



# wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 12:00 PM JST

PDB ID : 7EDJ  
EMDB ID : EMD-31073  
Title : Cryo-EM structure of SARS-CoV-2 S-UK variant (B.1.1.7) in complex with Angiotensin-converting enzyme 2 (ACE2) ectodomain  
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Wu, H.C.; Hsu, S.T.D.  
Deposited on : 2021-03-16  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

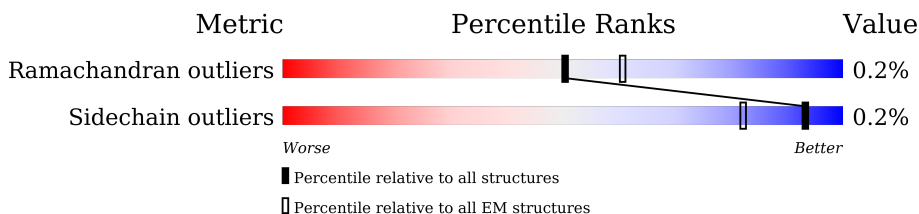
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

Mol	Chain	Length	Quality of chain
1	A	1286	
1	B	1286	
1	C	1286	
2	I	861	
2	J	861	
2	K	861	
3	D	2	
3	E	2	
3	F	2	


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

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Mol	Chain	Length	Quality of chain
3	i	2	 100%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 39565 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	1024	7992	5104	1329	1523	36	0	0
1	B	1016	7933	5070	1319	1508	36	0	0
1	C	1008	7878	5037	1308	1497	36	0	0

There are 330 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P0DTC2
A	-4	GLU	-	expression tag	UNP P0DTC2
A	-3	THR	-	expression tag	UNP P0DTC2
A	-2	ASP	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	LEU	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	TRP	-	expression tag	UNP P0DTC2
A	4	VAL	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	TRP	-	expression tag	UNP P0DTC2
A	9	VAL	-	expression tag	UNP P0DTC2
A	10	PRO	-	expression tag	UNP P0DTC2
A	11	GLY	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	14	GLY	-	expression tag	UNP P0DTC2
A	15	ASP	-	expression tag	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	TYR	ASN	conflict	UNP P0DTC2
A	567	ASP	ALA	conflict	UNP P0DTC2
A	611	GLY	ASP	conflict	UNP P0DTC2
A	678	HIS	PRO	conflict	UNP P0DTC2
A	680	ALA	ARG	conflict	UNP P0DTC2
A	682	ALA	ARG	conflict	UNP P0DTC2
A	713	ILE	THR	conflict	UNP P0DTC2
A	979	ALA	SER	conflict	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1115	HIS	ASP	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
B	-5	MET	-	initiating methionine	UNP P0DTC2
B	-4	GLU	-	expression tag	UNP P0DTC2
B	-3	THR	-	expression tag	UNP P0DTC2
B	-2	ASP	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	LEU	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	TRP	-	expression tag	UNP P0DTC2
B	4	VAL	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	TRP	-	expression tag	UNP P0DTC2
B	9	VAL	-	expression tag	UNP P0DTC2
B	10	PRO	-	expression tag	UNP P0DTC2
B	11	GLY	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	14	GLY	-	expression tag	UNP P0DTC2
B	15	ASP	-	expression tag	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	498	TYR	ASN	conflict	UNP P0DTC2
B	567	ASP	ALA	conflict	UNP P0DTC2
B	611	GLY	ASP	conflict	UNP P0DTC2
B	678	HIS	PRO	conflict	UNP P0DTC2
B	680	ALA	ARG	conflict	UNP P0DTC2
B	682	ALA	ARG	conflict	UNP P0DTC2
B	713	ILE	THR	conflict	UNP P0DTC2
B	979	ALA	SER	conflict	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1115	HIS	ASP	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-5	MET	-	initiating methionine	UNP P0DTC2
C	-4	GLU	-	expression tag	UNP P0DTC2
C	-3	THR	-	expression tag	UNP P0DTC2
C	-2	ASP	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	LEU	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	TRP	-	expression tag	UNP P0DTC2
C	4	VAL	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	TRP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	VAL	-	expression tag	UNP P0DTC2
C	10	PRO	-	expression tag	UNP P0DTC2
C	11	GLY	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	14	GLY	-	expression tag	UNP P0DTC2
C	15	ASP	-	expression tag	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	498	TYR	ASN	conflict	UNP P0DTC2
C	567	ASP	ALA	conflict	UNP P0DTC2
C	611	GLY	ASP	conflict	UNP P0DTC2
C	678	HIS	PRO	conflict	UNP P0DTC2
C	680	ALA	ARG	conflict	UNP P0DTC2
C	682	ALA	ARG	conflict	UNP P0DTC2
C	713	ILE	THR	conflict	UNP P0DTC2
C	979	ALA	SER	conflict	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1115	HIS	ASP	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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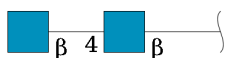
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1269	LEU	-	expression tag	UNP P0DTC2
C	1270	ASN	-	expression tag	UNP P0DTC2
C	1271	MET	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	THR	-	expression tag	UNP P0DTC2
C	1274	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 a protein called Angiotensin-converting enzyme 2 (ACE2) ectodomain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	J	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	K	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

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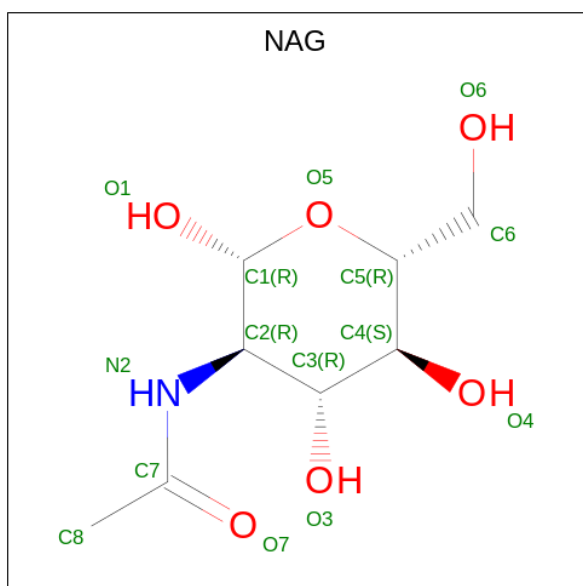
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	L	2	28	16	2	10	0	0
3	M	2	28	16	2	10	0	0
3	N	2	28	16	2	10	0	0
3	O	2	28	16	2	10	0	0
3	P	2	28	16	2	10	0	0
3	Q	2	28	16	2	10	0	0
3	R	2	28	16	2	10	0	0
3	S	2	28	16	2	10	0	0
3	T	2	28	16	2	10	0	0
3	U	2	28	16	2	10	0	0
3	V	2	28	16	2	10	0	0
3	W	2	28	16	2	10	0	0
3	X	2	28	16	2	10	0	0
3	Y	2	28	16	2	10	0	0
3	Z	2	28	16	2	10	0	0
3	a	2	28	16	2	10	0	0
3	b	2	28	16	2	10	0	0
3	c	2	28	16	2	10	0	0
3	d	2	28	16	2	10	0	0
3	e	2	28	16	2	10	0	0
3	f	2	28	16	2	10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			84	48	6	30	
4	B	1	Total	C	N	O	0
			84	48	6	30	

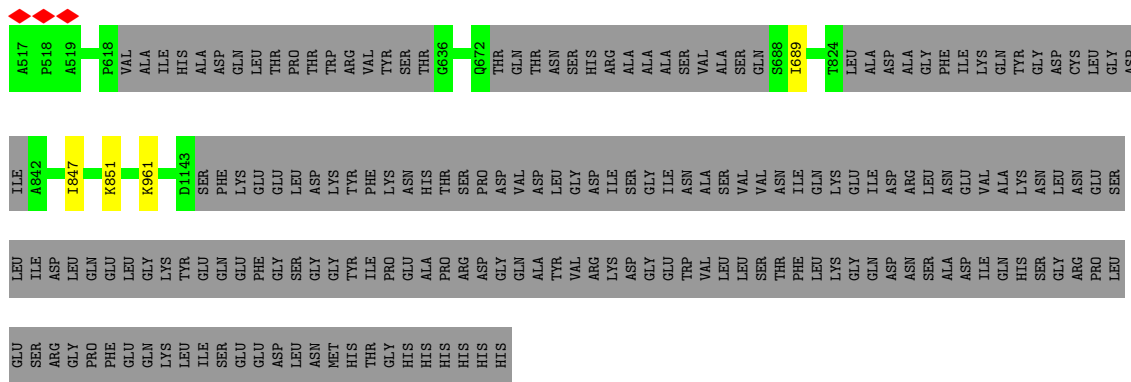
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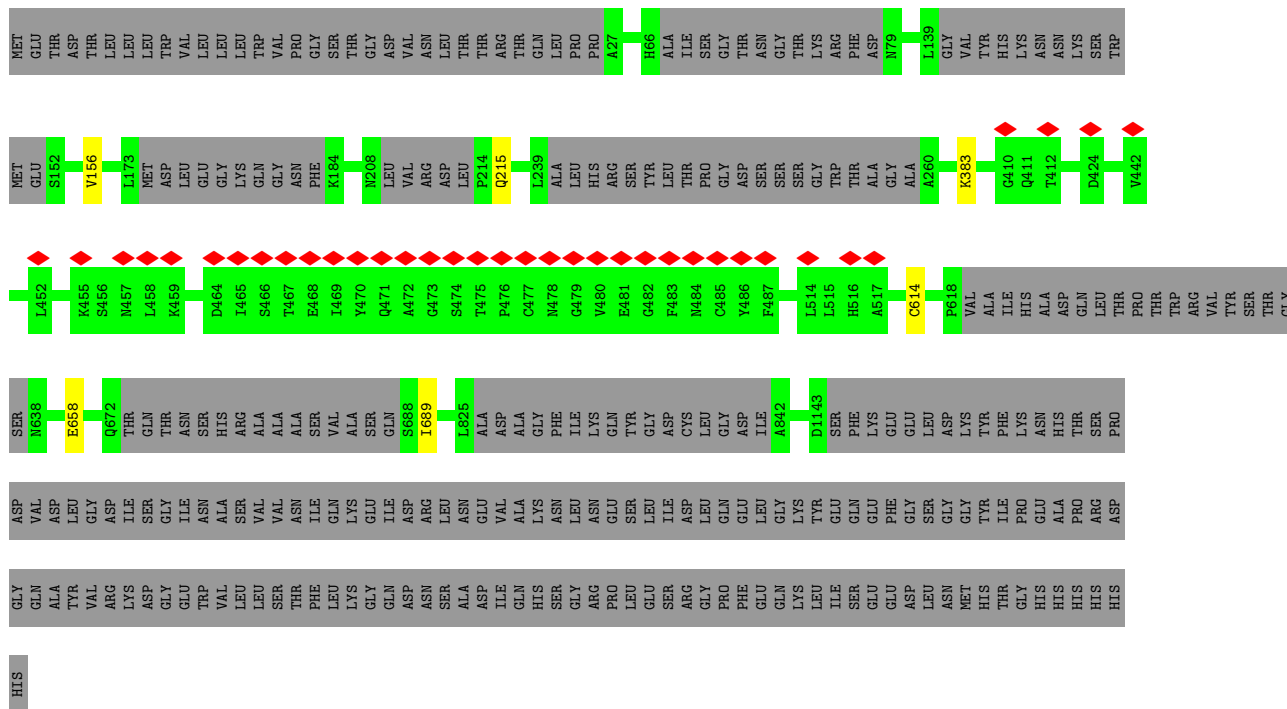
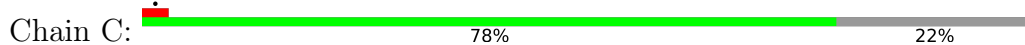
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	Total 84	C 48	N 6	O 30	0
4	B	1	Total 84	C 48	N 6	O 30	0
4	B	1	Total 84	C 48	N 6	O 30	0
4	B	1	Total 84	C 48	N 6	O 30	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	C	1	Total 98	C 56	N 7	O 35	0
4	I	1	Total 84	C 48	N 6	O 30	0
4	I	1	Total 84	C 48	N 6	O 30	0
4	I	1	Total 84	C 48	N 6	O 30	0
4	I	1	Total 84	C 48	N 6	O 30	0
4	I	1	Total 84	C 48	N 6	O 30	0
4	I	1	Total 84	C 48	N 6	O 30	0
4	J	1	Total 14	C 8	N 1	O 5	0



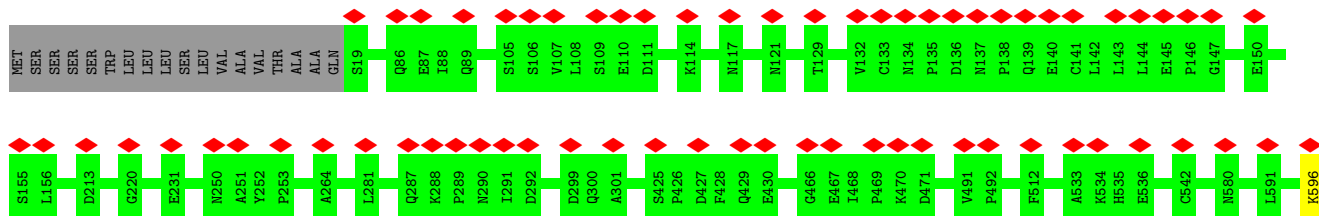




• Molecule 1: Spike glycoprotein

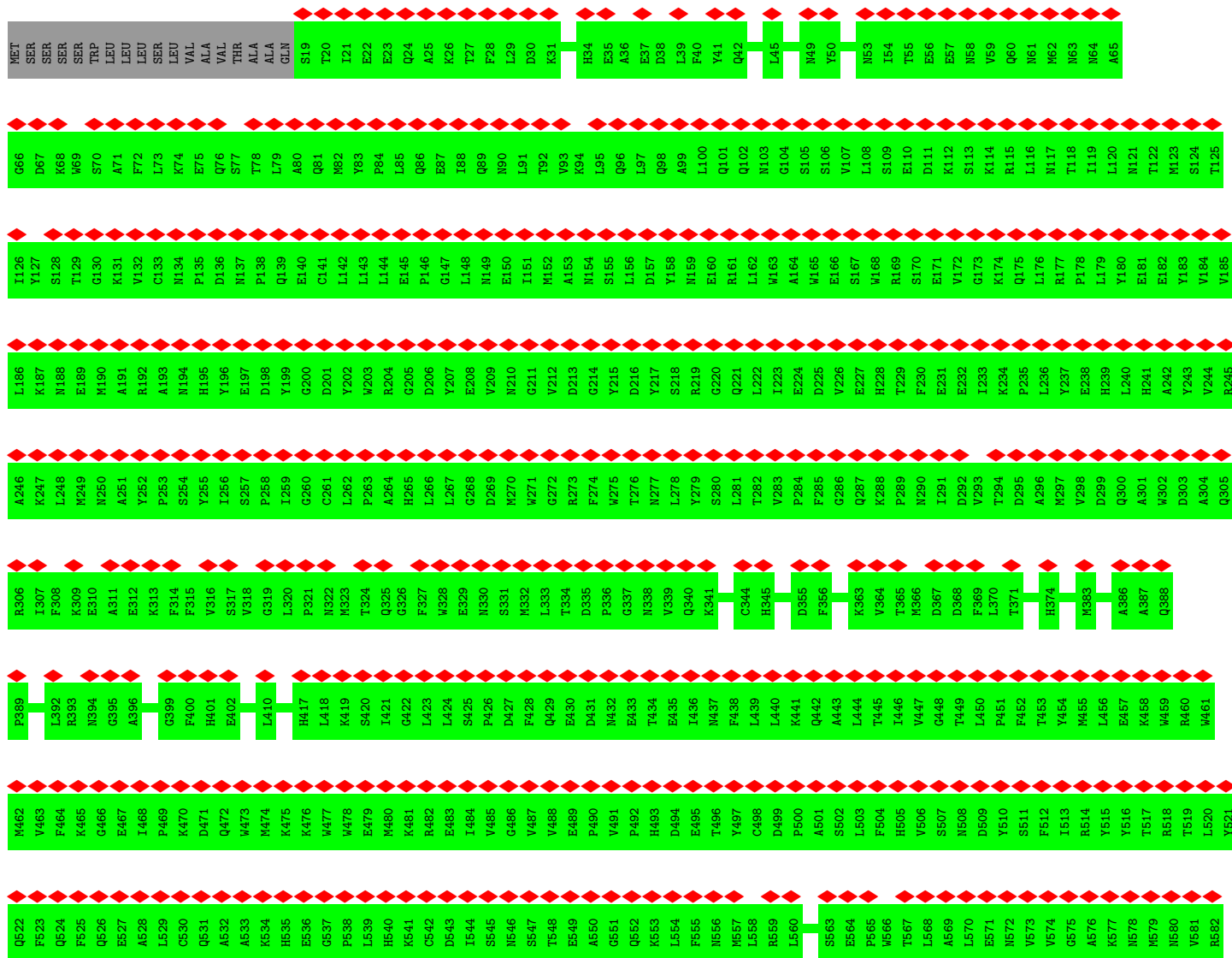


• Molecule 2: Angiotensin-converting enzyme 2 (ACE2) ectodomain





● Molecule 2: Angiotensin-converting enzyme 2 (ACE2) ectodomain





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

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

LEU  
TYR  
LYS

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

Chain D:  50%  
100%

  
NAG1  
NAG2

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

Chain E:  100%

NAG1  
NAG2

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

Chain F:  100%

NAG1  
NAG2

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

Chain G:  100%

NAG1  
NAG2

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

Chain H:  50%  
50%

NAG1  
NAG2

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

Chain L:  100%

  
MAG1  
MAG2

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

Chain M:  100%

  
MAG1  
MAG2

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

Chain N:  50% 50%

  
MAG1  
MAG2

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

Chain O:  100%

  
MAG1  
MAG2

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

Chain P:  50% 50%

  
MAG1  
MAG2

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

Chain Q:  100%

  
MAG1  
MAG2

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

Chain R:  100%

MAG1  
MAG2

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

Chain S:  100%

MAG1  
MAG2

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

Chain T:  50% 50%

MAG1  
MAG2

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

Chain U:  50% 50%

MAG1  
MAG2

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

Chain V:  100%

MAG1  
MAG2

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

Chain W:  100%

MAG1  
MAG2

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

Chain X:  50% 100%



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

Chain Y:  100%



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

Chain Z:  100%




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

Chain a:  50%  
100%



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

Chain b:  100%



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

Chain c:  100%



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

Chain d:  50%  
100%





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

Chain e:  100%



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

Chain f:  100%



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

Chain g:  50% 50%



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

Chain h:  100%



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

Chain i:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	460280	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	3.115	Depositor
Minimum map value	-1.813	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.37	0/8172	0.53	0/11119
1	B	0.38	0/8113	0.52	0/11039
1	C	0.37	0/8057	0.52	0/10961
2	I	0.25	0/4999	0.45	0/6792
2	J	0.24	0/4999	0.44	0/6792
2	K	0.24	0/4999	0.45	0/6792
All	All	0.33	0/39339	0.50	0/53495

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	614	CYS	Peptide
1	C	658	GLU	Peptide

### 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1008/1286 (78%)	908 (90%)	98 (10%)	2 (0%)	47	77
1	B	1000/1286 (78%)	913 (91%)	84 (8%)	3 (0%)	41	71
1	C	990/1286 (77%)	898 (91%)	89 (9%)	3 (0%)	41	71
2	I	594/861 (69%)	556 (94%)	38 (6%)	0	100	100
2	J	594/861 (69%)	559 (94%)	35 (6%)	0	100	100
2	K	594/861 (69%)	558 (94%)	36 (6%)	0	100	100
All	All	4780/6441 (74%)	4392 (92%)	380 (8%)	8 (0%)	50	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	814	PHE
1	B	847	ILE
1	C	156	VAL
1	B	100	ARG
1	B	689	ILE

### 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	893/1115 (80%)	892 (100%)	1 (0%)	93	97
1	B	886/1115 (80%)	884 (100%)	2 (0%)	93	97
1	C	880/1115 (79%)	879 (100%)	1 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	526/752 (70%)	525 (100%)	1 (0%)	93	97
2	J	526/752 (70%)	525 (100%)	1 (0%)	93	97
2	K	526/752 (70%)	523 (99%)	3 (1%)	86	91
All	All	4237/5601 (76%)	4228 (100%)	9 (0%)	93	97

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	192	ARG
2	K	596	LYS
1	C	383	LYS
2	I	596	LYS
2	J	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	24	GLN
2	J	380	GLN
2	K	374	HIS
1	B	419	ASN
1	A	419	ASN

### 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
3	NAG	D	1	3,1	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	D	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	E	1	3,1	14,14,15	0.45	0	17,19,21	0.55	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	F	1	3,1	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.58	0	17,19,21	0.44	0
3	NAG	G	1	3,1	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	H	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	1.45	2 (11%)
3	NAG	H	2	3	14,14,15	0.18	0	17,19,21	0.44	0
3	NAG	L	1	3,1	14,14,15	0.31	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.24	0	17,19,21	0.40	0
3	NAG	M	1	3,1	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	N	1	3,1	14,14,15	0.21	0	17,19,21	1.20	2 (11%)
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	O	1	3,1	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	O	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	P	1	3,1	14,14,15	0.39	0	17,19,21	1.26	1 (5%)
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	Q	1	3,1	14,14,15	0.34	0	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	0.24	0	17,19,21	0.59	0
3	NAG	R	1	3,1	14,14,15	0.30	0	17,19,21	0.56	0
3	NAG	R	2	3	14,14,15	0.19	0	17,19,21	0.38	0
3	NAG	S	1	3,1	14,14,15	0.17	0	17,19,21	0.44	0
3	NAG	S	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	T	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	T	2	3	14,14,15	0.43	0	17,19,21	1.25	1 (5%)
3	NAG	U	1	3,1	14,14,15	0.74	1 (7%)	17,19,21	1.26	1 (5%)
3	NAG	U	2	3	14,14,15	0.20	0	17,19,21	0.49	0
3	NAG	V	1	3,1	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	V	2	3	14,14,15	0.20	0	17,19,21	0.38	0
3	NAG	W	1	3,1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	W	2	3	14,14,15	0.35	0	17,19,21	0.56	0
3	NAG	X	1	3,1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	X	2	3	14,14,15	0.27	0	17,19,21	0.39	0
3	NAG	Y	1	3,1	14,14,15	0.25	0	17,19,21	0.40	0
3	NAG	Y	2	3	14,14,15	0.17	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	Z	1	3,1	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	Z	2	3	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	a	1	3,1	14,14,15	0.36	0	17,19,21	0.45	0
3	NAG	a	2	3	14,14,15	0.25	0	17,19,21	0.38	0
3	NAG	b	1	3,1	14,14,15	0.28	0	17,19,21	1.18	2 (11%)
3	NAG	b	2	3	14,14,15	0.32	0	17,19,21	0.59	1 (5%)
3	NAG	c	1	3,1	14,14,15	0.25	0	17,19,21	0.53	0
3	NAG	c	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	d	1	3,1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	d	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	e	1	3,1	14,14,15	0.26	0	17,19,21	0.42	0
3	NAG	e	2	3	14,14,15	0.23	0	17,19,21	0.47	0
3	NAG	f	1	3,1	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	f	2	3	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	g	1	3,1	14,14,15	0.46	0	17,19,21	0.78	1 (5%)
3	NAG	g	2	3	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	h	1	3,1	14,14,15	0.35	0	17,19,21	0.36	0
3	NAG	h	2	3	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	i	1	3,1	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	i	2	3	14,14,15	0.26	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
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	f	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	h	2	3	-	1/6/23/26	0/1/1/1
3	NAG	i	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	i	2	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	C1-C2	2.84	1.56	1.52
3	U	1	NAG	O5-C1	2.38	1.47	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1	NAG	C1-O5-C5	4.90	118.84	112.19
3	P	1	NAG	C1-O5-C5	4.70	118.56	112.19
3	H	1	NAG	C1-O5-C5	4.63	118.47	112.19
3	T	2	NAG	C2-N2-C7	4.31	129.04	122.90
3	N	1	NAG	C1-O5-C5	3.74	117.25	112.19

There are no chirality outliers.

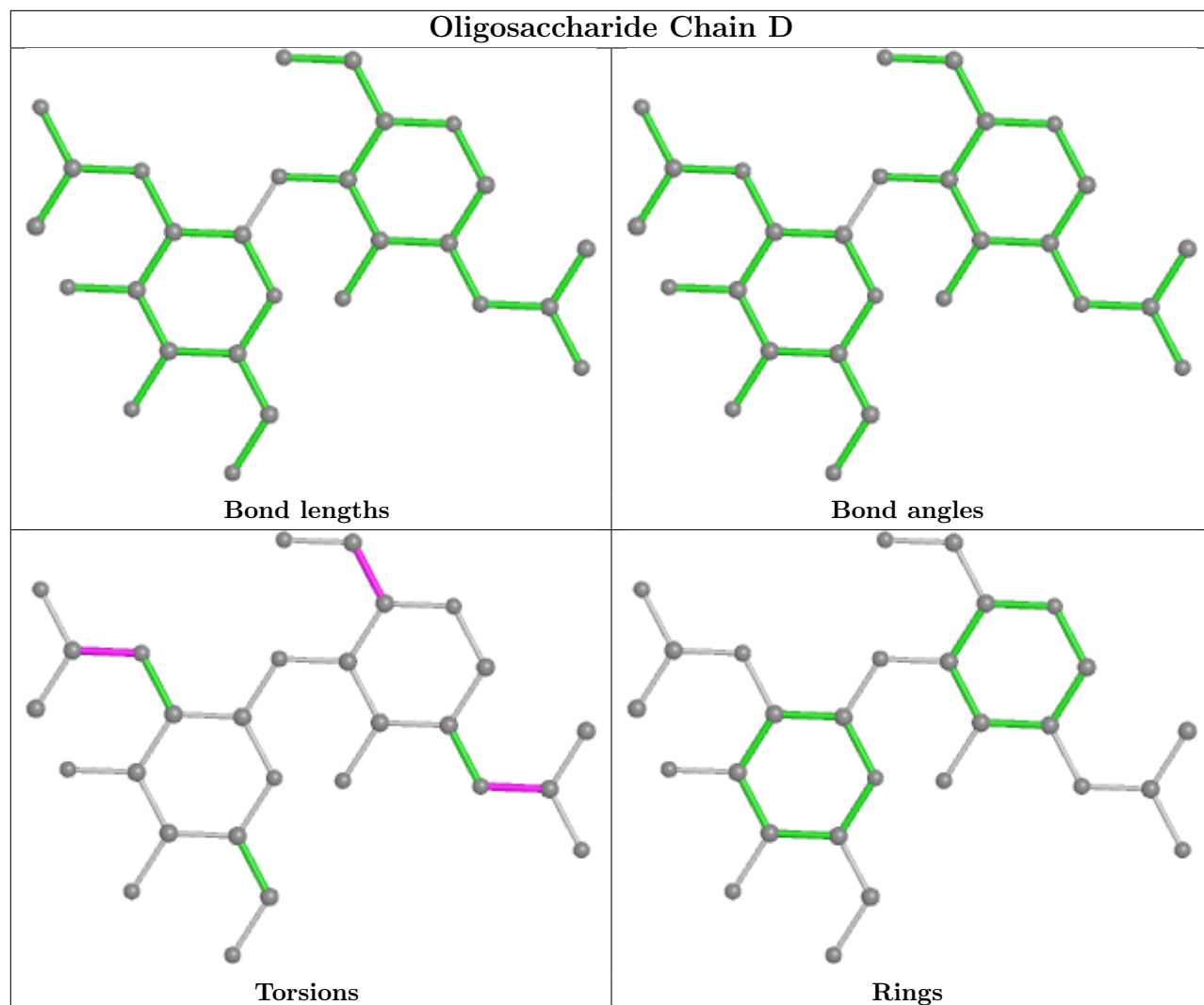
5 of 97 torsion outliers are listed below:

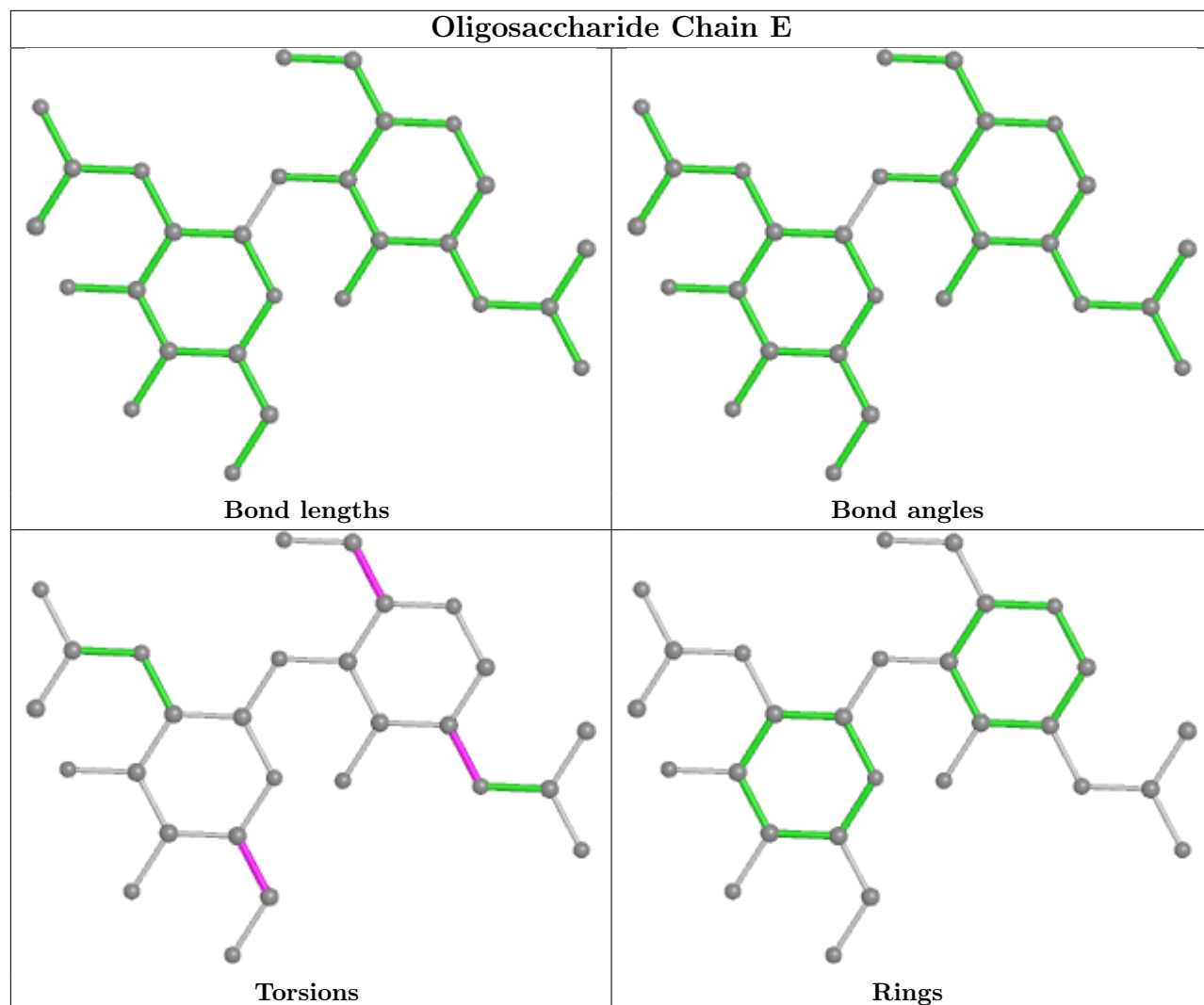
Mol	Chain	Res	Type	Atoms
3	N	2	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6

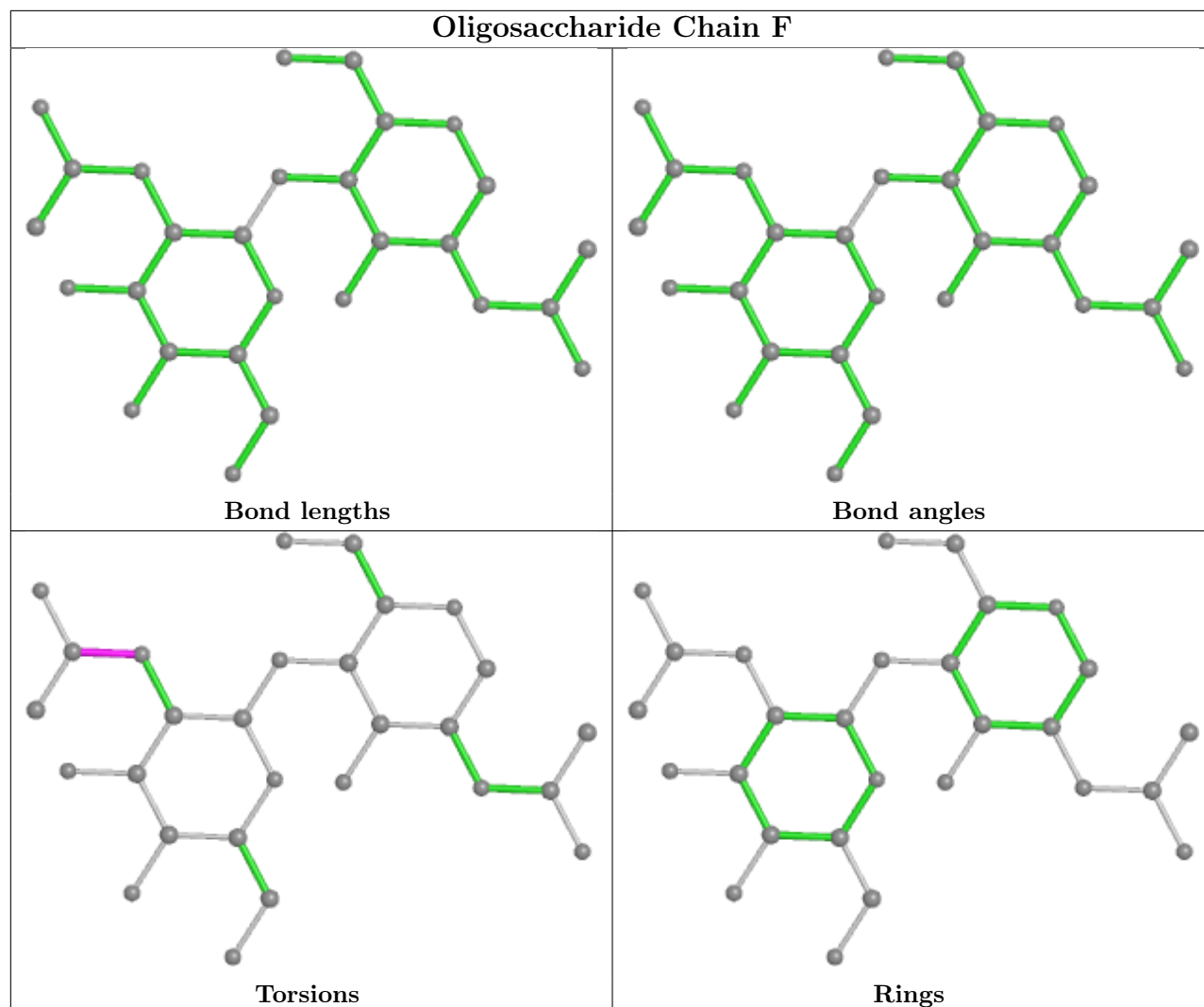
There are no ring outliers.

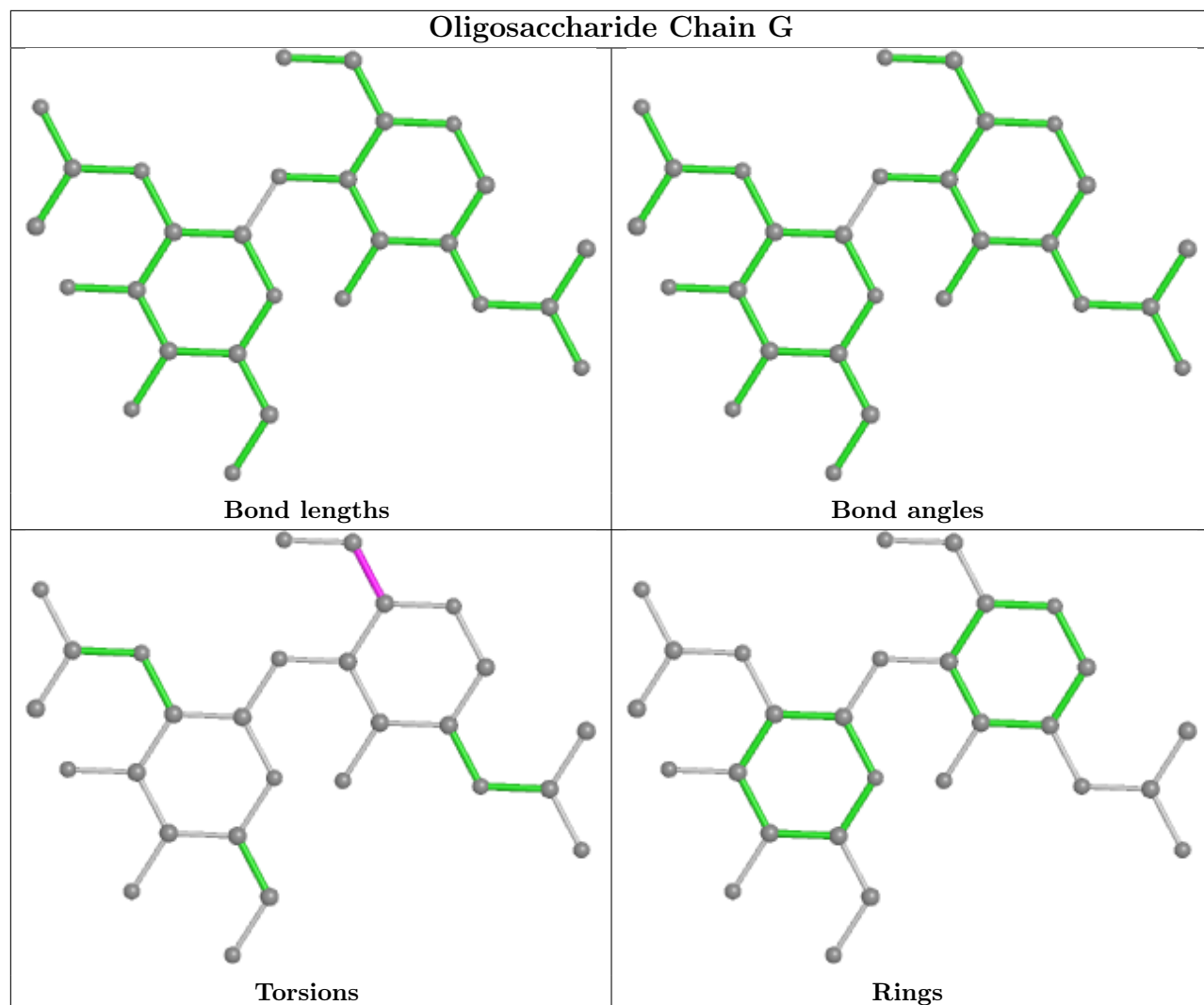
No monomer is involved in short contacts.

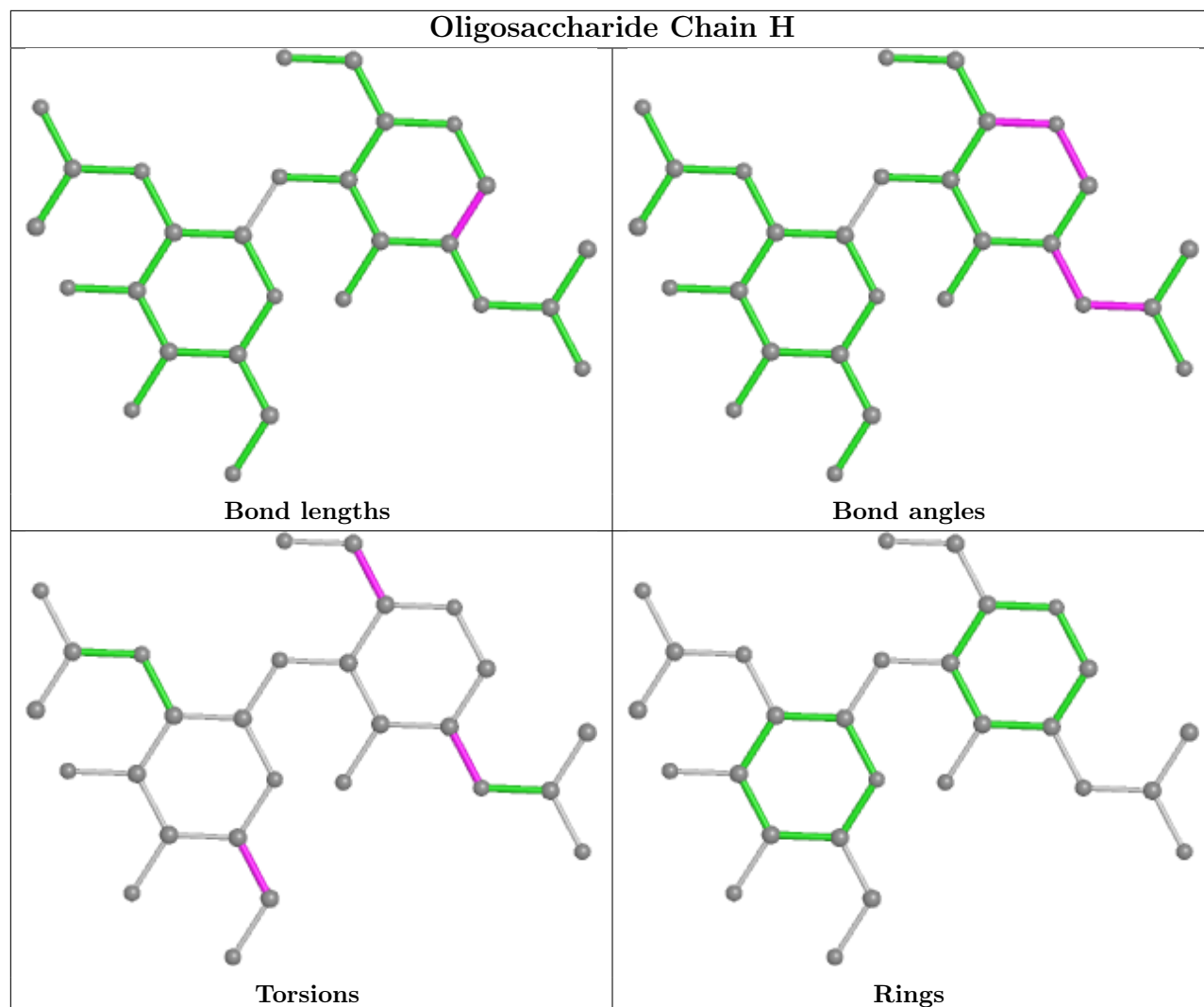
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

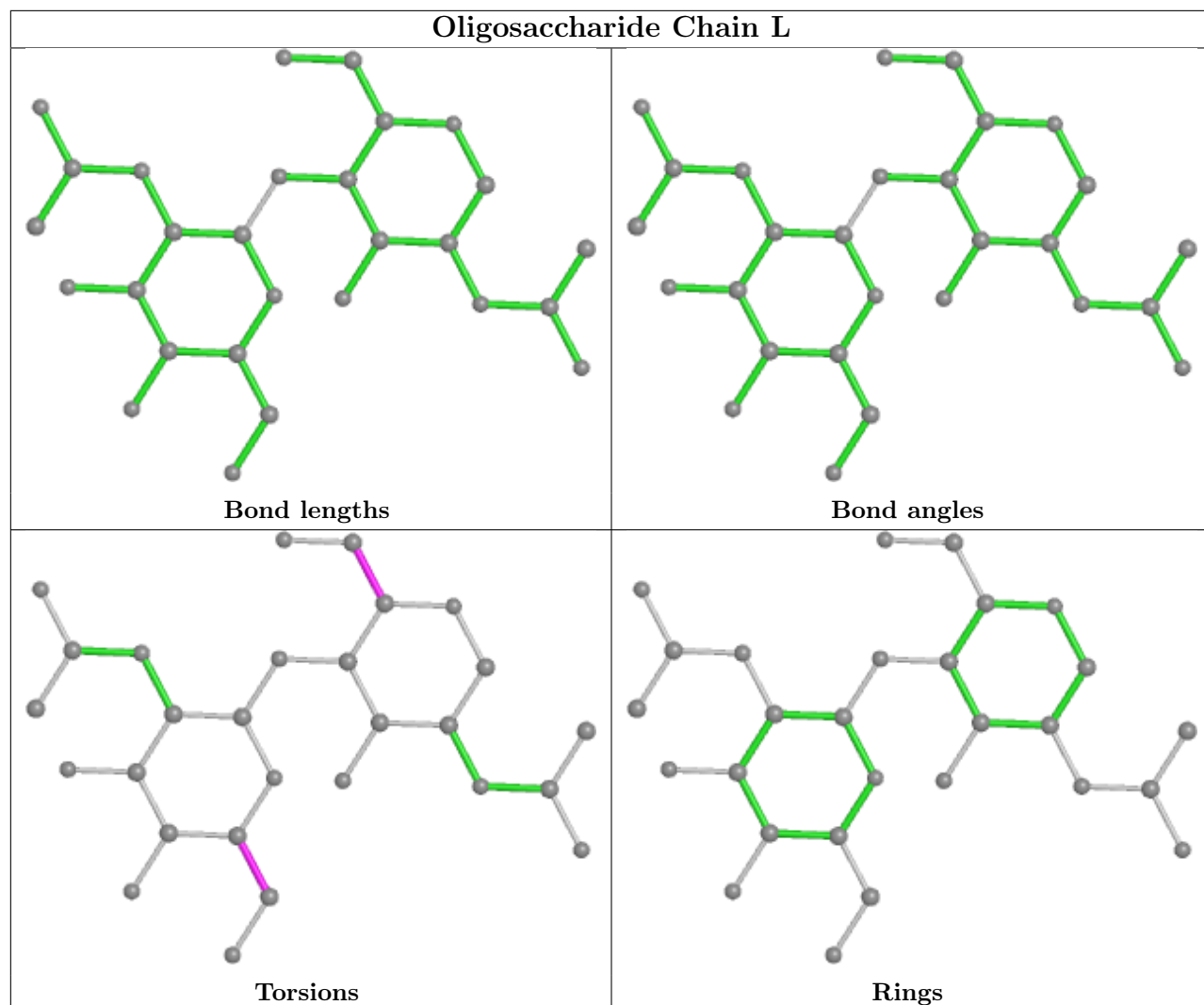


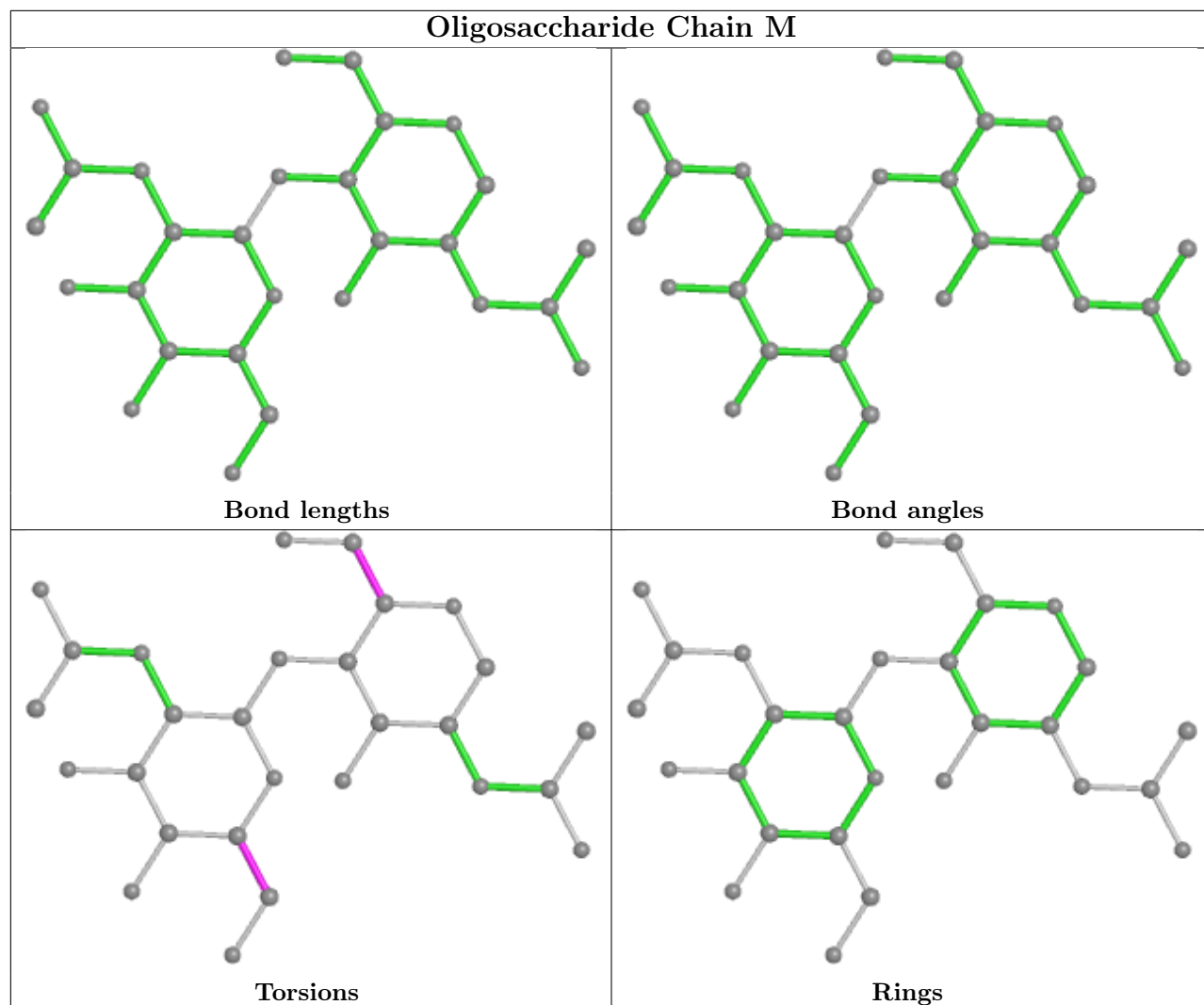




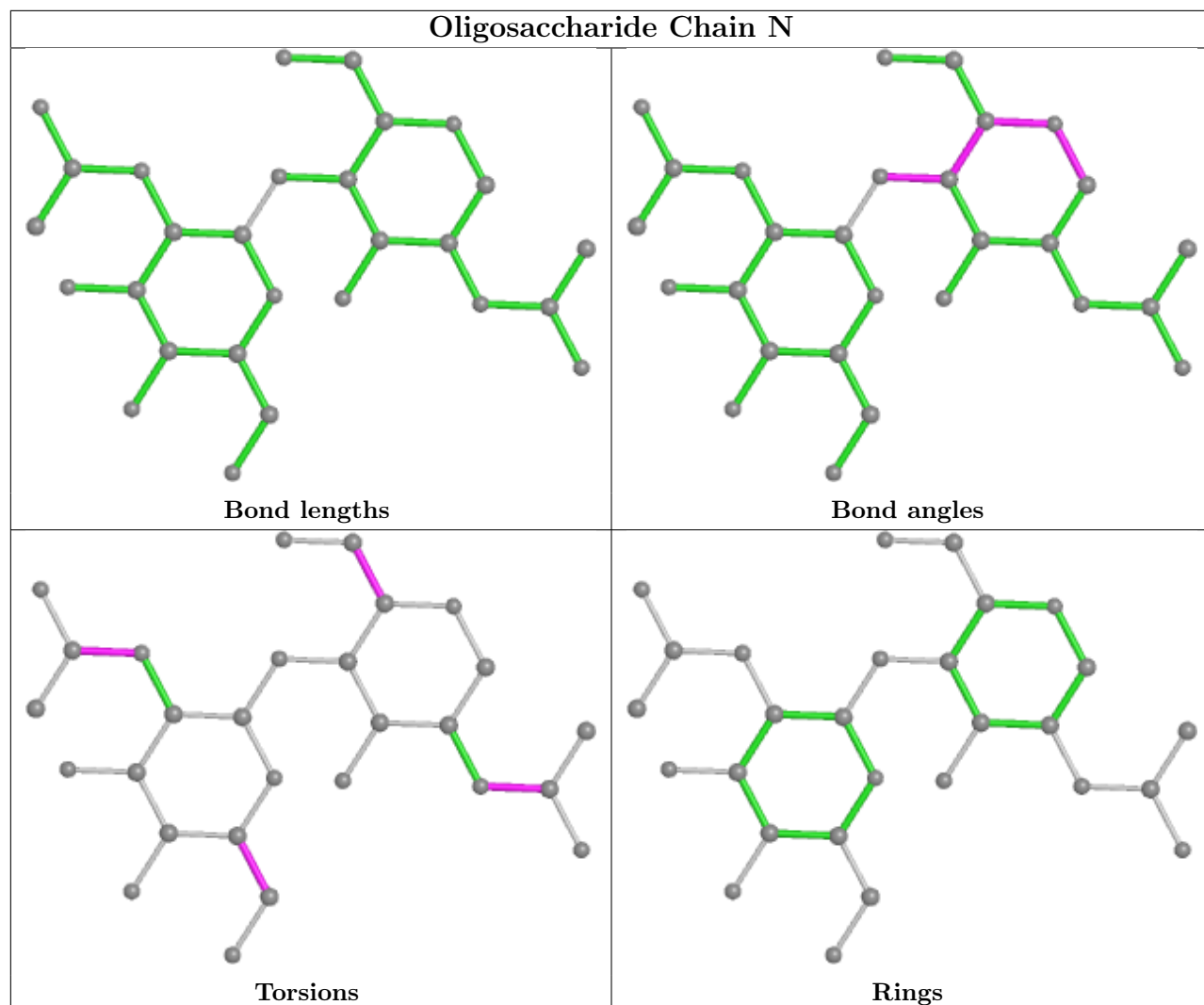


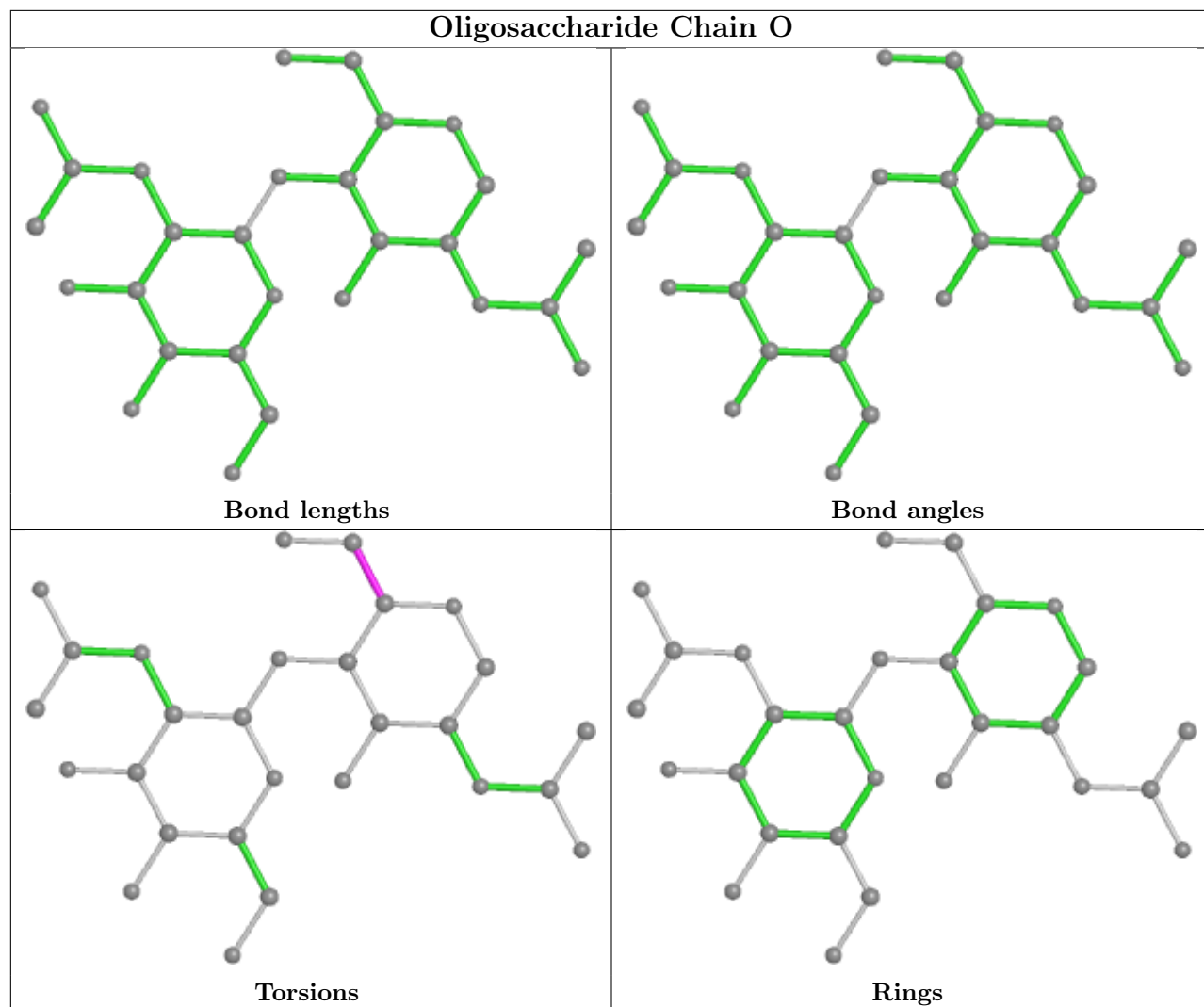


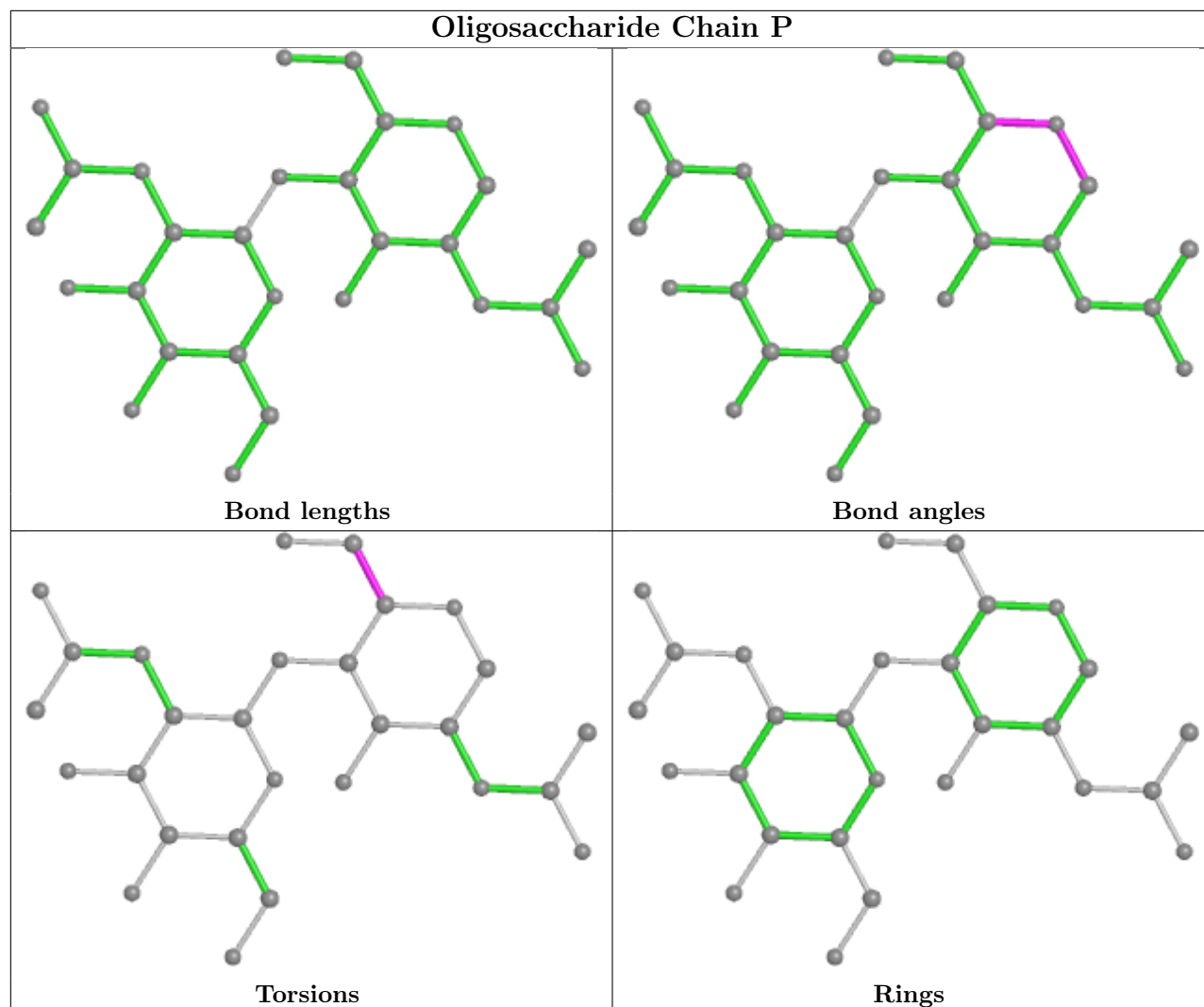


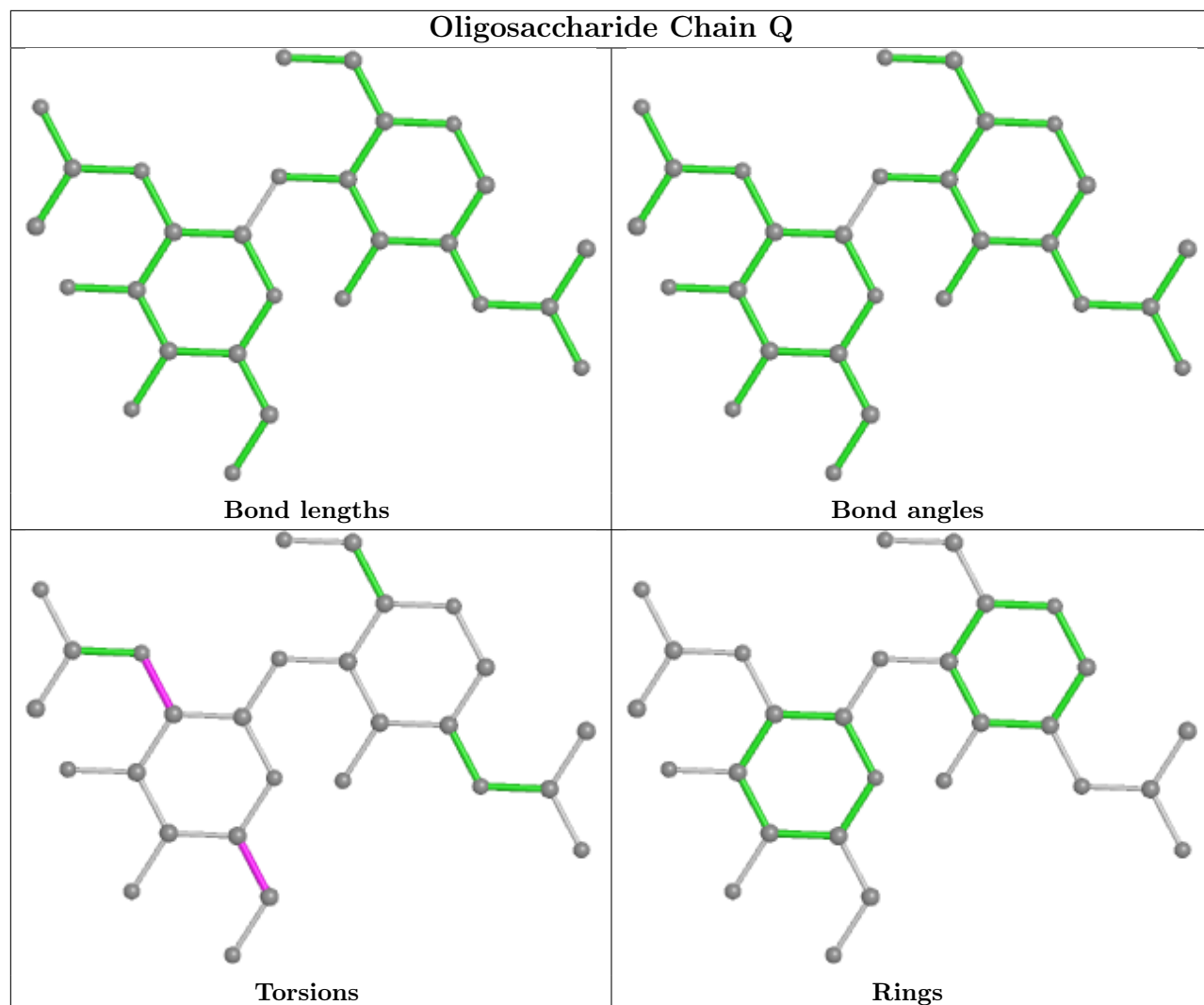


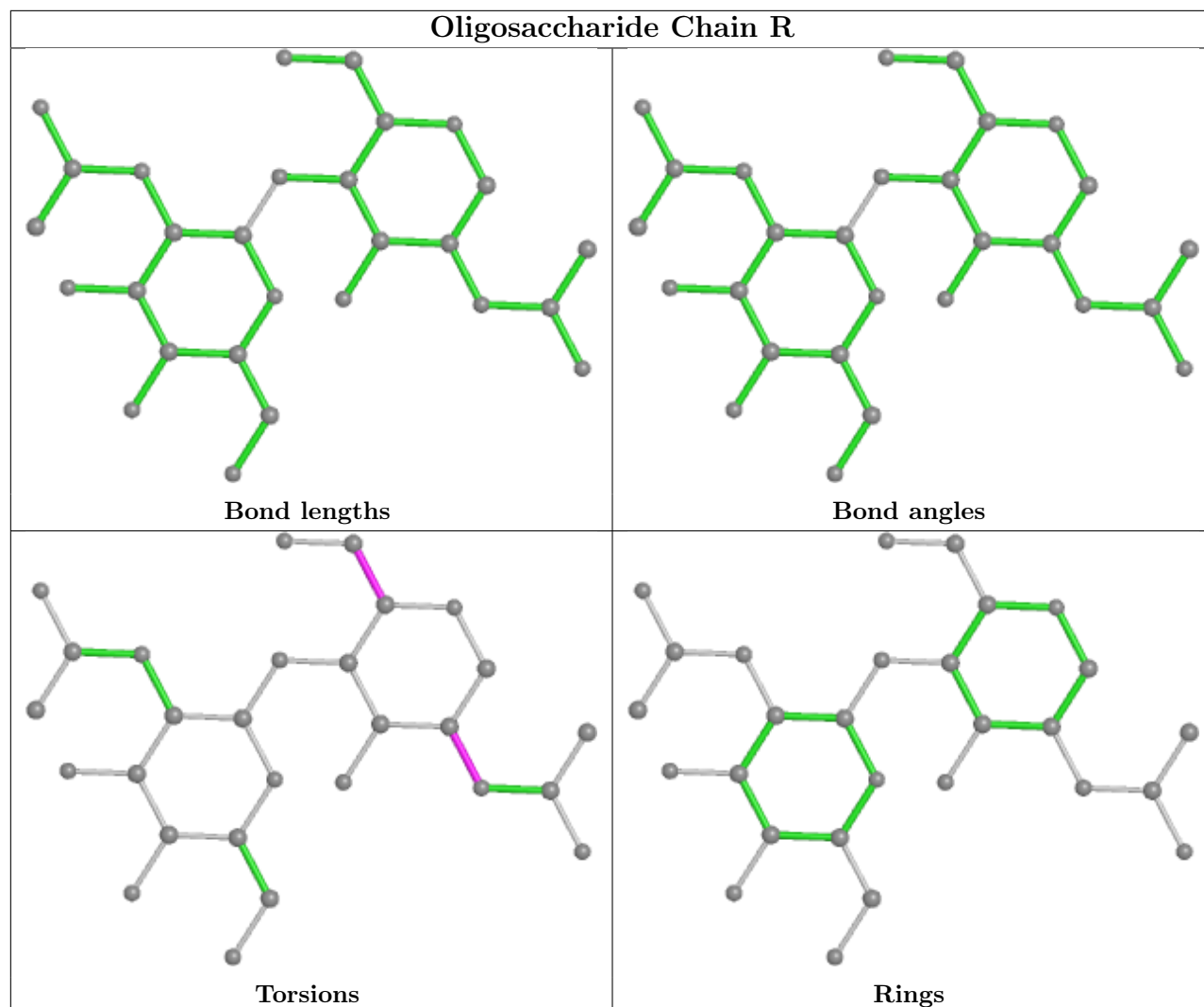


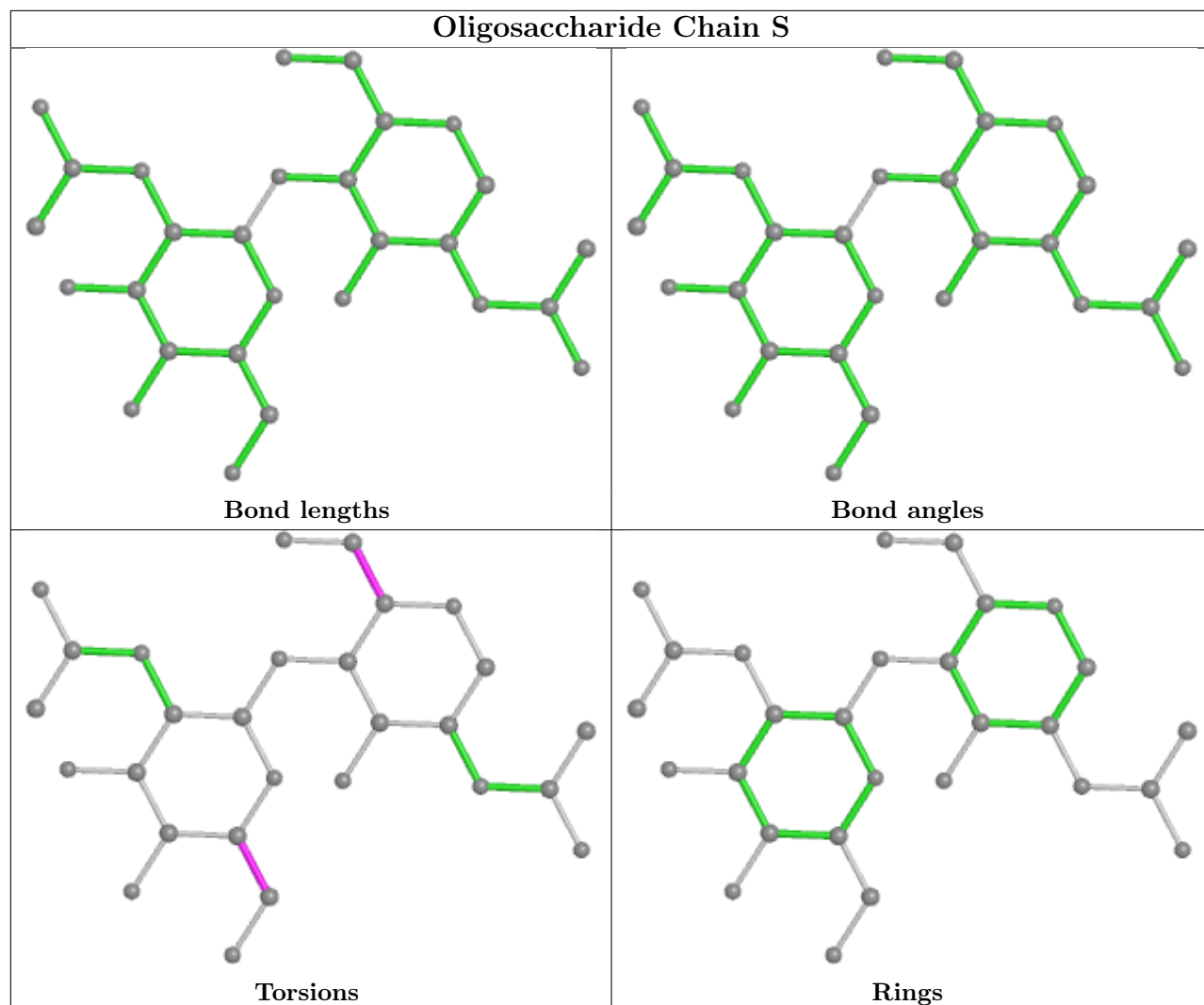


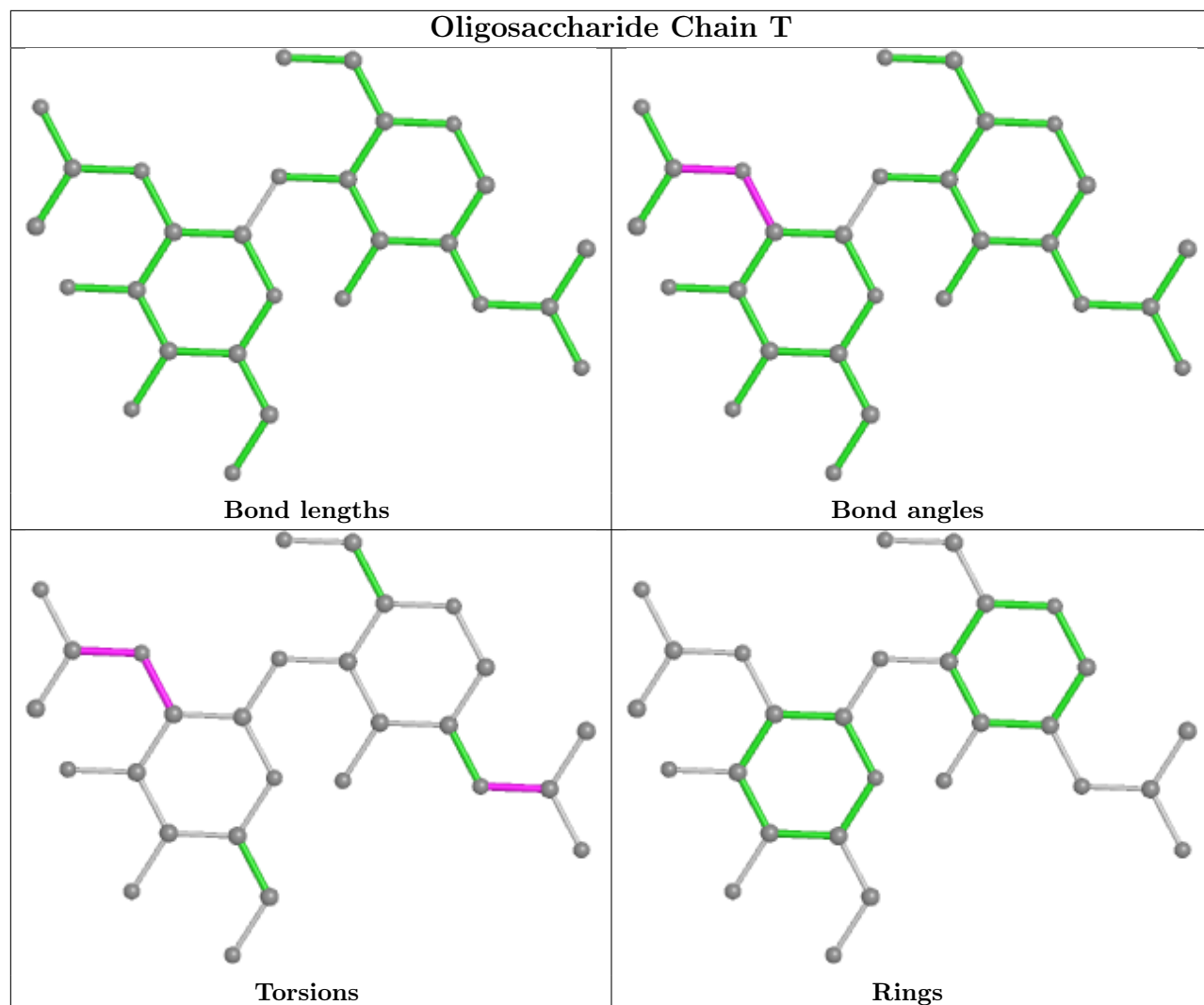


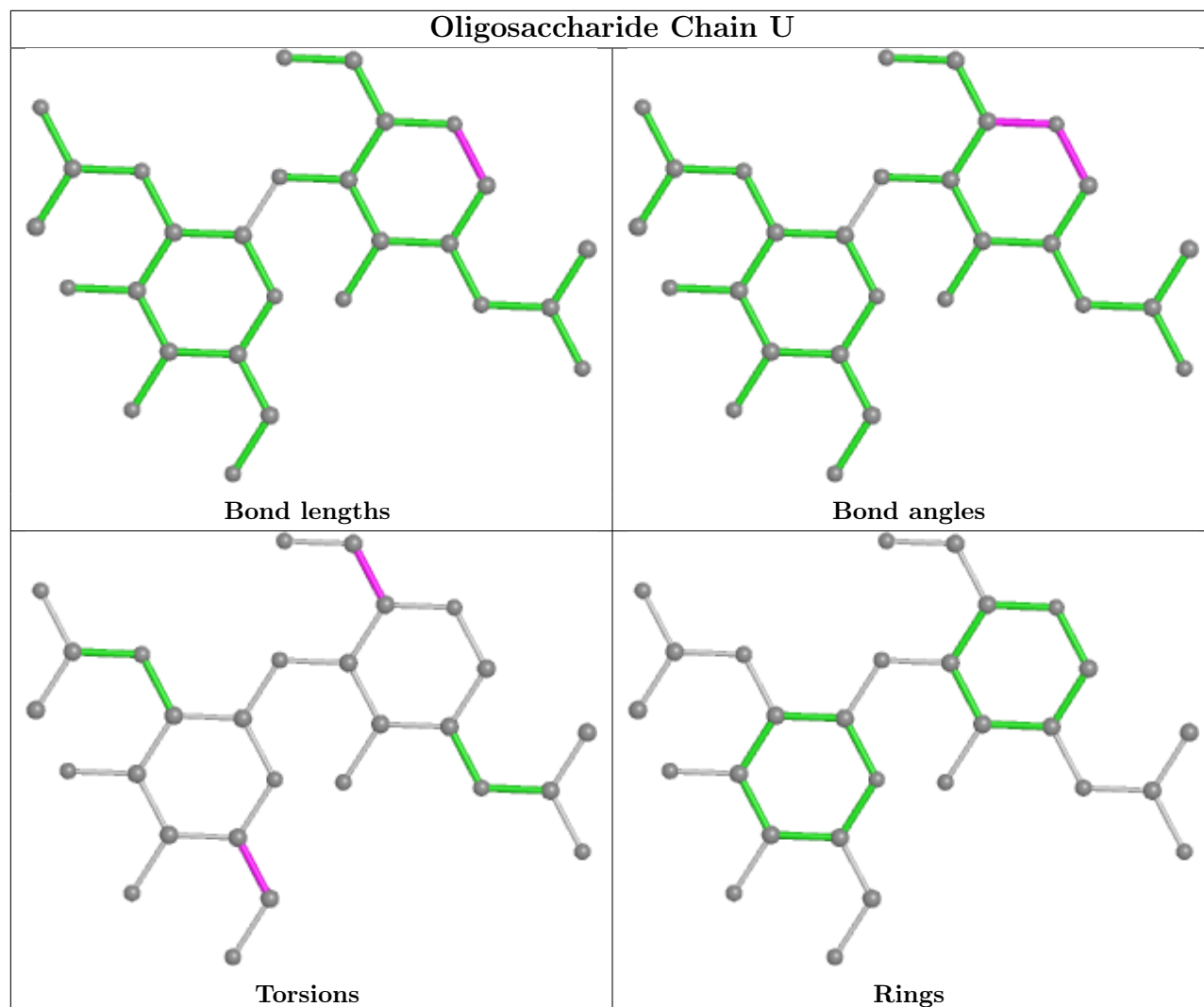




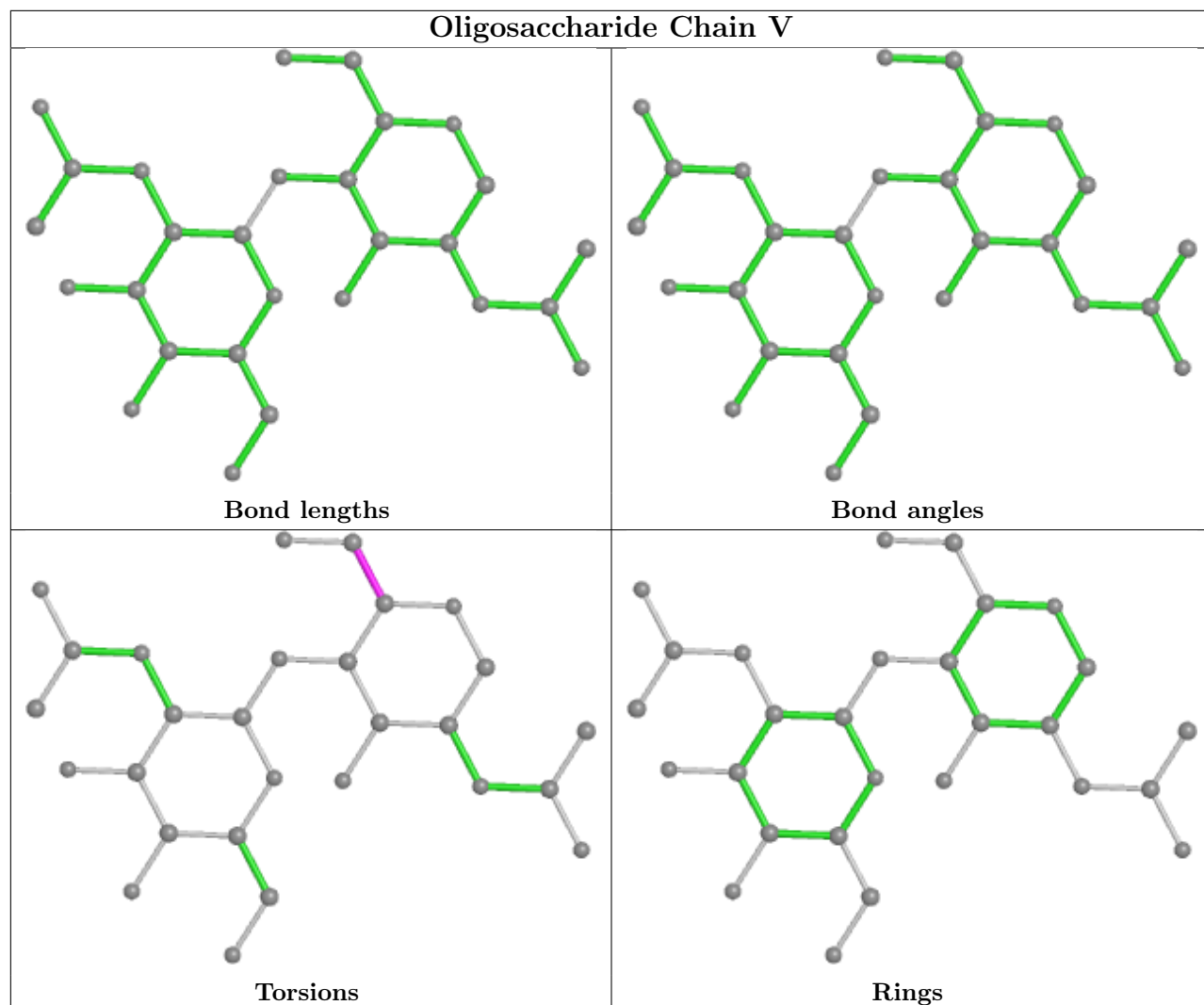


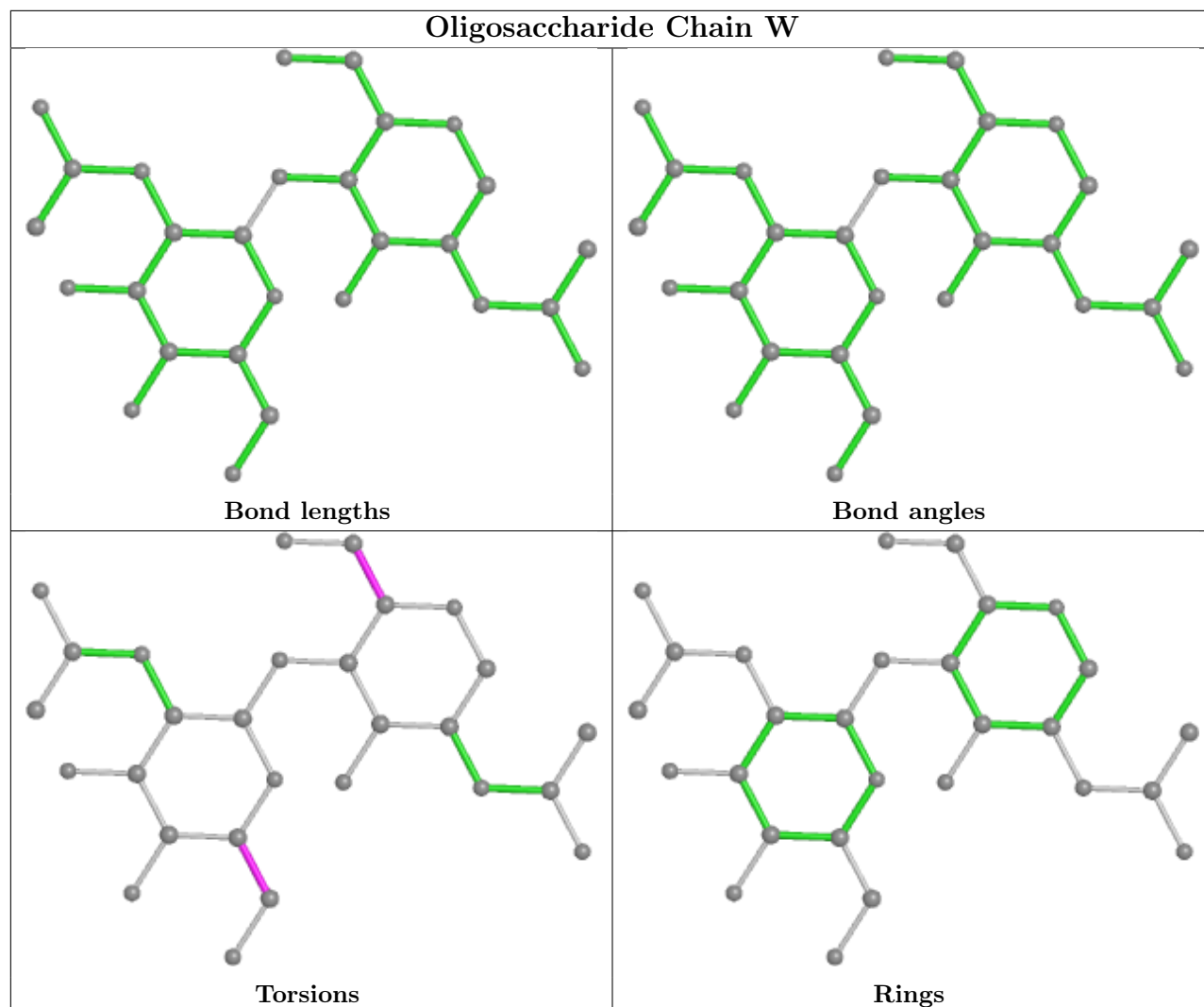


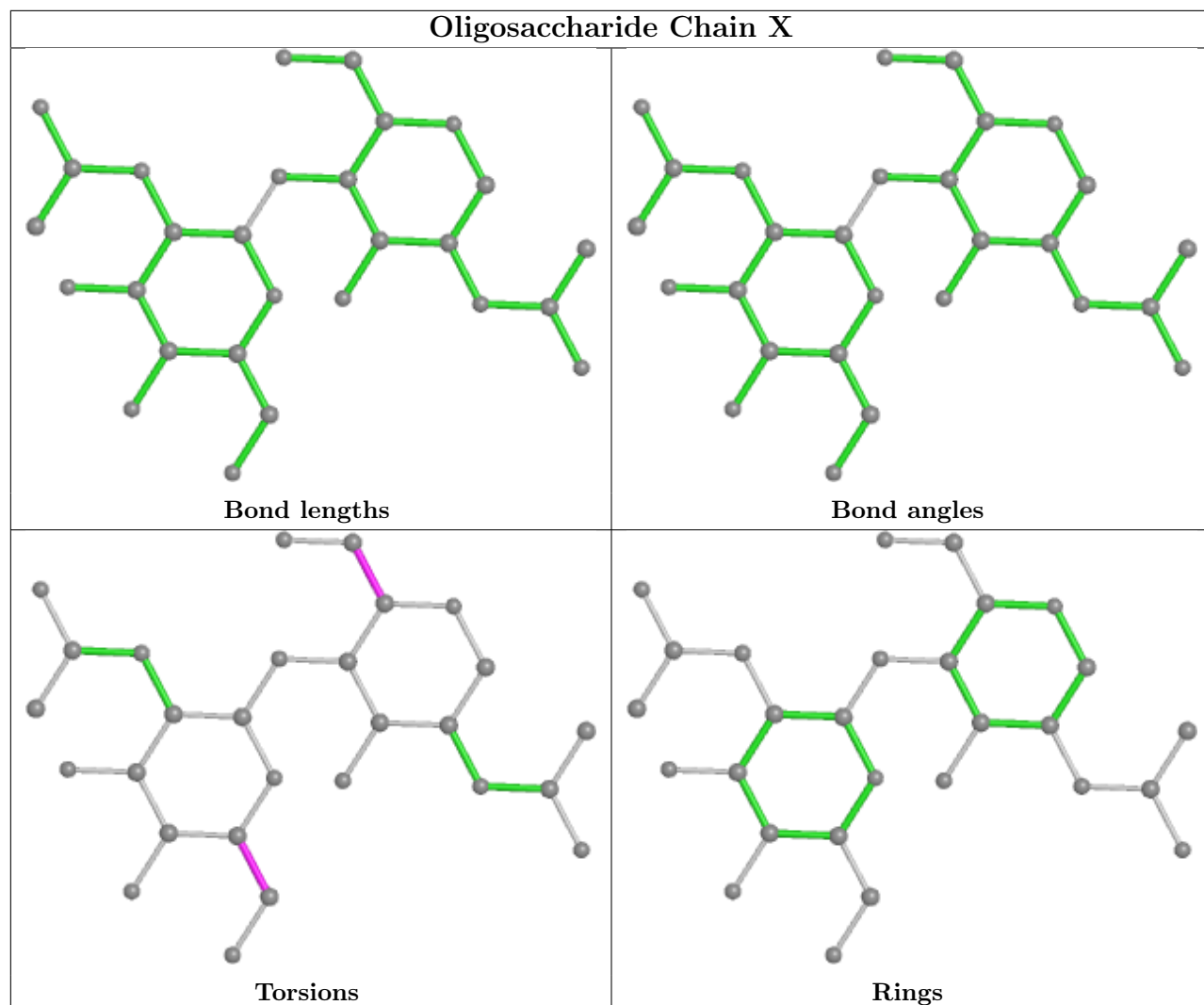


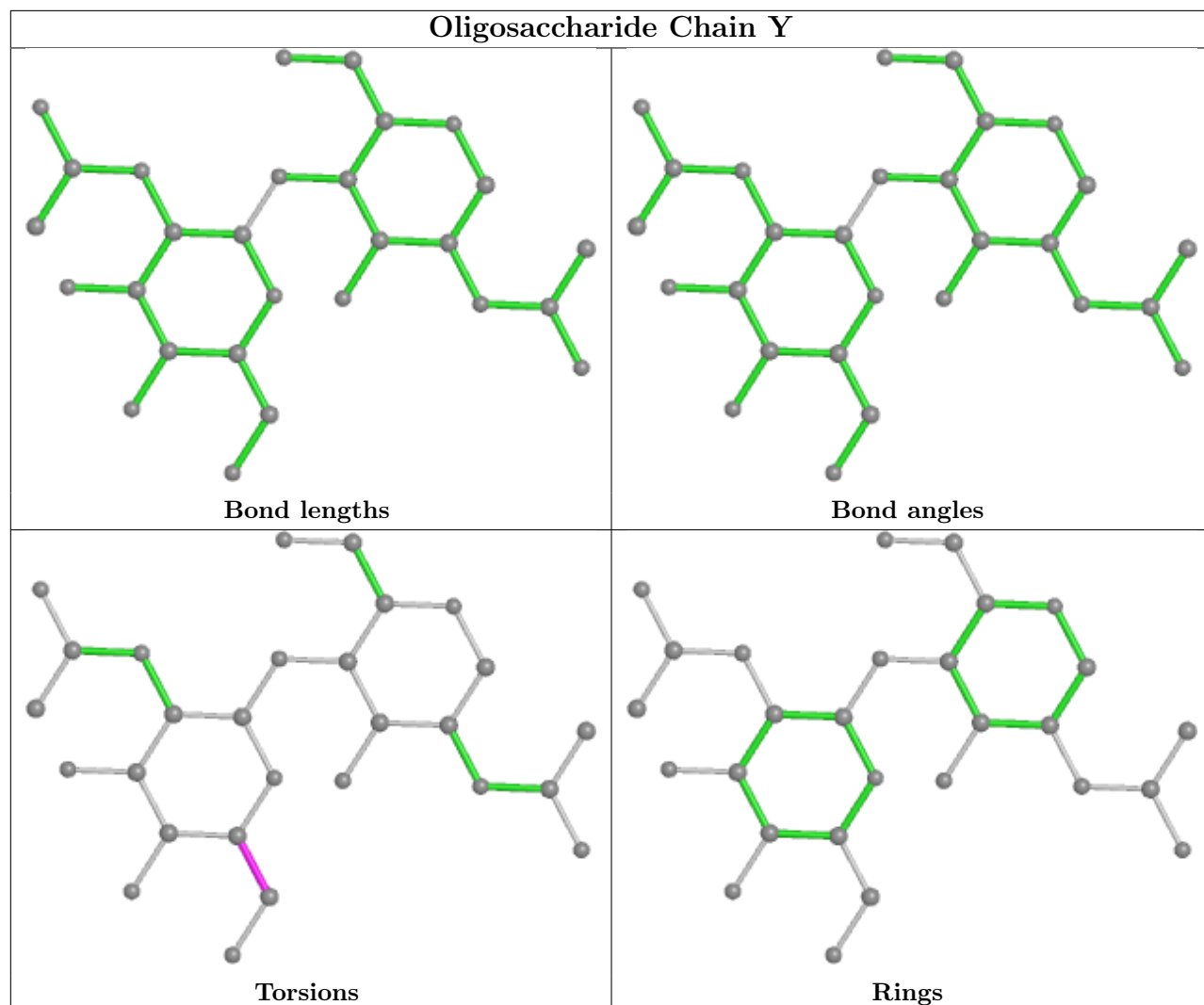


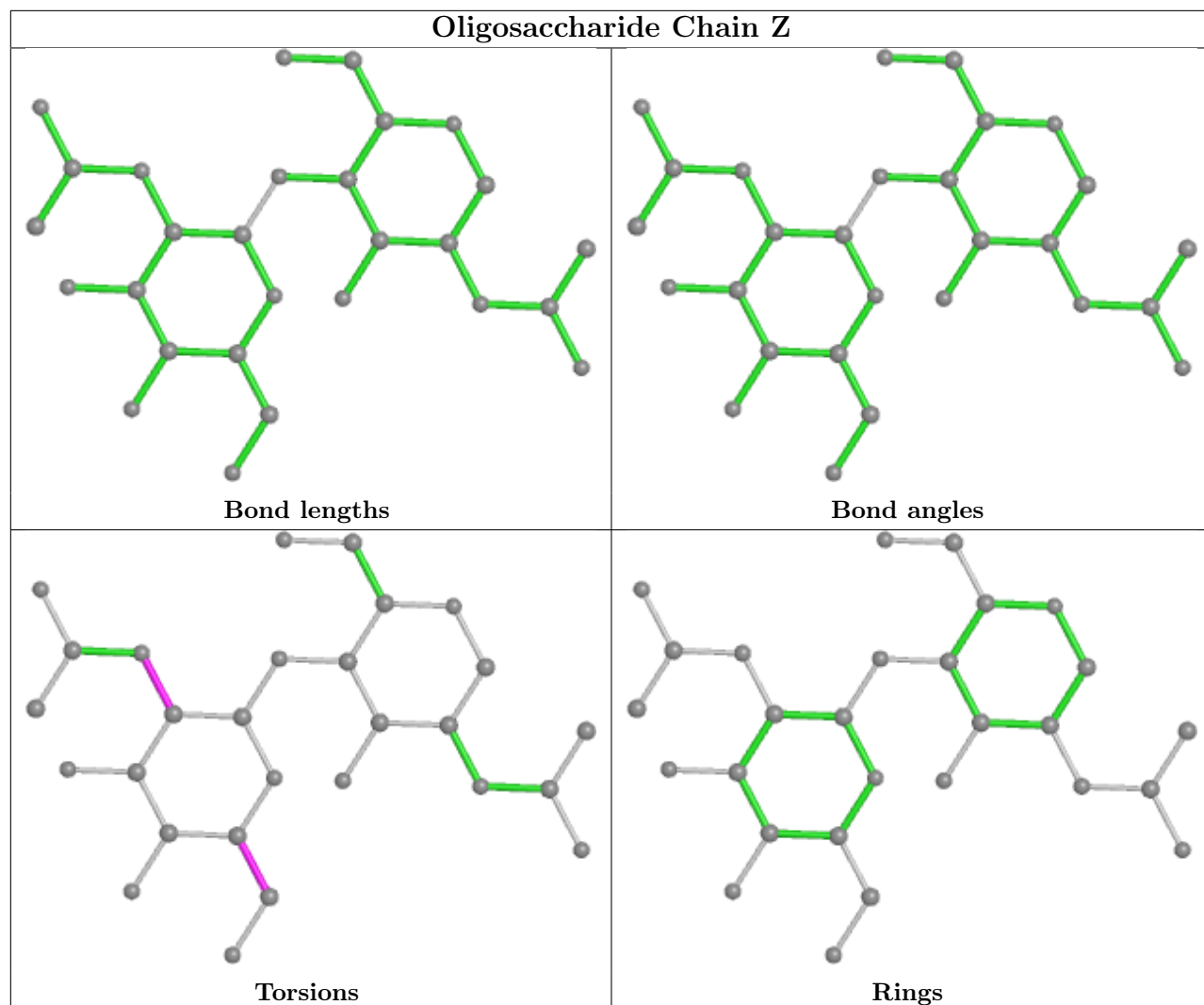


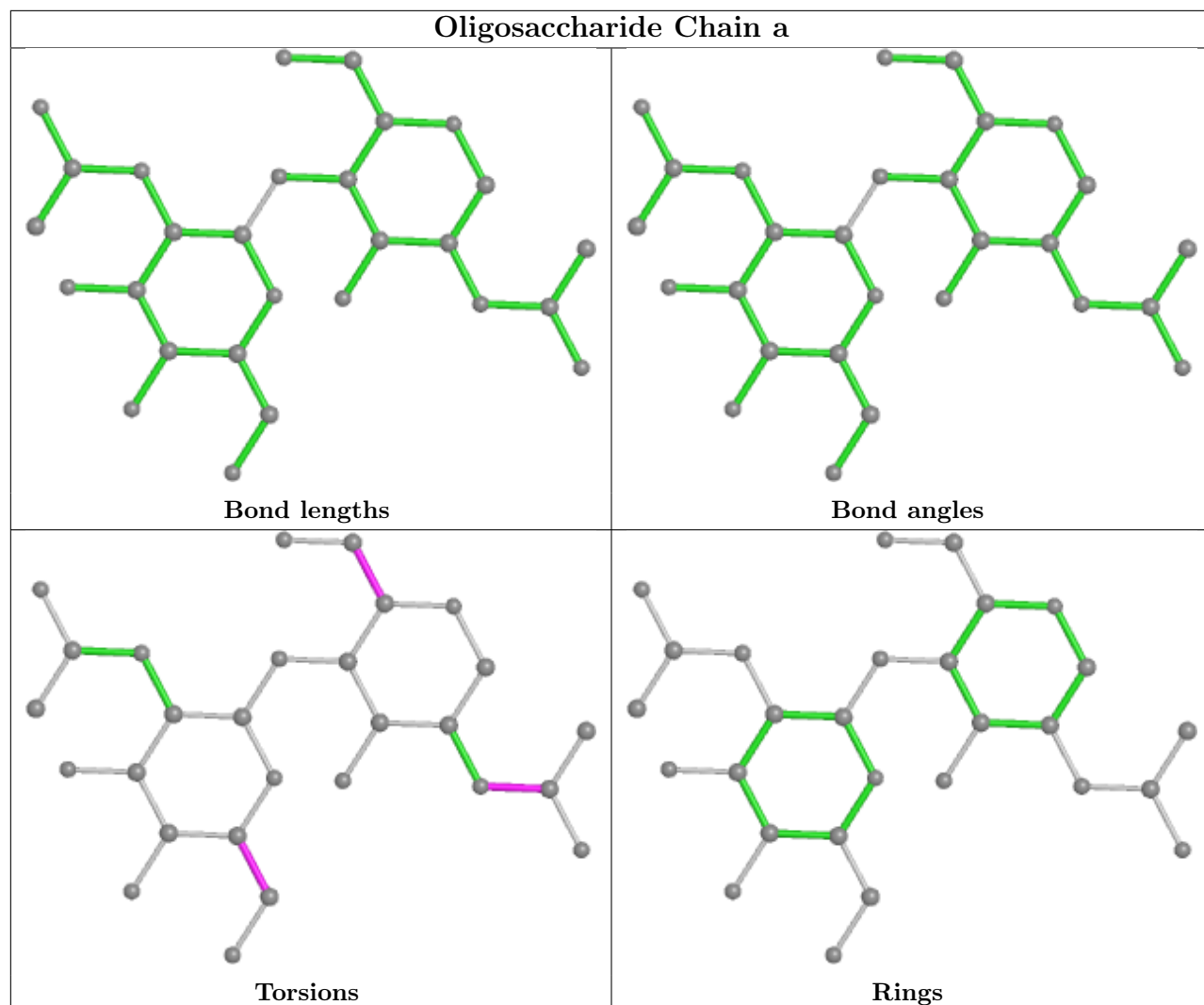


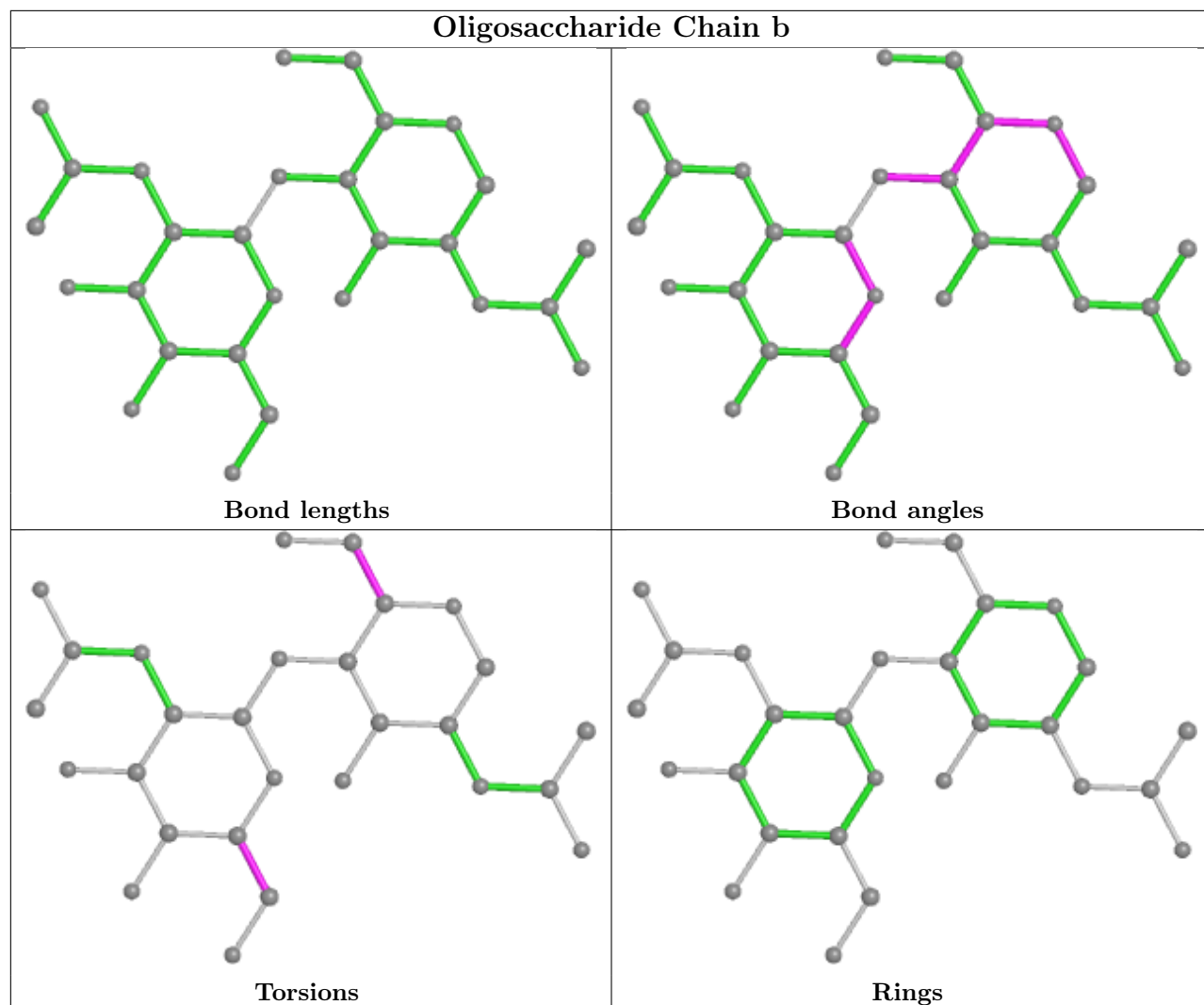


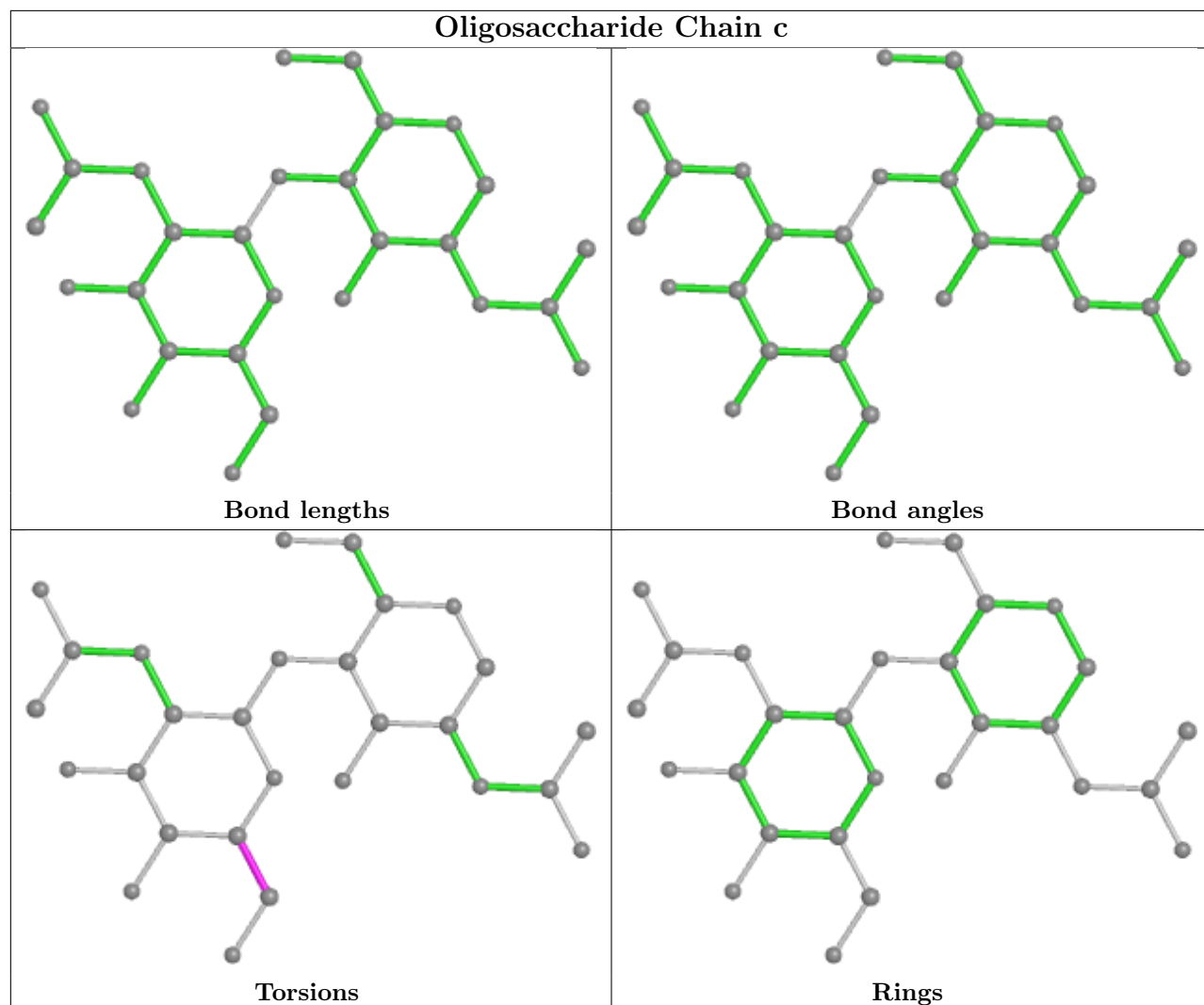




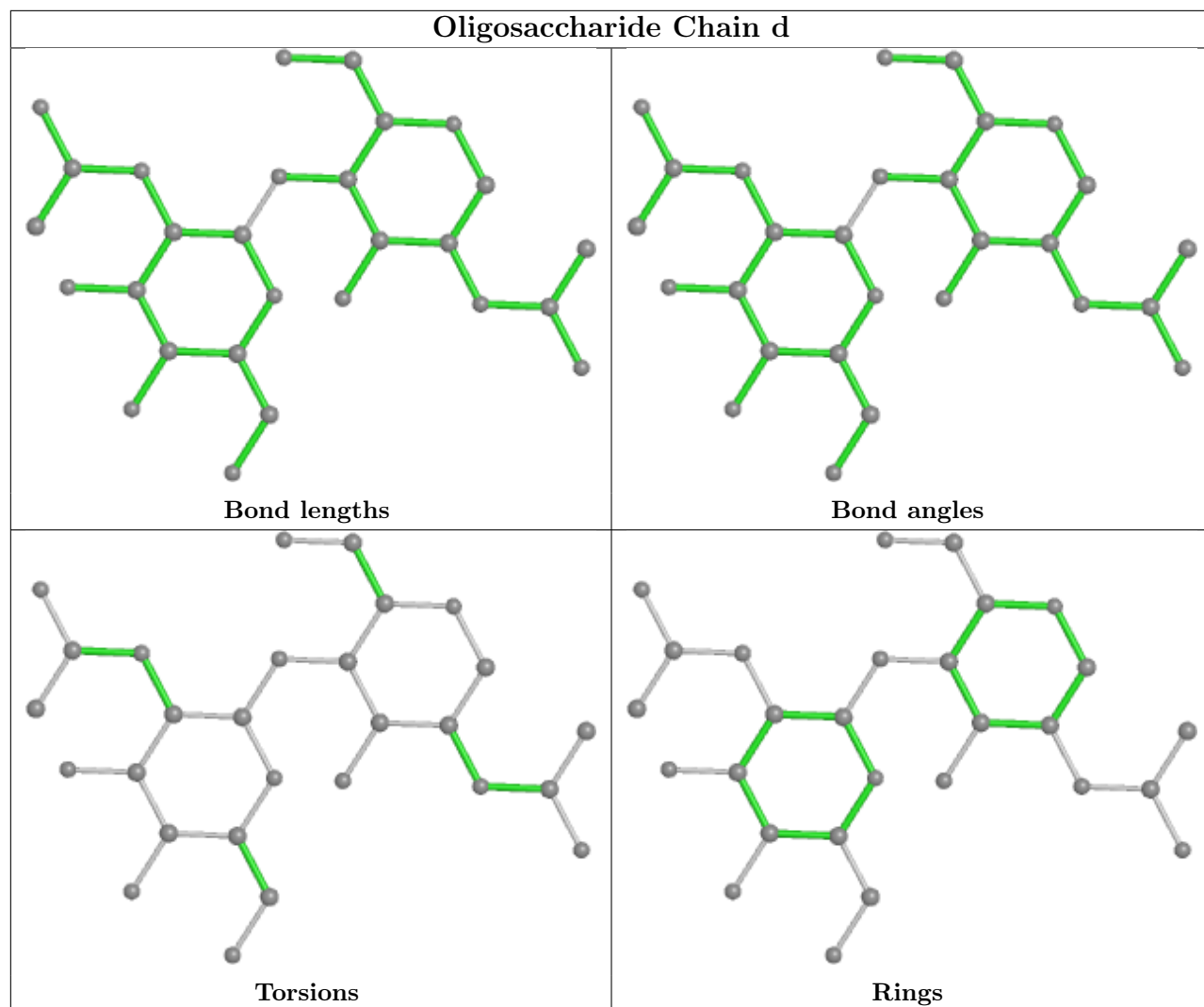


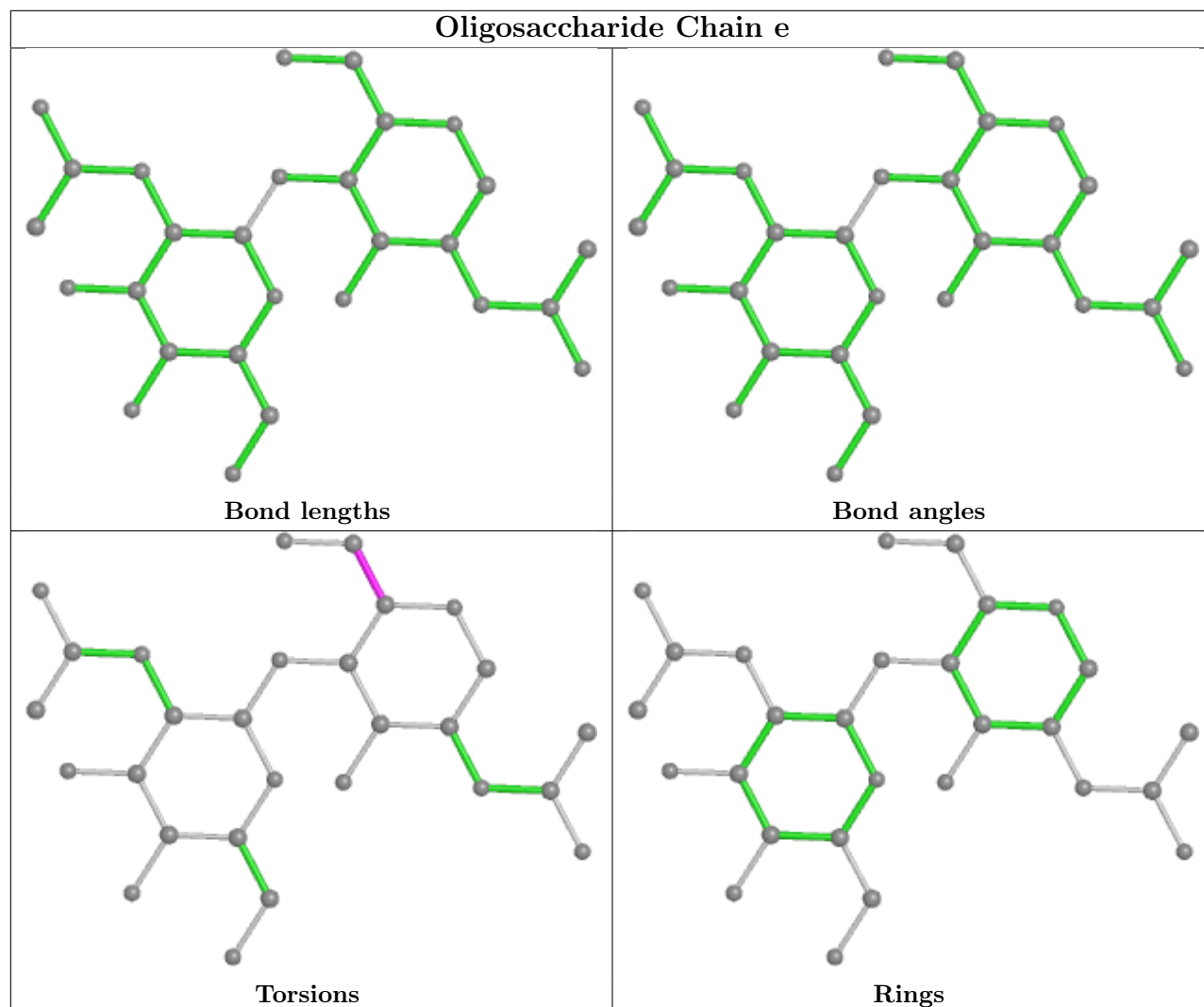


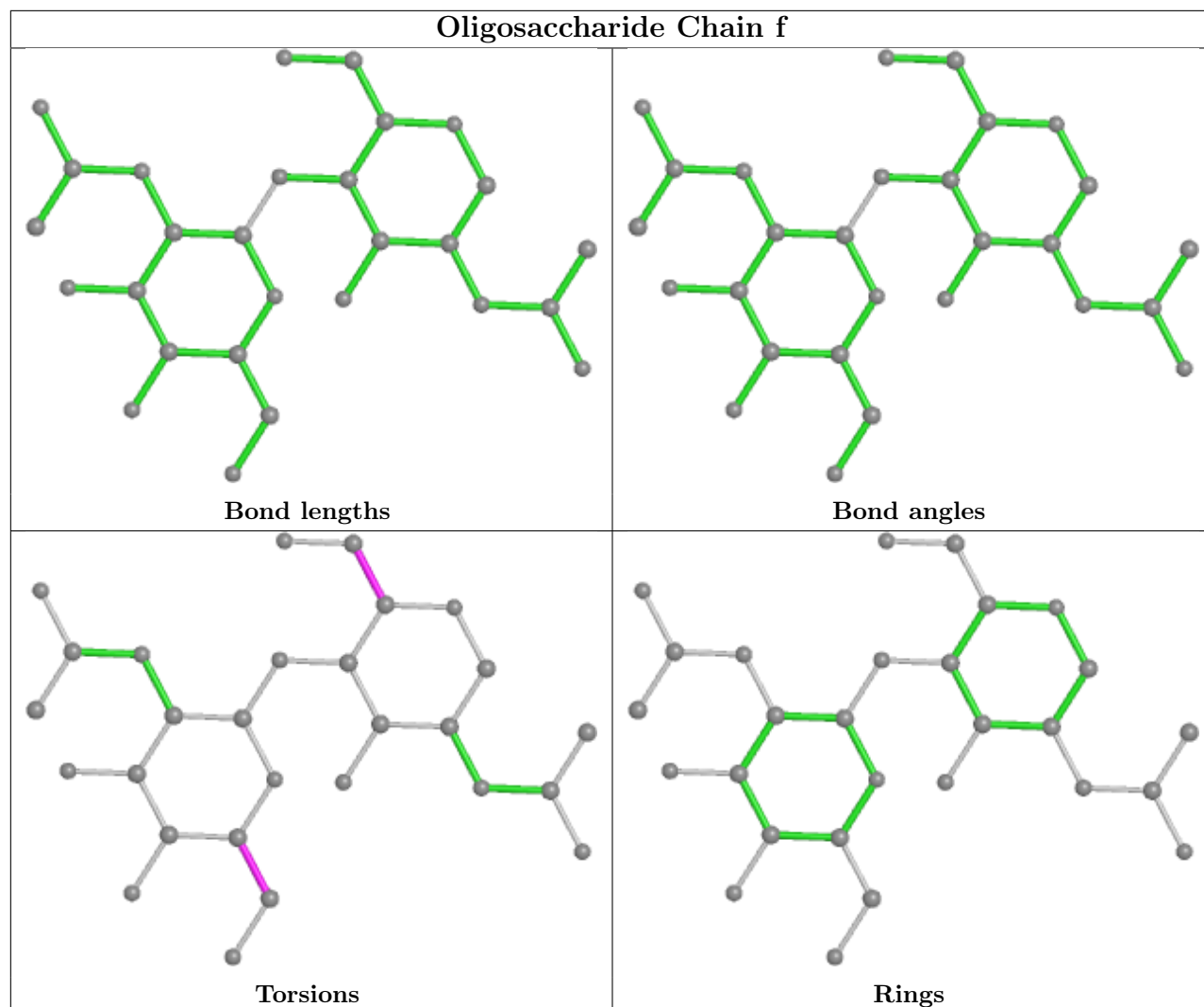


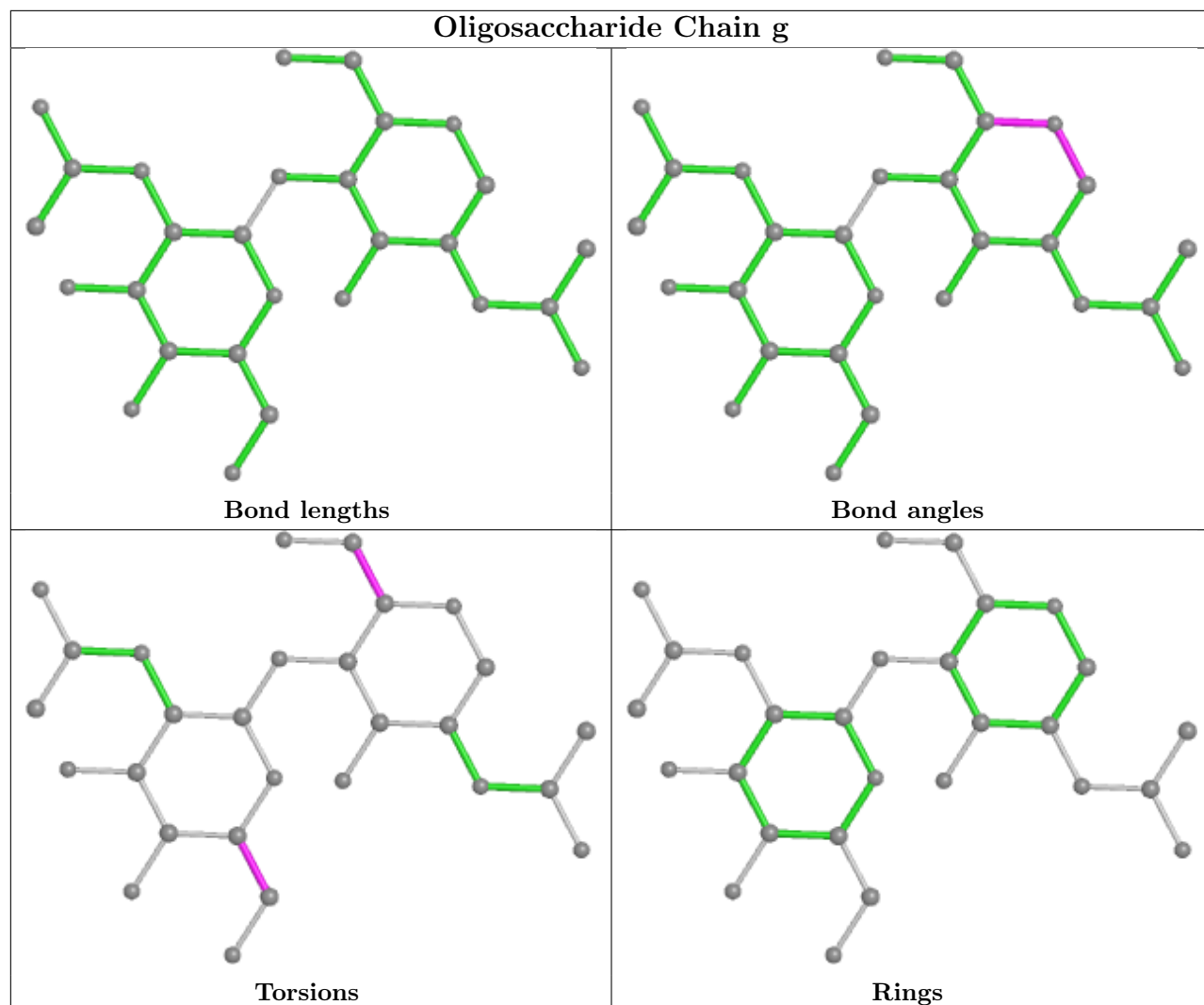


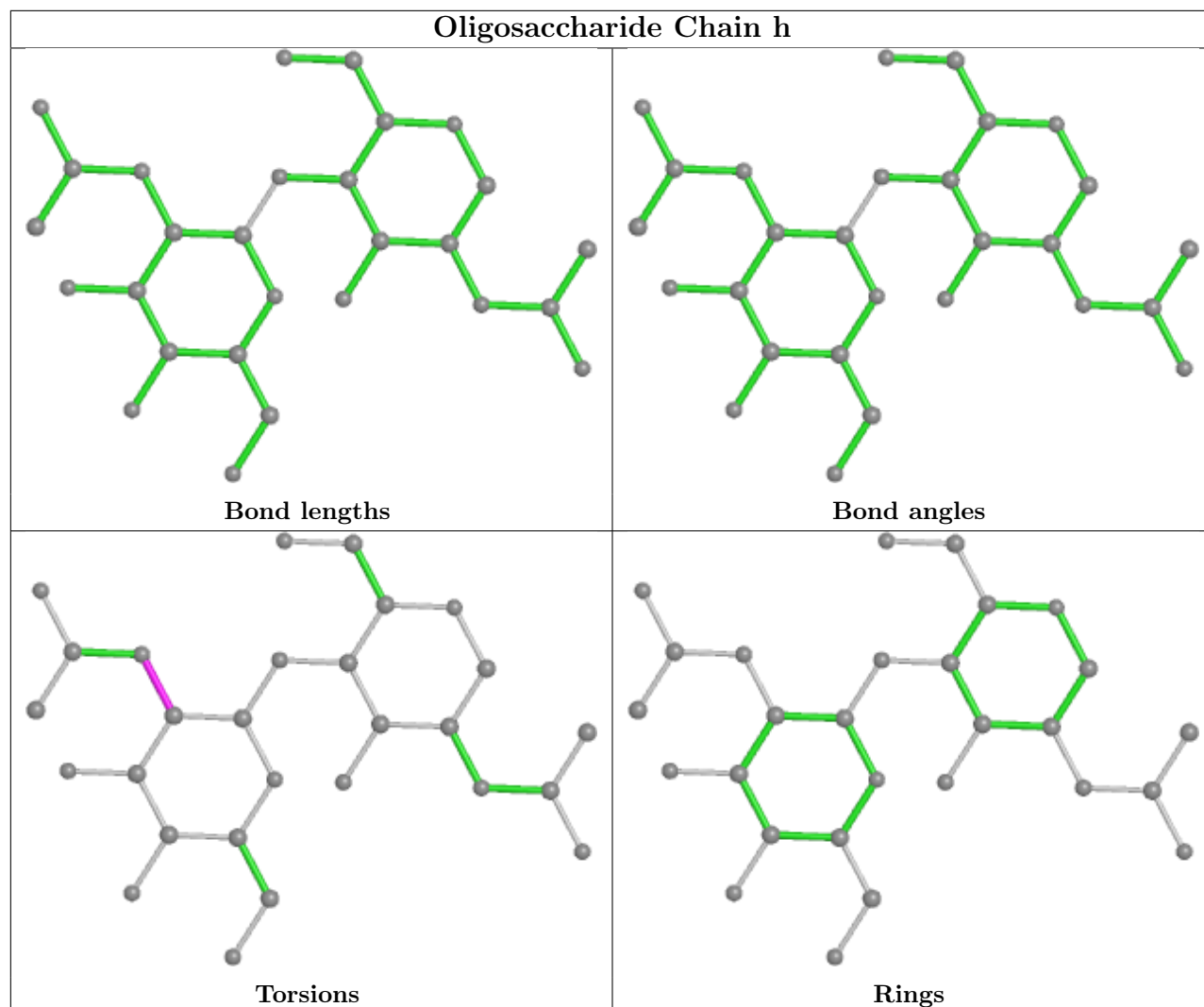


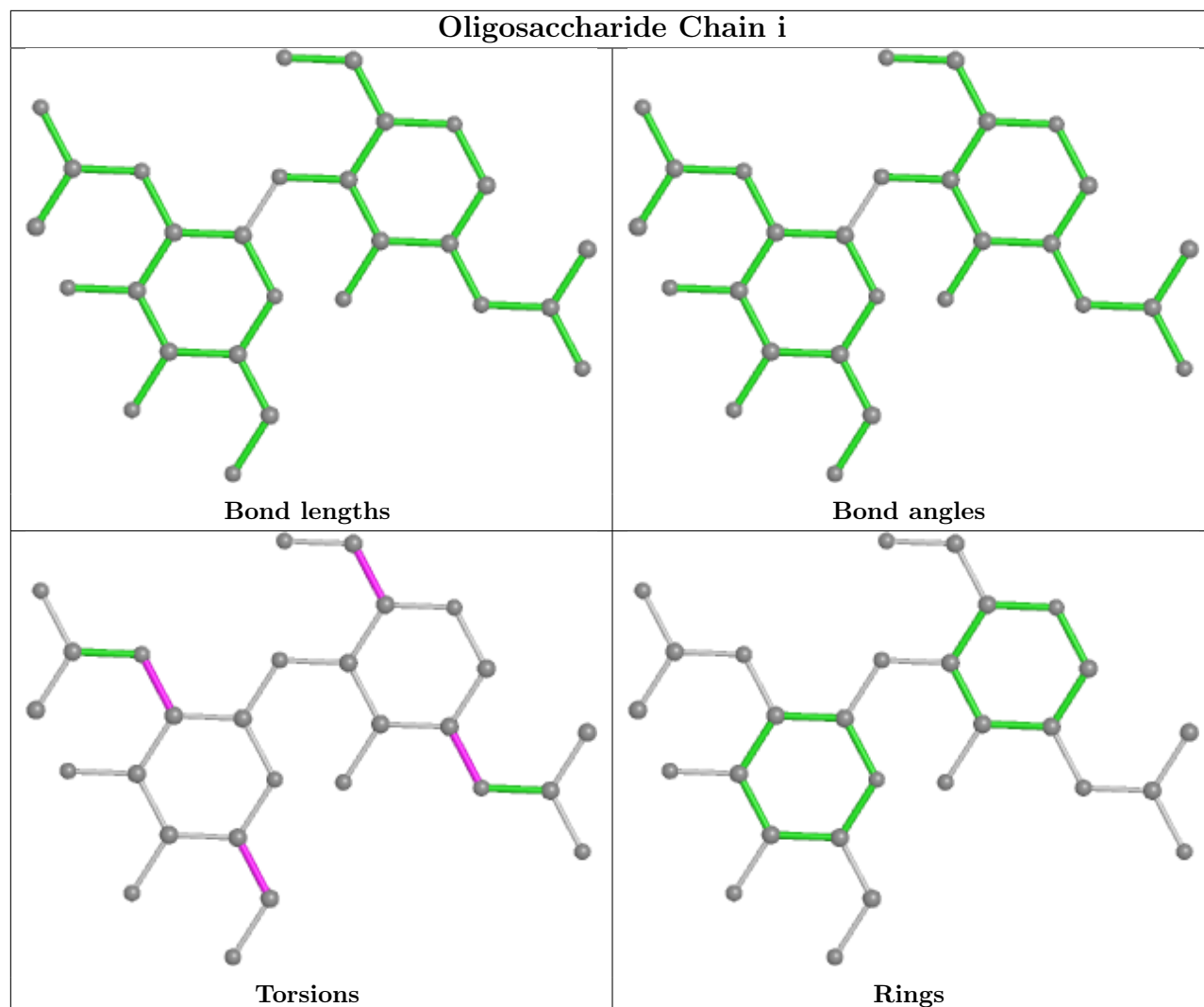












## 5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	C	2007	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	I	1003	2	14,14,15	0.19	0	17,19,21	0.37	0
4	NAG	C	2006	1	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	I	1004	2	14,14,15	0.23	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	2005	1	14,14,15	0.25	0	17,19,21	0.50	0
4	NAG	B	2001	1	14,14,15	0.46	0	17,19,21	0.62	0
4	NAG	B	2002	1	14,14,15	0.44	0	17,19,21	0.69	1 (5%)
4	NAG	A	2003	-	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	I	1006	2	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	I	1002	2	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	A	2002	1	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	C	2003	1	14,14,15	0.46	0	17,19,21	1.22	1 (5%)
4	NAG	C	2002	1	14,14,15	0.18	0	17,19,21	0.60	0
4	NAG	C	2004	1	14,14,15	0.25	0	17,19,21	0.45	0
4	NAG	A	2004	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	A	2006	1	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	B	2006	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	I	1005	2	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	J	1001	2	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	I	1001	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	2003	1	14,14,15	0.16	0	17,19,21	0.48	0
4	NAG	C	2005	1	14,14,15	0.29	0	17,19,21	0.36	0
4	NAG	C	2001	1	14,14,15	0.28	0	17,19,21	0.44	0
4	NAG	A	2005	1	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	B	2004	1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	A	2001	1	14,14,15	0.52	0	17,19,21	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1003	2	-	2/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1004	2	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2003	-	-	1/6/23/26	0/1/1/1
4	NAG	I	1006	2	-	0/6/23/26	0/1/1/1
4	NAG	I	1002	2	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	I	1005	2	-	0/6/23/26	0/1/1/1
4	NAG	J	1001	2	-	1/6/23/26	0/1/1/1
4	NAG	I	1001	2	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2003	NAG	C2-N2-C7	4.27	128.98	122.90
4	B	2002	NAG	C1-O5-C5	2.28	115.28	112.19

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2001	NAG	O5-C5-C6-O6
4	B	2002	NAG	C4-C5-C6-O6
4	I	1004	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.



## 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.

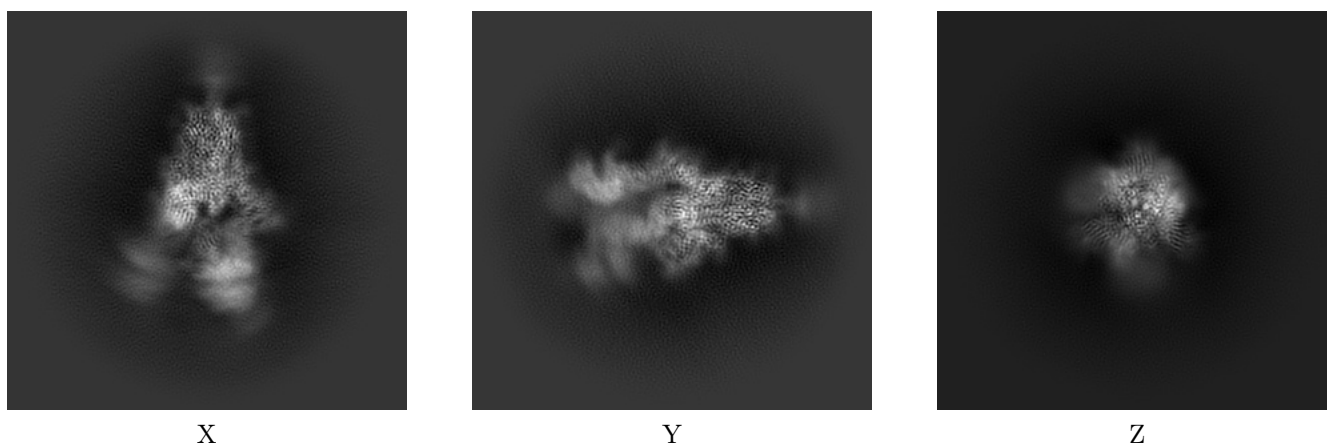
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31073. 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](#)

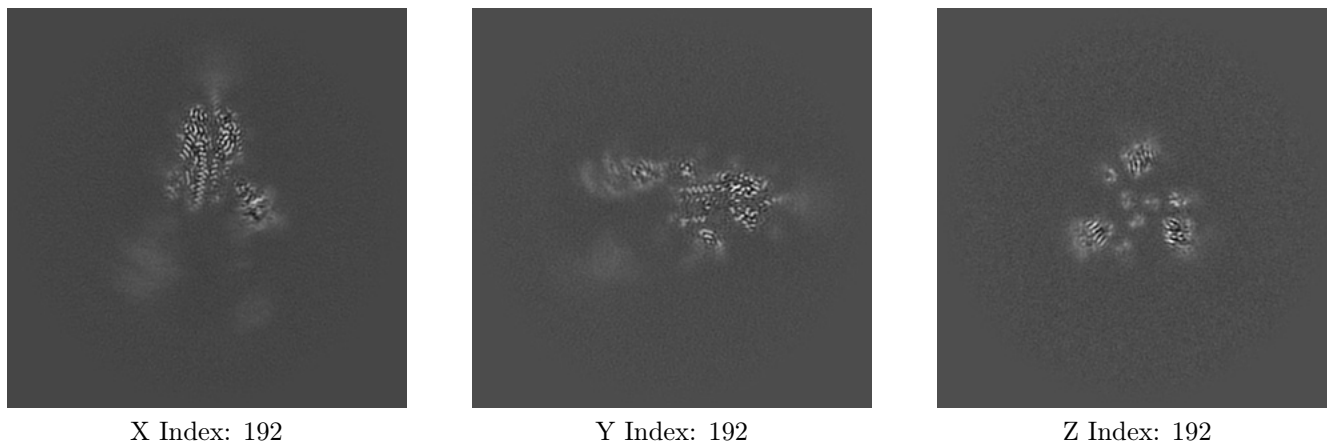
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

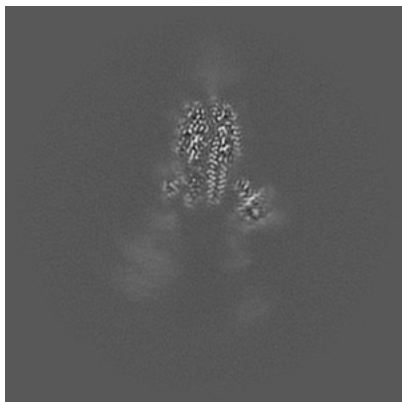
#### 6.2.1 Primary map



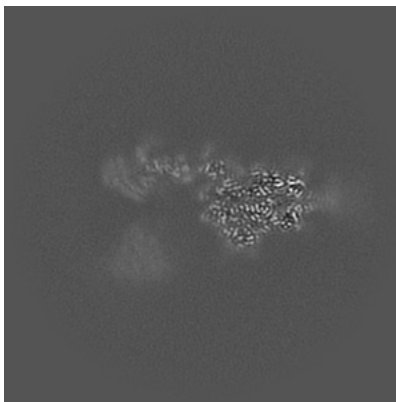
The images above show central slices of the map in three orthogonal directions.

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

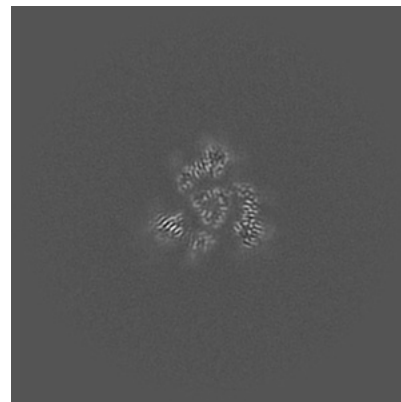
### 6.3.1 Primary map



X Index: 188



Y Index: 201

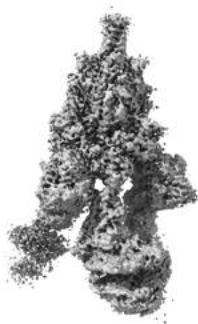


Z Index: 203

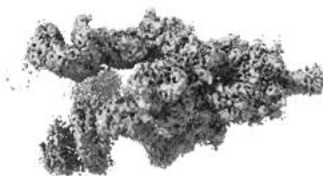
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

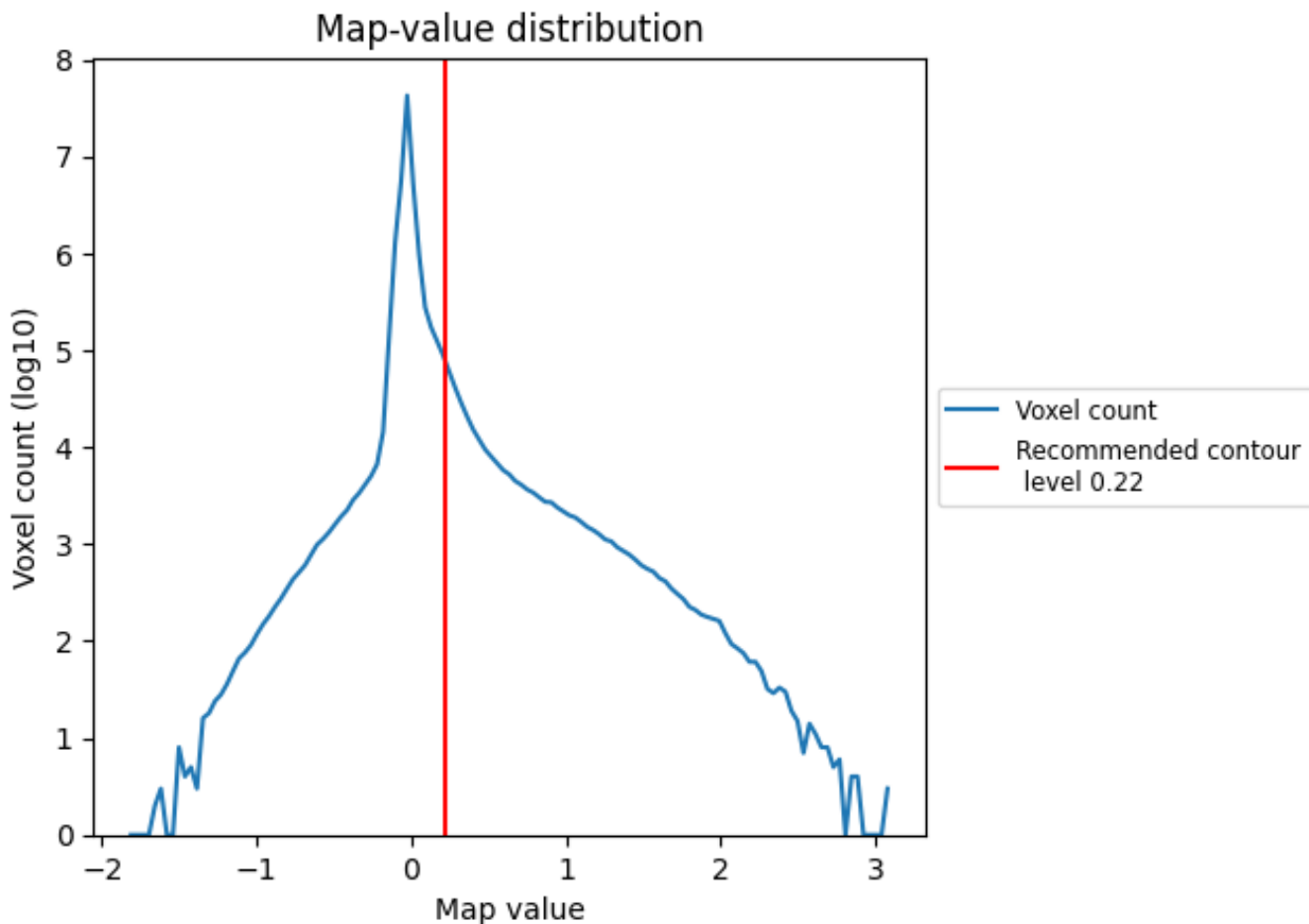
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

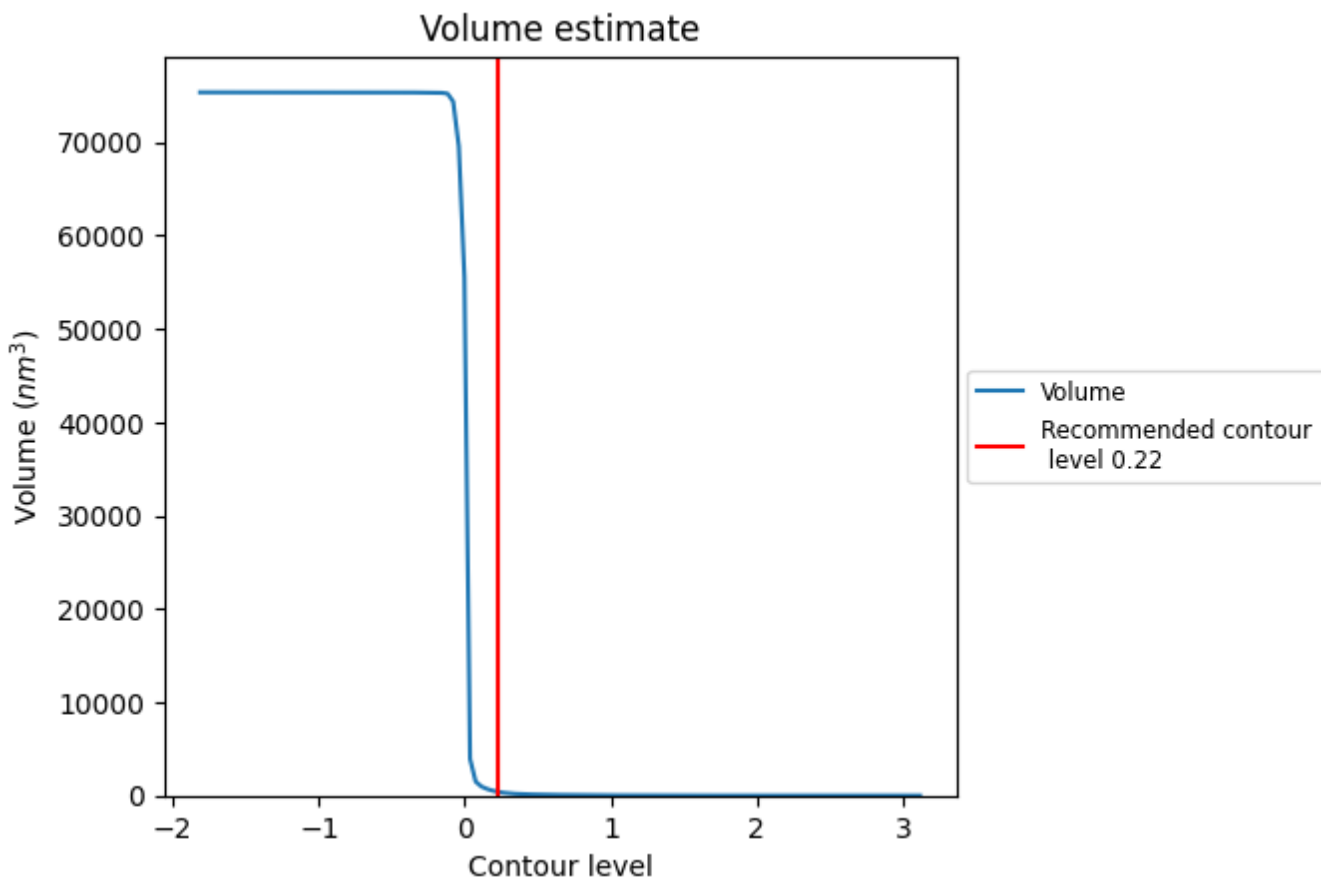
This section contains the results of statistical analysis of the map.

### 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.

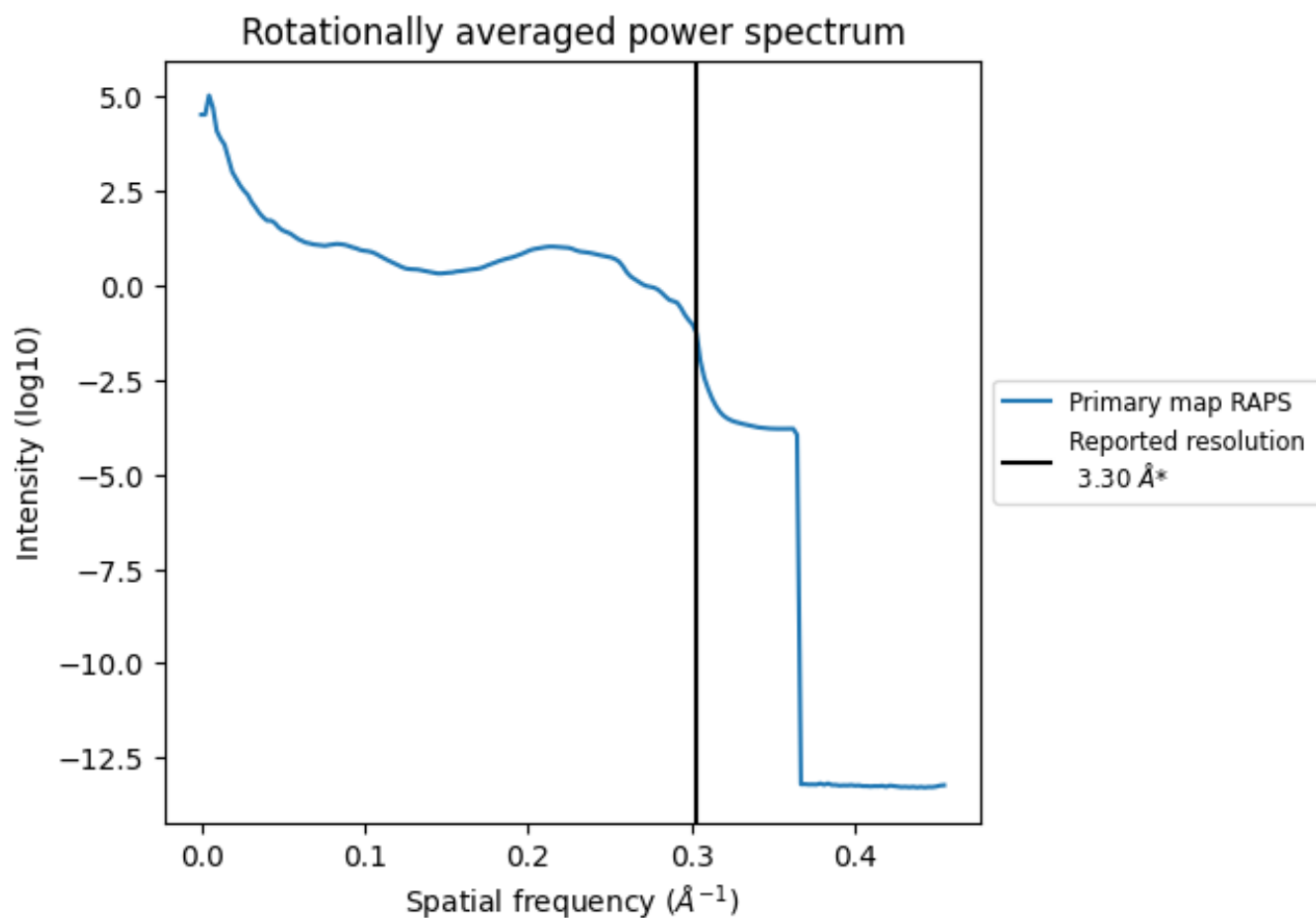
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 420  $\text{nm}^3$ ; this corresponds to an approximate mass of 379 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 0.303 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

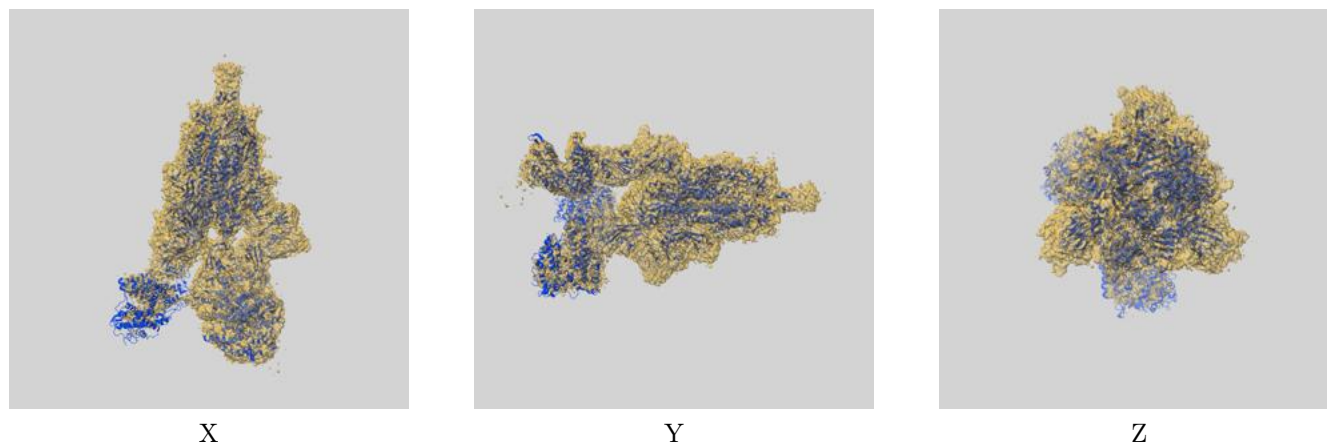
This section was not generated. No FSC curve or half-maps provided.



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

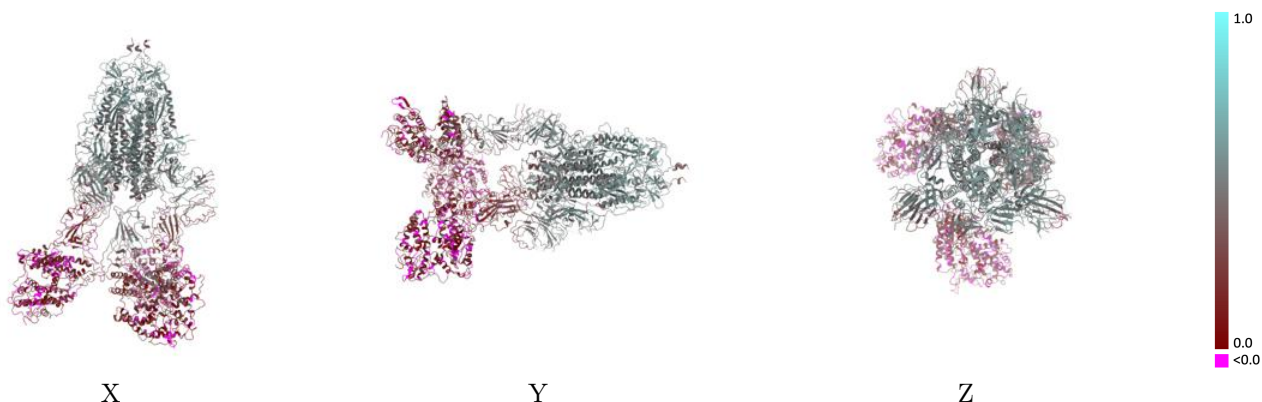
This section contains information regarding the fit between EMDB map EMD-31073 and PDB model 7EDJ. Per-residue inclusion information can be found in section 3 on page 17.

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



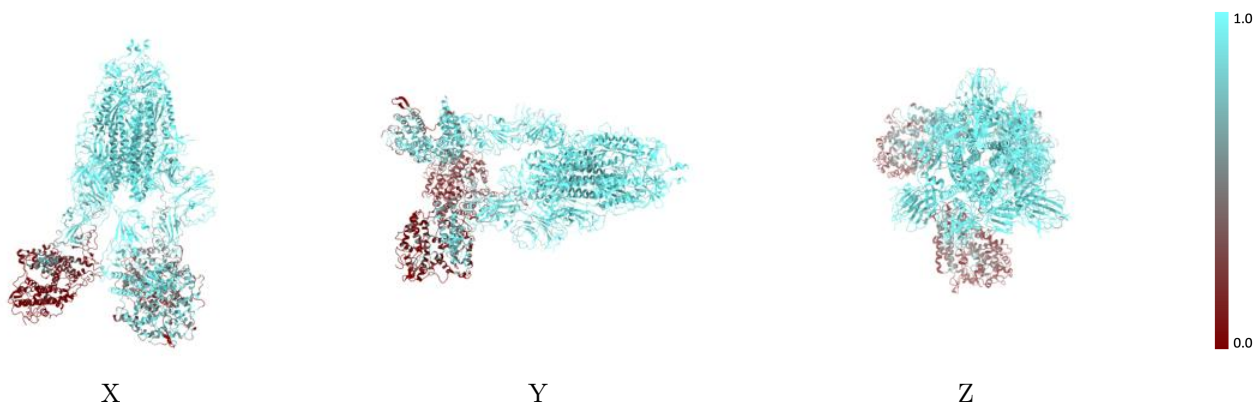
The images above show the 3D surface view of the map at the recommended contour level 0.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



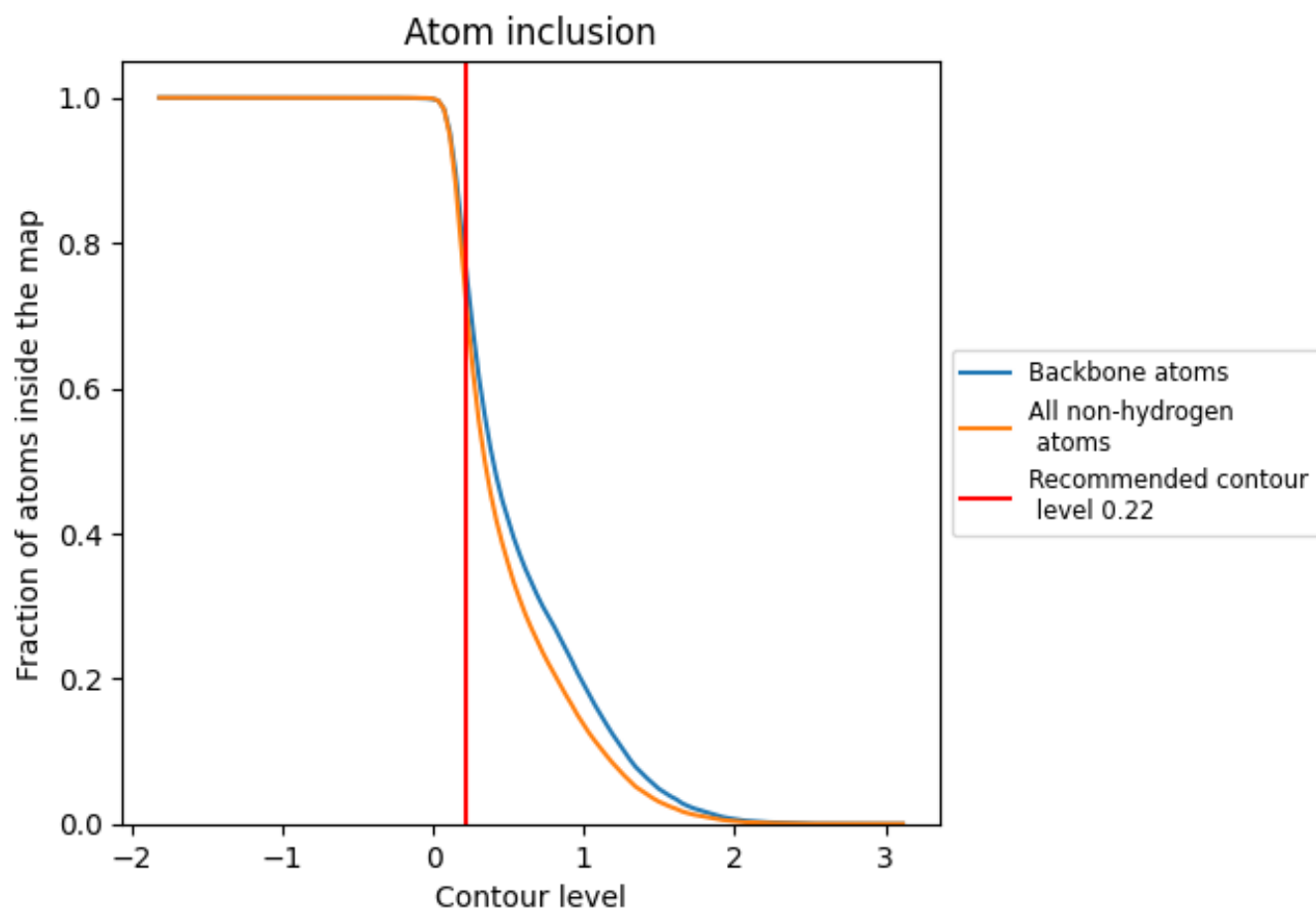
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.22).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7195	 0.3340
A	 0.9482	 0.4750
B	 0.8831	 0.4290
C	 0.9088	 0.4360
D	 0.6429	 0.2970
E	 0.8571	 0.3910
F	 0.9286	 0.3900
G	 0.8571	 0.3710
H	 0.7857	 0.3540
I	 0.7320	 0.2030
J	 0.1336	 0.1140
K	 0.3188	 0.1180
L	 0.9286	 0.5060
M	 0.8571	 0.4040
N	 0.6071	 0.3450
O	 0.9643	 0.5090
P	 0.8571	 0.3030
Q	 0.7857	 0.2250
R	 0.6429	 0.3740
S	 0.8214	 0.4320
T	 0.9286	 0.4350
U	 0.6786	 0.3880
V	 0.8571	 0.4750
W	 0.9286	 0.3960
X	 0.5714	 0.3960
Y	 0.9286	 0.4360
Z	 0.8571	 0.4680
a	 0.5357	 0.2540
b	 0.7500	 0.2650
c	 0.8571	 0.3790
d	 0.6071	 0.3770
e	 0.7143	 0.4620
f	 0.9286	 0.4480
g	 0.6786	 0.3890
h	 0.8929	 0.4510
i	 0.8214	 0.3870

