



wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 02:16 PM JST

PDB ID : 7V8C
EMDB ID : EMD-31798
Title : Cryo-EM structure of SARS-CoV-2 S-Beta variant (B.1.351), Cleavable form, one RBD-up conformation
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Hsu, S.T.D.
Deposited on : 2021-08-22
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

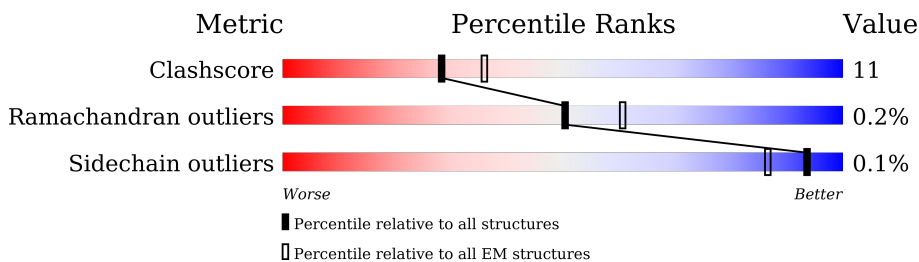
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	1280	
1	B	1280	
1	C	1280	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 25197 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
			Total	C	N	O	S		
1	A	1026	8016	5121	1331	1527	37	0	0
1	B	1032	8072	5159	1342	1534	37	0	0
1	C	1030	8059	5150	1340	1532	37	0	0

There are 261 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	conflict	UNP P0DTC2
A	80	ALA	ASP	conflict	UNP P0DTC2
A	215	GLY	ASP	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	243	ILE	ARG	conflict	UNP P0DTC2
A	414	ASN	LYS	conflict	UNP P0DTC2
A	481	LYS	GLU	conflict	UNP P0DTC2
A	498	TYR	ASN	conflict	UNP P0DTC2
A	611	GLY	ASP	conflict	UNP P0DTC2
A	698	VAL	ALA	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P0DTC2
B	80	ALA	ASP	conflict	UNP P0DTC2
B	215	GLY	ASP	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	243	ILE	ARG	conflict	UNP P0DTC2
B	414	ASN	LYS	conflict	UNP P0DTC2
B	481	LYS	GLU	conflict	UNP P0DTC2
B	498	TYR	ASN	conflict	UNP P0DTC2
B	611	GLY	ASP	conflict	UNP P0DTC2
B	698	VAL	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P0DTC2
C	80	ALA	ASP	conflict	UNP P0DTC2
C	215	GLY	ASP	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	243	ILE	ARG	conflict	UNP P0DTC2
C	414	ASN	LYS	conflict	UNP P0DTC2
C	481	LYS	GLU	conflict	UNP P0DTC2
C	498	TYR	ASN	conflict	UNP P0DTC2
C	611	GLY	ASP	conflict	UNP P0DTC2
C	698	VAL	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0

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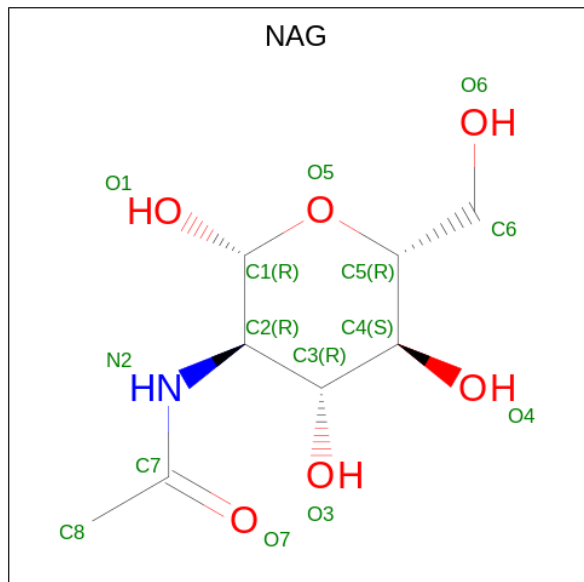
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0
2	K	2	28	16	2	10	0	0
2	L	2	28	16	2	10	0	0
2	M	2	28	16	2	10	0	0
2	N	2	28	16	2	10	0	0
2	O	2	28	16	2	10	0	0
2	P	2	28	16	2	10	0	0
2	Q	2	28	16	2	10	0	0
2	R	2	28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	b	2	Total 28	C 16	N 2	O 10	0	0
2	c	2	Total 28	C 16	N 2	O 10	0	0
2	d	2	Total 28	C 16	N 2	O 10	0	0
2	e	2	Total 28	C 16	N 2	O 10	0	0
2	f	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	Total 70	C 40	N 5	O 25	0
3	A	1	Total 70	C 40	N 5	O 25	0
3	A	1	Total 70	C 40	N 5	O 25	0
3	A	1	Total 70	C 40	N 5	O 25	0
3	A	1	Total 70	C 40	N 5	O 25	0
3	B	1	Total 84	C 48	N 6	O 30	0

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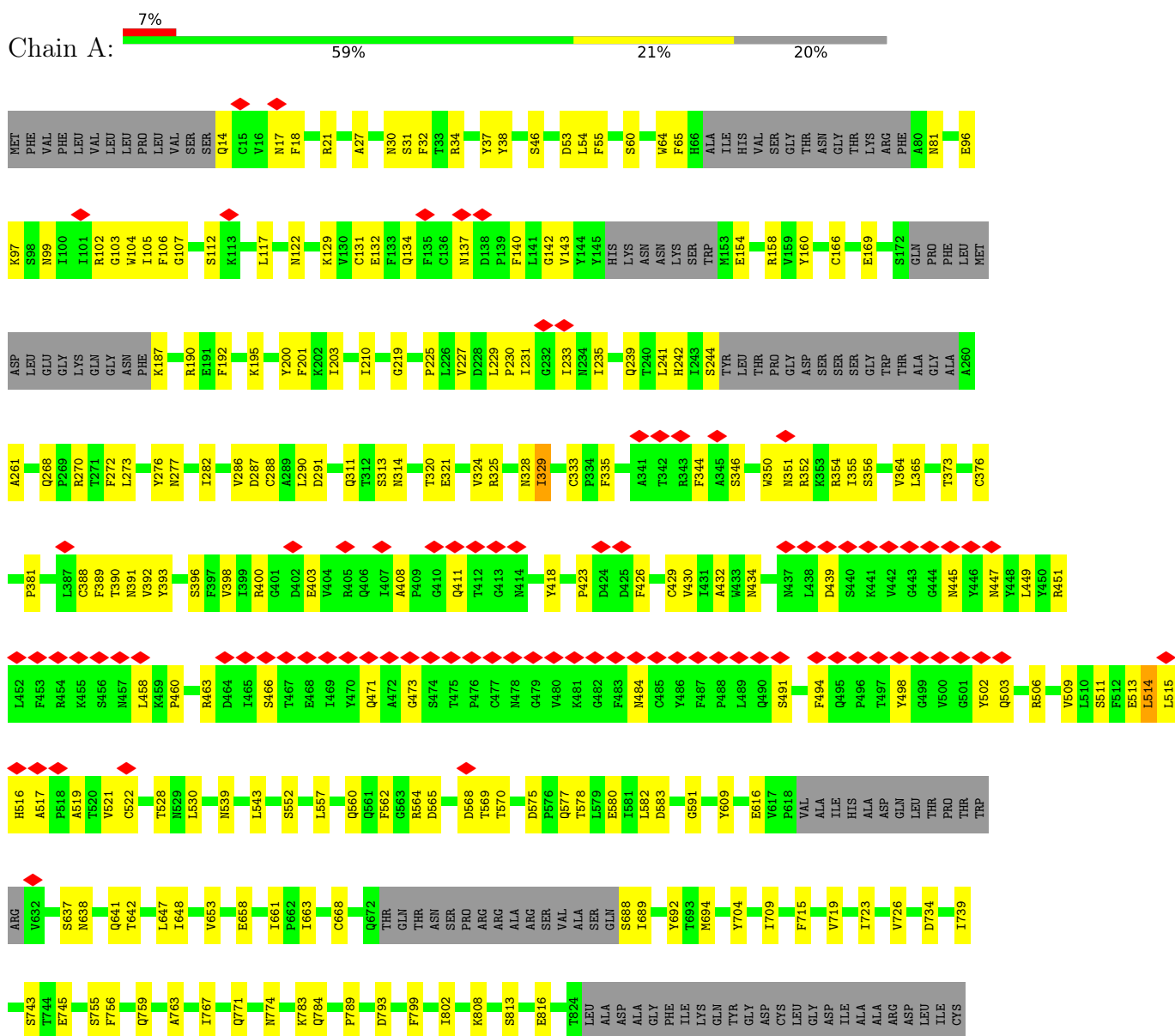
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	Total 84	48	6	30	0
3	B	1	Total 84	48	6	30	0
3	B	1	Total 84	48	6	30	0
3	B	1	Total 84	48	6	30	0
3	B	1	Total 84	48	6	30	0
3	C	1	Total 84	48	6	30	0
3	C	1	Total 84	48	6	30	0
3	C	1	Total 84	48	6	30	0
3	C	1	Total 84	48	6	30	0
3	C	1	Total 84	48	6	30	0
3	C	1	Total 84	48	6	30	0

3 Residue-property plots [i](#)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

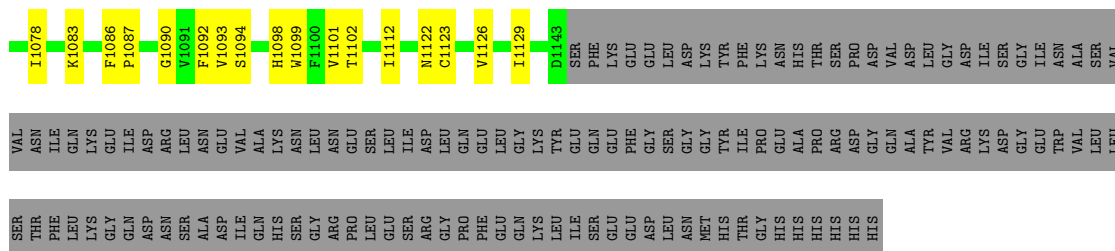


ALA	GLN	LYS	F852	L855	L862	T863	D864	E865	M866	G877	T880	S881	L891	H892	P894	H897	R902	F903	Q910	N911	V912	L913	L919	Q923	L966	N967	K961	L963	S964	D976	L977	S979	R980	K983	E987	I994	L998	T1003						
Q1007	R1016	K1025	R1036	F1039	L1046	G1066	V1057	V1058	V1062	A1077	K1083	A1084	H1085	F1086	P1087	V1091	F1092	V1093	V1101	F1106	E1108	I1112	V1119	N1122	C1123	I1129	N1132	T1133	V1134	Y1135	P1140	E1141	L1142	D1143	SER	PHE	LYS	GLU	GLU					
LEU	ASP	TYR	PHE	LYS	ASN	HIS	THR	THR	PRO	ARG	ASP	PRO	VAL	ASP	GLY	VAL	VAL	ASN	ILE	GLN	LYS	ILE	ASP	GLY	GLU	GLU	GLU	GLY	GLY	GLN	GLY	TYR	LEU	GLN	GLN	PHE	GLU	PHE	GLU	GLY				
SER	GLY	TYR	ILE	PRO	GLU	ALA	PRO	ARG	ASP	GLY	ALA	TYR	VAL	ARG	LYS	ILE	ASP	GLY	GLU	TRP	VAL	ALA	LEU	VAL	SER	VAL	GLU	ARG	GLY	PRO	PHE	GLN	GLY	GLN	LEU	ILE	SER	GLU	GLU	GLU	ASP			
LEU	ASN	MET	HIS	THR	GLY	HIS	HIS	HIS	HIS	HIS																																		

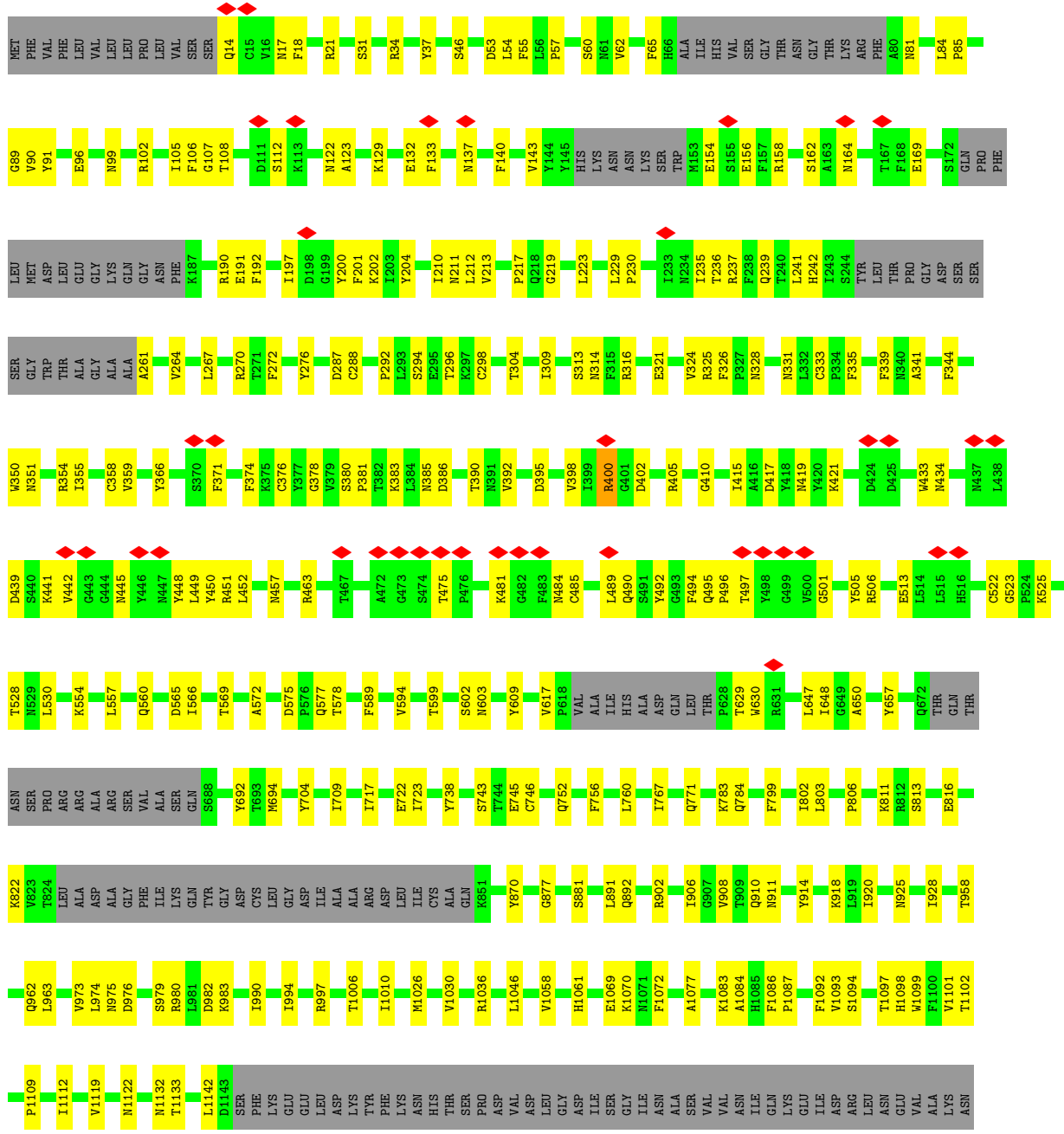
● Molecule 1: Spike glycoprotein



MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	LEU	VAL	SER	Q14	C15	V16	N17	F18	T19	T20	R21	T22	Q23	T29	S46	F55	T63	W64	F65	H66	ILE	ILE	HIS	VAL	SER	GLY	THR	ASN	GLY	ARG	PRO	LEU	LEU	ARG	PHE	N81	Y91	F92	A93	E96	M99	I100	I101				
W104	I105	G107	T108	S112	K113	L114	Q115	I119	M122	A123	T124	I128	K129	V130	C131	E132	F133	Q134	F135	M137	Y144	Y145	HIS	LYS	ASN	ASN	LEU	THR	PRO	GLY	ASP	SER	SER	SER	GLY	TRP	M153	R158	S161	N164	M165	C166	T167	F168	E169	S172	GLN	PRO	PHE	LEU	MET	ASP	LEU	GLU	GLY
LYS	GLN	GLY	ASN	K187	M188	L189	R190	E191	F192	Y200	K206	L216	S221	D228	L229	P230	I231	T236	R237	T240	L241	S244	TYR	LEU	LEU	THR	PRO	GLY	ASP	SER	SER	SER	GLY	TRP	THR	ALA	ALA	ALA	A260	A261	A261	R270	T271	F272	Y276	D287	C288	A289	L290						
D291	P292	S294	T304	K307	S313	T320	R325	N328	C333	F339	T342	R343	F344	A349	W350	R354	L355	S356	N357	C358	Y366	F371	S372	K375	C376	Y377	G378	V379	S380	P381	T382	K383	C388	F389	T390	N391	V392	Y393	S396	I399	R400														
G401	R405	Q411	M419	K421	D424	A432	W433	M436	D439	V442	G443	G444	M445	N447	Y448	L449	R450	Y451	L452	F453	P460	R463	S466	T467	E468	I469	Y470	Q471	A472	G473	S474	T475	P476	C477	N478	G479	V480	K481	G482	F483	M484	C485	Y486	F487	P488	L489									
Q490	S491	Y492	G493	F494	Q495	P496	T497	Q503	R506	L514	L515	H516	A517	P518	A519	T520	V521	C522	S527	K532	N533	K534	C535	V536	N541	D575	P576	Q577	E580	I581	L582	V592	P597	A472	G598	T599	M600	S602	Q604	V605	T615	E616	V617	P618	VAL	ALA	ILE								
HIS	ALA	ASP	GLN	LEU	THR	P628	T629	W630	S634	V639	T642	R643	T648	M655	S656	V657	D660	I661	P662	I663	L667	C668	Q672	THR	GLY	GLN	THR	THR	ASN	SER	PRO	ARG	ALA	ALA	ARG	VAL	VAL	ALA	ALA	GLN	S688	M694	S695	L696	V605	T615	I709	A710	E722	I723					
V726	W733	D734	E745	W748	L751	S755	Q759	E777	Q781	D793	F799	Q801	I802	V823	T824	L825	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	ARG	ASP	LEU	ILE	S695	L696	ALA	ALA	S708	I709	A710	L861	L862	T863							
I867	G877	T880	S881	L891	P894	M897	G898	M899	A900	Y901	Q910	N911	Y912	L913	N925	I928	I931	Q932	L956	G968	V973	D976	R980	L981	V984	E985	T1003	Q1007	M1026	V1030	P1054	H1055	G1056	V1057	V1058	H1061	L1069																		



• Molecule 1: Spike glycoprotein



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

GLY
ARG
PRO
LEU
SER
ARG
GLY
PRO
PHE
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLY
ASP
LEU
ASN
MET
HIS
THR
GLY
HIS
HIS
PRO
HIS
HIS
ASP
HIS
HIS

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




MAG1
MAG2

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




MAG1
MAG2

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



MAG1
MAG2

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




MAG1
MAG2

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



MAG1
MAG2

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





- 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:  50% 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:  50% 50% 50%



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



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



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



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



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



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





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



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



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



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



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



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





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

Chain b:  100%



- 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:  50%
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:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	392357	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
Maximum map value	2.988	Depositor
Minimum map value	-1.348	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	0.32	0/8198	0.49	1/11156 (0.0%)
1	B	0.32	0/8257	0.50	0/11236
1	C	0.33	0/8244	0.50	0/11218
All	All	0.32	0/24699	0.50	1/33610 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	LEU	CB-CG-CD2	-5.05	102.41	111.00

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	8016	0	7812	197	0
1	B	8072	0	7872	169	0
1	C	8059	0	7859	192	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
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	2	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	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	1	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	2	0
2	a	28	0	25	0	0
2	b	28	0	25	0	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
3	A	70	0	65	1	0
3	B	84	0	78	3	0
3	C	84	0	78	1	0
All	All	25197	0	24489	523	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 11.

The worst 5 of 523 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:B:46:SER:HA	1:B:276:TYR:O	1.74	0.87
1:A:46:SER:HA	1:A:276:TYR:O	1.76	0.86
1:A:230:PRO:O	1:C:354:ARG:NH1	2.11	0.81
1:C:84:LEU:HD12	1:C:85:PRO:HD2	1.61	0.81
1:B:449:LEU:HD21	1:B:489:LEU:HB3	1.61	0.81

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%)	952 (94%)	57 (6%)	1 (0%)	51	82
1	B	1016/1280 (79%)	938 (92%)	77 (8%)	1 (0%)	51	82
1	C	1014/1280 (79%)	938 (92%)	73 (7%)	3 (0%)	41	72
All	All	3040/3840 (79%)	2828 (93%)	207 (7%)	5 (0%)	50	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ILE
1	B	985	GLU
1	C	617	VAL
1	C	321	GLU
1	C	90	VAL

5.3.2 Protein sidechains [i](#)

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	898/1113 (81%)	898 (100%)	0	100	100
1	B	904/1113 (81%)	904 (100%)	0	100	100
1	C	903/1113 (81%)	901 (100%)	2 (0%)	93	98
All	All	2705/3339 (81%)	2703 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	400	ARG
1	C	405	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	910	GLN
1	C	17	ASN
1	C	910	GLN
1	C	137	ASN
1	A	1007	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](#)

58 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.49	0	17,19,21	0.66	0
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.59	0
2	NAG	E	1	2,1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	E	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	F	1	2,1	14,14,15	0.51	0	17,19,21	1.19	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	F	2	2	14,14,15	0.18	0	17,19,21	0.41	0
2	NAG	G	1	2,1	14,14,15	0.25	0	17,19,21	0.38	0
2	NAG	G	2	2	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	H	1	2,1	14,14,15	0.32	0	17,19,21	0.44	0
2	NAG	H	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	I	1	2,1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	I	2	2	14,14,15	0.18	0	17,19,21	0.39	0
2	NAG	J	1	2,1	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	J	2	2	14,14,15	0.18	0	17,19,21	0.46	0
2	NAG	K	1	2,1	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	K	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	L	1	2,1	14,14,15	0.33	0	17,19,21	0.43	0
2	NAG	L	2	2	14,14,15	0.16	0	17,19,21	0.42	0
2	NAG	M	1	2,1	14,14,15	0.27	0	17,19,21	0.38	0
2	NAG	M	2	2	14,14,15	0.21	0	17,19,21	0.47	0
2	NAG	N	1	2,1	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	N	2	2	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	O	1	2	14,14,15	0.42	0	17,19,21	1.26	1 (5%)
2	NAG	O	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	P	1	2,1	14,14,15	0.28	0	17,19,21	0.50	0
2	NAG	P	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	Q	1	2,1	14,14,15	0.28	0	17,19,21	0.39	0
2	NAG	Q	2	2	14,14,15	0.27	0	17,19,21	0.49	0
2	NAG	R	1	2,1	14,14,15	0.23	0	17,19,21	0.56	0
2	NAG	R	2	2	14,14,15	0.22	0	17,19,21	0.37	0
2	NAG	S	1	2,1	14,14,15	0.39	0	17,19,21	0.40	0
2	NAG	S	2	2	14,14,15	0.18	0	17,19,21	0.47	0
2	NAG	T	1	2,1	14,14,15	0.29	0	17,19,21	0.42	0
2	NAG	T	2	2	14,14,15	0.17	0	17,19,21	0.47	0
2	NAG	U	1	2,1	14,14,15	0.29	0	17,19,21	0.41	0
2	NAG	U	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	V	1	2,1	14,14,15	0.63	1 (7%)	17,19,21	0.68	0
2	NAG	V	2	2	14,14,15	0.26	0	17,19,21	0.59	1 (5%)
2	NAG	W	1	2,1	14,14,15	0.35	0	17,19,21	0.39	0
2	NAG	W	2	2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	X	1	2,1	14,14,15	0.43	0	17,19,21	0.39	0
2	NAG	X	2	2	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	Y	1	2,1	14,14,15	0.37	0	17,19,21	0.41	0
2	NAG	Y	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	Z	1	2,1	14,14,15	0.23	0	17,19,21	0.56	0
2	NAG	Z	2	2	14,14,15	0.48	0	17,19,21	0.49	0
2	NAG	a	1	2,1	14,14,15	0.38	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	a	2	2	14,14,15	0.18	0	17,19,21	0.47	0
2	NAG	b	1	2,1	14,14,15	0.22	0	17,19,21	0.50	0
2	NAG	b	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	c	1	2,1	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	c	2	2	14,14,15	0.18	0	17,19,21	0.40	0
2	NAG	d	1	2,1	14,14,15	0.44	0	17,19,21	0.64	0
2	NAG	d	2	2	14,14,15	0.23	0	17,19,21	0.38	0
2	NAG	e	1	2,1	14,14,15	0.40	0	17,19,21	0.43	0
2	NAG	e	2	2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	f	1	2,1	14,14,15	0.29	0	17,19,21	0.37	0
2	NAG	f	2	2	14,14,15	0.19	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
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	1/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	4/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	1	NAG	O5-C1	-2.16	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	NAG	C2-N2-C7	4.30	129.02	122.90
2	F	1	NAG	C2-N2-C7	4.17	128.84	122.90
2	V	2	NAG	C1-O5-C5	2.03	114.95	112.19

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

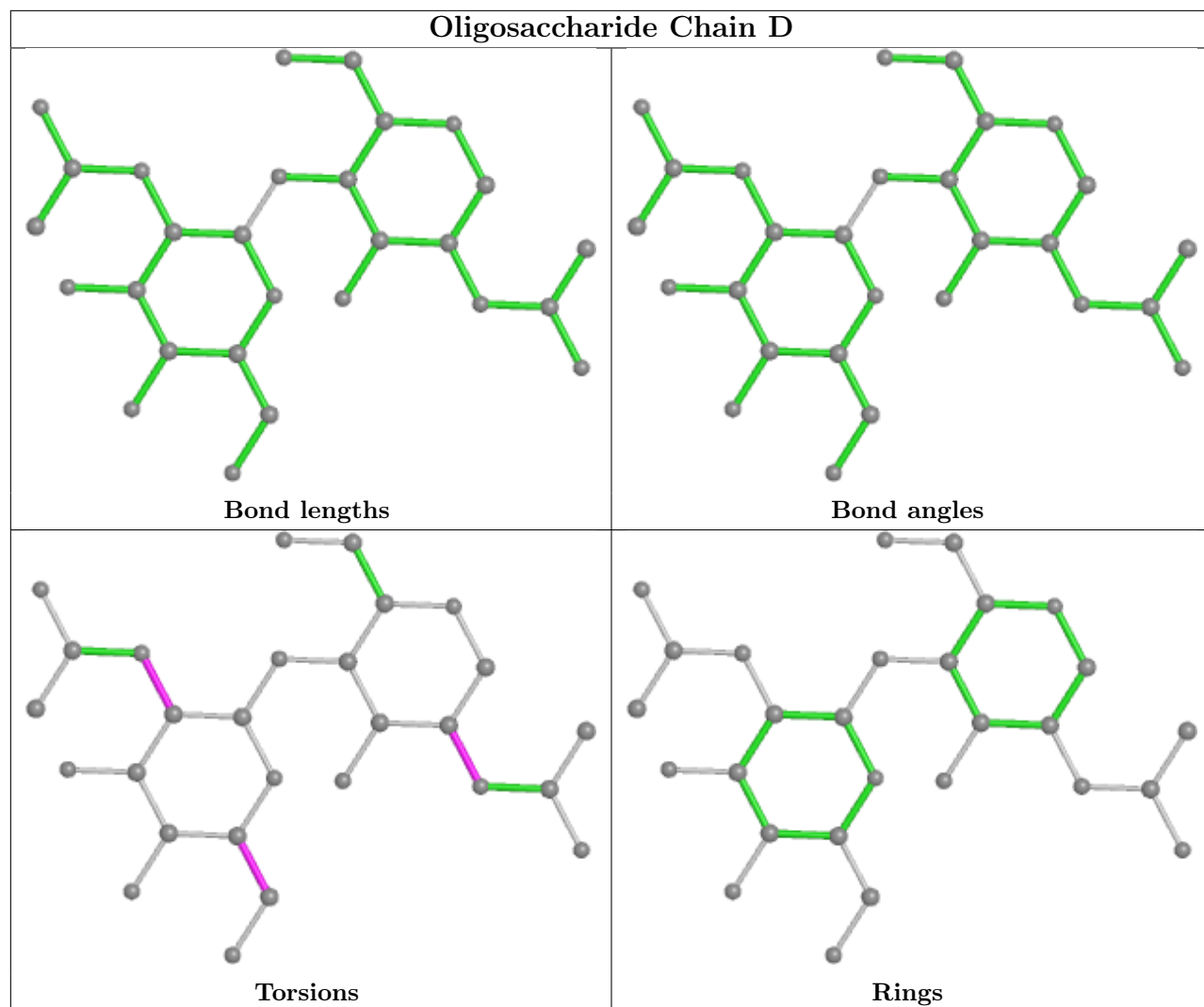
Mol	Chain	Res	Type	Atoms
2	X	1	NAG	O5-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6

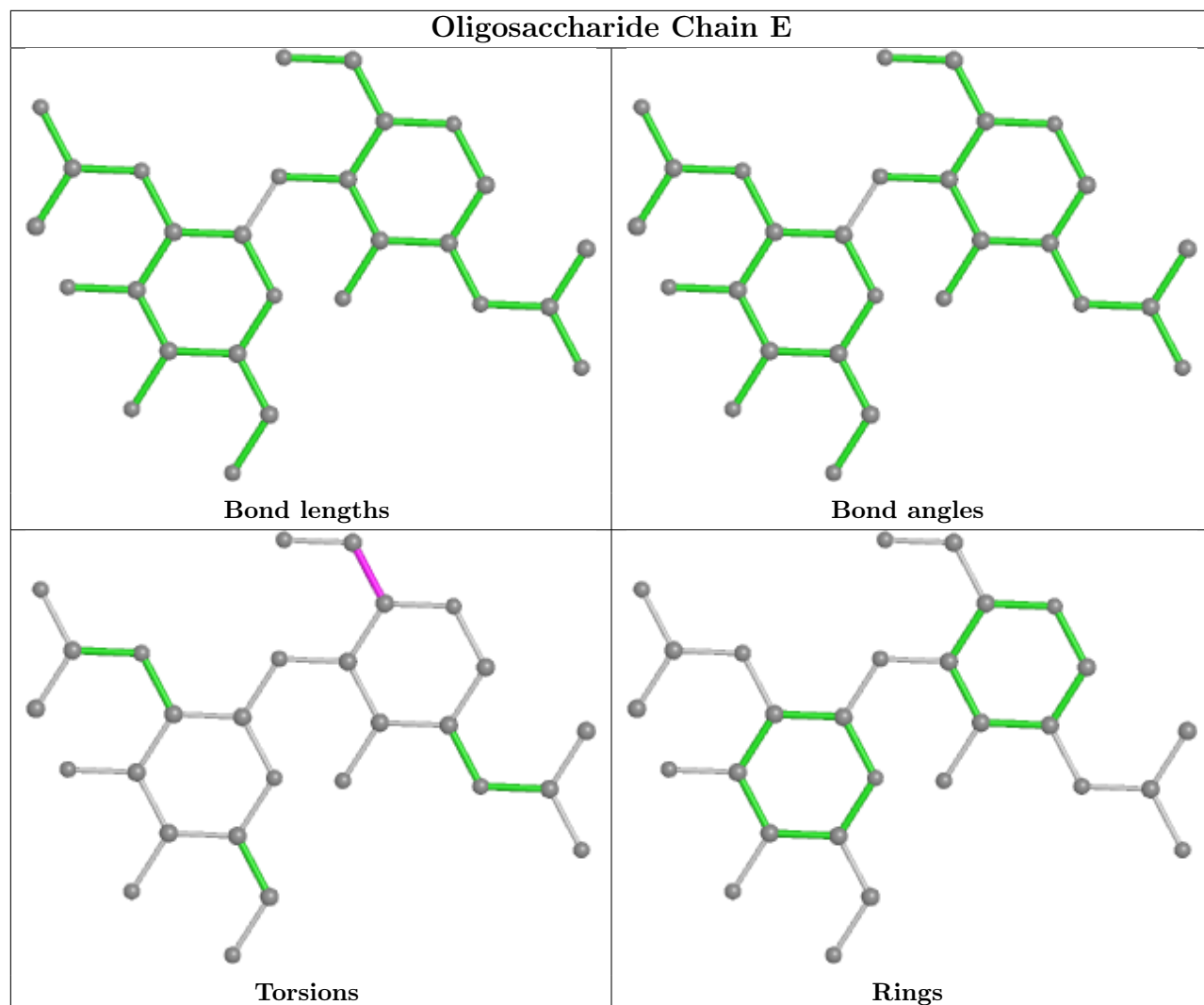
There are no ring outliers.

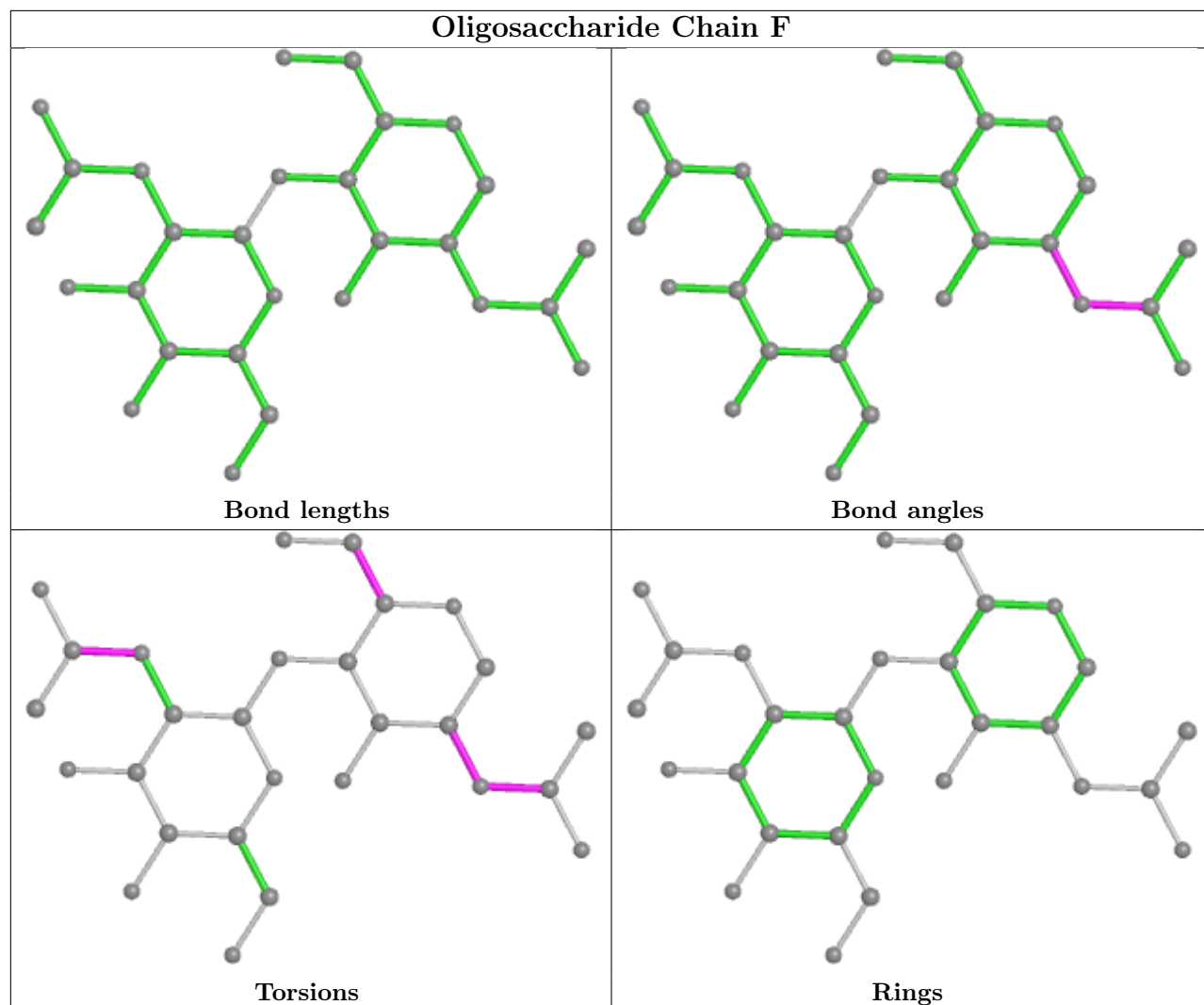
7 monomers are involved in 7 short contacts:

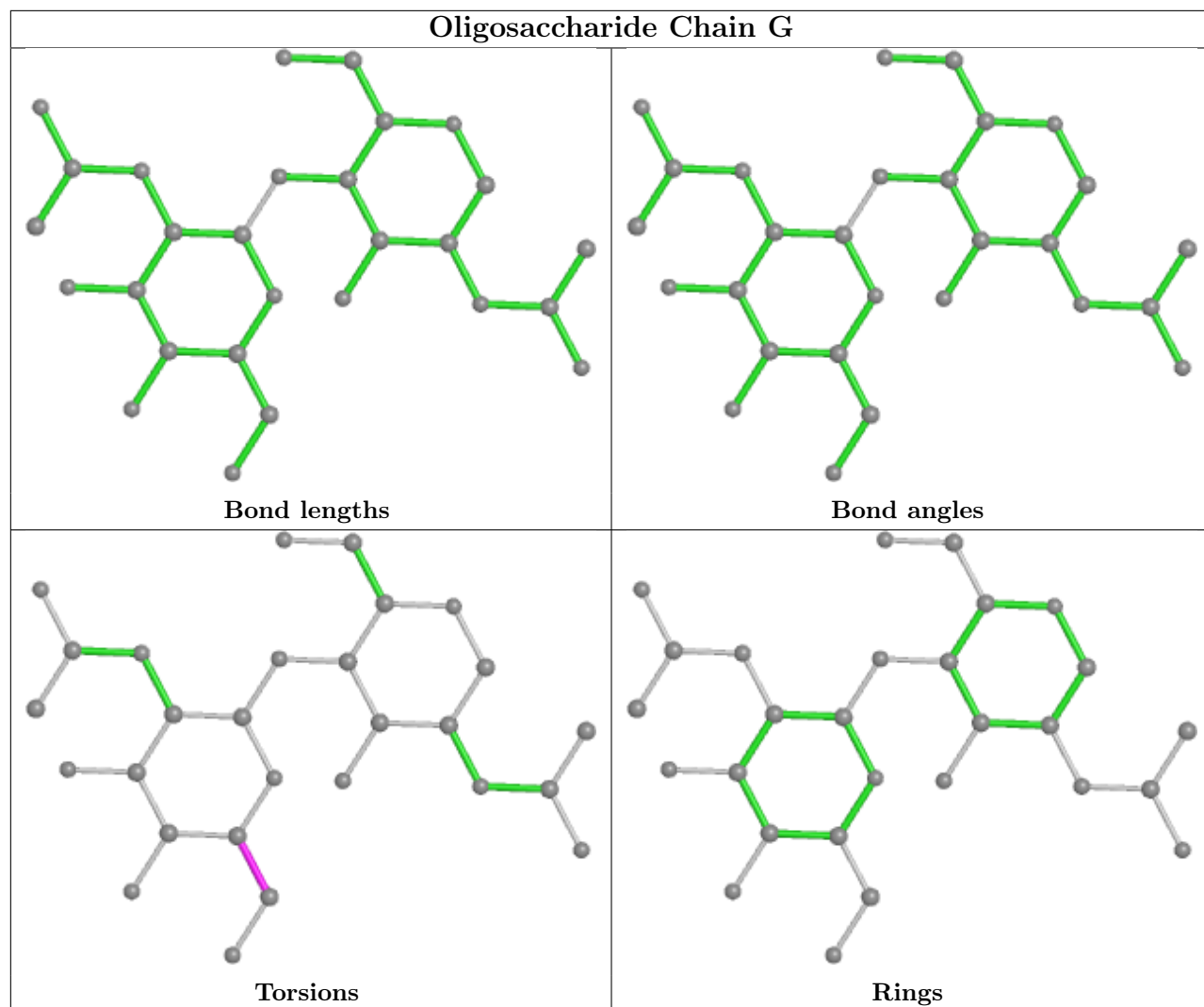
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	2	NAG	1	0
2	Z	1	NAG	2	0
2	F	1	NAG	1	0
2	Z	2	NAG	1	0
2	O	1	NAG	2	0
2	Q	1	NAG	1	0
2	O	2	NAG	1	0

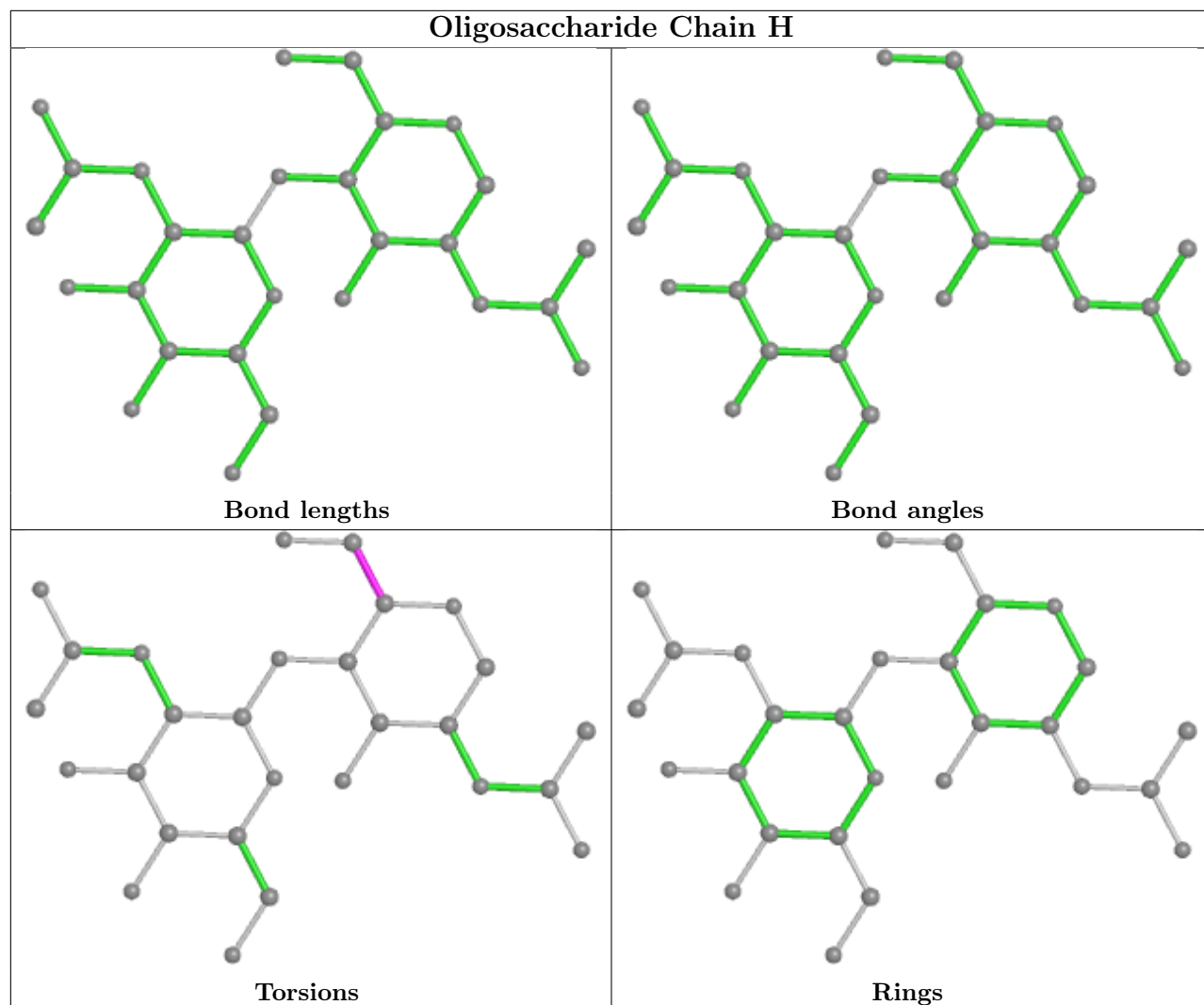
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

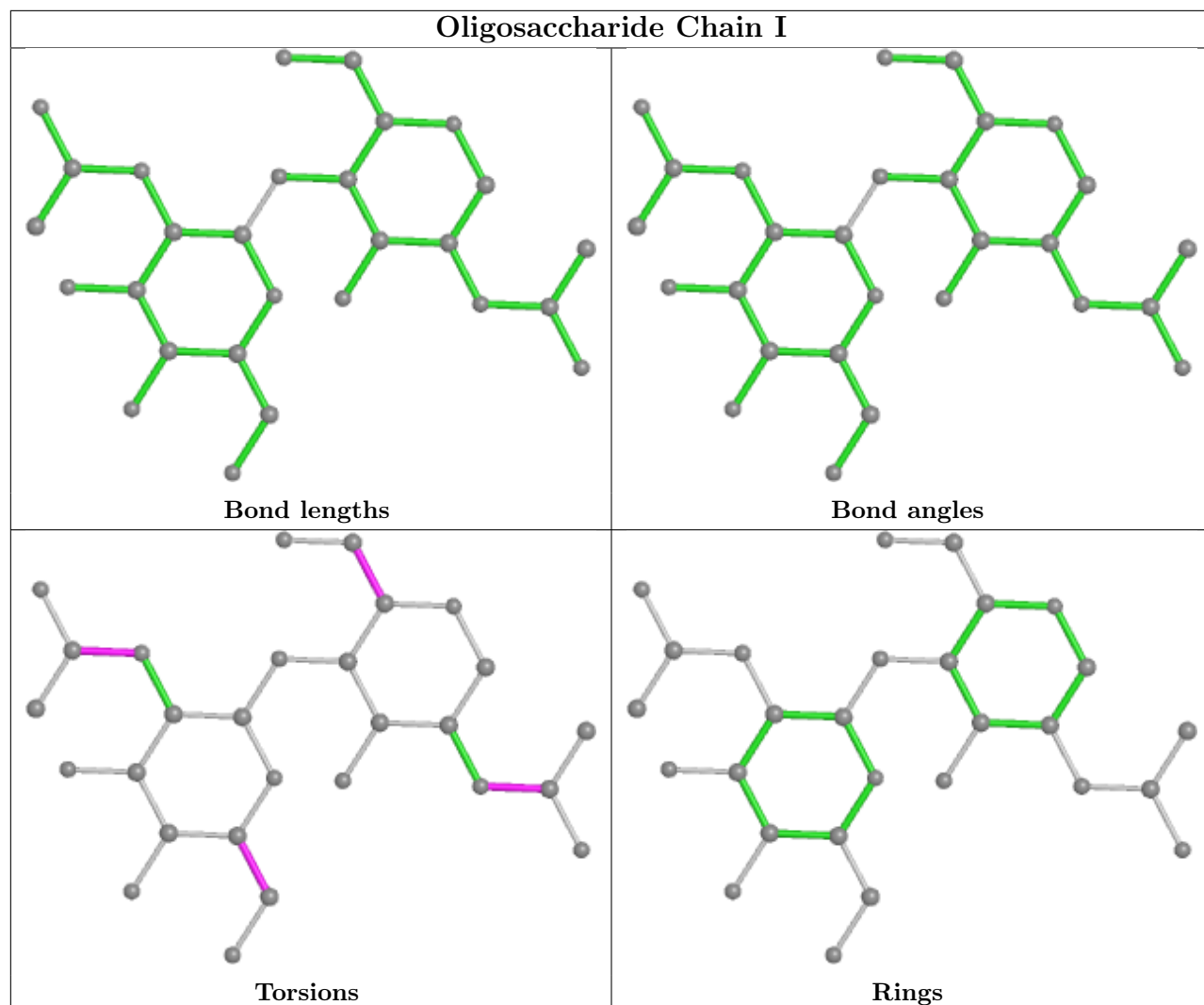


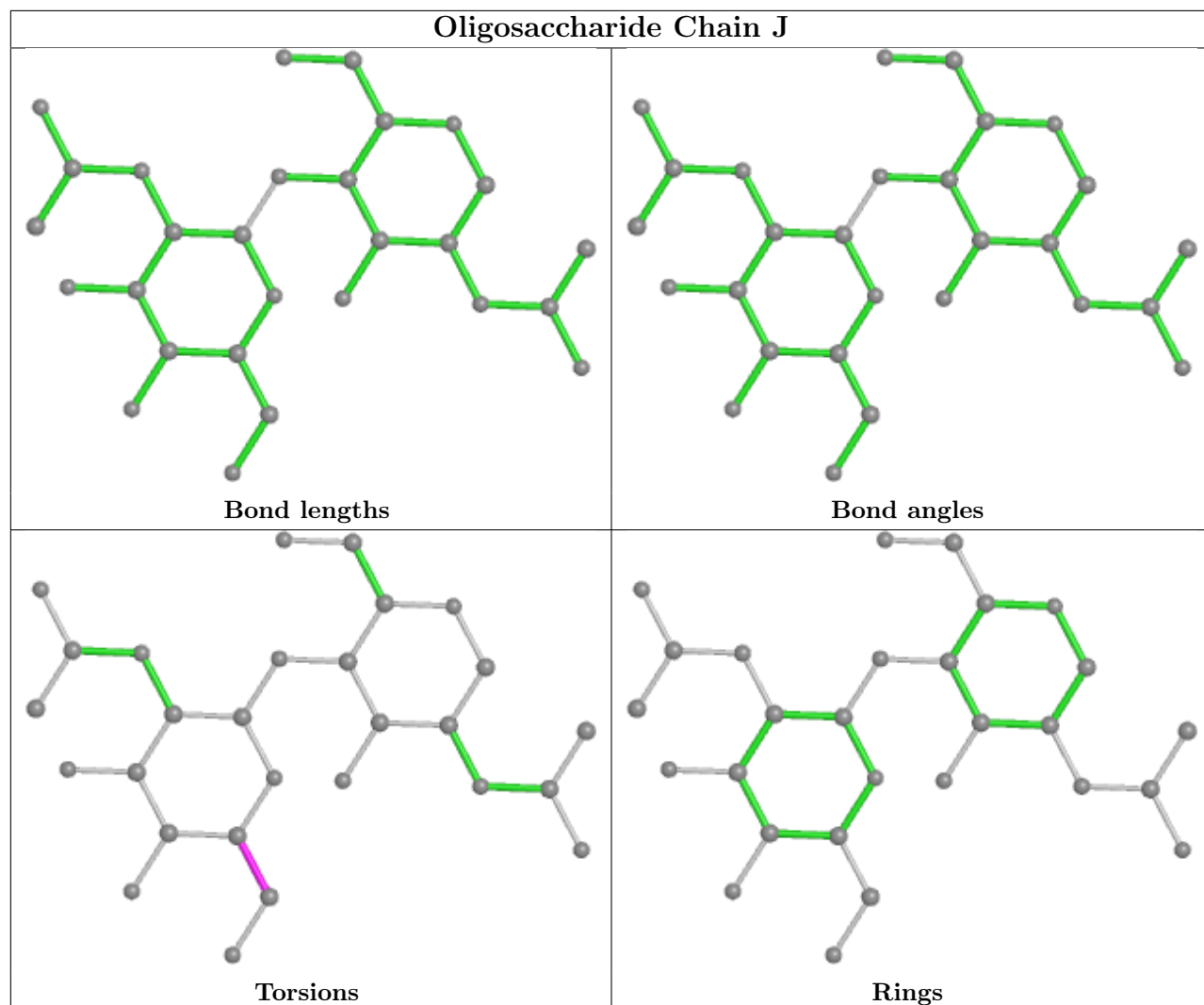


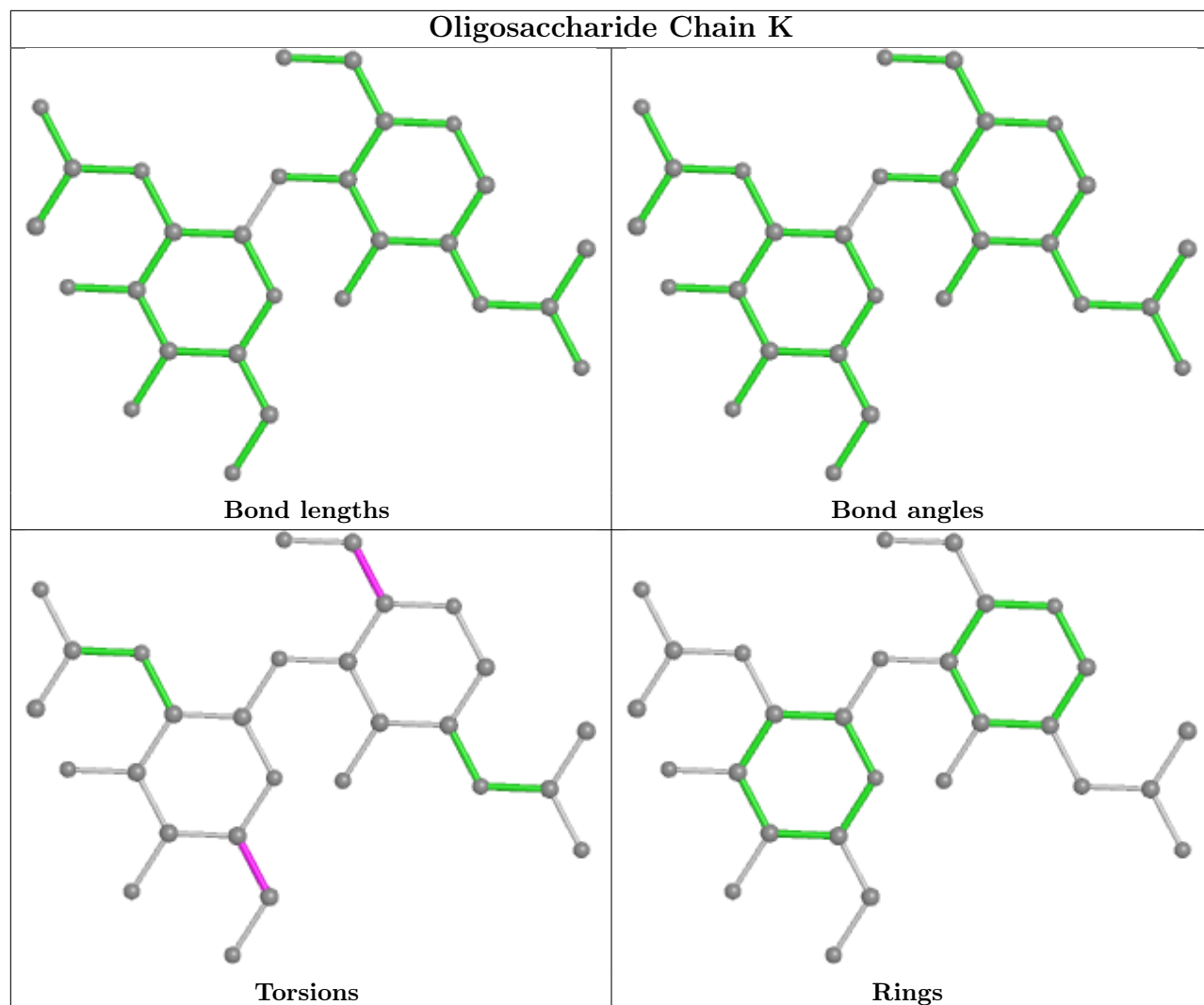


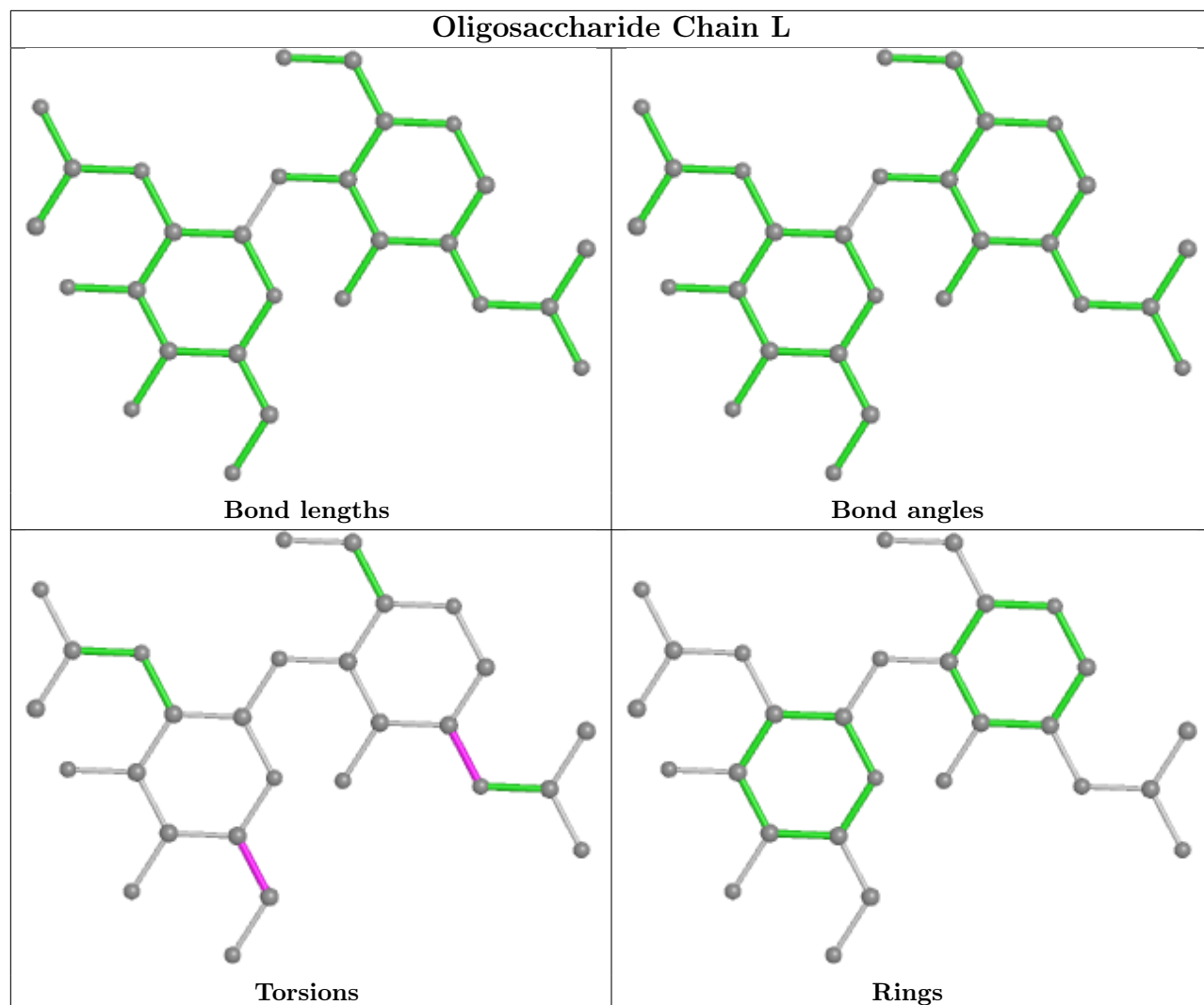


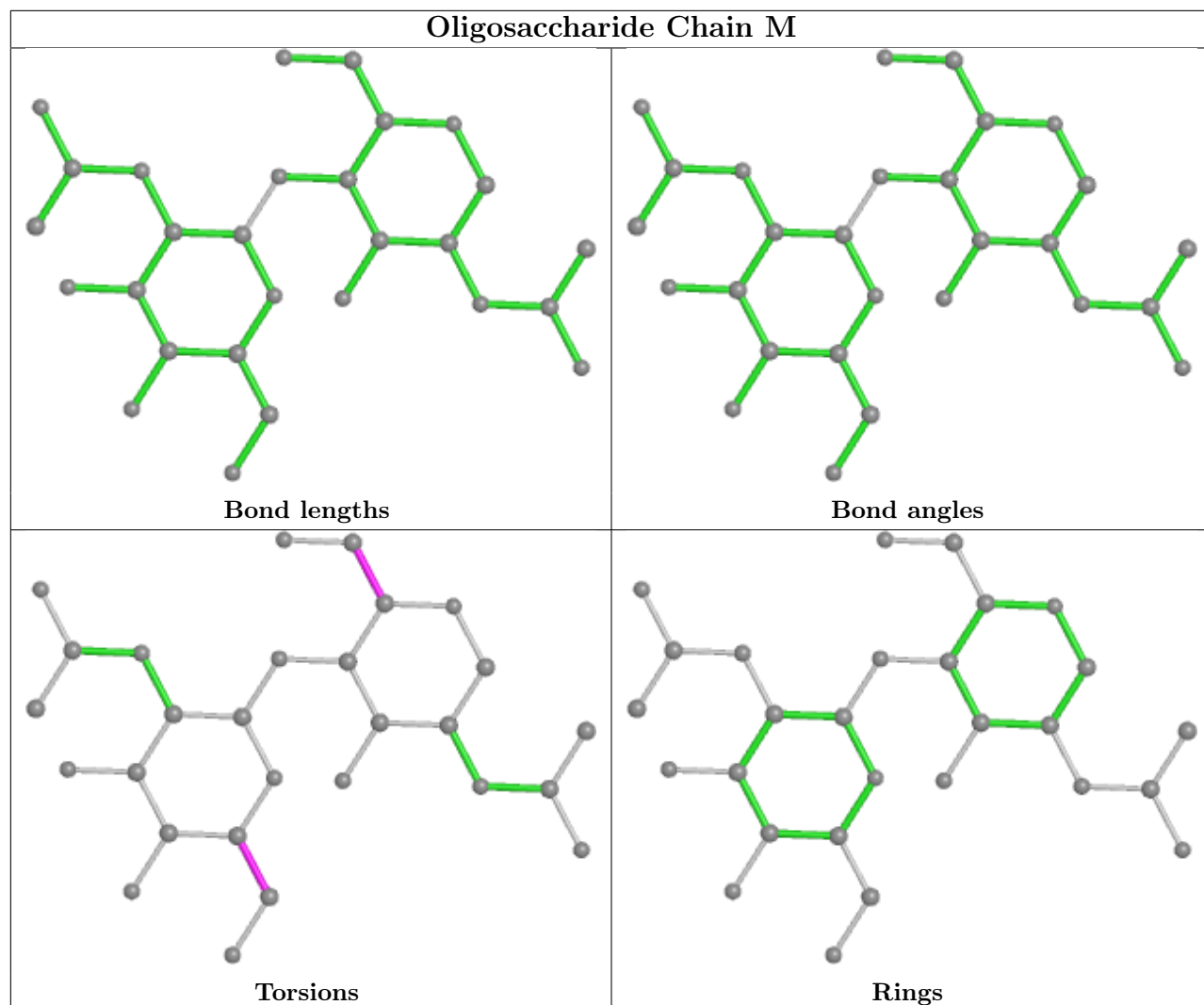


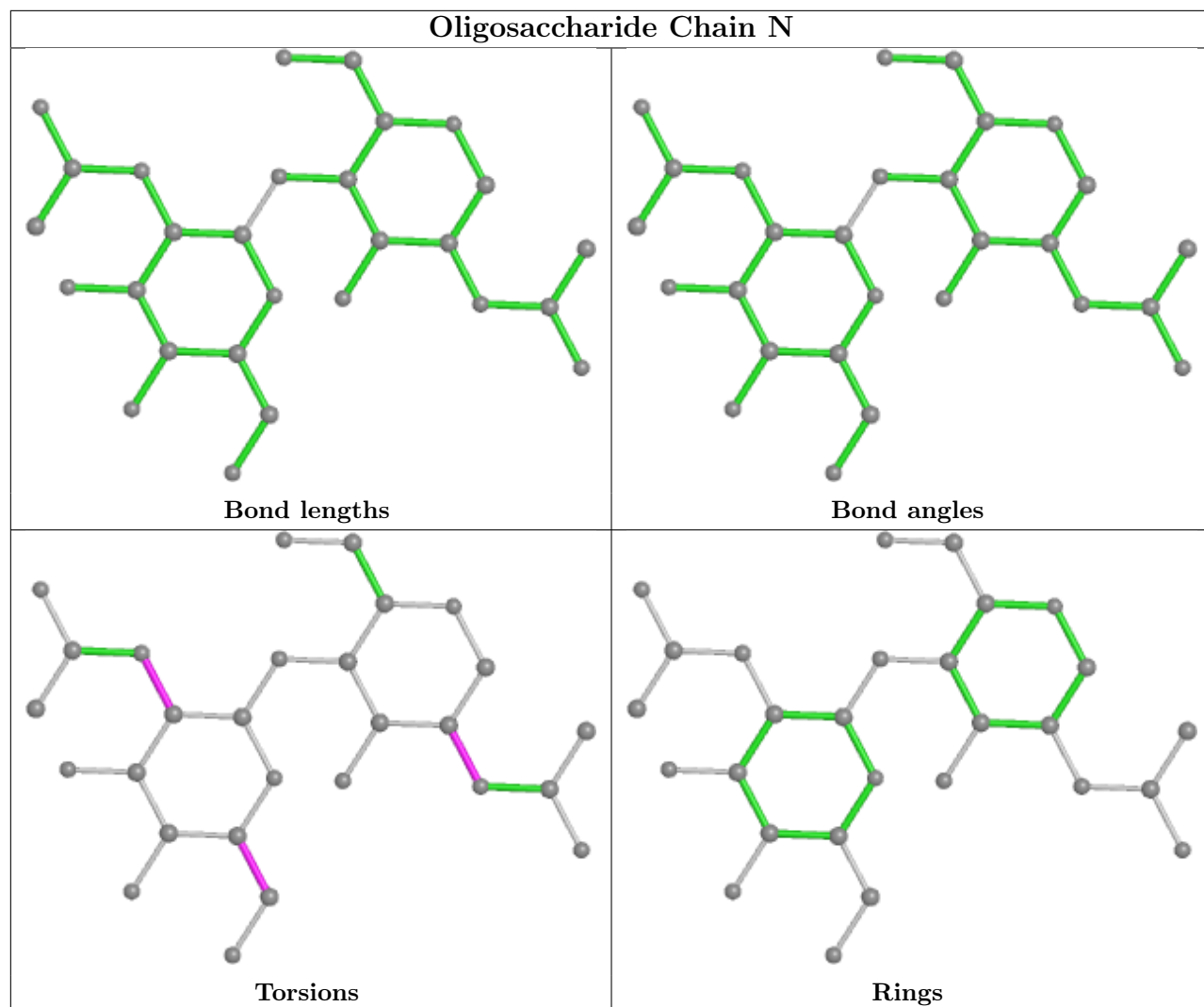


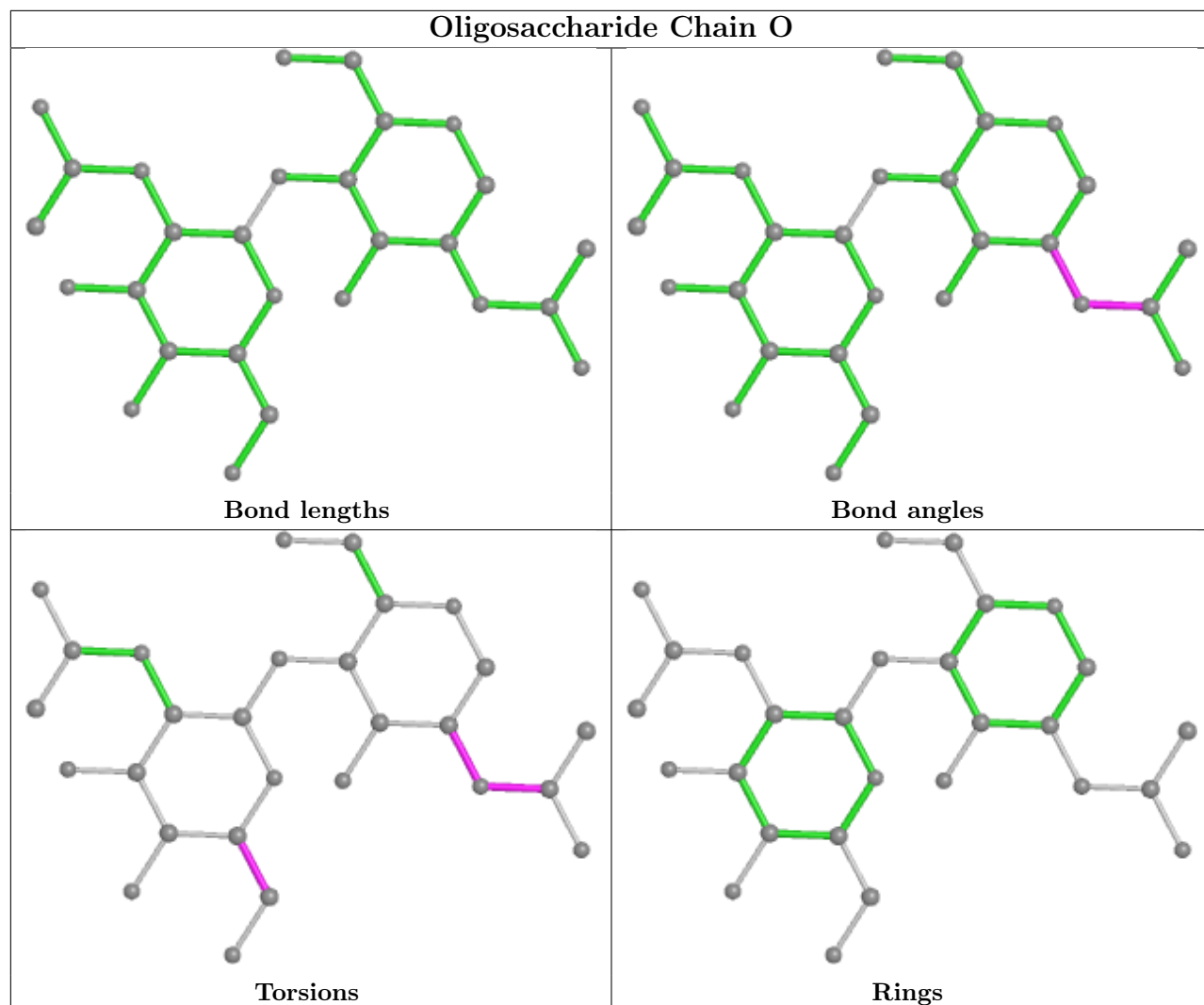


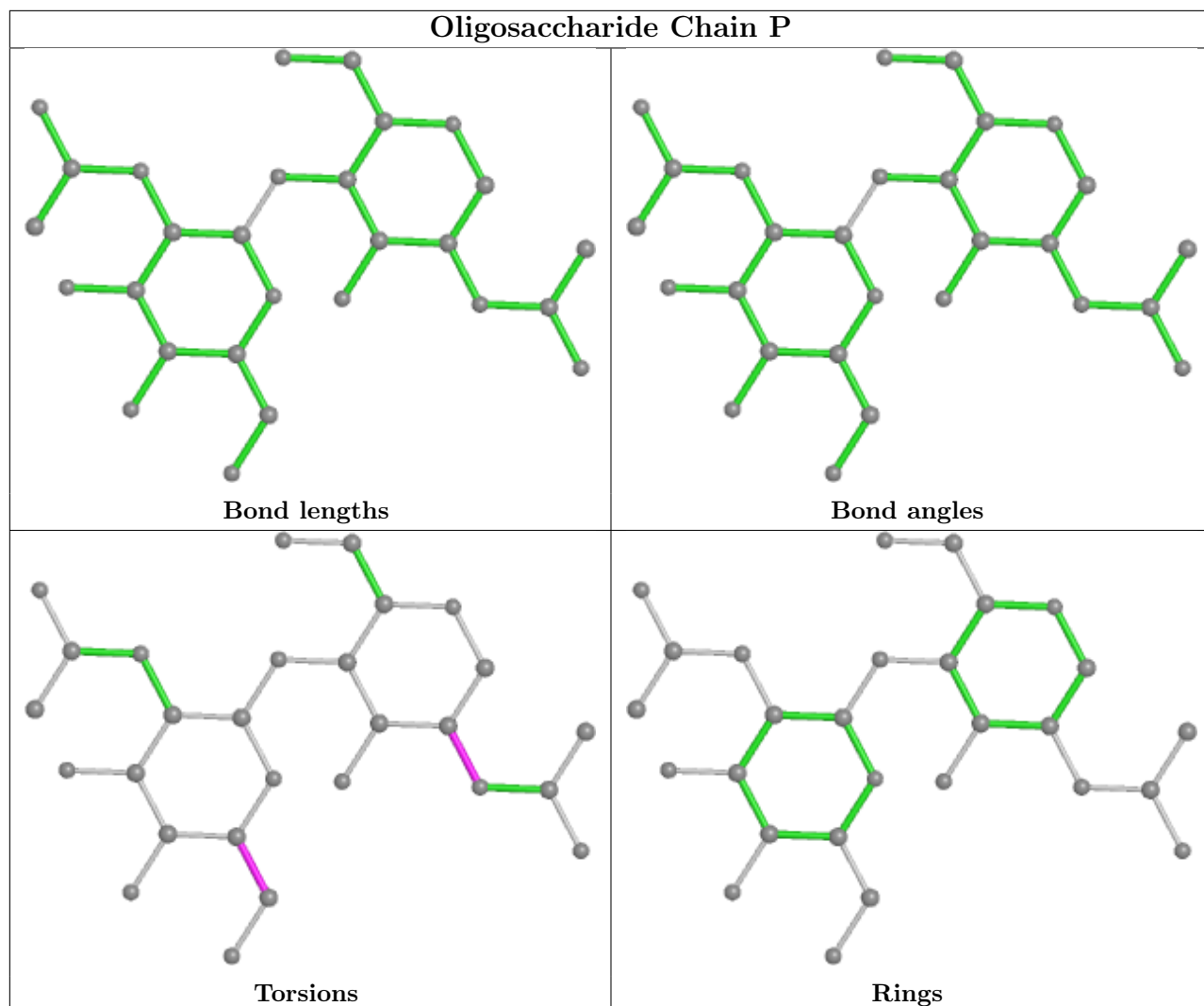


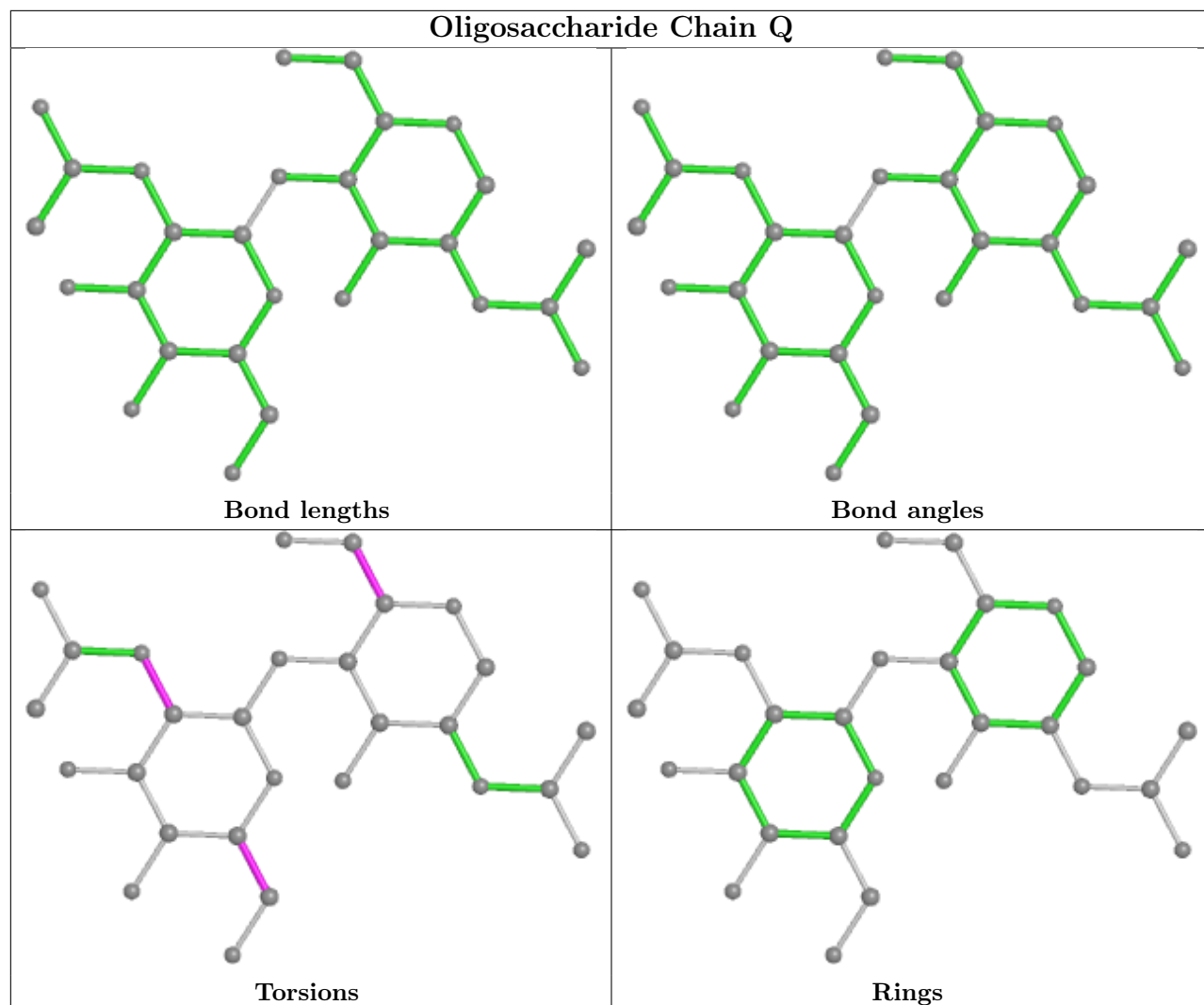


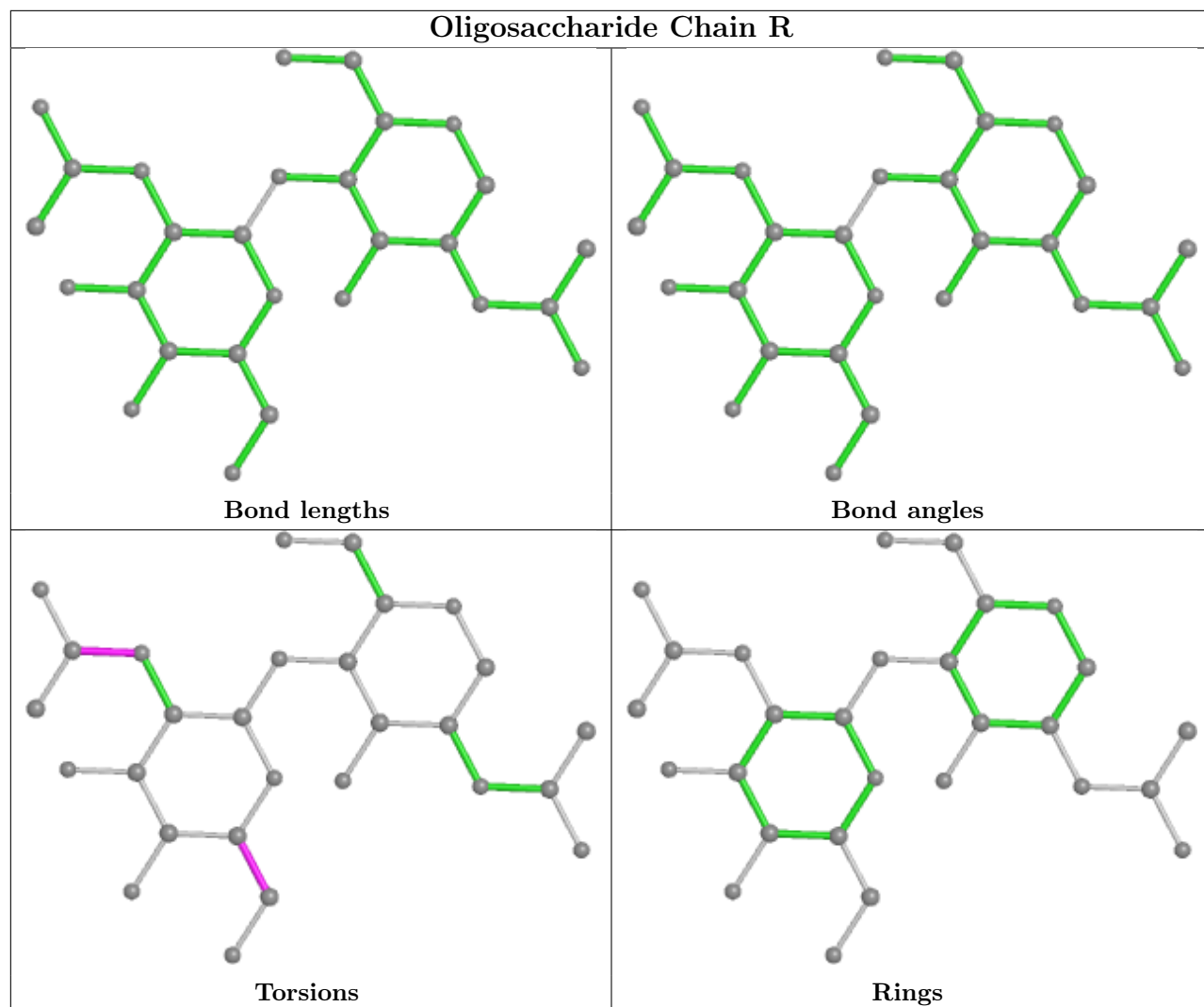


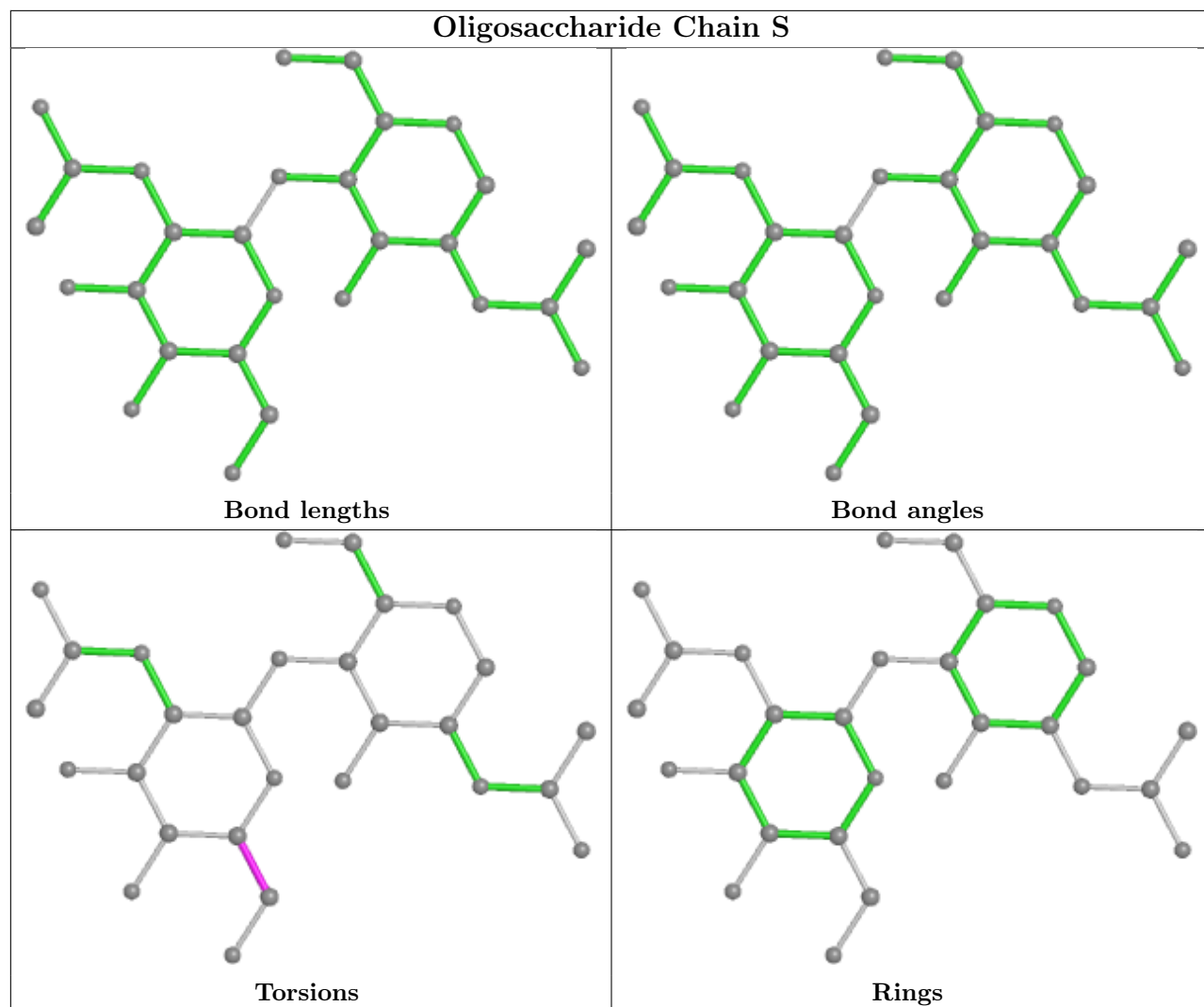


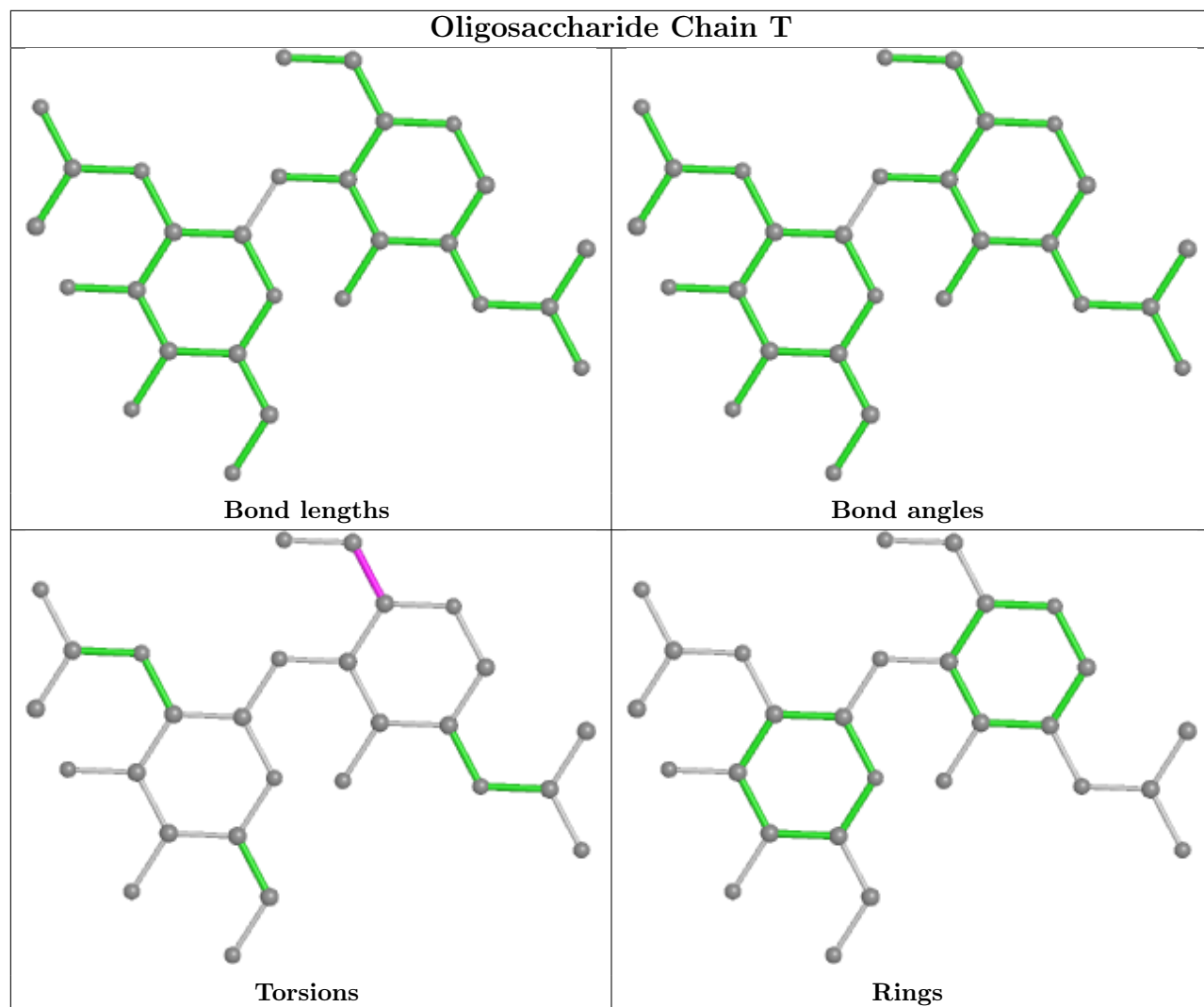


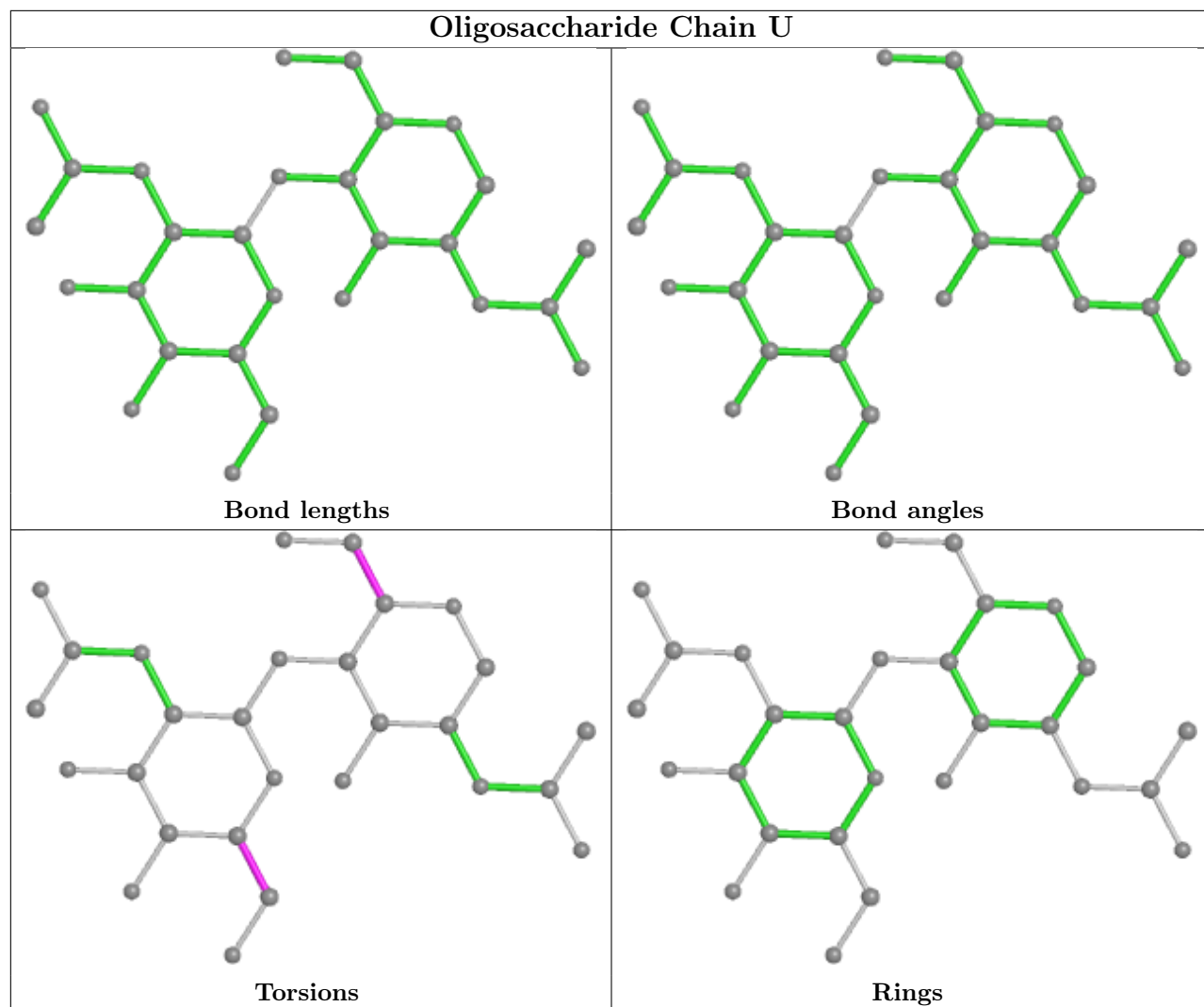


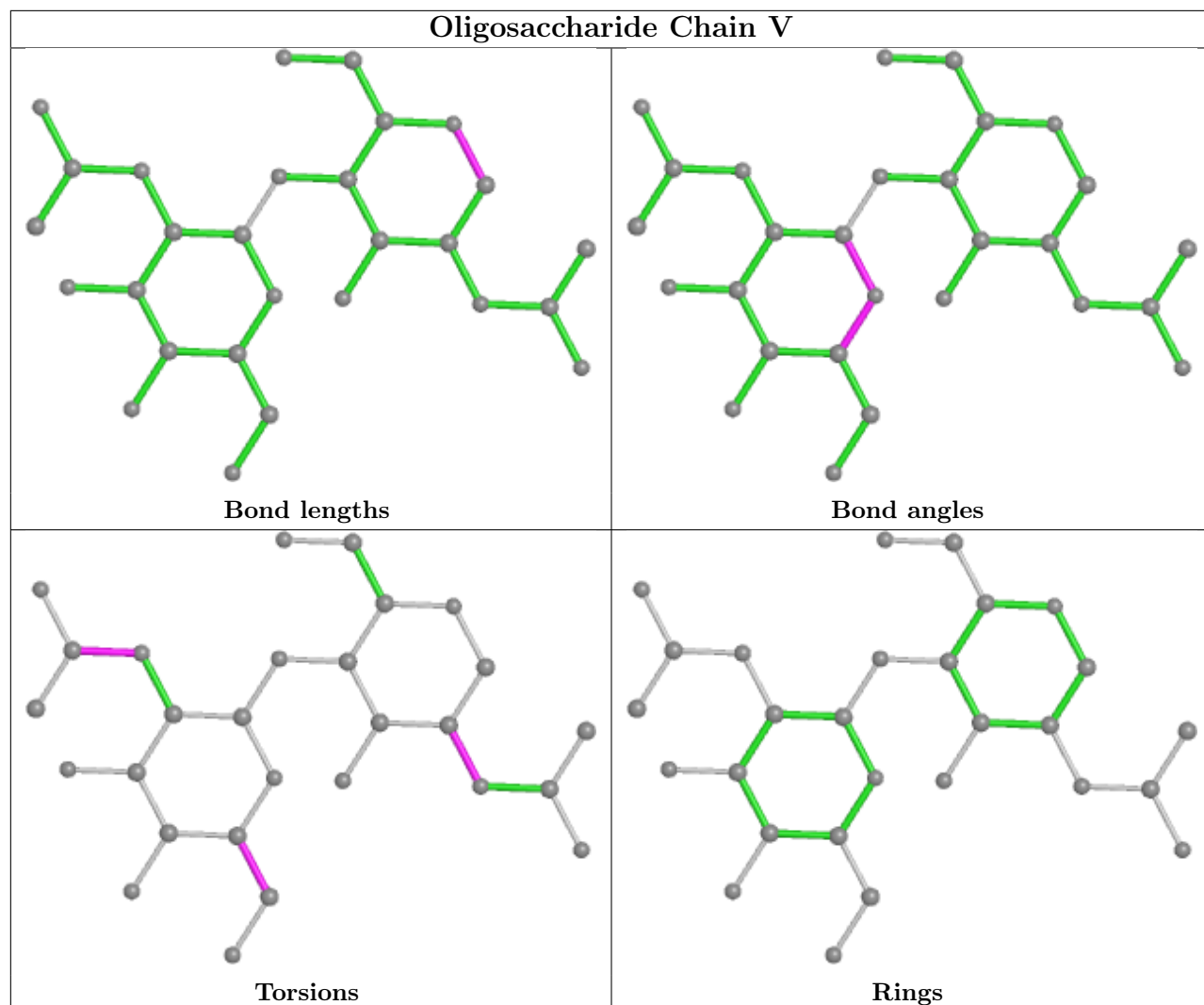


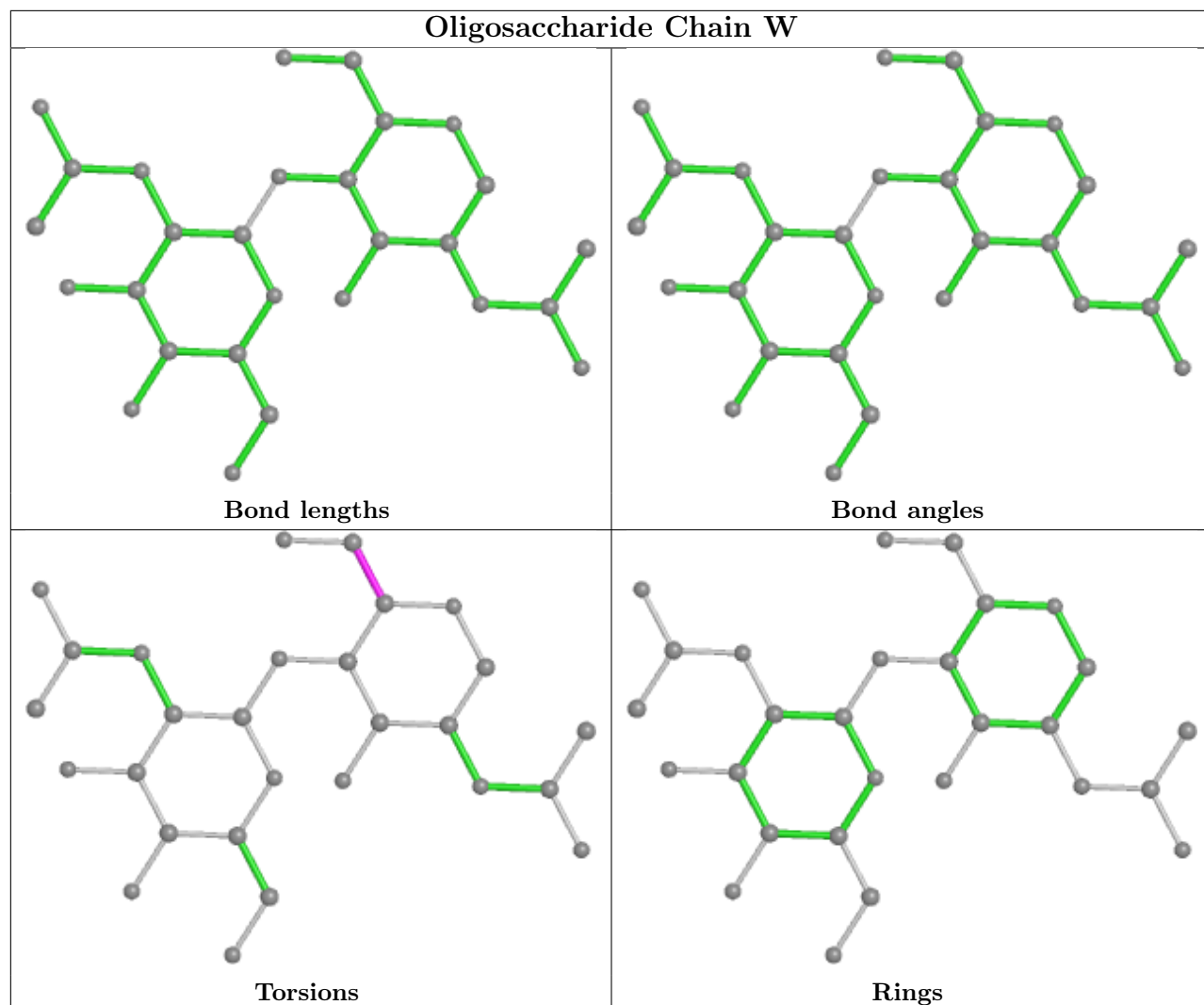


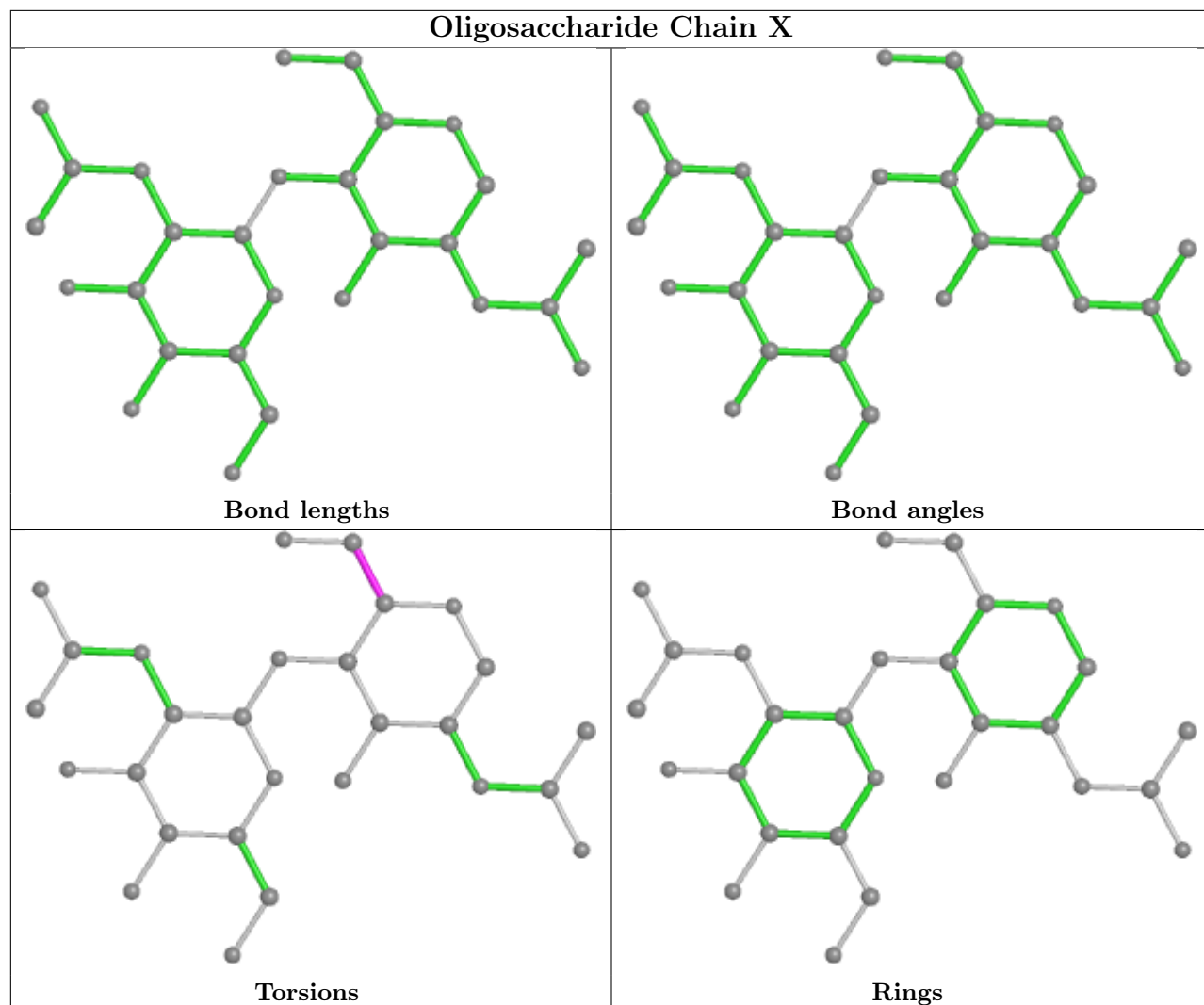


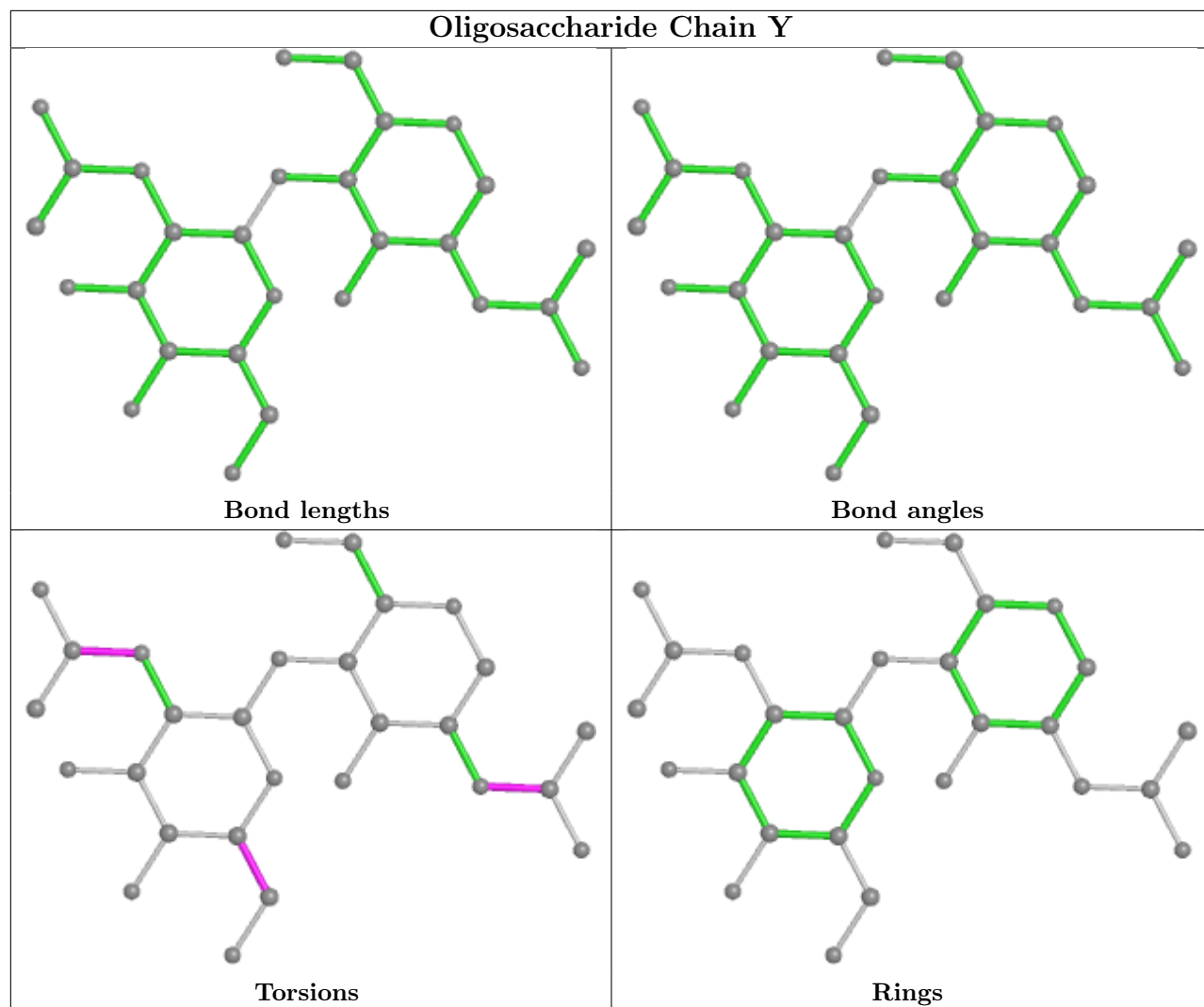


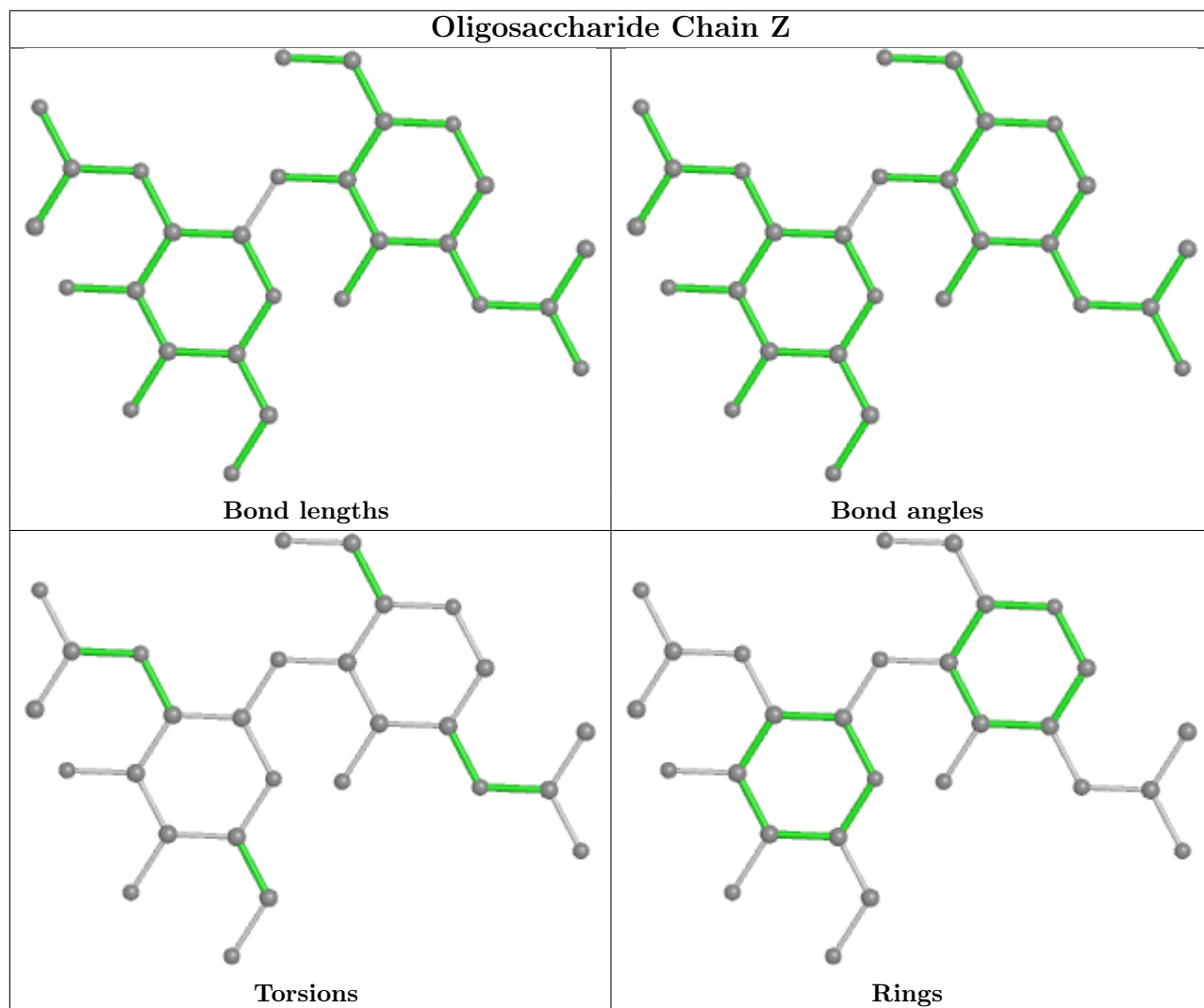


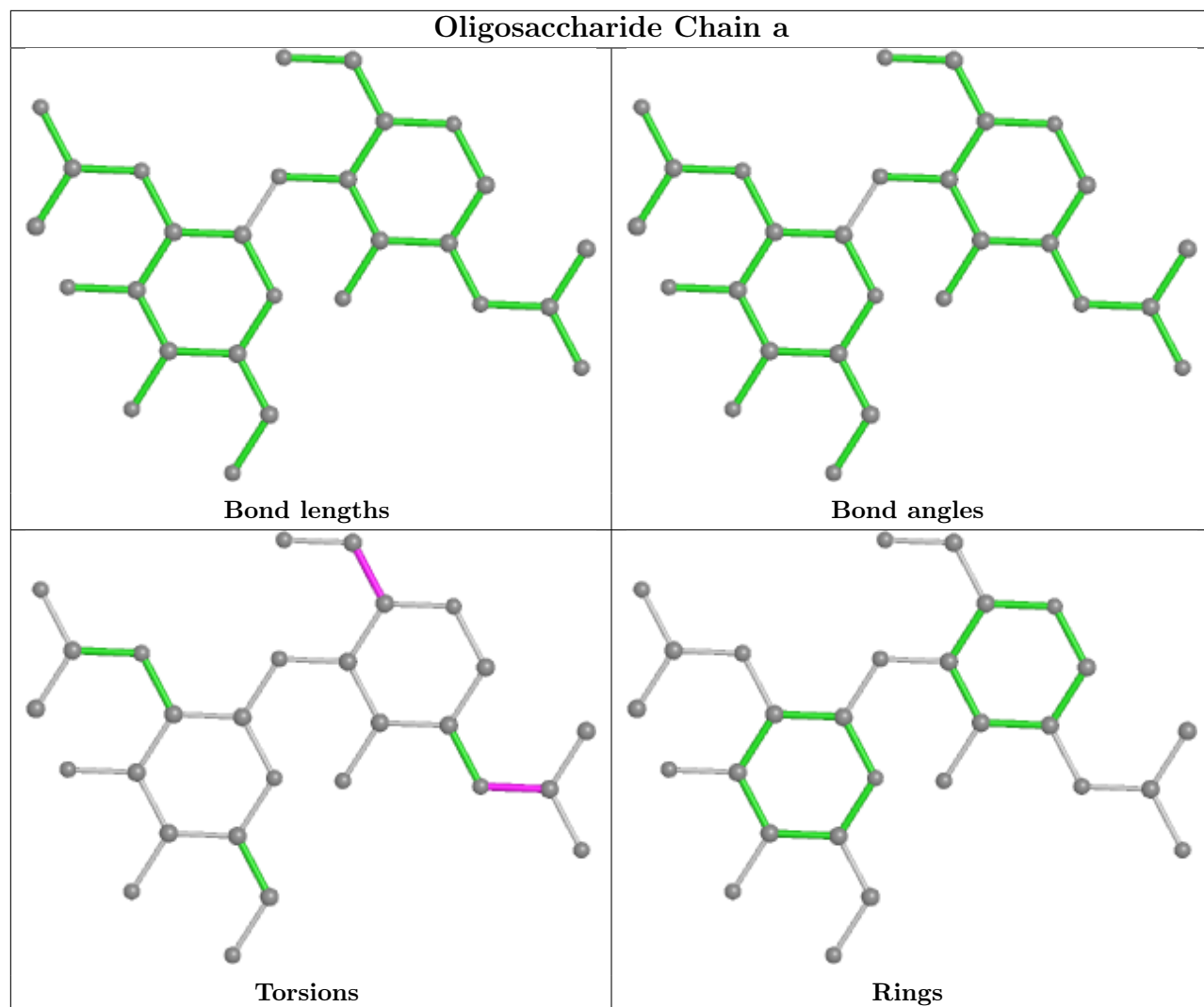


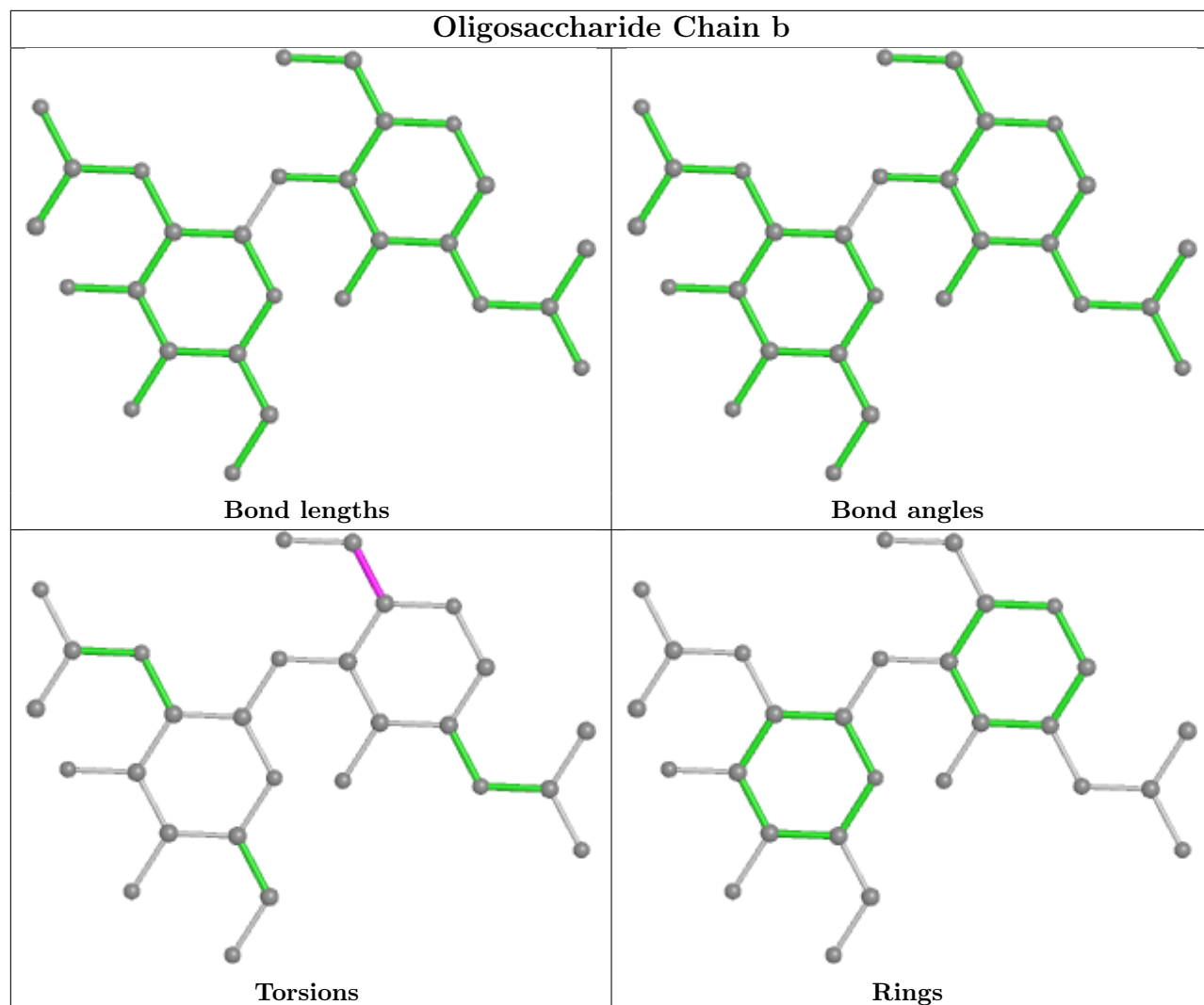


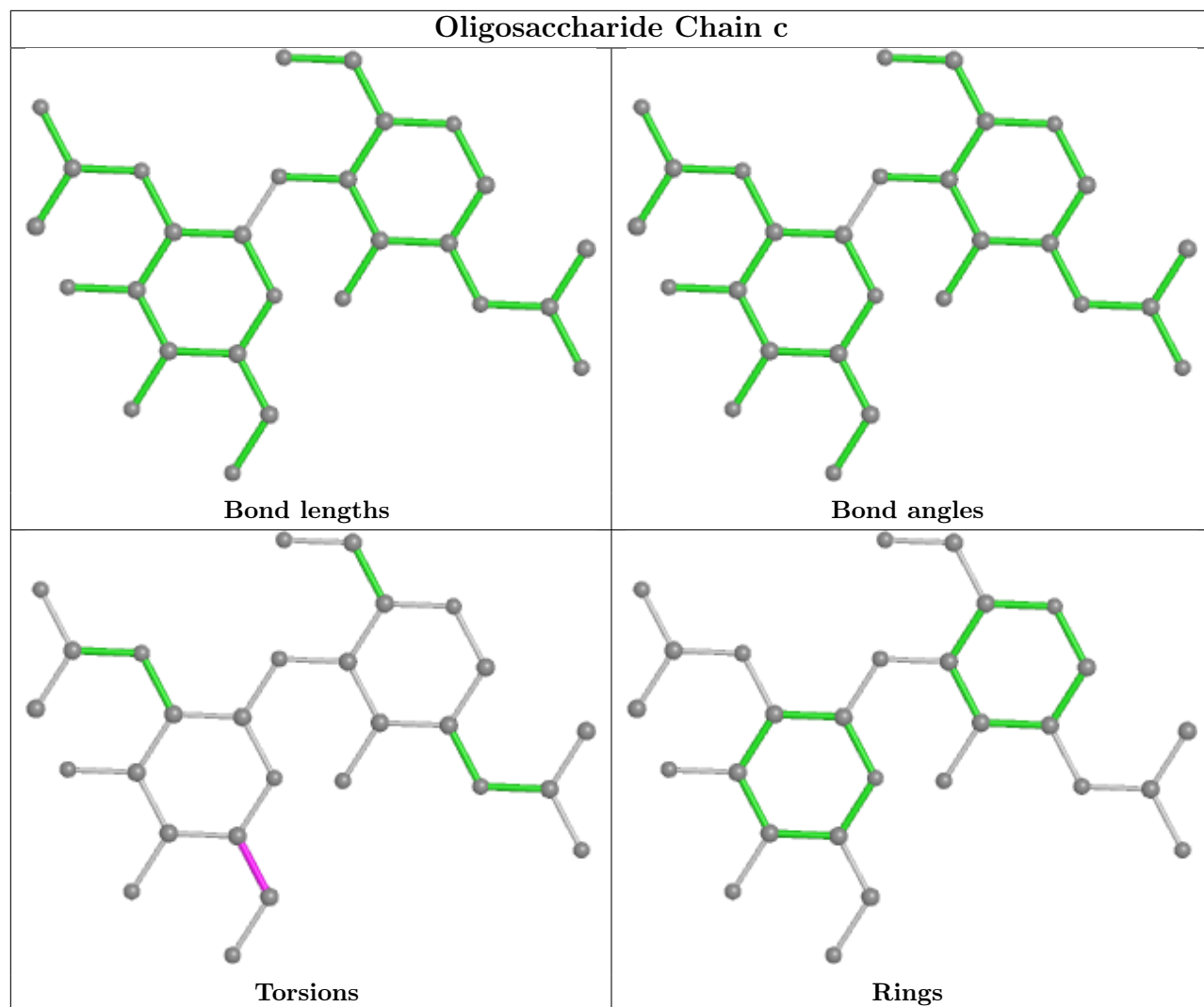


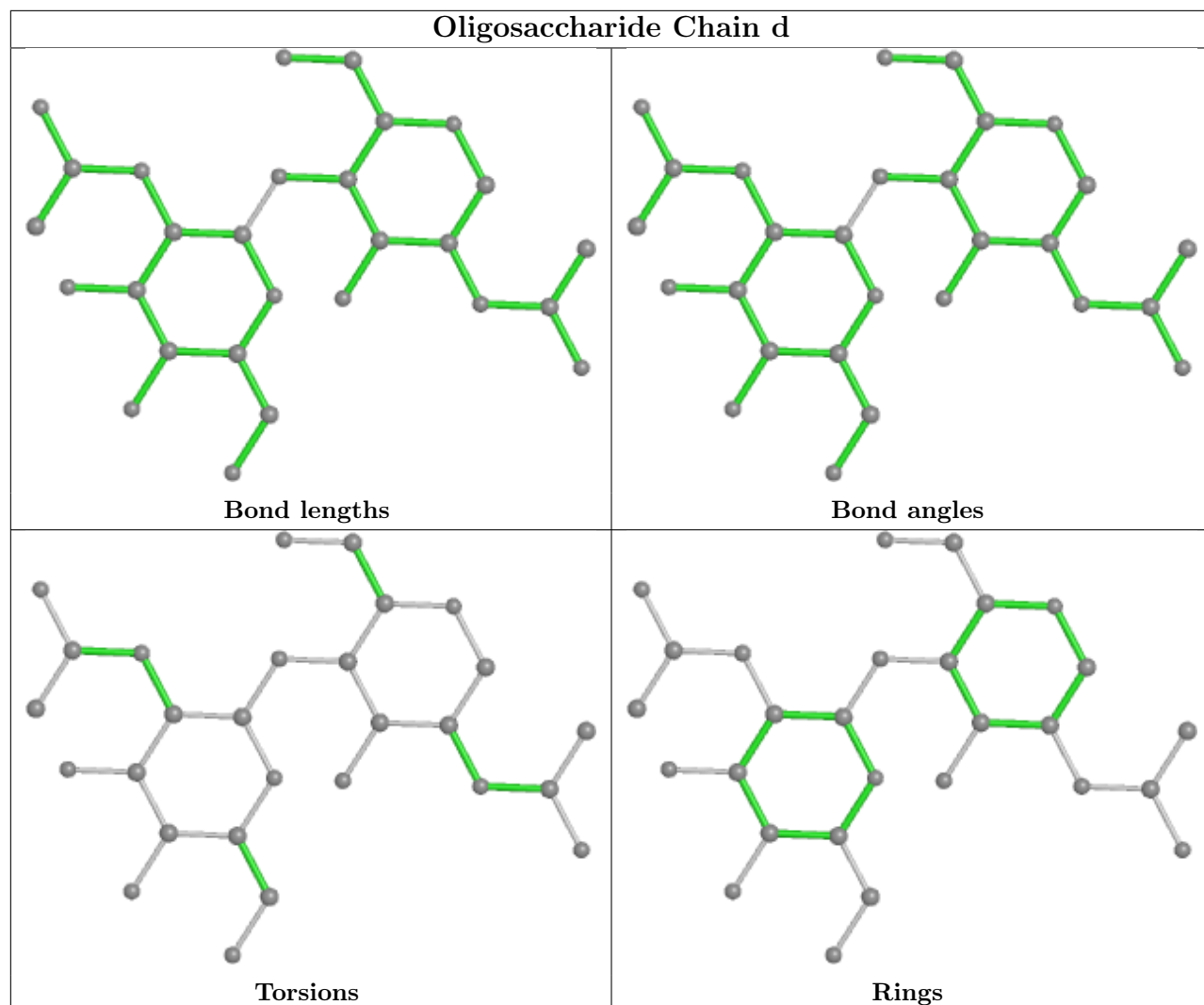


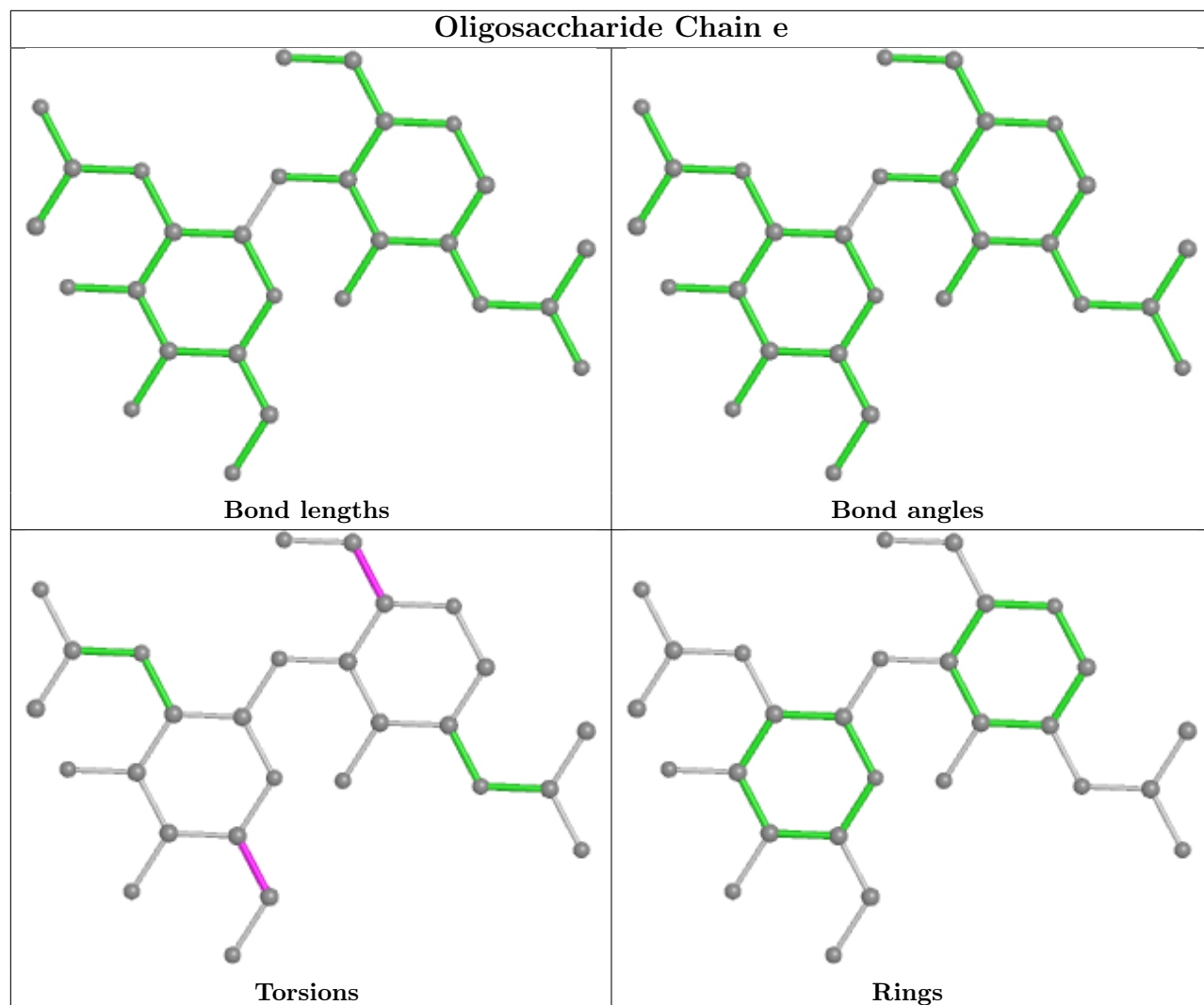


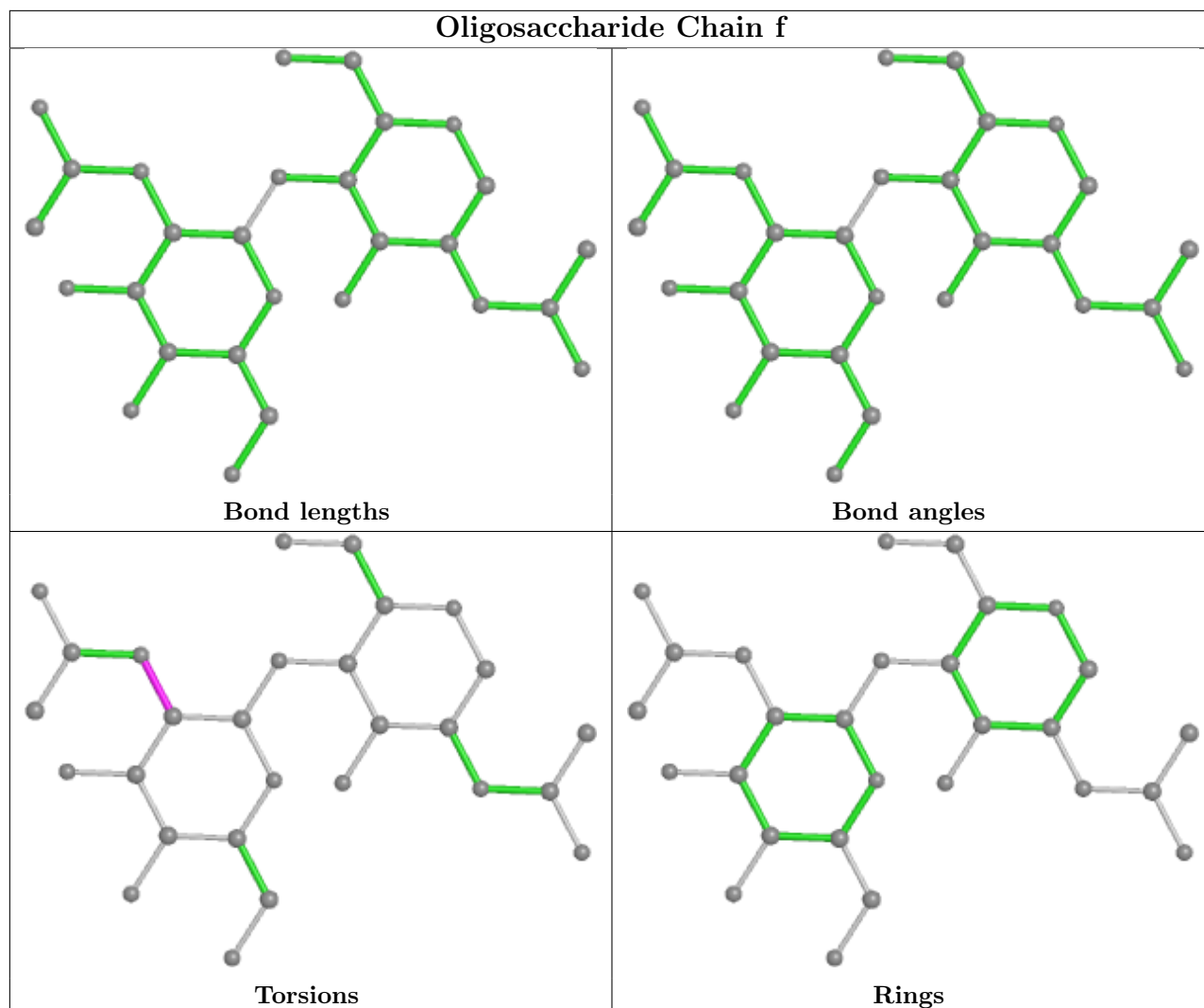












5.6 Ligand geometry [i](#)

17 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	C	2004	1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	A	2004	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	C	2006	1	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	B	2004	1	14,14,15	0.21	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	2006	1	14,14,15	0.21	0	17,19,21	0.58	0
3	NAG	C	2003	1	14,14,15	0.16	0	17,19,21	0.37	0
3	NAG	A	2002	-	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	B	2005	1	14,14,15	0.19	0	17,19,21	0.40	0
3	NAG	C	2005	1	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	B	2002	1	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	C	2001	1	14,14,15	0.32	0	17,19,21	0.36	0
3	NAG	C	2002	1	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	B	2003	1	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	A	2001	1	14,14,15	0.21	0	17,19,21	0.79	1 (5%)
3	NAG	A	2003	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	B	2001	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	2005	1	14,14,15	0.24	0	17,19,21	0.46	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	C	2004	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
3	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2006	1	-	3/6/23/26	0/1/1/1
3	NAG	C	2003	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2002	-	-	2/6/23/26	0/1/1/1
3	NAG	B	2005	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	2002	1	-	4/6/23/26	0/1/1/1
3	NAG	C	2001	1	-	3/6/23/26	0/1/1/1
3	NAG	C	2002	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2003	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2005	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	NAG	C1-O5-C5	2.41	115.46	112.19

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2005	NAG	C4-C5-C6-O6
3	C	2003	NAG	C4-C5-C6-O6
3	A	2002	NAG	O5-C5-C6-O6
3	B	2003	NAG	O5-C5-C6-O6
3	A	2002	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2005	NAG	1	0
3	B	2002	NAG	1	0
3	C	2002	NAG	1	0
3	B	2001	NAG	1	0
3	A	2005	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.

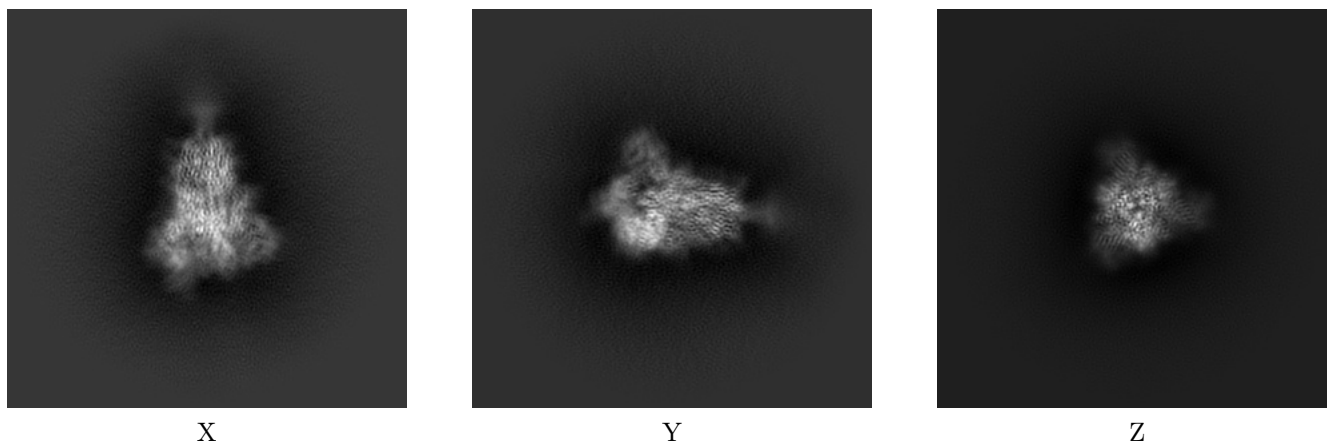
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31798. 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 [i](#)

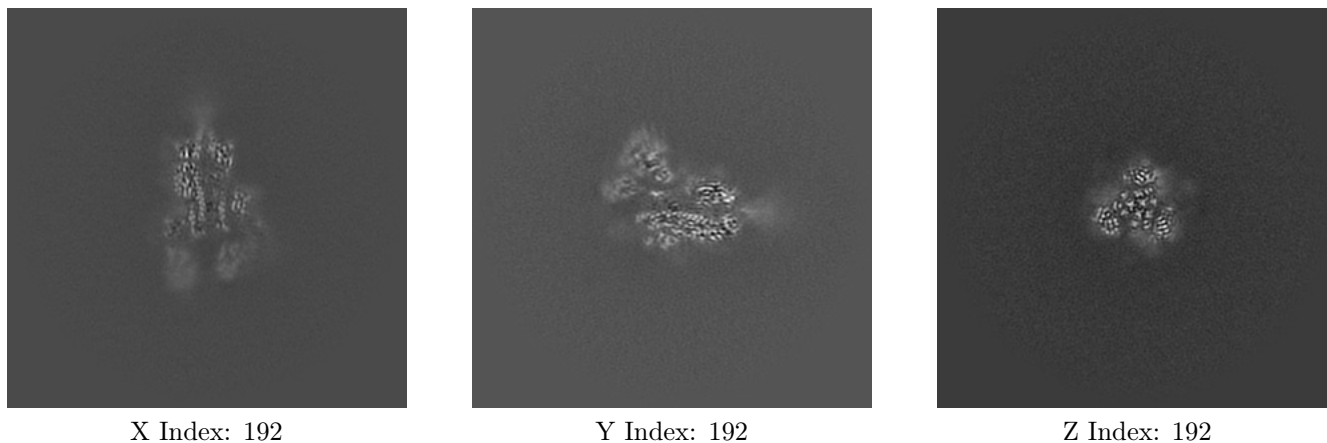
6.1.1 Primary map



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

6.2 Central slices [i](#)

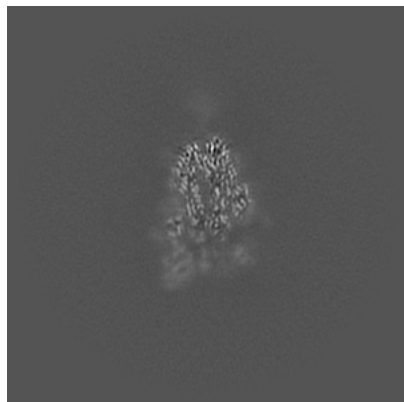
6.2.1 Primary map



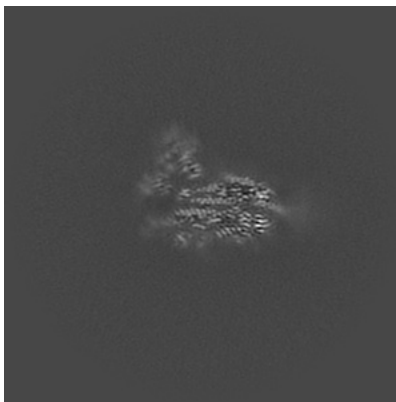
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

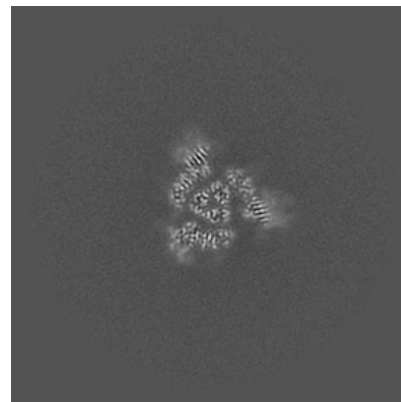
6.3.1 Primary map



X Index: 201



Y Index: 196



Z Index: 171

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

6.4 Orthogonal surface views [i](#)

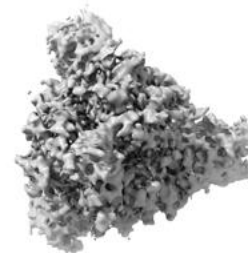
6.4.1 Primary map



X



Y



Z

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.

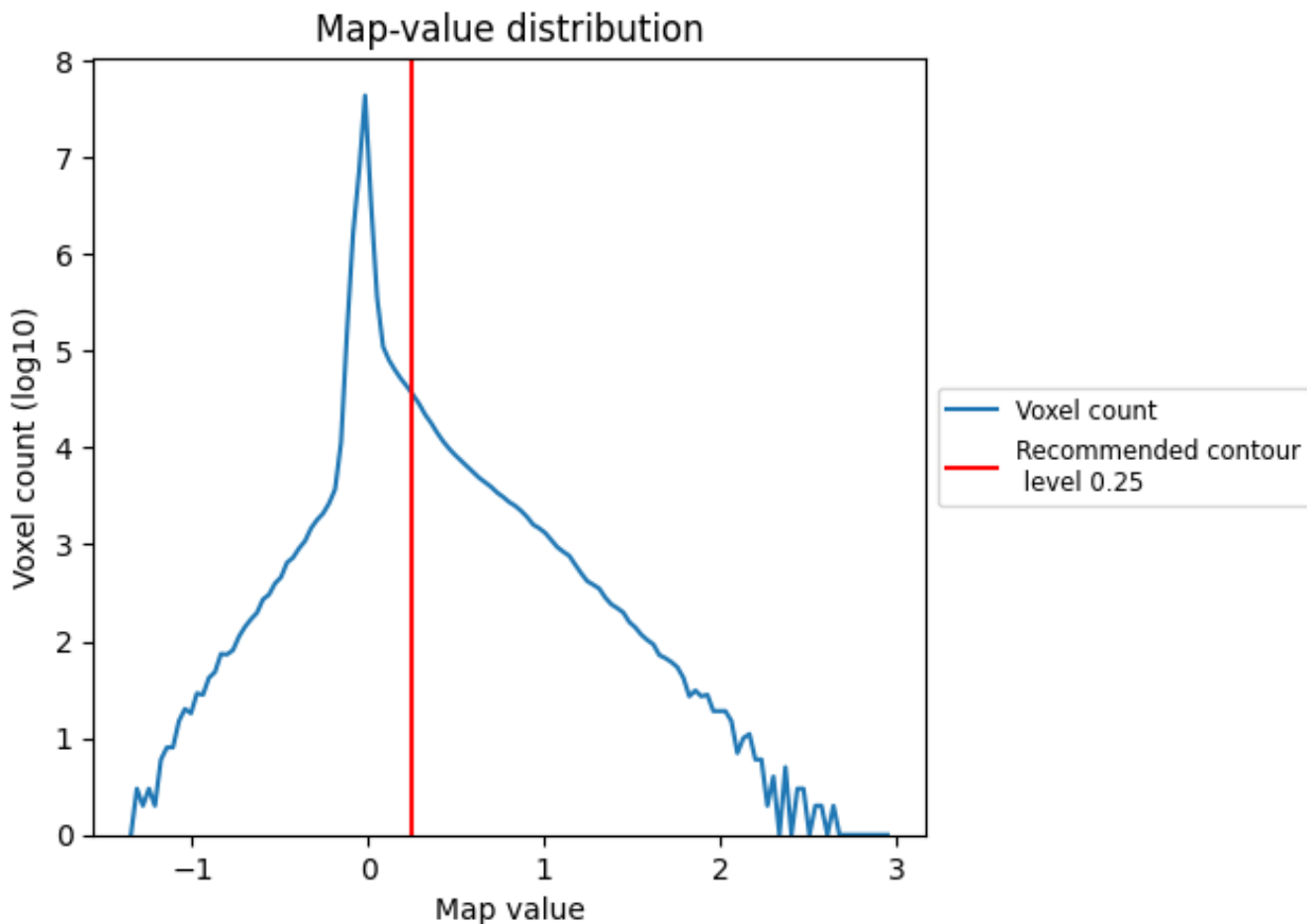
6.5 Mask visualisation

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

7 Map analysis [i](#)

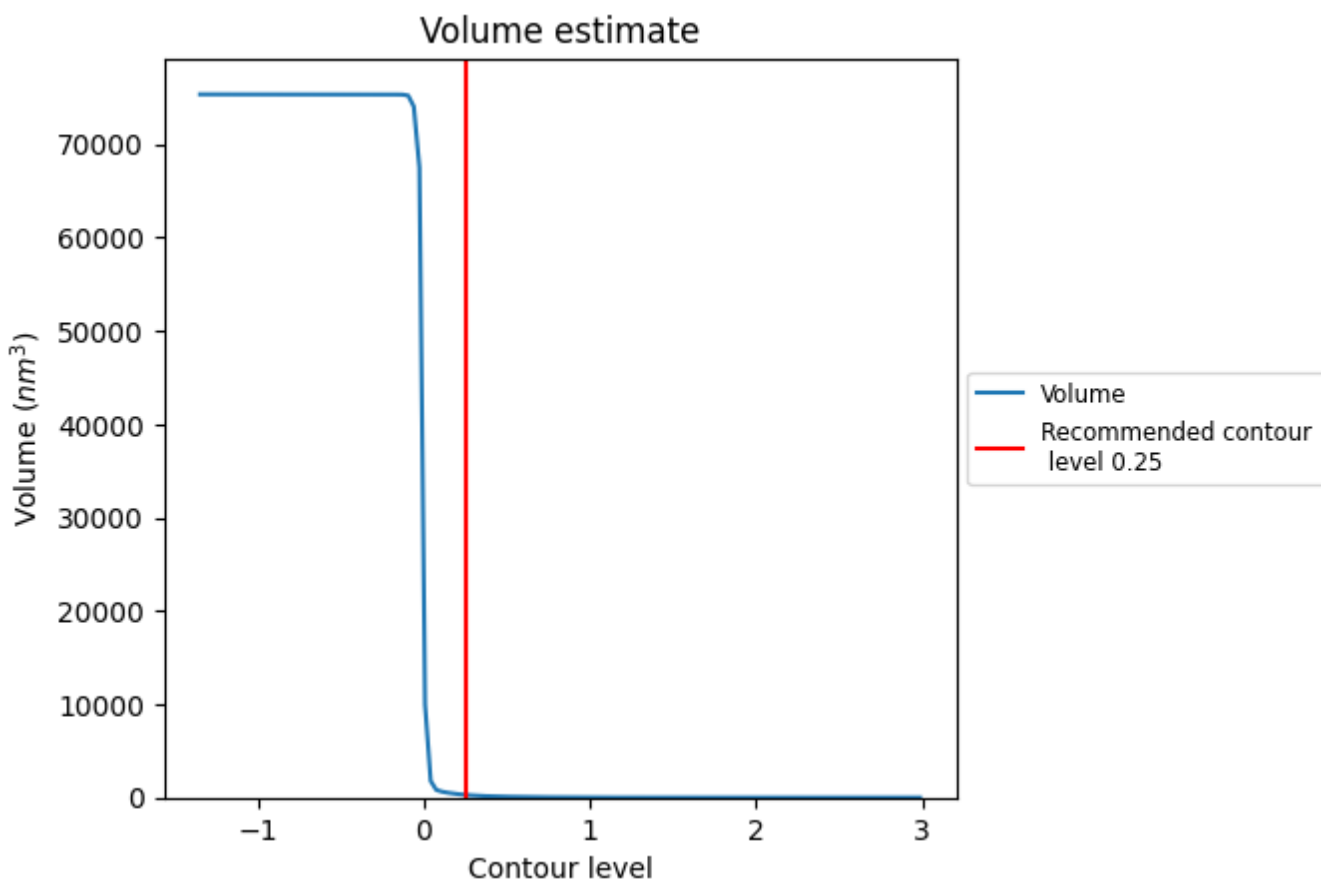
This section contains the results of statistical analysis of the map.

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.

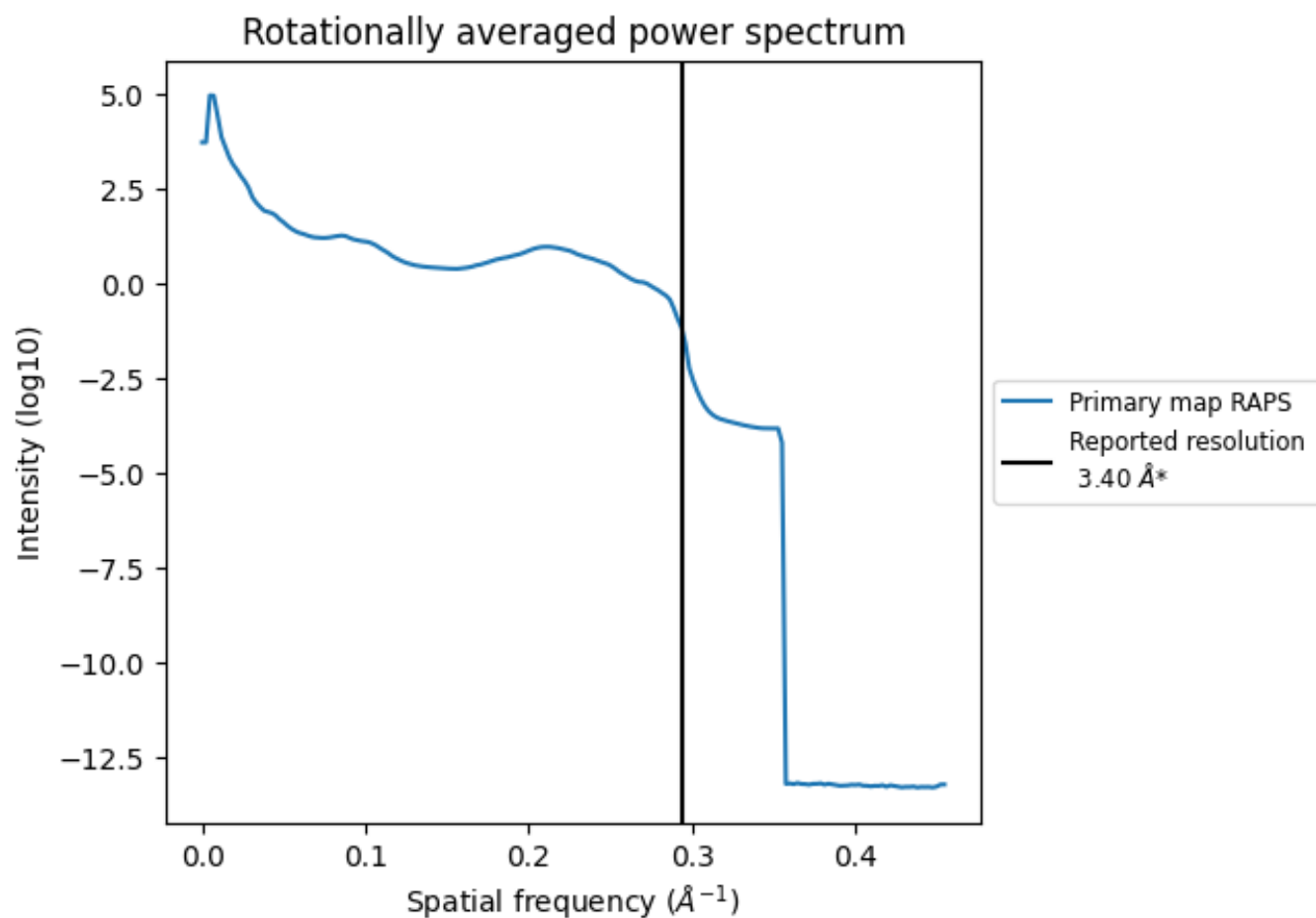
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 288 nm³; this corresponds to an approximate mass of 260 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

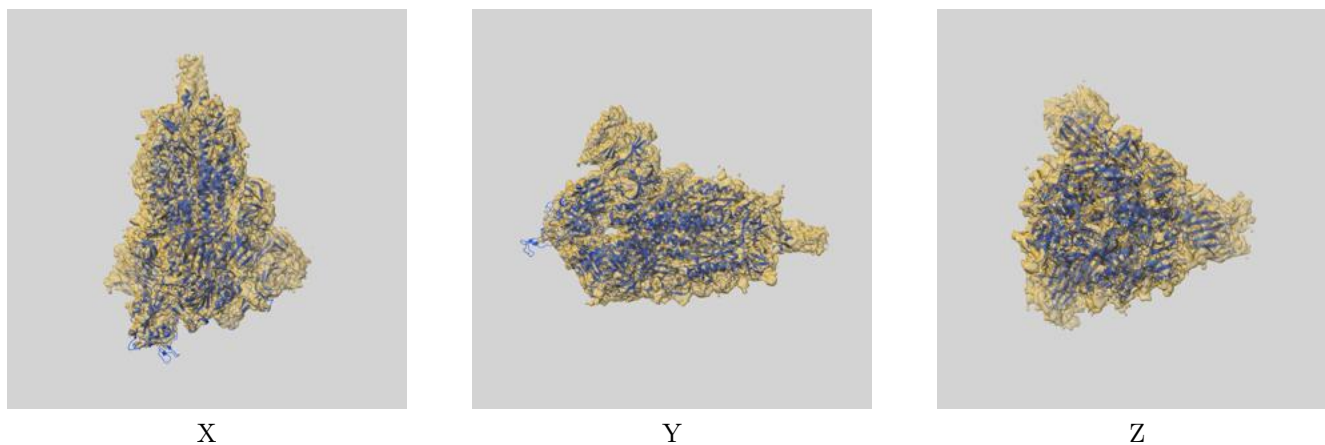
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31798 and PDB model 7V8C. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



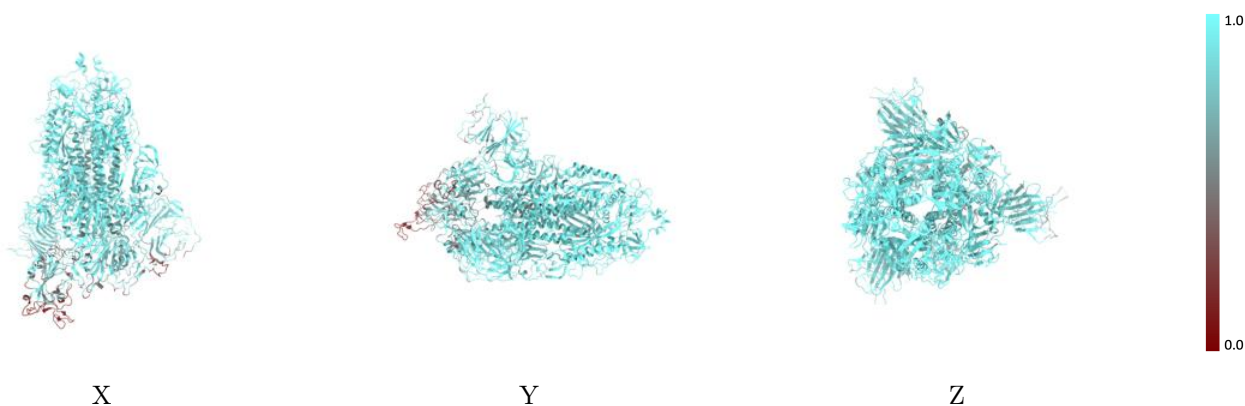
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



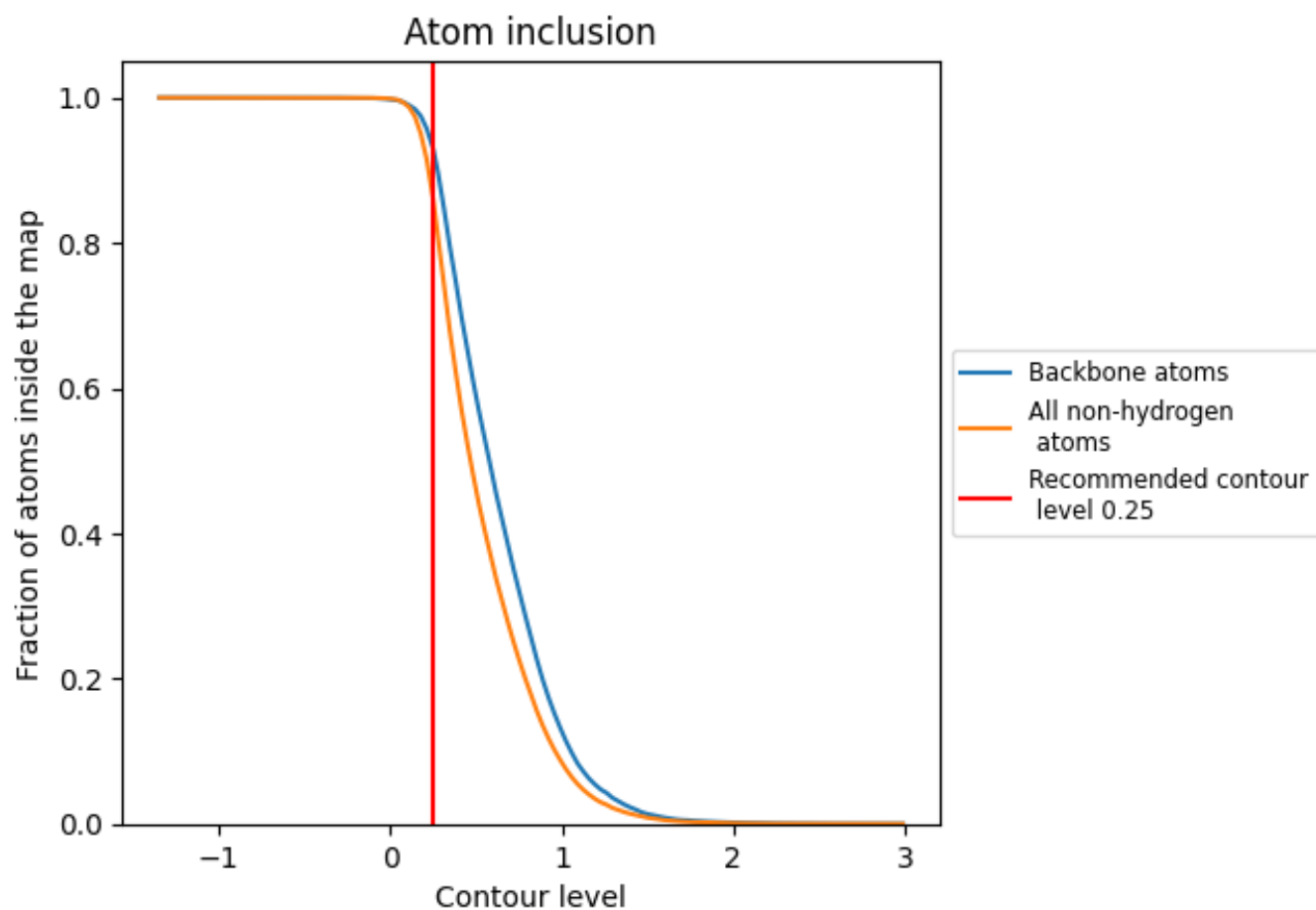
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 86% 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	 0.8575	 0.3870
A	 0.8356	 0.3700
B	 0.8801	 0.3970
C	 0.8801	 0.3950
D	 0.1071	 0.2830
E	 0.4286	 0.3600
F	 0.5357	 0.2610
G	 0.2857	 0.2600
H	 0.6786	 0.3520
I	 0.6429	 0.4930
J	 0.8571	 0.4550
K	 0.8214	 0.3590
L	 0.6071	 0.3500
M	 0.8571	 0.4420
N	 0.7857	 0.4530
O	 0.5000	 0.2890
P	 0.3571	 0.3110
Q	 0.3214	 0.3400
R	 0.4643	 0.3180
S	 0.5714	 0.4080
T	 0.9643	 0.4660
U	 0.8214	 0.3680
V	 0.4643	 0.2900
W	 0.9286	 0.4770
X	 0.8571	 0.4360
Y	 0.3929	 0.2420
Z	 0.2143	 0.2050
a	 0.6429	 0.3800
b	 0.9286	 0.4820
c	 0.8214	 0.4350
d	 0.6071	 0.3200
e	 0.8929	 0.4380
f	 0.7857	 0.4180

