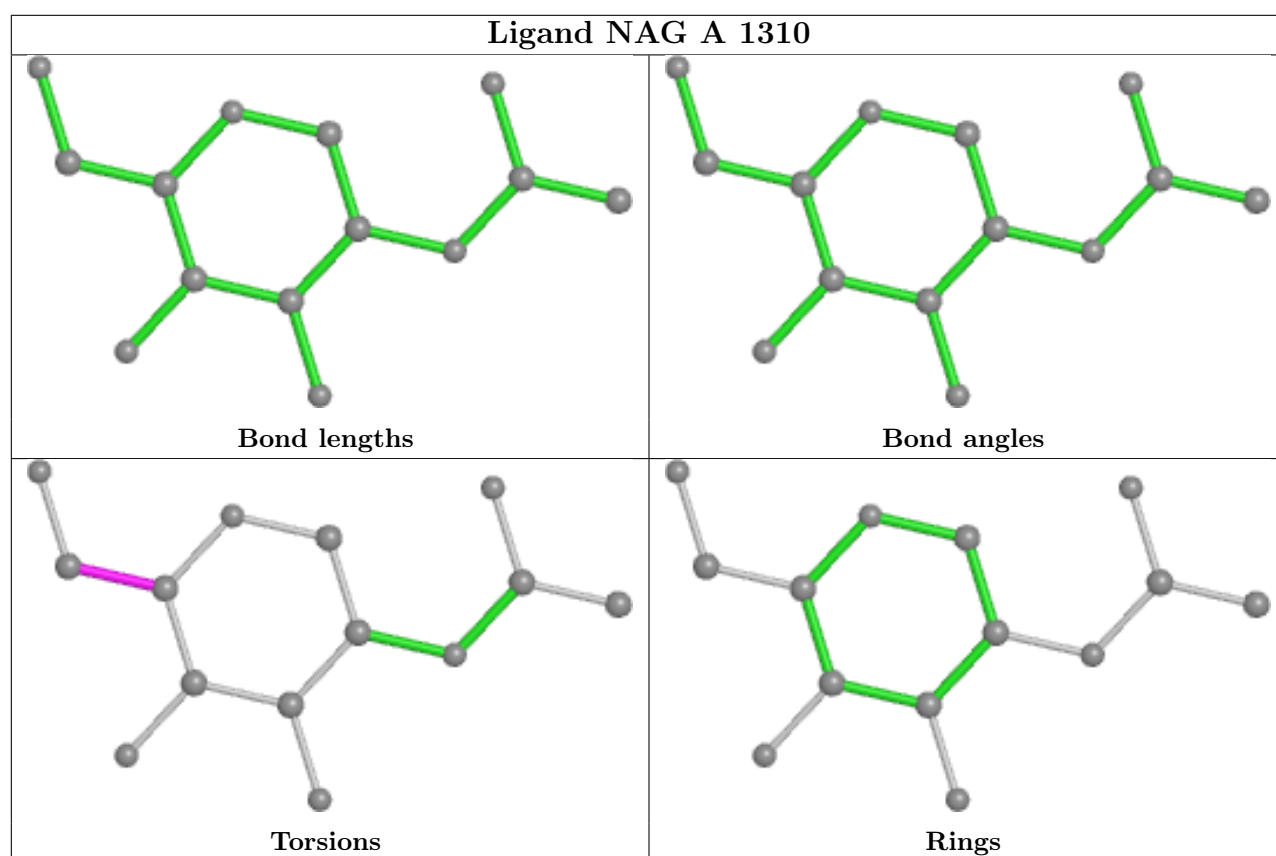
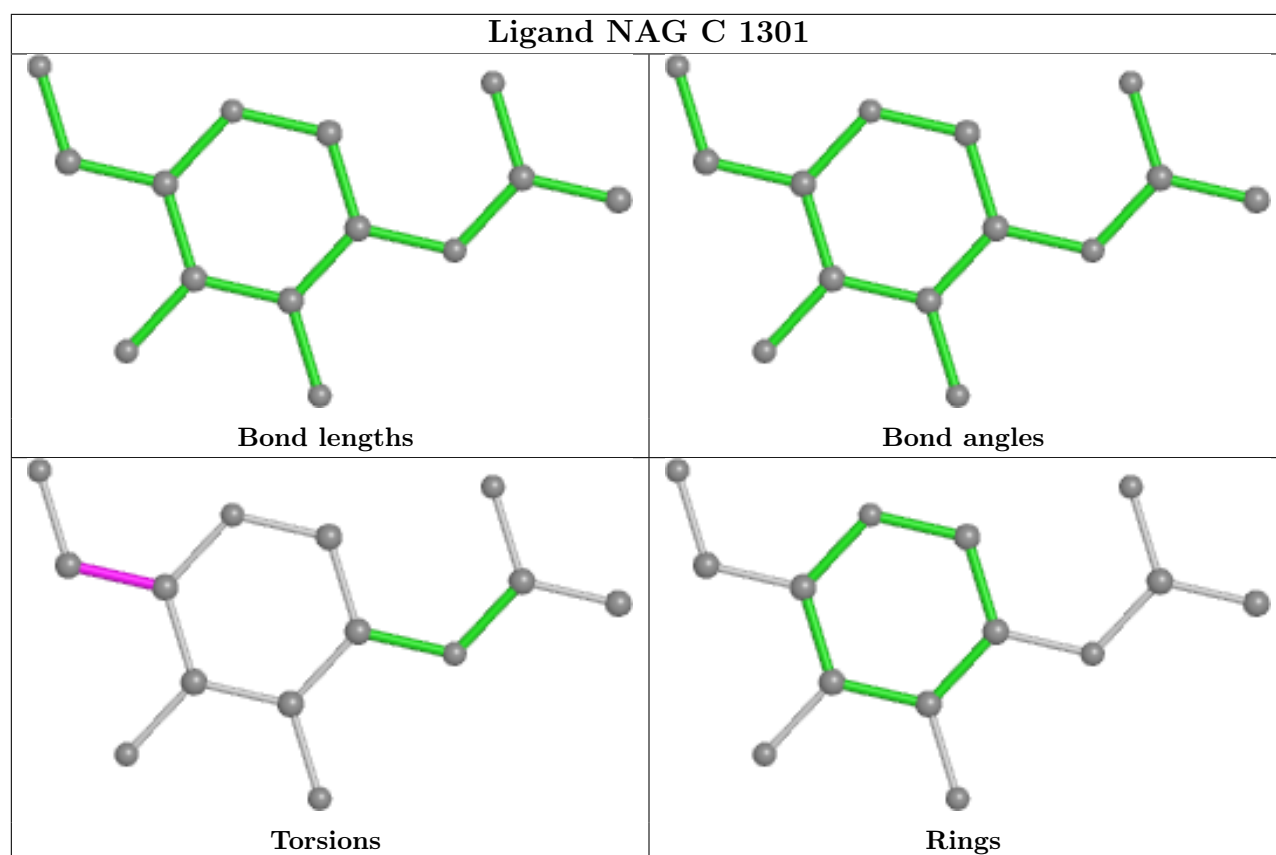


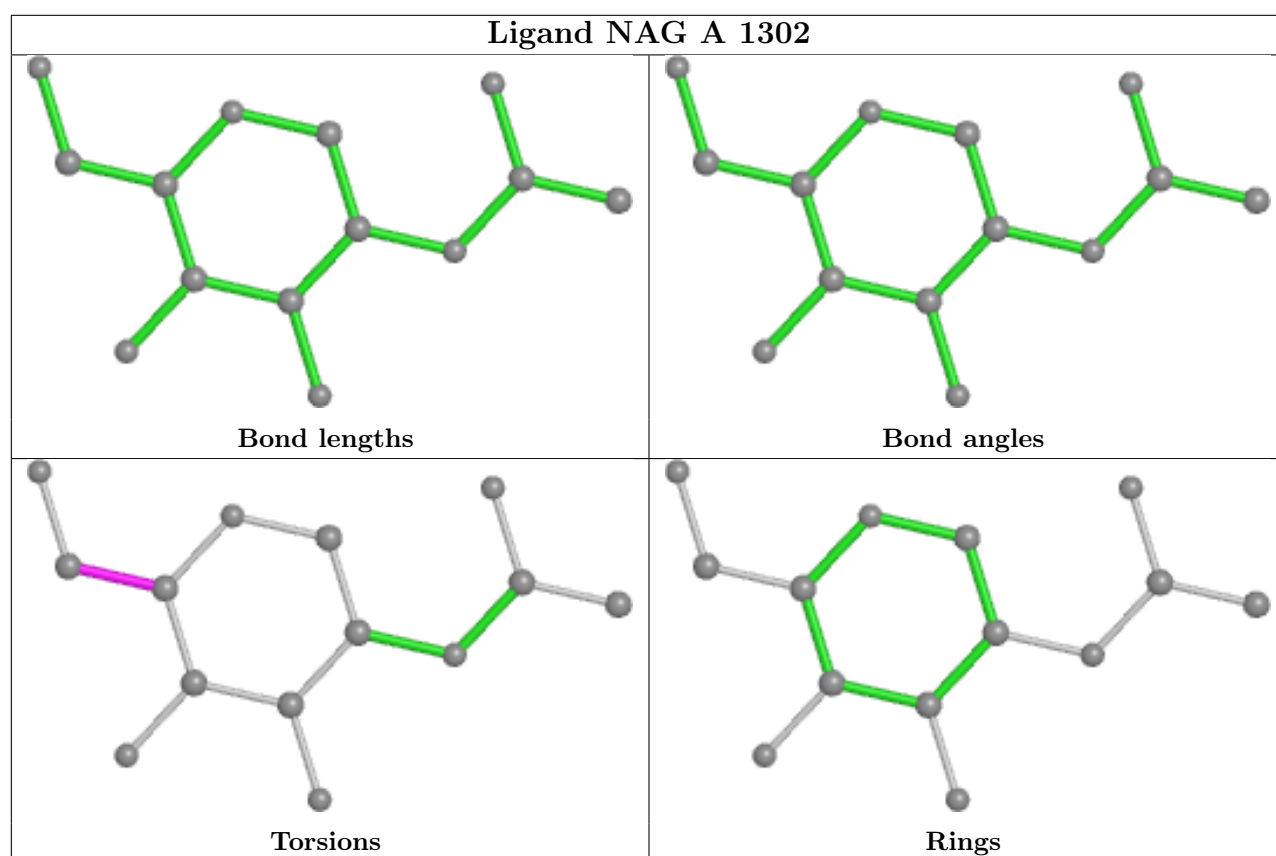
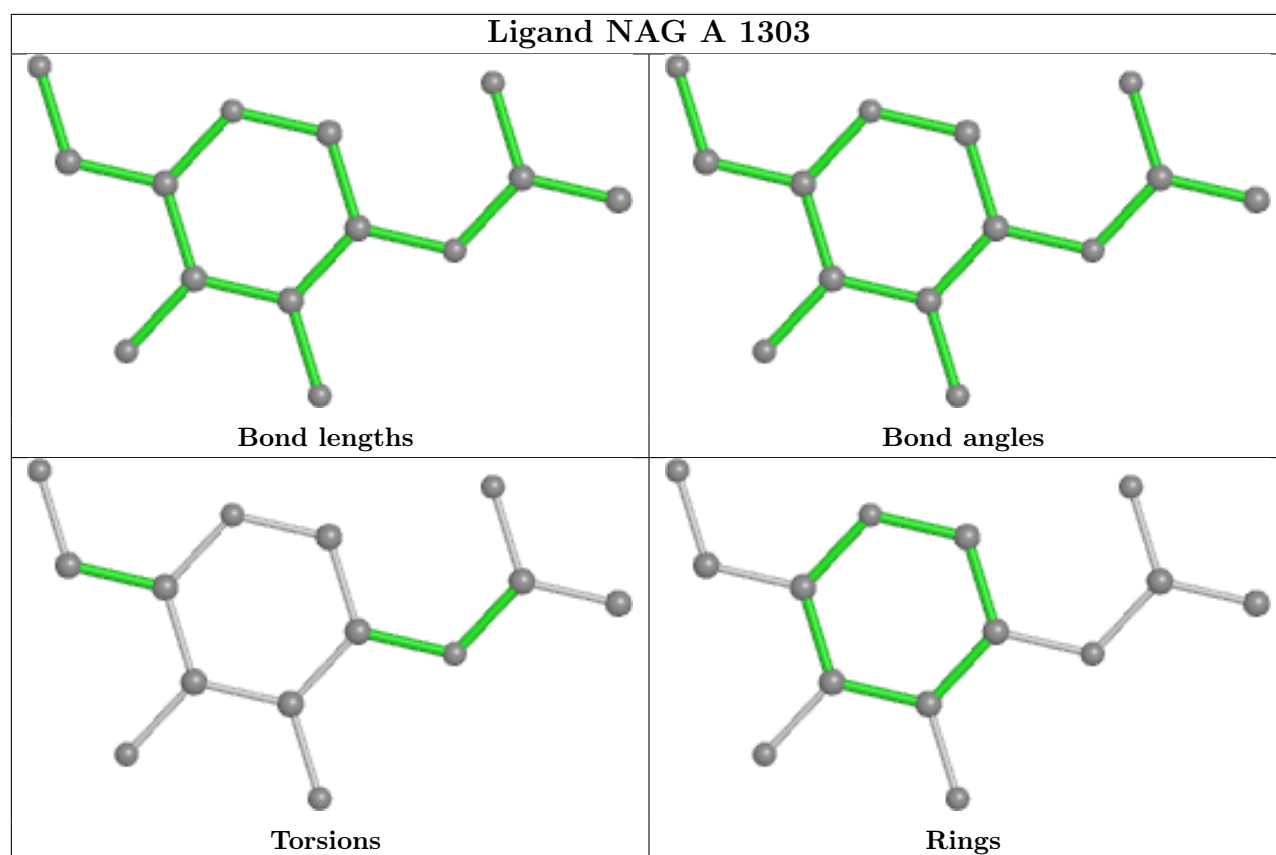
Ligand NAG B 1307

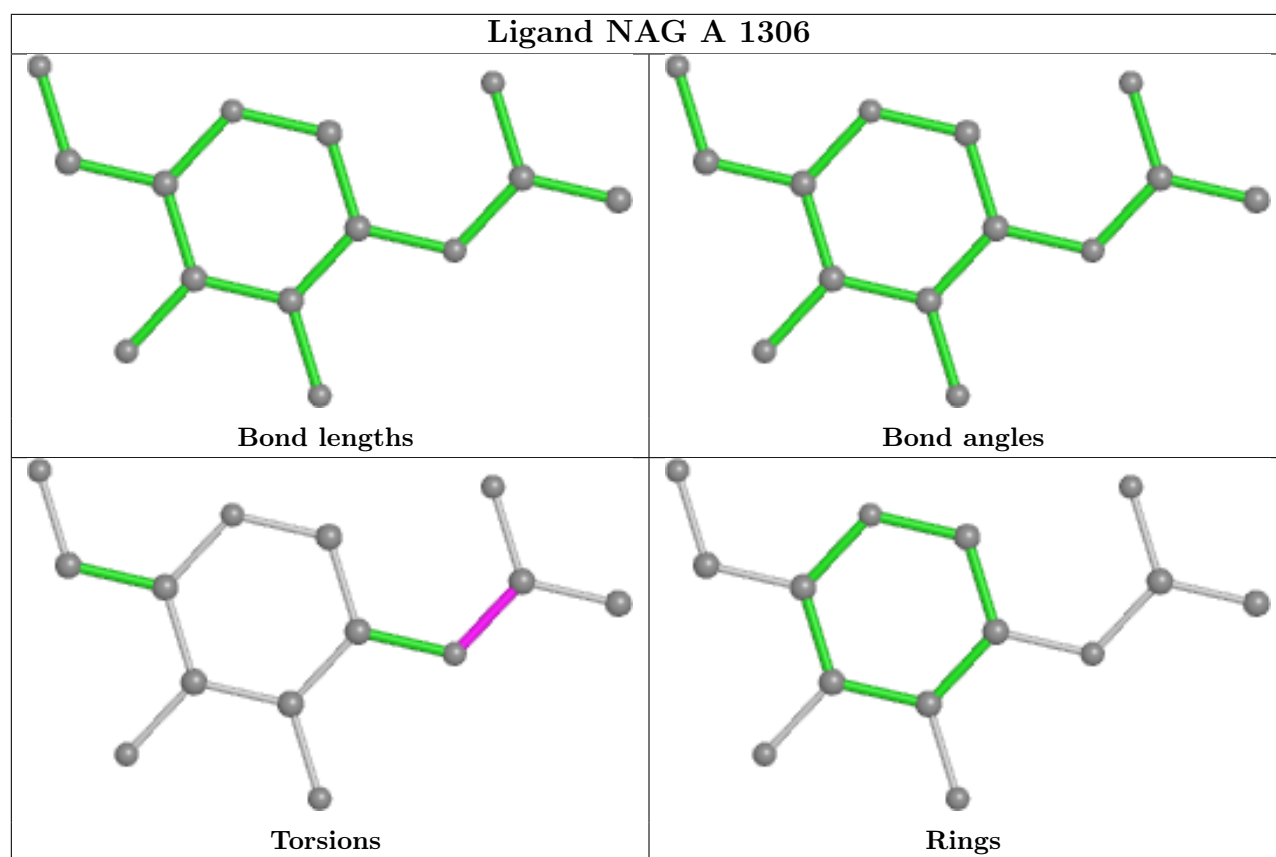












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.