



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 06:52 AM JST

PDB ID : 7Y1Y  
EMDB ID : EMD-33575  
Title : S-ECD (Omicron BA.2) in complex with PD of ACE2  
Authors : Li, Y.N.; Shen, Y.P.; Zhang, Y.Y.; Yan, R.H.  
Deposited on : 2022-06-09  
Resolution : 3.30 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](mailto: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>.

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

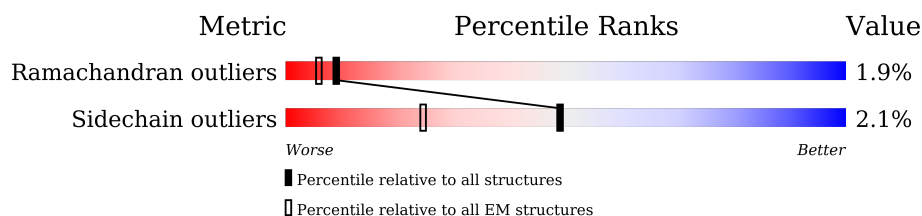
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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.




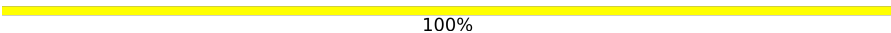


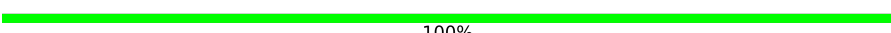








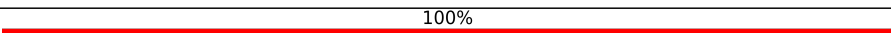



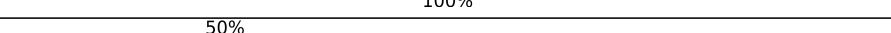

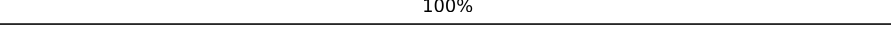
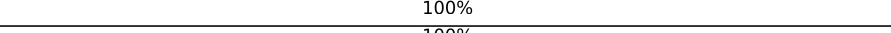
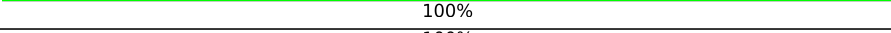
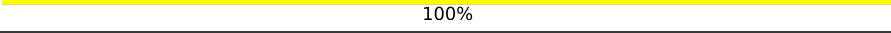

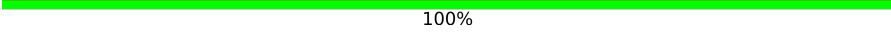
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1268	 7% 76% 21%
1	B	1268	 8% 75% 21%
1	C	1268	 1% 75% 21%
2	D	624	 63% 94% 2%
2	F	624	 80% 94% 2%
2	H	624	 28% 94% 2%
3	E	2	 100%
3	G	2	 50% 100%
3	I	2	 100%

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Mol	Chain	Length	Quality of chain
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	
3	d	2	
3	e	2	
3	f	2	
3	g	2	
3	h	2	

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Mol	Chain	Length	Quality of chain
3	i	2	100%
			<div><div></div></div>
3	j	2	100%
			<div><div></div></div>
3	k	2	100%
			<div><div></div></div>
3	l	2	100%
			<div><div></div></div>
3	m	2	100%
			<div><div></div></div>
3	n	2	100%
			<div><div></div></div>
3	o	2	100%
			<div><div></div></div>
3	p	2	100%
			<div><div></div></div>
3	q	2	100%
			<div><div></div></div>
3	r	2	100%
			<div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39556 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	999	Total	C	N	O	S	0	0
			7834	5016	1302	1480	36		
1	B	998	Total	C	N	O	S	0	0
			7828	5013	1301	1478	36		
1	C	998	Total	C	N	O	S	0	0
			7828	5013	1301	1478	36		

There are 306 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	26	SER	PRO	variant	UNP P0DTC2
A	27	SER	ALA	variant	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	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	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	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	GLU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	SER	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLU	-	expression tag	UNP P0DTC2
A	1244	VAL	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	ALA	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	SER	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	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	GLY	-	expression tag	UNP P0DTC2
A	1260	SER	-	expression tag	UNP P0DTC2
A	1261	VAL	-	expression tag	UNP P0DTC2
A	1262	GLU	-	expression tag	UNP P0DTC2
A	1263	ASP	-	expression tag	UNP P0DTC2
A	1264	TYR	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	ASP	-	expression tag	UNP P0DTC2
A	1267	ASP	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2
A	1269	ASP	-	expression tag	UNP P0DTC2
A	1270	LYS	-	expression tag	UNP P0DTC2
B	21	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	26	SER	PRO	variant	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	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	493	ARG	GLN	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	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	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	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	SER	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLU	-	expression tag	UNP P0DTC2
B	1244	VAL	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	ALA	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	SER	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	SER	-	expression tag	UNP P0DTC2
B	1261	VAL	-	expression tag	UNP P0DTC2
B	1262	GLU	-	expression tag	UNP P0DTC2
B	1263	ASP	-	expression tag	UNP P0DTC2
B	1264	TYR	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	ASP	-	expression tag	UNP P0DTC2
B	1267	ASP	-	expression tag	UNP P0DTC2
B	1268	ASP	-	expression tag	UNP P0DTC2
B	1269	ASP	-	expression tag	UNP P0DTC2
B	1270	LYS	-	expression tag	UNP P0DTC2
C	21	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	26	SER	PRO	variant	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
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	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	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	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	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	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1241	SER	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLU	-	expression tag	UNP P0DTC2
C	1244	VAL	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	ALA	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	SER	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	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	GLY	-	expression tag	UNP P0DTC2
C	1260	SER	-	expression tag	UNP P0DTC2
C	1261	VAL	-	expression tag	UNP P0DTC2
C	1262	GLU	-	expression tag	UNP P0DTC2
C	1263	ASP	-	expression tag	UNP P0DTC2
C	1264	TYR	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	ASP	-	expression tag	UNP P0DTC2
C	1267	ASP	-	expression tag	UNP P0DTC2
C	1268	ASP	-	expression tag	UNP P0DTC2
C	1269	ASP	-	expression tag	UNP P0DTC2
C	1270	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	F	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	H	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP Q9BYF1
D	1	GLY	-	expression tag	UNP Q9BYF1
D	2	VAL	-	expression tag	UNP Q9BYF1
D	3	LYS	-	expression tag	UNP Q9BYF1
D	4	VAL	-	expression tag	UNP Q9BYF1
D	5	LEU	-	expression tag	UNP Q9BYF1
D	6	PHE	-	expression tag	UNP Q9BYF1
D	7	ALA	-	expression tag	UNP Q9BYF1
D	8	LEU	-	expression tag	UNP Q9BYF1
D	9	ILE	-	expression tag	UNP Q9BYF1
D	10	CYS	-	expression tag	UNP Q9BYF1
D	11	ILE	-	expression tag	UNP Q9BYF1
D	12	ALA	-	expression tag	UNP Q9BYF1
D	13	VAL	-	expression tag	UNP Q9BYF1
D	14	ALA	-	expression tag	UNP Q9BYF1
D	15	GLU	-	expression tag	UNP Q9BYF1
D	16	ALA	-	expression tag	UNP Q9BYF1
D	17	GLY	-	expression tag	UNP Q9BYF1
D	18	THR	-	expression tag	UNP Q9BYF1
D	616	ASP	-	expression tag	UNP Q9BYF1
D	617	TYR	-	expression tag	UNP Q9BYF1
D	618	LYS	-	expression tag	UNP Q9BYF1
D	619	ASP	-	expression tag	UNP Q9BYF1
D	620	ASP	-	expression tag	UNP Q9BYF1
D	621	ASP	-	expression tag	UNP Q9BYF1
D	622	ASP	-	expression tag	UNP Q9BYF1
D	623	LYS	-	expression tag	UNP Q9BYF1
F	0	MET	-	initiating methionine	UNP Q9BYF1
F	1	GLY	-	expression tag	UNP Q9BYF1
F	2	VAL	-	expression tag	UNP Q9BYF1
F	3	LYS	-	expression tag	UNP Q9BYF1
F	4	VAL	-	expression tag	UNP Q9BYF1
F	5	LEU	-	expression tag	UNP Q9BYF1
F	6	PHE	-	expression tag	UNP Q9BYF1
F	7	ALA	-	expression tag	UNP Q9BYF1
F	8	LEU	-	expression tag	UNP Q9BYF1
F	9	ILE	-	expression tag	UNP Q9BYF1
F	10	CYS	-	expression tag	UNP Q9BYF1
F	11	ILE	-	expression tag	UNP Q9BYF1
F	12	ALA	-	expression tag	UNP Q9BYF1
F	13	VAL	-	expression tag	UNP Q9BYF1
F	14	ALA	-	expression tag	UNP Q9BYF1
F	15	GLU	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	16	ALA	-	expression tag	UNP Q9BYF1
F	17	GLY	-	expression tag	UNP Q9BYF1
F	18	THR	-	expression tag	UNP Q9BYF1
F	616	ASP	-	expression tag	UNP Q9BYF1
F	617	TYR	-	expression tag	UNP Q9BYF1
F	618	LYS	-	expression tag	UNP Q9BYF1
F	619	ASP	-	expression tag	UNP Q9BYF1
F	620	ASP	-	expression tag	UNP Q9BYF1
F	621	ASP	-	expression tag	UNP Q9BYF1
F	622	ASP	-	expression tag	UNP Q9BYF1
F	623	LYS	-	expression tag	UNP Q9BYF1
H	0	MET	-	initiating methionine	UNP Q9BYF1
H	1	GLY	-	expression tag	UNP Q9BYF1
H	2	VAL	-	expression tag	UNP Q9BYF1
H	3	LYS	-	expression tag	UNP Q9BYF1
H	4	VAL	-	expression tag	UNP Q9BYF1
H	5	LEU	-	expression tag	UNP Q9BYF1
H	6	PHE	-	expression tag	UNP Q9BYF1
H	7	ALA	-	expression tag	UNP Q9BYF1
H	8	LEU	-	expression tag	UNP Q9BYF1
H	9	ILE	-	expression tag	UNP Q9BYF1
H	10	CYS	-	expression tag	UNP Q9BYF1
H	11	ILE	-	expression tag	UNP Q9BYF1
H	12	ALA	-	expression tag	UNP Q9BYF1
H	13	VAL	-	expression tag	UNP Q9BYF1
H	14	ALA	-	expression tag	UNP Q9BYF1
H	15	GLU	-	expression tag	UNP Q9BYF1
H	16	ALA	-	expression tag	UNP Q9BYF1
H	17	GLY	-	expression tag	UNP Q9BYF1
H	18	THR	-	expression tag	UNP Q9BYF1
H	616	ASP	-	expression tag	UNP Q9BYF1
H	617	TYR	-	expression tag	UNP Q9BYF1
H	618	LYS	-	expression tag	UNP Q9BYF1
H	619	ASP	-	expression tag	UNP Q9BYF1
H	620	ASP	-	expression tag	UNP Q9BYF1
H	621	ASP	-	expression tag	UNP Q9BYF1
H	622	ASP	-	expression tag	UNP Q9BYF1
H	623	LYS	-	expression tag	UNP Q9BYF1

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



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

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		
3	l	2	Total	C	N	O	0	0
			28	16	2	10		
3	m	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		
3	p	2	Total	C	N	O	0	0
			28	16	2	10		
3	q	2	Total	C	N	O	0	0
			28	16	2	10		
3	r	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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).





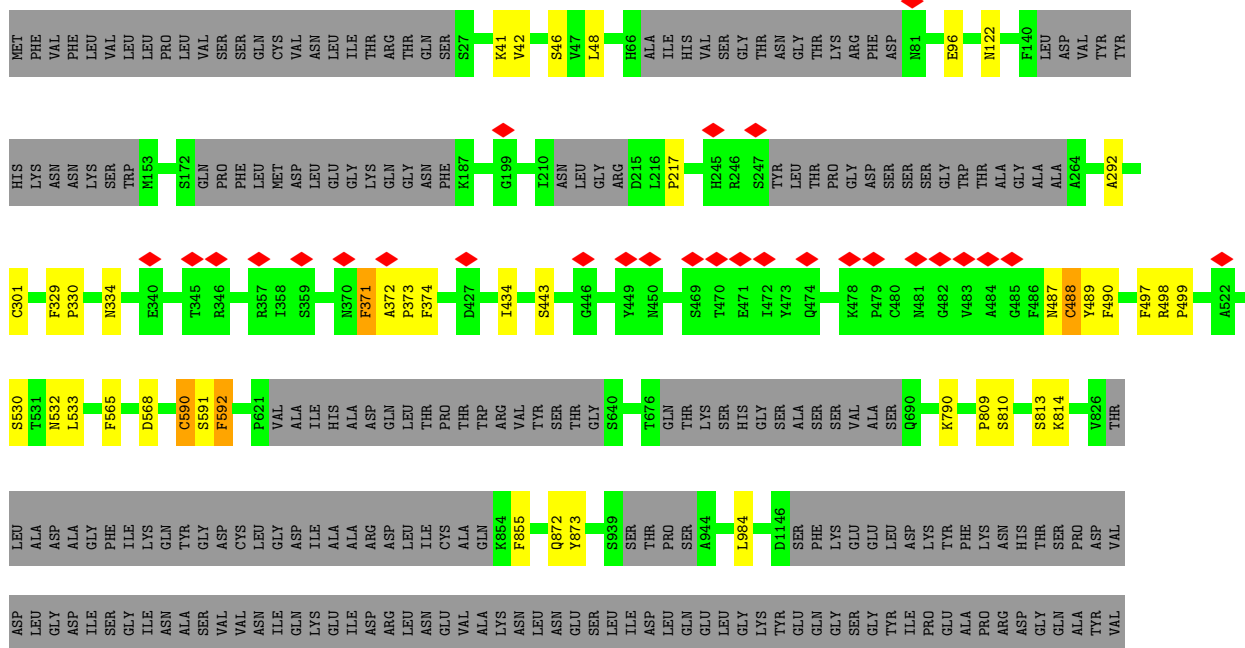
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4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

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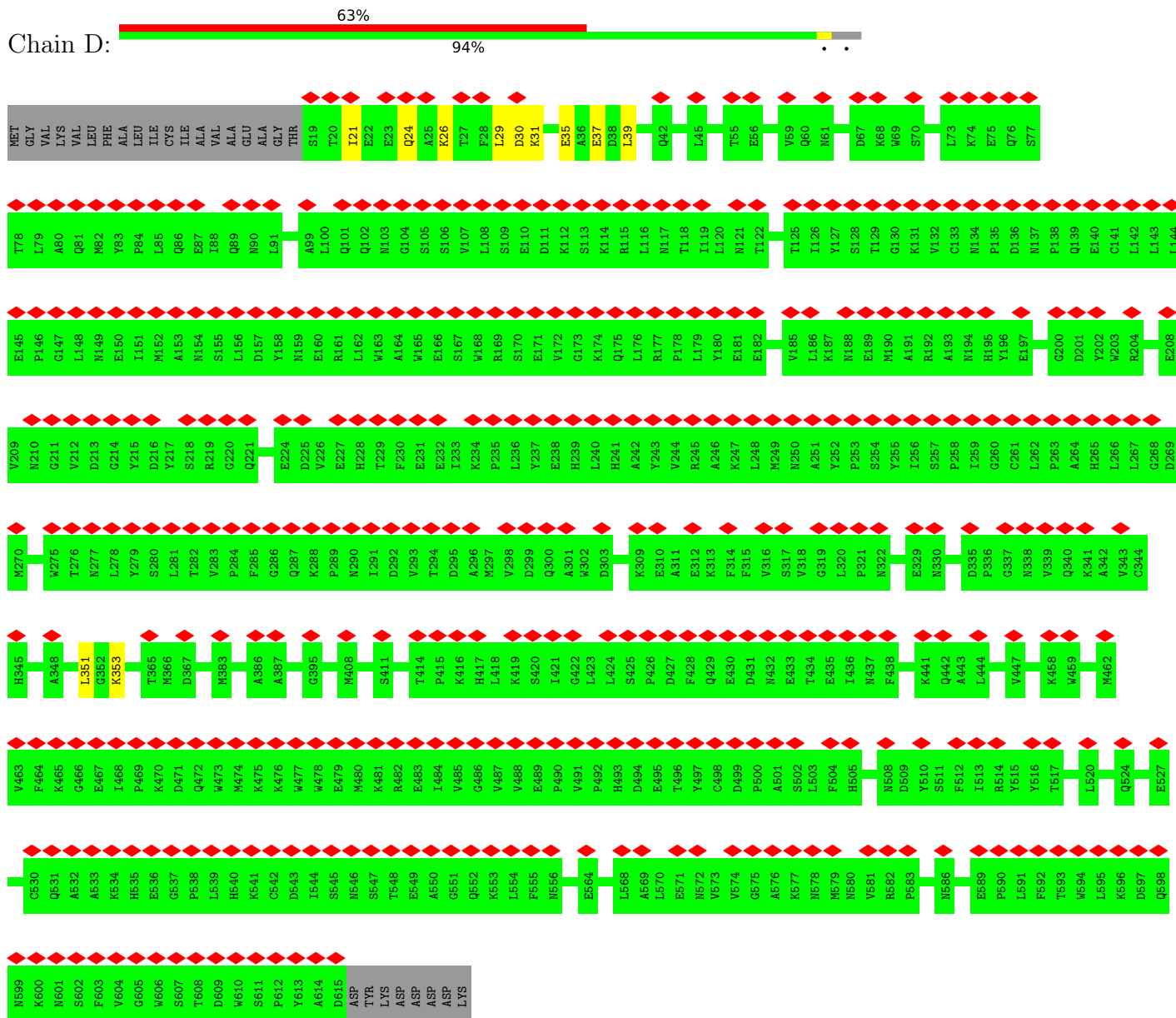
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

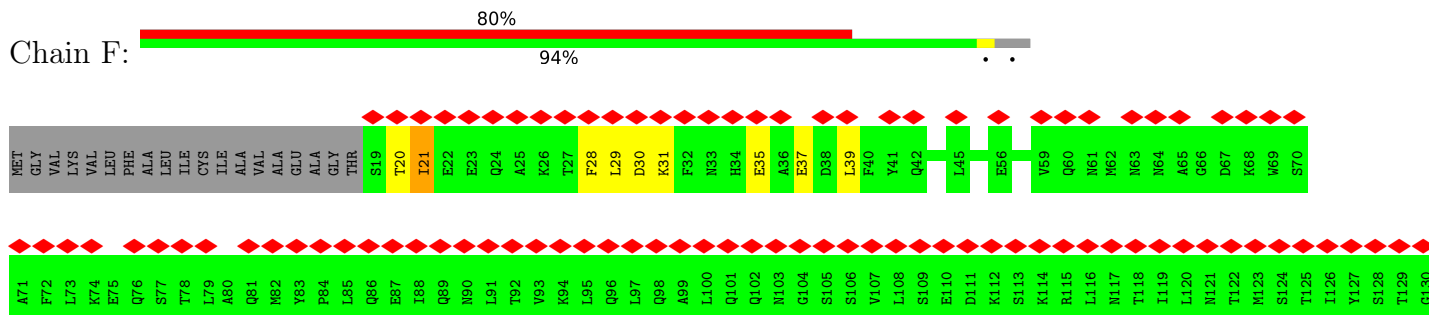


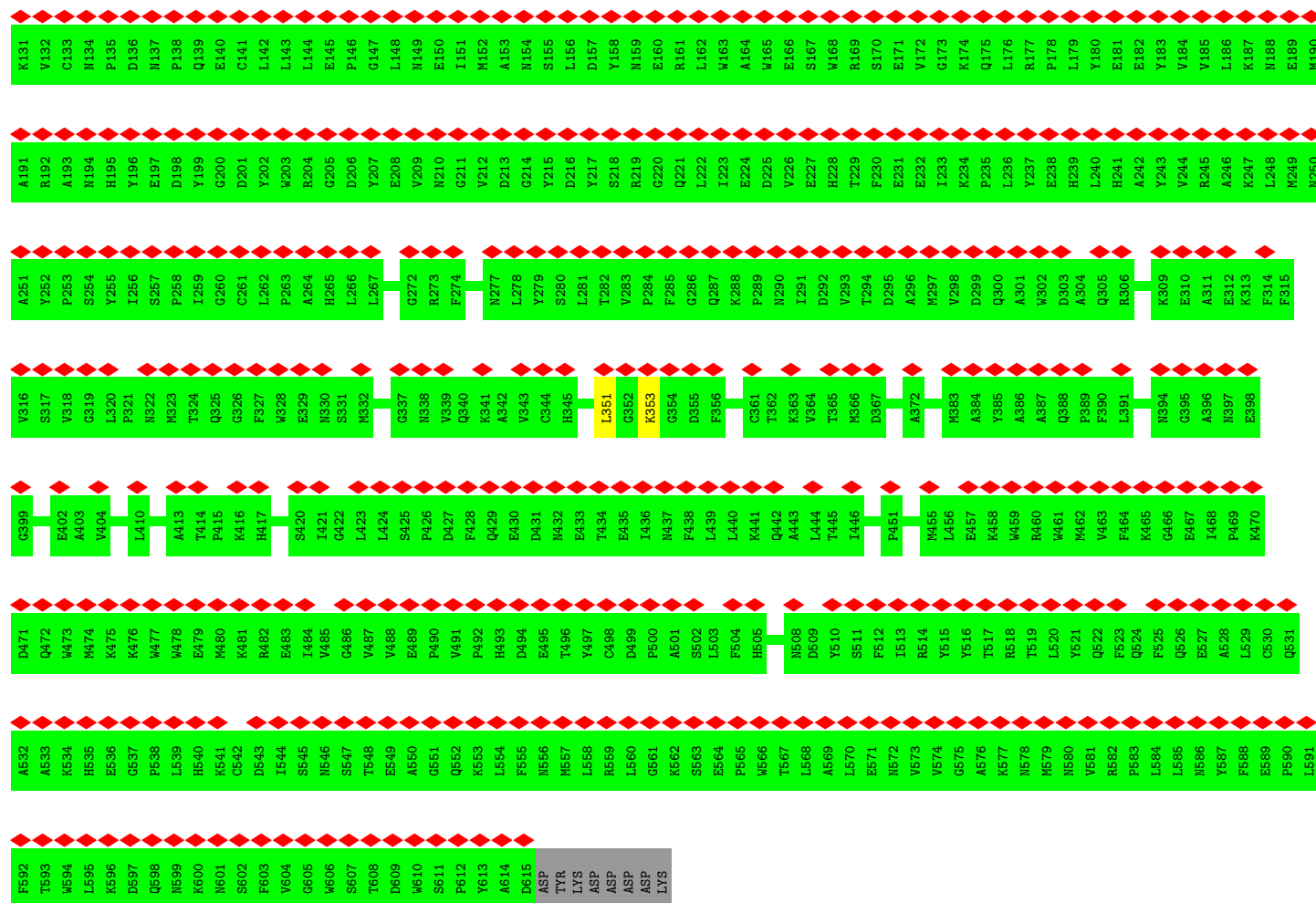


Chain D:



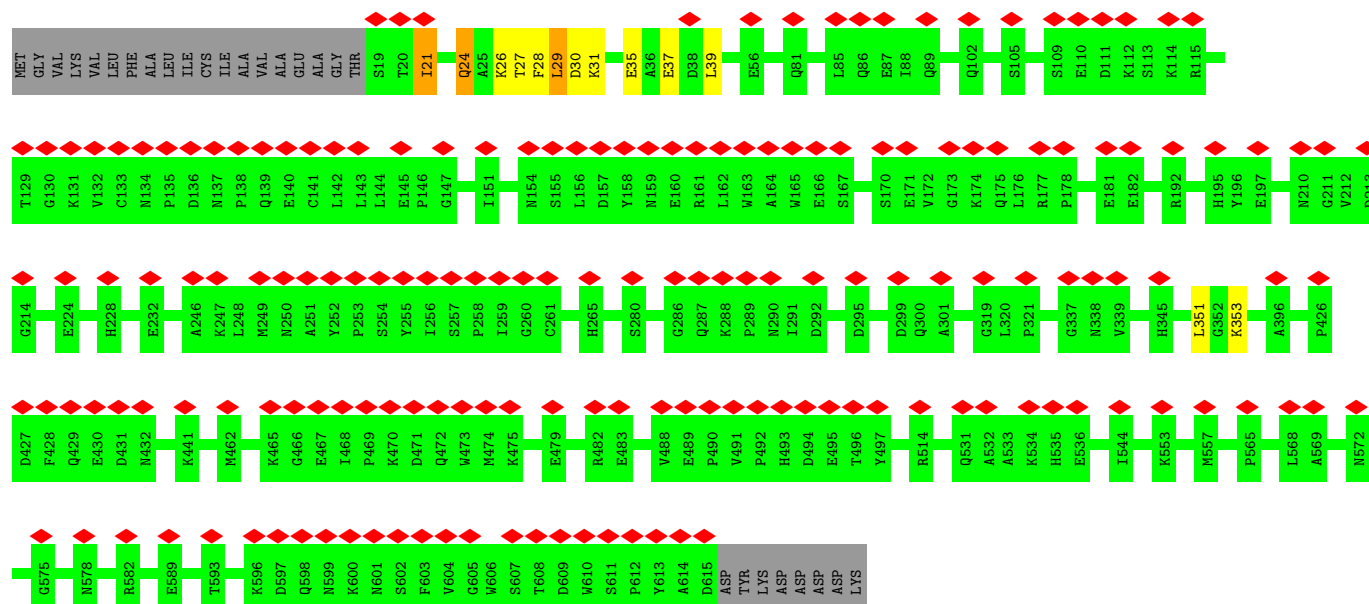
Chain F:





• Molecule 2: Processed angiotensin-converting enzyme 2

Chain H: 28% 94%



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

Chain E:  100%



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

Chain G:  50% 100%



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

Chain I:  100%



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

Chain J:  50% 50%



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

Chain K:  100%



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

Chain L:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  100%



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

Chain O:  50% 100%



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

Chain P:  50% 100%



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

Chain Q:  50% 50%



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

Chain R:  50% 50%



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

Chain S:  100%





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

Chain T:  100%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  100%  
 100%



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

Chain X:  50%  
 50%  50%



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

Chain Y:  50%  50%



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

Chain Z:  100%



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

Chain a:  50% 50%



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

Chain b:  100%



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

Chain c:  100%



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

Chain d:  100% 100%



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

Chain e:  100% 100%



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



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



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



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



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



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





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



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



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



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



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



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131412	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.150	Depositor
Minimum map value	-1.757	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	0.56	0/8017	0.56	0/10903
1	B	0.55	0/8011	0.55	0/10895
1	C	0.55	0/8011	0.55	0/10895
2	D	0.31	0/5007	0.44	0/6803
2	F	0.31	0/5007	0.44	0/6803
2	H	0.31	0/5007	0.44	0/6803
All	All	0.47	0/39060	0.51	0/53102

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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	979/1268 (77%)	887 (91%)	70 (7%)	22 (2%)	5	26
1	B	978/1268 (77%)	872 (89%)	78 (8%)	28 (3%)	3	22
1	C	978/1268 (77%)	879 (90%)	73 (8%)	26 (3%)	4	22
2	D	595/624 (95%)	555 (93%)	37 (6%)	3 (0%)	25	56
2	F	595/624 (95%)	553 (93%)	38 (6%)	4 (1%)	19	50
2	H	595/624 (95%)	549 (92%)	40 (7%)	6 (1%)	13	42
All	All	4720/5676 (83%)	4295 (91%)	336 (7%)	89 (2%)	9	29

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	THR
1	A	533	LEU
1	A	590	CYS
1	A	591	SER
1	A	855	PHE
1	B	28	TYR
1	B	46	SER
1	B	292	ALA
1	B	319	ARG
1	B	372	ALA
1	B	374	PHE
1	B	488	CYS
1	B	498	ARG
1	B	530	SER
1	B	590	CYS
1	B	591	SER
1	C	46	SER
1	C	292	ALA
1	C	371	PHE
1	C	372	ALA
1	C	373	PRO
1	C	488	CYS
1	C	499	PRO
1	C	568	ASP
1	C	591	SER
1	C	984	LEU
2	F	20	THR
2	F	21	ILE
2	H	21	ILE
1	A	41	LYS

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Mol	Chain	Res	Type
1	A	42	VAL
1	A	46	SER
1	A	96	GLU
1	A	332	ILE
1	A	530	SER
1	A	701	ALA
1	B	41	LYS
1	B	96	GLU
1	B	318	PHE
1	B	373	PRO
1	B	497	PHE
1	B	527	PRO
1	B	533	LEU
1	C	41	LYS
1	C	96	GLU
1	C	498	ARG
1	C	590	CYS
1	C	814	LYS
1	C	855	PHE
2	D	21	ILE
2	D	351	LEU
2	F	351	LEU
2	H	27	THR
2	H	351	LEU
1	A	48	LEU
1	A	330	PRO
1	A	497	PHE
1	A	797	PHE
1	B	48	LEU
1	B	473	TYR
1	B	695	TYR
1	B	700	GLY
1	C	48	LEU
1	C	330	PRO
1	C	374	PHE
1	C	487	ASN
1	C	810	SER
2	H	24	GLN
1	A	217	PRO
1	A	372	ALA
1	A	798	GLY
1	B	217	PRO

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Mol	Chain	Res	Type
1	B	531	THR
1	C	217	PRO
1	C	592	PHE
1	C	813	SER
2	H	29	LEU
1	A	495	TYR
1	A	532	ASN
1	B	42	VAL
1	B	333	THR
1	C	42	VAL
2	D	353	LYS
2	F	353	LYS
2	H	353	LYS
1	A	373	PRO
1	C	809	PRO
1	B	742	ILE
1	B	330	PRO

### 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	877/1105 (79%)	856 (98%)	21 (2%)	44	68
1	B	876/1105 (79%)	855 (98%)	21 (2%)	44	68
1	C	876/1105 (79%)	856 (98%)	20 (2%)	45	68
2	D	527/548 (96%)	519 (98%)	8 (2%)	60	77
2	F	527/548 (96%)	519 (98%)	8 (2%)	60	77
2	H	527/548 (96%)	517 (98%)	10 (2%)	52	72
All	All	4210/4959 (85%)	4122 (98%)	88 (2%)	49	70

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER

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Mol	Chain	Res	Type
1	A	61	ASN
1	A	122	ASN
1	A	291	CYS
1	A	296	LEU
1	A	298	GLU
1	A	300	LYS
1	A	301	CYS
1	A	302	THR
1	A	328	ARG
1	A	329	PHE
1	A	334	ASN
1	A	442	ASP
1	A	443	SER
1	A	498	ARG
1	A	529	LYS
1	A	531	THR
1	A	532	ASN
1	A	588	THR
1	A	591	SER
1	A	1074	ASN
1	B	27	SER
1	B	28	TYR
1	B	62	VAL
1	B	122	ASN
1	B	297	SER
1	B	301	CYS
1	B	317	ASN
1	B	318	PHE
1	B	328	ARG
1	B	329	PHE
1	B	332	ILE
1	B	488	CYS
1	B	528	LYS
1	B	529	LYS
1	B	531	THR
1	B	588	THR
1	B	592	PHE
1	B	655	TYR
1	B	695	TYR
1	B	702	GLU
1	B	1074	ASN
1	C	122	ASN

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Mol	Chain	Res	Type
1	C	301	CYS
1	C	329	PHE
1	C	334	ASN
1	C	371	PHE
1	C	434	ILE
1	C	443	SER
1	C	488	CYS
1	C	489	TYR
1	C	490	PHE
1	C	497	PHE
1	C	530	SER
1	C	532	ASN
1	C	533	LEU
1	C	565	PHE
1	C	590	CYS
1	C	592	PHE
1	C	790	LYS
1	C	872	GLN
1	C	873	TYR
2	D	24	GLN
2	D	26	LYS
2	D	29	LEU
2	D	30	ASP
2	D	31	LYS
2	D	35	GLU
2	D	37	GLU
2	D	39	LEU
2	F	21	ILE
2	F	28	PHE
2	F	29	LEU
2	F	30	ASP
2	F	31	LYS
2	F	35	GLU
2	F	37	GLU
2	F	39	LEU
2	H	21	ILE
2	H	24	GLN
2	H	26	LYS
2	H	28	PHE
2	H	29	LEU
2	H	30	ASP
2	H	31	LYS

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Mol	Chain	Res	Type
2	H	35	GLU
2	H	37	GLU
2	H	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	A	477	ASN
1	A	690	GLN
1	B	321	GLN
1	B	417	ASN
1	B	477	ASN
1	B	487	ASN
1	B	580	GLN
1	B	1002	GLN
1	C	370	ASN
1	C	417	ASN
1	C	477	ASN
1	C	487	ASN
1	C	675	GLN
1	C	992	GLN
1	C	1005	GLN
2	D	101	GLN
2	D	137	ASN
2	D	210	ASN
2	D	277	ASN
2	D	394	ASN
2	D	442	GLN
2	D	472	GLN
2	D	599	ASN
2	F	101	GLN
2	F	137	ASN
2	F	210	ASN
2	F	277	ASN
2	F	394	ASN
2	F	442	GLN
2	F	472	GLN
2	F	599	ASN
2	H	24	GLN
2	H	101	GLN
2	H	137	ASN

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Mol	Chain	Res	Type
2	H	210	ASN
2	H	277	ASN
2	H	325	GLN
2	H	394	ASN
2	H	442	GLN
2	H	472	GLN
2	H	599	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 ⓘ

76 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	E	1	3,1	14,14,15	0.54	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	G	1	3,1	14,14,15	0.45	0	17,19,21	0.43	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	I	1	3,1	14,14,15	0.30	0	17,19,21	0.61	0
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	0.48	0
3	NAG	J	1	3,1	14,14,15	0.37	0	17,19,21	0.72	0
3	NAG	J	2	3	14,14,15	0.28	0	17,19,21	1.30	2 (11%)
3	NAG	K	1	3,1	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
3	NAG	K	2	3	14,14,15	0.37	0	17,19,21	1.41	3 (17%)
3	NAG	L	1	3,1	14,14,15	0.71	1 (7%)	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	L	2	3	14,14,15	0.29	0	17,19,21	0.64	0
3	NAG	M	1	3,1	14,14,15	0.24	0	17,19,21	0.69	1 (5%)
3	NAG	M	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	N	1	3,1	14,14,15	0.51	0	17,19,21	0.52	0
3	NAG	N	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	O	1	3,1	14,14,15	0.43	0	17,19,21	0.44	0
3	NAG	O	2	3	14,14,15	0.20	0	17,19,21	0.48	0
3	NAG	P	1	3,1	14,14,15	0.30	0	17,19,21	0.39	0
3	NAG	P	2	3	14,14,15	0.36	0	17,19,21	0.36	0
3	NAG	Q	1	3,1	14,14,15	0.33	0	17,19,21	1.14	1 (5%)
3	NAG	Q	2	3	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	R	1	3,1	14,14,15	0.34	0	17,19,21	0.69	1 (5%)
3	NAG	R	2	3	14,14,15	0.23	0	17,19,21	0.40	0
3	NAG	S	1	3,1	14,14,15	0.28	0	17,19,21	0.62	0
3	NAG	S	2	3	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	T	1	3,1	14,14,15	0.76	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	T	2	3	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
3	NAG	U	1	3,1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	U	2	3	14,14,15	0.27	0	17,19,21	0.37	0
3	NAG	V	1	3,1	14,14,15	0.53	0	17,19,21	0.49	0
3	NAG	V	2	3	14,14,15	0.24	0	17,19,21	0.59	0
3	NAG	W	1	3,1	14,14,15	0.44	0	17,19,21	0.44	0
3	NAG	W	2	3	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	X	1	3,1	14,14,15	0.23	0	17,19,21	1.37	1 (5%)
3	NAG	X	2	3	14,14,15	0.17	0	17,19,21	0.50	0
3	NAG	Y	1	3,1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
3	NAG	Y	2	3	14,14,15	0.39	0	17,19,21	0.46	0
3	NAG	Z	1	3,1	14,14,15	0.39	0	17,19,21	0.41	0
3	NAG	Z	2	3	14,14,15	0.21	0	17,19,21	0.74	0
3	NAG	a	1	3,1	14,14,15	0.37	0	17,19,21	0.48	0
3	NAG	a	2	3	14,14,15	0.58	0	17,19,21	1.30	1 (5%)
3	NAG	b	1	3,1	14,14,15	0.63	1 (7%)	17,19,21	0.42	0
3	NAG	b	2	3	14,14,15	0.34	0	17,19,21	1.36	2 (11%)
3	NAG	c	1	3,1	14,14,15	0.40	0	17,19,21	0.45	0
3	NAG	c	2	3	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	d	1	2,3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	d	2	3	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	e	1	2,3	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
3	NAG	e	2	3	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
3	NAG	f	1	2,3	14,14,15	0.23	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	f	2	3	14,14,15	0.41	0	17,19,21	1.25	1 (5%)
3	NAG	g	1	2,3	14,14,15	0.19	0	17,19,21	0.48	0
3	NAG	g	2	3	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	h	1	2,3	14,14,15	0.71	1 (7%)	17,19,21	0.65	0
3	NAG	h	2	3	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	i	1	2,3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	i	2	3	14,14,15	0.31	0	17,19,21	0.38	0
3	NAG	j	1	2,3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	j	2	3	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	k	1	2,3	14,14,15	0.21	0	17,19,21	0.58	0
3	NAG	k	2	3	14,14,15	0.42	0	17,19,21	1.25	1 (5%)
3	NAG	l	1	2,3	14,14,15	0.18	0	17,19,21	0.48	0
3	NAG	l	2	3	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	m	1	2,3	14,14,15	0.69	1 (7%)	17,19,21	0.65	0
3	NAG	m	2	3	14,14,15	0.20	0	17,19,21	0.52	0
3	NAG	n	1	2,3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	n	2	3	14,14,15	0.30	0	17,19,21	0.37	0
3	NAG	o	1	2,3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	o	2	3	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	p	1	2,3	14,14,15	0.24	0	17,19,21	0.57	0
3	NAG	p	2	3	14,14,15	0.41	0	17,19,21	1.25	1 (5%)
3	NAG	q	1	2,3	14,14,15	0.18	0	17,19,21	0.48	0
3	NAG	q	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	r	1	2,3	14,14,15	0.69	1 (7%)	17,19,21	0.66	0
3	NAG	r	2	3	14,14,15	0.21	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	a	2	3	-	0/6/23/26	0/1/1/1
3	NAG	b	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	b	2	3	-	0/6/23/26	0/1/1/1
3	NAG	c	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	2/6/23/26	0/1/1/1
3	NAG	e	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	f	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	5/6/23/26	0/1/1/1
3	NAG	g	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	i	2	3	-	2/6/23/26	0/1/1/1
3	NAG	j	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	NAG	k	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	k	2	3	-	5/6/23/26	0/1/1/1
3	NAG	l	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	NAG	m	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	2/6/23/26	0/1/1/1
3	NAG	n	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	n	2	3	-	2/6/23/26	0/1/1/1
3	NAG	o	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	o	2	3	-	2/6/23/26	0/1/1/1
3	NAG	p	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	p	2	3	-	5/6/23/26	0/1/1/1
3	NAG	q	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	r	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C1	-2.77	1.39	1.43
3	L	1	NAG	O5-C1	-2.59	1.39	1.43
3	h	1	NAG	O5-C1	-2.56	1.39	1.43
3	r	1	NAG	O5-C1	-2.50	1.39	1.43
3	m	1	NAG	O5-C1	-2.49	1.39	1.43
3	K	1	NAG	O5-C1	-2.31	1.40	1.43
3	b	1	NAG	O5-C1	-2.15	1.40	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	1	NAG	C2-N2-C7	4.71	129.61	122.90
3	K	2	NAG	C2-N2-C7	4.47	129.27	122.90
3	b	2	NAG	C2-N2-C7	4.33	129.07	122.90
3	a	2	NAG	C2-N2-C7	4.31	129.04	122.90
3	k	2	NAG	C2-N2-C7	4.30	129.03	122.90
3	f	2	NAG	C2-N2-C7	4.27	128.99	122.90
3	p	2	NAG	C2-N2-C7	4.27	128.98	122.90
3	J	2	NAG	C2-N2-C7	4.23	128.93	122.90
3	Q	1	NAG	C1-O5-C5	3.32	116.69	112.19
3	K	2	NAG	C1-C2-N2	2.43	114.64	110.49
3	T	1	NAG	O4-C4-C3	-2.40	104.80	110.35
3	J	2	NAG	C1-C2-N2	2.35	114.51	110.49
3	e	1	NAG	C8-C7-N2	2.30	119.99	116.10
3	e	2	NAG	C8-C7-N2	2.29	119.97	116.10
3	R	1	NAG	C1-O5-C5	2.26	115.25	112.19
3	b	2	NAG	C1-C2-N2	2.24	114.32	110.49
3	Y	1	NAG	C1-O5-C5	2.24	115.23	112.19
3	M	1	NAG	C1-O5-C5	2.09	115.03	112.19
3	T	2	NAG	C1-O5-C5	2.06	114.98	112.19
3	K	2	NAG	C1-O5-C5	2.05	114.97	112.19
3	e	2	NAG	C2-N2-C7	-2.05	119.99	122.90
3	e	1	NAG	C2-N2-C7	-2.05	119.99	122.90

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	f	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	p	2	NAG	O5-C5-C6-O6
3	d	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	i	2	NAG	C4-C5-C6-O6
3	l	2	NAG	C4-C5-C6-O6
3	n	2	NAG	C4-C5-C6-O6
3	q	2	NAG	C4-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	m	2	NAG	O5-C5-C6-O6
3	r	2	NAG	O5-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	k	2	NAG	C4-C5-C6-O6
3	m	1	NAG	C4-C5-C6-O6
3	p	2	NAG	C4-C5-C6-O6
3	r	1	NAG	C4-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	i	2	NAG	O5-C5-C6-O6
3	n	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
3	q	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	f	2	NAG	C8-C7-N2-C2
3	f	2	NAG	O7-C7-N2-C2
3	k	2	NAG	C8-C7-N2-C2
3	k	2	NAG	O7-C7-N2-C2
3	p	2	NAG	C8-C7-N2-C2
3	p	2	NAG	O7-C7-N2-C2
3	h	2	NAG	C4-C5-C6-O6
3	m	2	NAG	C4-C5-C6-O6
3	r	2	NAG	C4-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	j	1	NAG	O5-C5-C6-O6
3	m	1	NAG	O5-C5-C6-O6
3	o	1	NAG	O5-C5-C6-O6
3	r	1	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	l	1	NAG	O5-C5-C6-O6
3	q	1	NAG	O5-C5-C6-O6
3	n	1	NAG	C4-C5-C6-O6
3	d	1	NAG	C4-C5-C6-O6
3	i	1	NAG	C4-C5-C6-O6
3	j	2	NAG	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	l	1	NAG	C4-C5-C6-O6
3	q	1	NAG	C4-C5-C6-O6
3	d	1	NAG	O5-C5-C6-O6

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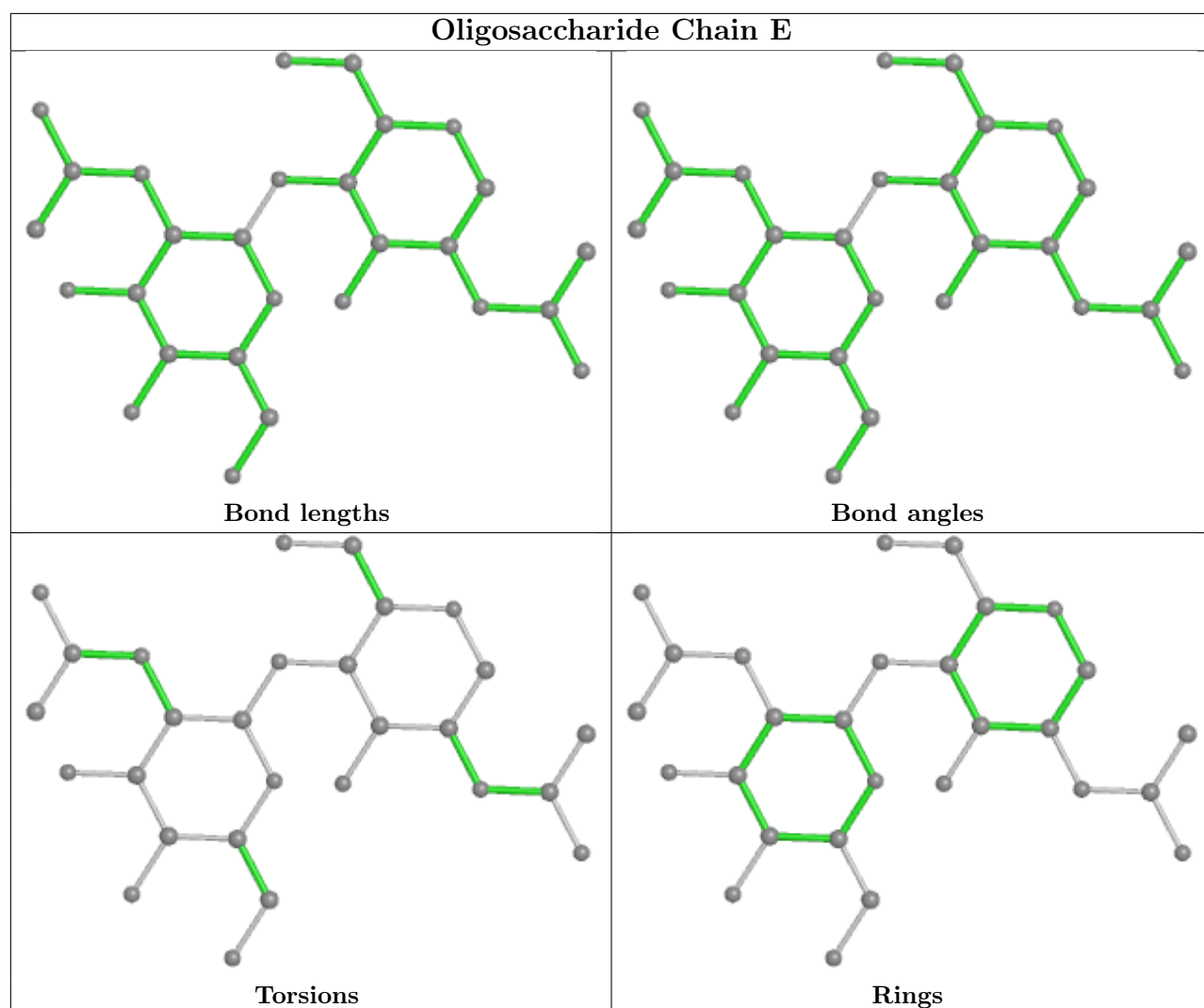
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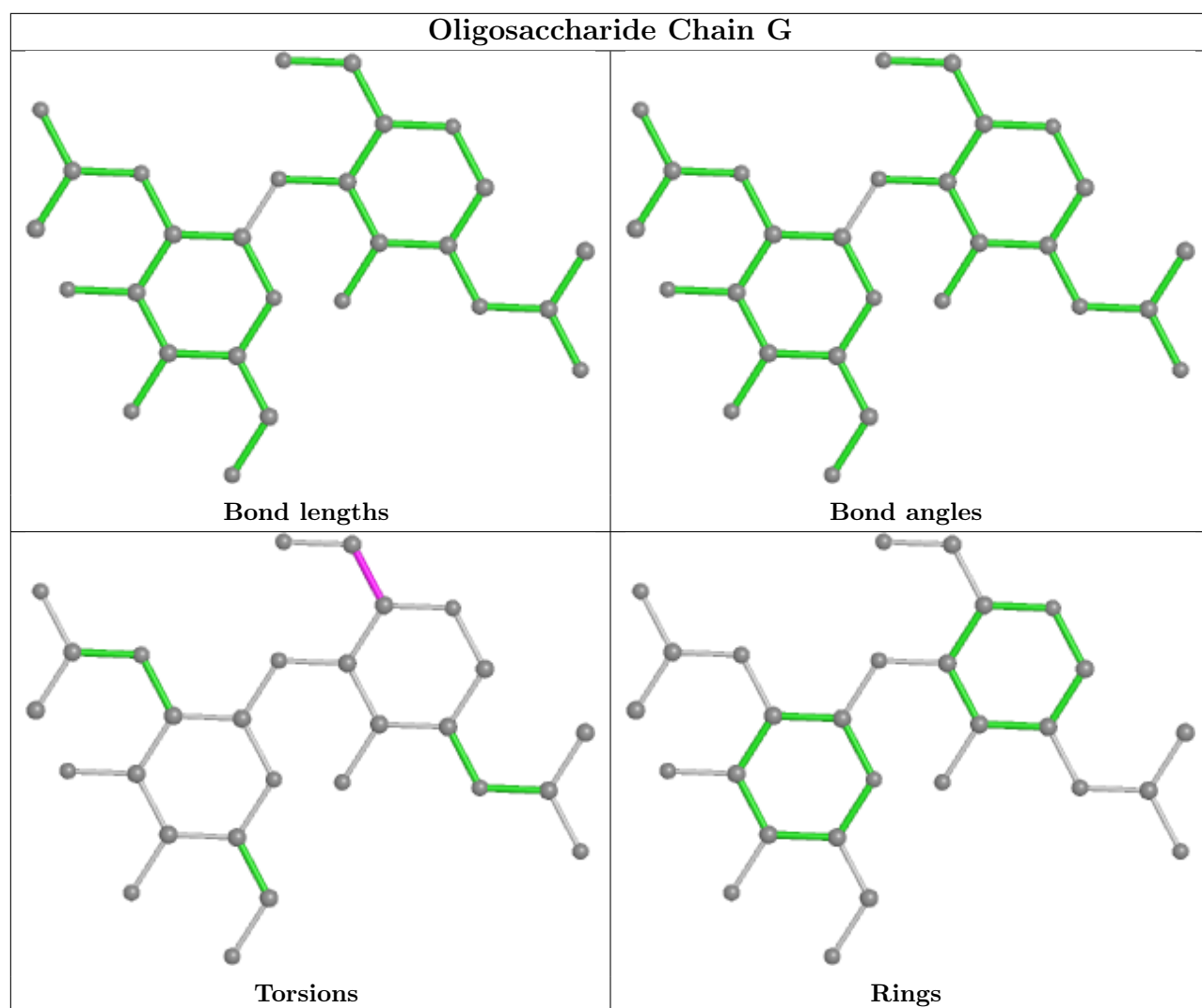
Mol	Chain	Res	Type	Atoms
3	i	1	NAG	O5-C5-C6-O6
3	n	1	NAG	O5-C5-C6-O6
3	j	1	NAG	C4-C5-C6-O6
3	o	1	NAG	C4-C5-C6-O6
3	o	2	NAG	C4-C5-C6-O6
3	j	2	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	f	2	NAG	C3-C2-N2-C7
3	k	2	NAG	C3-C2-N2-C7
3	p	2	NAG	C3-C2-N2-C7

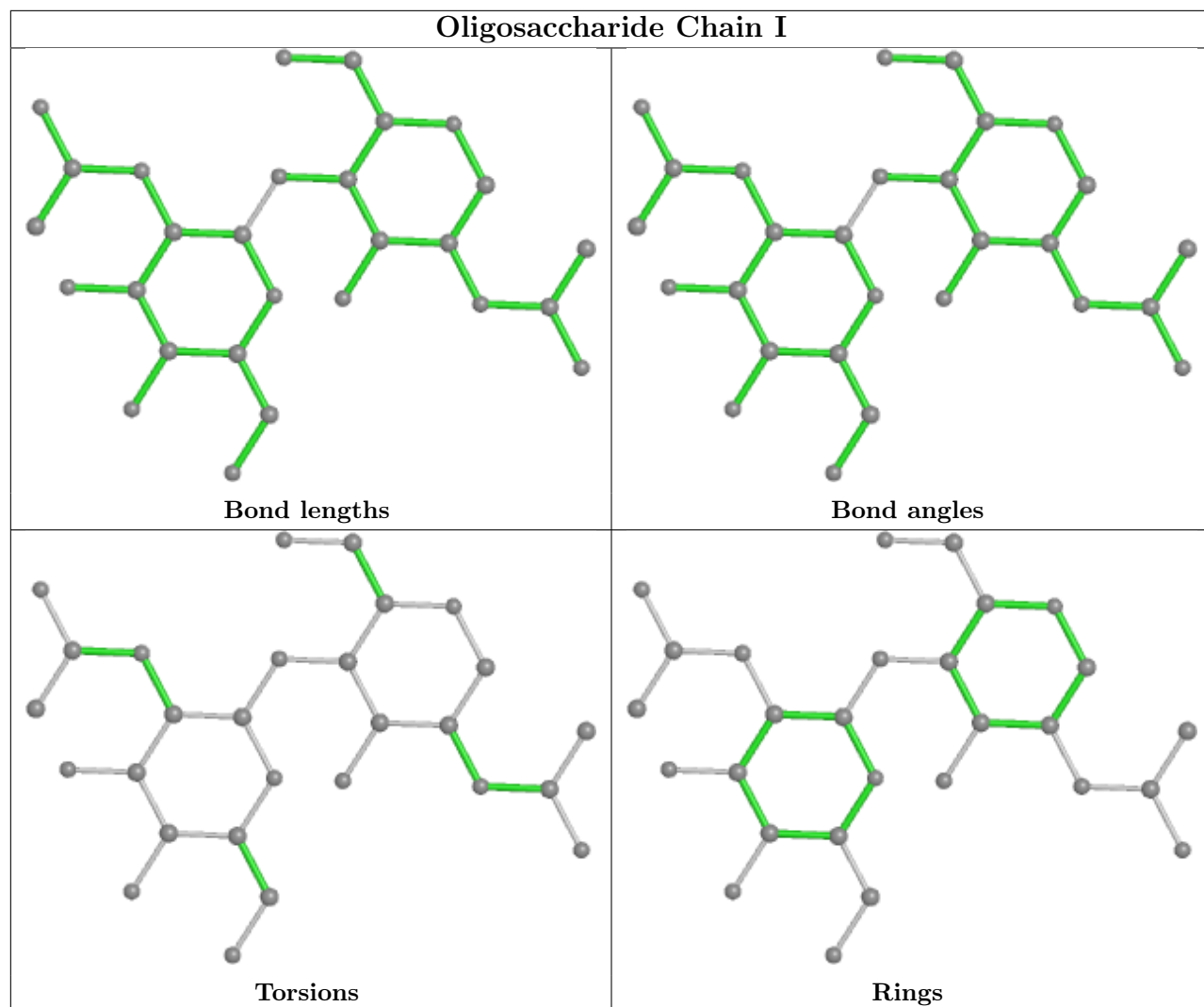
There are no ring outliers.

No monomer is involved in short contacts.

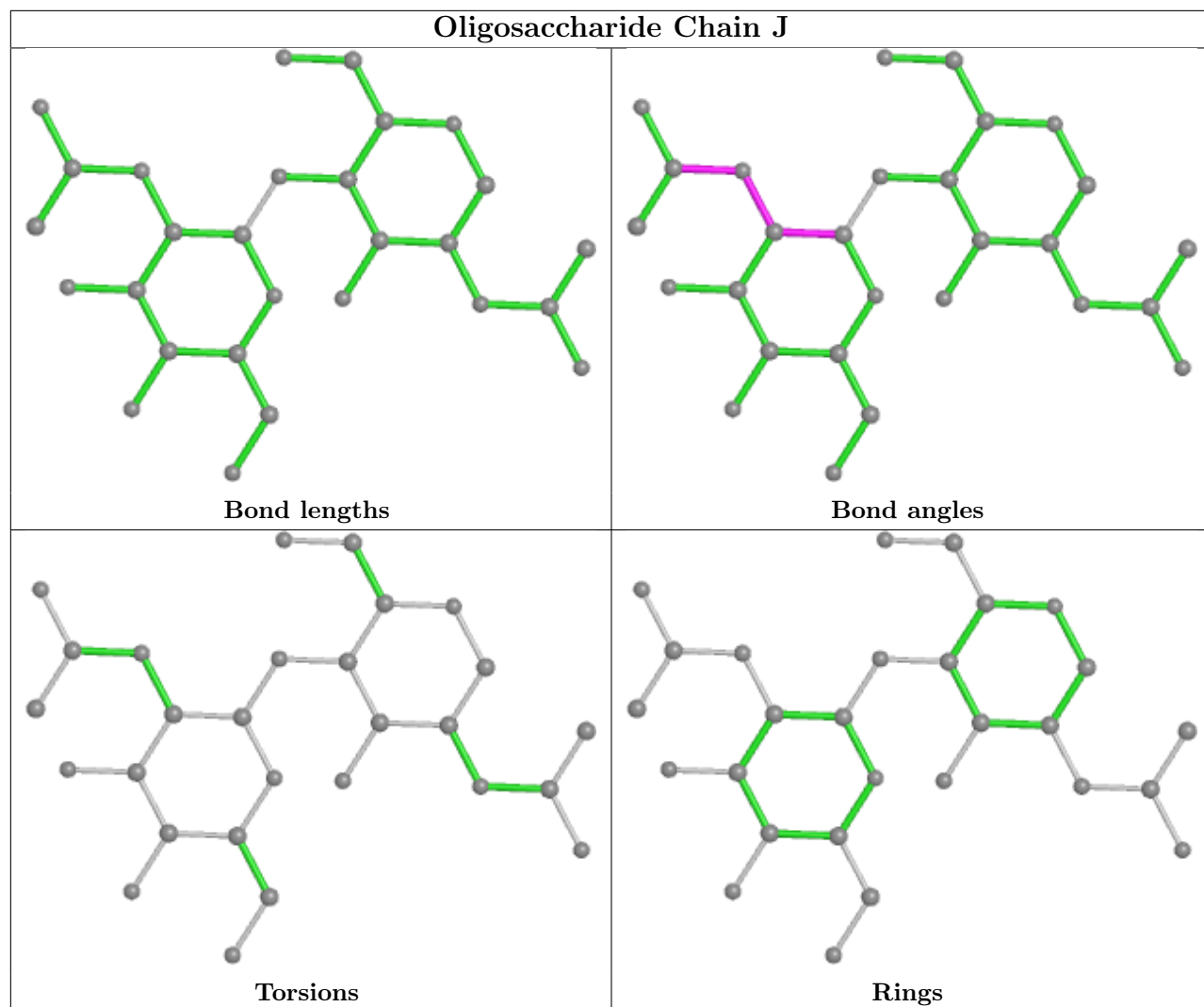
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

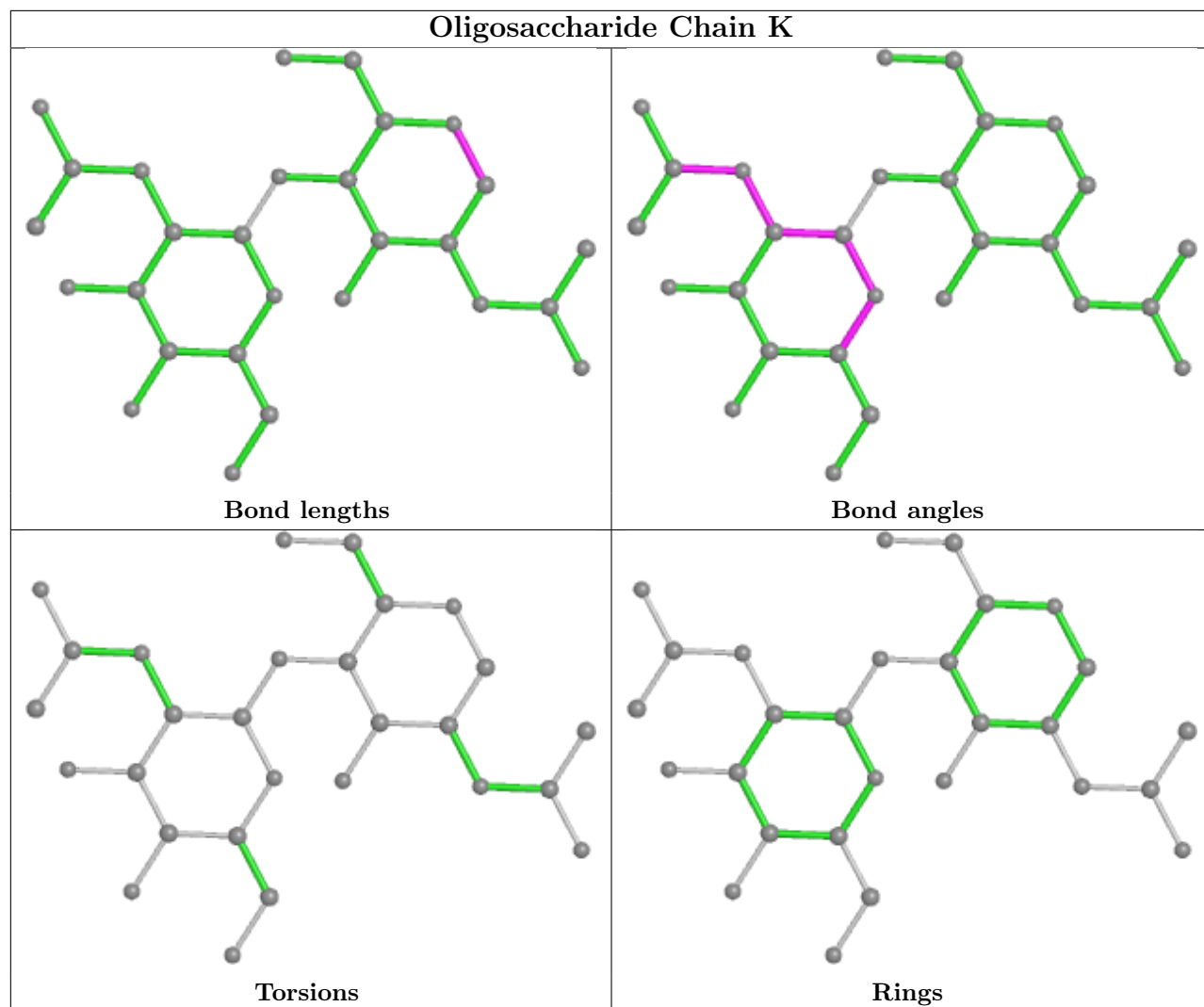


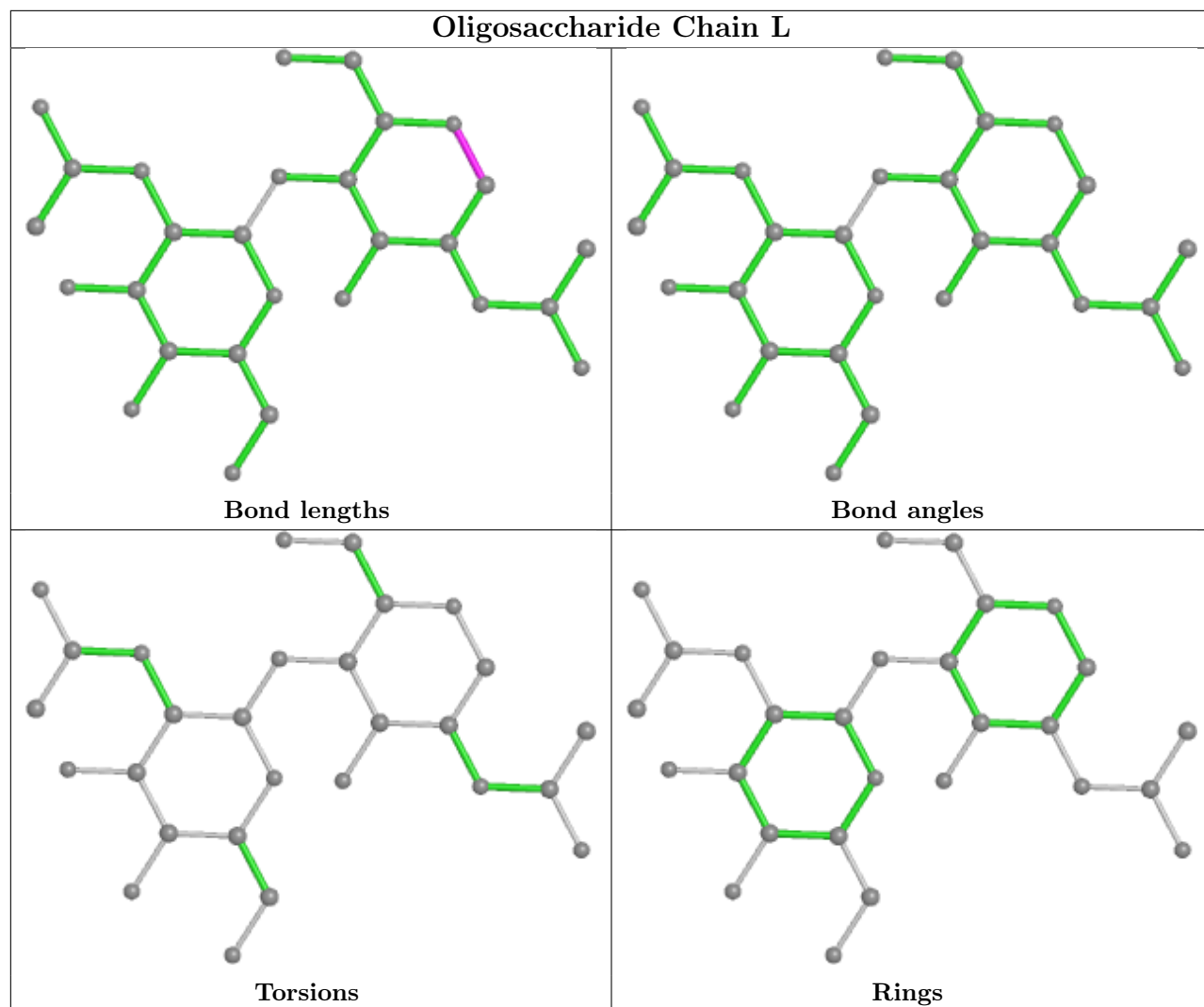


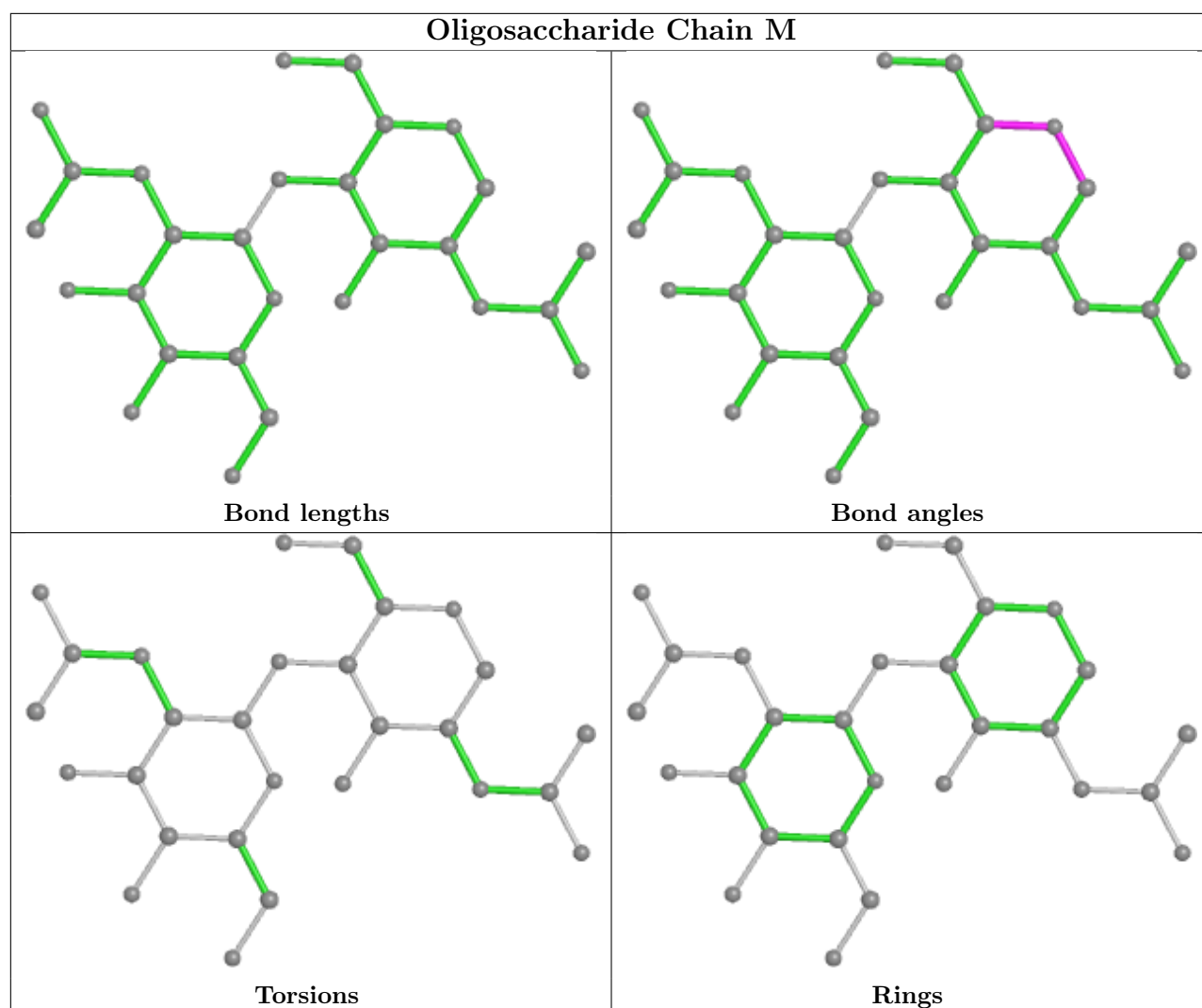


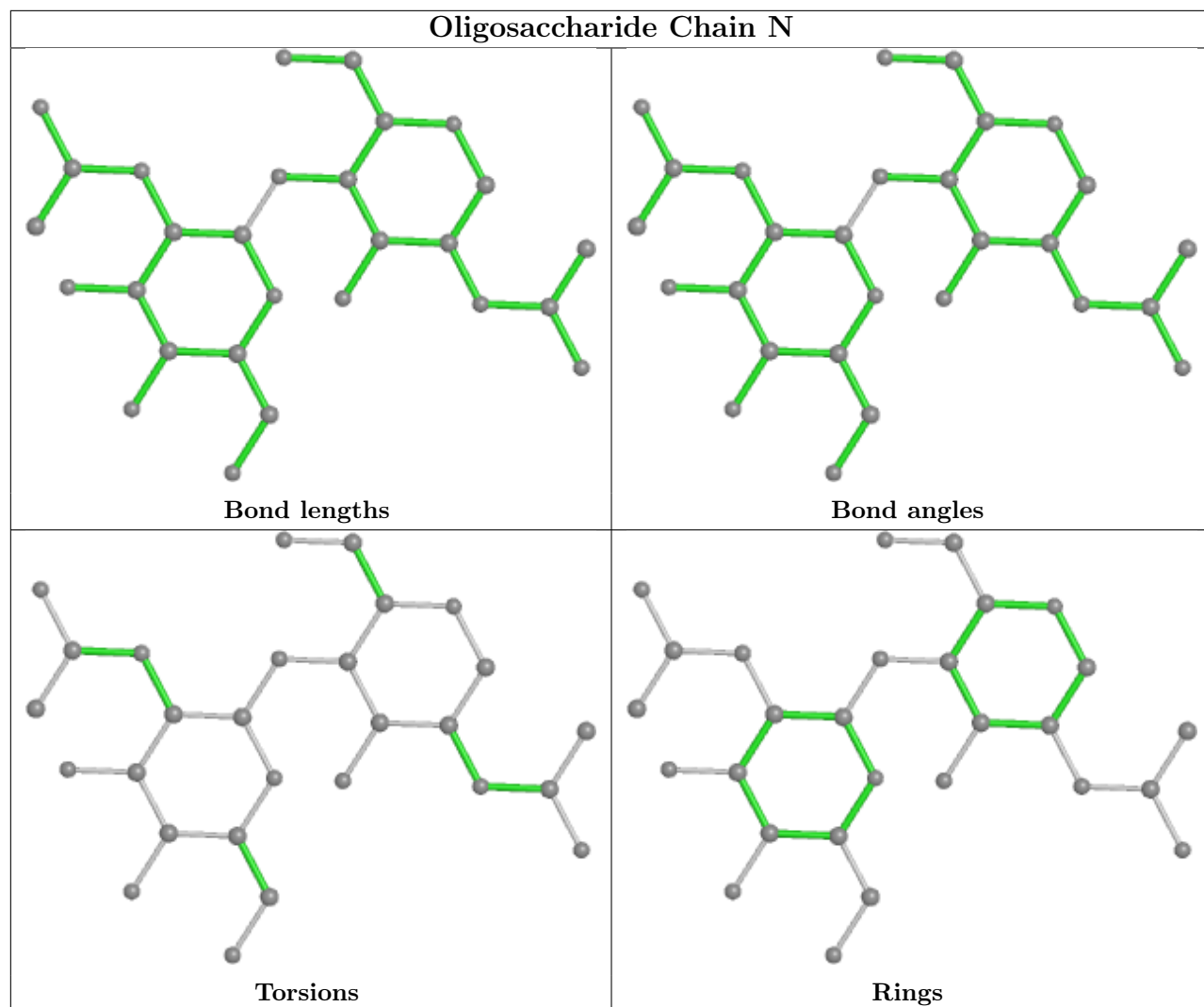


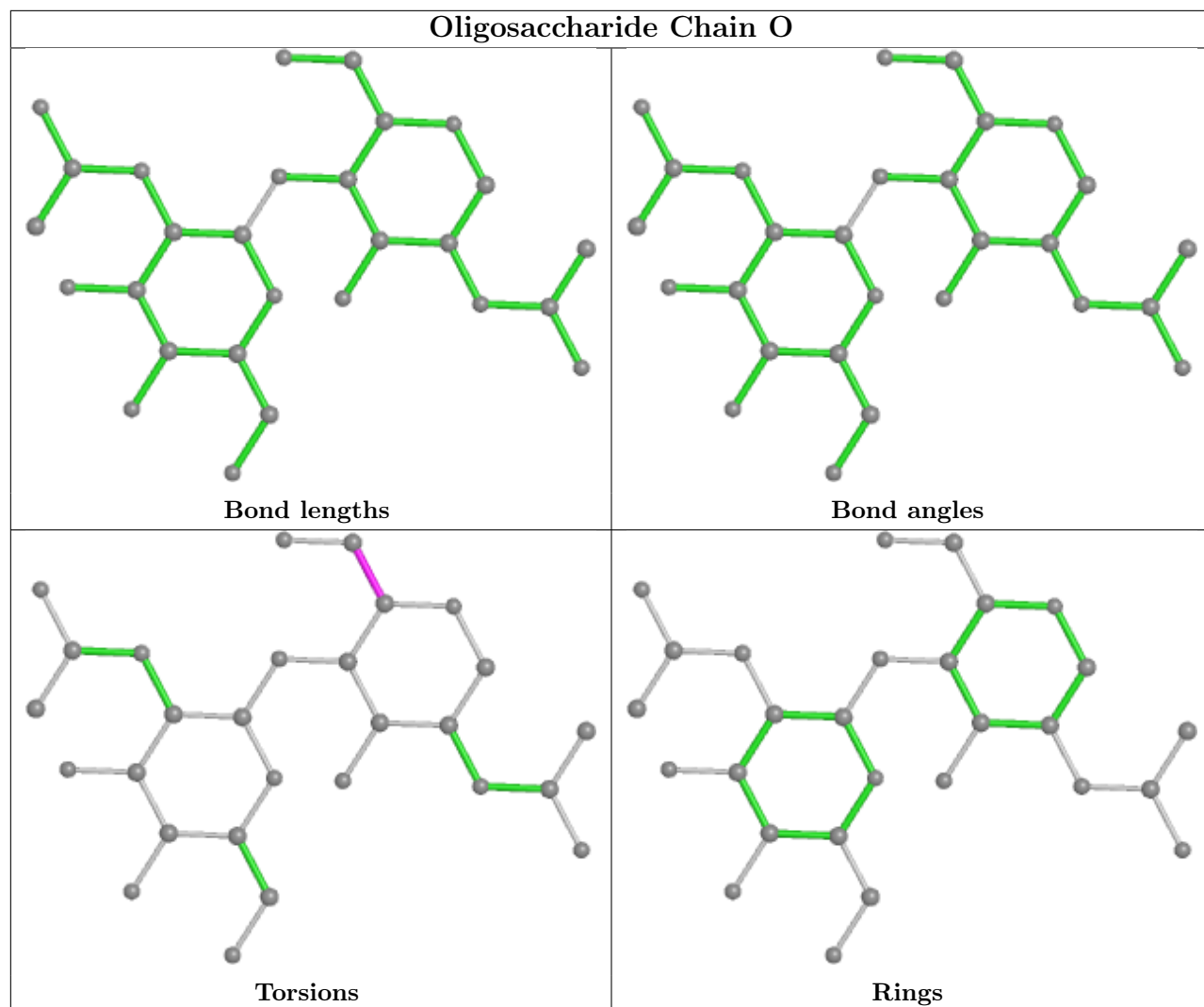


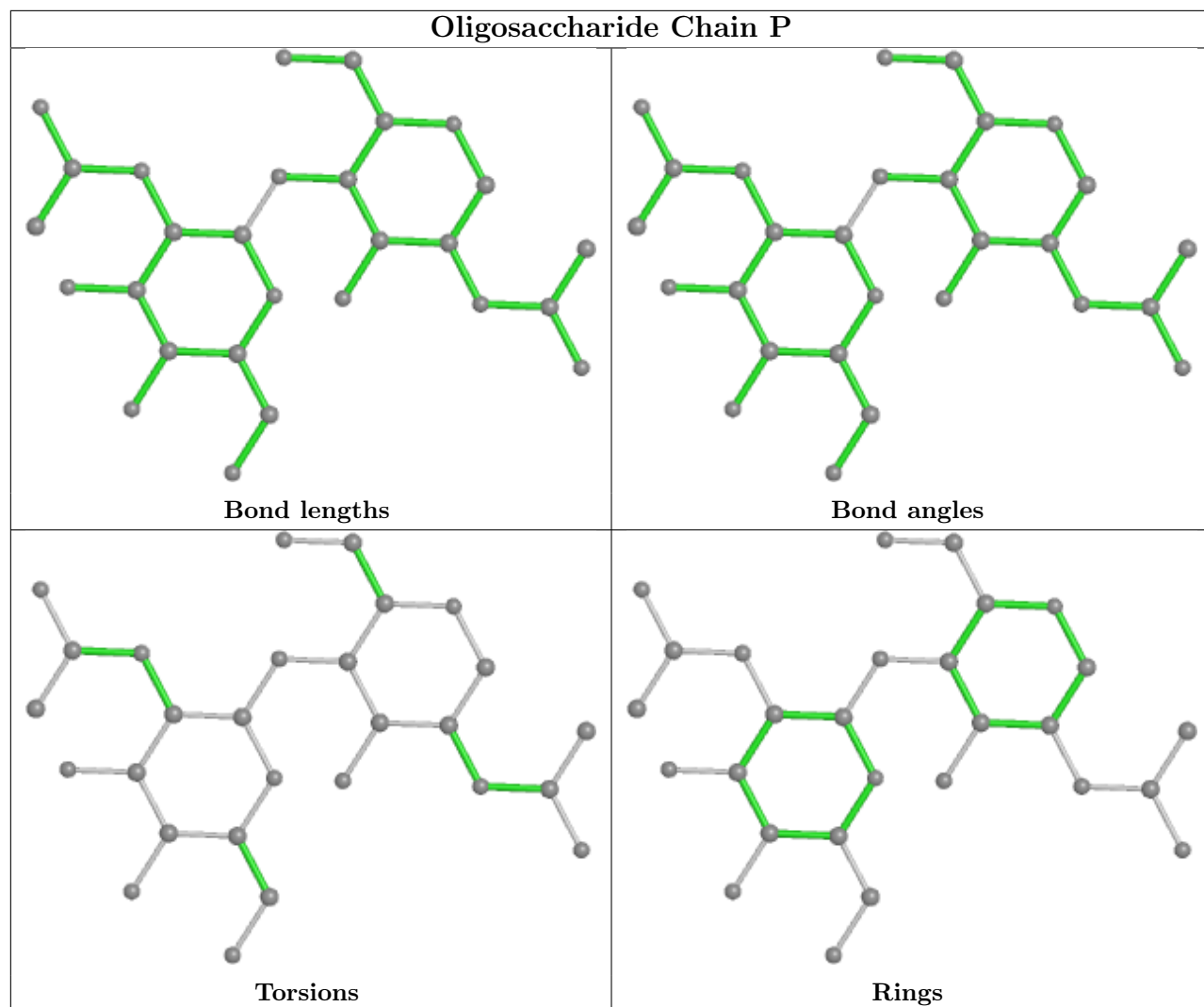


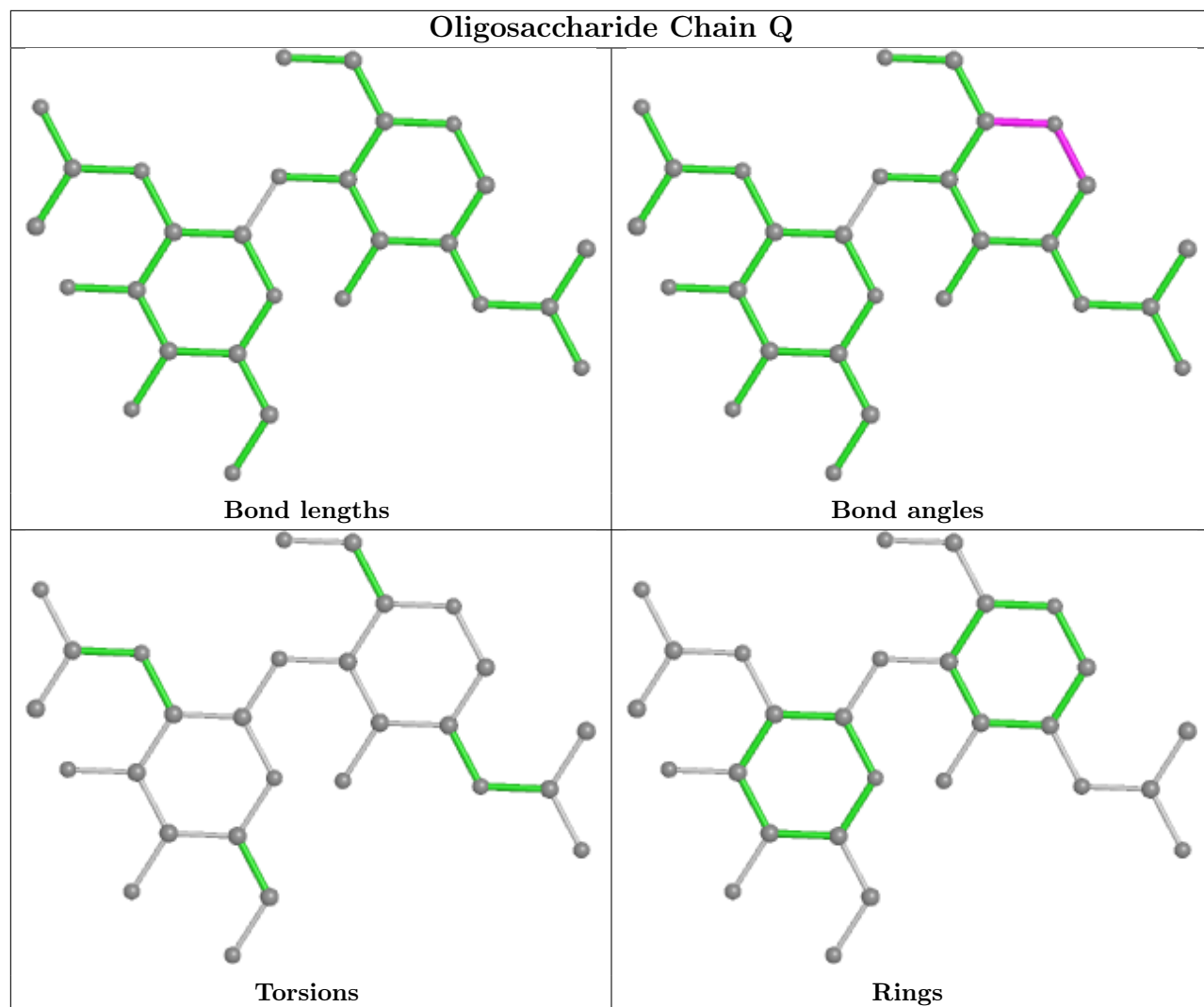




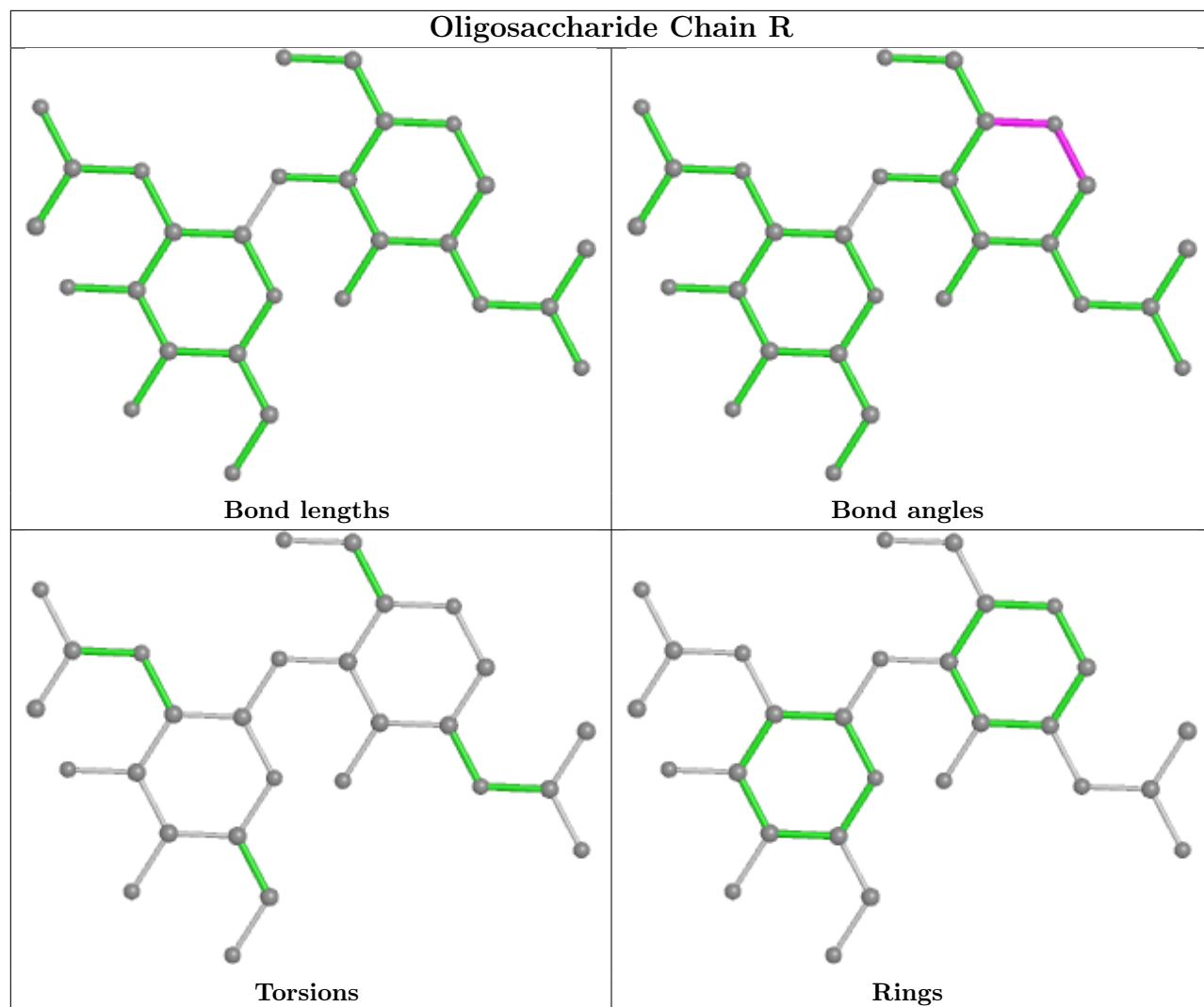


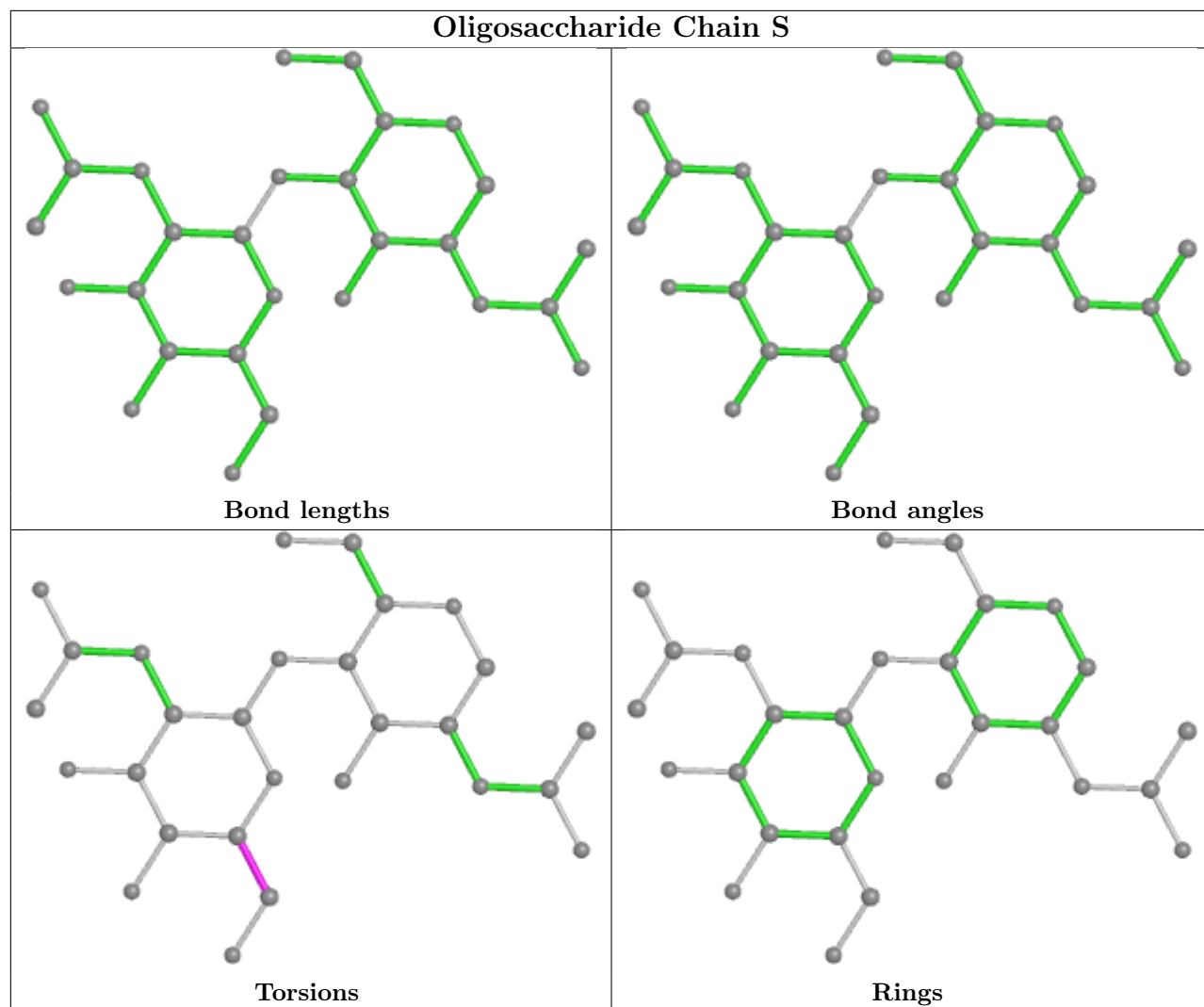


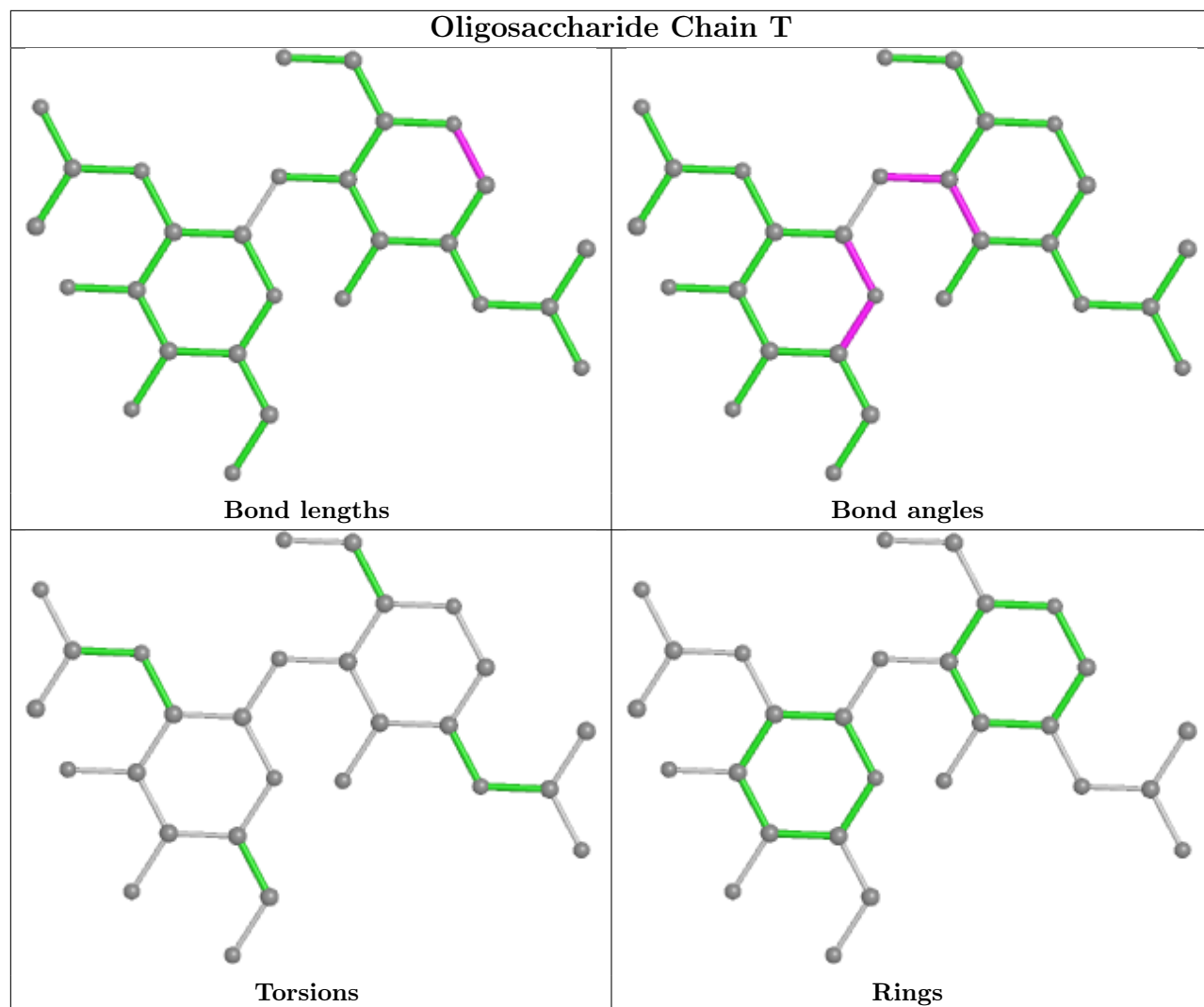


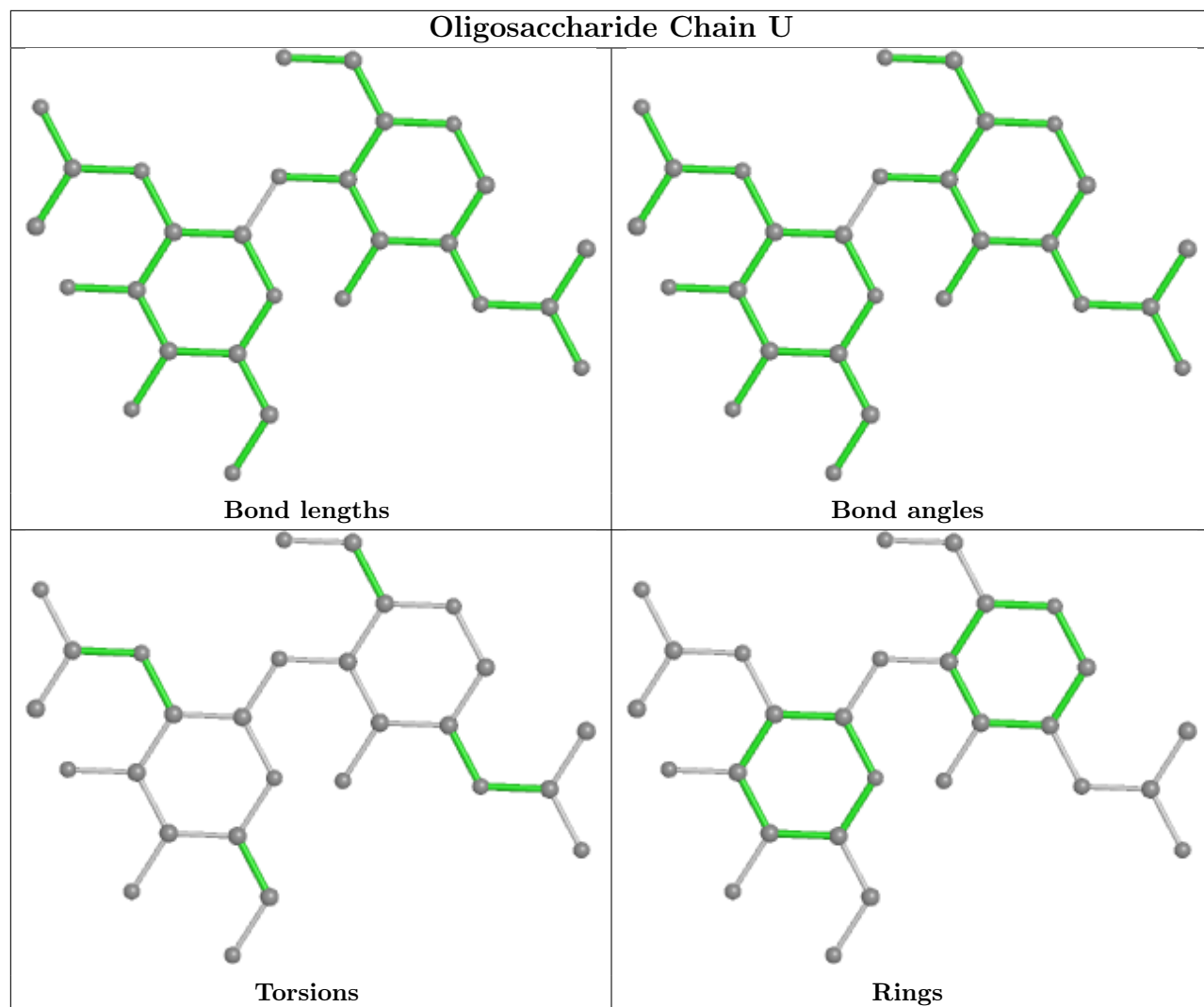


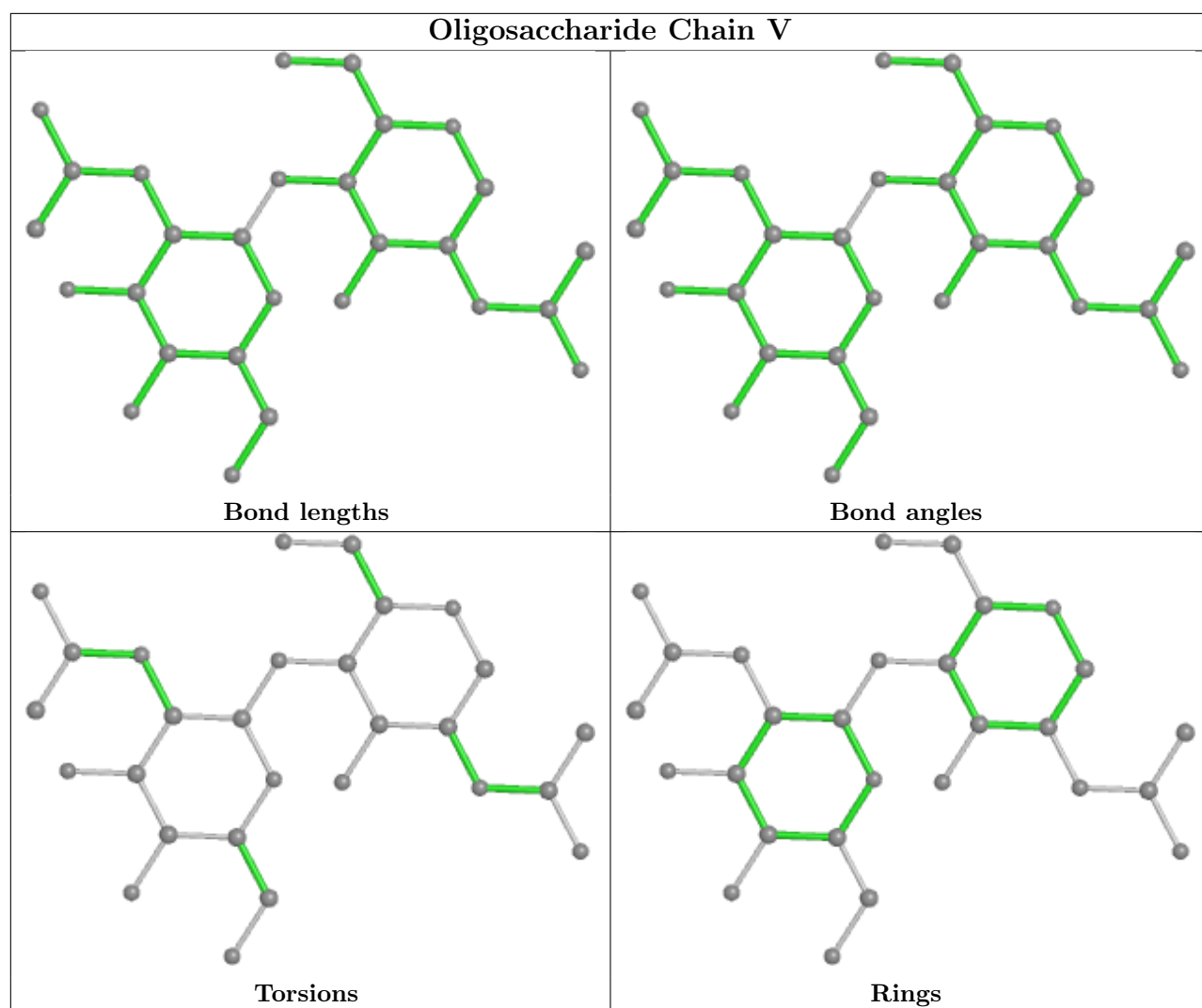


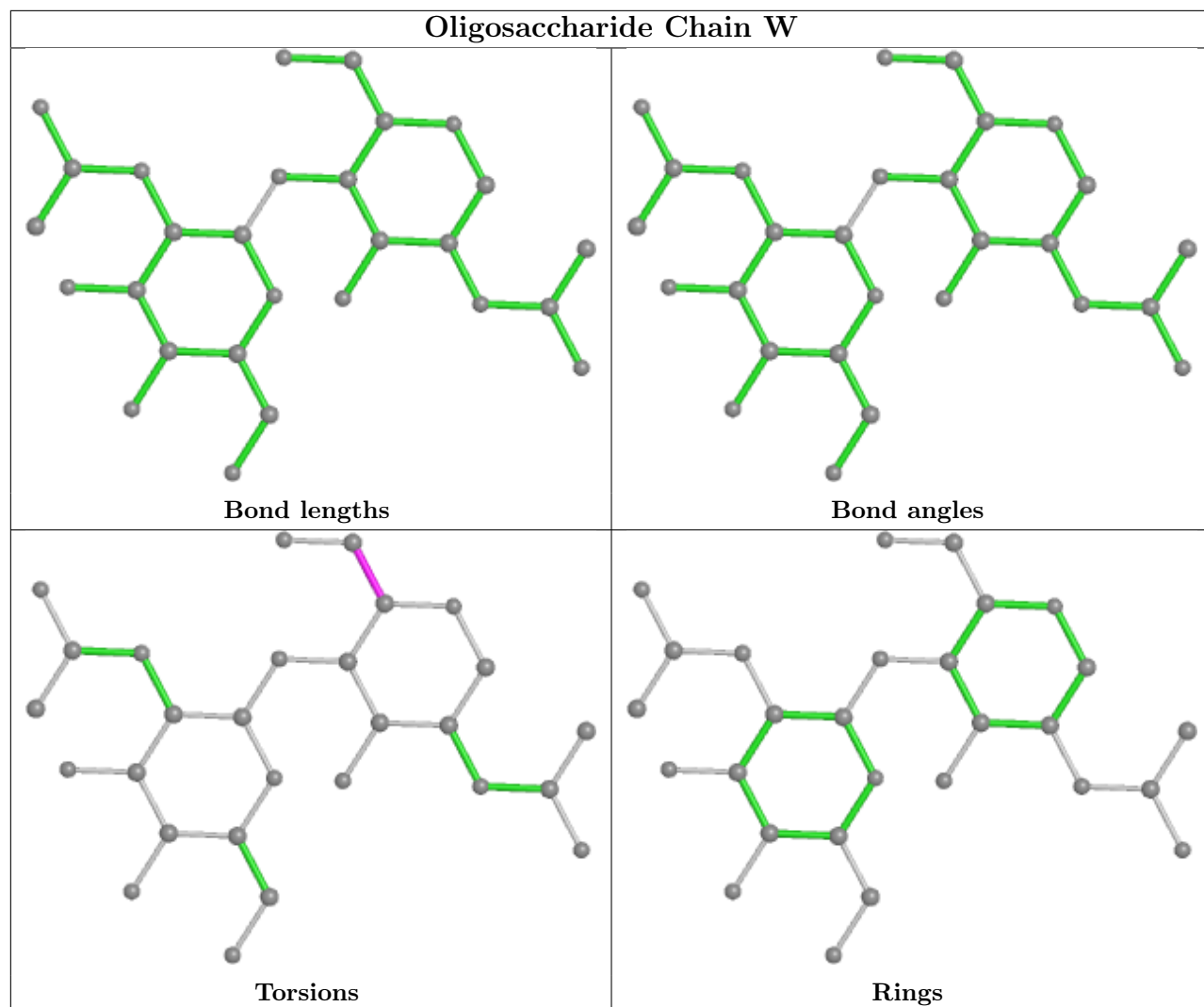


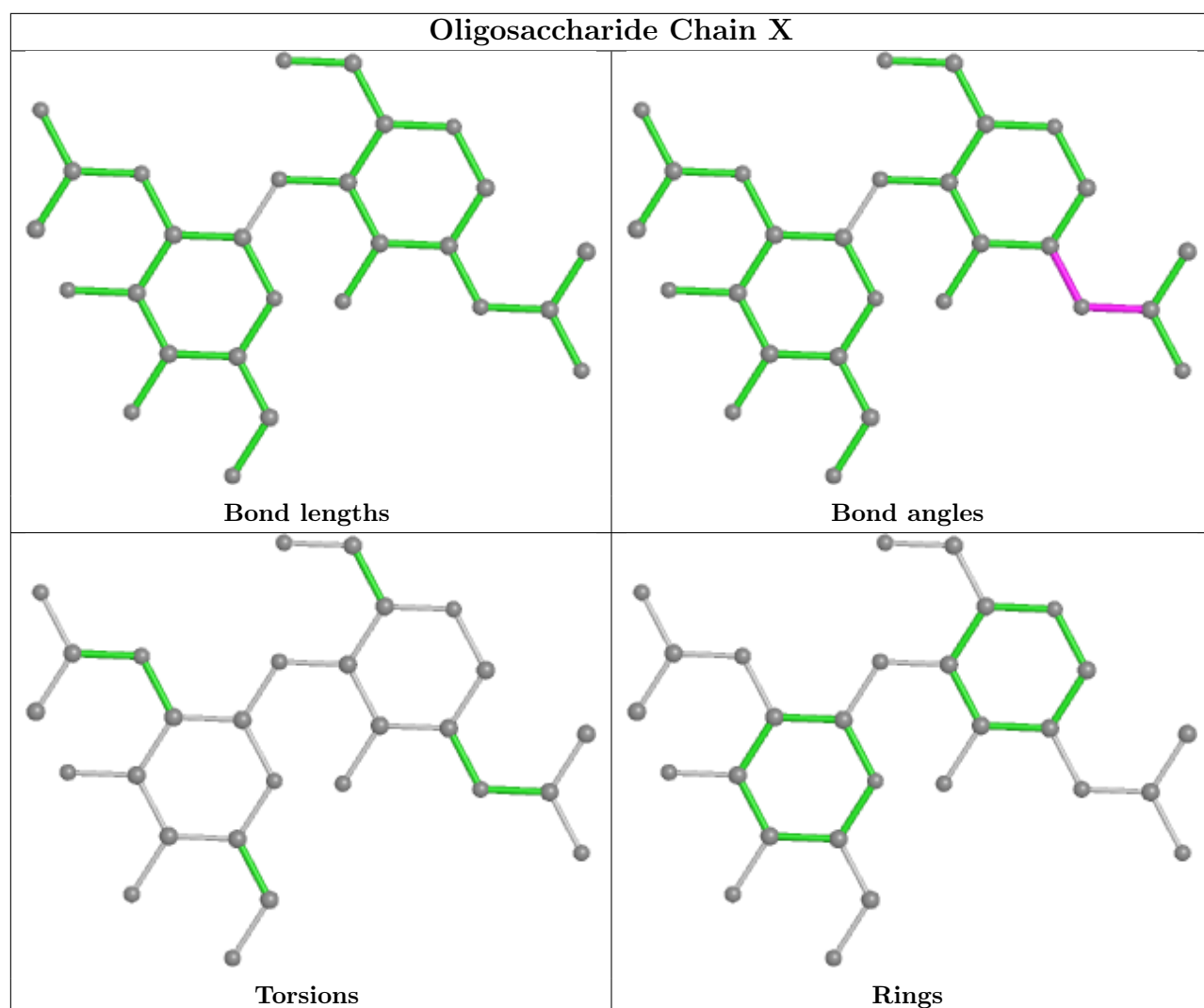


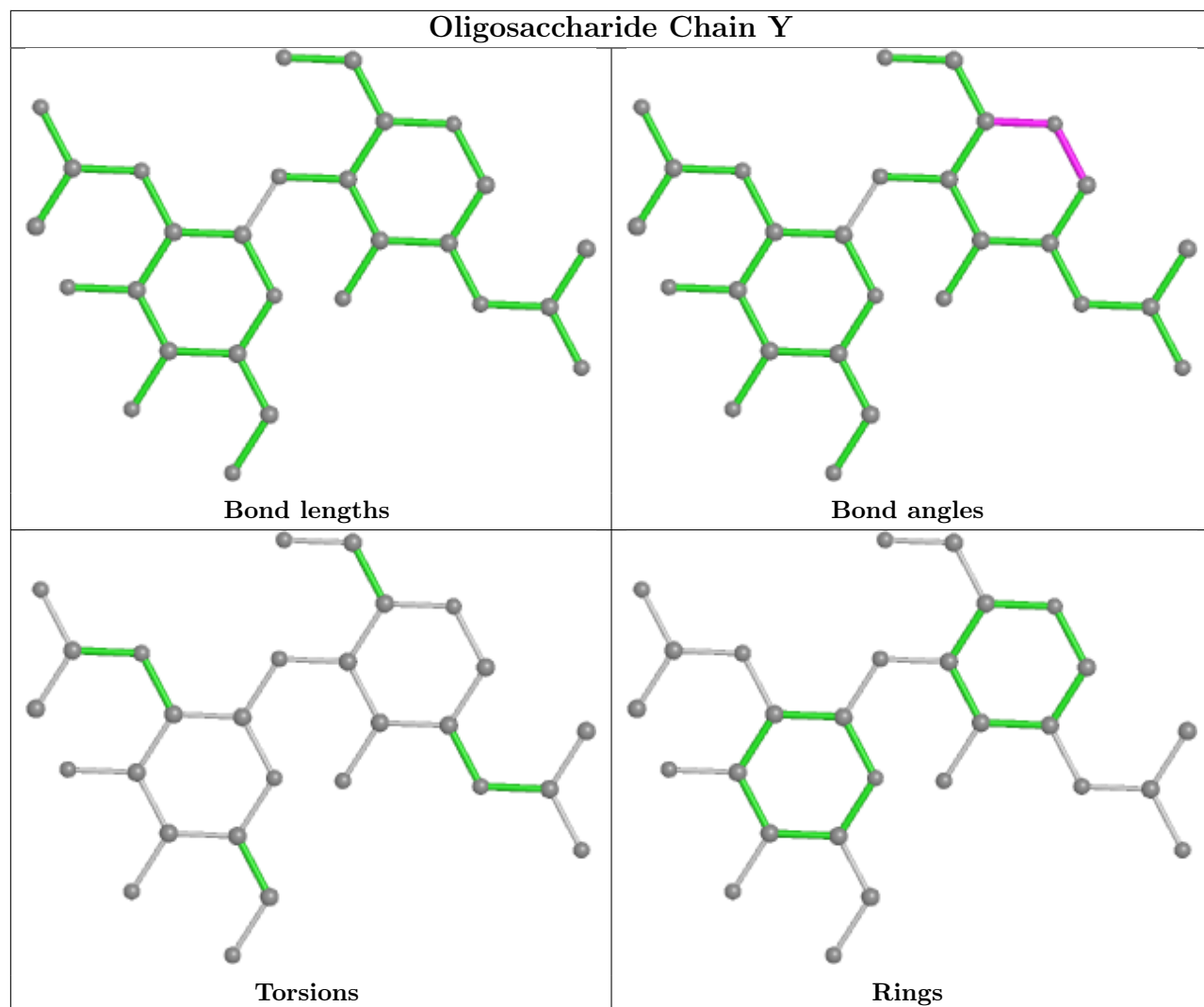




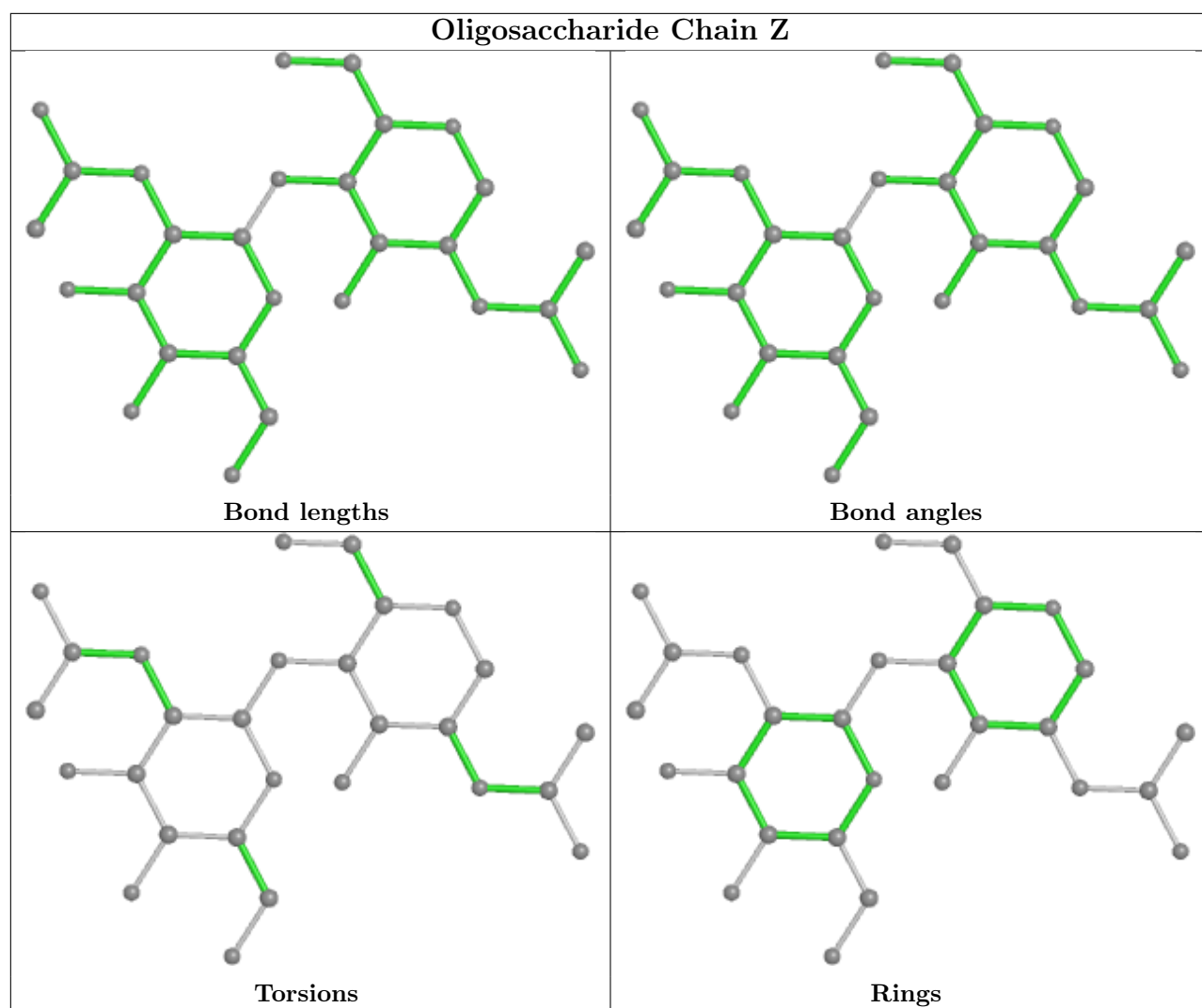


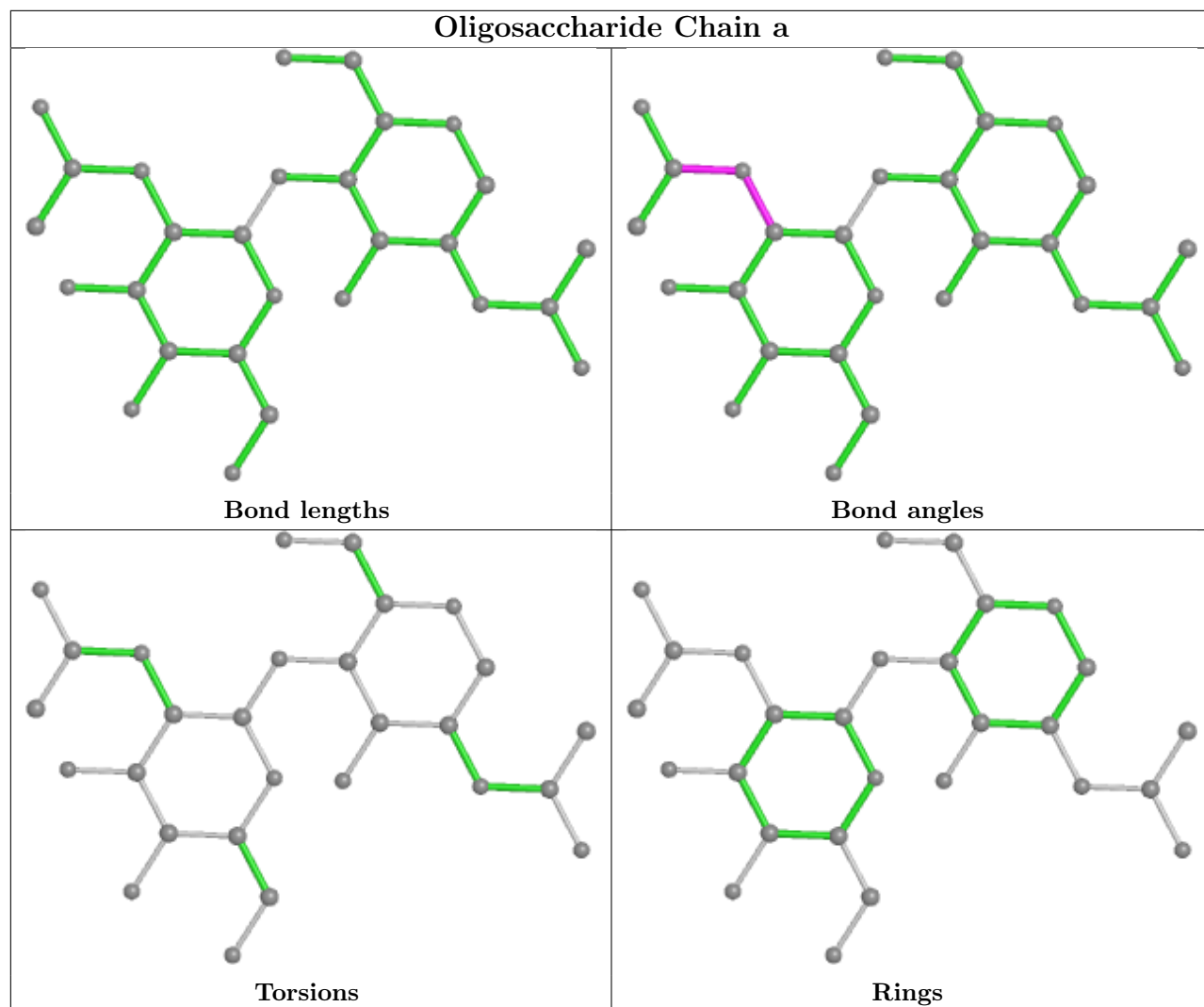


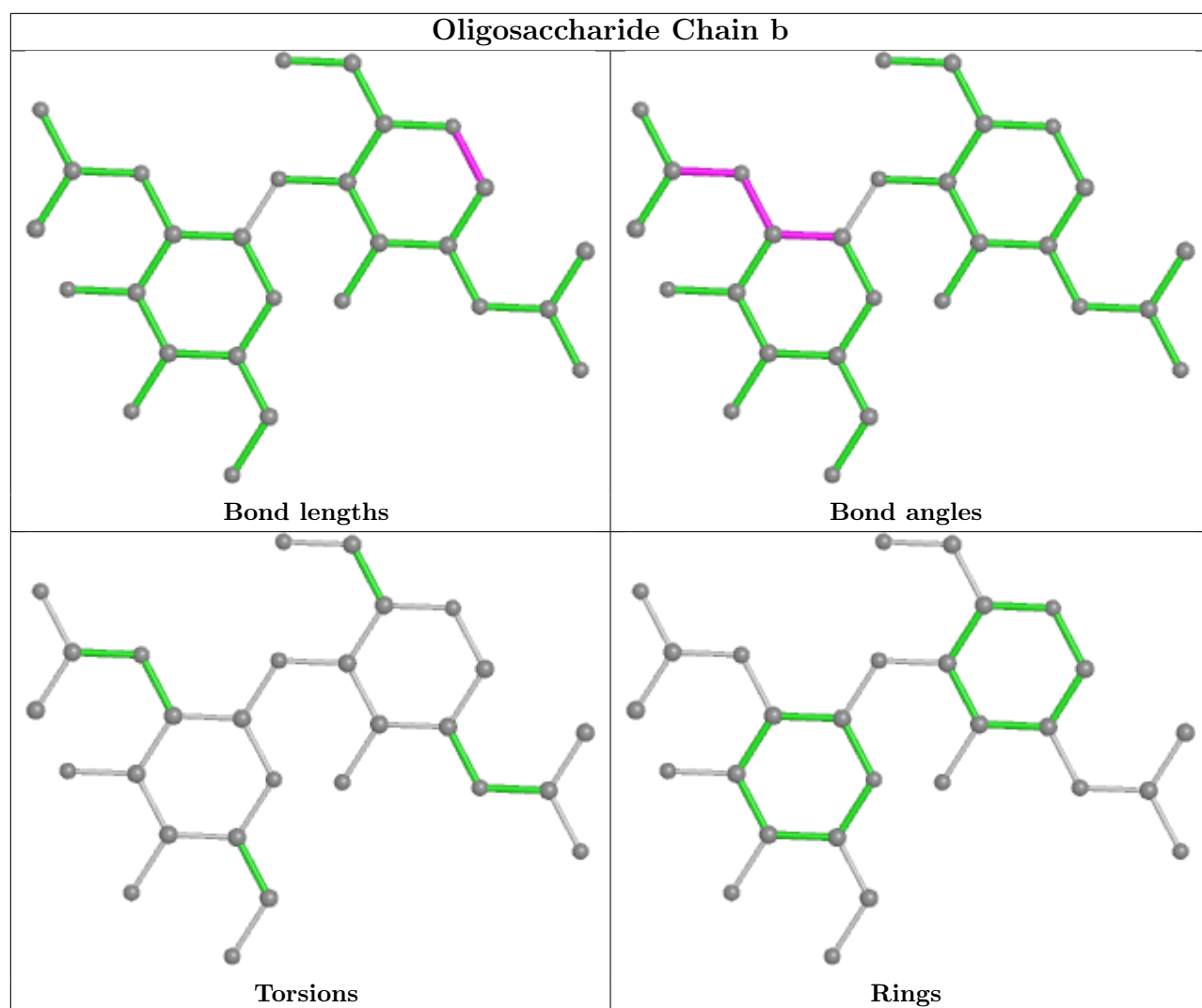


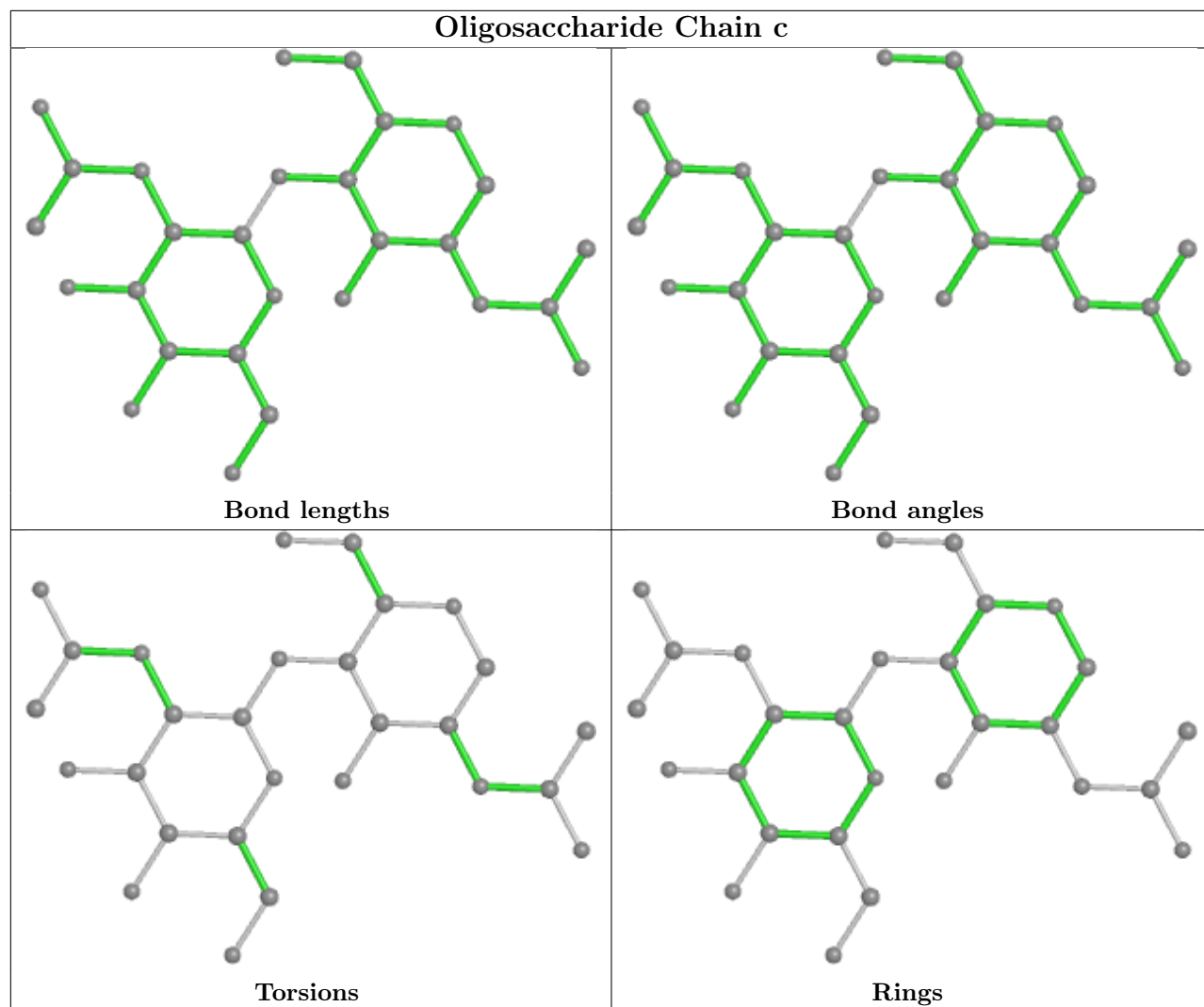


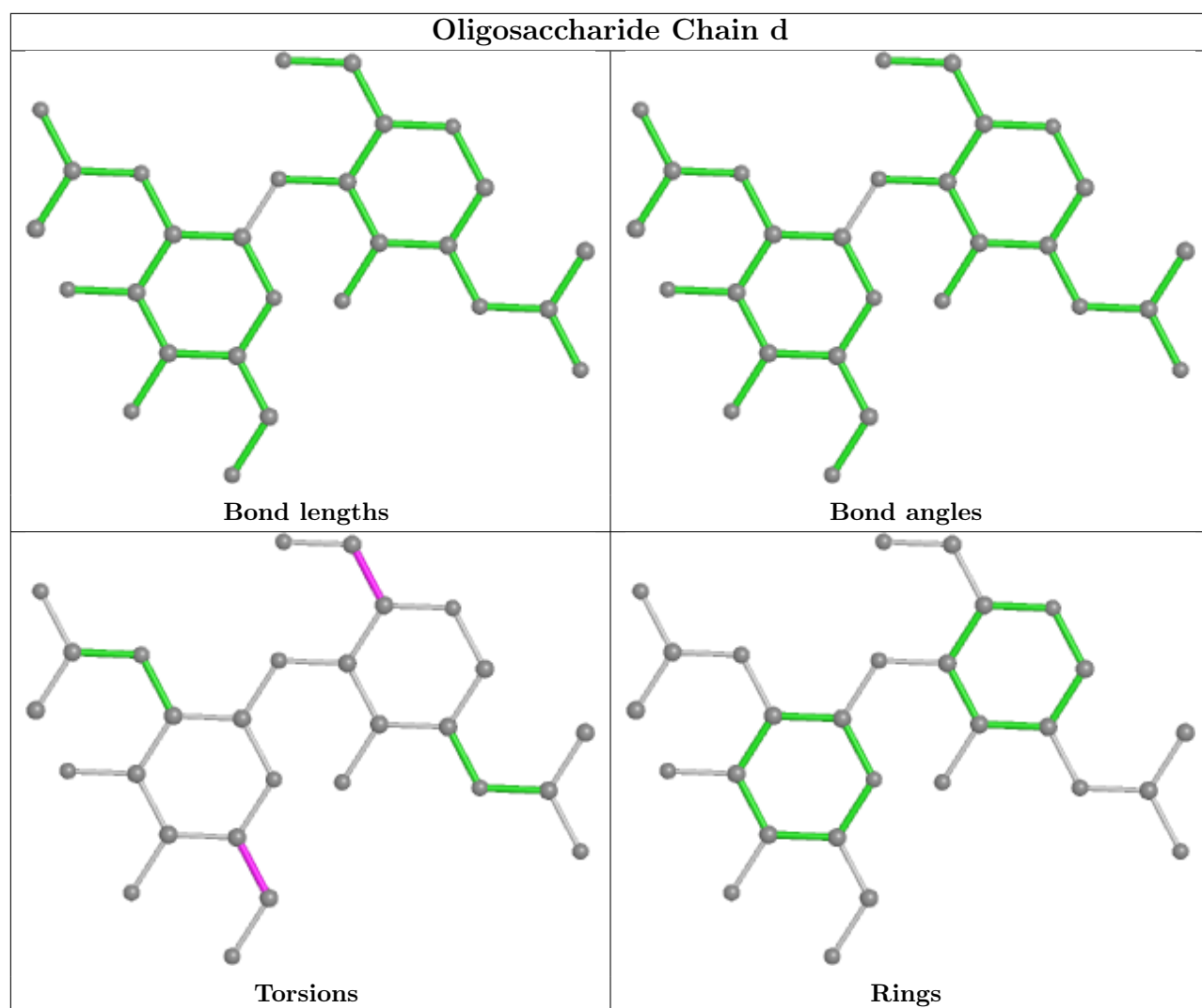


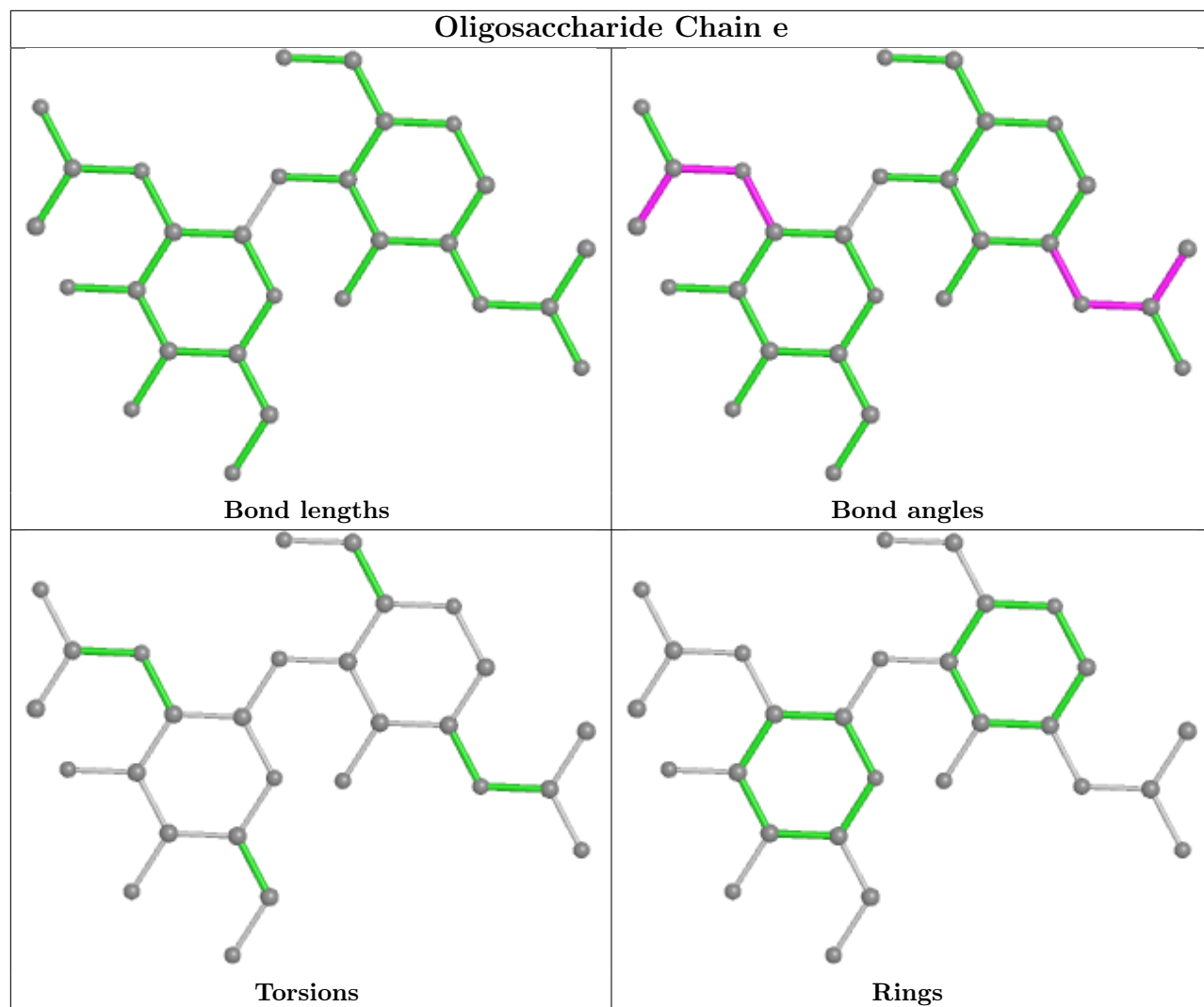


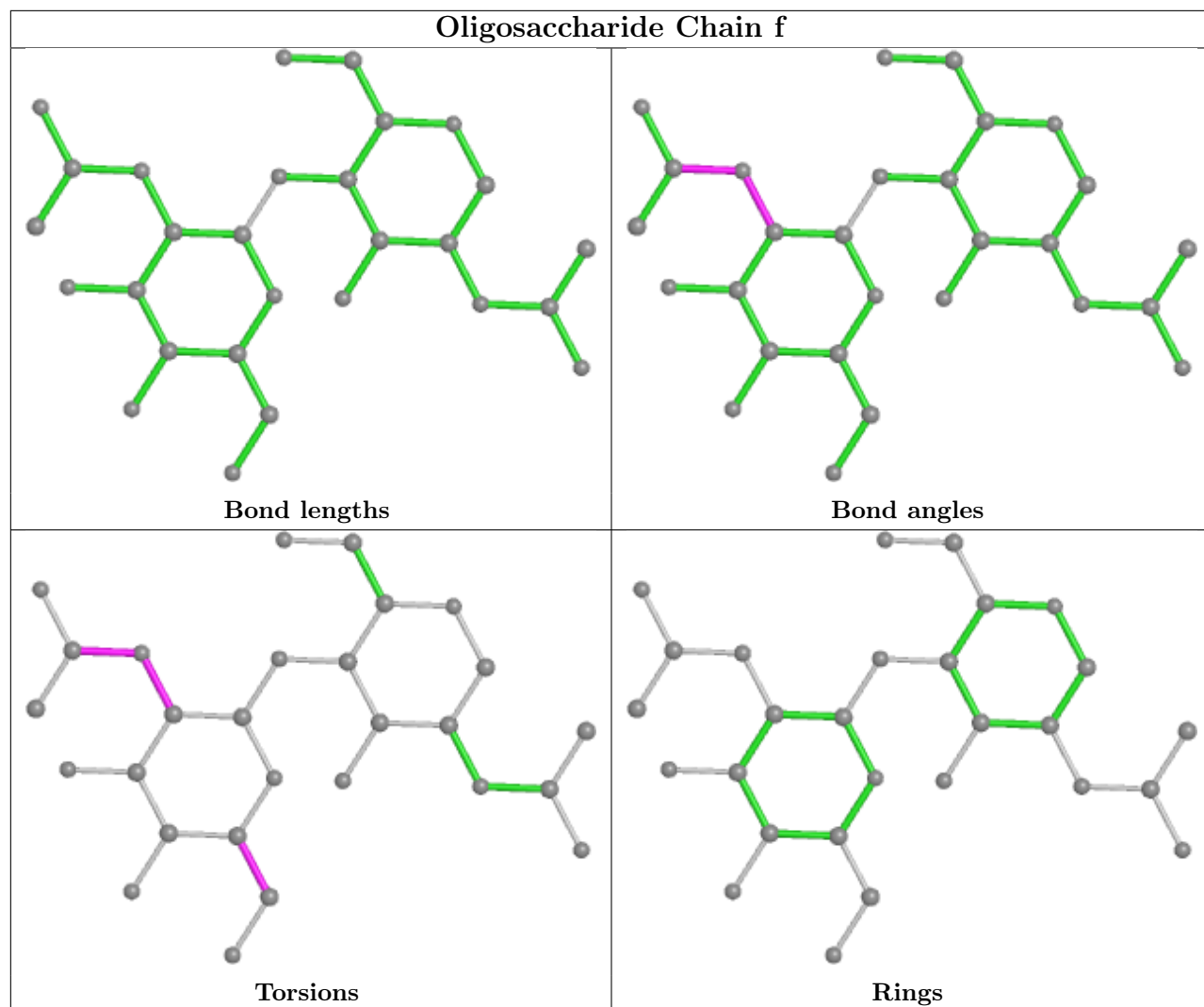


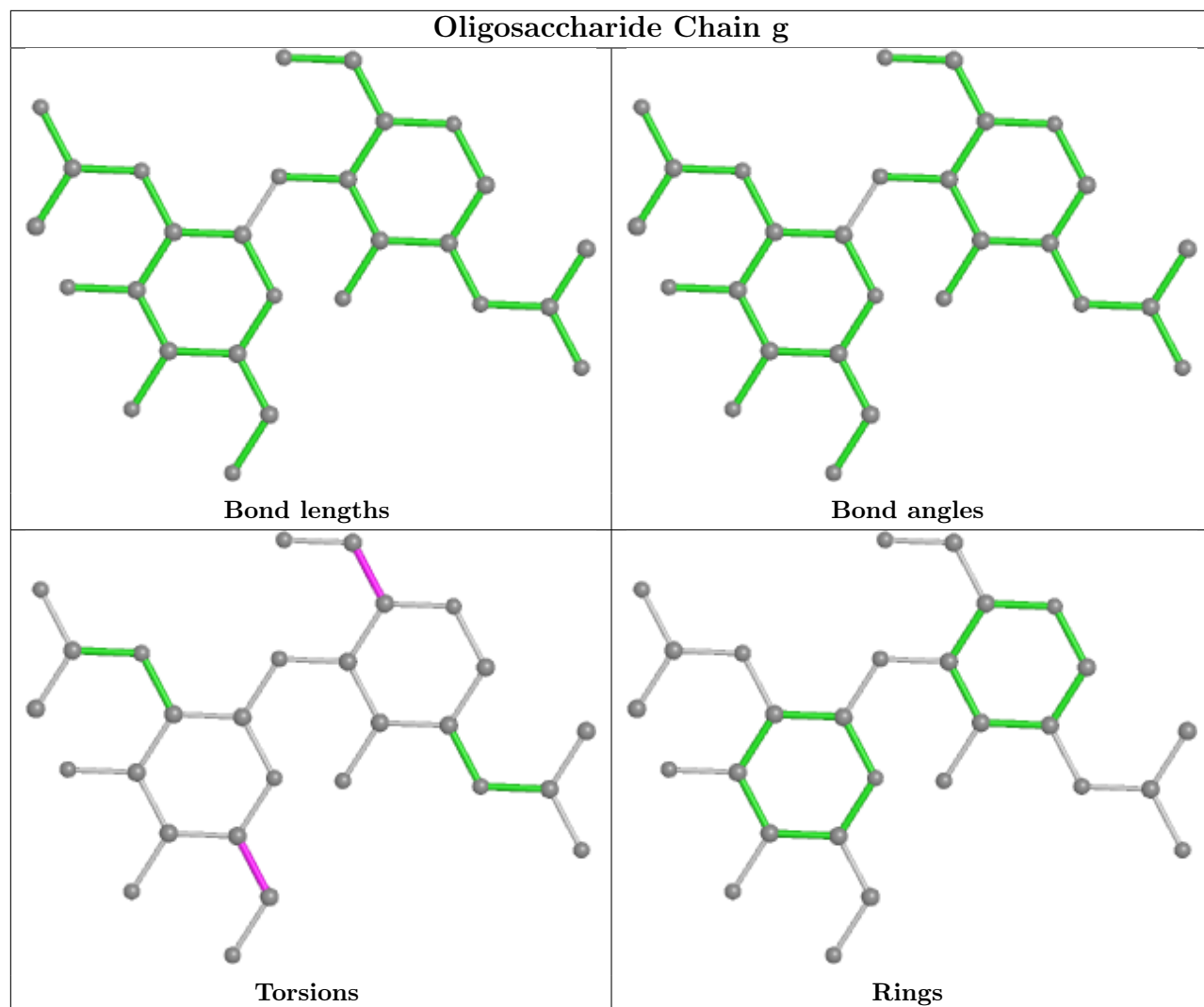




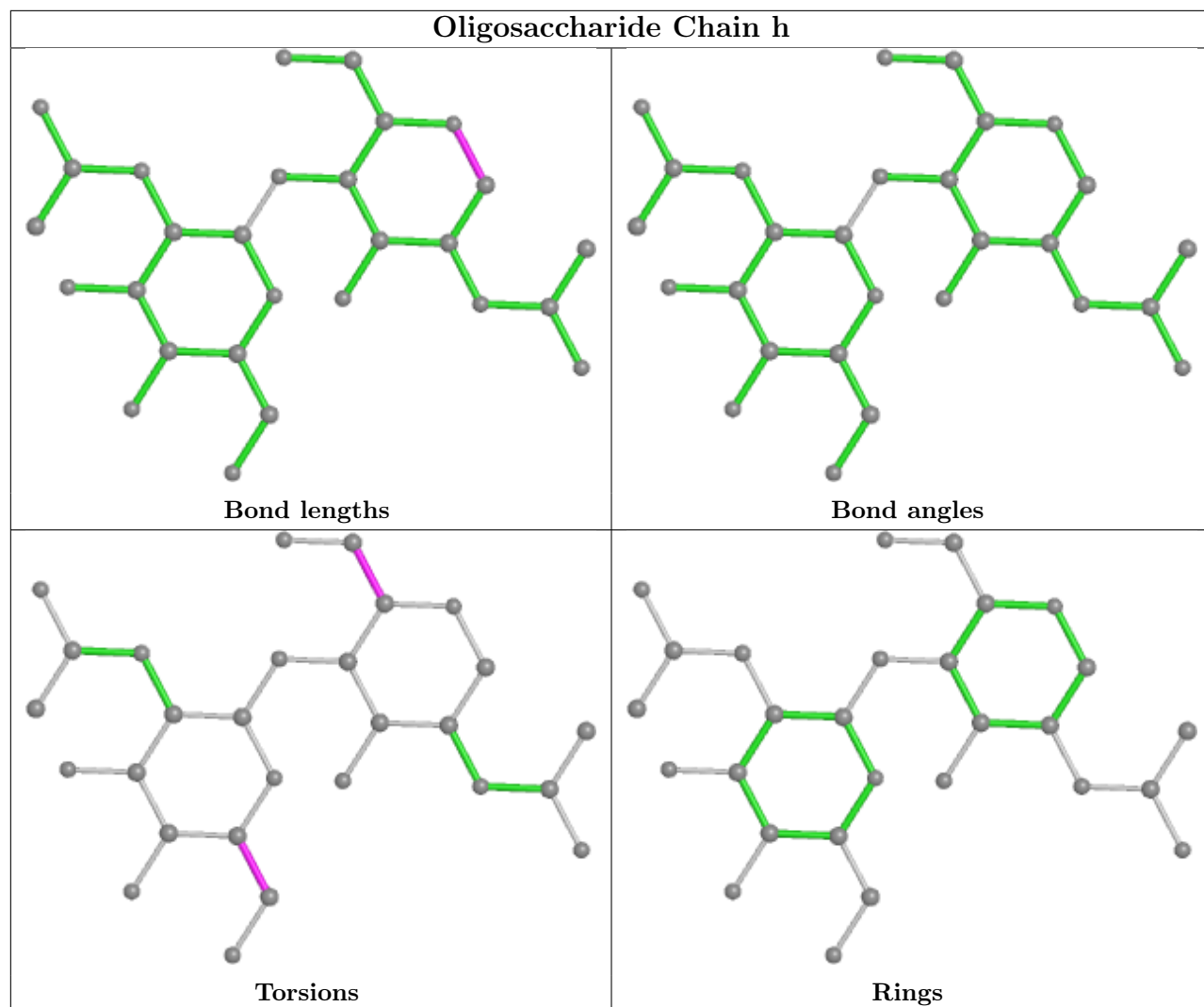


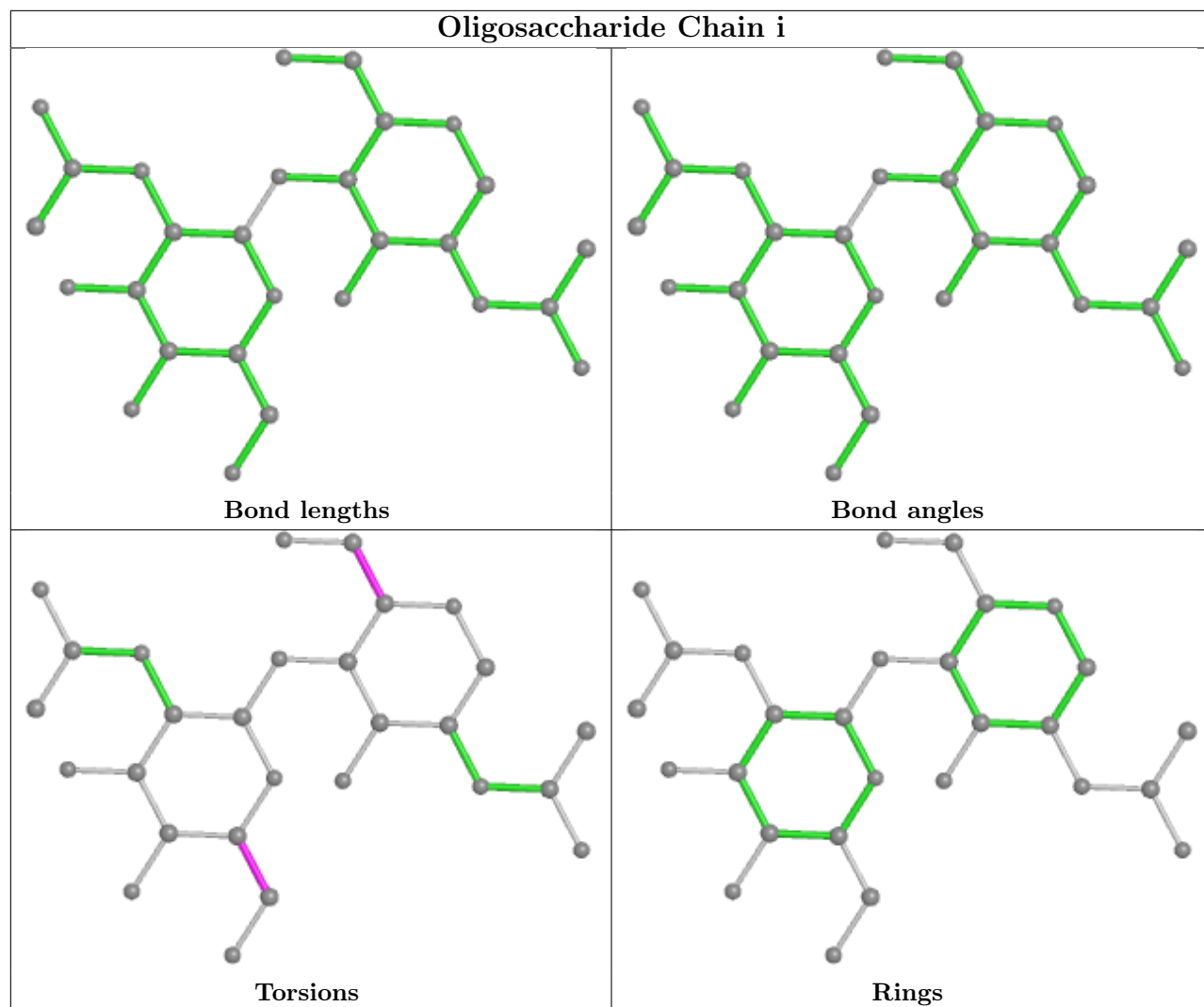


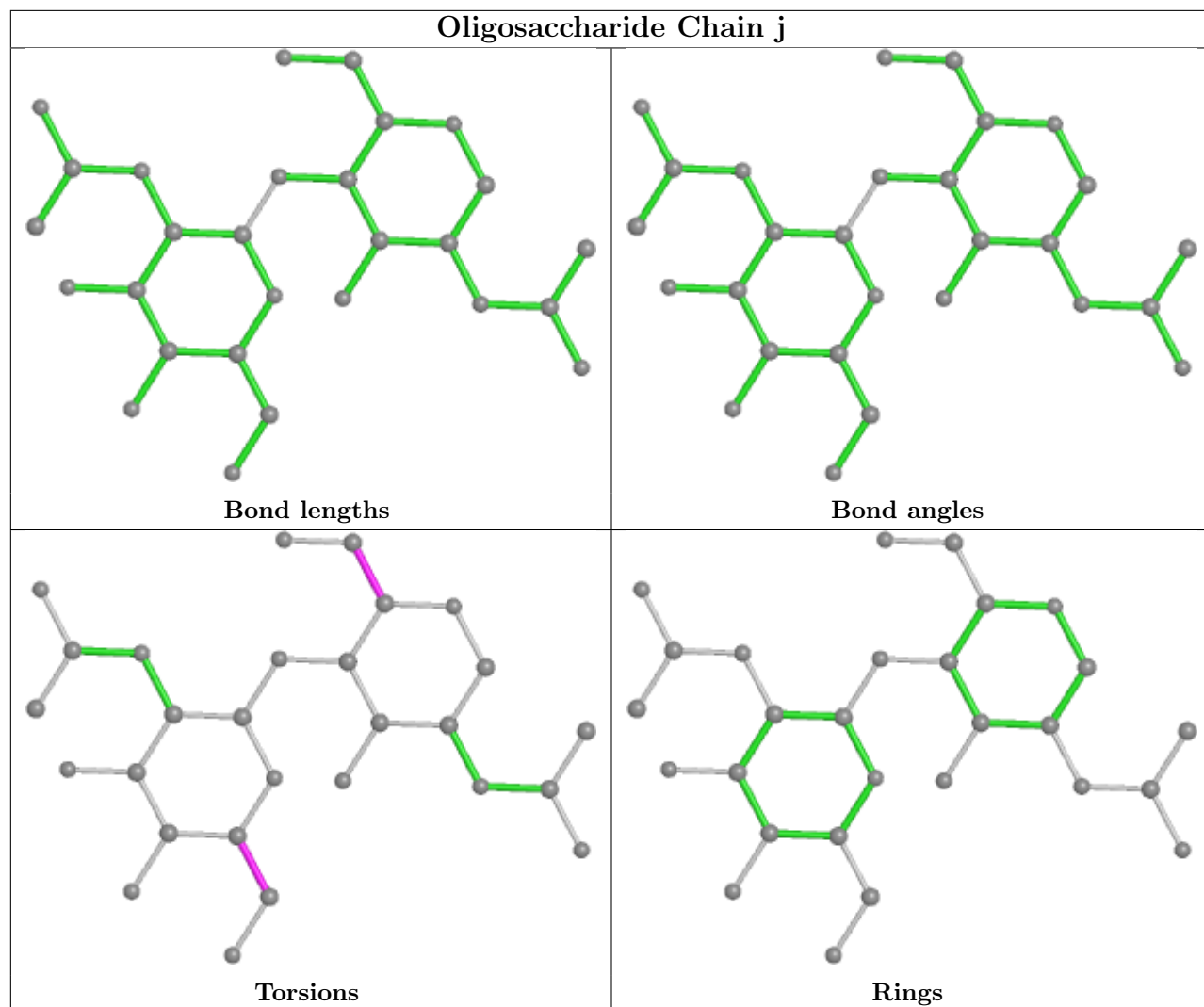


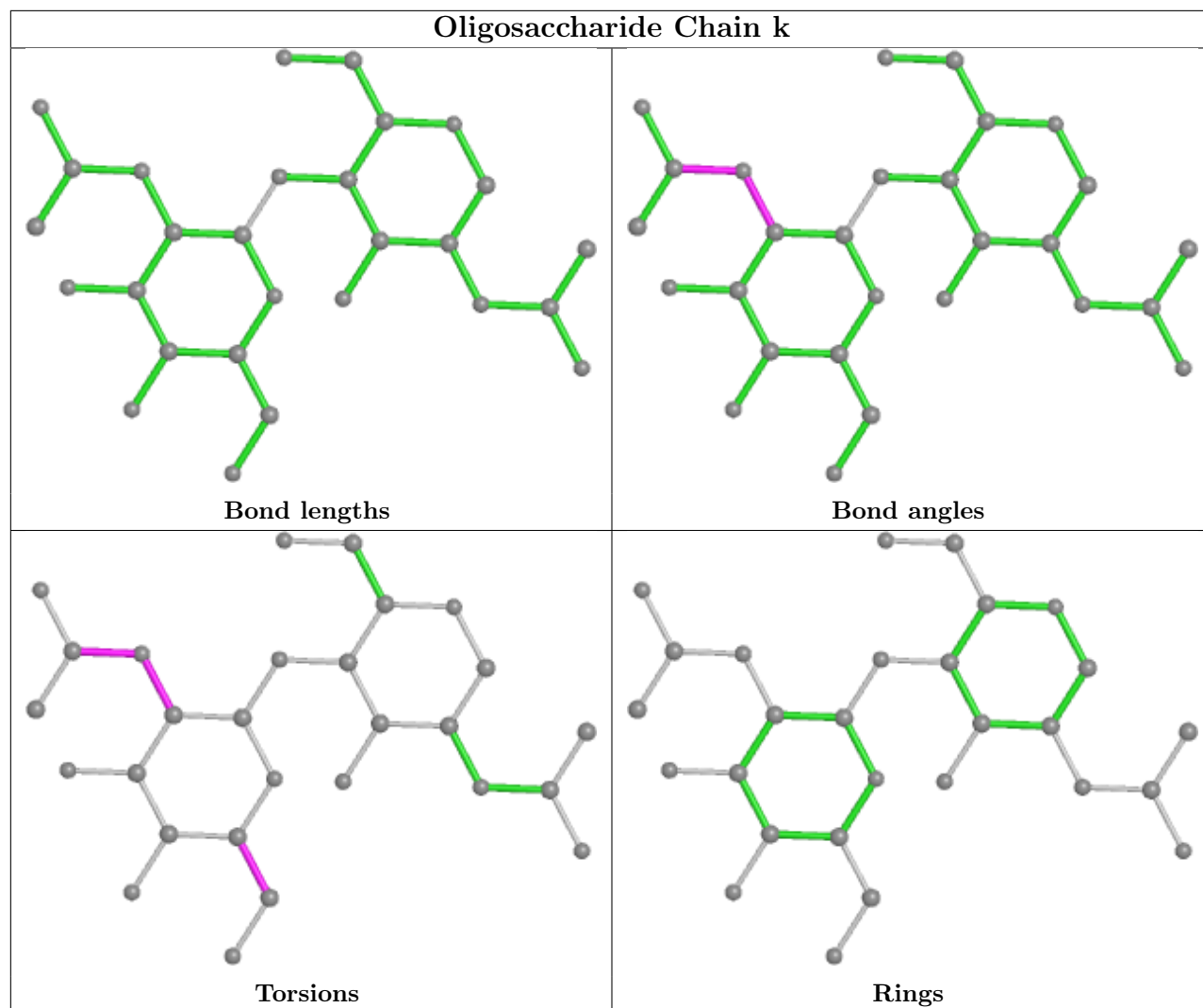


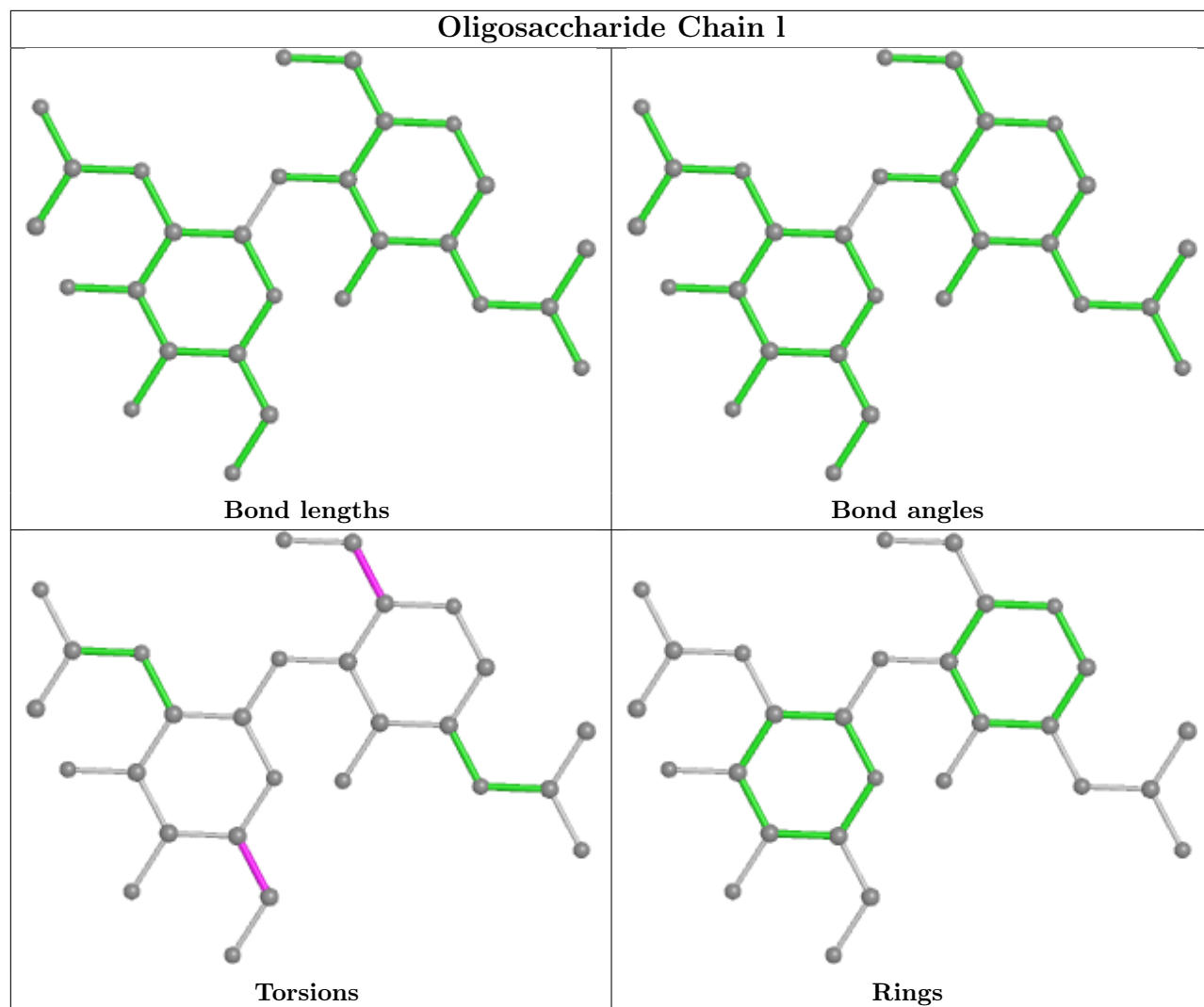


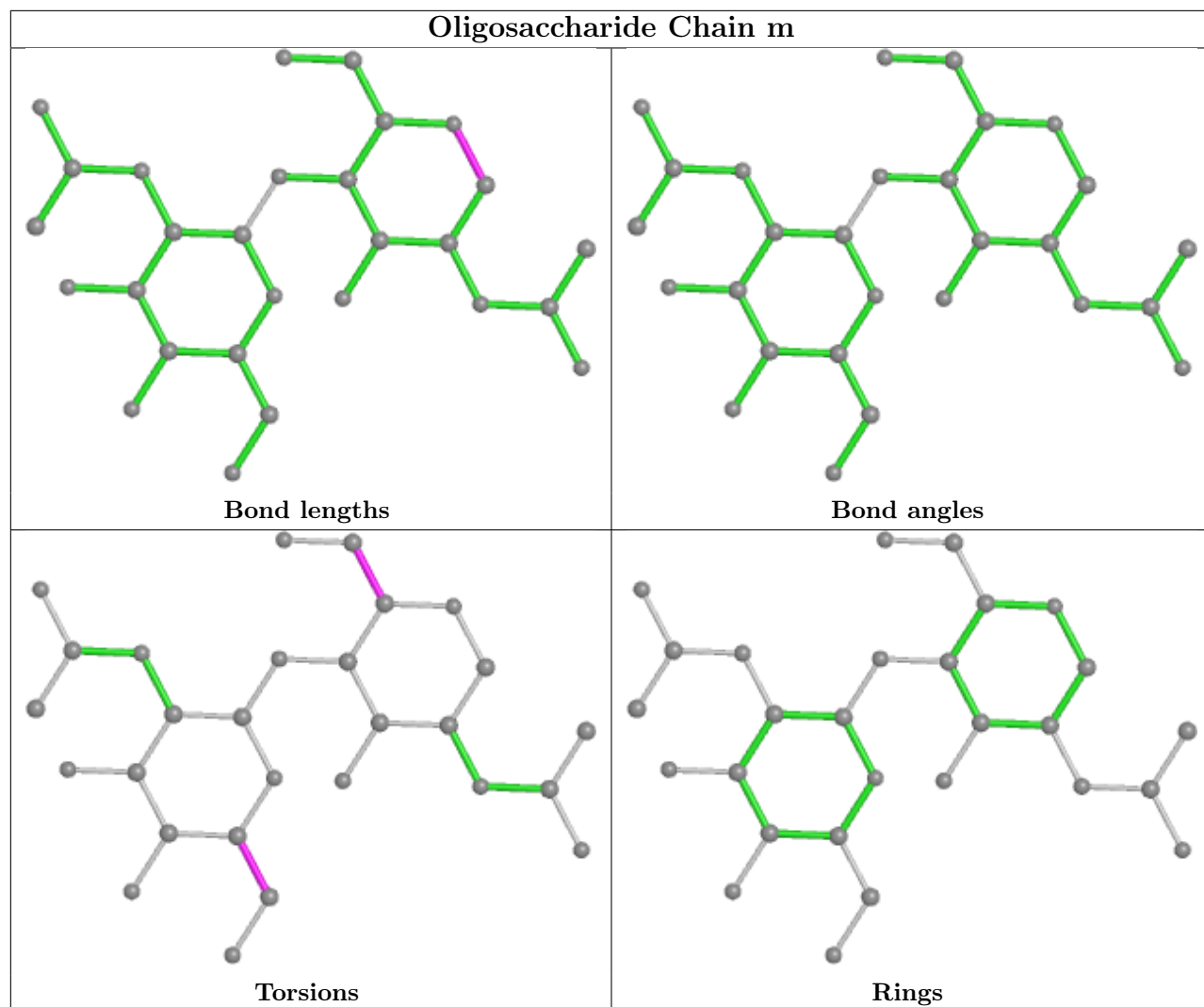


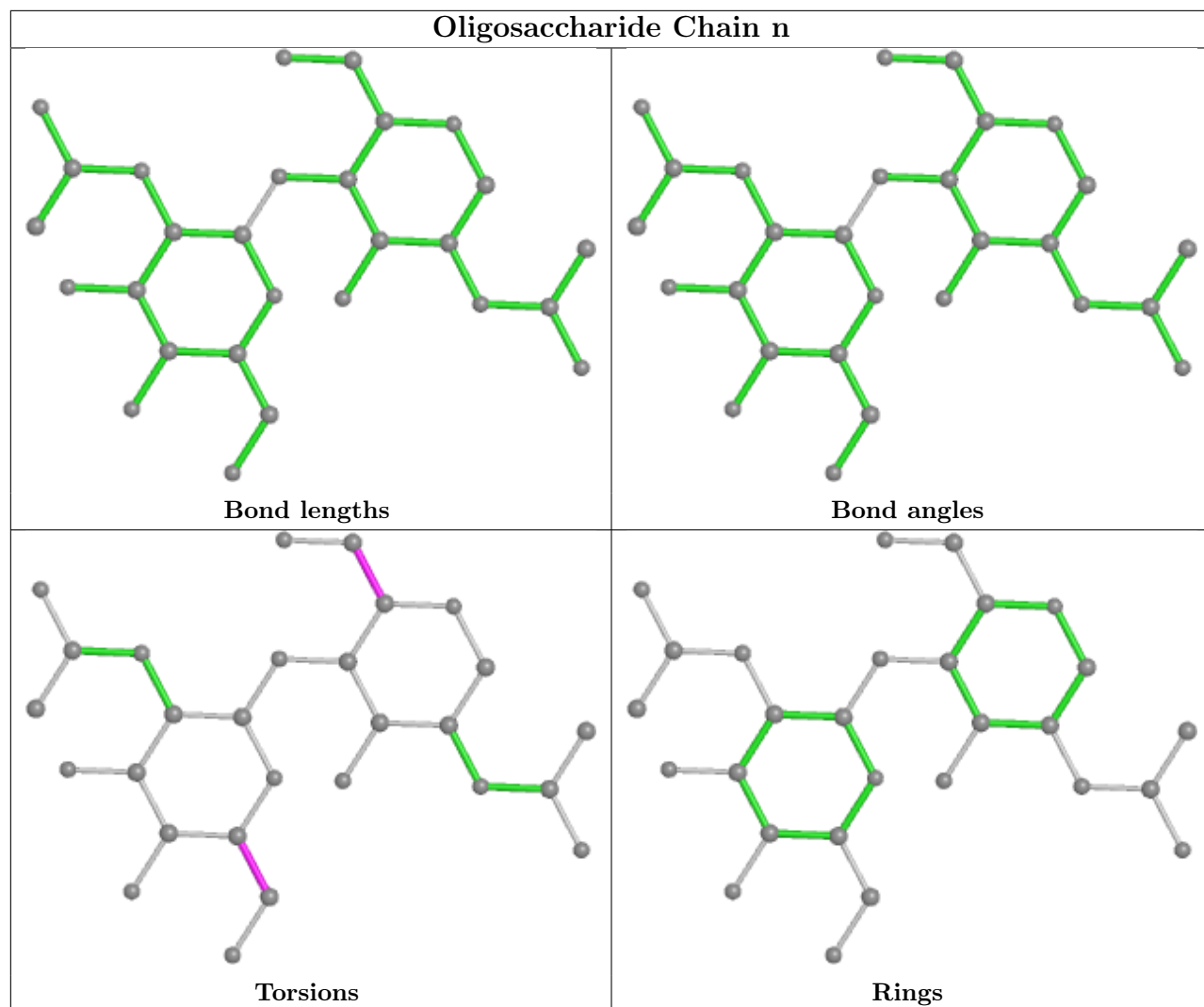


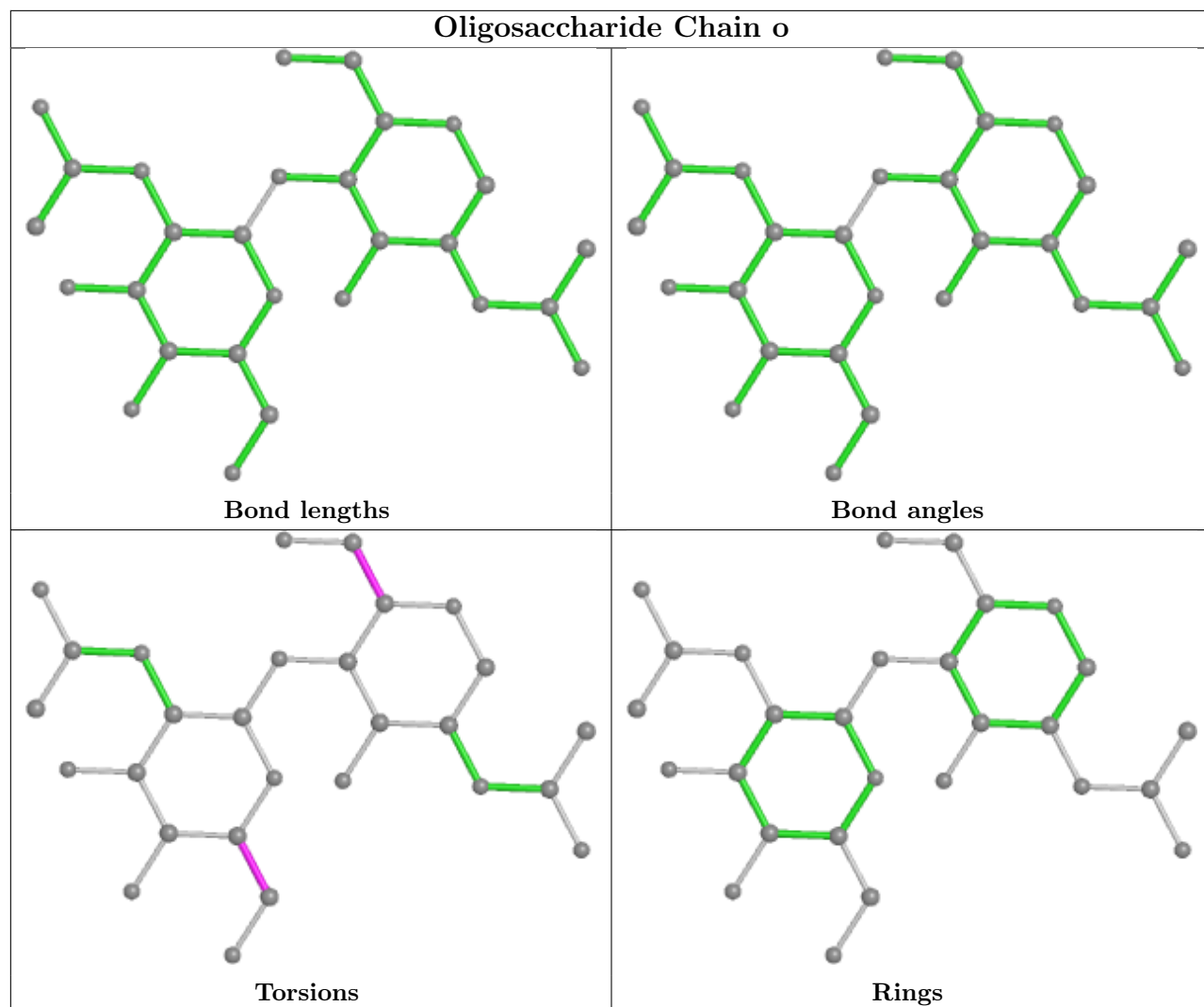




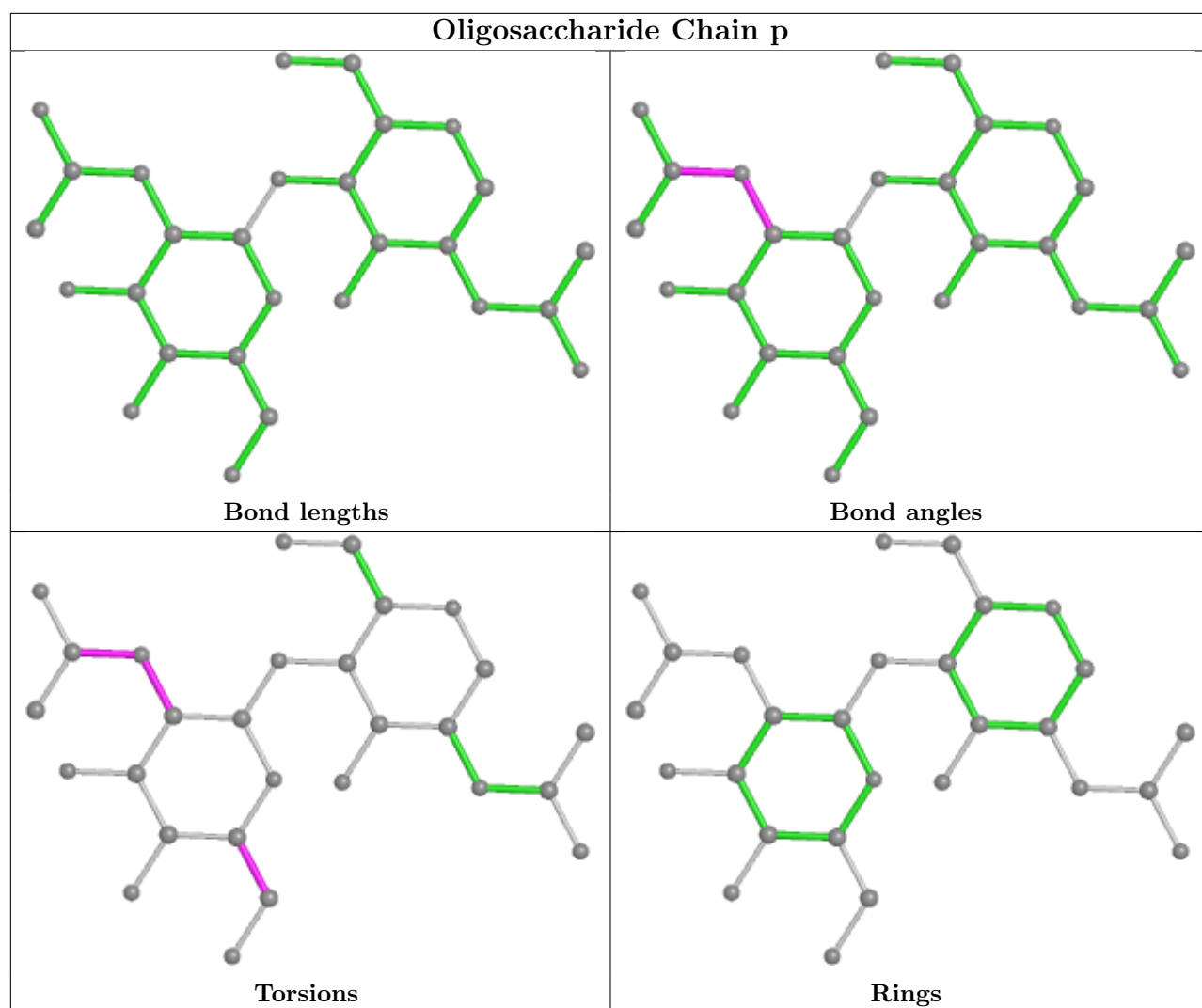


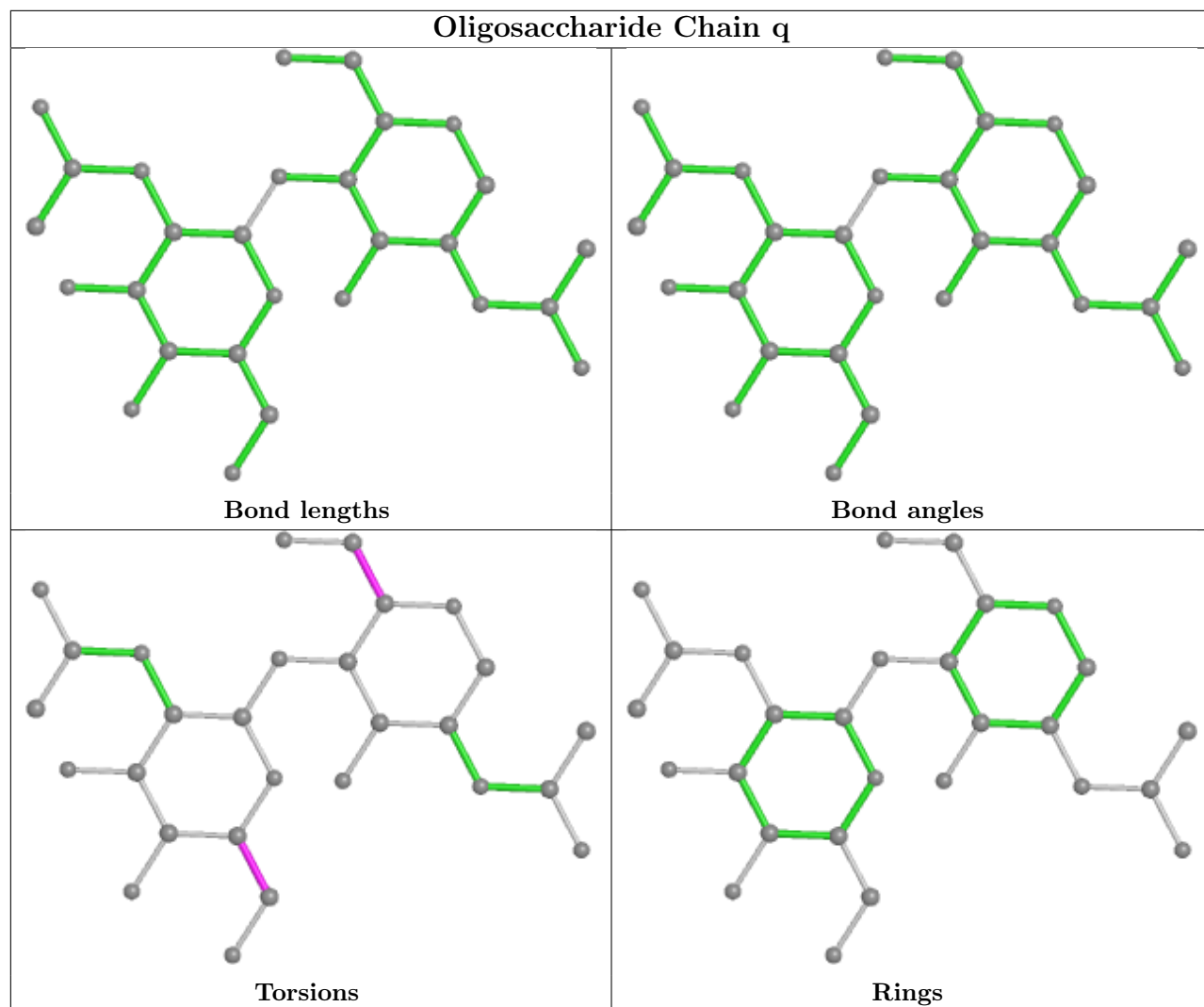


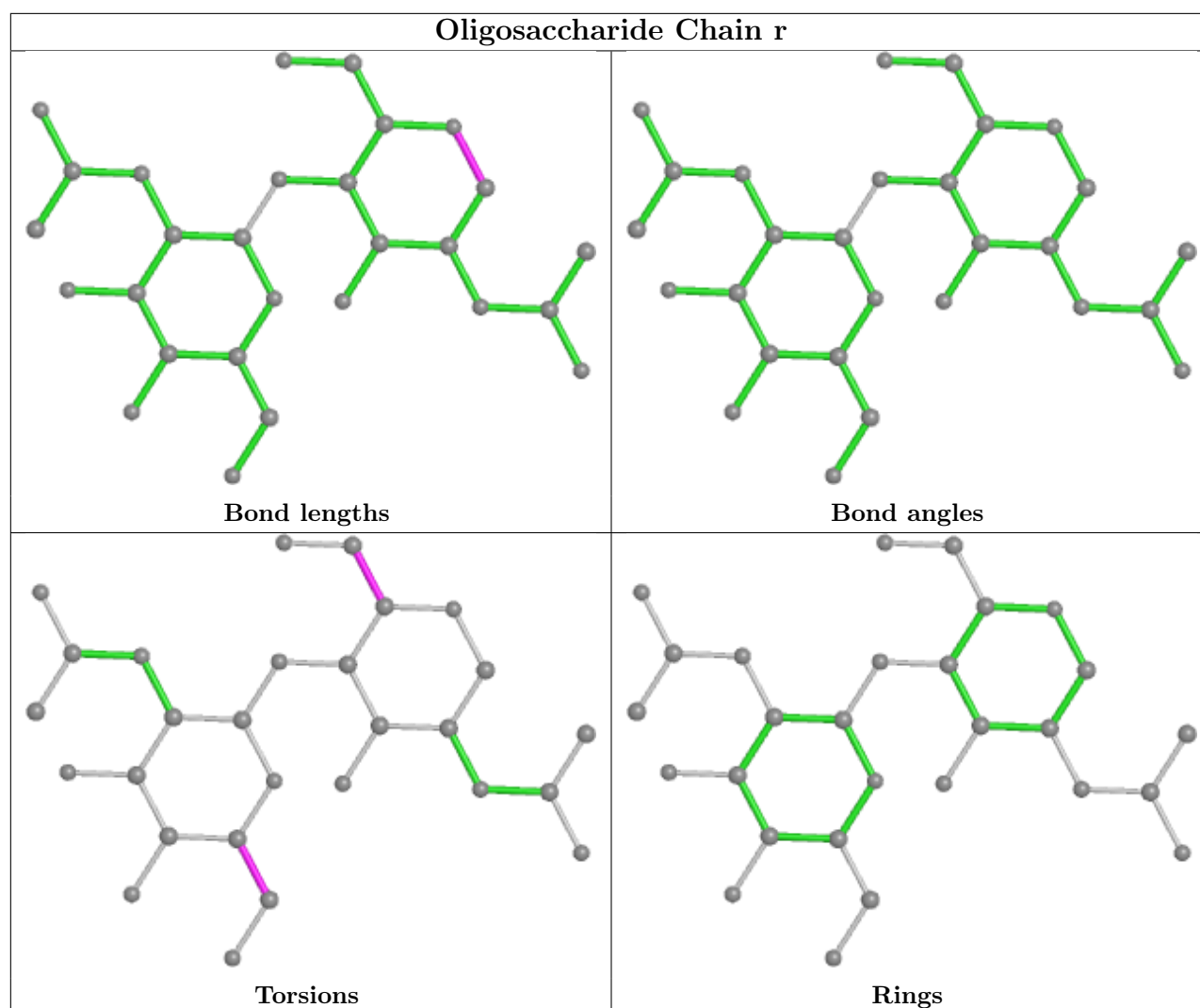












## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
4	NAG	F	701	2	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	A	1404	1	14,14,15	0.48	0	17,19,21	0.53	0
4	NAG	B	1402	1	14,14,15	0.21	0	17,19,21	0.63	0
4	NAG	C	1408	1	14,14,15	0.31	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1407	1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	A	1401	1	14,14,15	0.29	0	17,19,21	0.32	0
4	NAG	A	1403	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	D	701	2	14,14,15	0.26	0	17,19,21	0.51	0
4	NAG	B	1405	1	14,14,15	0.60	0	17,19,21	1.28	1 (5%)
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	C	1401	1	14,14,15	0.27	0	17,19,21	0.33	0
4	NAG	C	1403	1	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
4	NAG	A	1405	1	14,14,15	0.61	0	17,19,21	1.26	1 (5%)
4	NAG	B	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	C	1406	1	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	A	1406	1	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.40	0
4	NAG	B	1401	1	14,14,15	0.28	0	17,19,21	0.32	0
4	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1405	1	14,14,15	0.61	0	17,19,21	1.27	1 (5%)
4	NAG	C	1404	1	14,14,15	0.48	0	17,19,21	0.53	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	B	1406	1	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	A	1409	1	14,14,15	0.49	0	17,19,21	0.35	0
4	NAG	A	1407	1	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	B	1404	1	14,14,15	0.48	0	17,19,21	0.53	0
4	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	H	701	2	14,14,15	0.28	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	701	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	D	701	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
4	NAG	H	701	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1405	NAG	C2-N2-C7	4.40	129.17	122.90
4	C	1405	NAG	C2-N2-C7	4.39	129.16	122.90
4	A	1405	NAG	C2-N2-C7	4.35	129.10	122.90
4	C	1403	NAG	C8-C7-N2	2.28	119.95	116.10
4	C	1403	NAG	C2-N2-C7	-2.07	119.95	122.90

There are no chirality outliers.

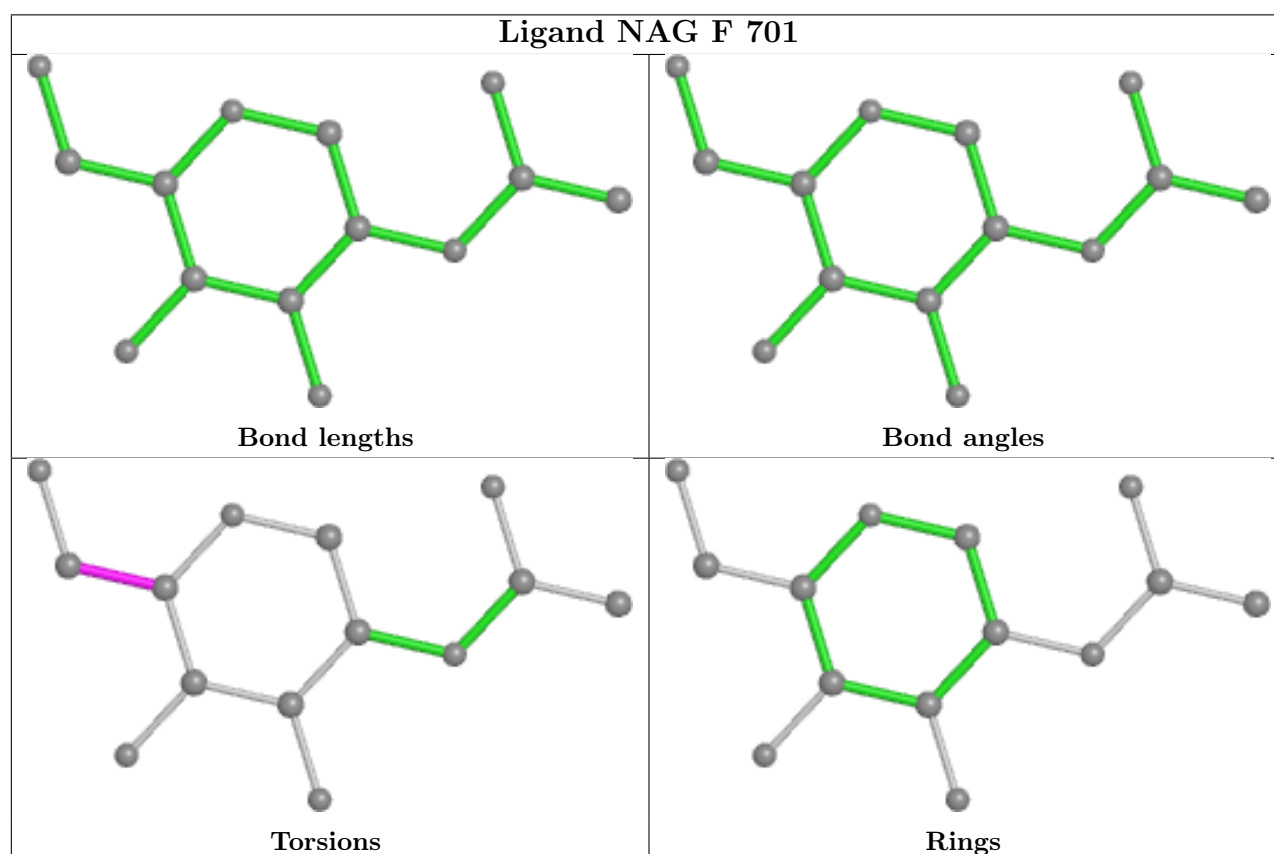
All (6) torsion outliers are listed below:

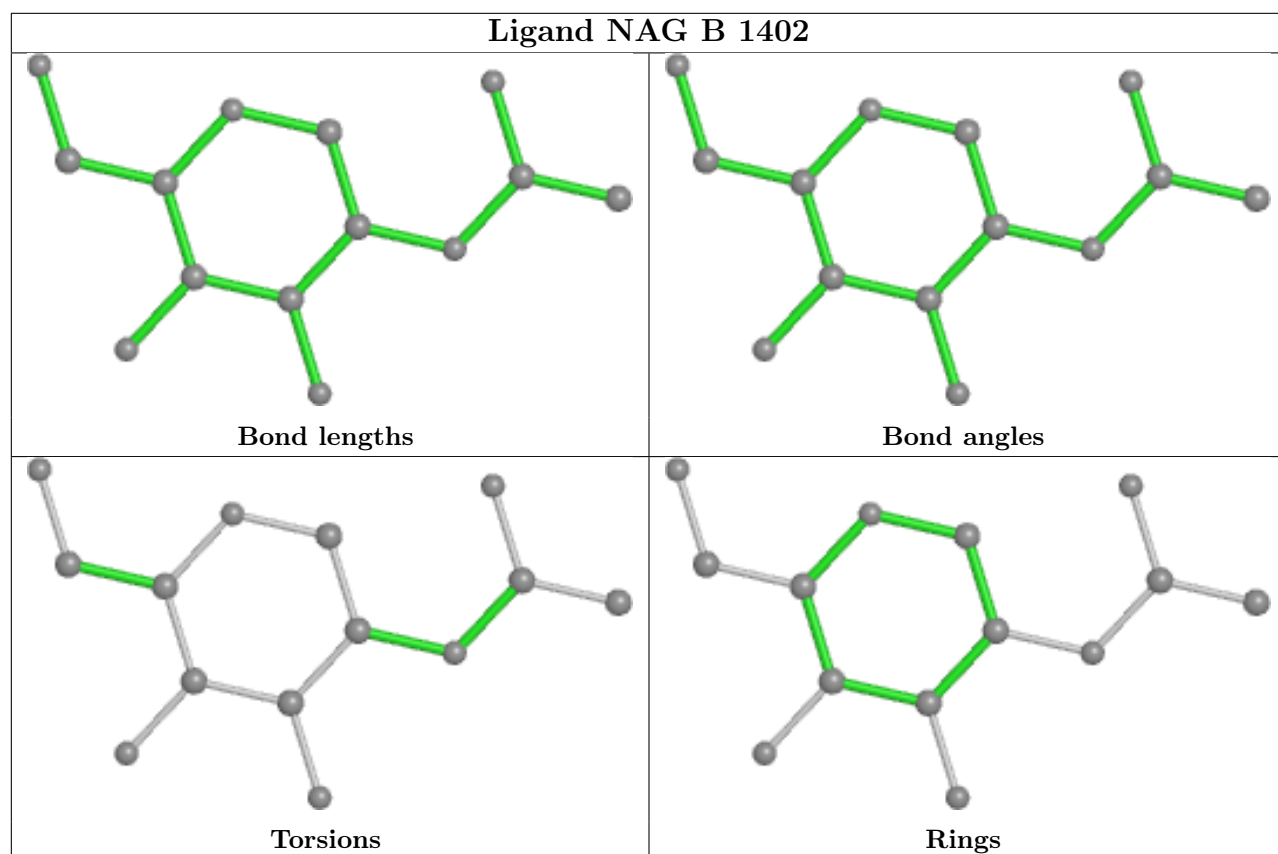
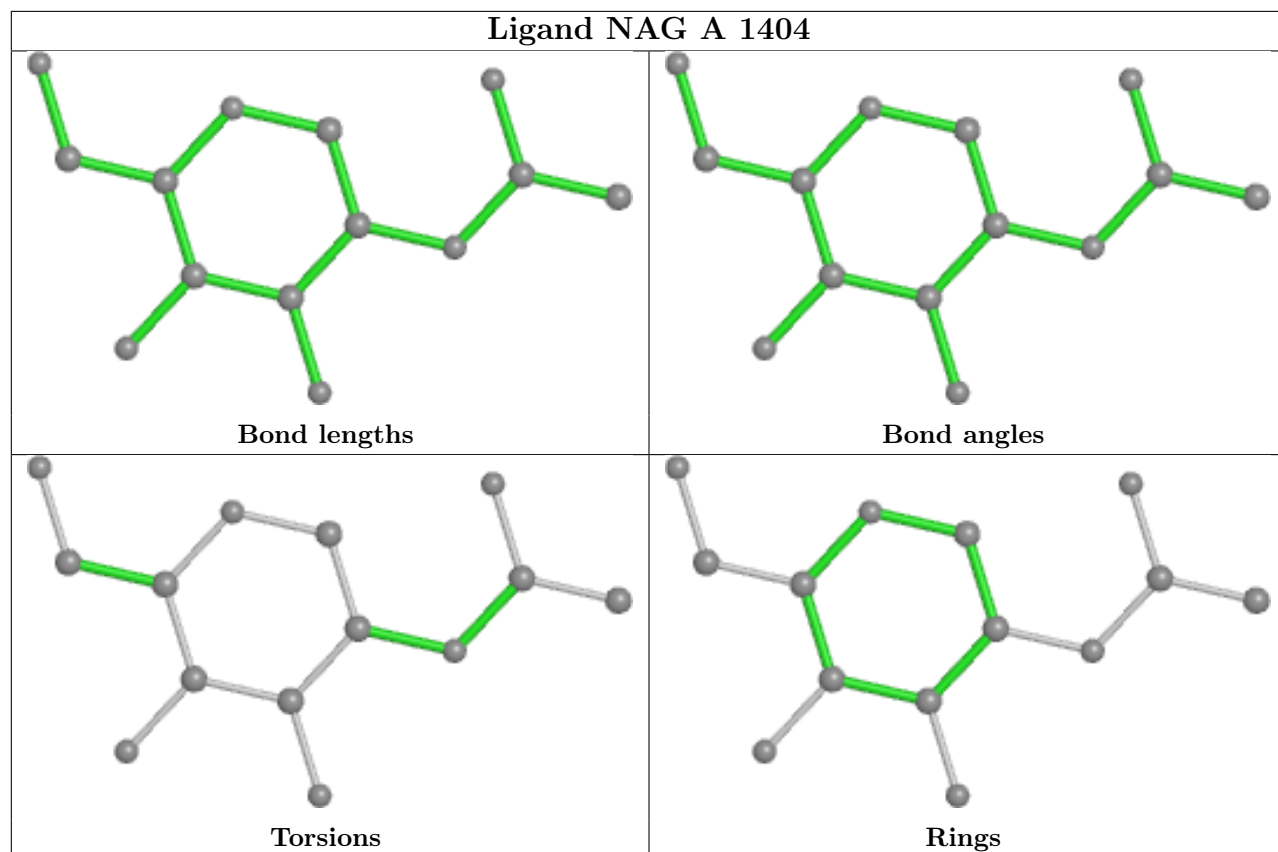
Mol	Chain	Res	Type	Atoms
4	D	701	NAG	O5-C5-C6-O6
4	F	701	NAG	O5-C5-C6-O6
4	H	701	NAG	O5-C5-C6-O6
4	D	701	NAG	C4-C5-C6-O6
4	F	701	NAG	C4-C5-C6-O6
4	H	701	NAG	C4-C5-C6-O6

There are no ring outliers.

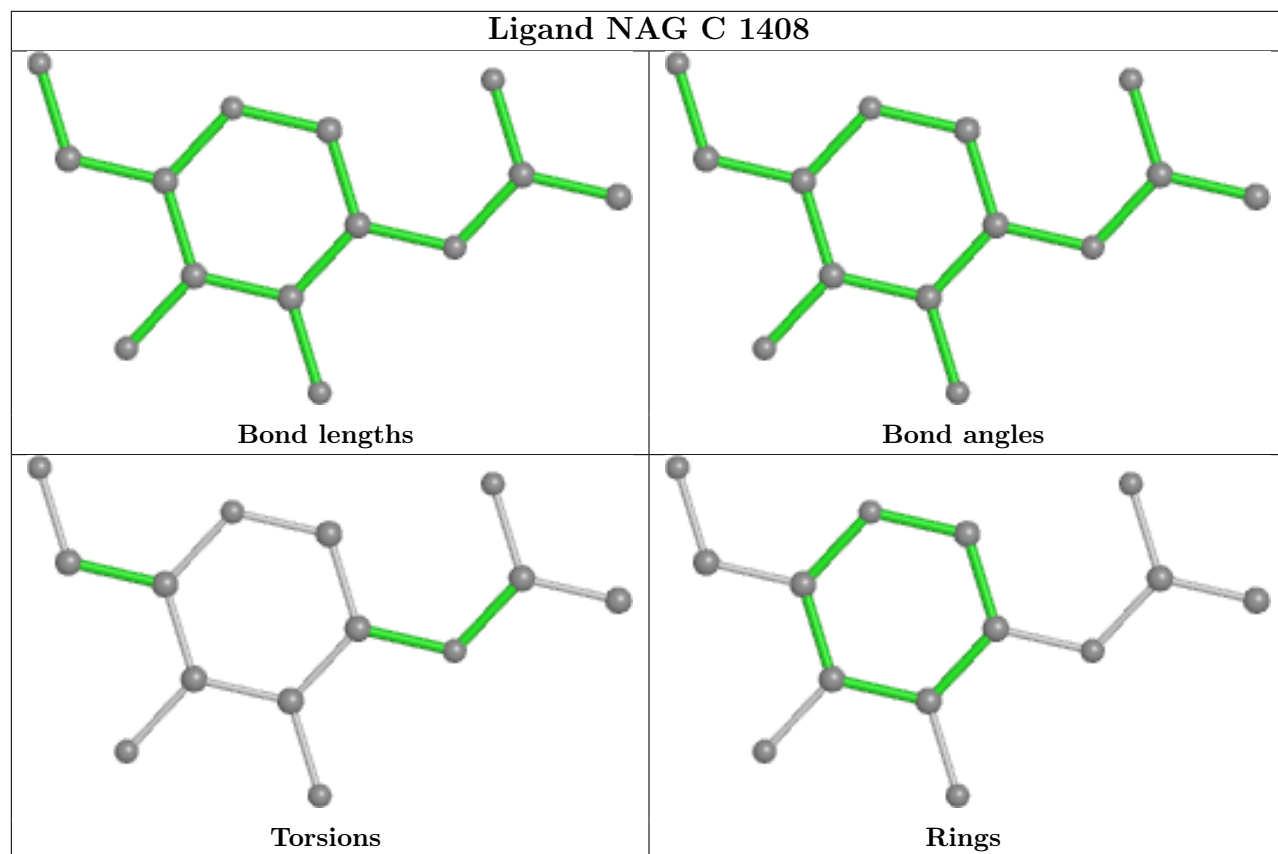
No monomer is involved in short contacts.

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.

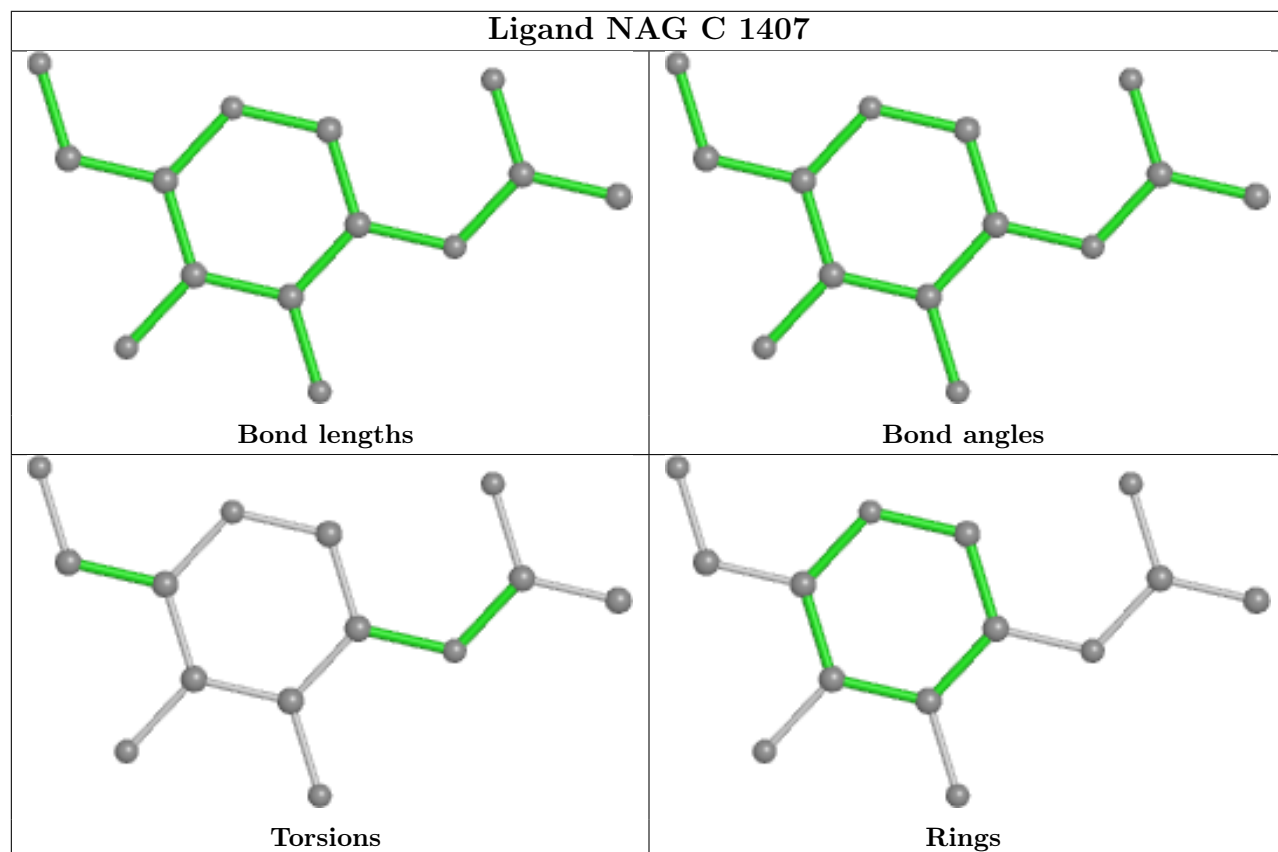




## Ligand NAG C 1408

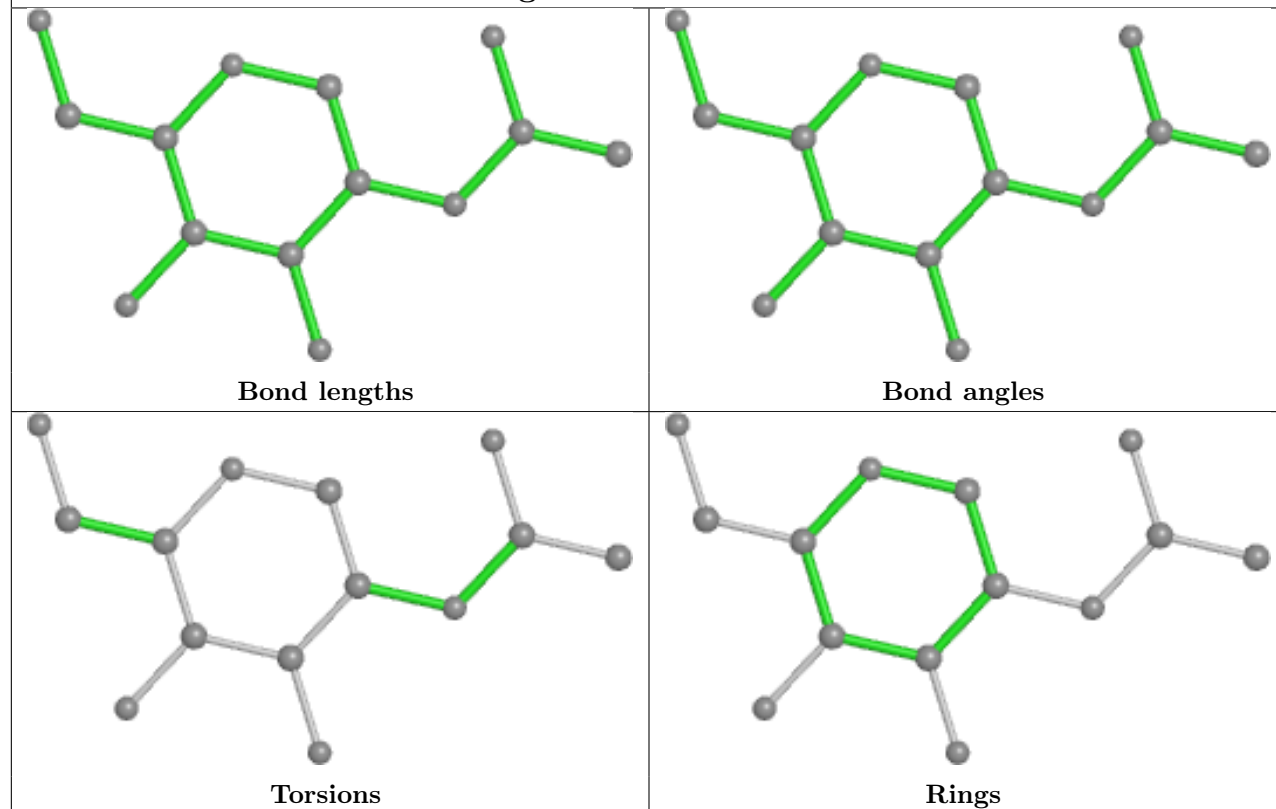


## Ligand NAG C 1407

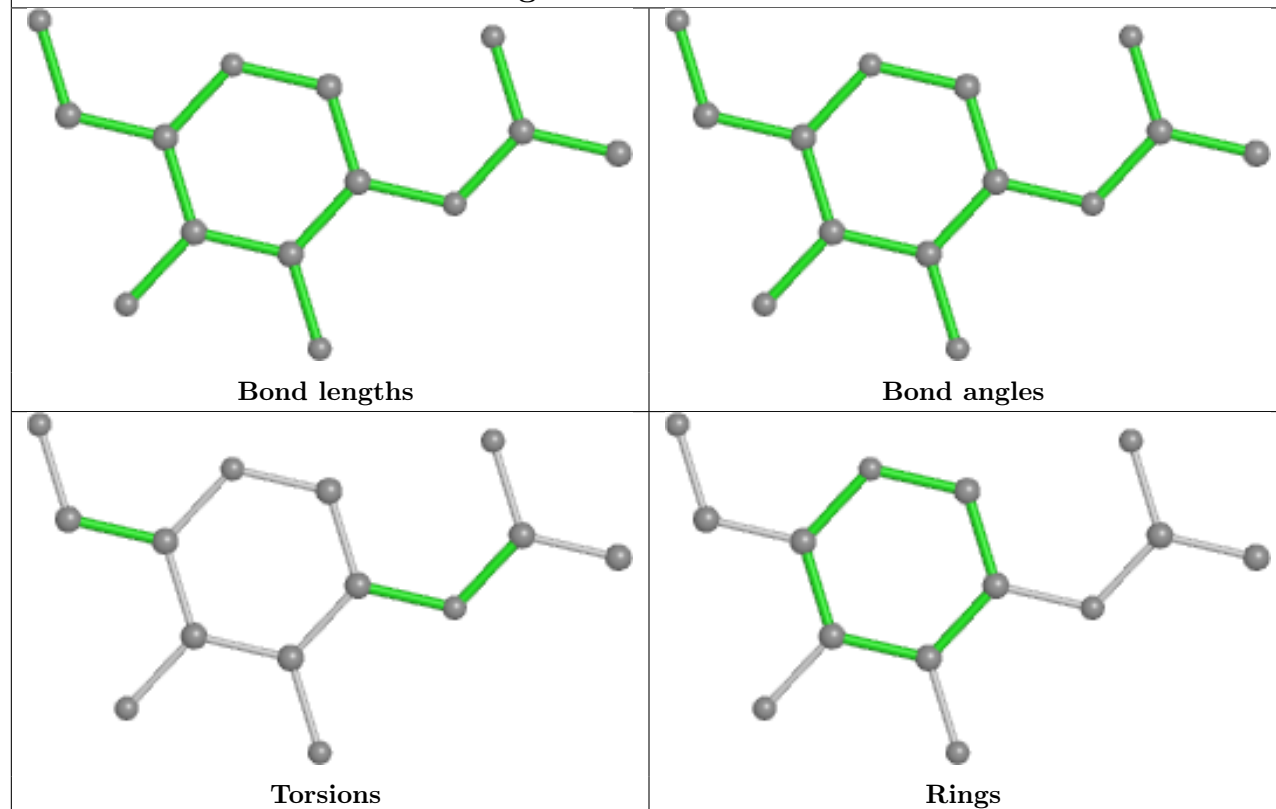


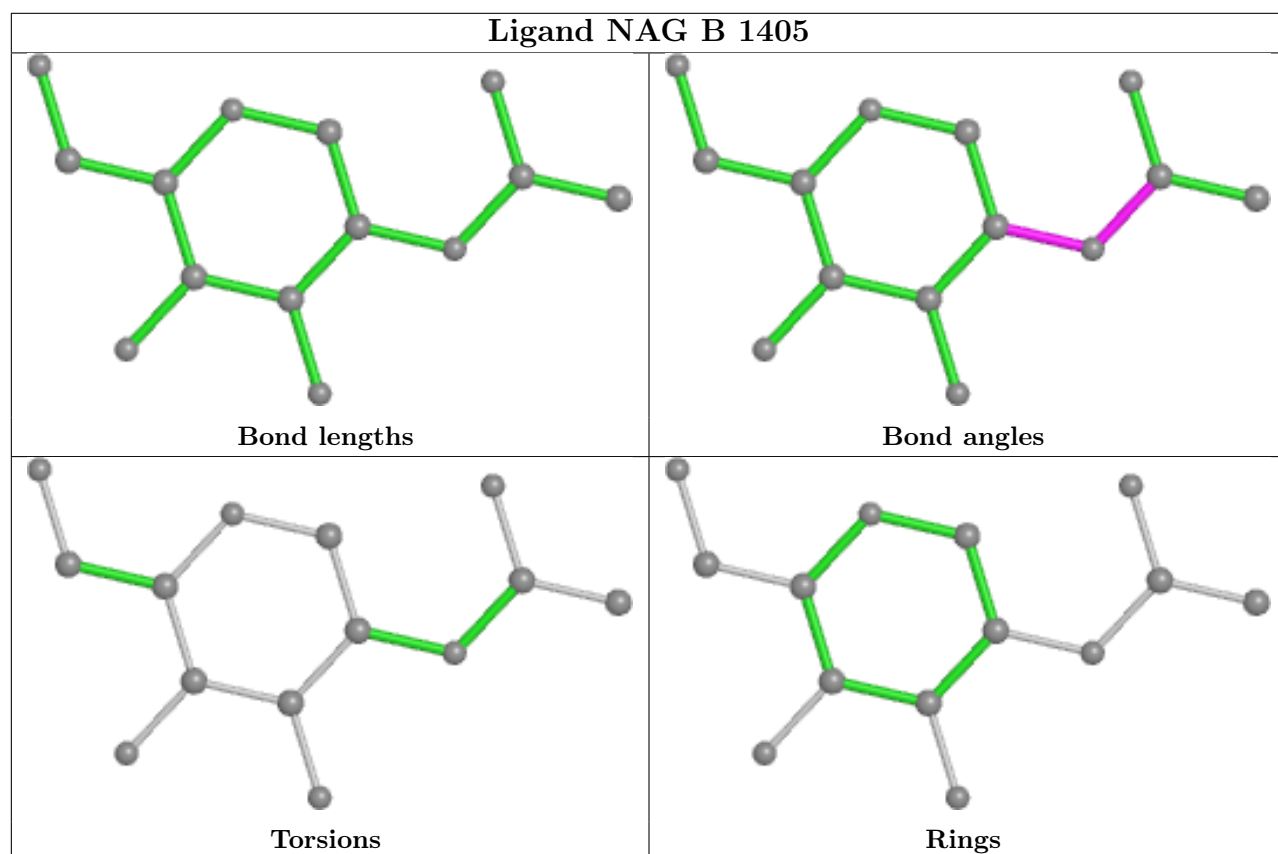
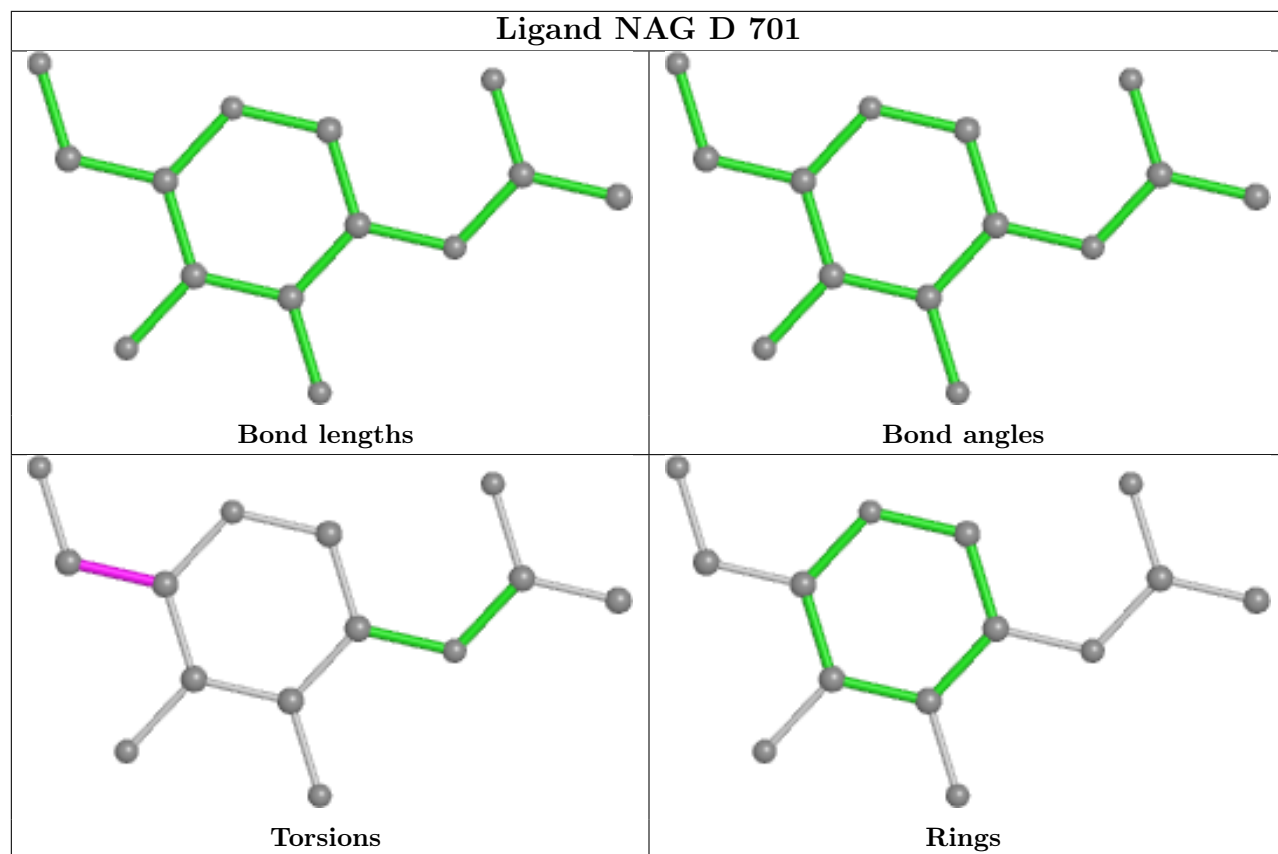


## Ligand NAG A 1401

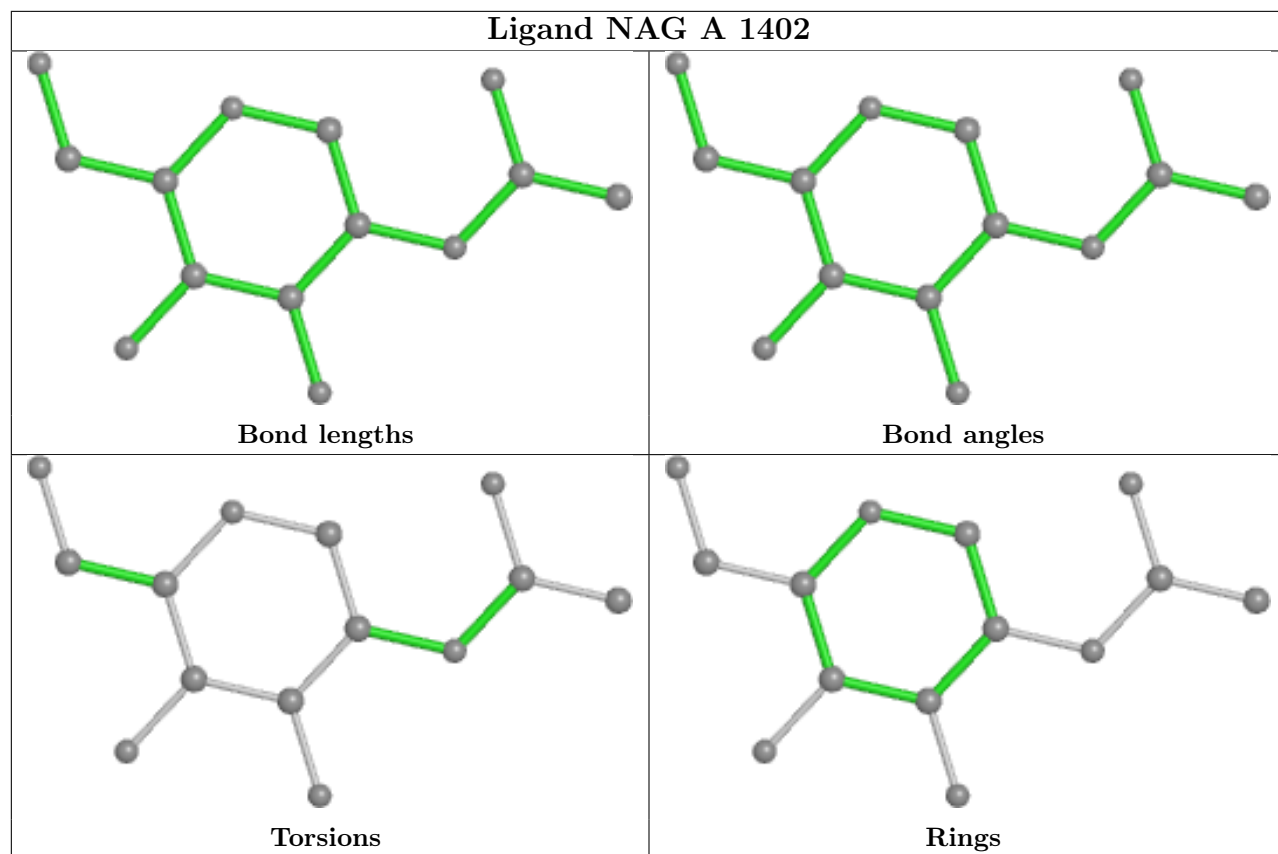


## Ligand NAG A 1403

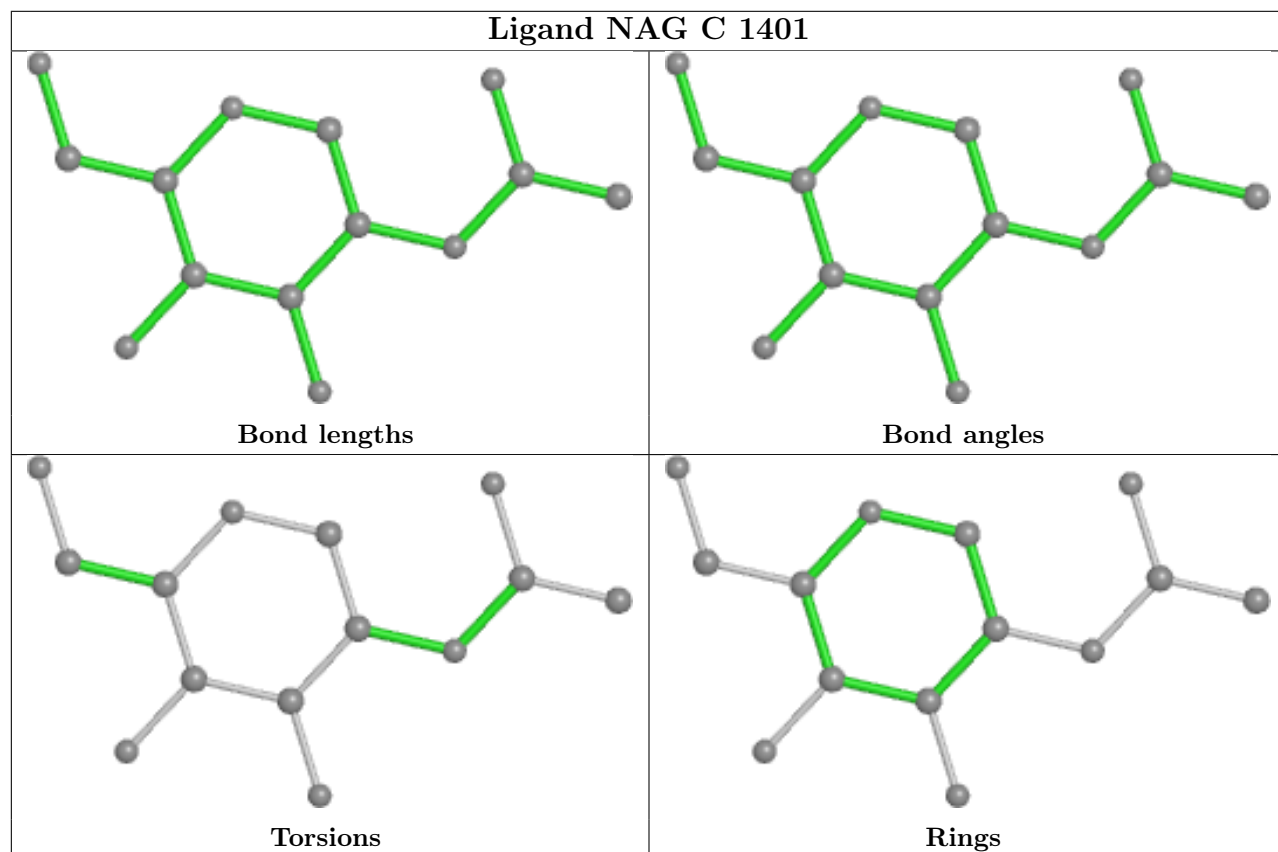




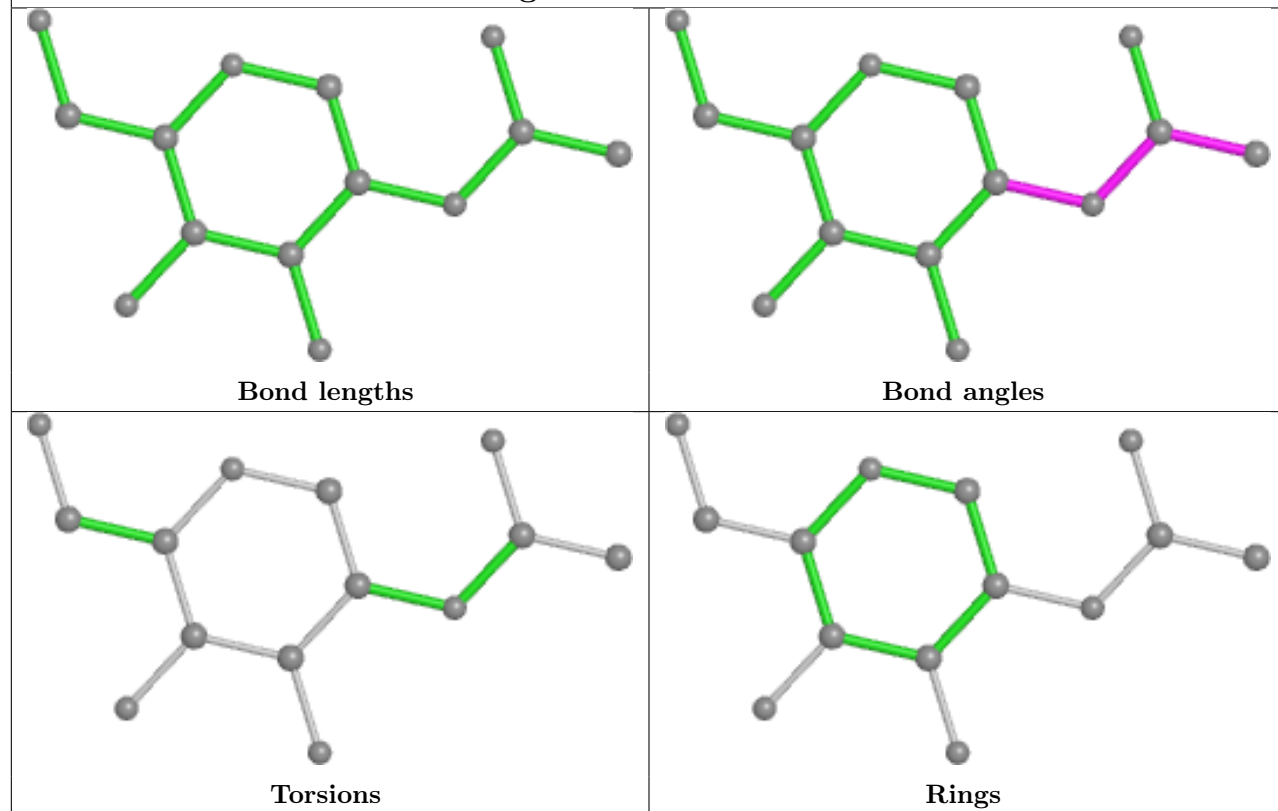
## Ligand NAG A 1402



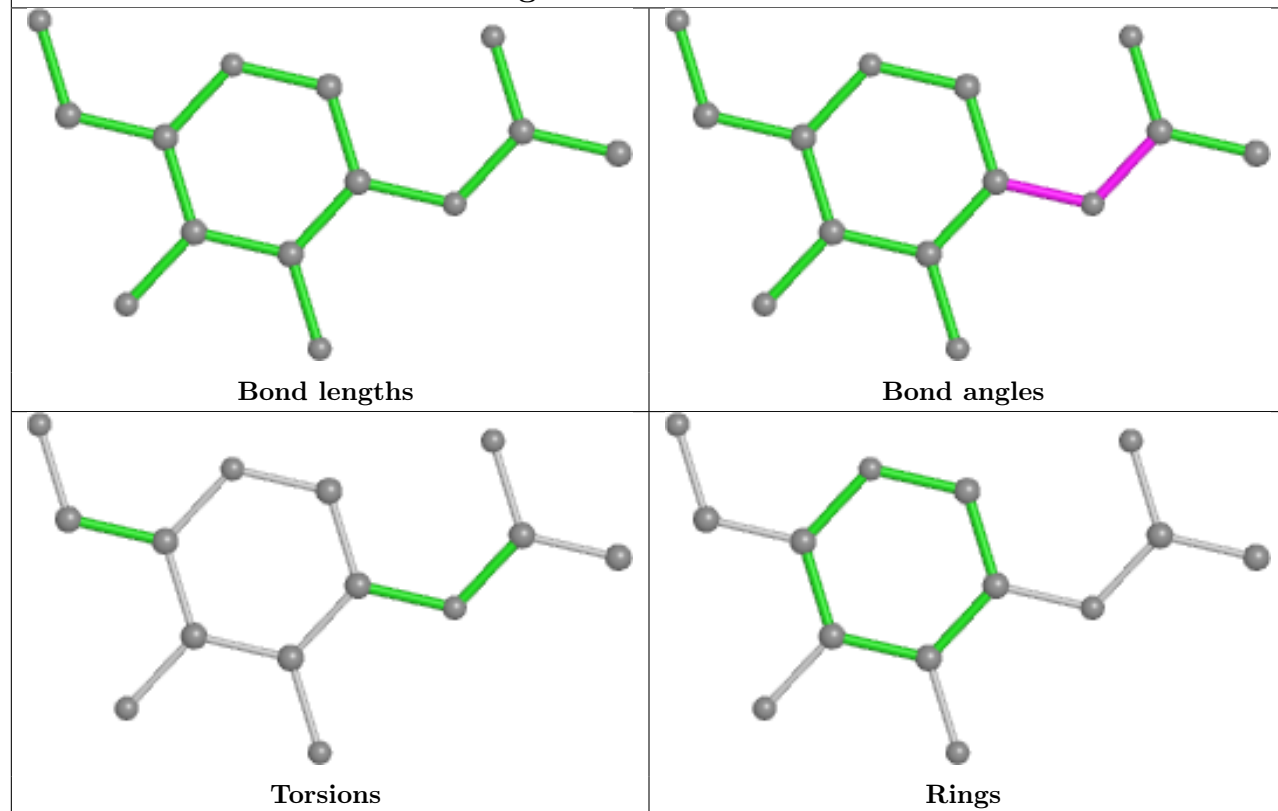
## Ligand NAG C 1401



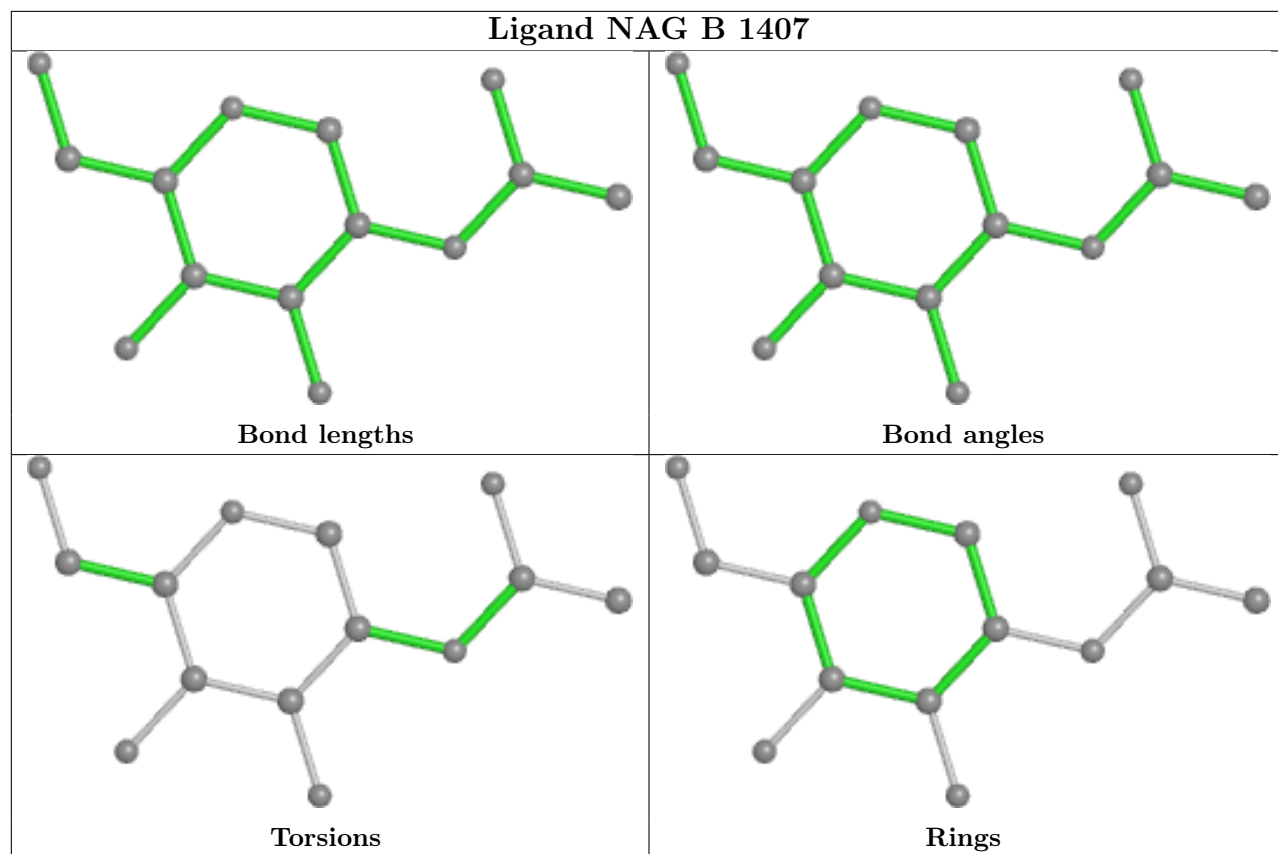
## Ligand NAG C 1403



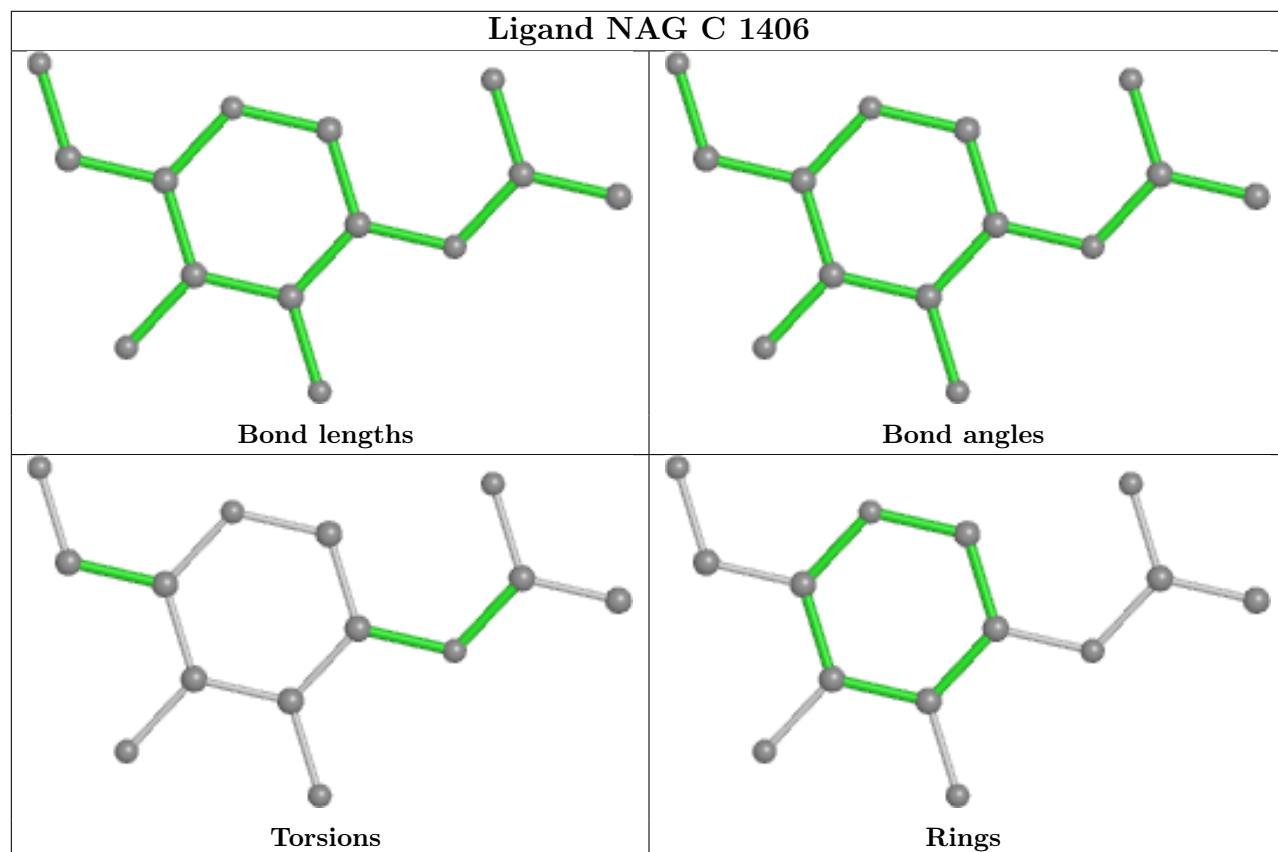
## Ligand NAG A 1405



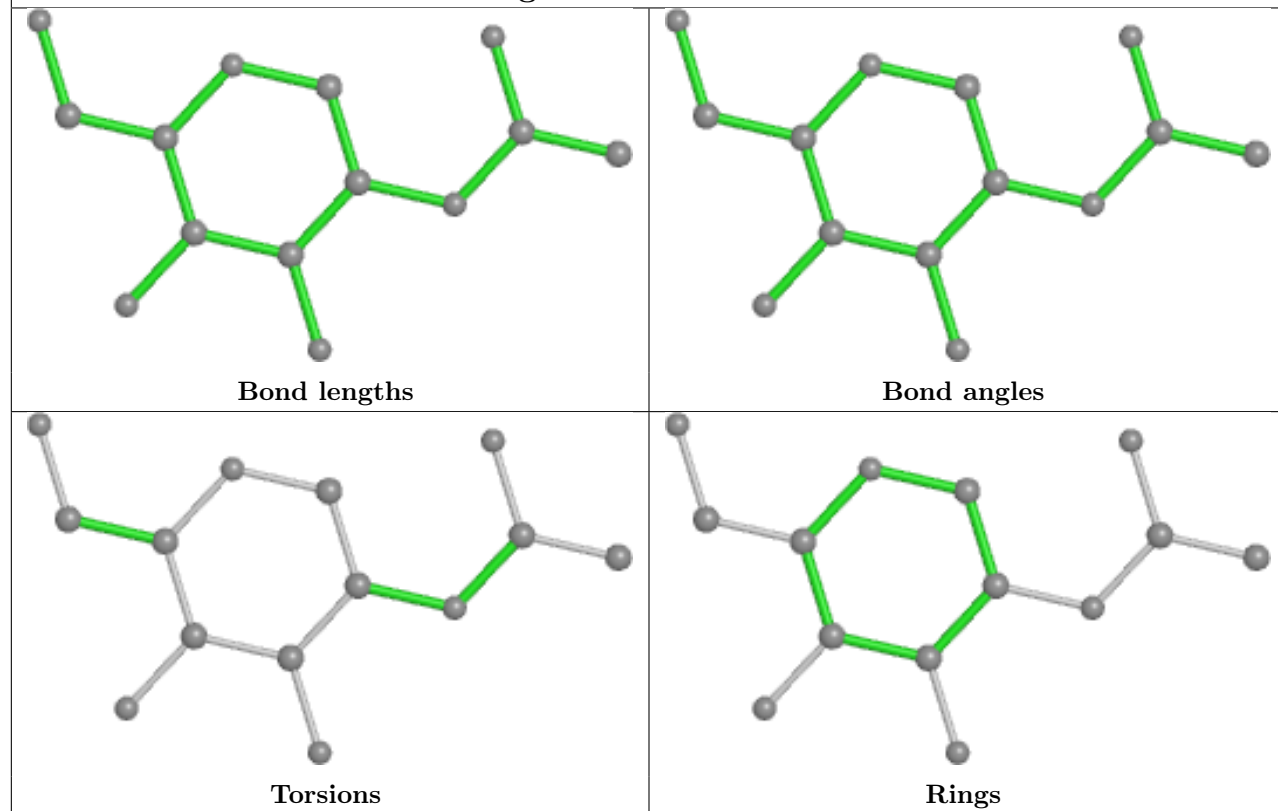
## Ligand NAG B 1407



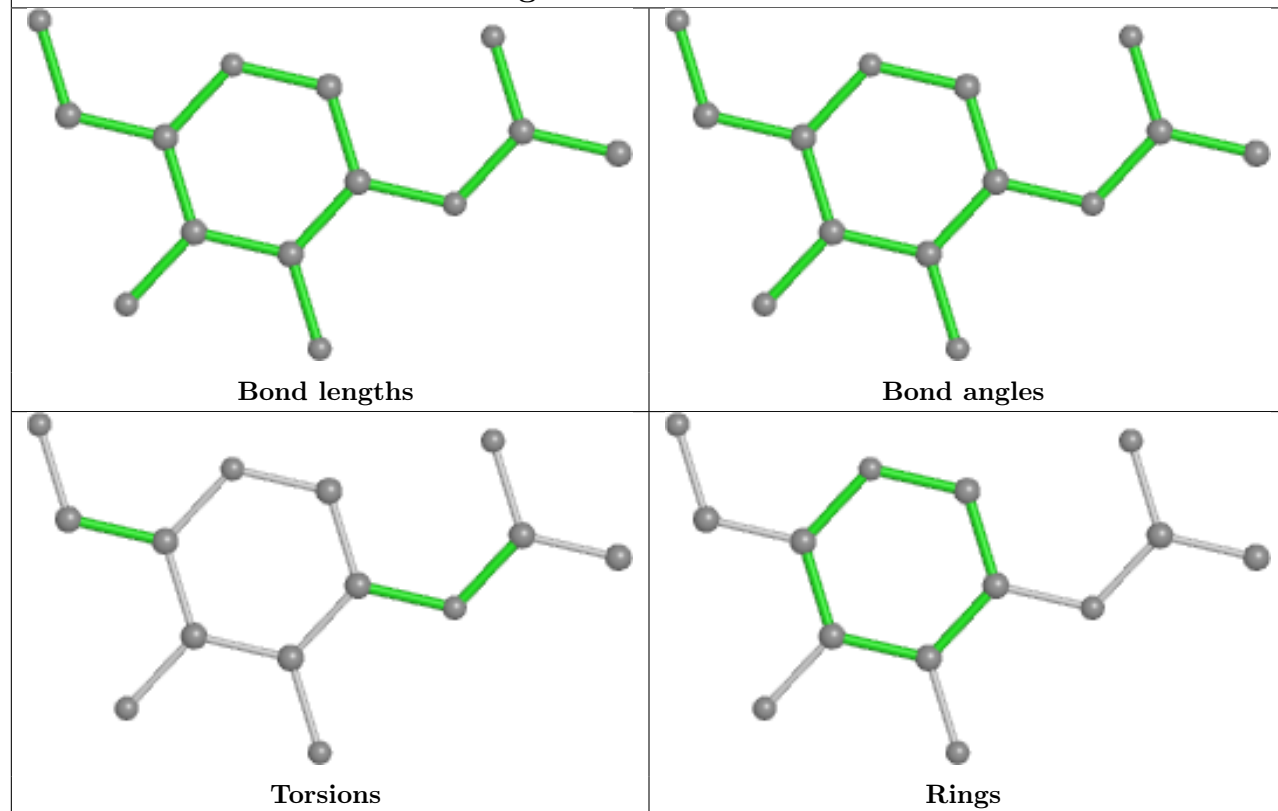
## Ligand NAG C 1406



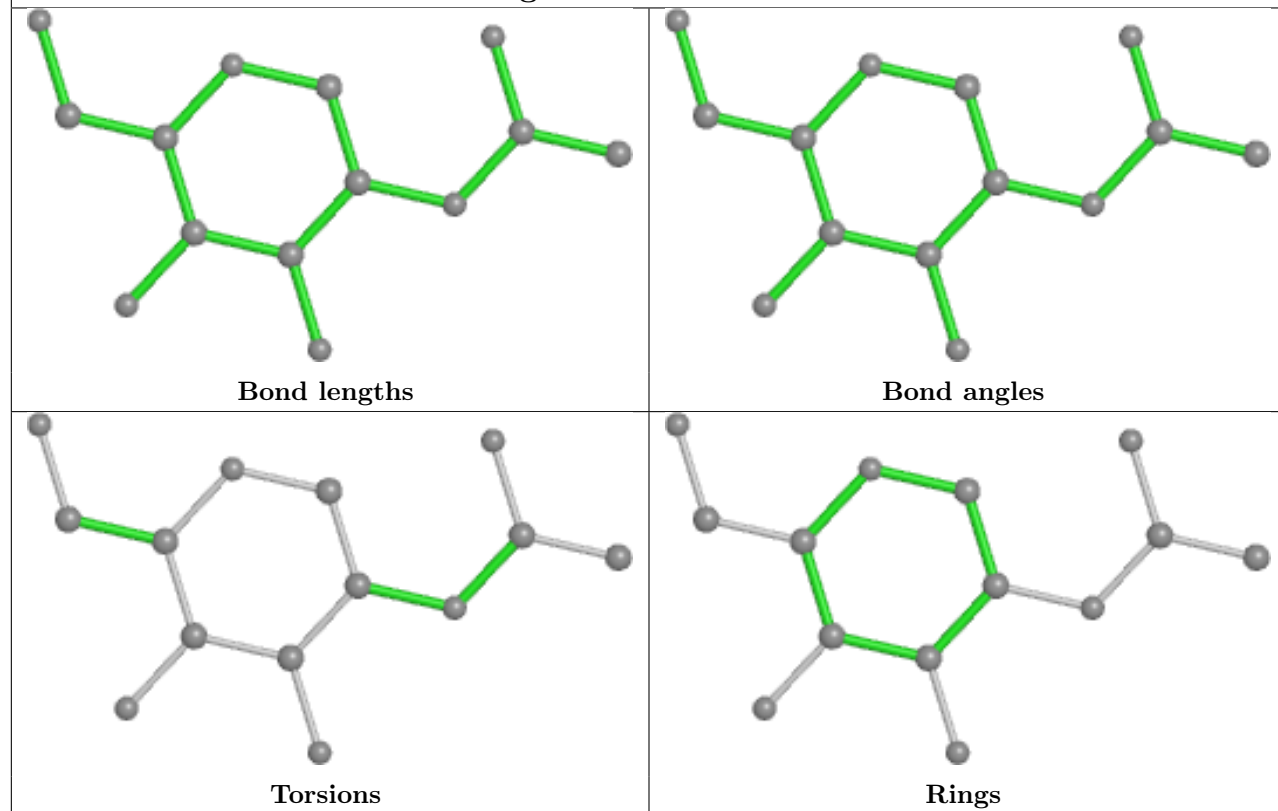
## Ligand NAG A 1406



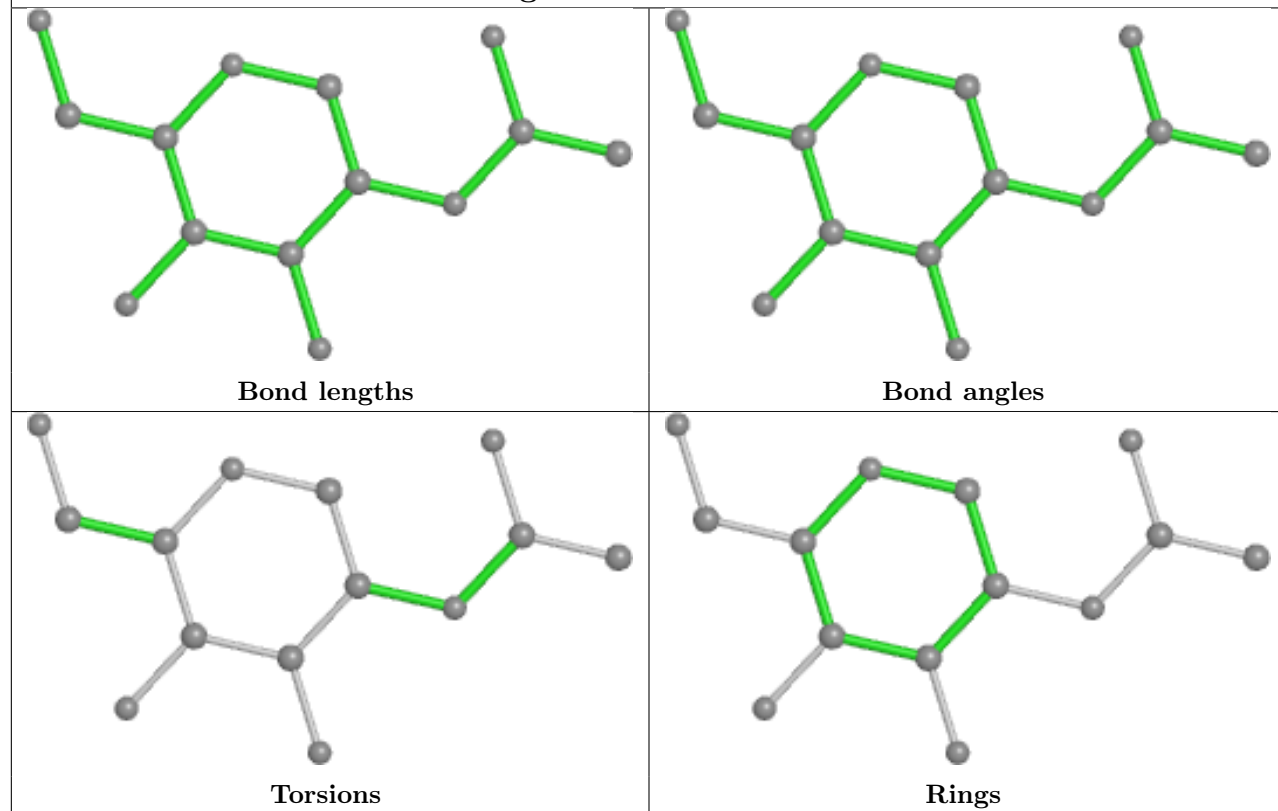
## Ligand NAG A 1408



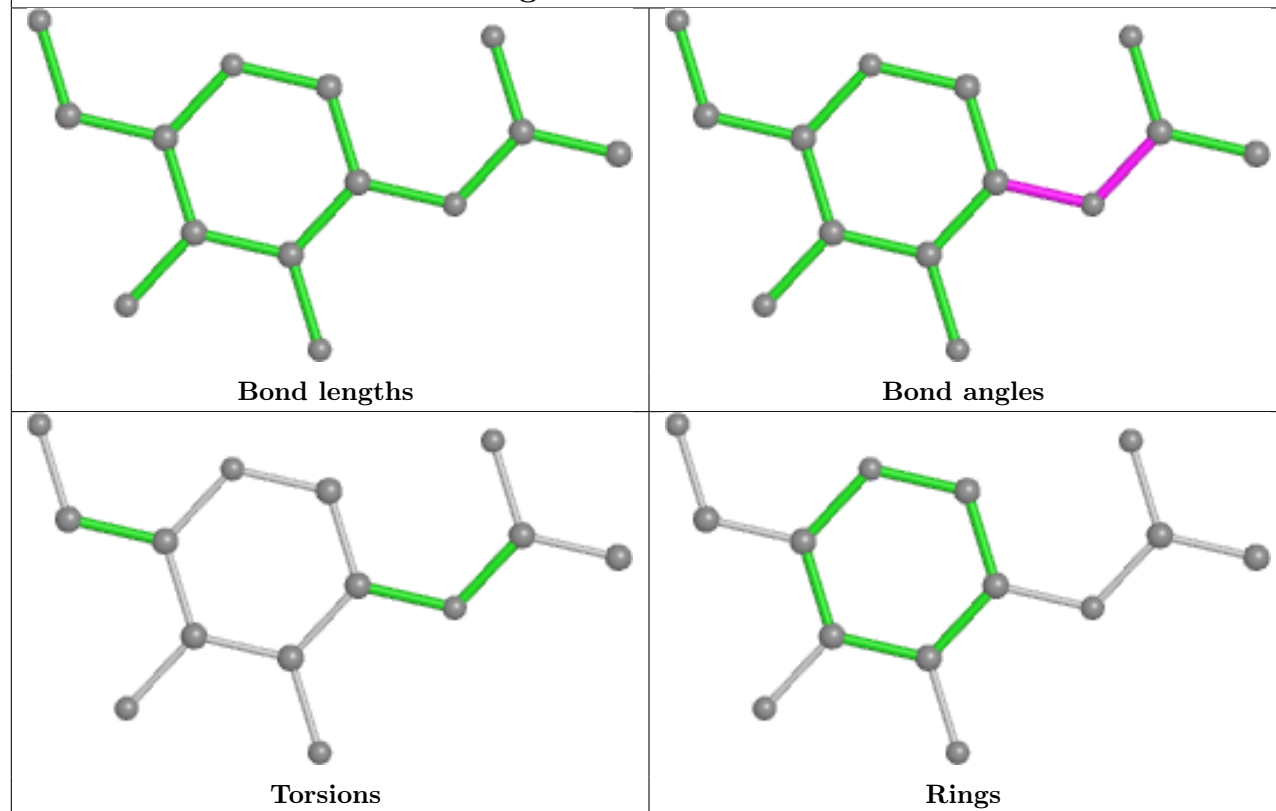
## Ligand NAG B 1401



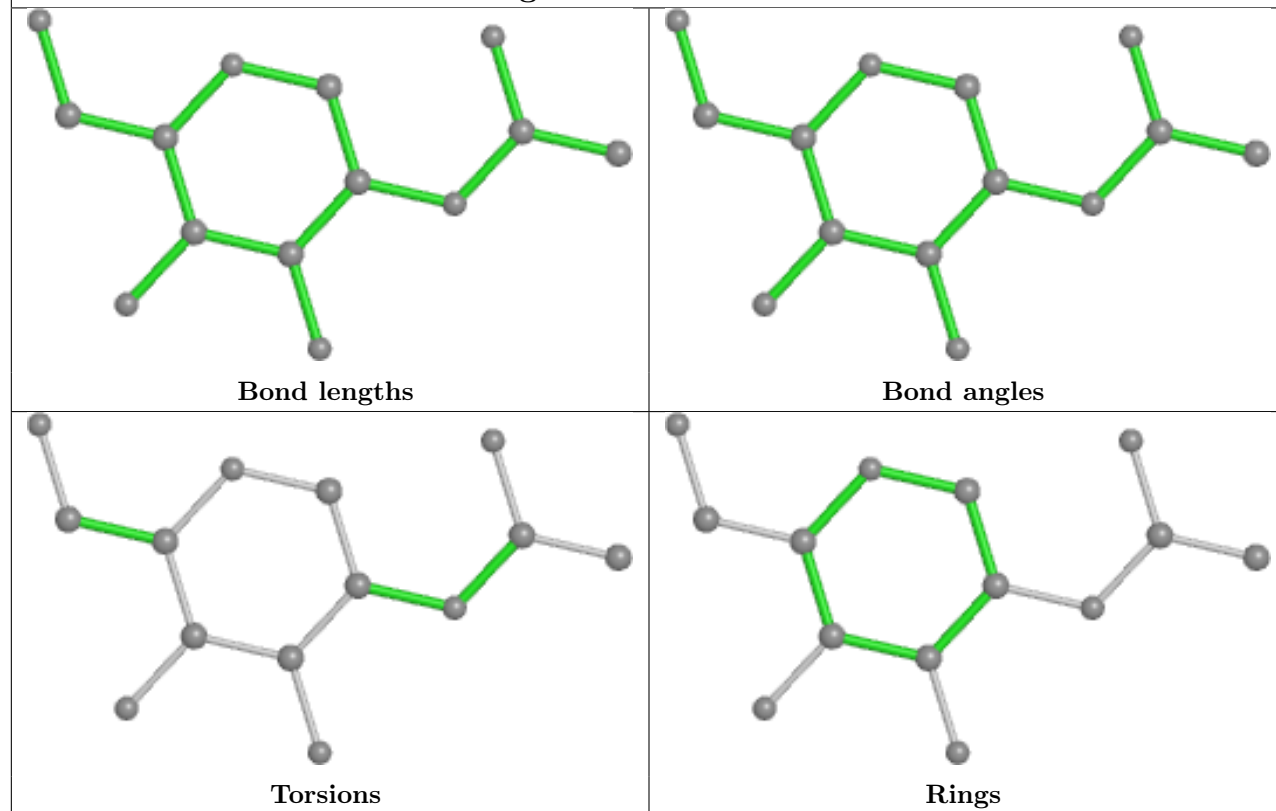
## Ligand NAG B 1403



## Ligand NAG C 1405

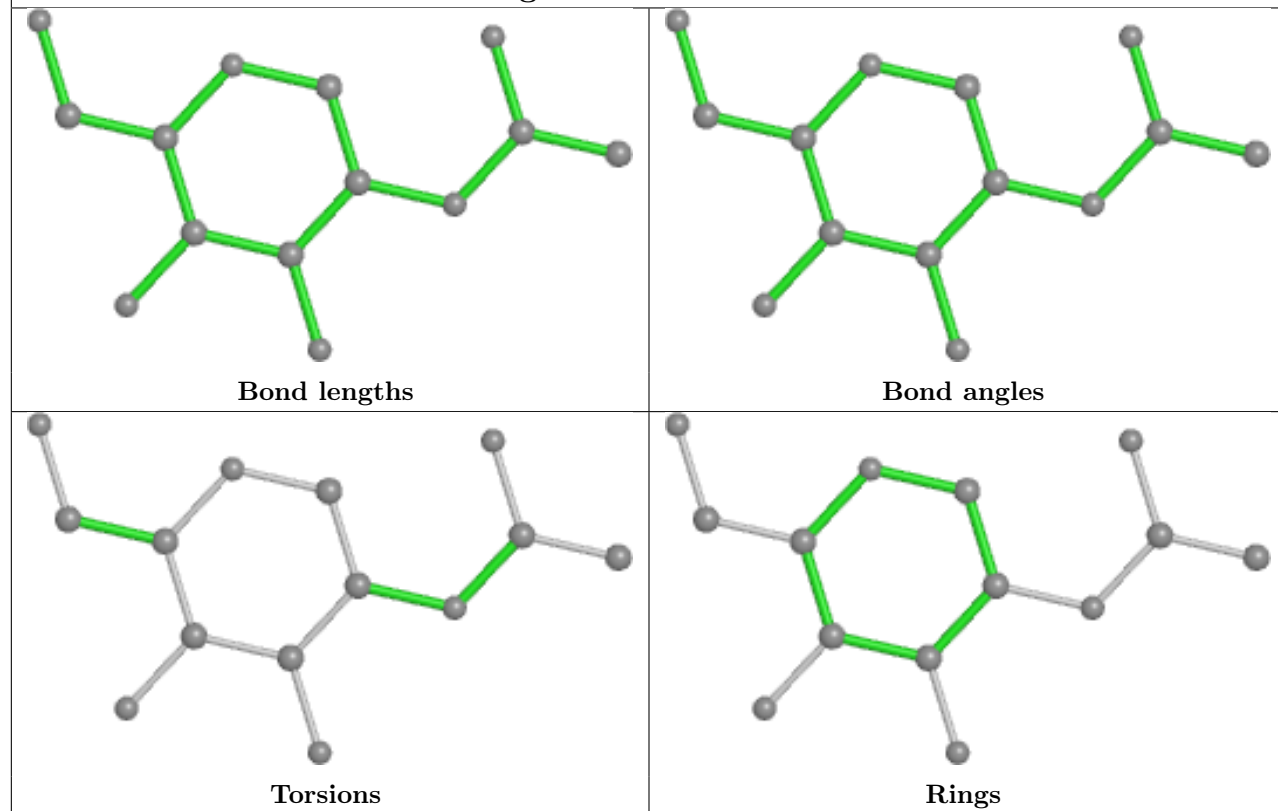


## Ligand NAG C 1404

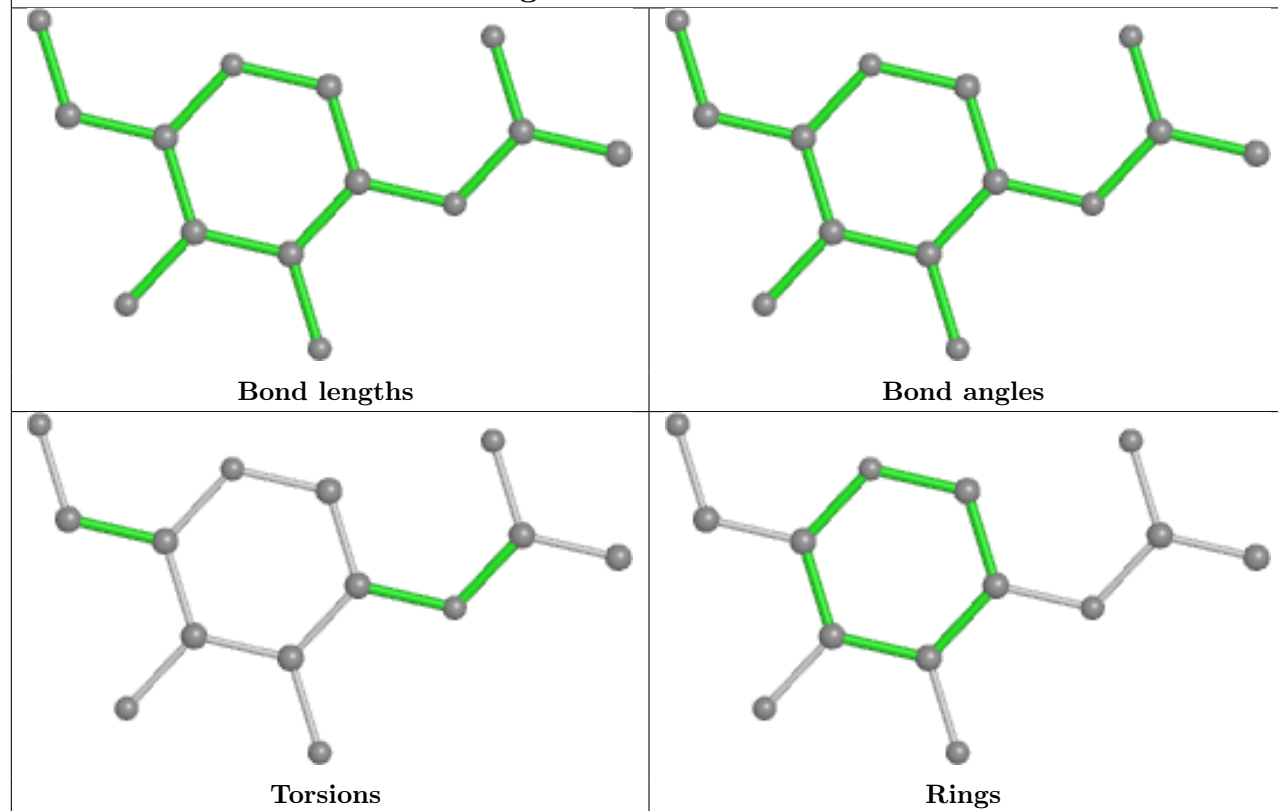


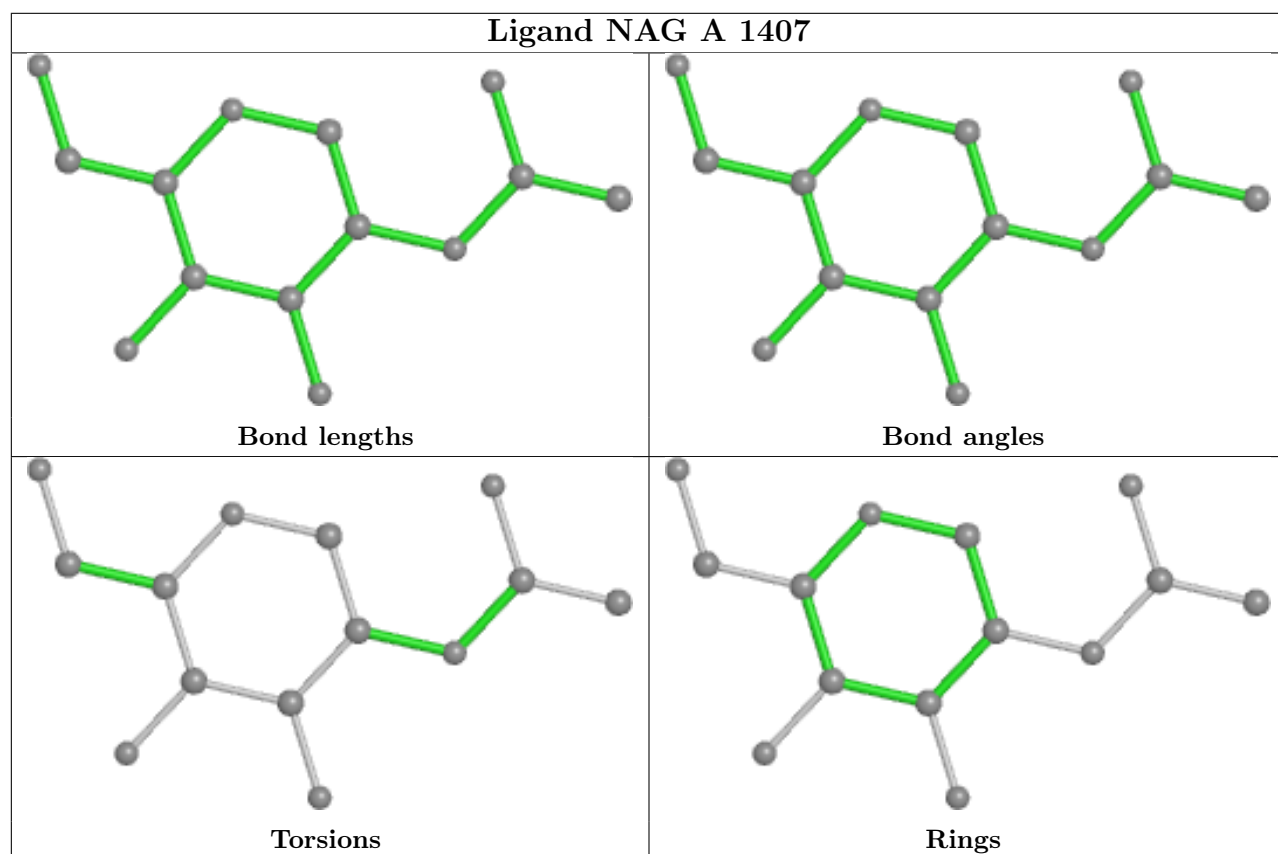
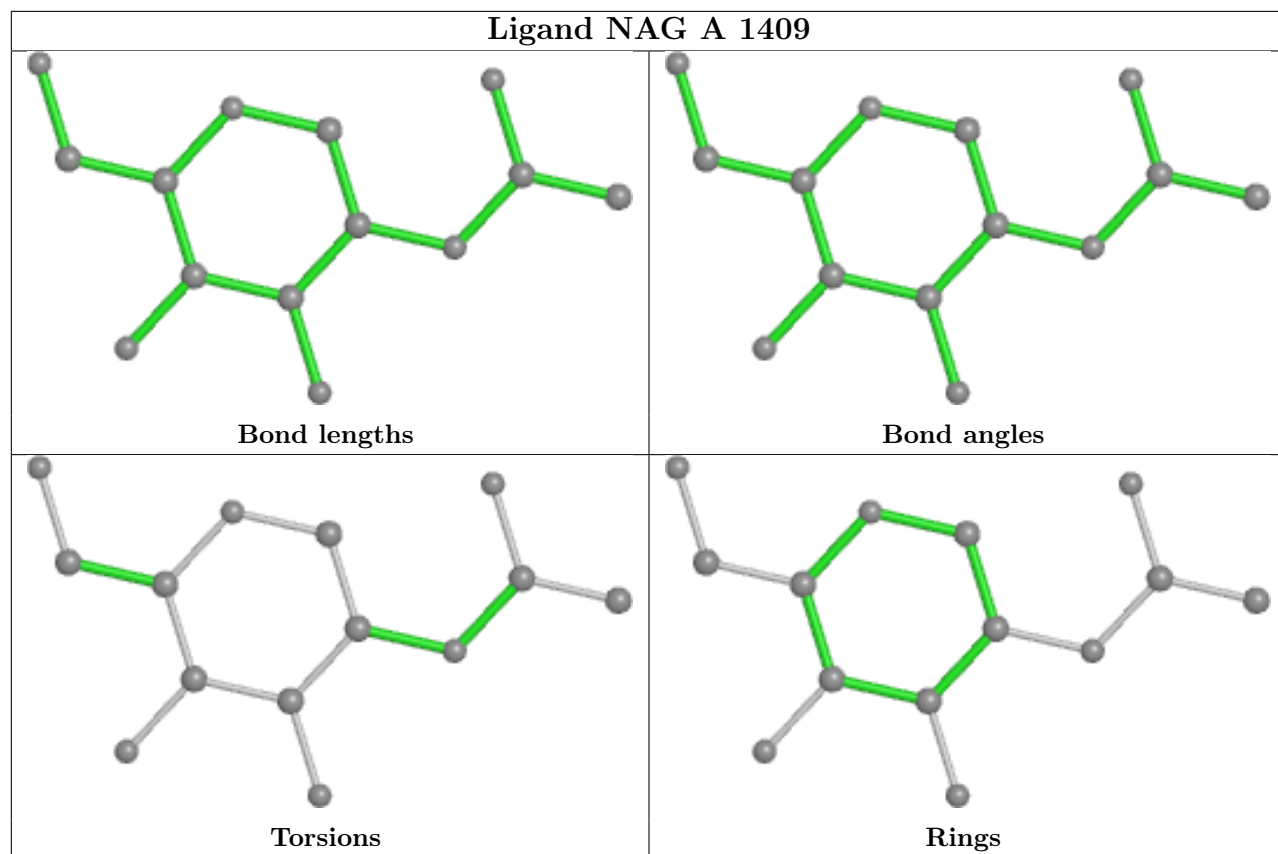


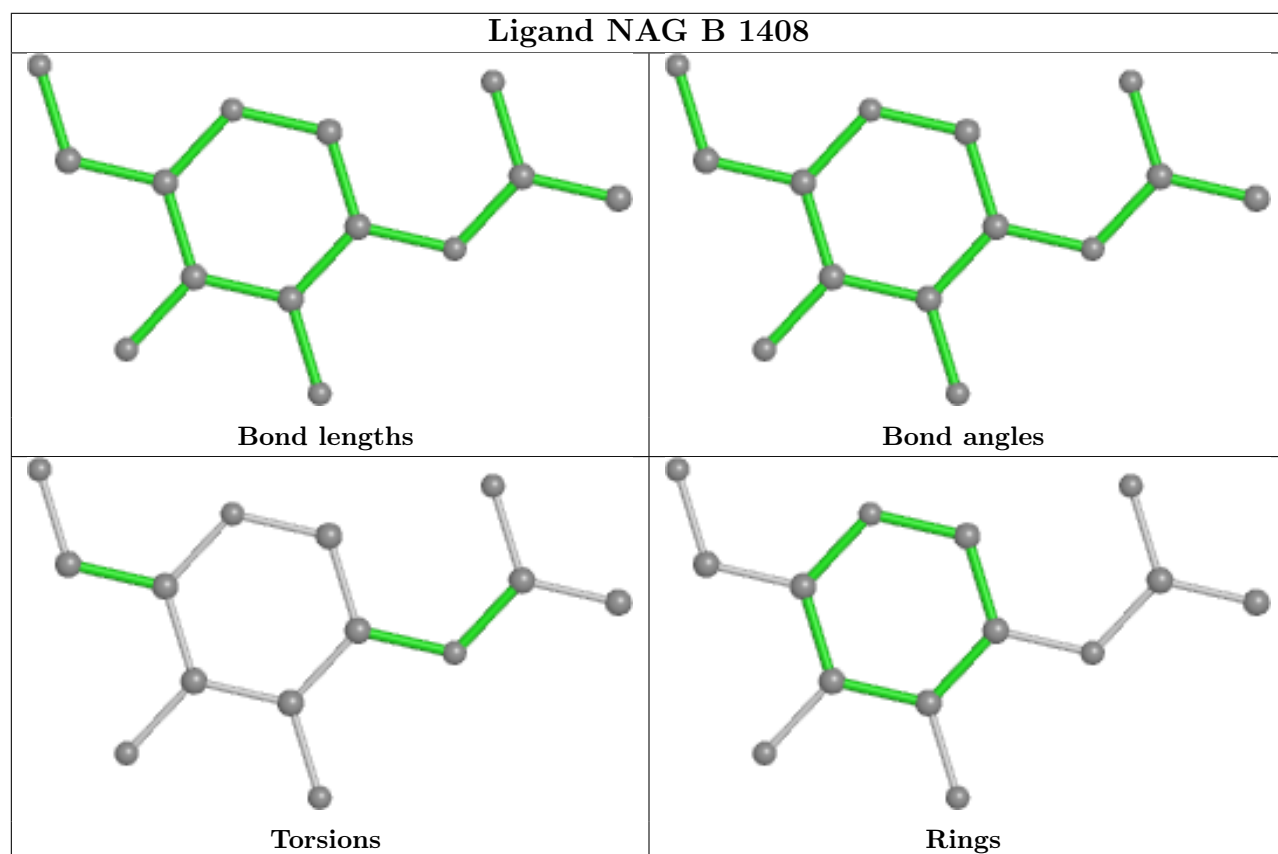
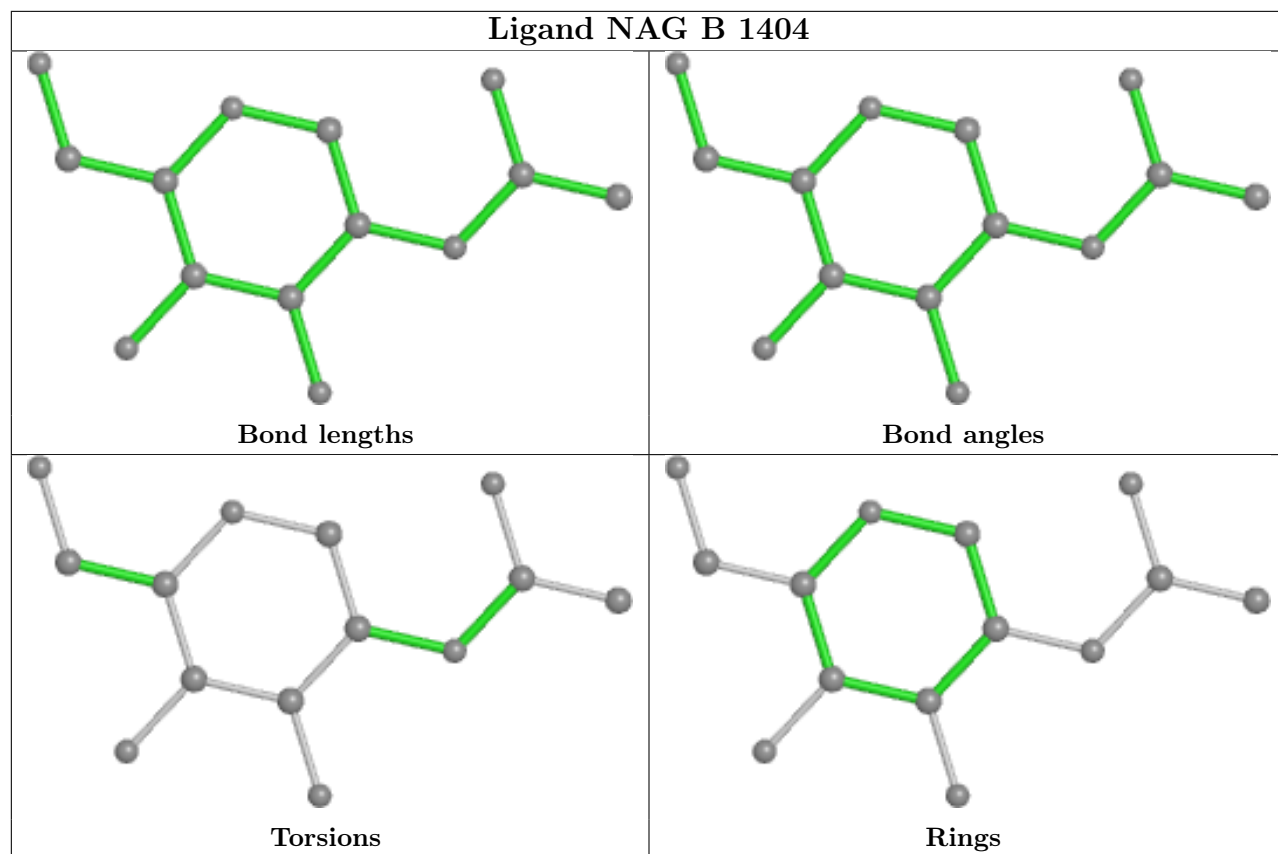
## Ligand NAG C 1402

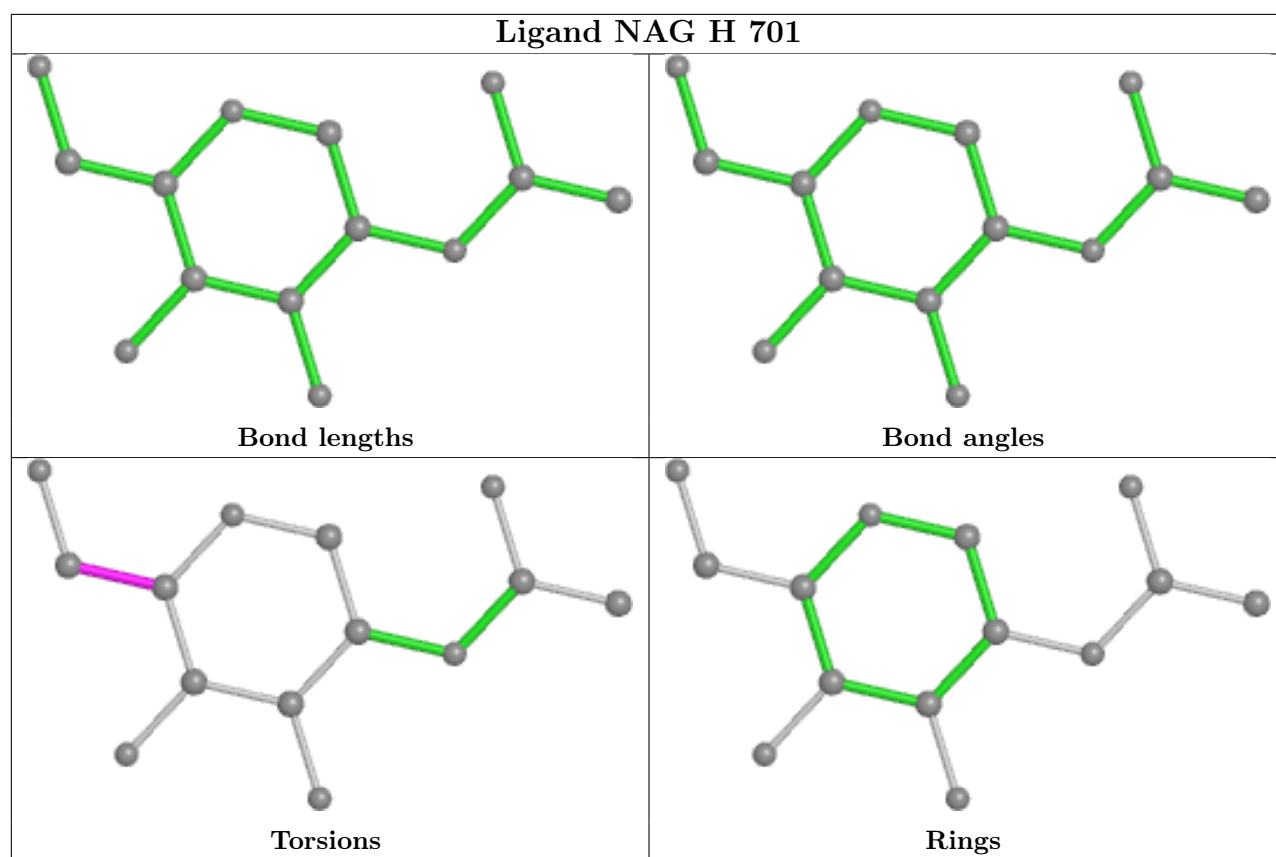


## Ligand NAG B 1406









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

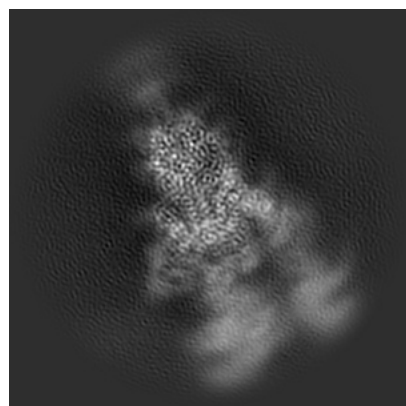
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33575. These allow visual inspection of the internal detail of the map and identification of artifacts.

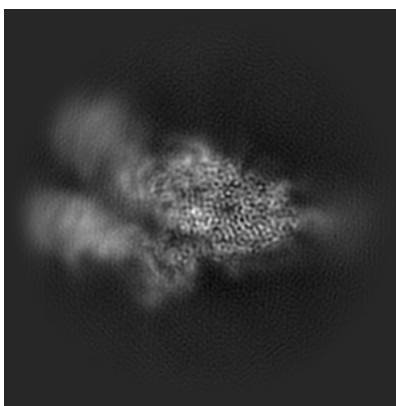
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

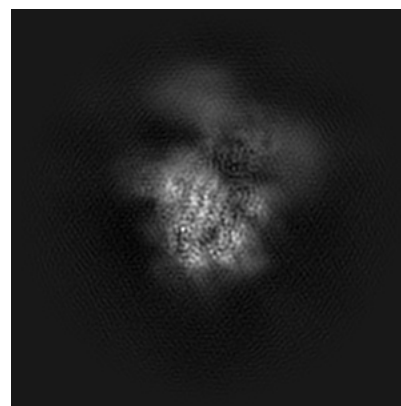
#### 6.1.1 Primary map



X

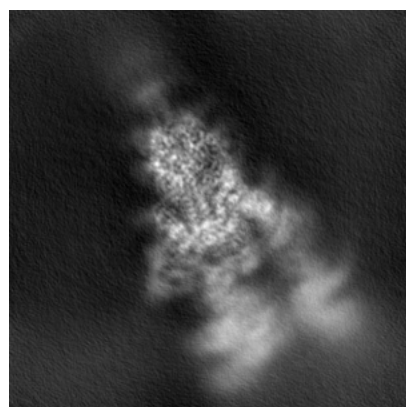


Y

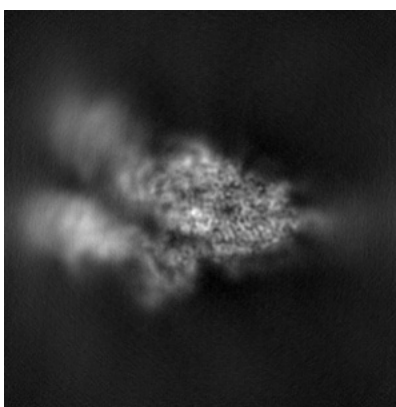


Z

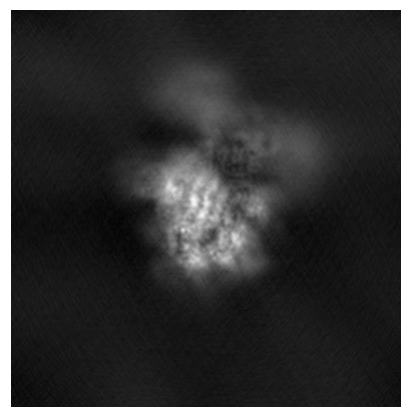
#### 6.1.2 Raw map



X



Y

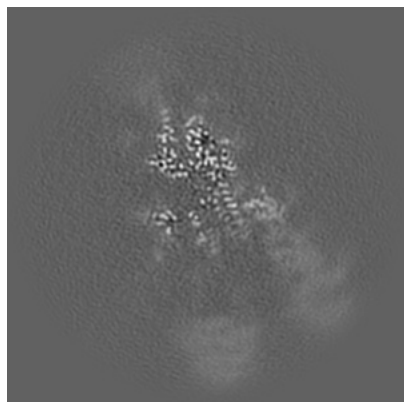


Z

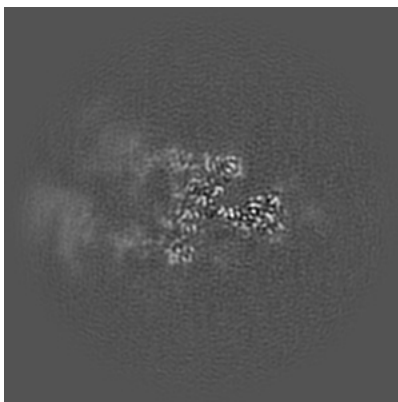
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

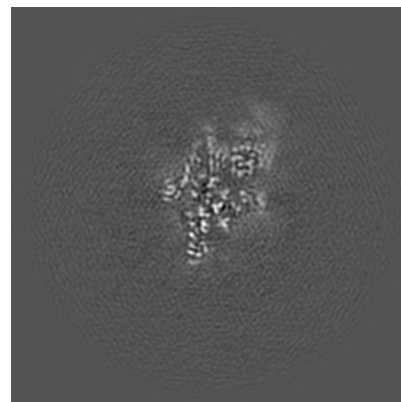
### 6.2.1 Primary map



X Index: 144

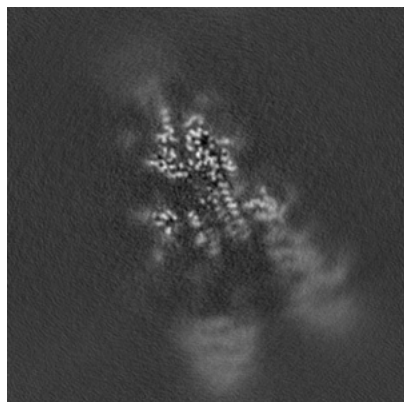


Y Index: 144

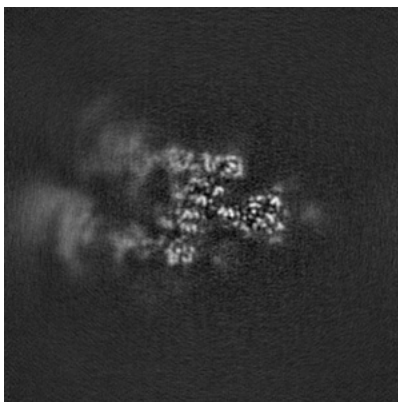


Z Index: 144

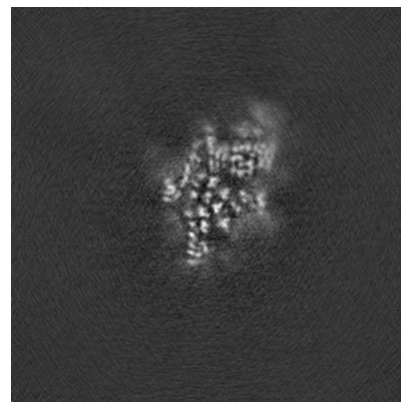
### 6.2.2 Raw map



X Index: 144



Y Index: 144

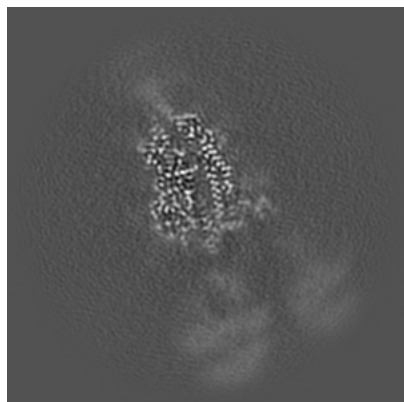


Z Index: 144

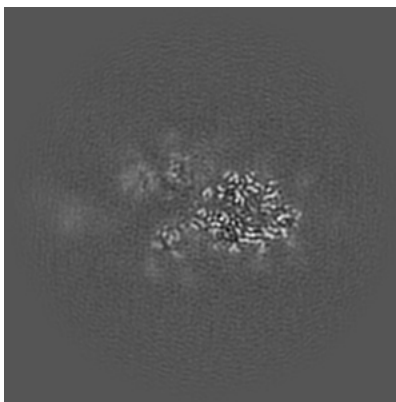
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

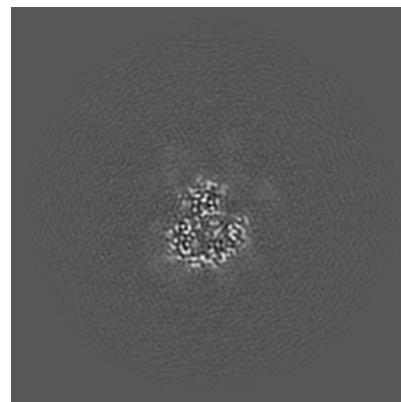
### 6.3.1 Primary map



X Index: 131

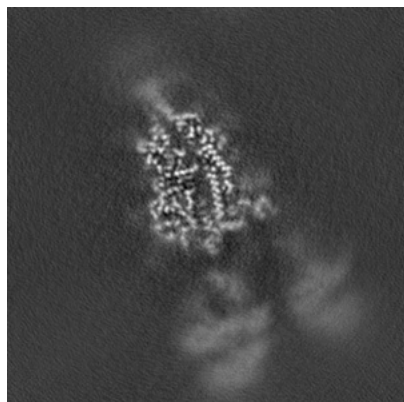


Y Index: 130

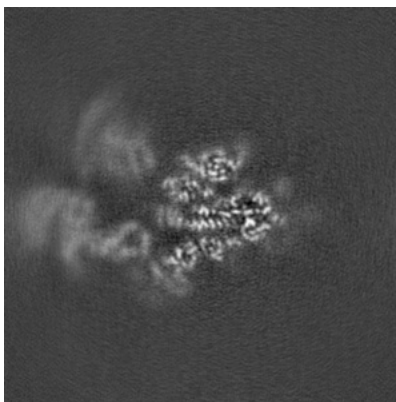


Z Index: 176

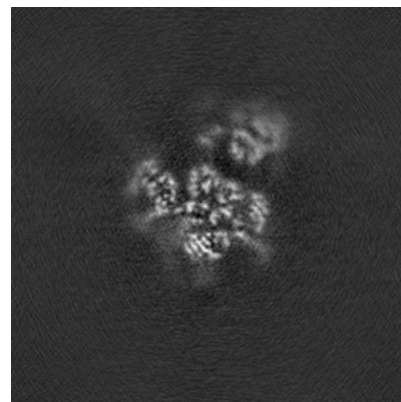
### 6.3.2 Raw map



X Index: 131



Y Index: 152



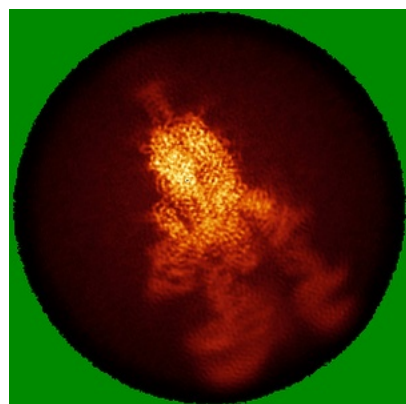
Z Index: 132

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

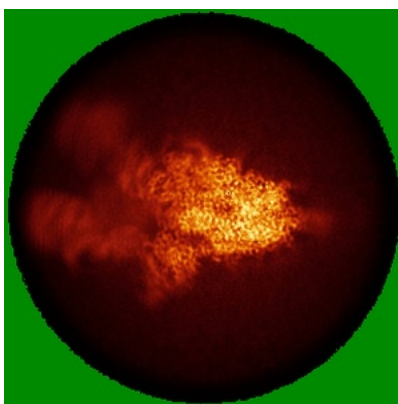


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

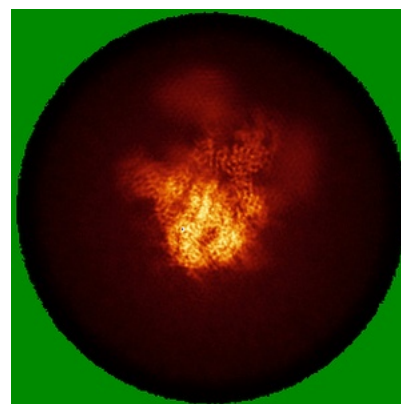
### 6.4.1 Primary map



X

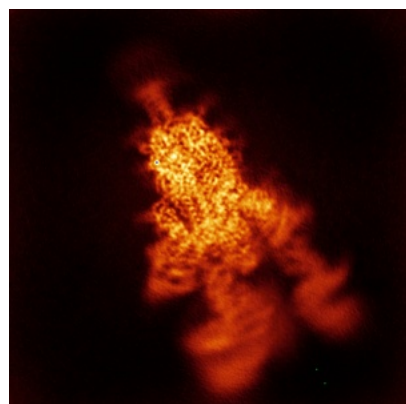


Y

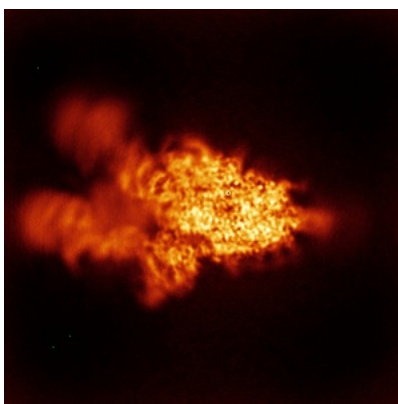


Z

### 6.4.2 Raw map



X



Y



Z

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



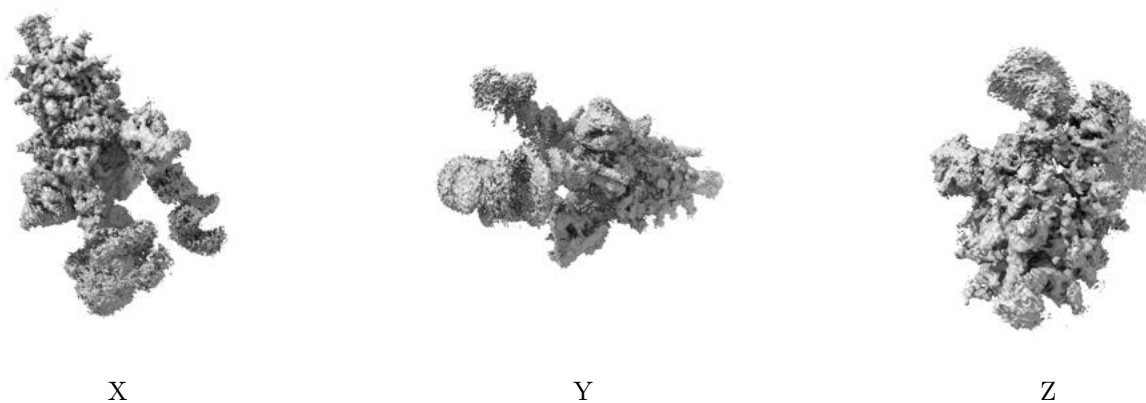
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

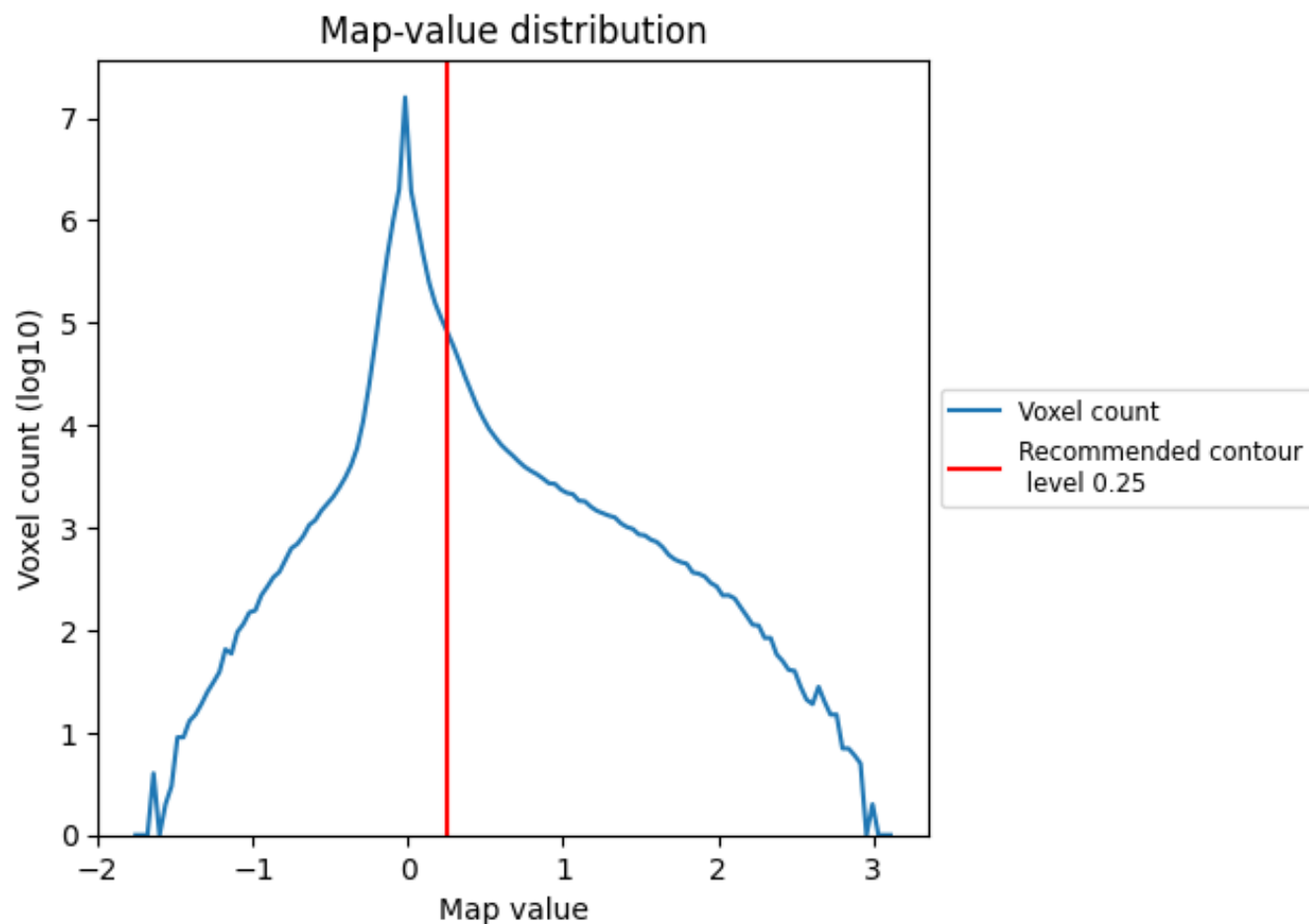
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

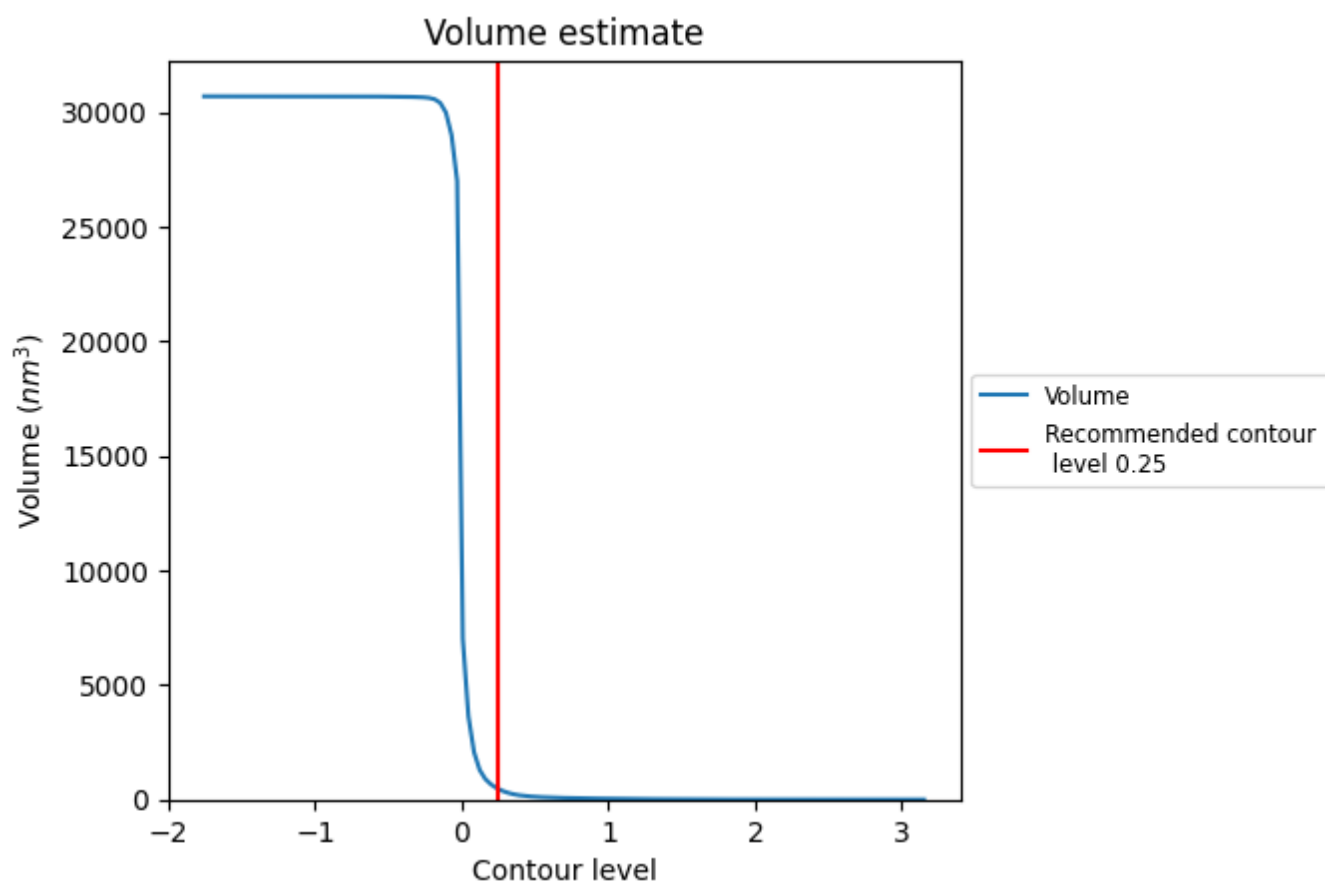
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

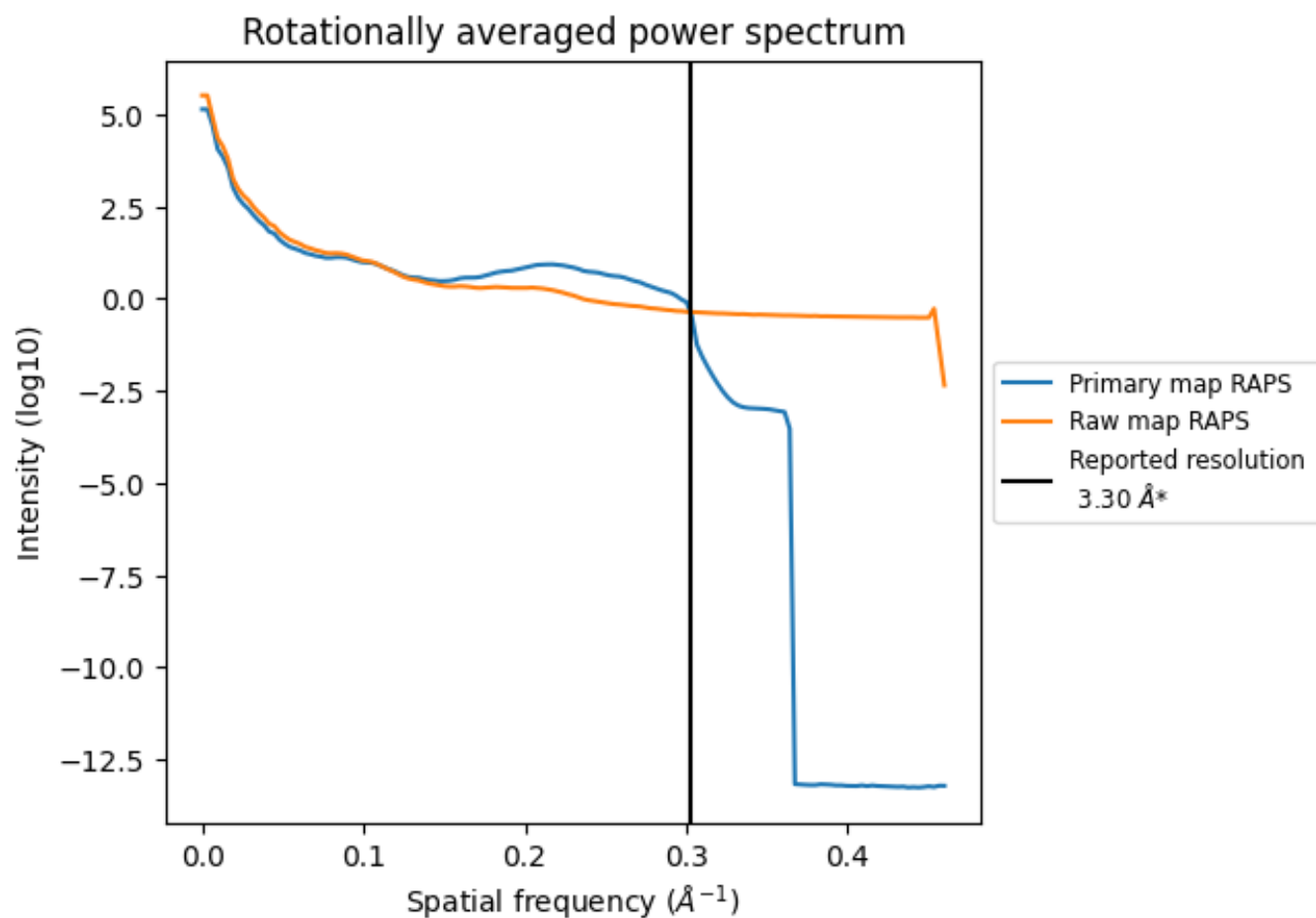
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 461  $\text{nm}^3$ ; this corresponds to an approximate mass of 416 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

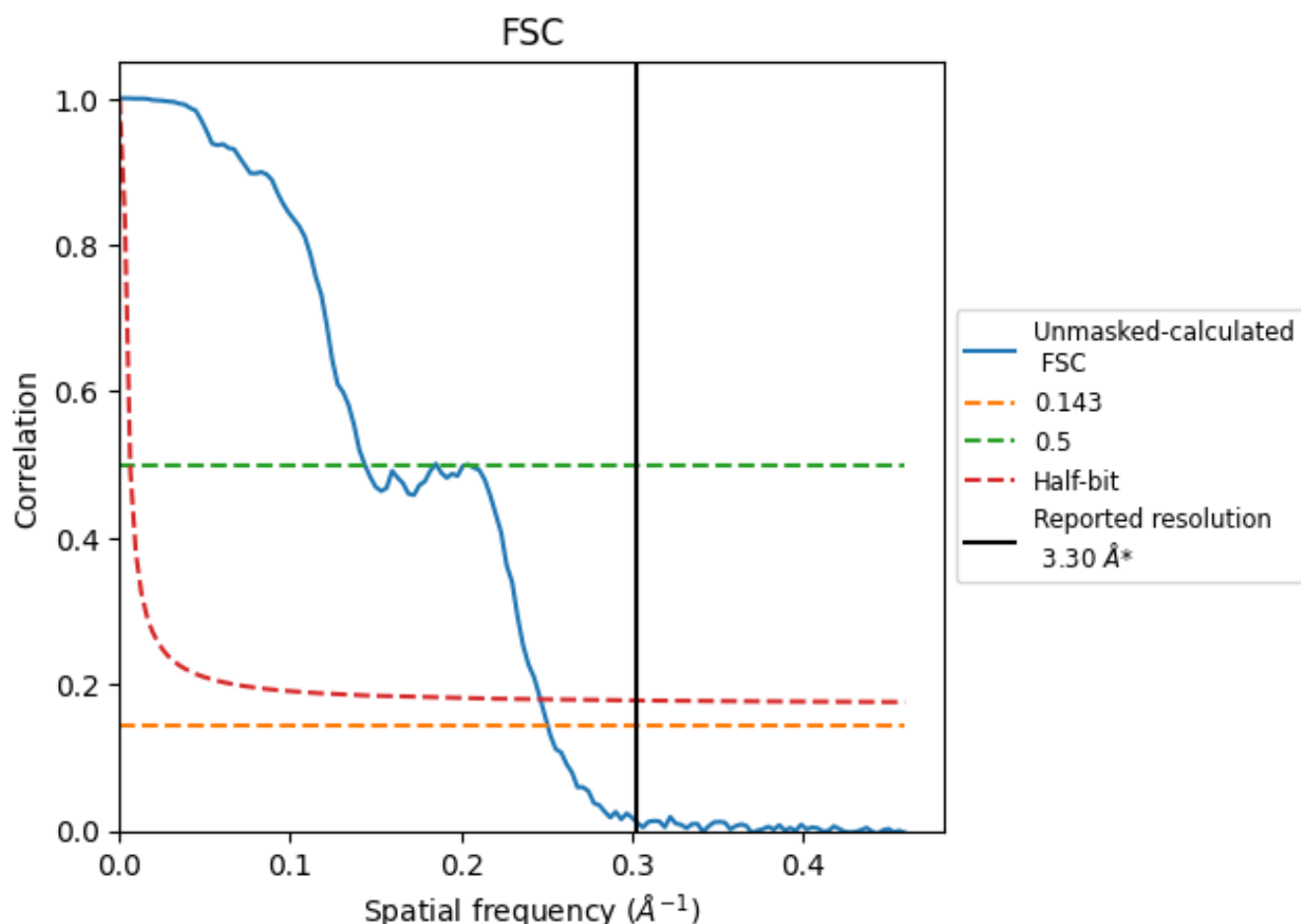


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

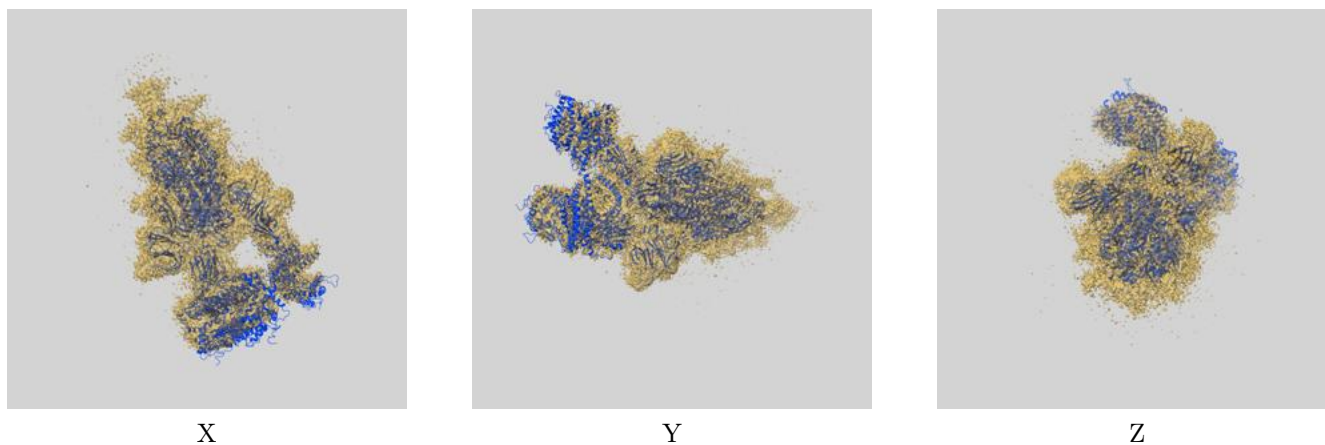
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	6.96	4.06

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

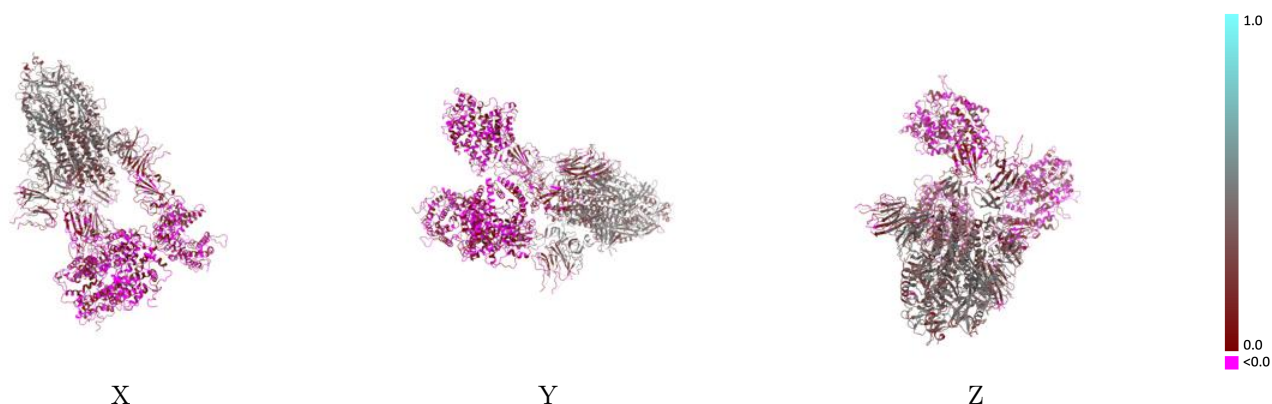
This section contains information regarding the fit between EMDB map EMD-33575 and PDB model 7Y1Y. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

### 9.1 Map-model overlay [i](#)



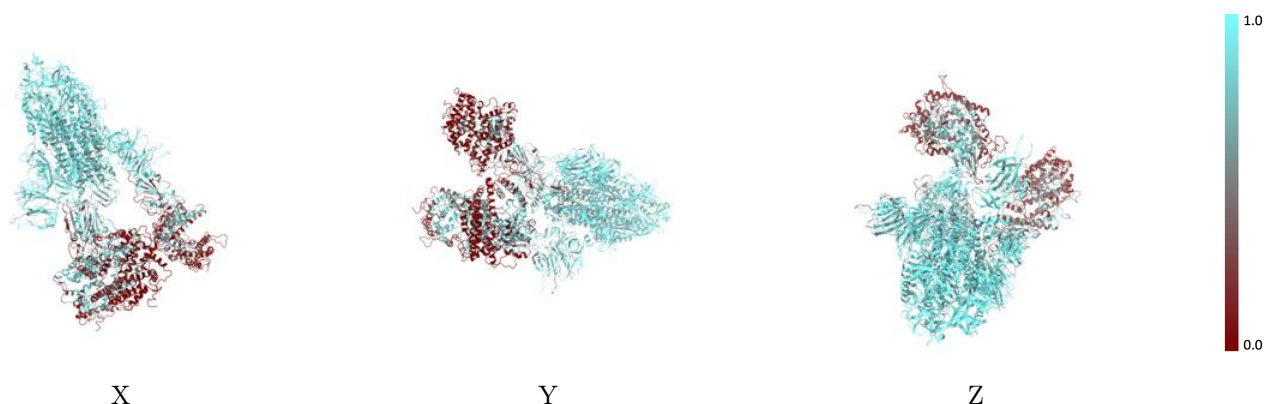
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

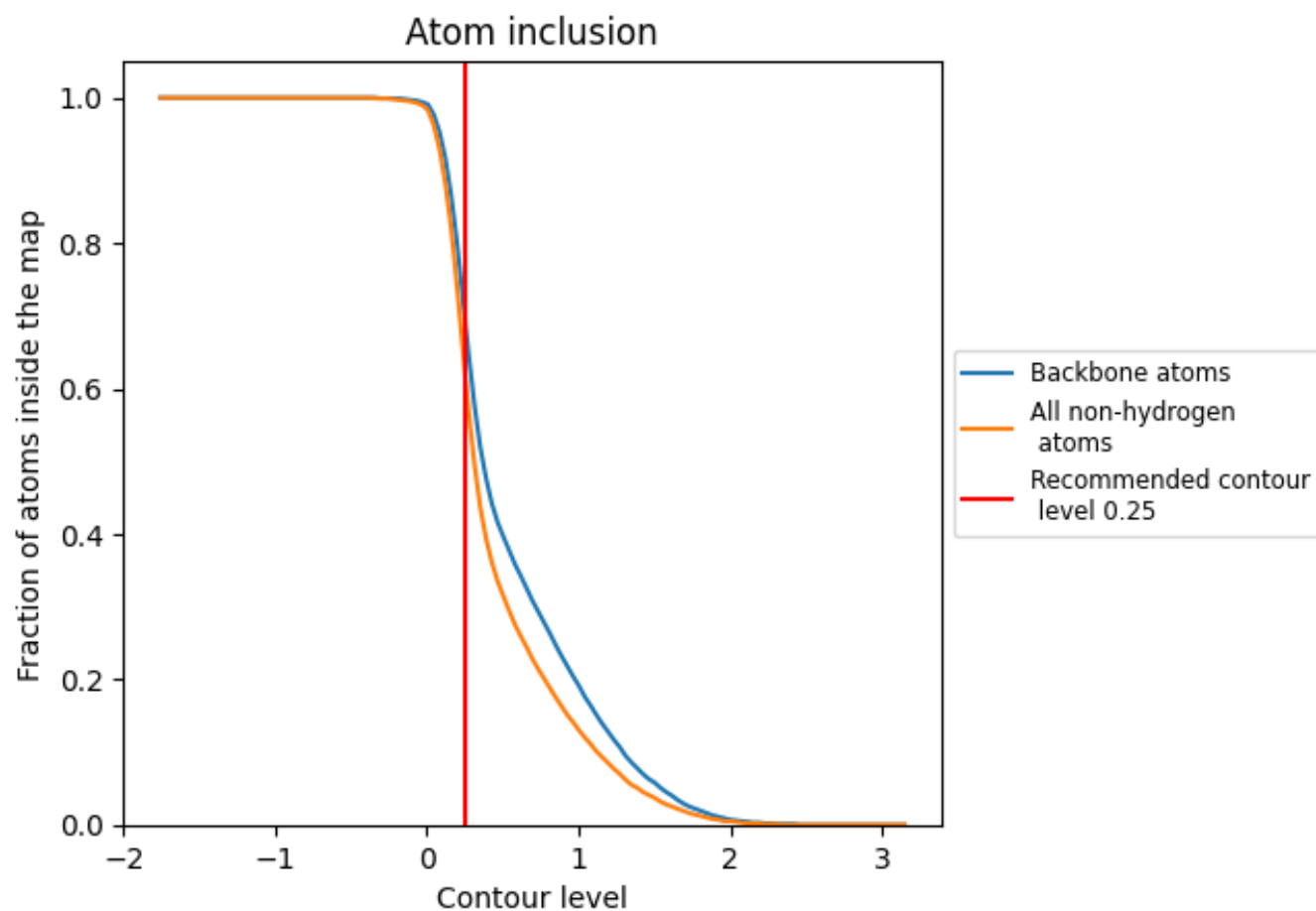
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6220	 0.1840
A	 0.7750	 0.2730
B	 0.7660	 0.2740
C	 0.8350	 0.3040
D	 0.2880	 0.0220
E	 0.7860	 0.2970
F	 0.1730	 0.0180
G	 0.2860	 0.1360
H	 0.6130	 0.0320
I	 0.9290	 0.3790
J	 0.7140	 0.1390
K	 0.7140	 0.2820
L	 0.8570	 0.2680
M	 0.8570	 0.3030
N	 0.7140	 0.2070
O	 0.2140	 -0.0420
P	 0.4640	 0.1950
Q	 0.8210	 0.2810
R	 0.8930	 0.2760
S	 0.6430	 0.3270
T	 0.9290	 0.3550
U	 0.9290	 0.3600
V	 0.7860	 0.3900
W	 0.1790	 0.0020
X	 0.4640	 -0.0020
Y	 0.8930	 0.3670
Z	 0.7860	 0.1470
a	 0.6070	 0.3260
b	 0.8930	 0.3230
c	 0.7860	 0.3070
d	 0.1430	 -0.0440
e	 0.0000	 0.0540
f	 0.0000	 0.1250
g	 0.0000	 -0.1140
h	 0.0000	 0.0440



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Chain	Atom inclusion	Q-score
i	 0.2500	 0.0980
j	 0.0000	 -0.0680
k	 0.0000	 -0.1180
l	 0.0000	 -0.0160
m	 0.0000	 0.0210
n	 0.1790	 -0.0030
o	 0.1070	 0.1090
p	 0.0710	 -0.1280
q	 0.0000	 0.0160
r	 0.2500	 0.0390