



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:08 PM UTC

PDB ID : 7V76 / pdb_00007v76
EMDB ID : EMD-31760
Title : Cryo-EM structure of SARS-CoV-2 S-Beta variant (B.1.351), uncleavable form, one RBD-up conformation
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Hsu, S.T.D.
Deposited on : 2021-08-21
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

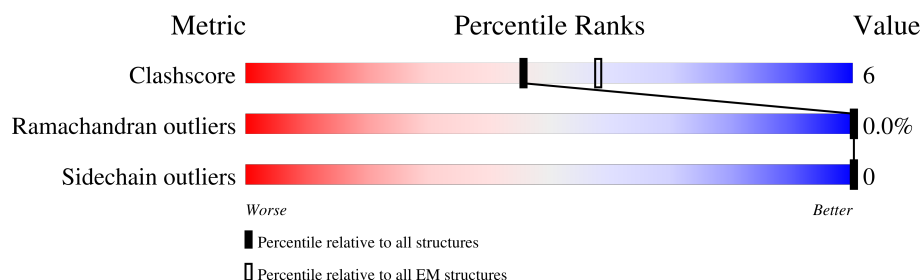
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1280	67% 13% 20%
1	B	1280	68% 12% 19%
1	C	1280	65% 15% 20%
2	D	2	50% 50%
2	E	2	50% 50%
2	F	2	100%
2	G	2	50% 50%
2	H	2	50% 50%
2	I	2	100%

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Mol	Chain	Length	Quality of chain
2	J	2	100%
2	K	2	100%
2	L	2	100%
2	M	2	100%
2	N	2	100%
2	O	2	100%
2	P	2	50%
2	Q	2	100%
2	R	2	100%
2	S	2	100%
2	T	2	100%
2	U	2	100%
2	V	2	100%
2	W	2	50%
2	X	2	100%
2	Y	2	100%
2	Z	2	100%
2	a	2	50%
2	b	2	50%
2	c	2	100%
2	d	2	100%
2	e	2	100%
2	f	2	50%
2	g	2	50%
2	h	2	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25219 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	1026	Total	C	N	O	S	0	0
			8014	5120	1330	1527	37		
1	B	1032	Total	C	N	O	S	0	0
			8070	5158	1341	1534	37		
1	C	1030	Total	C	N	O	S	0	0
			8057	5149	1339	1532	37		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	243	ILE	ARG	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	481	LYS	GLU	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	698	VAL	ALA	variant	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1206	GLU	-	expression tag	UNP P0DTC2
A	1207	PHE	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLN	-	expression tag	UNP P0DTC2
A	1241	ASP	-	expression tag	UNP P0DTC2
A	1242	ASN	-	expression tag	UNP P0DTC2
A	1243	SER	-	expression tag	UNP P0DTC2
A	1244	ALA	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	ILE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	HIS	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	ARG	-	expression tag	UNP P0DTC2
A	1252	PRO	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	SER	-	expression tag	UNP P0DTC2
A	1256	ARG	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	PRO	-	expression tag	UNP P0DTC2
A	1259	PHE	-	expression tag	UNP P0DTC2
A	1260	GLU	-	expression tag	UNP P0DTC2
A	1261	GLN	-	expression tag	UNP P0DTC2
A	1262	LYS	-	expression tag	UNP P0DTC2
A	1263	LEU	-	expression tag	UNP P0DTC2
A	1264	ILE	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLU	-	expression tag	UNP P0DTC2
A	1268	ASP	-	expression tag	UNP P0DTC2
A	1269	LEU	-	expression tag	UNP P0DTC2
A	1270	ASN	-	expression tag	UNP P0DTC2
A	1271	MET	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	THR	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	243	ILE	ARG	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	481	LYS	GLU	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	698	VAL	ALA	variant	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1206	GLU	-	expression tag	UNP P0DTC2
B	1207	PHE	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	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
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	LYS	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	GLN	-	expression tag	UNP P0DTC2
B	1241	ASP	-	expression tag	UNP P0DTC2
B	1242	ASN	-	expression tag	UNP P0DTC2
B	1243	SER	-	expression tag	UNP P0DTC2
B	1244	ALA	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	GLY	-	expression tag	UNP P0DTC2
B	1251	ARG	-	expression tag	UNP P0DTC2
B	1252	PRO	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLU	-	expression tag	UNP P0DTC2
B	1255	SER	-	expression tag	UNP P0DTC2
B	1256	ARG	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	PRO	-	expression tag	UNP P0DTC2
B	1259	PHE	-	expression tag	UNP P0DTC2
B	1260	GLU	-	expression tag	UNP P0DTC2
B	1261	GLN	-	expression tag	UNP P0DTC2
B	1262	LYS	-	expression tag	UNP P0DTC2
B	1263	LEU	-	expression tag	UNP P0DTC2
B	1264	ILE	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	GLU	-	expression tag	UNP P0DTC2
B	1268	ASP	-	expression tag	UNP P0DTC2
B	1269	LEU	-	expression tag	UNP P0DTC2
B	1270	ASN	-	expression tag	UNP P0DTC2
B	1271	MET	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	THR	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	HIS	-	expression tag	UNP P0DTC2
B	1277	HIS	-	expression tag	UNP P0DTC2
B	1278	HIS	-	expression tag	UNP P0DTC2
B	1279	HIS	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	243	ILE	ARG	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	481	LYS	GLU	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	698	VAL	ALA	variant	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1206	GLU	-	expression tag	UNP P0DTC2
C	1207	PHE	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	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	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	GLN	-	expression tag	UNP P0DTC2
C	1241	ASP	-	expression tag	UNP P0DTC2
C	1242	ASN	-	expression tag	UNP P0DTC2
C	1243	SER	-	expression tag	UNP P0DTC2
C	1244	ALA	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	ILE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	GLY	-	expression tag	UNP P0DTC2
C	1251	ARG	-	expression tag	UNP P0DTC2
C	1252	PRO	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLU	-	expression tag	UNP P0DTC2
C	1255	SER	-	expression tag	UNP P0DTC2
C	1256	ARG	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	PRO	-	expression tag	UNP P0DTC2
C	1259	PHE	-	expression tag	UNP P0DTC2
C	1260	GLU	-	expression tag	UNP P0DTC2
C	1261	GLN	-	expression tag	UNP P0DTC2
C	1262	LYS	-	expression tag	UNP P0DTC2
C	1263	LEU	-	expression tag	UNP P0DTC2
C	1264	ILE	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	GLU	-	expression tag	UNP P0DTC2
C	1268	ASP	-	expression tag	UNP P0DTC2
C	1269	LEU	-	expression tag	UNP P0DTC2
C	1270	ASN	-	expression tag	UNP P0DTC2
C	1271	MET	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	THR	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	HIS	-	expression tag	UNP P0DTC2
C	1277	HIS	-	expression tag	UNP P0DTC2
C	1278	HIS	-	expression tag	UNP P0DTC2
C	1279	HIS	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2

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



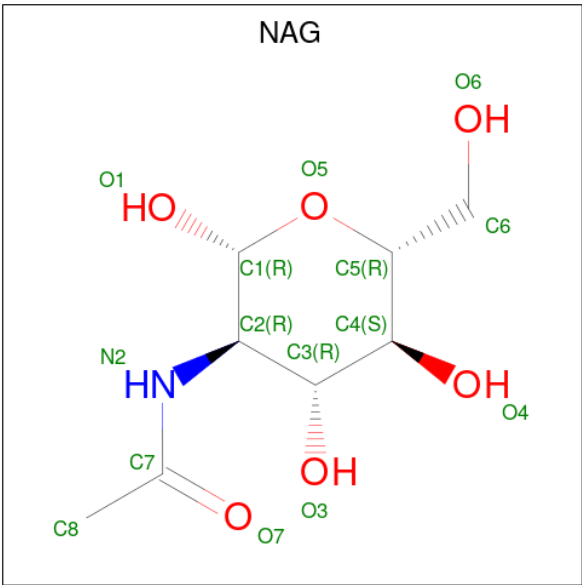
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	f	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	h	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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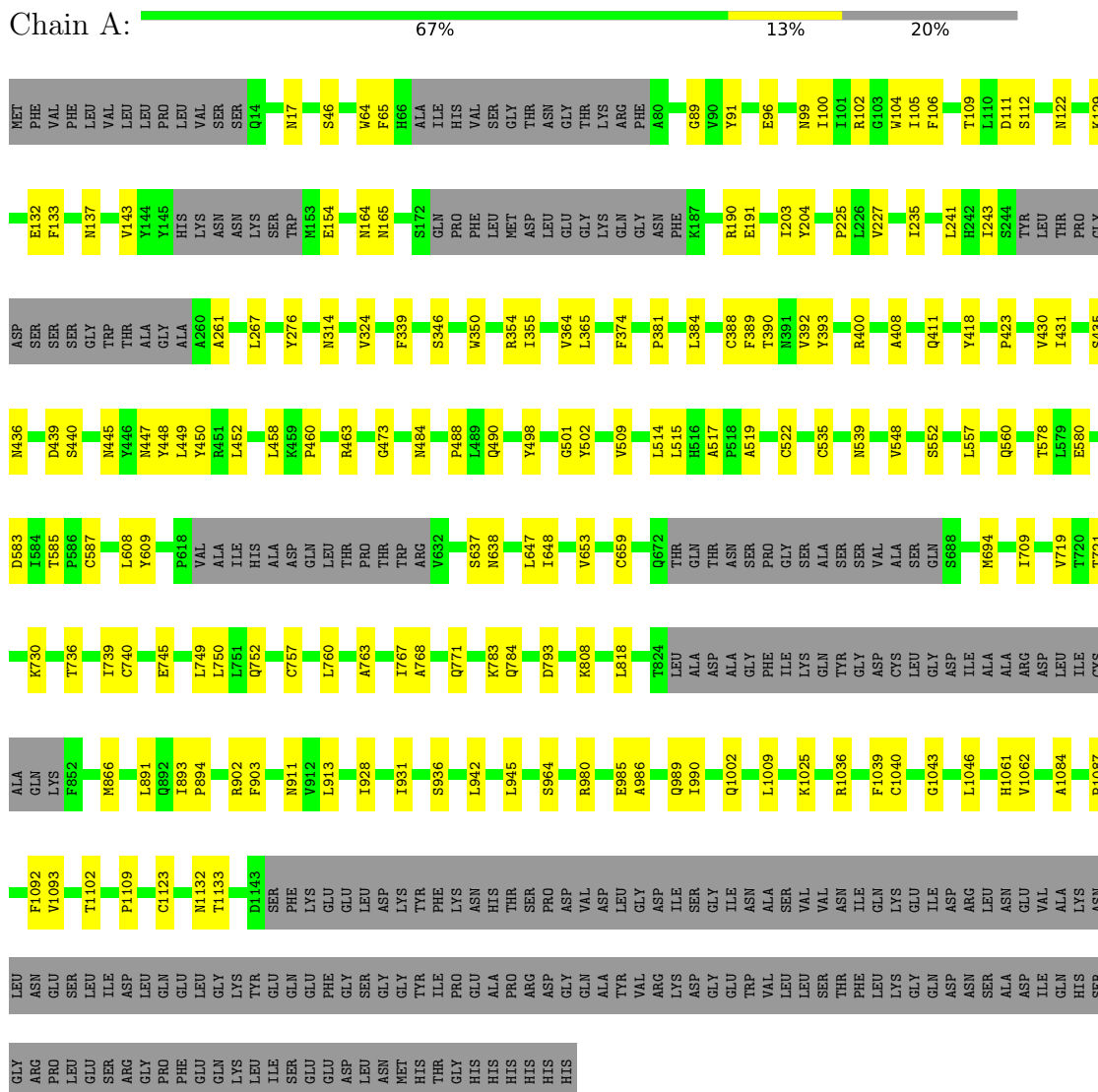
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	14	8	1	5	0

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

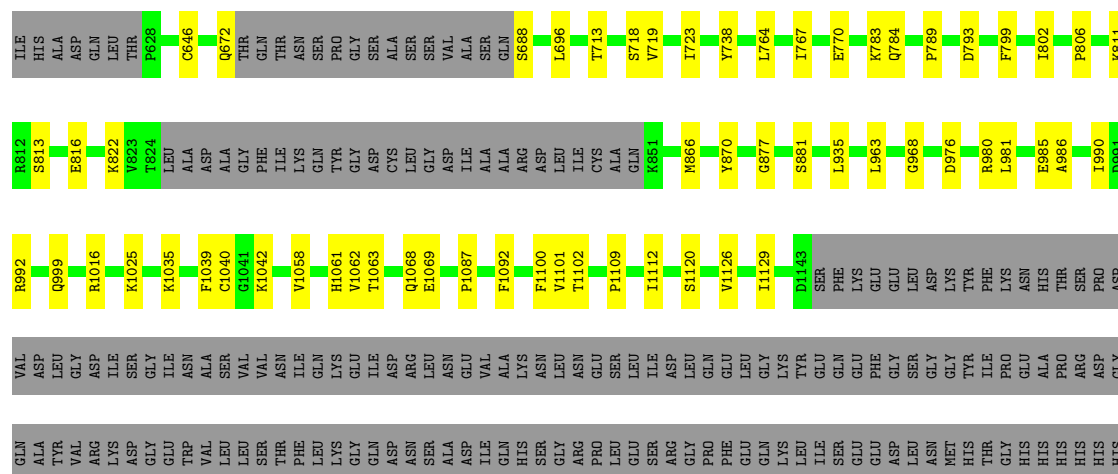


HIS	ALA	HIS	THR	HIS	GLY	SER	K526	V359	R190	S112	MET
HIS	PRO	HIS	THR	HIS	ASP	GLN	K527	V359	R190	S112	MET
HIS	ARG	HIS	SER	HIS	ILE	GLN	S688	T373	F194	I119	VAL
HIS	ASP	HIS	PRO	HIS	ALA	ALA	L696	K375	I203	N121	LEU
HIS	GLY	HIS	ASP	HIS	ARG	ARG	A703	C535	H207	T124	VAL
	GLN		VAL		ASP	ASP	A704	F381	I210	N125	LEU
	ALA		ASP		ASP	LEU	Y704	R574	P217	V126	LEU
	VAL		GLY		ASP	ILE	I709	D575	I210	N125	LEU
	ARG		ASP		CYS	GLY	V709	T390	P217	V127	VAL
	LYS		ILE		ALA	ILE	V719	N391	I210	N125	VAL
	ASP		SER		GLN	SER	I581	V392	I210	N125	SER
	GLY		GLY		R951	GLY	E722	R400	I235	K129	SER
	GLU		ILE		ILE	ILE	E723	T236	V130	C131	SER
	TRP		ASN		A887	TRP	I723	G401	R237	E132	Q14
	VAL		ALA		ALA	VAL	T596	D402	I243	S244	N17
	LEU		SER		T893	LEU	V726	E403	I244	N137	R21
	LEU		VAL		P894	VAL	S727	P597	H242	Y144	T22
	SER		VAL		N952	SER	M728	T601	S244	Y143	Q23
	THR		ASN		ASN	THR	D734	V605	TYR	Y144	S31
	PHE		ILE		GLN	ILE	T744	C614	LEU	Y145	S31
	LEU		GLN		D982	LEU	E745	T615	THR	HIS	S46
	LYS		LYS		P983	LYS	T744	E816	PRO	LYS	S46
	GLY		GLU		P984	GLY	E745	K421	GLY	ASN	S60
	GLN		ILE		Q1007	ILE	S755	V617	ASP	ASN	S60
	ASP		ASP		ASP	ASP	S755	P618	SER	LYS	S60
	ASN		ARG		ARG	ASN	Q759	P423	SER	LYS	S60
	SER		ASN		R1011	SER	Q759	VAL	SER	SER	W64
	ALA		ASN		ALA	ASN	K773	ALA	SER	TRP	F65
	ASP		GLU		L1046	GLU	K773	ILE	SER	GLY	H66
	ILE		VAL		M1047	VAL	E777	HIS	TRP	E154	H66
	GLN		ALA		S1048	ALA	E777	ALA	ALA	ALA	ALA
	HIS		LYS		F1049	LYS	F799	ASP	ALA	F157	ILE
	SER		ASN		LEU	ASN	K783	GLN	GLY	Y160	VAL
	GLY		LEU		G1056	LEU	Q784	LEU	ALA	Y160	VAL
	ARG		ASN		V1057	ASN	Q784	THR	A260	GLY	SER
	PRO		GLU		V1058	GLU	D793	P628	A261	N164	GLY
	LEU		SER		LEU	SER	F799	R451	Y276	N165	GLY
	GLU		LEU		H1061	LEU	F799	V639	K307	C166	THR
	SER		ILE		V1062	ASP	I802	K455	E169	E169	LYS
	ARG		ASP		K1083	LEU	P806	C646	K307	E169	LYS
	GLY		LEU		GLN	LEU	P806	L647	E169	E169	ARG
	PHE		GLU		V1093	GLY	K811	I648	S313	S172	PHE
	GLU		LEU		LEU	LEU	K811	D660	N314	GLN	ARG
	GLN		GLY		V1119	GLY	K811	D660	R325	PHE	ARG
	LYS		LYS		LYS	LYS	L825	Q672	R325	GLN	PHE
	LEU		TYR		D1143	TYR	ALA	THR	R325	LEU	ARG
	ILE		GLU		SER	GLY	ASP	GLN	R328	MET	PHE
	GLU		GLN		PHE	GLY	THR	THR	I329	LEU	ARG
	SER		GLU		LYS	GLY	ALA	ASN	T330	GLY	D88
	GLU		PHE		GLY	PHE	GLY	ASN	N331	LEU	G89
	GLU		GLY		GLU	GLY	PHE	SER	Y492	GLY	T95
	ASP		GLY		GLY	ILE	ILE	PRO	G493	GLY	T95
	LEU		SER		LEU	LYS	LYS	GLY	T342	LYS	N99
	ASN		GLY		ASP	GLN	TYR	GLY	W350	GLN	I100
	MET		GLY		LYS	GLY	ALA	SER	R506	GLY	I101
	HIS		TYR		TYR	TYR	ALA	ALA	R354	ASN	R102
	THR		ILE		PHE	ASP	GLY	SER	T355	PHE	G103
	GLY		PRO		LYS	CYS	ASP	SER	E513	K187	G107
	PRO		GLY		ASN	LEU	VAL	VAL	T355	N188	T102
	GLY		GLY		ALA	LEU	ALA	ALA	C358	L189	T102

• Molecule 1: Spike glycoprotein

Chain C:  65% 15% 20%

L458	S322	I210	K113	MET
Y470	I323	I210	L117	PHE
K481	V324	P217	L118	VAL
C485	R325	P225	N122	PHE
L489	F326	P230	A123	LEU
Y492	F335	I235	I128	LEU
G499	W350	Q239	K129	PRO
V500	I355	T240	V130	LEU
G501	F371	L241	C131	VAL
Y502	S372	H242	E132	SER
Q503	T373	I243	F135	Q14
	F374	S244	C136	N17
	V379	THR	N137	S31
V509	S380	LEU	F140	S46
E513	P381	THR	V143	S60
P518	T390	PRO	Y144	
A519	N391	GLY	Y145	
T520	V392	ASP	HIS	W64
K525	R400	SER	LYS	F65
C535	G401	SER	ASN	H66
V536	D402	GLY	ASN	ALA
N537	Q411	TRP	LYS	ILE
F538	M414	THR	SER	HIS
N539	I415	ALA	TRP	VAL
Q561		GLY	M153	SER
		ALA	E154	GLY
		A261	R158	THR
		Y266	C166	ASN
D565	P423	L274	E169	GLY
I566	D424	K275	S172	THR
T569	D425	Y276	GLN	LYS
	F426	I282	PRO	ARG
Q577	V430	T283	PHE	PHE
C587	I431	D284	LEU	
S588	W432	D291	MET	N87
F589	M434	P292	ASP	Y91
V594	S435	T296	LEU	K97
T599	D439	T299	GLY	S98
S602	N445	F303	LYS	N99
N603	L449	T304	GLM	I100
Y609	Y450	S313	GLY	I101
V617	R451	N314	ASN	R102
P618	L452	R316	PHE	F106
VAL	F453		K137	T109
	R454		LYS	L110
	V657		GLY	D111
			ASP	S112
			GLY	
			LEU	
			GLY	
			GLM	
			GLY	
			ASN	
			PHE	



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

Chain D: 50% 50%



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

Chain E: 50% 50%



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

Chain F: 100%



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

Chain G: 50% 50%



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

Chain H: 50% 50%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain T:  100%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  50% 50%



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

Chain X:  100%



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

Chain Y:  100%



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

Chain Z:  100%



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

Chain a:  50% 50%



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

Chain b:  50% 50%



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

Chain c:  100%



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

Chain d:  100%



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

Chain e:  100%



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

Chain f:  50% 50%



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

Chain g:  50% 50%



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

Chain h:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	306270	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
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	0.11	0/8198	0.28	0/11159
1	B	0.11	0/8257	0.29	0/11239
1	C	0.11	0/8244	0.30	0/11221
All	All	0.11	0/24699	0.29	0/33619

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	8014	0	7803	99	0
1	B	8070	0	7863	101	0
1	C	8057	0	7851	117	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	2	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	2	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	1	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
2	f	28	0	25	0	0
2	g	28	0	25	1	0
2	h	28	0	25	0	0
3	A	56	0	52	2	0
3	B	84	0	78	1	0
3	C	70	0	65	0	0
All	All	25219	0	24487	309	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (309) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:HE1	1:A:261:ALA:HB1	1.47	0.78
1:A:381:PRO:HA	1:A:384:LEU:HD23	1.70	0.72
1:B:46:SER:HA	1:B:276:TYR:O	1.91	0.70
1:B:64:TRP:HE1	1:B:261:ALA:HB1	1.58	0.69
1:C:400:ARG:NH1	1:C:501:GLY:O	2.21	0.69
1:B:722:GLU:OE2	1:B:1061:HIS:NE2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:TRP:HE1	1:C:261:ALA:HB1	1.58	0.68
1:C:31:SER:HB3	1:C:60:SER:H	1.58	0.68
1:A:355:ILE:HB	1:A:392:VAL:HB	1.75	0.67
1:A:1084:ALA:HB2	1:A:1123:CYS:HB3	1.76	0.67
1:A:866:MET:HG2	1:C:696:LEU:HD21	1.76	0.67
1:B:696:LEU:HD21	1:C:866:MET:HG2	1.78	0.66
1:B:112:SER:HA	1:B:132:GLU:HB3	1.78	0.65
1:C:46:SER:HA	1:C:276:TYR:O	1.97	0.65
1:A:439:ASP:O	1:A:445:ASN:ND2	2.28	0.64
1:A:783:LYS:HG3	1:A:784:GLN:HG3	1.80	0.63
1:A:986:ALA:O	1:A:990:ILE:HG12	1.99	0.63
1:A:143:VAL:HG12	1:A:154:GLU:HG3	1.80	0.63
1:A:911:ASN:ND2	1:C:1120:SER:OG	2.32	0.63
1:B:17:ASN:OD1	1:B:137:ASN:ND2	2.33	0.62
1:C:144:TYR:OH	1:C:158:ARG:NH2	2.32	0.62
1:C:296:THR:HG21	1:C:594:VAL:HG21	1.81	0.62
2:P:1:NAG:H83	2:P:1:NAG:H3	1.82	0.62
1:A:46:SER:HA	1:A:276:TYR:O	2.00	0.62
1:C:449:LEU:HD11	1:C:489:LEU:HB3	1.82	0.61
1:C:770:GLU:OE2	1:C:1016:ARG:NH1	2.32	0.61
1:A:112:SER:HA	1:A:132:GLU:HB3	1.83	0.60
1:A:721:THR:HG23	1:A:931:ILE:HD11	1.84	0.60
1:C:99:ASN:OD1	1:C:190:ARG:NH2	2.35	0.60
1:A:552:SER:HB3	1:A:583:ASP:HB2	1.83	0.59
1:C:713:THR:OG1	1:C:1068:GLN:O	2.16	0.59
1:A:515:LEU:HD23	1:A:517:ALA:H	1.67	0.59
1:A:1002:GLN:OE1	1:C:999:GLN:NE2	2.35	0.59
1:B:165:ASN:HB3	2:P:1:NAG:C7	2.32	0.59
1:C:210:ILE:HG12	1:C:217:PRO:HG3	1.84	0.59
1:C:65:PHE:O	1:C:261:ALA:HA	2.03	0.59
1:B:450:TYR:HE1	1:B:490:GLN:HE21	1.51	0.58
1:A:350:TRP:O	1:A:463:ARG:NH2	2.34	0.58
1:C:783:LYS:HG3	1:C:784:GLN:HG3	1.86	0.58
1:A:346:SER:OG	1:A:449:LEU:O	2.22	0.58
1:B:704:TYR:HB3	1:C:789:PRO:HG3	1.86	0.57
1:B:423:PRO:HG2	1:B:426:PHE:HB2	1.86	0.57
1:C:313:SER:OG	1:C:314:ASN:N	2.37	0.57
1:A:767:ILE:O	1:A:771:GLN:HG2	2.04	0.57
1:B:31:SER:HB3	1:B:60:SER:H	1.69	0.57
1:C:81:ASN:ND2	1:C:240:THR:O	2.36	0.57
1:B:615:THR:OG1	1:B:616:GLU:OE1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:SER:O	1:B:759:GLN:NE2	2.38	0.57
1:A:980:ARG:HG2	1:C:379:VAL:HG12	1.87	0.57
1:C:129:LYS:HZ1	1:C:169:GLU:HB3	1.69	0.57
1:C:565:ASP:OD1	1:C:569:THR:OG1	2.23	0.56
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.88	0.56
1:C:355:ILE:HB	1:C:392:VAL:HB	1.87	0.56
1:C:400:ARG:HD3	1:C:402:ASP:H	1.69	0.56
1:B:719:VAL:HG22	1:B:1062:VAL:HG22	1.86	0.56
1:C:316:ARG:HG2	1:C:589:PHE:HB2	1.87	0.56
1:A:324:VAL:HG23	1:A:539:ASN:HB3	1.88	0.56
1:A:557:LEU:HD12	1:A:560:GLN:HE22	1.71	0.56
1:C:374:PHE:HE2	1:C:381:PRO:HB3	1.70	0.56
1:A:423:PRO:HD3	1:A:460:PRO:HB3	1.88	0.56
1:B:601:THR:HA	3:B:2005:NAG:H82	1.88	0.56
1:A:389:PHE:HD1	1:A:514:LEU:HB2	1.70	0.55
1:A:653:VAL:HA	3:A:2004:NAG:H82	1.87	0.55
1:C:17:ASN:OD1	1:C:137:ASN:ND2	2.40	0.55
1:B:119:ILE:HG12	1:B:128:ILE:HG12	1.88	0.55
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.90	0.54
1:A:314:ASN:ND2	1:B:734:ASP:OD2	2.40	0.54
1:A:757:CYS:HA	1:A:760:LEU:HB2	1.90	0.54
1:B:373:THR:HB	1:B:375:LYS:NZ	2.22	0.54
1:A:408:ALA:HB3	1:A:411:GLN:HG3	1.89	0.54
1:A:445:ASN:OD1	1:A:447:ASN:ND2	2.40	0.54
1:C:430:VAL:HG12	1:C:509:VAL:HG12	1.90	0.54
1:C:518:PRO:HG3	1:C:561:GLN:HG3	1.88	0.54
1:C:877:GLY:O	1:C:881:SER:OG	2.25	0.54
1:C:91:TYR:OH	1:C:191:GLU:OE2	2.25	0.54
1:A:767:ILE:HD11	1:A:1009:LEU:HD23	1.90	0.53
1:C:122:ASN:OD1	1:C:123:ALA:N	2.33	0.53
2:b:2:NAG:H83	2:b:2:NAG:H3	1.88	0.53
1:B:893:ILE:HD12	1:B:894:PRO:HD2	1.90	0.53
1:C:986:ALA:O	1:C:990:ILE:HG12	2.09	0.53
1:B:783:LYS:HG3	1:B:784:GLN:HG3	1.89	0.53
1:C:143:VAL:HG12	1:C:154:GLU:HG3	1.89	0.53
1:C:499:GLY:O	1:C:503:GLN:NE2	2.40	0.53
1:B:421:LYS:HZ3	1:B:458:LEU:HB2	1.72	0.53
1:A:203:ILE:HB	1:A:227:VAL:HG12	1.91	0.52
1:B:374:PHE:HE1	1:B:381:PRO:HB3	1.73	0.52
1:B:354:ARG:NH1	1:C:230:PRO:O	2.42	0.52
1:A:65:PHE:O	1:A:261:ALA:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:HG12	1:B:217:PRO:HG3	1.91	0.52
1:C:292:PRO:O	1:C:296:THR:HG23	2.09	0.52
1:C:723:ILE:HG13	1:C:1058:VAL:HG22	1.92	0.52
1:B:491:SER:OG	1:B:492:TYR:N	2.41	0.52
1:C:799:PHE:HD1	1:C:802:ILE:HD11	1.74	0.52
1:B:355:ILE:HB	1:B:392:VAL:HB	1.92	0.52
1:B:1083:LYS:HD2	1:B:1119:VAL:HG21	1.90	0.52
1:B:660:ASP:OD1	1:B:660:ASP:N	2.42	0.52
1:B:574:ARG:HB3	1:B:581:ILE:HG22	1.91	0.52
1:C:565:ASP:OD1	1:C:566:ILE:N	2.41	0.52
1:C:153:MET:N	1:C:153:MET:SD	2.83	0.51
1:C:424:ASP:OD1	1:C:425:ASP:N	2.43	0.51
1:A:109:THR:OG1	1:A:111:ASP:OD1	2.28	0.51
1:B:723:ILE:HG12	1:B:1058:VAL:HG22	1.91	0.51
1:A:719:VAL:HG22	1:A:1062:VAL:HG22	1.92	0.51
1:A:129:LYS:HD3	1:A:133:PHE:HZ	1.75	0.51
1:A:339:PHE:HB2	2:H:1:NAG:H82	1.91	0.51
1:B:373:THR:OG1	1:B:432:ALA:HB3	2.10	0.51
1:A:739:ILE:HD11	1:A:750:LEU:HD22	1.93	0.51
1:A:164:ASN:OD1	1:A:165:ASN:N	2.41	0.51
1:C:390:THR:OG1	1:C:513:GLU:OE2	2.25	0.51
1:C:414:ASN:OD1	1:C:415:ILE:N	2.44	0.51
1:C:87:ASN:HB2	1:C:266:TYR:HE1	1.75	0.51
1:C:602:SER:OG	1:C:603:ASN:N	2.44	0.51
1:A:354:ARG:NH1	1:A:393:TYR:OH	2.44	0.50
1:B:46:SER:CA	1:B:276:TYR:O	2.58	0.50
1:B:439:ASP:OD1	1:B:448:TYR:OH	2.29	0.50
1:C:457:ASN:OD1	1:C:458:LEU:N	2.39	0.50
1:C:976:ASP:HB3	1:C:980:ARG:HH12	1.77	0.50
1:A:1102:THR:HG22	1:A:1109:PRO:HA	1.93	0.50
1:B:108:THR:O	1:B:237:ARG:NH1	2.44	0.50
1:B:726:VAL:HG22	1:B:1056:GLY:HA2	1.92	0.50
1:B:358:CYS:HB2	1:B:521:VAL:HG23	1.93	0.50
1:C:968:GLY:HA3	1:C:992:ARG:HH21	1.76	0.50
1:C:1101:VAL:HG13	1:C:1112:ILE:HG12	1.93	0.50
1:B:709:ILE:HD11	1:B:1093:VAL:HG12	1.93	0.50
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.93	0.50
1:B:21:ARG:O	1:B:23:GLN:NE2	2.45	0.49
1:B:164:ASN:OD1	1:B:165:ASN:N	2.41	0.49
1:B:100:ILE:HG23	1:B:243:ILE:HD13	1.94	0.49
1:B:143:VAL:HG12	1:B:154:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:LEU:HD23	1:C:282:ILE:HD13	1.92	0.49
1:B:129:LYS:HG2	1:B:169:GLU:HG3	1.93	0.49
1:B:380:SER:N	1:C:980:ARG:O	2.41	0.49
1:C:451:ARG:HH22	1:C:454:ARG:HG3	1.77	0.49
1:C:976:ASP:HB3	1:C:980:ARG:NH1	2.27	0.49
1:A:902:ARG:NH1	1:A:1046:LEU:O	2.43	0.49
1:A:763:ALA:O	1:A:767:ILE:HG12	2.13	0.49
1:C:738:TYR:CE2	1:C:963:LEU:HD11	2.47	0.49
1:A:389:PHE:CD1	1:A:514:LEU:HB2	2.47	0.49
1:C:719:VAL:HG22	1:C:1062:VAL:HG22	1.94	0.48
1:C:325:ARG:NH2	1:C:577:GLN:OE1	2.42	0.48
1:C:373:THR:HB	1:C:432:ALA:HB3	1.96	0.48
1:A:105:ILE:HG13	1:A:241:LEU:HD21	1.94	0.48
1:A:89:GLY:HA3	1:A:267:LEU:HD12	1.96	0.48
1:B:194:PHE:HD1	1:B:203:ILE:HG12	1.79	0.48
1:A:608:LEU:HD12	1:A:647:LEU:HD13	1.96	0.48
1:A:637:SER:OG	1:A:638:ASN:N	2.47	0.48
1:A:985:GLU:O	1:A:989:GLN:HG2	2.13	0.48
1:B:703:ALA:HB2	2:W:2:NAG:H62	1.96	0.48
1:C:806:PRO:O	1:C:811:LYS:NZ	2.43	0.48
1:B:983:PRO:N	1:B:984:PRO:HD2	2.29	0.47
1:A:1087:PRO:HD3	1:A:1092:PHE:HE2	1.78	0.47
1:B:402:ASP:OD1	1:B:402:ASP:N	2.45	0.47
1:A:730:LYS:HE3	1:A:768:ALA:HB1	1.97	0.47
1:C:408:ALA:HB3	1:C:411:GLN:HG3	1.97	0.47
1:A:104:TRP:HB3	1:A:106:PHE:HE1	1.79	0.47
1:C:1025:LYS:NZ	1:C:1039:PHE:O	2.48	0.47
1:B:342:THR:O	1:B:506:ARG:NH2	2.47	0.47
1:A:1040:CYS:HB2	1:A:1061:HIS:CE1	2.49	0.47
1:A:452:LEU:N	1:A:488:PRO:O	2.44	0.47
1:A:1132:ASN:OD1	1:A:1133:THR:N	2.38	0.47
1:B:83:VAL:HG11	1:B:237:ARG:HH21	1.80	0.47
1:C:102:ARG:NH2	1:C:122:ASN:O	2.48	0.47
1:C:82:PRO:O	1:C:239:GLN:NE2	2.47	0.47
1:C:106:PHE:HB3	1:C:235:ILE:HG21	1.97	0.47
1:B:107:GLY:HA2	1:B:235:ILE:HG22	1.95	0.47
1:B:408:ALA:HB3	1:B:411:GLN:HG3	1.96	0.47
1:C:335:PHE:HE1	1:C:355:ILE:HD13	1.80	0.46
2:E:1:NAG:H4	2:E:2:NAG:H2	1.68	0.46
1:A:498:TYR:HD2	1:A:502:TYR:HB3	1.79	0.46
1:B:88:ASP:OD1	1:B:89:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ASN:HD21	1:B:451:ARG:H	1.64	0.46
1:C:400:ARG:NH1	1:C:502:TYR:HA	2.30	0.46
1:A:793:ASP:N	1:A:793:ASP:OD1	2.48	0.46
1:A:578:THR:OG1	1:A:580:GLU:OE2	2.33	0.46
1:C:46:SER:CA	1:C:276:TYR:O	2.62	0.46
1:C:350:TRP:H	1:C:350:TRP:CD1	2.33	0.46
1:C:1102:THR:HG22	1:C:1109:PRO:HA	1.97	0.46
1:B:799:PHE:HD1	1:B:802:ILE:HD11	1.80	0.46
1:C:423:PRO:HG2	1:C:426:PHE:HB2	1.98	0.46
1:A:891:LEU:HD21	1:C:1069:GLU:HG2	1.97	0.46
1:B:421:LYS:HE2	1:B:457:ASN:HB3	1.97	0.46
1:A:928:ILE:O	1:A:931:ILE:HG22	2.16	0.46
1:B:374:PHE:CE1	1:B:381:PRO:HB3	2.51	0.46
1:B:1046:LEU:HB2	1:B:1062:VAL:O	2.16	0.46
1:B:451:ARG:HG3	1:B:488:PRO:HB2	1.97	0.46
1:C:981:LEU:HD12	1:C:985:GLU:HG3	1.97	0.46
1:A:535:CYS:HB2	1:A:587:CYS:HB3	1.73	0.45
1:A:808:LYS:HE3	1:A:808:LYS:HB2	1.79	0.45
1:B:17:ASN:HA	1:B:137:ASN:HD21	1.81	0.45
1:A:418:TYR:HA	1:A:458:LEU:HD23	1.97	0.45
1:B:639:VAL:HG22	1:B:648:ILE:HG12	1.97	0.45
1:B:793:ASP:OD1	1:B:793:ASP:N	2.46	0.45
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.28	0.45
1:C:1100:PHE:HZ	2:g:1:NAG:H62	1.82	0.45
1:B:614:CYS:HB2	1:B:646:CYS:HB3	1.81	0.45
1:C:112:SER:HA	1:C:132:GLU:HB3	1.98	0.45
1:B:65:PHE:O	1:B:261:ALA:HA	2.17	0.45
1:B:1007:GLN:HB3	1:B:1011:ARG:HH12	1.81	0.45
1:C:439:ASP:O	1:C:445:ASN:ND2	2.45	0.45
1:A:388:CYS:HB3	1:A:522:CYS:HB3	1.32	0.45
1:B:773:LYS:NZ	1:B:777:GLU:OE1	2.48	0.45
1:C:326:PHE:HE2	1:C:525:LYS:HD3	1.82	0.45
1:C:481:LYS:HA	1:C:485:CYS:HB2	1.98	0.45
1:C:1126:VAL:HB	1:C:1129:ILE:HD11	1.98	0.45
1:A:1043:GLY:HA2	1:B:887:ALA:HB1	1.99	0.45
1:C:296:THR:HA	1:C:299:THR:HG22	1.99	0.45
1:A:1025:LYS:NZ	1:A:1039:PHE:O	2.50	0.45
1:B:307:LYS:HG3	1:B:597:PRO:HA	1.99	0.45
1:C:304:THR:HA	1:C:599:THR:HG21	1.99	0.45
1:A:659:CYS:HB2	1:A:694:MET:HG2	1.99	0.44
1:B:744:THR:OG1	1:B:745:GLU:OE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:VAL:HG22	1:A:509:VAL:HG22	1.98	0.44
1:A:100:ILE:HG23	1:A:243:ILE:HD13	2.00	0.44
1:B:350:TRP:O	1:B:463:ARG:NH2	2.40	0.44
1:C:326:PHE:O	1:C:577:GLN:NE2	2.50	0.44
1:A:400:ARG:NH1	1:A:501:GLY:O	2.50	0.44
1:A:364:VAL:HG13	1:A:365:LEU:HD12	1.98	0.44
1:B:313:SER:OG	1:B:314:ASN:N	2.50	0.44
1:B:806:PRO:O	1:B:811:LYS:NZ	2.45	0.44
1:C:764:LEU:HD23	1:C:767:ILE:HD11	1.99	0.44
1:A:91:TYR:OH	1:A:191:GLU:OE2	2.27	0.44
1:A:350:TRP:CZ2	1:A:463:ARG:HB2	2.53	0.44
1:B:331:ASN:O	1:B:359:VAL:HG22	2.18	0.44
1:C:131:CYS:HB3	1:C:166:CYS:HB3	1.06	0.44
1:C:718:SER:OG	1:C:1063:THR:OG1	2.36	0.44
1:A:893:ILE:HD12	1:A:894:PRO:HD2	2.00	0.43
1:A:942:LEU:HD23	1:A:945:LEU:HD12	1.99	0.43
1:B:325:ARG:NH1	1:B:530:LEU:HD23	2.33	0.43
1:B:328:ASN:OD1	1:B:329:ILE:N	2.51	0.43
1:B:1047:MET:HE2	1:B:1049:PHE:CZ	2.53	0.43
1:C:118:LEU:HD11	1:C:135:PHE:HZ	1.84	0.43
1:A:374:PHE:CD1	1:A:431:ILE:HG12	2.54	0.43
2:W:1:NAG:O3	2:W:2:NAG:N2	2.51	0.43
1:A:609:TYR:HE2	1:A:648:ILE:HD12	1.83	0.43
1:C:1042:LYS:H	1:C:1063:THR:HG21	1.83	0.43
1:A:390:THR:HA	1:A:519:ALA:HA	2.00	0.43
1:A:818:LEU:HD21	1:A:936:SER:HB2	2.00	0.43
1:C:324:VAL:HG22	1:C:539:ASN:HB3	1.99	0.43
1:C:535:CYS:HB2	1:C:587:CYS:HB3	1.70	0.43
1:C:284:ASP:HB3	1:C:303:PHE:CE2	2.54	0.43
1:C:1087:PRO:HD3	1:C:1092:PHE:HE2	1.83	0.43
1:B:99:ASN:HB2	1:B:102:ARG:HH22	1.84	0.43
1:C:140:PHE:HB3	1:C:242:HIS:HB3	2.01	0.43
1:A:436:ASN:O	1:A:440:SER:OG	2.23	0.43
1:B:526:LYS:NZ	1:B:527:SER:H	2.17	0.43
1:C:100:ILE:HG23	1:C:243:ILE:HD13	2.01	0.43
1:C:935:LEU:HD23	1:C:935:LEU:HA	1.86	0.42
1:A:548:VAL:HG12	1:A:585:THR:O	2.20	0.42
1:A:903:PHE:CD2	1:A:913:LEU:HB2	2.54	0.42
1:A:473:GLY:H	1:A:484:ASN:HB3	1.84	0.42
1:A:709:ILE:HD11	1:A:1093:VAL:HG12	2.00	0.42
1:A:104:TRP:N	1:A:241:LEU:HD23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:HG23	1:B:125:ASN:H	1.84	0.42
1:A:1036:ARG:H	1:A:1036:ARG:HG2	1.60	0.42
1:B:728:MET:HB2	1:B:952:ASN:HD21	1.84	0.42
1:B:131:CYS:HB3	1:B:166:CYS:HB3	1.08	0.42
1:B:373:THR:HB	1:B:375:LYS:HZ3	1.81	0.42
1:B:1047:MET:HE2	1:B:1049:PHE:CE1	2.55	0.42
1:C:1035:LYS:HB3	1:C:1035:LYS:HE3	1.83	0.42
1:A:452:LEU:HD22	1:A:490:GLN:HG3	2.02	0.42
1:B:400:ARG:HB2	1:B:403:GLU:HG3	2.02	0.42
1:C:1040:CYS:HB2	1:C:1061:HIS:CE1	2.55	0.42
1:C:335:PHE:CE1	1:C:355:ILE:HD13	2.55	0.42
1:B:190:ARG:HG2	1:B:207:HIS:CE1	2.55	0.41
1:B:1007:GLN:HB3	1:B:1011:ARG:NH1	2.35	0.41
1:C:371:PHE:HA	1:C:433:TRP:HB3	2.01	0.41
1:C:609:TYR:HB2	1:C:646:CYS:SG	2.60	0.41
1:B:121:ASN:HA	1:B:126:VAL:HG12	2.02	0.41
1:B:596:THR:HB	1:B:605:VAL:HG12	2.01	0.41
1:C:822:LYS:HD2	1:C:822:LYS:HA	1.80	0.41
1:A:99:ASN:HB3	1:A:102:ARG:NH2	2.35	0.41
1:B:439:ASP:OD2	1:B:506:ARG:NE	2.48	0.41
1:C:204:TYR:CD1	1:C:225:PRO:HA	2.55	0.41
1:A:736:THR:O	1:A:740:CYS:HB2	2.21	0.41
1:B:99:ASN:OD1	1:B:190:ARG:NH2	2.53	0.41
1:B:95:THR:HB	1:B:189:LEU:HD13	2.01	0.41
1:B:455:LYS:HE2	1:B:455:LYS:HB2	1.93	0.41
1:B:745:GLU:OE1	1:B:745:GLU:N	2.47	0.41
1:C:97:LYS:O	1:C:100:ILE:HG12	2.21	0.41
1:B:575:ASP:OD1	1:B:575:ASP:N	2.42	0.41
1:B:696:LEU:HD22	1:C:870:TYR:CZ	2.55	0.41
1:B:982:ASP:C	1:B:984:PRO:HD2	2.45	0.41
1:C:453:PHE:HB3	1:C:470:TYR:CD1	2.55	0.41
1:C:793:ASP:OD1	1:C:793:ASP:N	2.53	0.41
1:A:745:GLU:H	1:A:745:GLU:CD	2.29	0.41
1:C:813:SER:OG	1:C:816:GLU:HG3	2.21	0.41
1:B:103:GLY:C	1:B:241:LEU:HD23	2.46	0.41
1:C:291:ASP:HB2	1:C:292:PRO:HD2	2.03	0.41
1:C:400:ARG:HB2	1:C:492:TYR:CE1	2.56	0.41
1:A:439:ASP:OD1	1:A:448:TYR:OH	2.30	0.41
1:B:143:VAL:HA	1:B:154:GLU:HG2	2.03	0.41
1:C:322:SER:HA	1:C:537:ASN:O	2.20	0.41
1:C:672:GLN:HG2	1:C:688:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:LEU:O	1:A:752:GLN:HG2	2.21	0.40
1:A:17:ASN:OD1	1:A:137:ASN:ND2	2.44	0.40
1:A:204:TYR:CD1	1:A:225:PRO:HA	2.55	0.40
1:A:435:SER:OG	1:A:439:ASP:OD2	2.34	0.40
1:A:450:TYR:HE2	1:A:452:LEU:HD13	1.87	0.40
1:C:113:LYS:HE2	1:C:113:LYS:HB3	1.94	0.40
1:A:122:ASN:OD1	3:A:2002:NAG:N2	2.54	0.40
1:B:535:CYS:HB2	1:B:587:CYS:HB3	1.79	0.40
1:A:964:SER:O	1:A:964:SER:OG	2.30	0.40
1:B:157:PHE:HE1	1:B:160:TYR:HE1	1.70	0.40
1:C:118:LEU:O	1:C:128:ILE:HA	2.21	0.40
1:C:390:THR:HG22	1:C:520:THR:H	1.86	0.40
1:A:96:GLU:HG2	1:A:190:ARG:HD2	2.04	0.40
1:B:390:THR:HG22	1:B:513:GLU:OE2	2.22	0.40
1:B:493:GLY:O	1:B:502:TYR:OH	2.21	0.40
1:C:434:ASN:OD1	1:C:435:SER:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1010/1280 (79%)	971 (96%)	39 (4%)	0	100	100
1	B	1016/1280 (79%)	965 (95%)	51 (5%)	0	100	100
1	C	1014/1280 (79%)	967 (95%)	46 (4%)	1 (0%)	48	79
All	All	3040/3840 (79%)	2903 (96%)	136 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	617	VAL

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	898/1112 (81%)	898 (100%)	0	100	100
1	B	904/1112 (81%)	904 (100%)	0	100	100
1	C	903/1112 (81%)	903 (100%)	0	100	100
All	All	2705/3336 (81%)	2705 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	188	ASN
1	A	391	ASN
1	A	447	ASN
1	A	490	GLN
1	A	533	ASN
1	A	604	GLN
1	A	911	ASN
1	A	1002	GLN
1	B	17	ASN
1	B	115	GLN
1	B	125	ASN
1	B	137	ASN
1	B	218	GLN
1	B	239	GLN
1	B	436	ASN
1	B	771	GLN
1	B	801	GLN
1	B	898	GLN
1	B	910	GLN
1	B	911	ASN
1	B	916	ASN
1	B	952	ASN
1	B	1103	GLN

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Mol	Chain	Res	Type
1	C	134	GLN
1	C	537	ASN
1	C	561	GLN
1	C	761	ASN
1	C	771	GLN
1	C	957	ASN
1	C	999	GLN
1	C	1139	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

62 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.67	1 (7%)	17,19,21	0.88	0
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.63	0
2	NAG	E	1	1,2	14,14,15	0.84	1 (7%)	17,19,21	1.27	1 (5%)
2	NAG	E	2	2	14,14,15	0.42	0	17,19,21	0.41	0
2	NAG	F	1	1,2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	F	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	G	1	1,2	14,14,15	0.64	1 (7%)	17,19,21	1.40	1 (5%)
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.42	0
2	NAG	H	1	1,2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	H	2	2	14,14,15	0.24	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	1	1,2	14,14,15	0.28	0	17,19,21	0.51	0
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	J	1	1,2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	J	2	2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	K	1	1,2	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	K	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	L	1	1,2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	L	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	M	1	1,2	14,14,15	0.28	0	17,19,21	0.52	0
2	NAG	M	2	2	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	N	1	1,2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	N	2	2	14,14,15	0.25	0	17,19,21	0.54	0
2	NAG	O	1	1,2	14,14,15	0.24	0	17,19,21	0.56	0
2	NAG	O	2	2	14,14,15	0.28	0	17,19,21	0.54	0
2	NAG	P	1	1,2	14,14,15	0.82	1 (7%)	17,19,21	1.44	3 (17%)
2	NAG	P	2	2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	Q	1	1,2	14,14,15	0.25	0	17,19,21	0.53	0
2	NAG	Q	2	2	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	R	1	1,2	14,14,15	0.27	0	17,19,21	0.45	0
2	NAG	R	2	2	14,14,15	0.29	0	17,19,21	0.55	0
2	NAG	S	1	1,2	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	S	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	T	1	1,2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	T	2	2	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	U	1	1,2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	U	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	V	1	1,2	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	V	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	W	1	1,2	14,14,15	0.53	0	17,19,21	0.83	1 (5%)
2	NAG	W	2	2	14,14,15	0.21	0	17,19,21	0.56	0
2	NAG	X	1	1,2	14,14,15	0.17	0	17,19,21	0.44	0
2	NAG	X	2	2	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	Y	1	1,2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	Y	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	Z	1	1,2	14,14,15	0.22	0	17,19,21	0.53	0
2	NAG	Z	2	2	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	a	1	1,2	14,14,15	0.30	0	17,19,21	0.55	0
2	NAG	a	2	2	14,14,15	0.67	1 (7%)	17,19,21	0.48	0
2	NAG	b	1	1,2	14,14,15	0.29	0	17,19,21	0.54	0
2	NAG	b	2	2	14,14,15	0.49	0	17,19,21	1.33	2 (11%)
2	NAG	c	1	1,2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	c	2	2	14,14,15	0.22	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	d	1	1,2	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	d	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	e	1	1,2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	e	2	2	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	f	1	1,2	14,14,15	0.43	0	17,19,21	0.72	1 (5%)
2	NAG	f	2	2	14,14,15	0.26	0	17,19,21	0.39	0
2	NAG	g	1	1,2	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	g	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	h	1	1,2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	h	2	2	14,14,15	0.25	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
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	4/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	O	2	2	-	4/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	3/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	V	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	4/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	3/6/23/26	0/1/1/1
2	NAG	a	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	4/6/23/26	0/1/1/1
2	NAG	c	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	2/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	f	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	NAG	g	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	3.02	1.48	1.43
2	P	1	NAG	C1-C2	2.75	1.56	1.52
2	D	1	NAG	O5-C1	-2.31	1.39	1.43
2	a	2	NAG	C1-C2	2.28	1.55	1.52
2	G	1	NAG	O5-C1	2.16	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C1-O5-C5	5.51	119.57	112.19
2	E	1	NAG	C1-O5-C5	5.03	118.93	112.19
2	b	2	NAG	C2-N2-C7	4.58	129.04	122.90
2	P	1	NAG	C2-N2-C7	4.39	128.78	122.90
2	P	1	NAG	C1-O5-C5	2.73	115.84	112.19
2	f	1	NAG	C1-O5-C5	2.43	115.44	112.19
2	W	1	NAG	C1-O5-C5	2.19	115.12	112.19
2	b	2	NAG	C1-C2-N2	2.17	113.86	110.43
2	P	1	NAG	C1-C2-N2	2.11	113.76	110.43

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	X	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Q	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	P	1	NAG	C8-C7-N2-C2
2	P	1	NAG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
2	W	2	NAG	C8-C7-N2-C2
2	W	2	NAG	O7-C7-N2-C2
2	b	2	NAG	C8-C7-N2-C2
2	b	2	NAG	O7-C7-N2-C2
2	h	1	NAG	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	V	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	N	2	NAG	C1-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7
2	Q	1	NAG	C1-C2-N2-C7
2	R	2	NAG	C1-C2-N2-C7
2	Z	1	NAG	C1-C2-N2-C7
2	h	2	NAG	C1-C2-N2-C7

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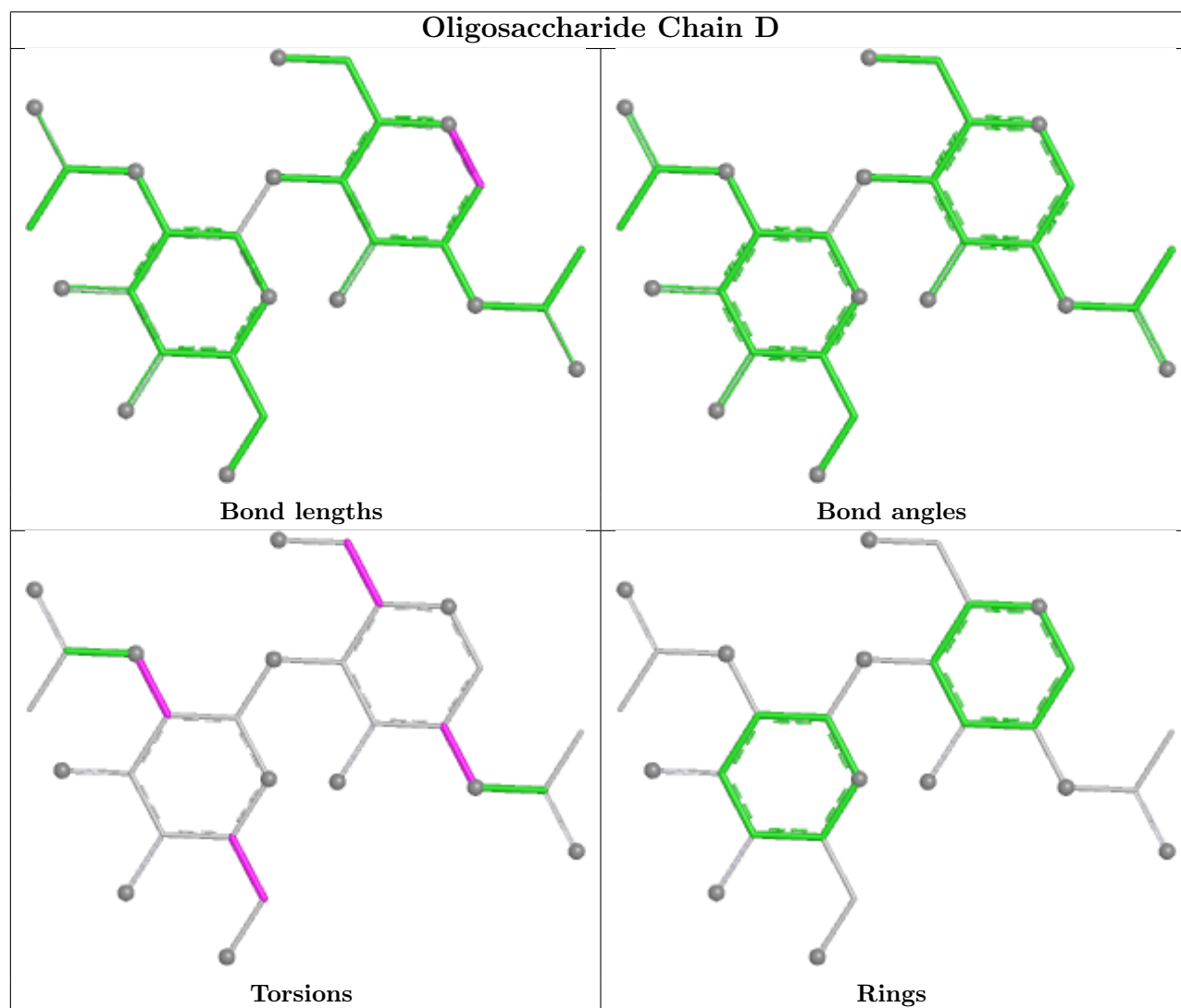
Mol	Chain	Res	Type	Atoms
2	g	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7
2	N	2	NAG	C3-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	P	1	NAG	C3-C2-N2-C7
2	Q	1	NAG	C3-C2-N2-C7
2	R	2	NAG	C3-C2-N2-C7
2	W	1	NAG	C3-C2-N2-C7
2	Z	1	NAG	C3-C2-N2-C7
2	h	2	NAG	C3-C2-N2-C7
2	F	2	NAG	O5-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C1-C2-N2-C7
2	O	1	NAG	C1-C2-N2-C7
2	P	1	NAG	C1-C2-N2-C7
2	W	1	NAG	C1-C2-N2-C7
2	Z	2	NAG	C1-C2-N2-C7
2	b	2	NAG	C1-C2-N2-C7
2	b	2	NAG	C3-C2-N2-C7
2	O	2	NAG	O5-C5-C6-O6

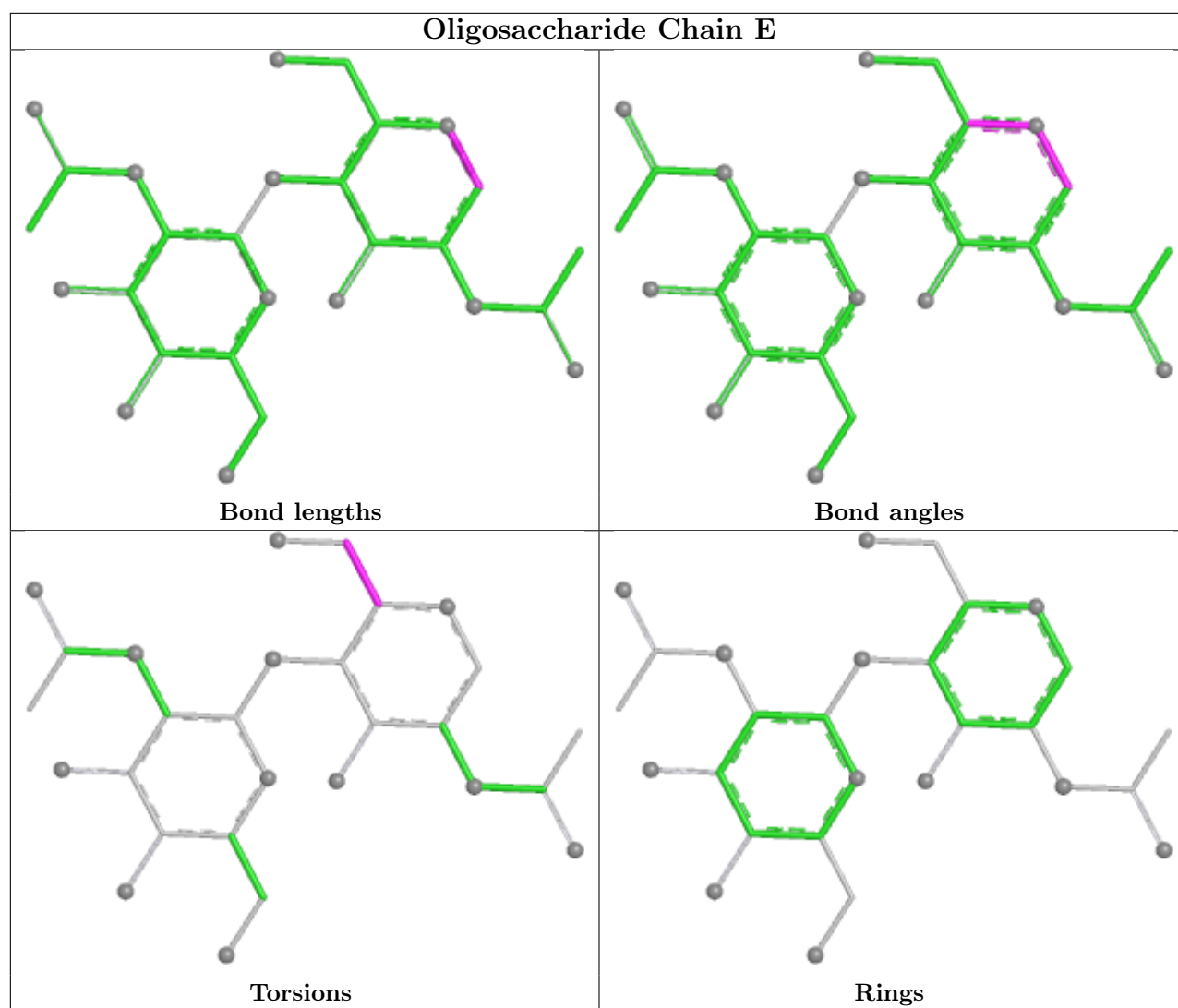
There are no ring outliers.

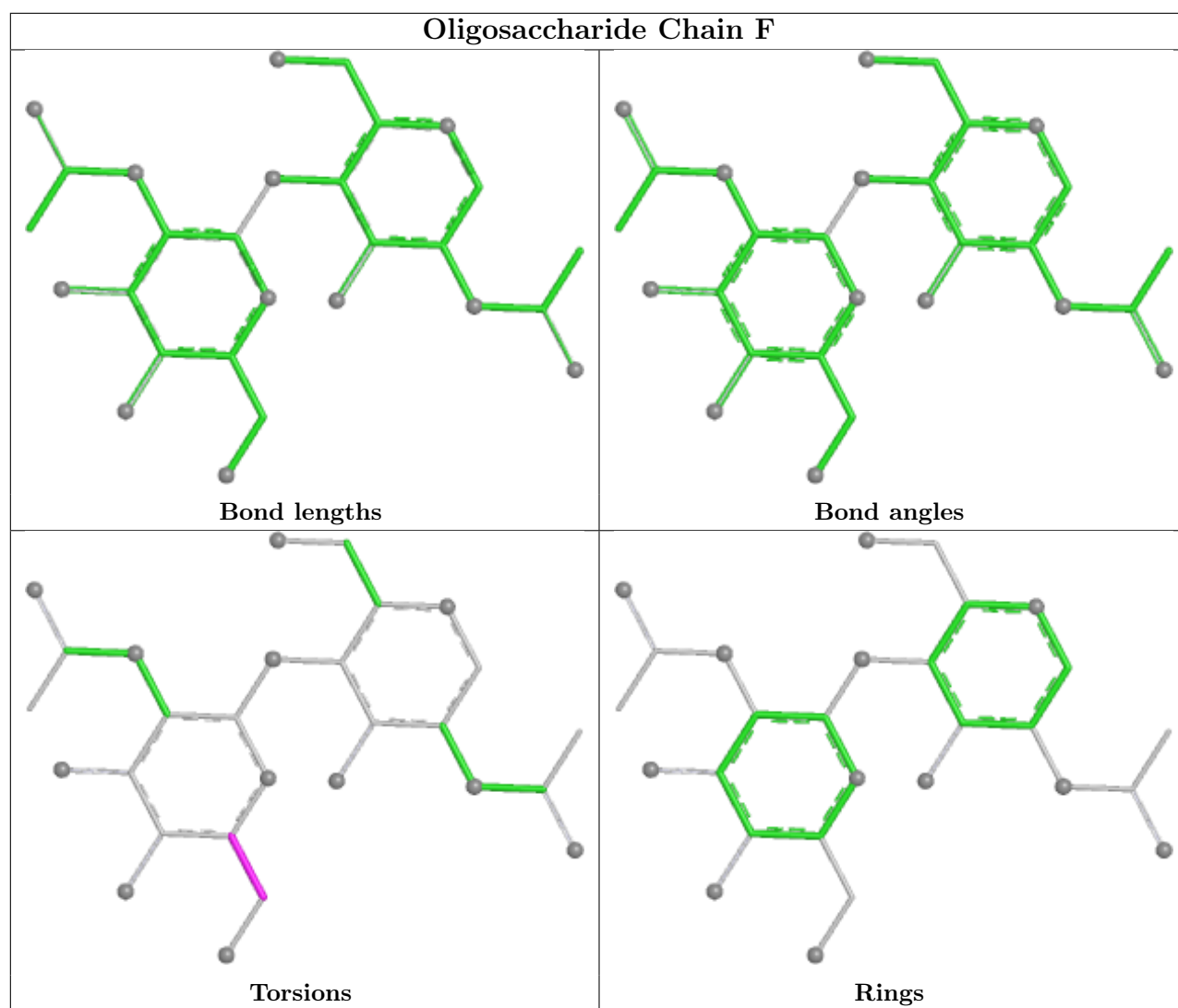
8 monomers are involved in 8 short contacts:

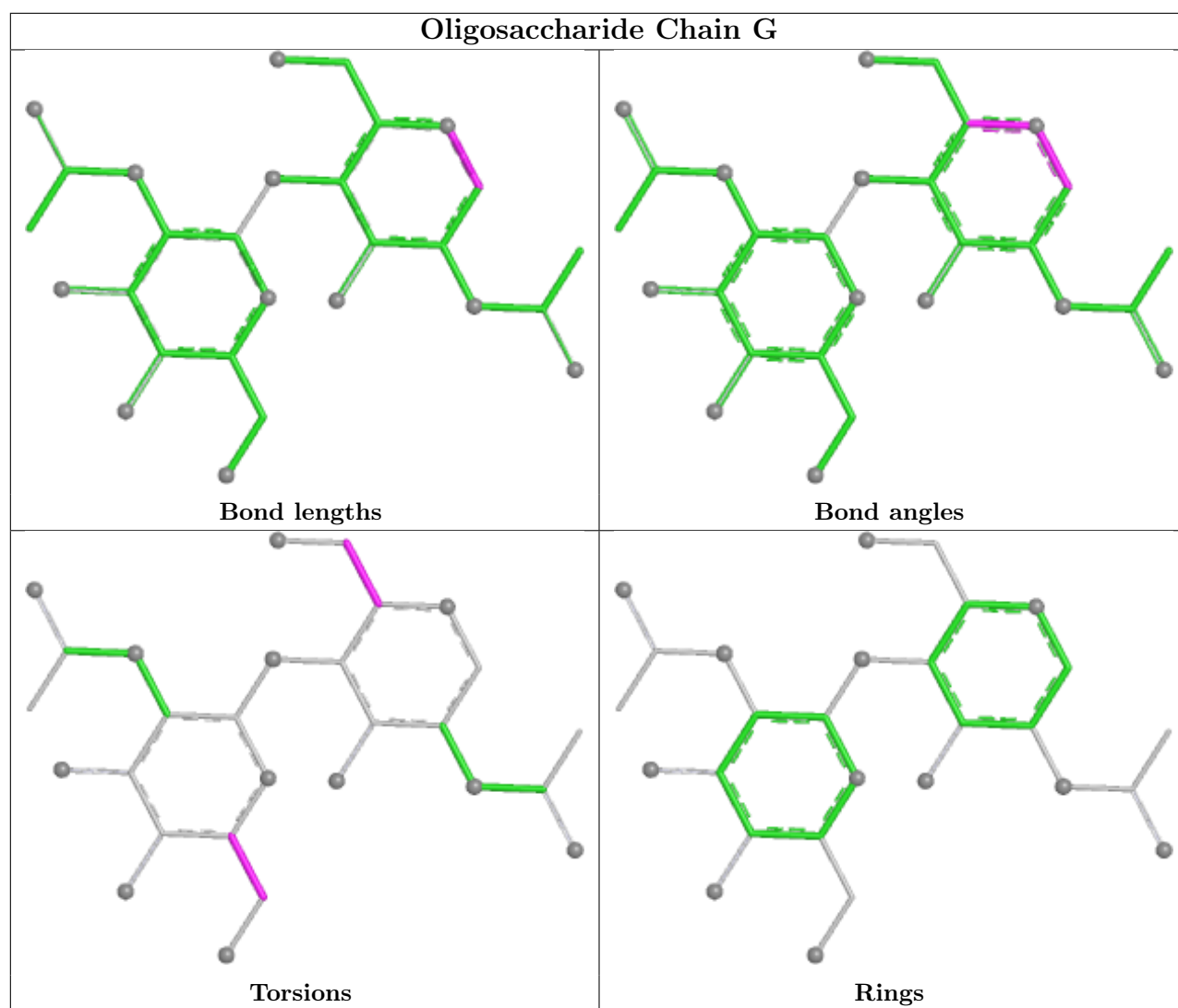
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	1	NAG	1	0
2	E	1	NAG	1	0
2	g	1	NAG	1	0
2	H	1	NAG	1	0
2	E	2	NAG	1	0
2	W	2	NAG	2	0
2	b	2	NAG	1	0
2	P	1	NAG	2	0

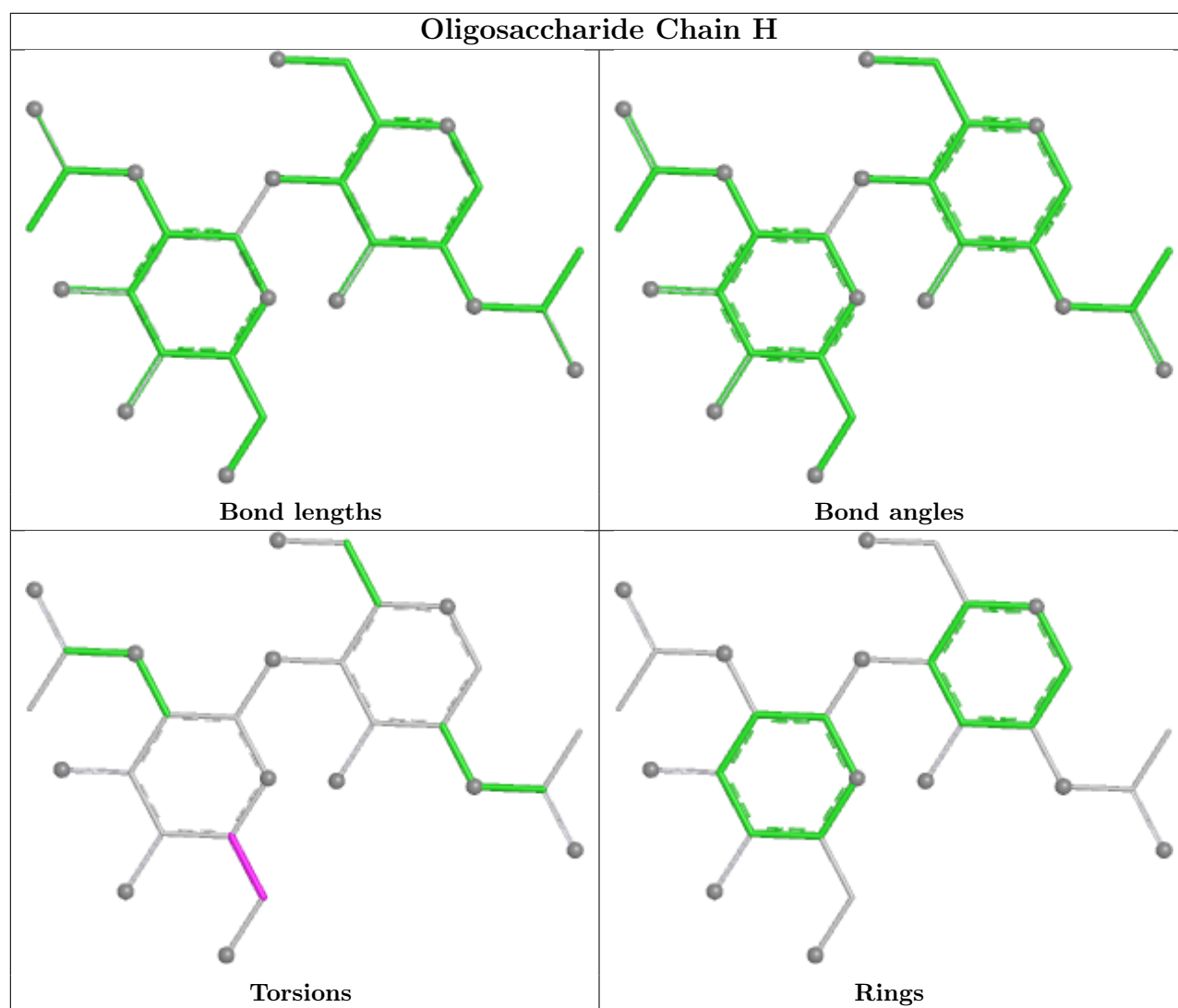
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

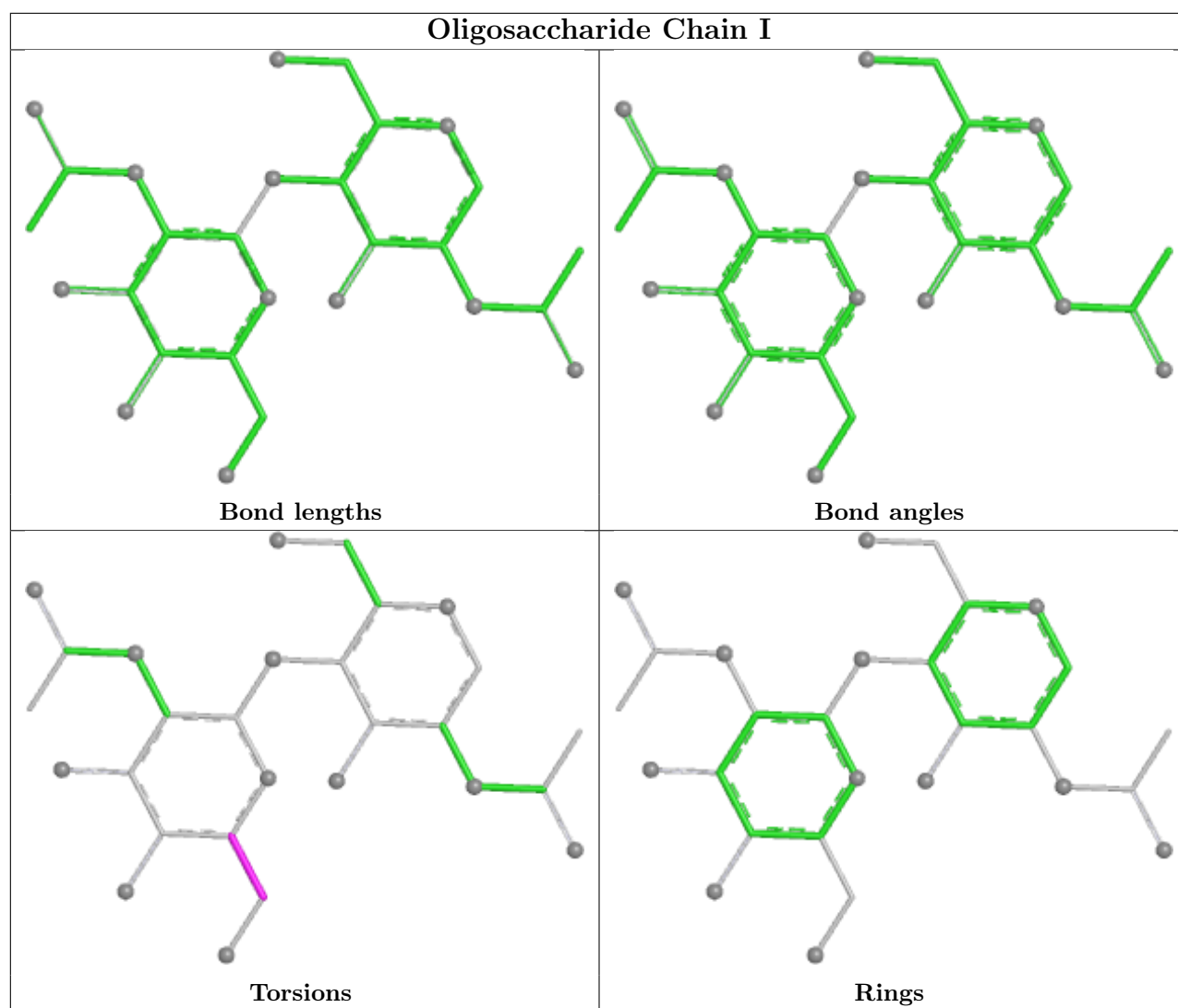


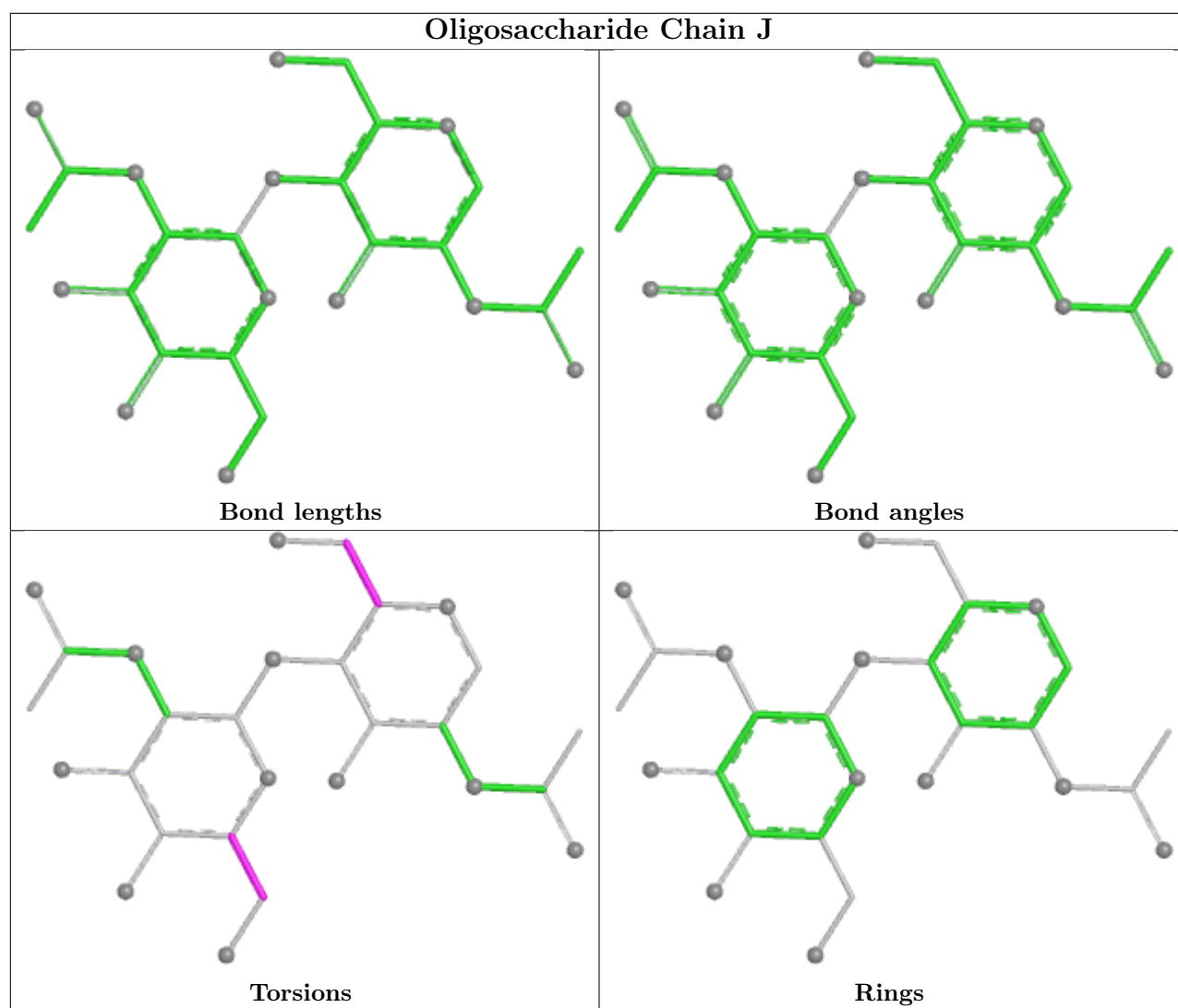


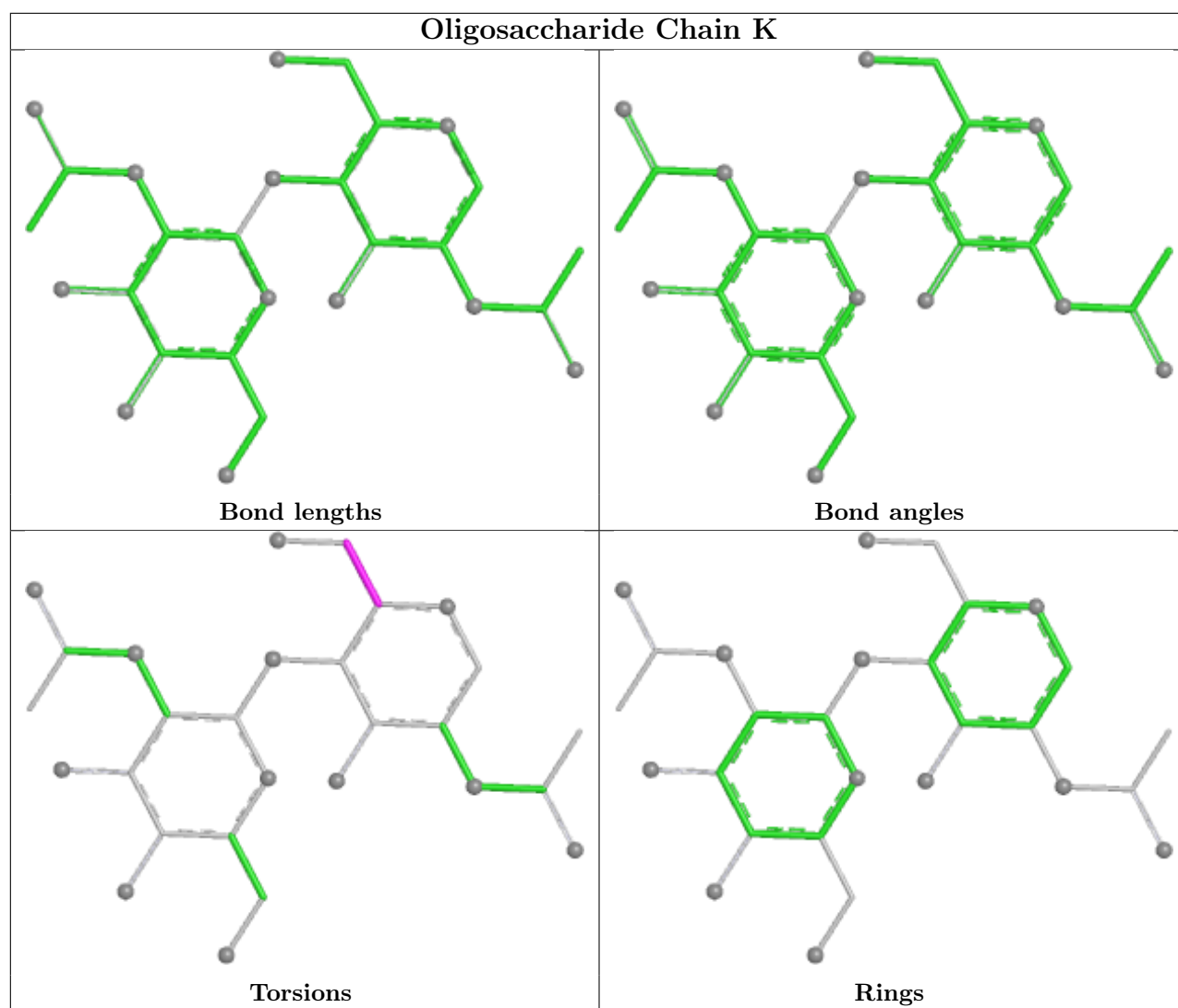


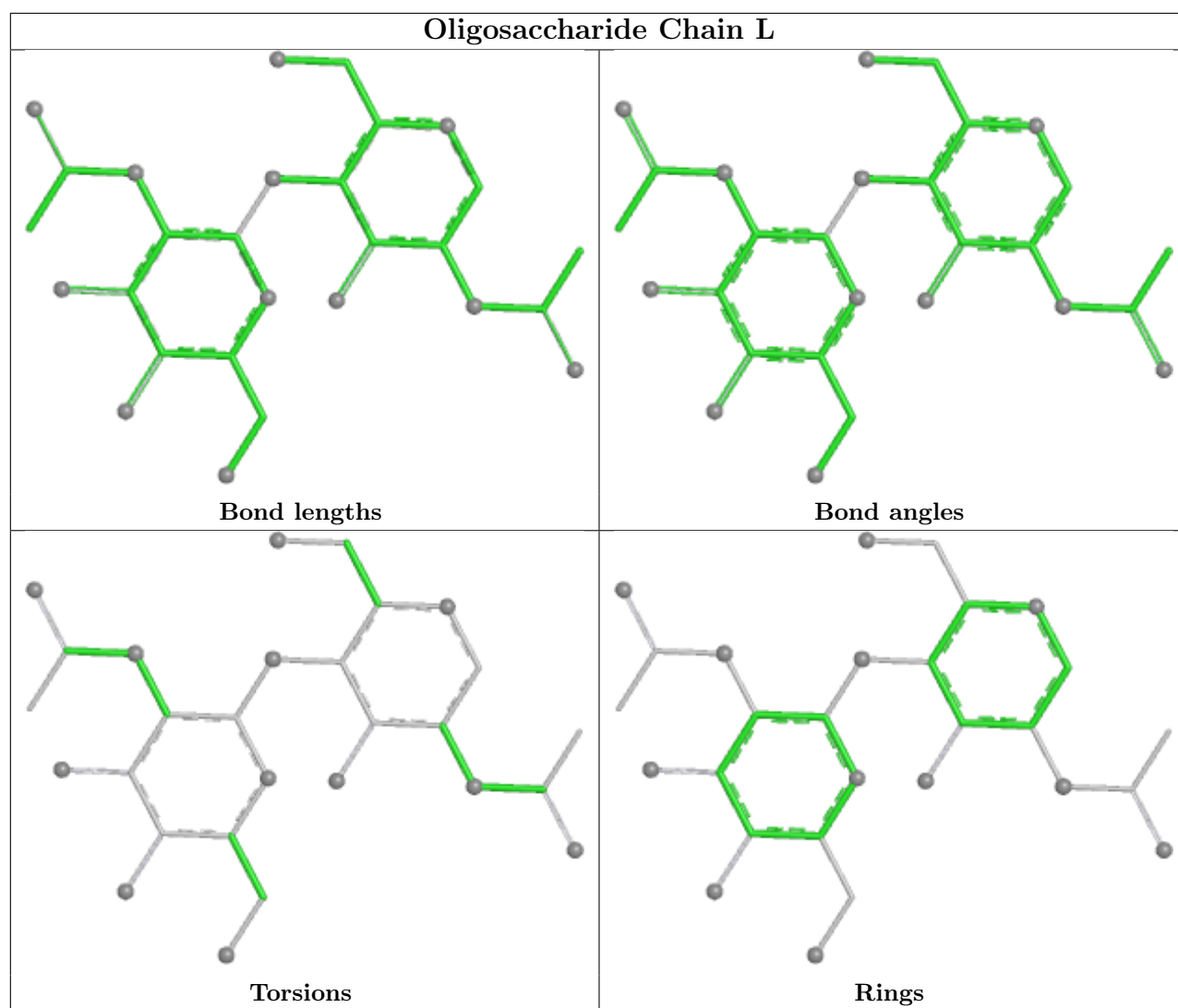


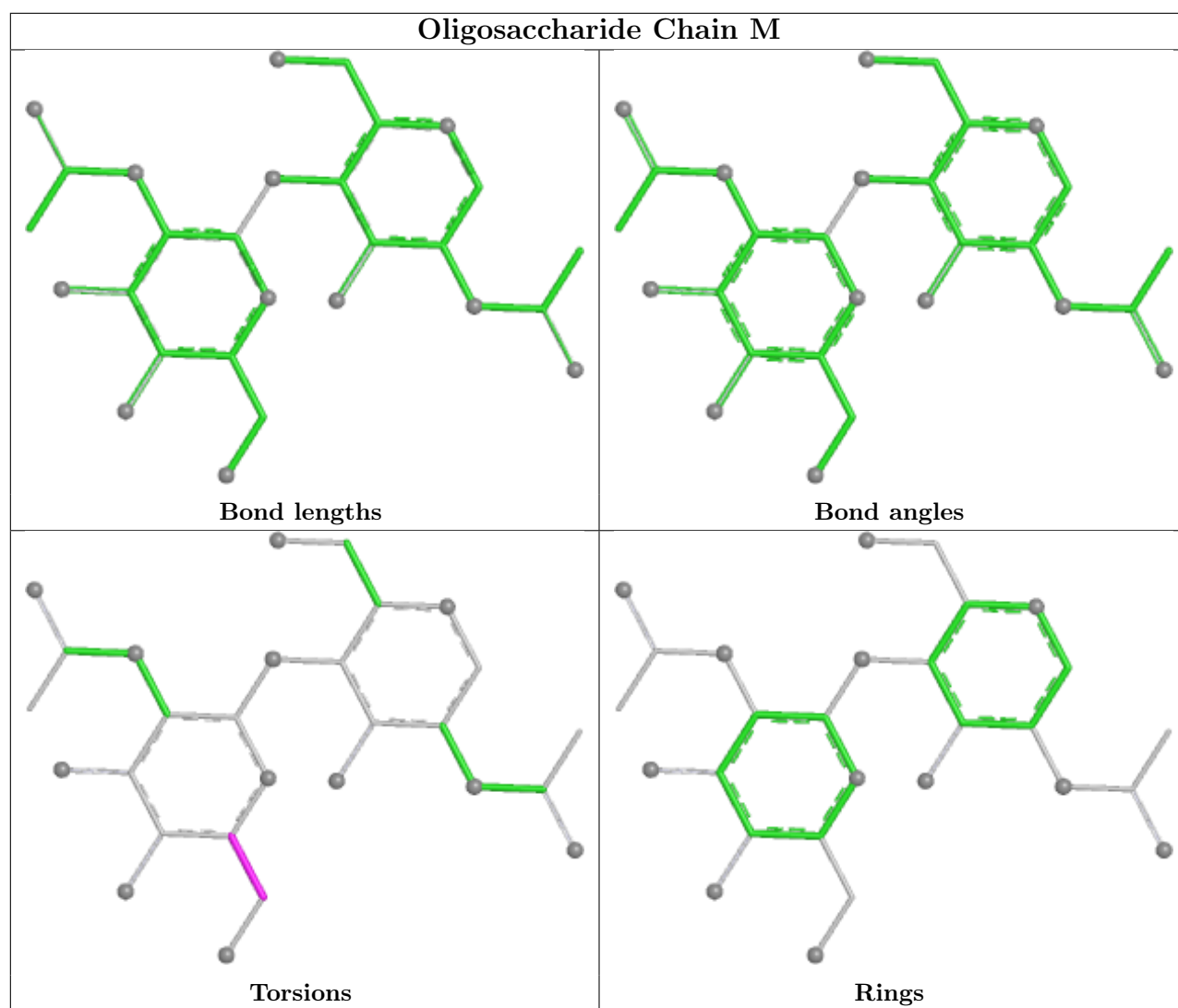


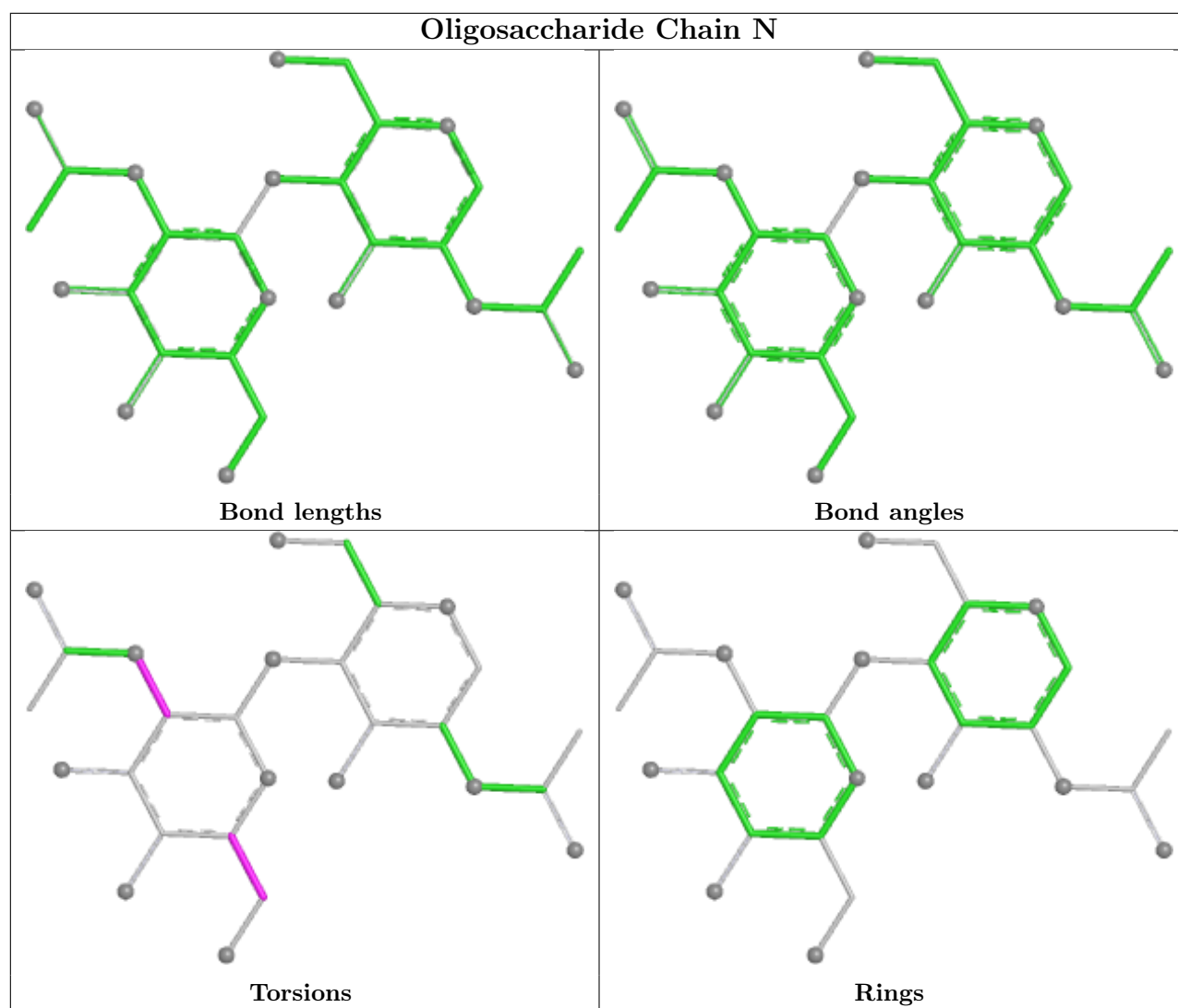


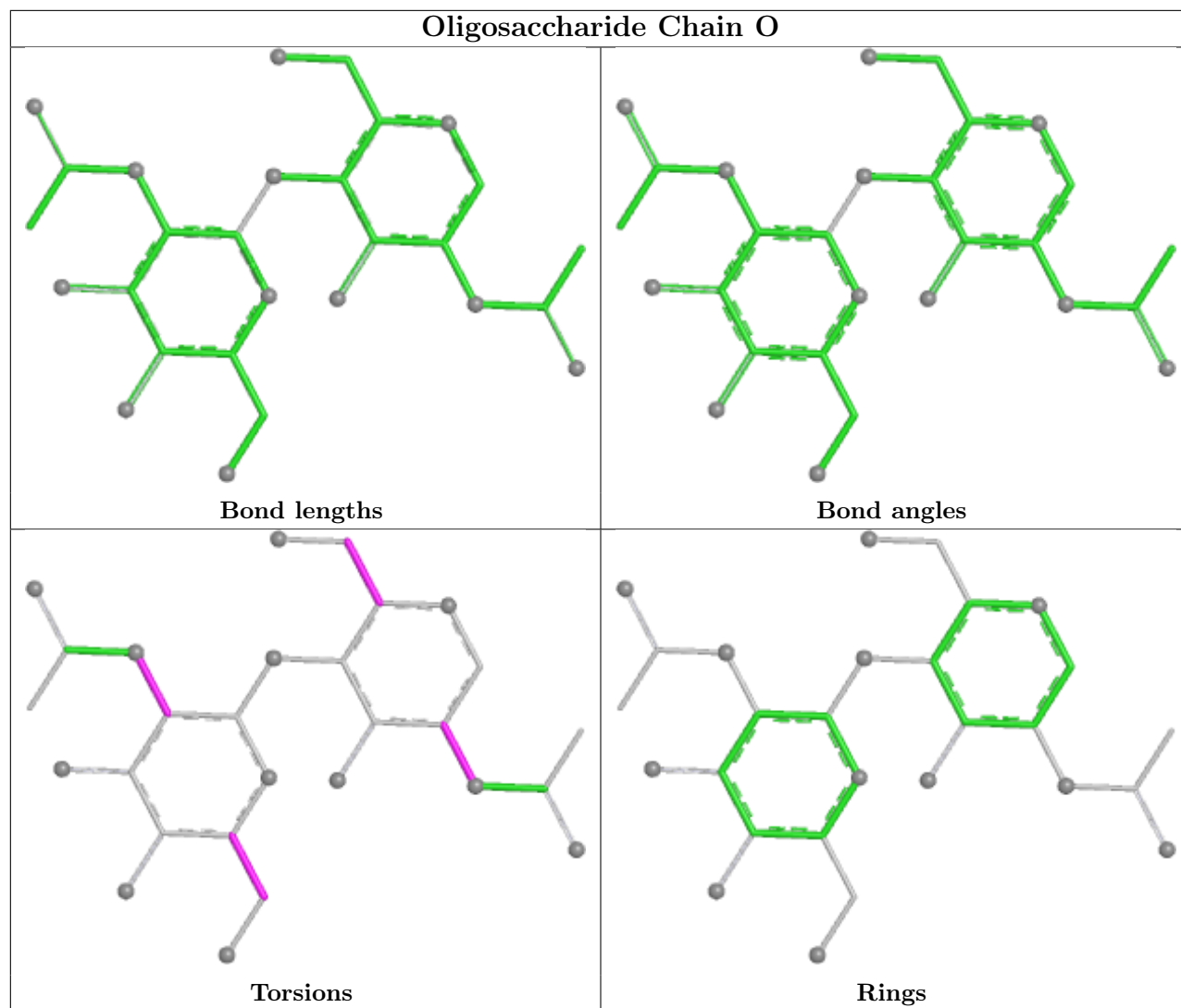


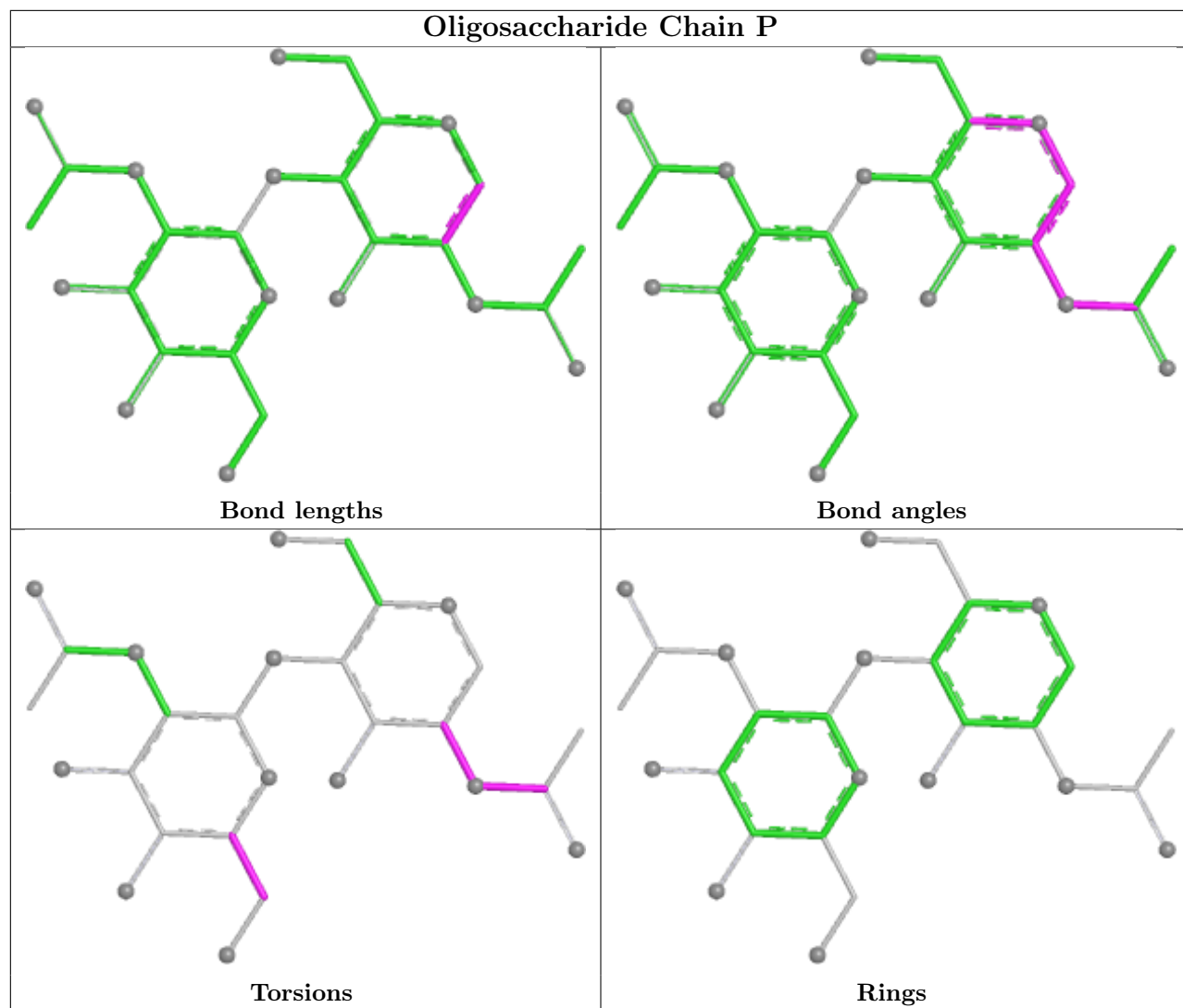


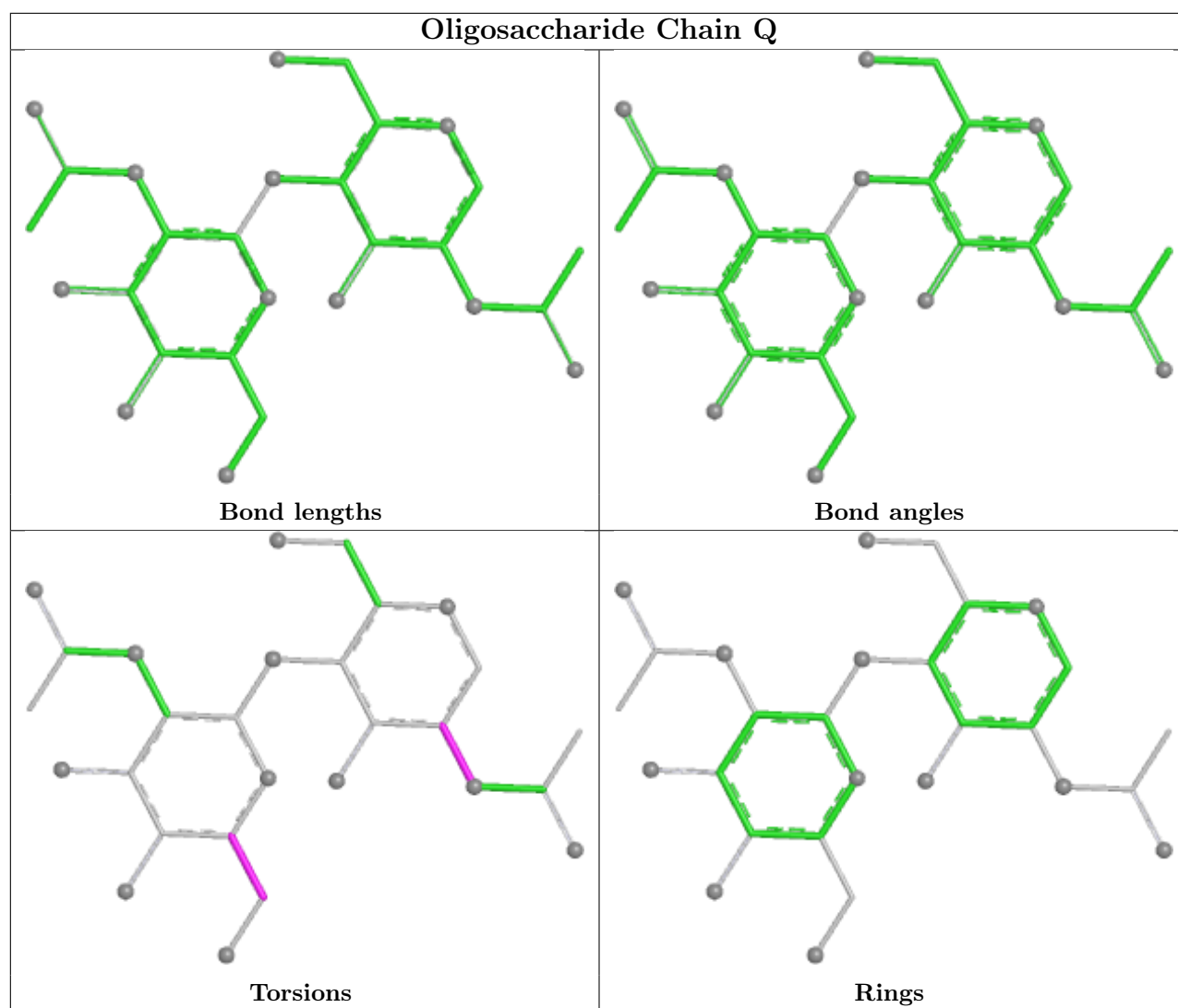


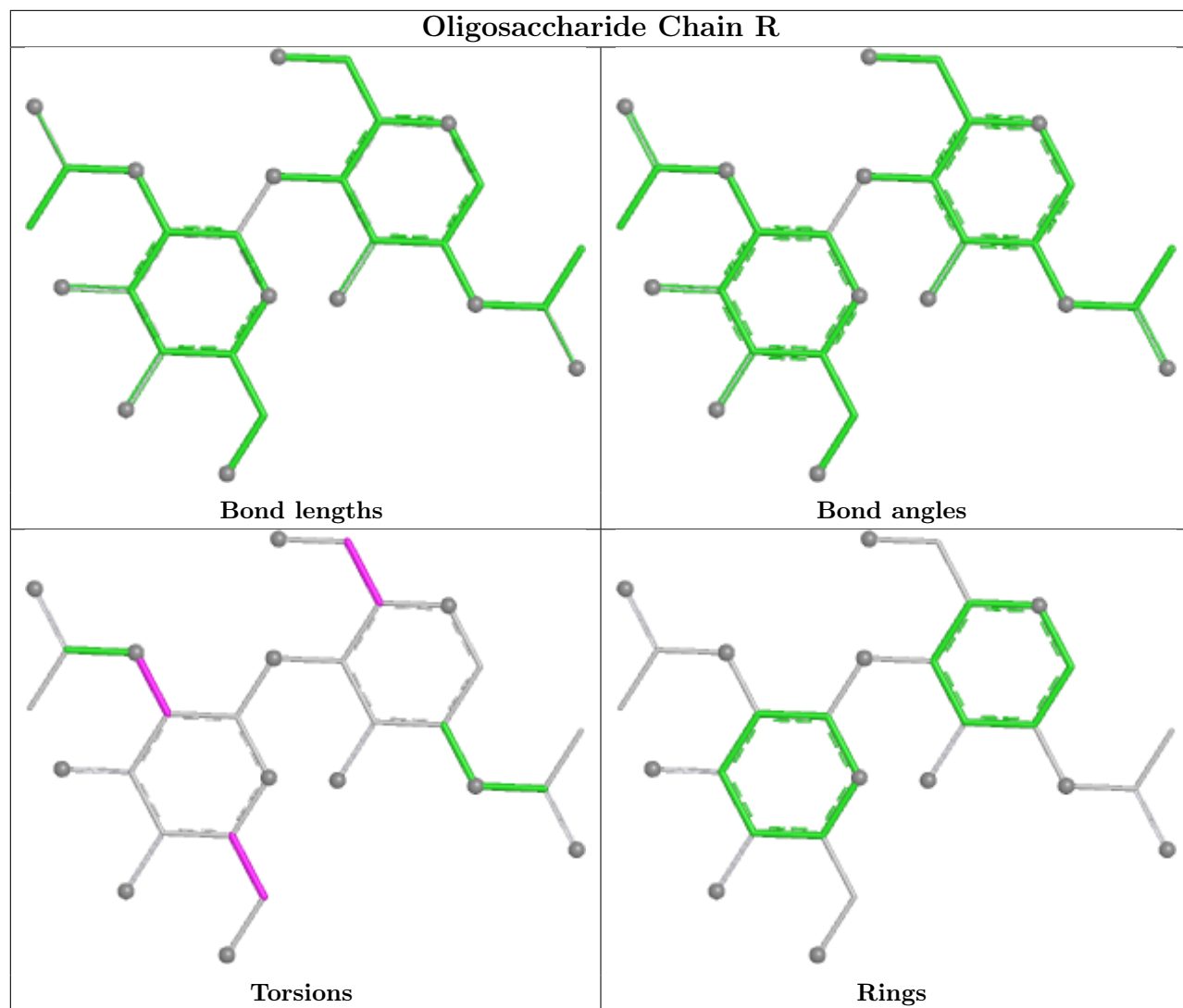


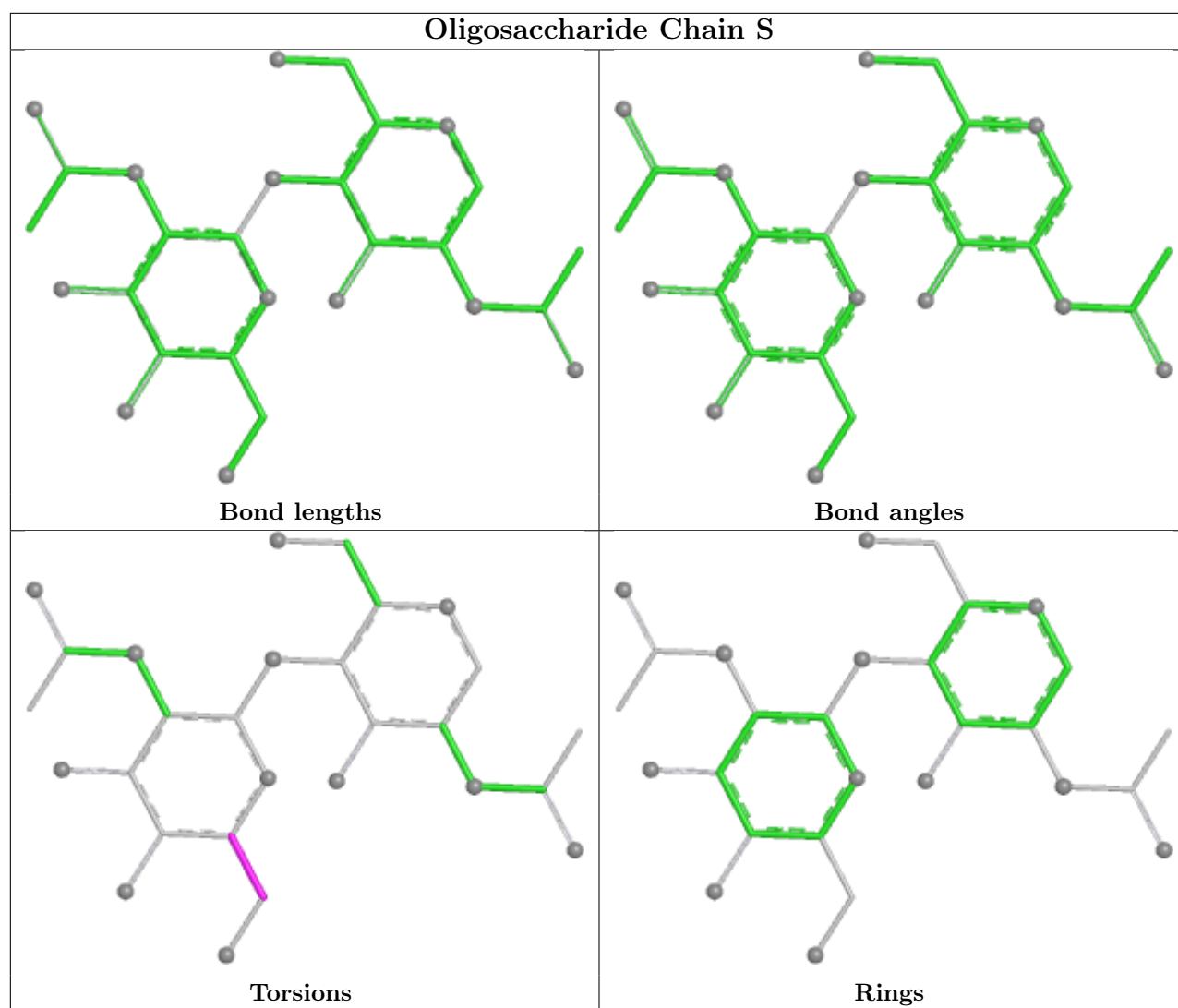


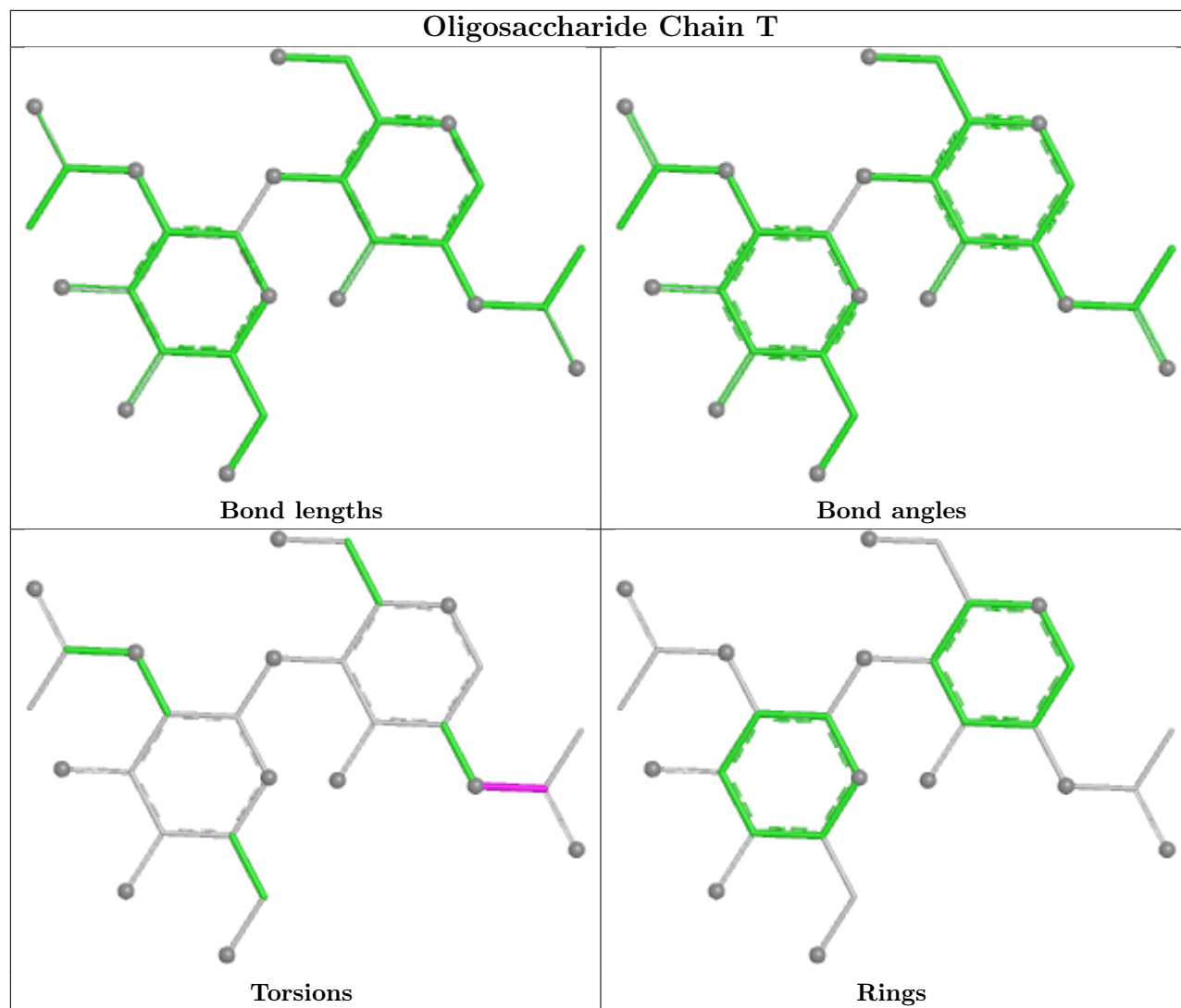


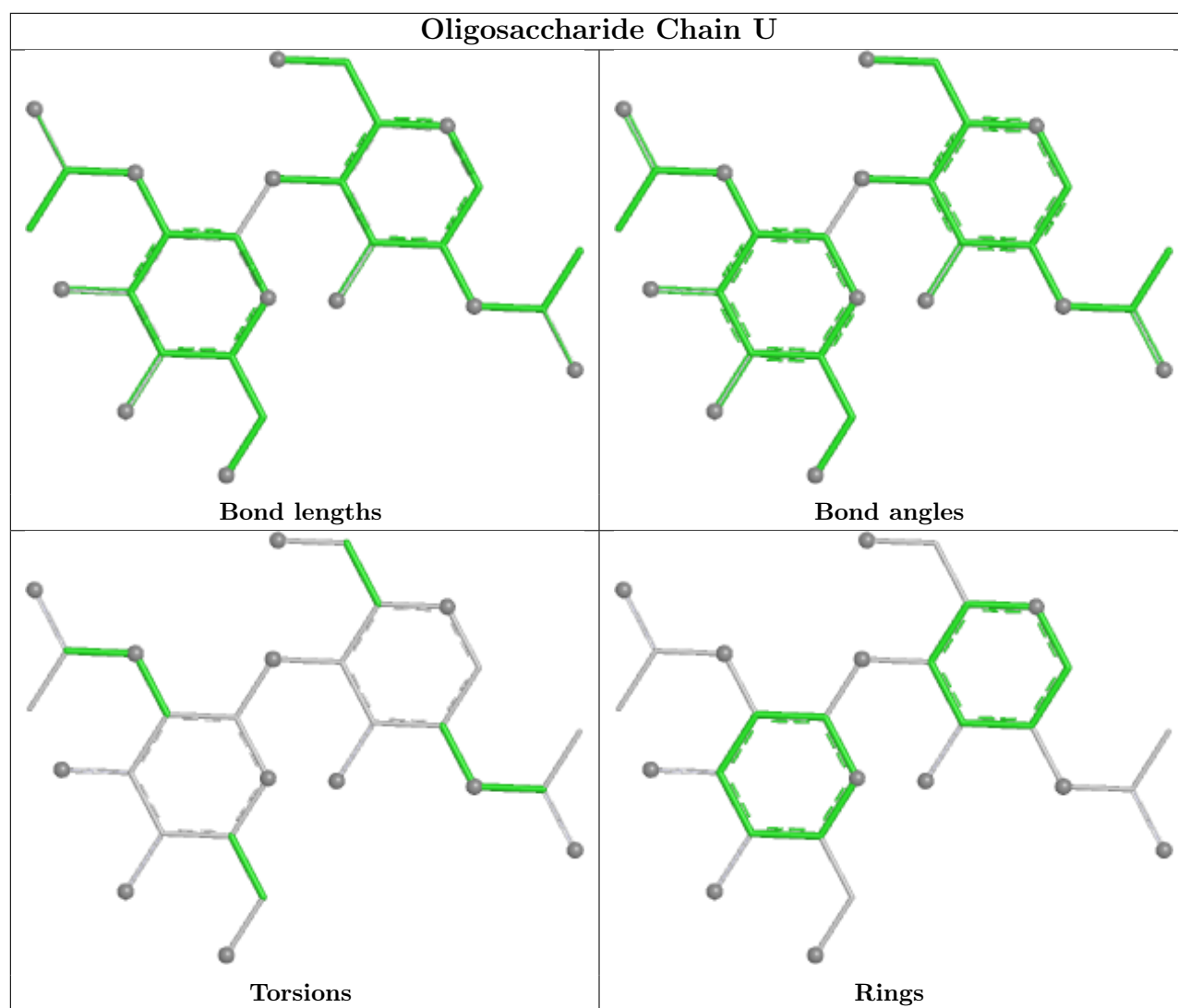


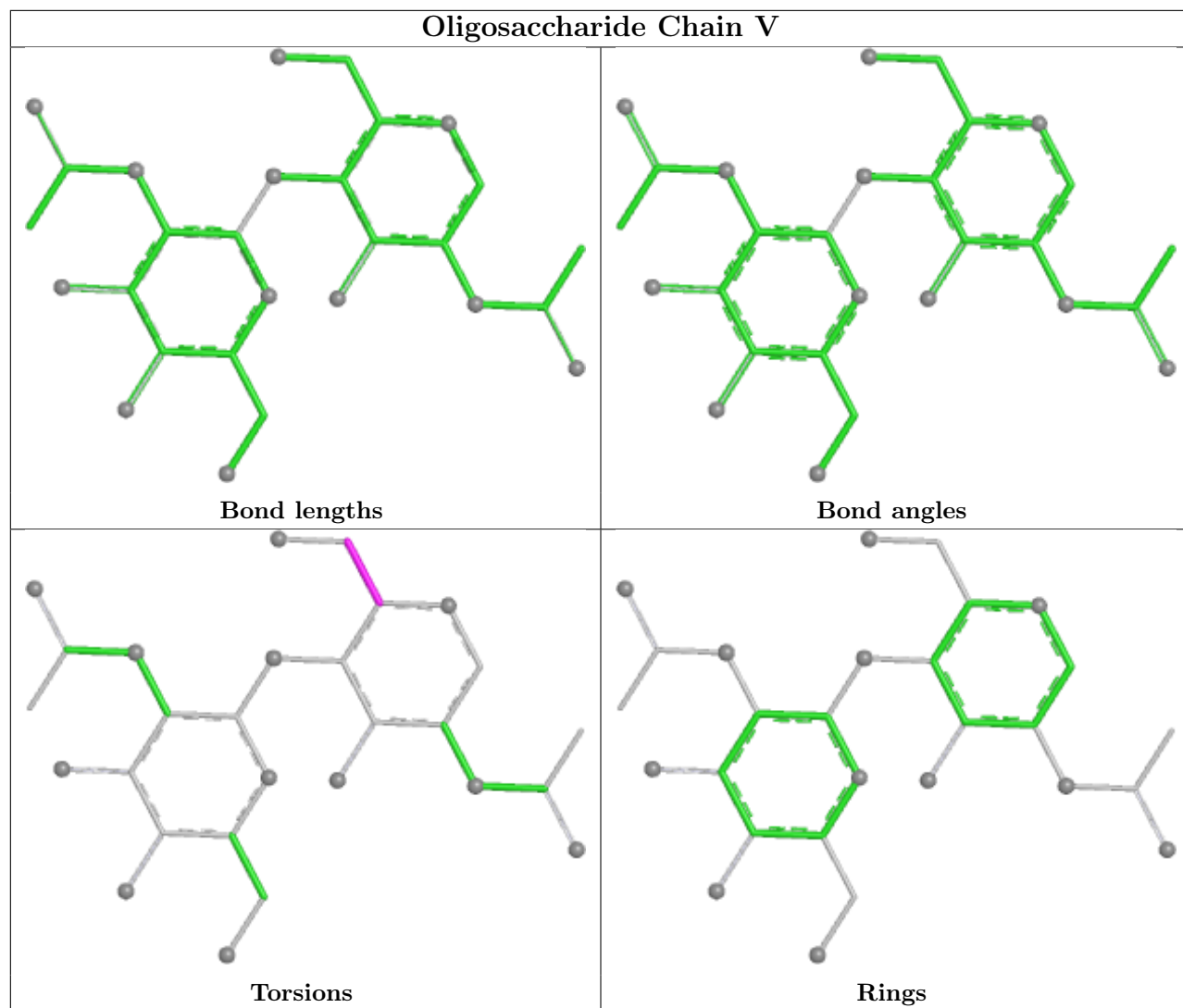


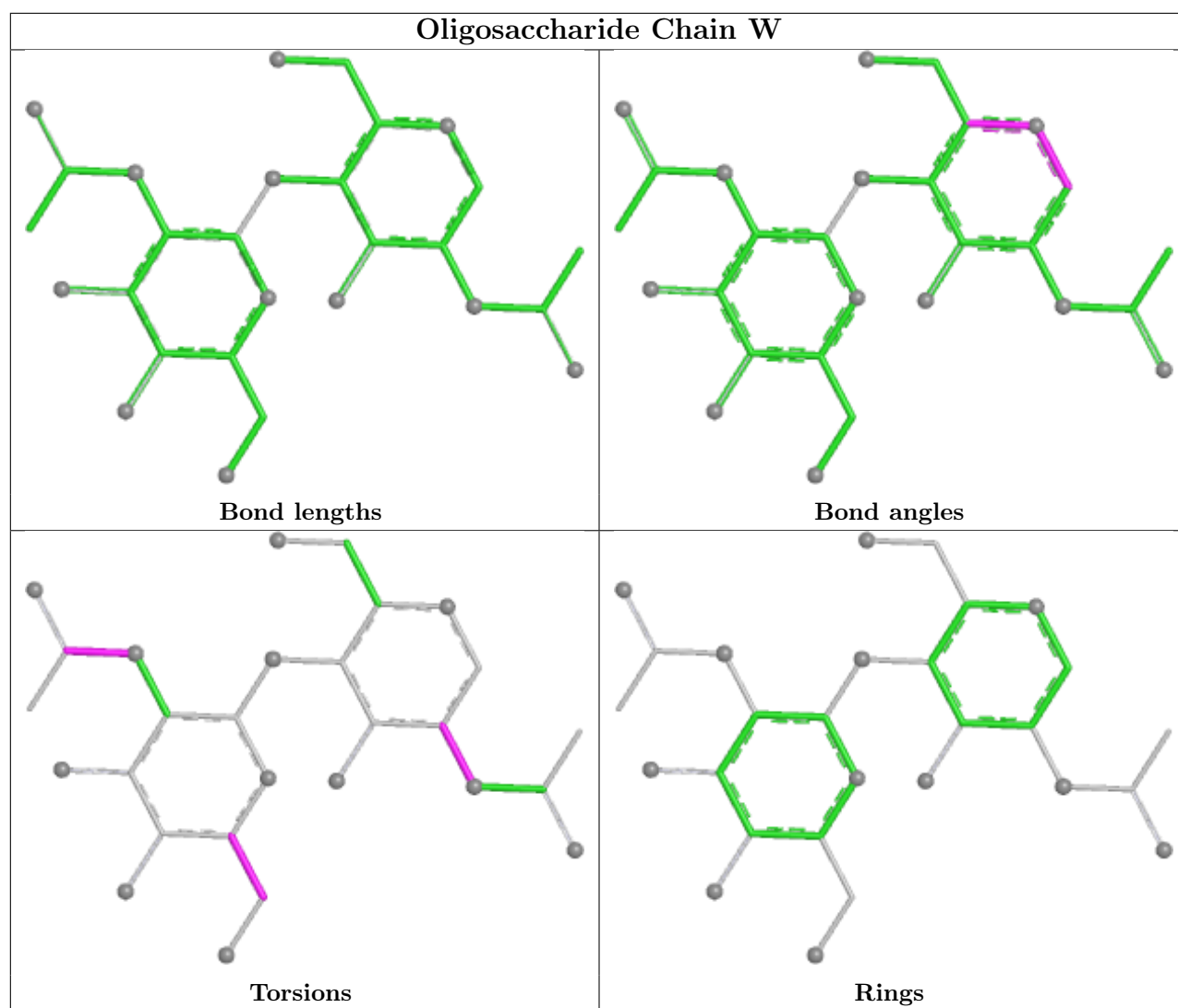


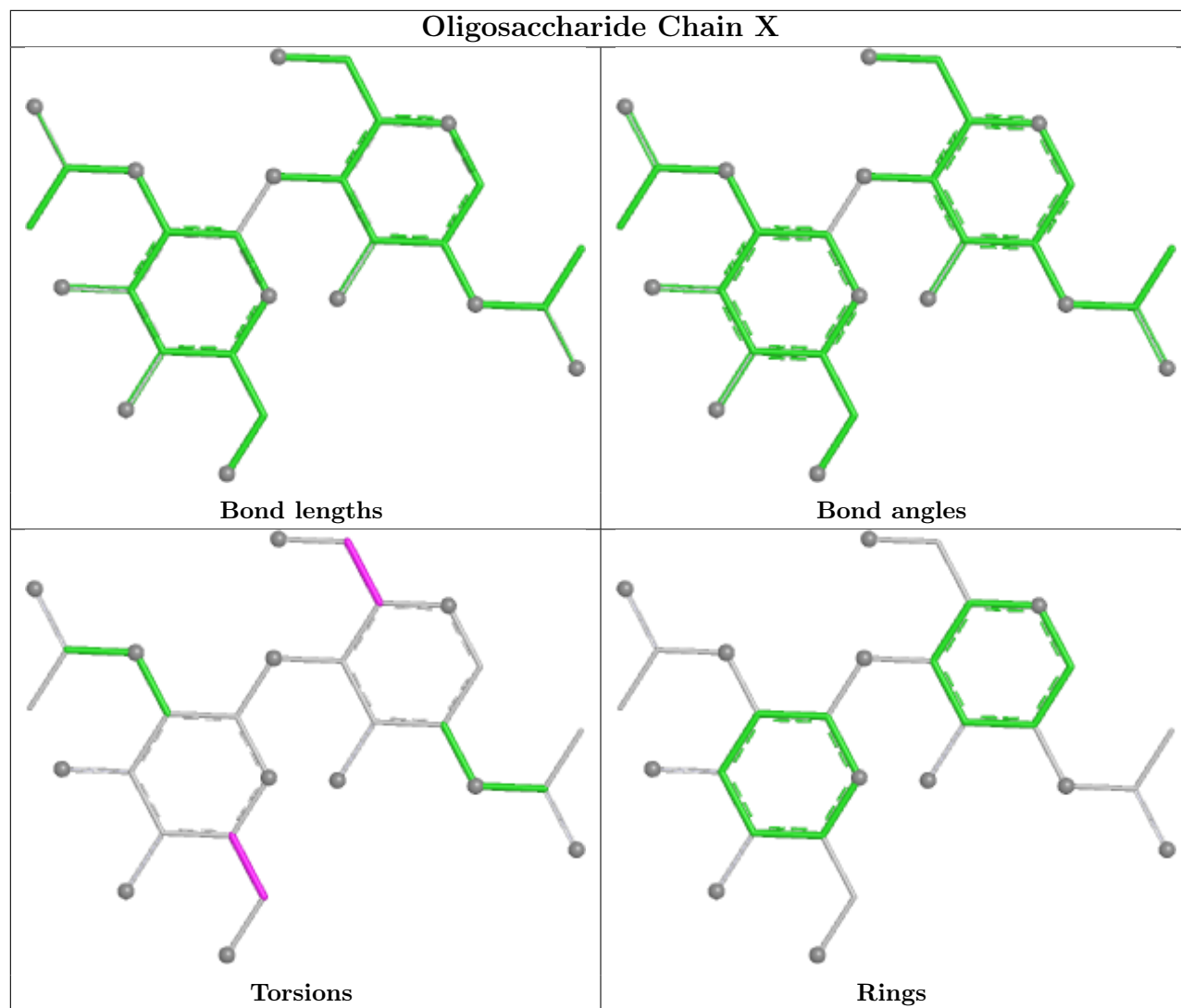


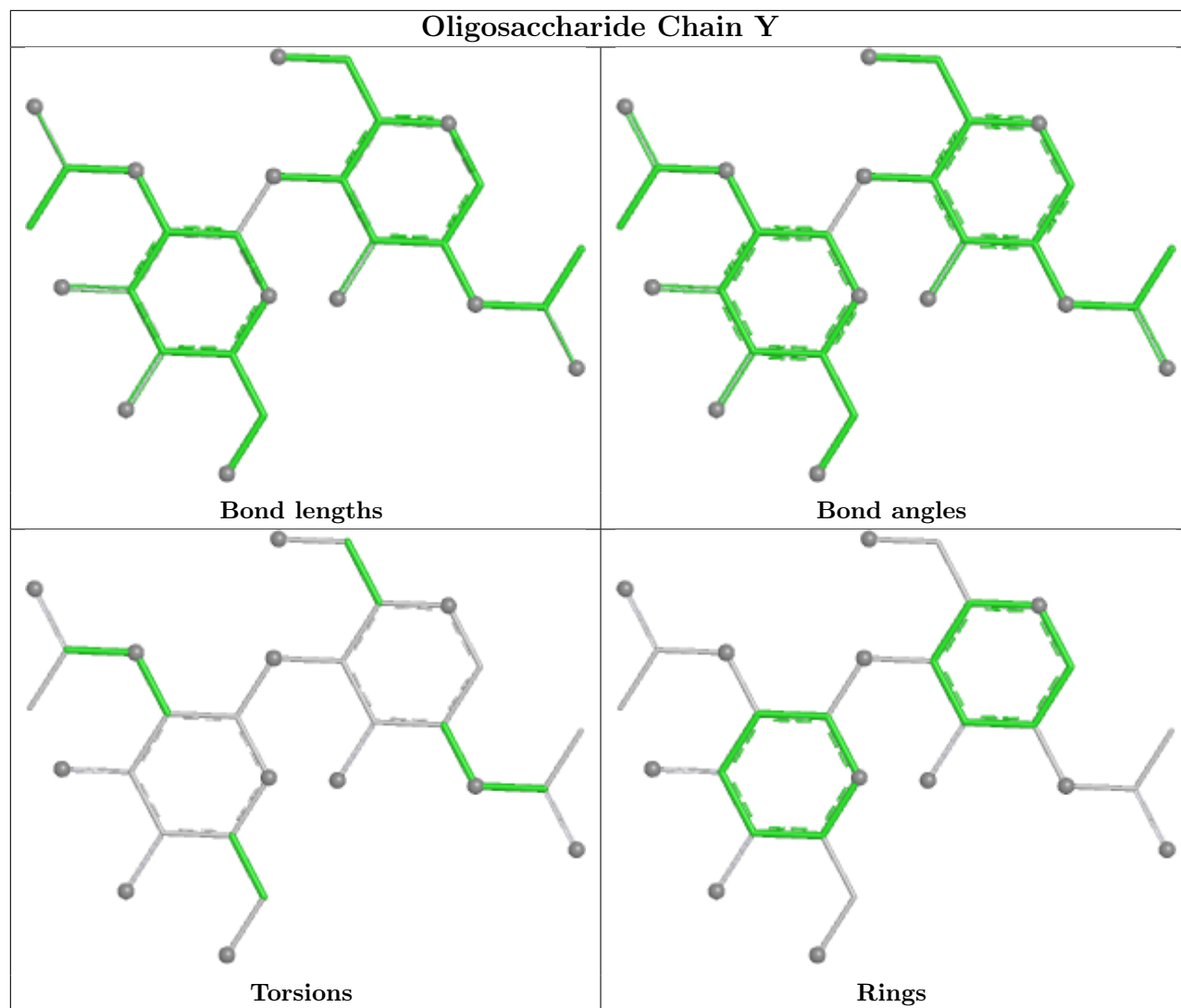


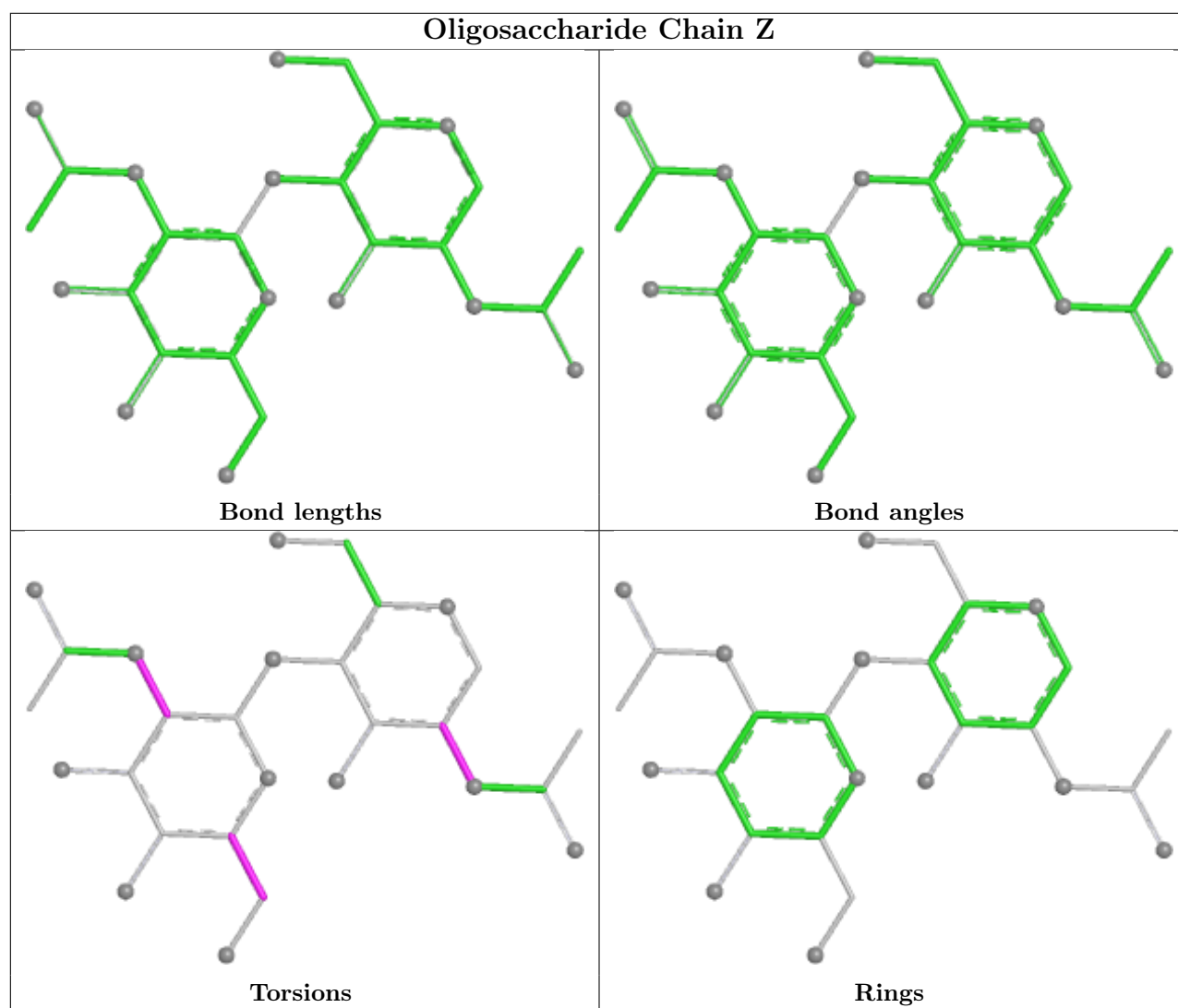


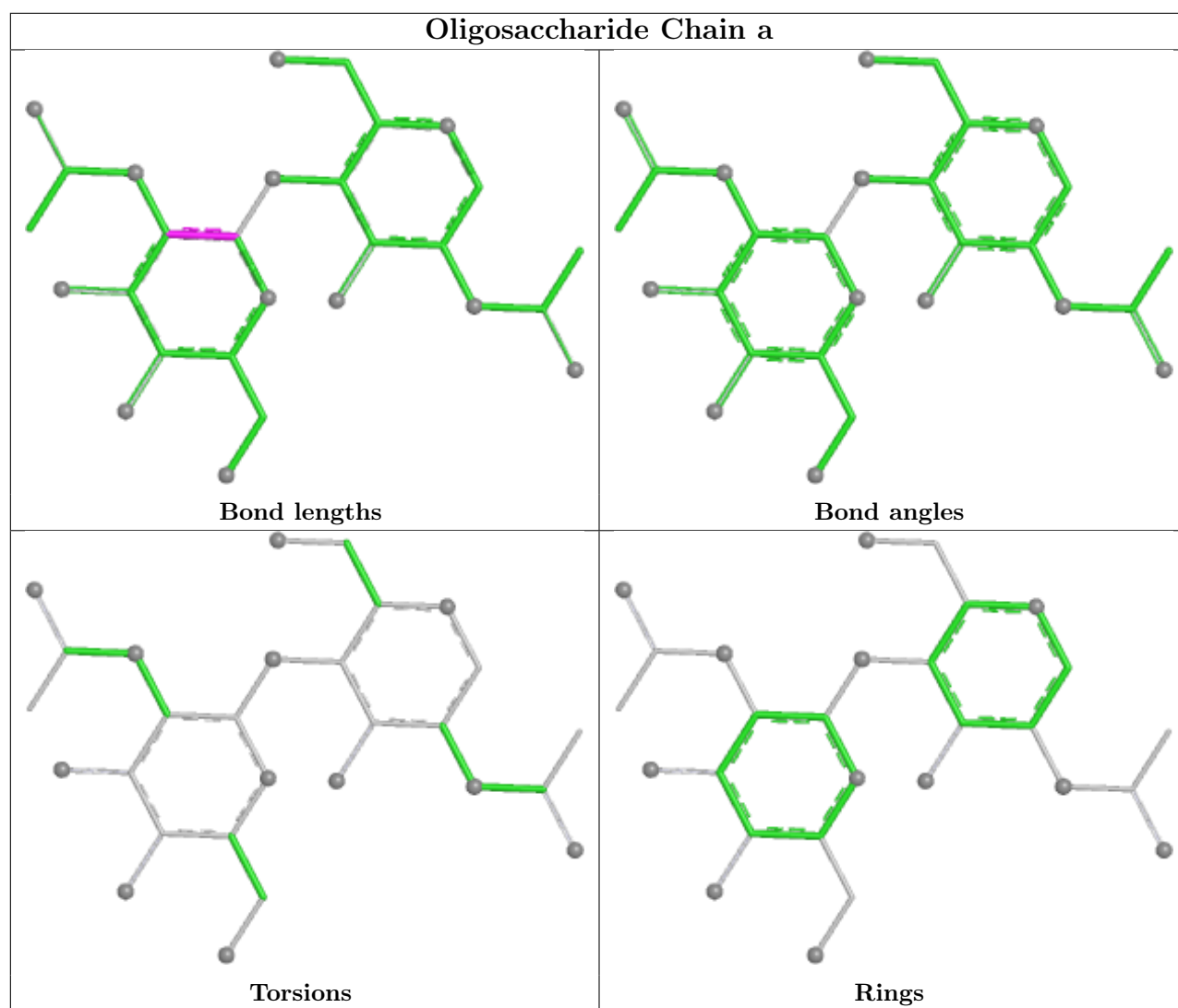


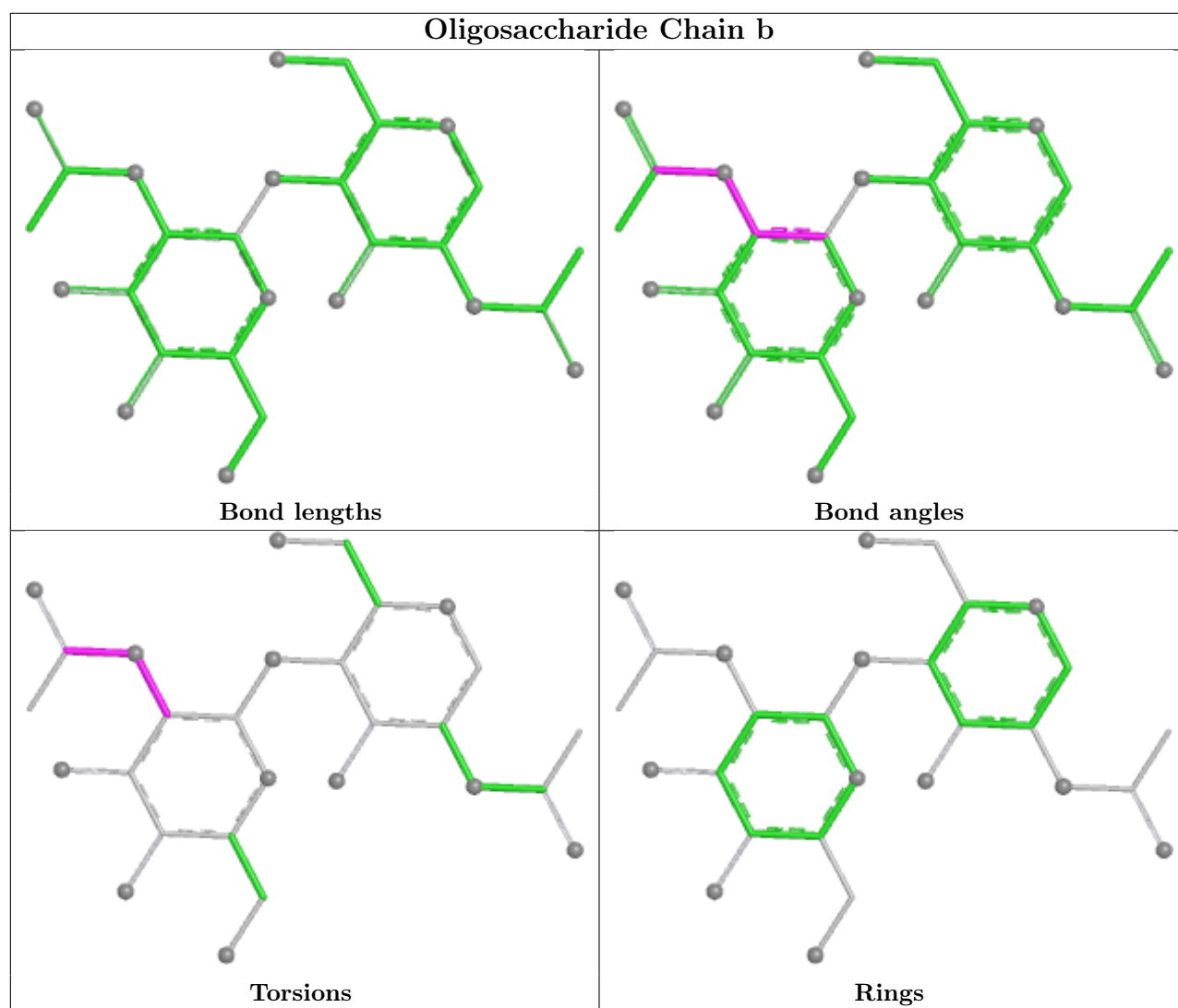


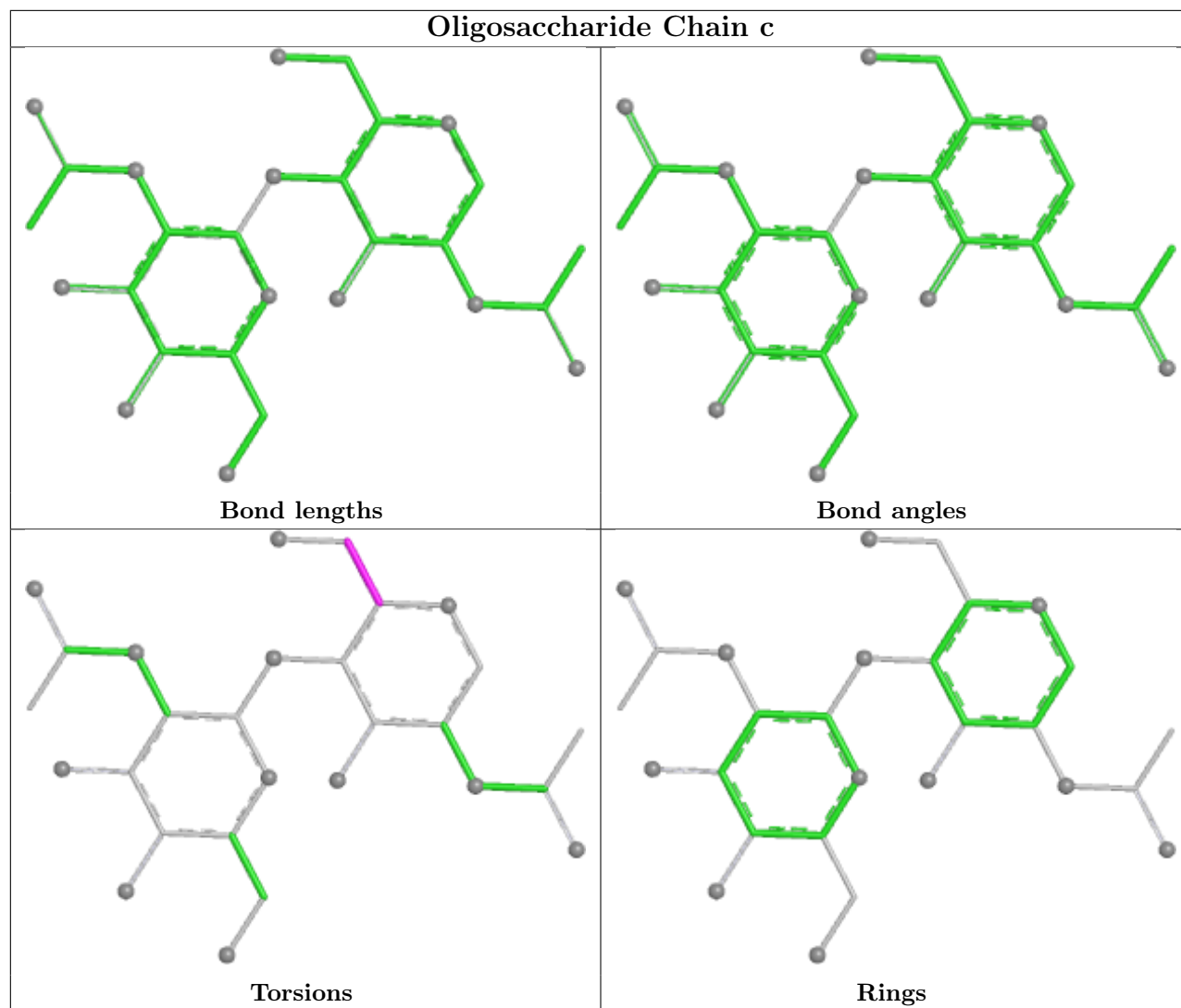


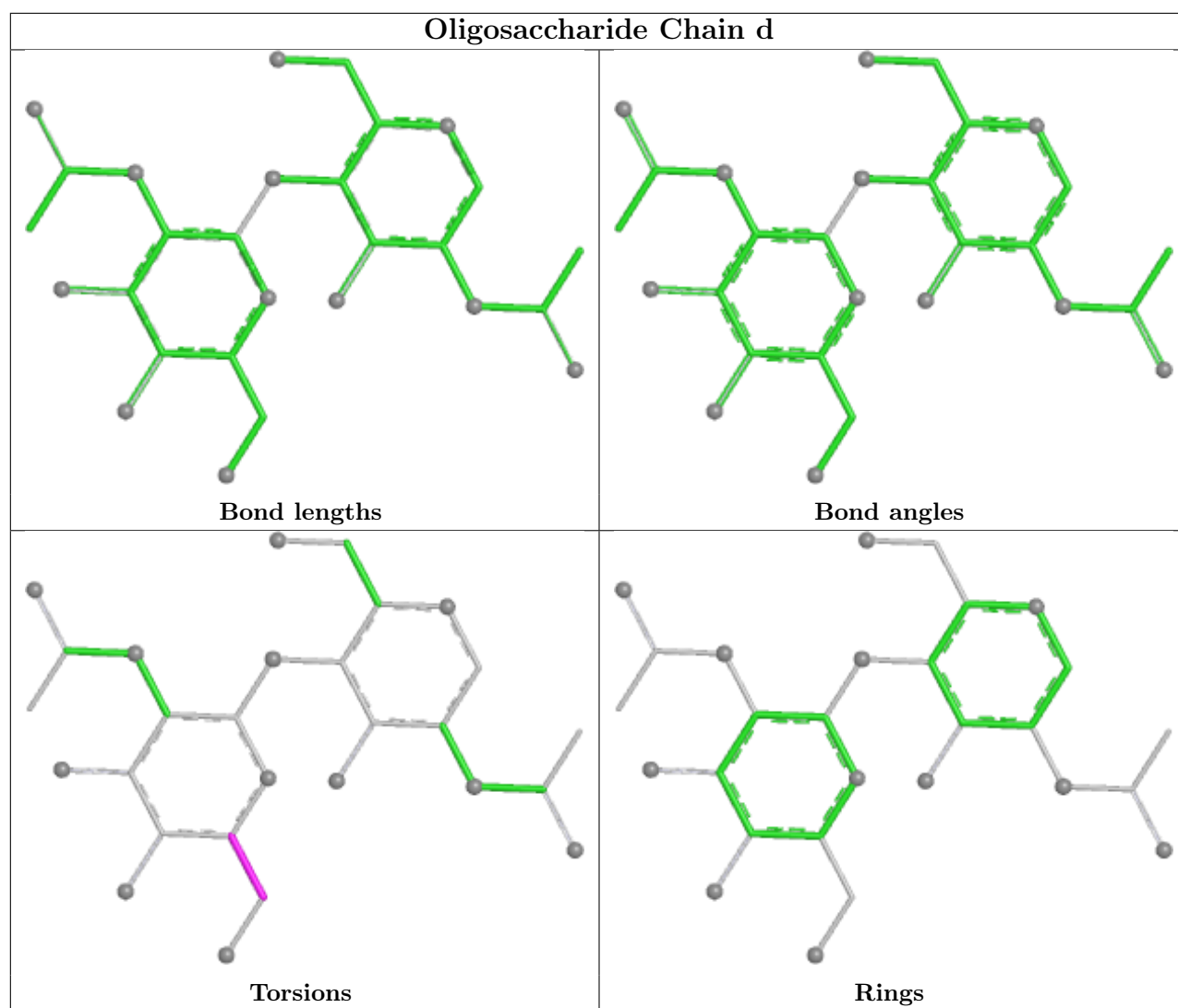


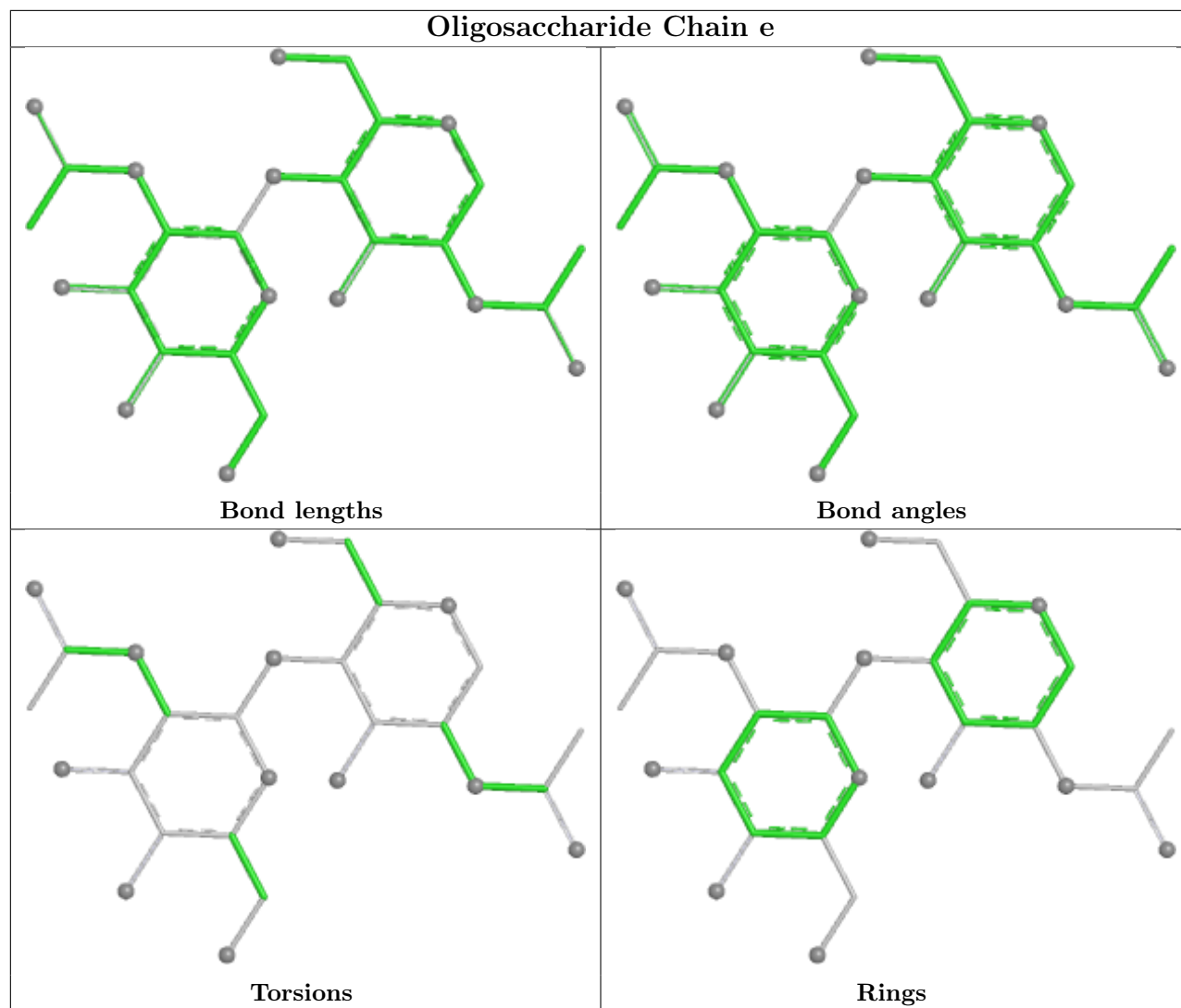


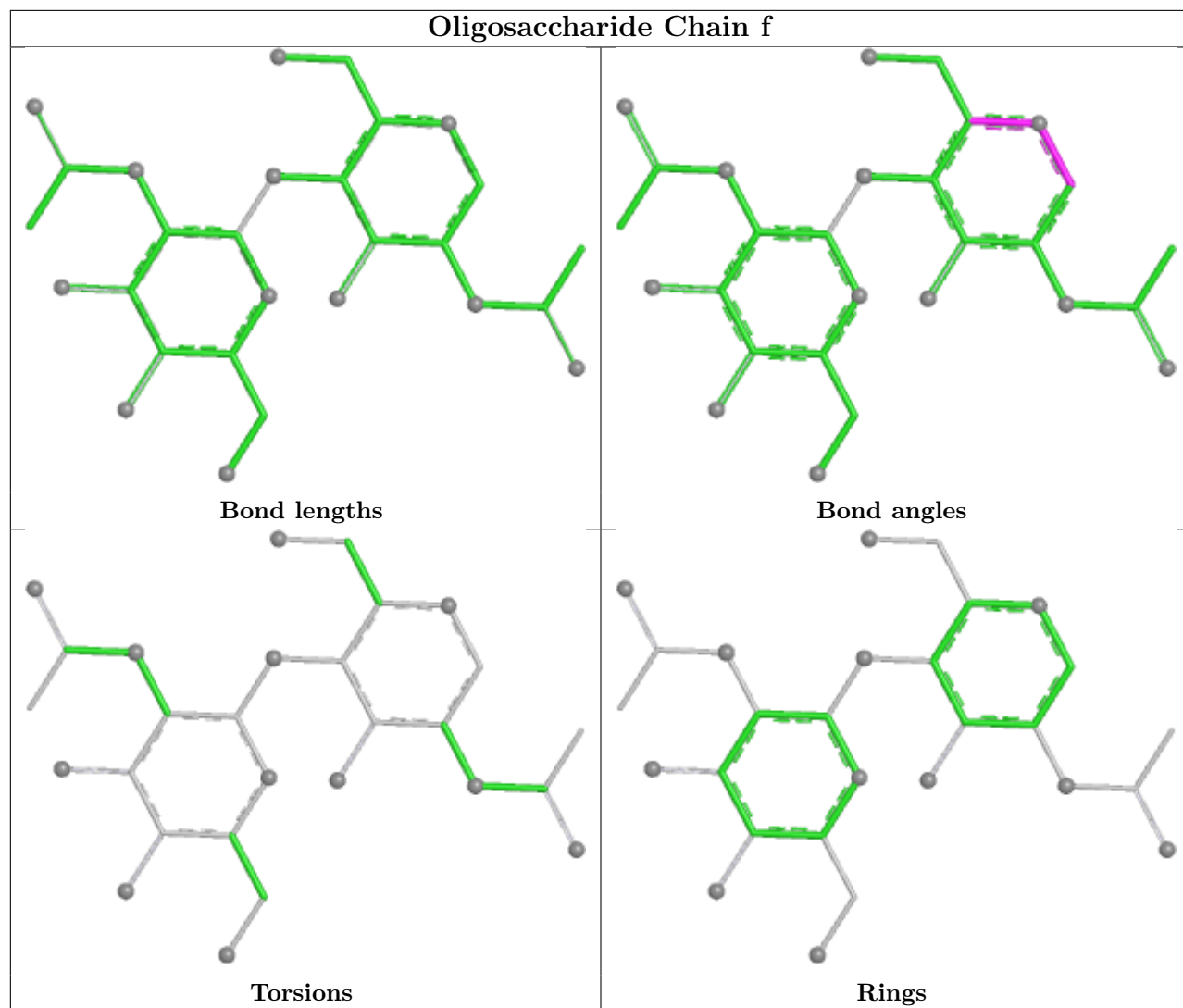


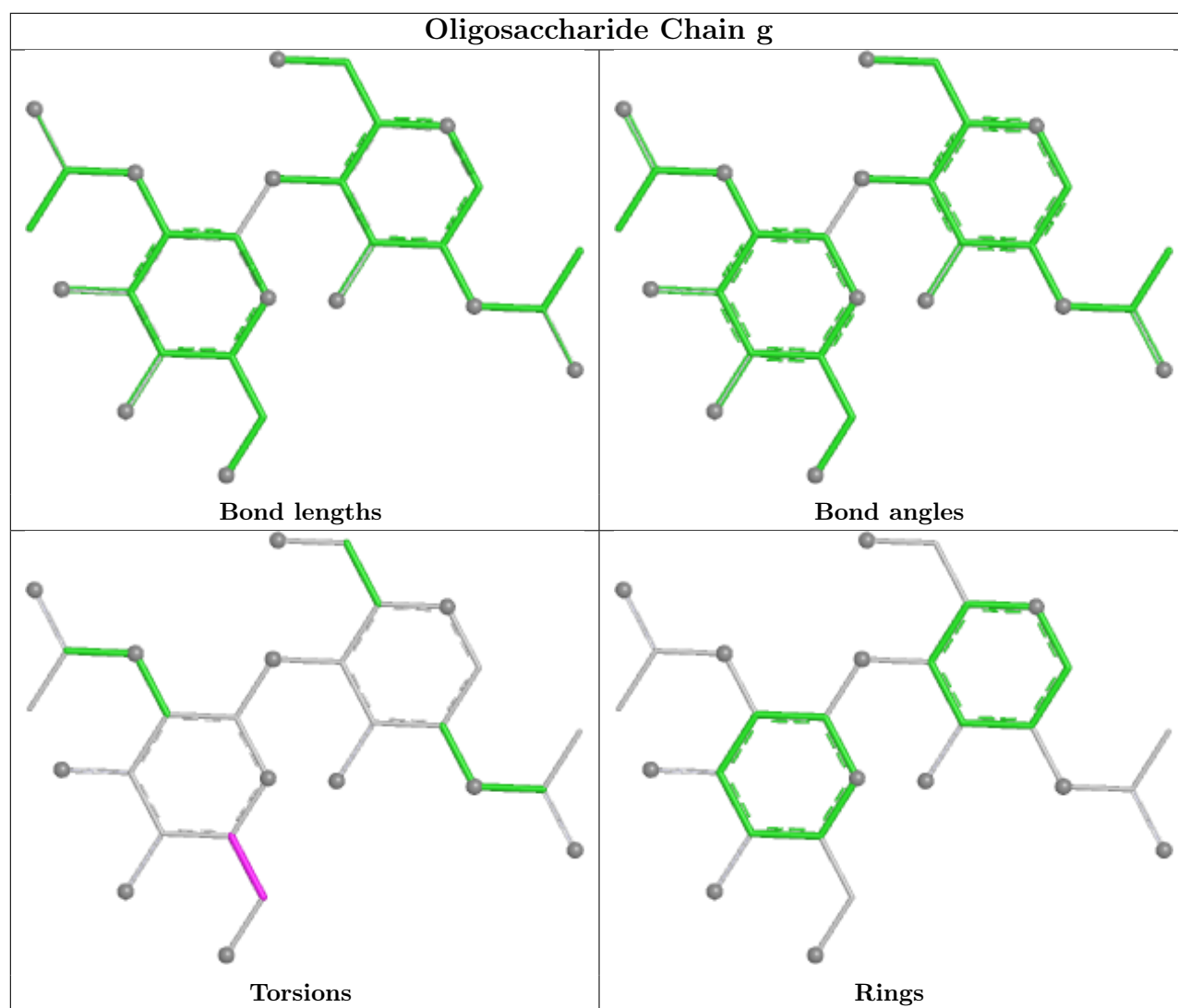


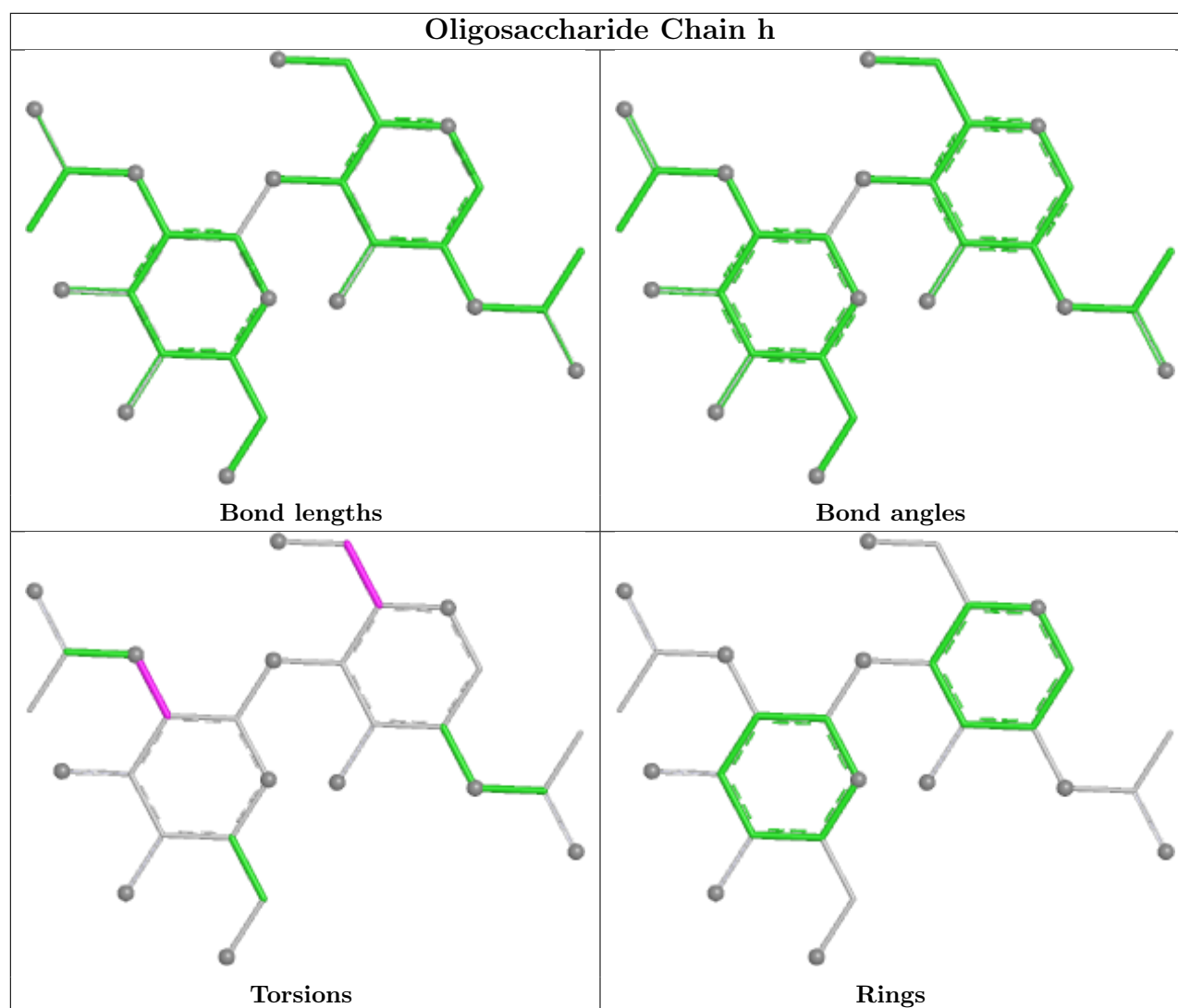












5.6 Ligand geometry [i](#)

15 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	$\# Z > 2$
3	NAG	B	2004	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	B	2003	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	B	2006	1	14,14,15	0.29	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2004	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	A	2001	1	14,14,15	0.29	0	17,19,21	0.64	0
3	NAG	C	2001	1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	C	2005	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	B	2005	1	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	B	2002	1	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	A	2004	1	14,14,15	0.39	0	17,19,21	0.38	0
3	NAG	A	2003	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	C	2002	1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	C	2003	1	14,14,15	0.19	0	17,19,21	0.44	0
3	NAG	A	2002	1	14,14,15	0.32	0	17,19,21	0.45	0
3	NAG	B	2001	1	14,14,15	0.25	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
3	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2003	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2006	1	-	4/6/23/26	0/1/1/1
3	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2005	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2004	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2001	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2004	NAG	C4-C5-C6-O6
3	C	2002	NAG	O5-C5-C6-O6
3	A	2002	NAG	O5-C5-C6-O6
3	C	2002	NAG	C4-C5-C6-O6
3	A	2004	NAG	O5-C5-C6-O6
3	A	2002	NAG	C4-C5-C6-O6
3	B	2001	NAG	C8-C7-N2-C2
3	B	2001	NAG	O7-C7-N2-C2
3	B	2002	NAG	C8-C7-N2-C2
3	B	2002	NAG	O7-C7-N2-C2
3	C	2003	NAG	C8-C7-N2-C2
3	C	2003	NAG	O7-C7-N2-C2
3	B	2006	NAG	O5-C5-C6-O6
3	C	2001	NAG	O5-C5-C6-O6
3	B	2001	NAG	O5-C5-C6-O6
3	B	2005	NAG	O5-C5-C6-O6
3	B	2006	NAG	C4-C5-C6-O6
3	C	2001	NAG	C4-C5-C6-O6
3	A	2001	NAG	C1-C2-N2-C7
3	B	2006	NAG	C1-C2-N2-C7
3	B	2001	NAG	C4-C5-C6-O6
3	A	2001	NAG	C3-C2-N2-C7
3	B	2006	NAG	C3-C2-N2-C7
3	B	2005	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2005	NAG	1	0
3	A	2004	NAG	1	0
3	A	2002	NAG	1	0

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

This section contains visualisations of the EMDB entry EMD-31760. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.