



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:58 PM UTC

PDB ID : 7V85 / pdb_00007v85
EMDB ID : EMD-31790
Title : Cryo-EM structure of SARS-CoV-2 S-Kappa variant (B.1.617.1) in complex with Angiotensin-converting enzyme 2 (ACE2) ectodomain, two ACE2-bound form
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Hsu, S.T.D.
Deposited on : 2021-08-22
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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

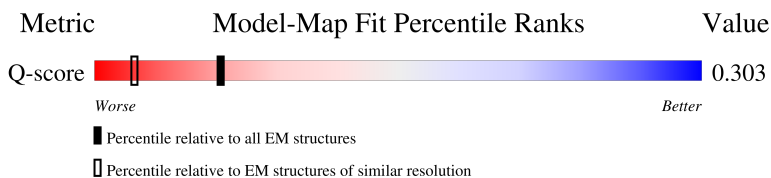
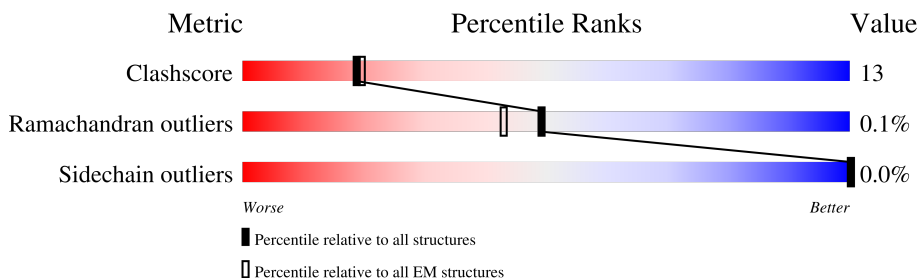
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1283	
1	B	1283	
1	C	1283	
2	F	861	

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Mol	Chain	Length	Quality of chain
2	H	861	
3	D	2	
3	E	2	
3	G	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	

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Mol	Chain	Length	Quality of chain
3	d	2	 100%
3	e	2	 100%
3	f	2	 100%
3	g	2	 100%
3	h	2	 100%
3	i	2	 100%
3	j	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35101 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	B	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		
1	C	1038	Total	C	N	O	S	0	0
			8109	5177	1351	1544	37		

There are 261 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ASP	GLY	variant	UNP P0DTC2
A	154	LYS	GLU	engineered mutation	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	484	GLN	GLU	engineered mutation	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1071	HIS	GLN	engineered mutation	UNP P0DTC2
A	1101	ASP	HIS	engineered mutation	UNP P0DTC2
A	1209	GLU	-	expression tag	UNP P0DTC2
A	1210	PHE	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	ILE	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	GLU	-	expression tag	UNP P0DTC2
A	1219	ALA	-	expression tag	UNP P0DTC2
A	1220	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1221	ARG	-	expression tag	UNP P0DTC2
A	1222	ASP	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLN	-	expression tag	UNP P0DTC2
A	1225	ALA	-	expression tag	UNP P0DTC2
A	1226	TYR	-	expression tag	UNP P0DTC2
A	1227	VAL	-	expression tag	UNP P0DTC2
A	1228	ARG	-	expression tag	UNP P0DTC2
A	1229	LYS	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLU	-	expression tag	UNP P0DTC2
A	1233	TRP	-	expression tag	UNP P0DTC2
A	1234	VAL	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	SER	-	expression tag	UNP P0DTC2
A	1238	THR	-	expression tag	UNP P0DTC2
A	1239	PHE	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	GLY	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	ASP	-	expression tag	UNP P0DTC2
A	1245	ASN	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	ALA	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ILE	-	expression tag	UNP P0DTC2
A	1250	GLN	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	SER	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	ARG	-	expression tag	UNP P0DTC2
A	1255	PRO	-	expression tag	UNP P0DTC2
A	1256	LEU	-	expression tag	UNP P0DTC2
A	1257	GLU	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ARG	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	PRO	-	expression tag	UNP P0DTC2
A	1262	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	LEU	-	expression tag	UNP P0DTC2
A	1267	ILE	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLU	-	expression tag	UNP P0DTC2
A	1270	GLU	-	expression tag	UNP P0DTC2
A	1271	ASP	-	expression tag	UNP P0DTC2
A	1272	LEU	-	expression tag	UNP P0DTC2
A	1273	ASN	-	expression tag	UNP P0DTC2
A	1274	MET	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	THR	-	expression tag	UNP P0DTC2
A	1277	GLY	-	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
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	154	LYS	GLU	engineered mutation	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	484	GLN	GLU	engineered mutation	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1071	HIS	GLN	engineered mutation	UNP P0DTC2
B	1101	ASP	HIS	engineered mutation	UNP P0DTC2
B	1209	GLU	-	expression tag	UNP P0DTC2
B	1210	PHE	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	TYR	-	expression tag	UNP P0DTC2
B	1216	ILE	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1218	GLU	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	PRO	-	expression tag	UNP P0DTC2
B	1221	ARG	-	expression tag	UNP P0DTC2
B	1222	ASP	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLN	-	expression tag	UNP P0DTC2
B	1225	ALA	-	expression tag	UNP P0DTC2
B	1226	TYR	-	expression tag	UNP P0DTC2
B	1227	VAL	-	expression tag	UNP P0DTC2
B	1228	ARG	-	expression tag	UNP P0DTC2
B	1229	LYS	-	expression tag	UNP P0DTC2
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLU	-	expression tag	UNP P0DTC2
B	1233	TRP	-	expression tag	UNP P0DTC2
B	1234	VAL	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	THR	-	expression tag	UNP P0DTC2
B	1239	PHE	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	GLY	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	ASP	-	expression tag	UNP P0DTC2
B	1245	ASN	-	expression tag	UNP P0DTC2
B	1246	SER	-	expression tag	UNP P0DTC2
B	1247	ALA	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ILE	-	expression tag	UNP P0DTC2
B	1250	GLN	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	SER	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	ARG	-	expression tag	UNP P0DTC2
B	1255	PRO	-	expression tag	UNP P0DTC2
B	1256	LEU	-	expression tag	UNP P0DTC2
B	1257	GLU	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	PRO	-	expression tag	UNP P0DTC2
B	1262	PHE	-	expression tag	UNP P0DTC2
B	1263	GLU	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	LEU	-	expression tag	UNP P0DTC2
B	1267	ILE	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	GLU	-	expression tag	UNP P0DTC2
B	1270	GLU	-	expression tag	UNP P0DTC2
B	1271	ASP	-	expression tag	UNP P0DTC2
B	1272	LEU	-	expression tag	UNP P0DTC2
B	1273	ASN	-	expression tag	UNP P0DTC2
B	1274	MET	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	THR	-	expression tag	UNP P0DTC2
B	1277	GLY	-	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
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	154	LYS	GLU	engineered mutation	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	484	GLN	GLU	engineered mutation	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1071	HIS	GLN	engineered mutation	UNP P0DTC2
C	1101	ASP	HIS	engineered mutation	UNP P0DTC2
C	1209	GLU	-	expression tag	UNP P0DTC2
C	1210	PHE	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1215	TYR	-	expression tag	UNP P0DTC2
C	1216	ILE	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	GLU	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	PRO	-	expression tag	UNP P0DTC2
C	1221	ARG	-	expression tag	UNP P0DTC2
C	1222	ASP	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLN	-	expression tag	UNP P0DTC2
C	1225	ALA	-	expression tag	UNP P0DTC2
C	1226	TYR	-	expression tag	UNP P0DTC2
C	1227	VAL	-	expression tag	UNP P0DTC2
C	1228	ARG	-	expression tag	UNP P0DTC2
C	1229	LYS	-	expression tag	UNP P0DTC2
C	1230	ASP	-	expression tag	UNP P0DTC2
C	1231	GLY	-	expression tag	UNP P0DTC2
C	1232	GLU	-	expression tag	UNP P0DTC2
C	1233	TRP	-	expression tag	UNP P0DTC2
C	1234	VAL	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	THR	-	expression tag	UNP P0DTC2
C	1239	PHE	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	GLY	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	ASP	-	expression tag	UNP P0DTC2
C	1245	ASN	-	expression tag	UNP P0DTC2
C	1246	SER	-	expression tag	UNP P0DTC2
C	1247	ALA	-	expression tag	UNP P0DTC2
C	1248	ASP	-	expression tag	UNP P0DTC2
C	1249	ILE	-	expression tag	UNP P0DTC2
C	1250	GLN	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	SER	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	ARG	-	expression tag	UNP P0DTC2
C	1255	PRO	-	expression tag	UNP P0DTC2
C	1256	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1257	GLU	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ARG	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	PRO	-	expression tag	UNP P0DTC2
C	1262	PHE	-	expression tag	UNP P0DTC2
C	1263	GLU	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	LEU	-	expression tag	UNP P0DTC2
C	1267	ILE	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	GLU	-	expression tag	UNP P0DTC2
C	1270	GLU	-	expression tag	UNP P0DTC2
C	1271	ASP	-	expression tag	UNP P0DTC2
C	1272	LEU	-	expression tag	UNP P0DTC2
C	1273	ASN	-	expression tag	UNP P0DTC2
C	1274	MET	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	THR	-	expression tag	UNP P0DTC2
C	1277	GLY	-	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
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	596	Total	C	N	O	S	0	0
			4862	3111	805	917	29		
2	H	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.



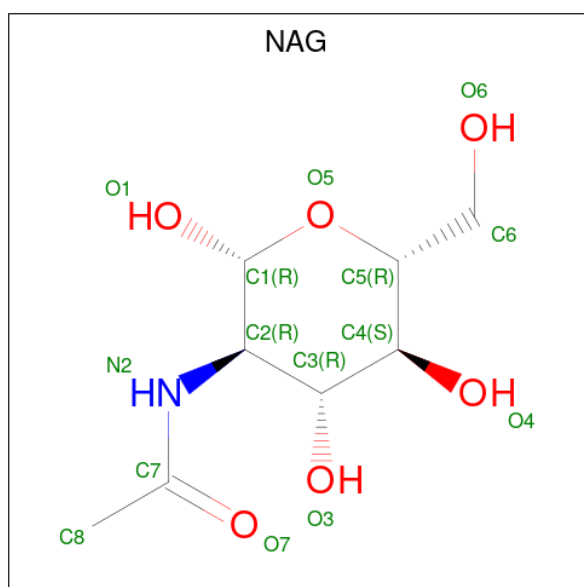
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	2	Total 28	C 16	N 2	O 10	0	0
3	E	2	Total 28	C 16	N 2	O 10	0	0
3	G	2	Total 28	C 16	N 2	O 10	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0
3	J	2	Total 28	C 16	N 2	O 10	0	0
3	K	2	Total 28	C 16	N 2	O 10	0	0
3	L	2	Total 28	C 16	N 2	O 10	0	0
3	M	2	Total 28	C 16	N 2	O 10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

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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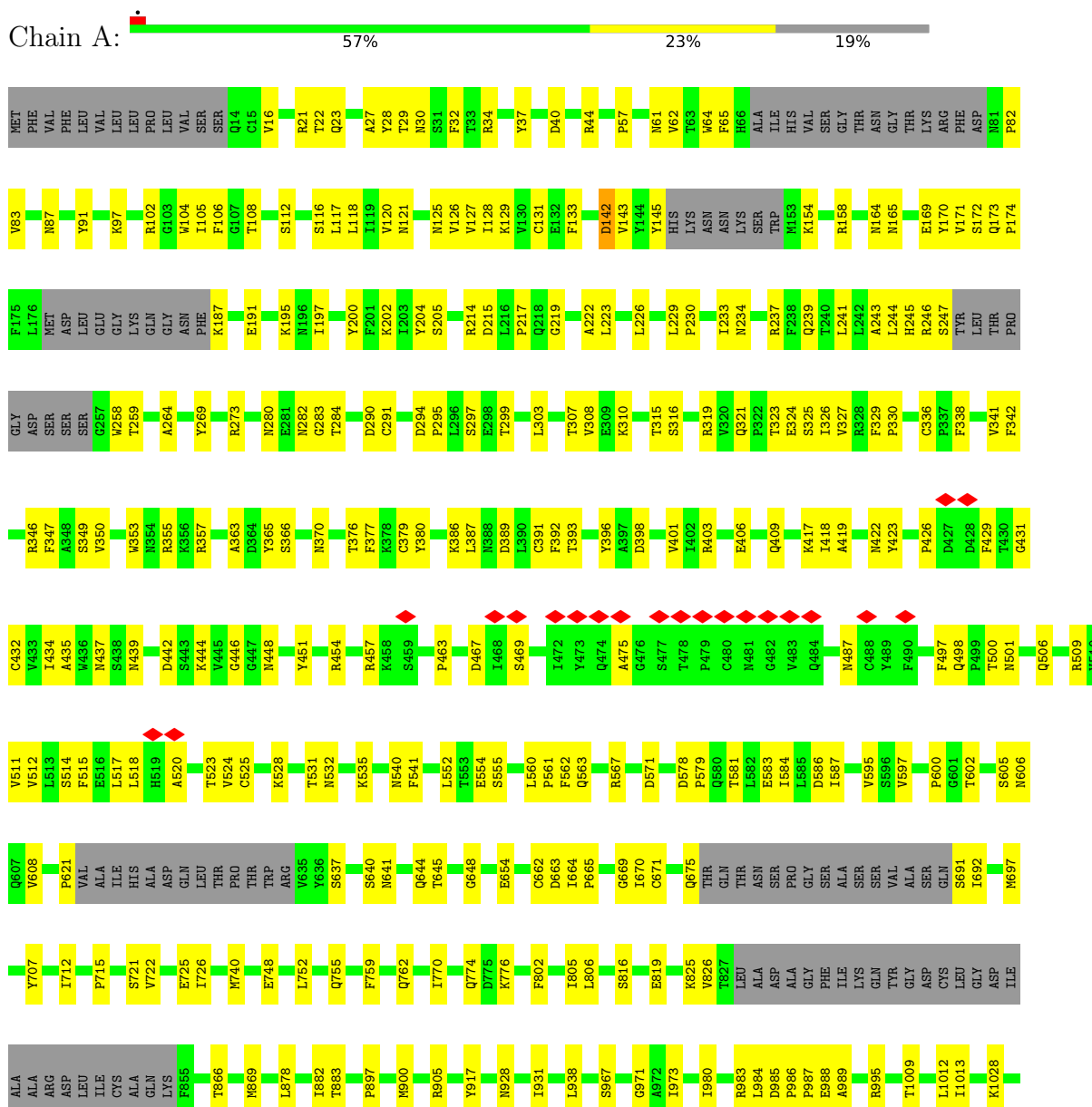
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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



F1042	GLY
L1049	ILE
M1050	ASN
S1051	ALA
F1052	SER
P1057	LEU
V1061	VAL
H1064	SER
V1065	THR
T1066	ASN
E1072	ILE
F1089	GLN
V1096	VAL
W1102	ALA
T1105	GLY
P1112	ASN
N1125	PRO
C1126	LEU
D1127	GLY
V1128	GLY
V1129	GLY
T1132	GLY
D1146	TYR
SER	GLY
PHE	GLN
LYS	GLU
GLU	PHE
GLY	GLY
LEU	SER
ASP	GLY
LYS	GLY
TYR	TYR
PHE	ILE
LYS	PRO
ASN	GLY
HIS	ALA
THR	PRO
SER	ARG
PRO	ASP
GLY	GLY
VAL	GLN
ALA	ALA
LEU	TYR
GLY	VAL
ASP	ARG
ILE	LYS
SER	ASP

GLY	GLY
GLU	TRP
TRP	VAL
ASN	PHE
ALA	LEU
SER	VAL
LEU	VAL
VAL	SER
SER	THR
THR	ASN
ASN	PHE
PHE	ILE
GLN	LYS
LYS	GLY
GLY	GLU
ILE	ILE
ASP	ASP
ASN	ASN
ALA	ALA
GLY	GLY
ASN	ASN
GLY	GLY
LEU	GLY
ASN	ASN
PRO	PRO
GLY	LEU
SER	GLY
ILE	ILE
SER	GLY
GLU	GLY
N30	GLY
S31	ILE
F32	ARG
V36	GLY
Y37	PRO
Y38	PHE
P39	GLY
D40	GLN
R44	LEU
V47	ILE
S60	SER
N61	GLY
V62	LEU
T63	ASN
W64	MET
F65	HIS
H66	THR
ILE	GLY
HIS	GLY
HIS	ALA
HIS	PRO
HIS	VAL
HIS	SER
HIS	ASP
HIS	GLY
HIS	GLN
HIS	VAL
HIS	ASN
HIS	GLY
HIS	THR
HIS	GLY
HIS	THR
HIS	LYS
HIS	ARG
HIS	ILE
HIS	LYS
HIS	ASP
HIS	SER

• Molecule 1: Spike glycoprotein

Chain B: 

MET	ASP
PHE	N81
VAL	P82
PHE	V83
LEU	L84
VAL	P85
VAL	S86
SER	P87
LEU	N87
PRO	D88
LEU	N89
VAL	L90
VAL	S91
SER	S92
SER	S93
GLY	W104
GLY	I105
LYS	F106
GLY	F107
GLY	T108
GLY	T109
GLY	L110
GLY	D111
GLY	S112
GLY	Q115
GLY	S116
GLY	L117
GLY	N121
GLY	N122
GLY	A123
GLY	T124
GLY	N125
GLY	V126
GLY	V127
GLY	I128
GLY	K129
GLY	V130
GLY	C131
GLY	E132
GLY	N137
GLY	L141
GLY	D142
GLY	V143
GLY	Y144
GLY	Y145
GLY	HIS
GLY	LYS
GLY	ASN
GLY	ASN
GLY	LYS
GLY	SER
GLY	TRP
GLY	M153
GLY	L244
GLY	H245
GLY	R246
GLY	F157
GLY	PHE

ASP	N81
ASP	P82
ASP	V83
ASP	L84
ASP	P85
ASP	S86
ASP	P87
ASP	N87
ASP	D88
ASP	N89
ASP	L90
ASP	S91
ASP	S92
ASP	S93
ASP	W104
ASP	I105
ASP	F106
ASP	F107
ASP	T108
ASP	T109
ASP	L110
ASP	D111
ASP	S112
ASP	Q115
ASP	S116
ASP	L117
ASP	N121
ASP	N122
ASP	A123
ASP	T124
ASP	N125
ASP	V126
ASP	V127
ASP	I128
ASP	K129
ASP	V130
ASP	C131
ASP	E132
ASP	N137
ASP	L141
ASP	D142
ASP	V143
ASP	Y144
ASP	Y145
ASP	HIS
ASP	LYS
ASP	ASN
ASP	ASN
ASP	LYS
ASP	SER
ASP	TRP
ASP	M153
ASP	L244
ASP	H245
ASP	R246
ASP	F157
ASP	PHE

N164	F168
F169	Y170
Y171	S172
Q173	P174
F175	L176
MET	ASP
LEU	GLU
GLY	GLY
LVS	GLN
GLN	GLY
ASN	ASN
PHE	K187
N188	L189
R190	K195
Y200	F201
K202	I203
Y204	P209
R214	F220
E224	P225
L226	V227
P230	I233
N234	I235
T236	R237
F238	Q239
T240	L244
H245	R246

SER
THR
PHE
PHE
LEU
LYS
GLY
GLN
ASP
ASN
GLN
ALA
SER
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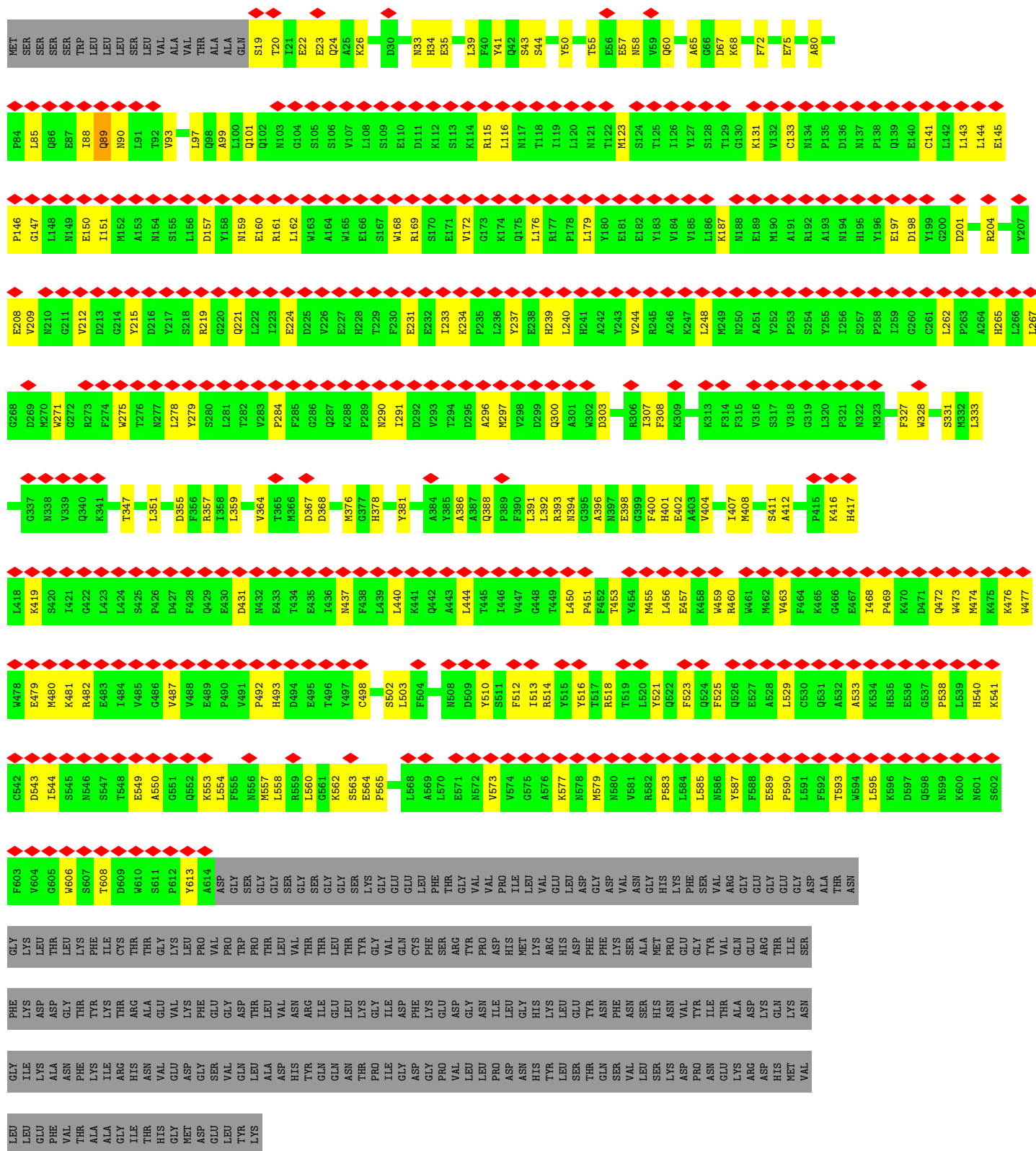
• Molecule 1: Spike glycoprotein



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• Molecule 2: Angiotensin-converting enzyme 2, Green fluorescent protein





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

Chain E:  50% 50%



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

Chain G:  100%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  100%



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

Chain N:  50% 50%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain R:  50% 100%



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

Chain S:  100%



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

Chain T:  100%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  100%



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

Chain X:  100%



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

Chain Y:  50% 50%



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

Chain Z:  100%



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

Chain a:  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:  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:  100%

NAG1
NAG2

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

Chain h:  100%

NAG1
NAG2

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

Chain i:  100%

NAG1
NAG2

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

Chain j:  100%

NAG1
NAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66721	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	1.614	Depositor
Minimum map value	-0.681	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.18	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	0.23	0/8295	0.38	0/11291
1	B	0.23	0/8295	0.37	1/11291 (0.0%)
1	C	0.23	0/8295	0.36	0/11291
2	F	0.12	0/4999	0.34	2/6792 (0.0%)
2	H	0.11	0/4999	0.30	0/6792
All	All	0.21	0/34883	0.36	3/47457 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	PRO	CA-N-CD	-5.21	104.70	112.00
2	F	89	GLN	CA-C-N	5.20	131.47	121.54
2	F	89	GLN	C-N-CA	5.20	131.47	121.54

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	8109	0	7900	233	0
1	B	8109	0	7900	207	0
1	C	8109	0	7903	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	4862	0	4639	148	0
2	H	4862	0	4639	131	0
3	D	28	0	25	1	0
3	E	28	0	25	1	0
3	G	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
3	i	28	0	25	0	0
3	j	28	0	25	0	0
4	A	56	0	52	3	0
4	B	56	0	52	1	0
4	C	70	0	65	3	0
All	All	35101	0	33925	889	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 13.

The worst 5 of 889 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:347:PHE:HB2	1:B:401:VAL:HG23	1.55	0.89
2:F:529:LEU:O	2:F:533:ALA:HB2	1.72	0.89
1:A:27:ALA:HB3	1:A:64:TRP:O	1.76	0.84
1:A:315:THR:HG22	1:A:316:SER:H	1.43	0.83
1:B:245:HIS:HE2	1:B:247:SER:HG	1.25	0.82

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	1022/1283 (80%)	947 (93%)	72 (7%)	3 (0%)	36	65
1	B	1022/1283 (80%)	948 (93%)	74 (7%)	0	100	100
1	C	1022/1283 (80%)	947 (93%)	74 (7%)	1 (0%)	48	75
2	F	594/861 (69%)	565 (95%)	29 (5%)	0	100	100
2	H	594/861 (69%)	556 (94%)	38 (6%)	0	100	100
All	All	4254/5571 (76%)	3963 (93%)	287 (7%)	4 (0%)	49	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1102	TRP
1	C	1102	TRP
1	A	214	ARG
1	A	142	ASP

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	907/1116 (81%)	907 (100%)	0	100	100
1	B	907/1116 (81%)	907 (100%)	0	100	100
1	C	907/1116 (81%)	907 (100%)	0	100	100
2	F	526/752 (70%)	526 (100%)	0	100	100
2	H	526/752 (70%)	525 (100%)	1 (0%)	87	88
All	All	3773/4852 (78%)	3772 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	397	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	98	GLN
2	H	102	GLN
2	F	139	GLN
2	F	524	GLN
2	H	305	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

62 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	D	1	3,1	14,14,15	0.57	0	17,19,21	0.59	0
3	NAG	D	2	3	14,14,15	0.43	0	17,19,21	1.32	2 (11%)
3	NAG	E	1	3,1	14,14,15	0.32	0	17,19,21	0.57	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.49	0
3	NAG	G	1	3,1	14,14,15	0.33	0	17,19,21	0.52	0
3	NAG	G	2	3	14,14,15	0.18	0	17,19,21	0.54	0
3	NAG	I	1	3,1	14,14,15	0.28	0	17,19,21	0.45	0
3	NAG	I	2	3	14,14,15	0.27	0	17,19,21	0.54	0
3	NAG	J	1	3,1	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	K	1	3,1	14,14,15	0.39	0	17,19,21	0.41	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.54	0
3	NAG	L	1	3,1	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	L	2	3	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	M	1	3,1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	M	2	3	14,14,15	0.17	0	17,19,21	0.50	0
3	NAG	N	1	3,1	14,14,15	1.26	1 (7%)	17,19,21	1.23	1 (5%)
3	NAG	N	2	3	14,14,15	0.20	0	17,19,21	0.49	0
3	NAG	O	1	3,1	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	O	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	P	1	3,1	14,14,15	0.18	0	17,19,21	0.39	0
3	NAG	P	2	3	14,14,15	0.32	0	17,19,21	0.39	0
3	NAG	Q	1	3,1	14,14,15	0.65	1 (7%)	17,19,21	0.74	0
3	NAG	Q	2	3	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	R	1	3,1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	R	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	S	1	3,1	14,14,15	0.33	0	17,19,21	0.57	0
3	NAG	S	2	3	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	T	1	3,1	14,14,15	0.31	0	17,19,21	0.42	0
3	NAG	T	2	3	14,14,15	0.19	0	17,19,21	0.49	0
3	NAG	U	1	3,1	14,14,15	0.19	0	17,19,21	0.53	0
3	NAG	U	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	V	1	3,1	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	V	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	W	1	3,1	14,14,15	0.38	0	17,19,21	0.48	0
3	NAG	W	2	3	14,14,15	0.17	0	17,19,21	0.47	0
3	NAG	X	1	3,1	14,14,15	0.31	0	17,19,21	0.44	0
3	NAG	X	2	3	14,14,15	0.20	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Y	1	3,1	14,14,15	1.09	1 (7%)	17,19,21	1.02	1 (5%)
3	NAG	Y	2	3	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	Z	1	3,1	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	Z	2	3	14,14,15	0.20	0	17,19,21	0.48	0
3	NAG	a	1	3,1	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	a	2	3	14,14,15	0.18	0	17,19,21	0.47	0
3	NAG	b	1	3,1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	b	2	3	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	c	1	3,1	14,14,15	0.23	0	17,19,21	0.37	0
3	NAG	c	2	3	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	d	1	3,1	14,14,15	0.27	0	17,19,21	0.61	0
3	NAG	d	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	e	1	3,1	14,14,15	0.32	0	17,19,21	0.49	0
3	NAG	e	2	3	14,14,15	0.18	0	17,19,21	0.47	0
3	NAG	f	1	3,1	14,14,15	0.22	0	17,19,21	0.55	0
3	NAG	f	2	3	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	g	1	3,1	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	g	2	3	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	h	1	3,1	14,14,15	0.45	0	17,19,21	0.92	1 (5%)
3	NAG	h	2	3	14,14,15	0.17	0	17,19,21	0.66	1 (5%)
3	NAG	i	1	3,1	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	i	2	3	14,14,15	0.16	0	17,19,21	0.43	0
3	NAG	j	1	3,1	14,14,15	0.17	0	17,19,21	0.51	0
3	NAG	j	2	3	14,14,15	0.18	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	6/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	2/6/23/26	0/1/1/1
3	NAG	e	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	e	2	3	-	2/6/23/26	0/1/1/1
3	NAG	f	1	3,1	-	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	-	0/6/23/26	0/1/1/1
3	NAG	h	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	h	2	3	-	0/6/23/26	0/1/1/1
3	NAG	i	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	i	2	3	-	0/6/23/26	0/1/1/1
3	NAG	j	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O5-C1	-4.24	1.36	1.43
3	Y	1	NAG	O5-C1	-3.46	1.37	1.43
3	Q	1	NAG	O5-C1	-2.05	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C2-N2-C7	4.53	128.97	122.90
3	N	1	NAG	C3-C4-C5	3.31	116.24	110.23
3	Y	1	NAG	C3-C4-C5	2.63	115.00	110.23
3	h	1	NAG	C1-O5-C5	2.50	115.54	112.19
3	D	2	NAG	C1-C2-N2	2.28	114.02	110.43

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6

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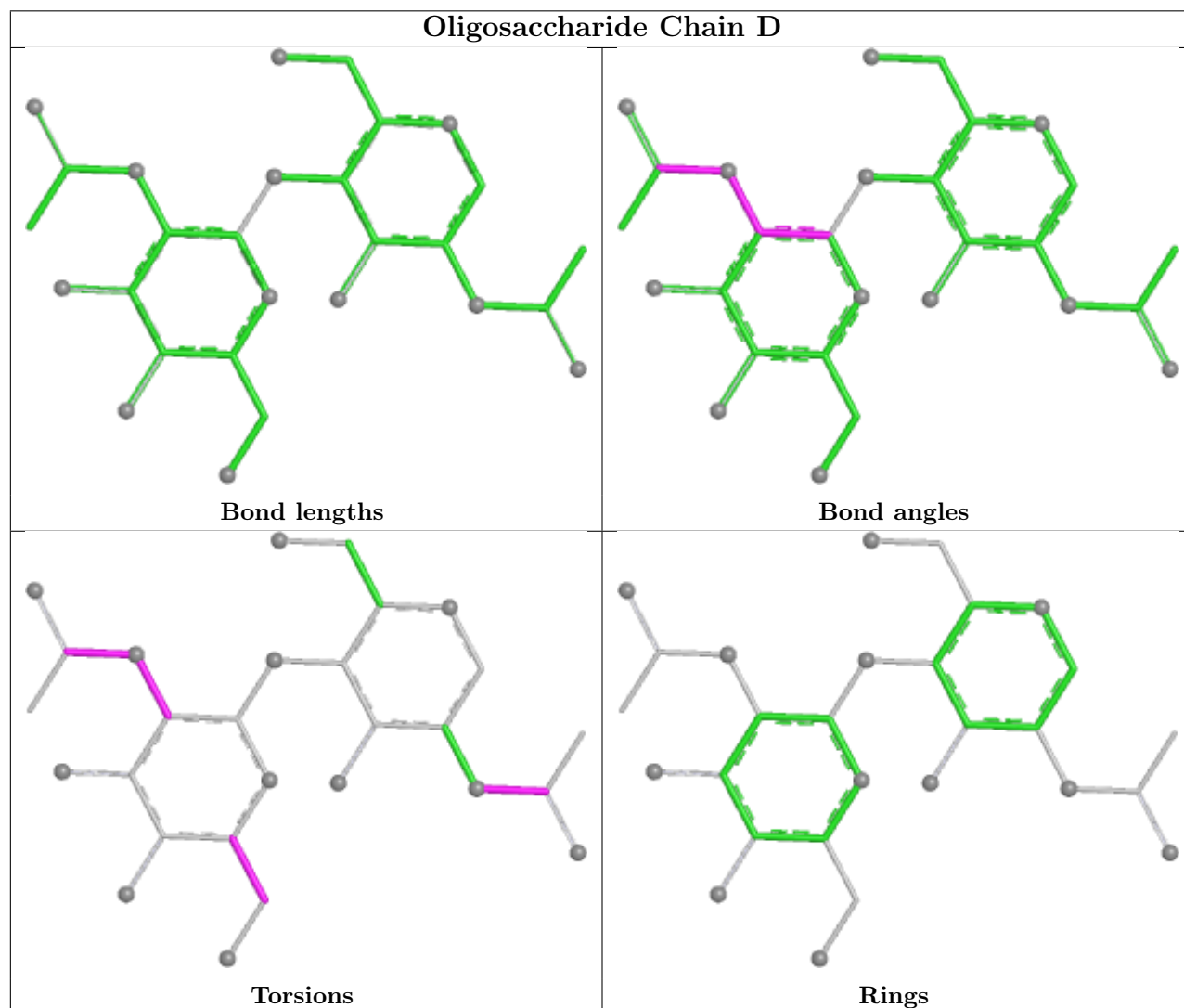
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6

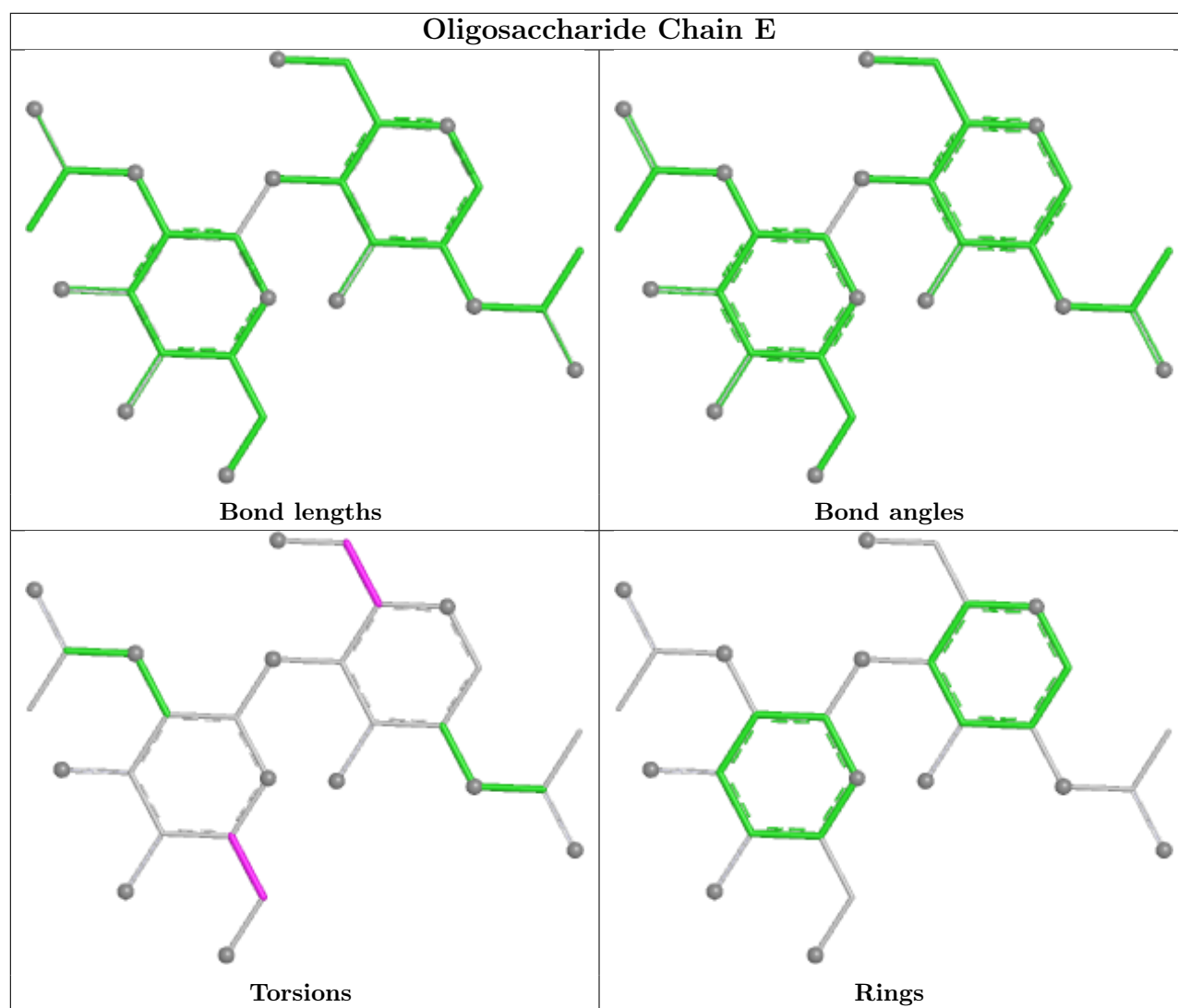
There are no ring outliers.

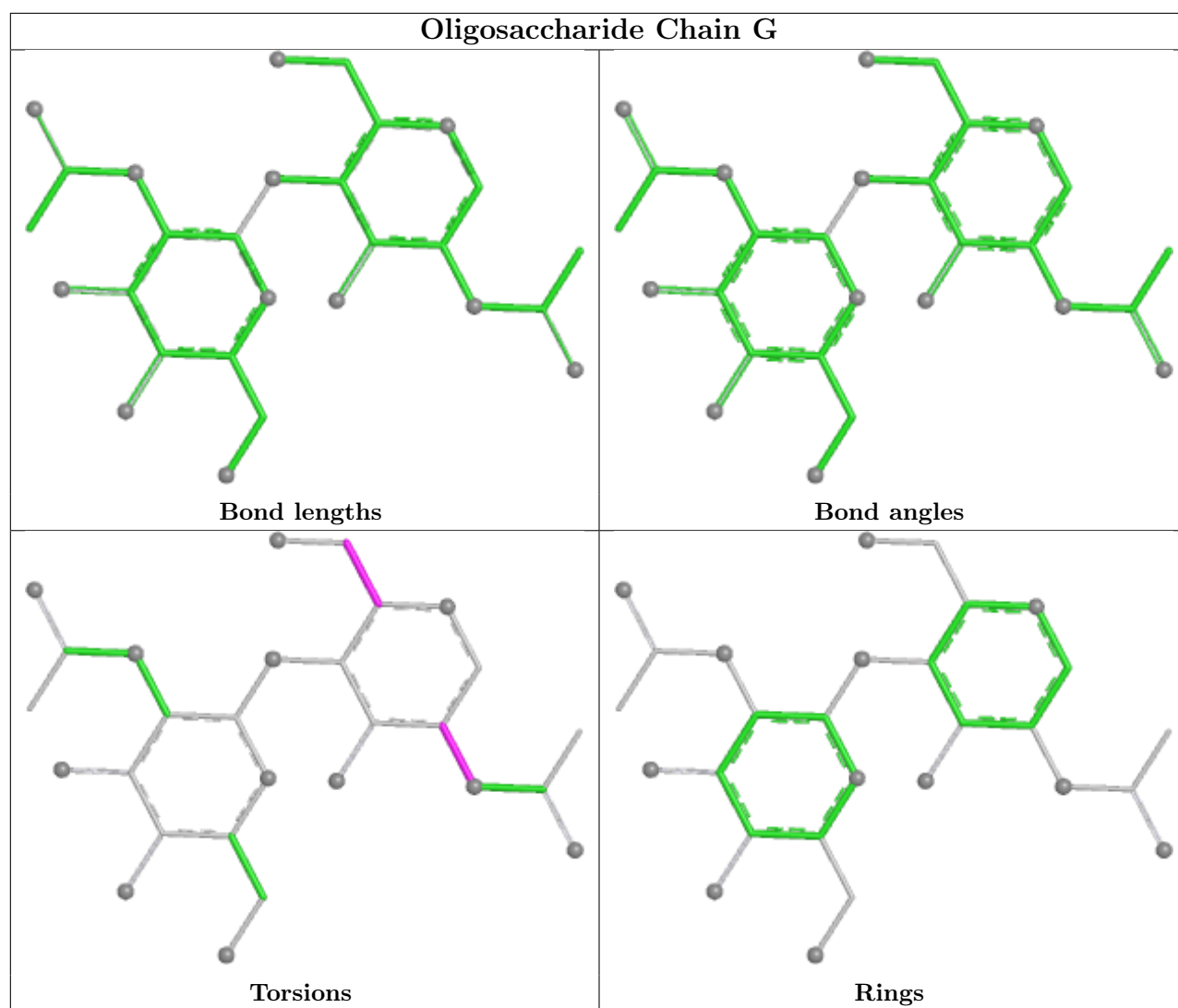
2 monomers are involved in 2 short contacts:

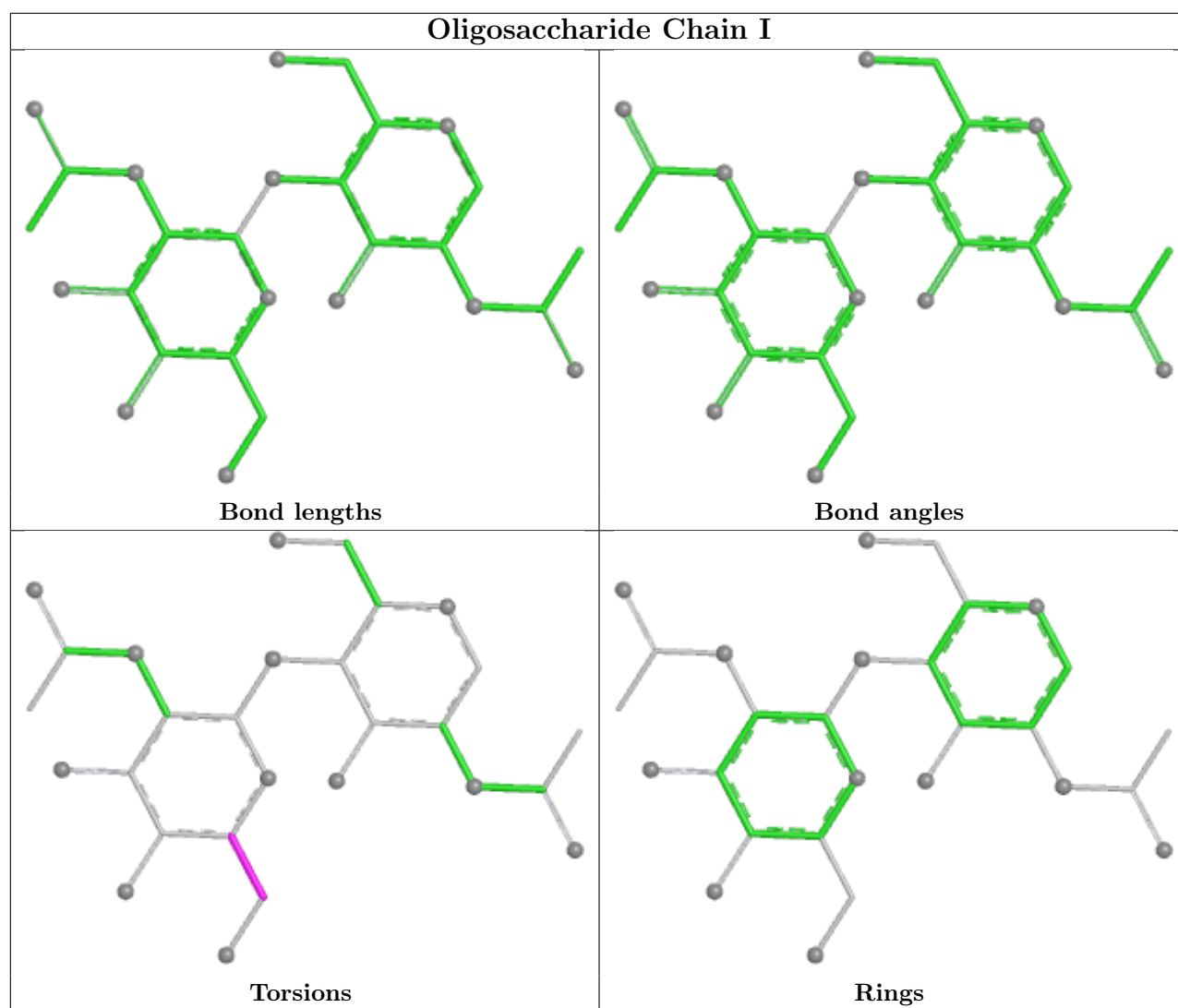
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	E	1	NAG	1	0

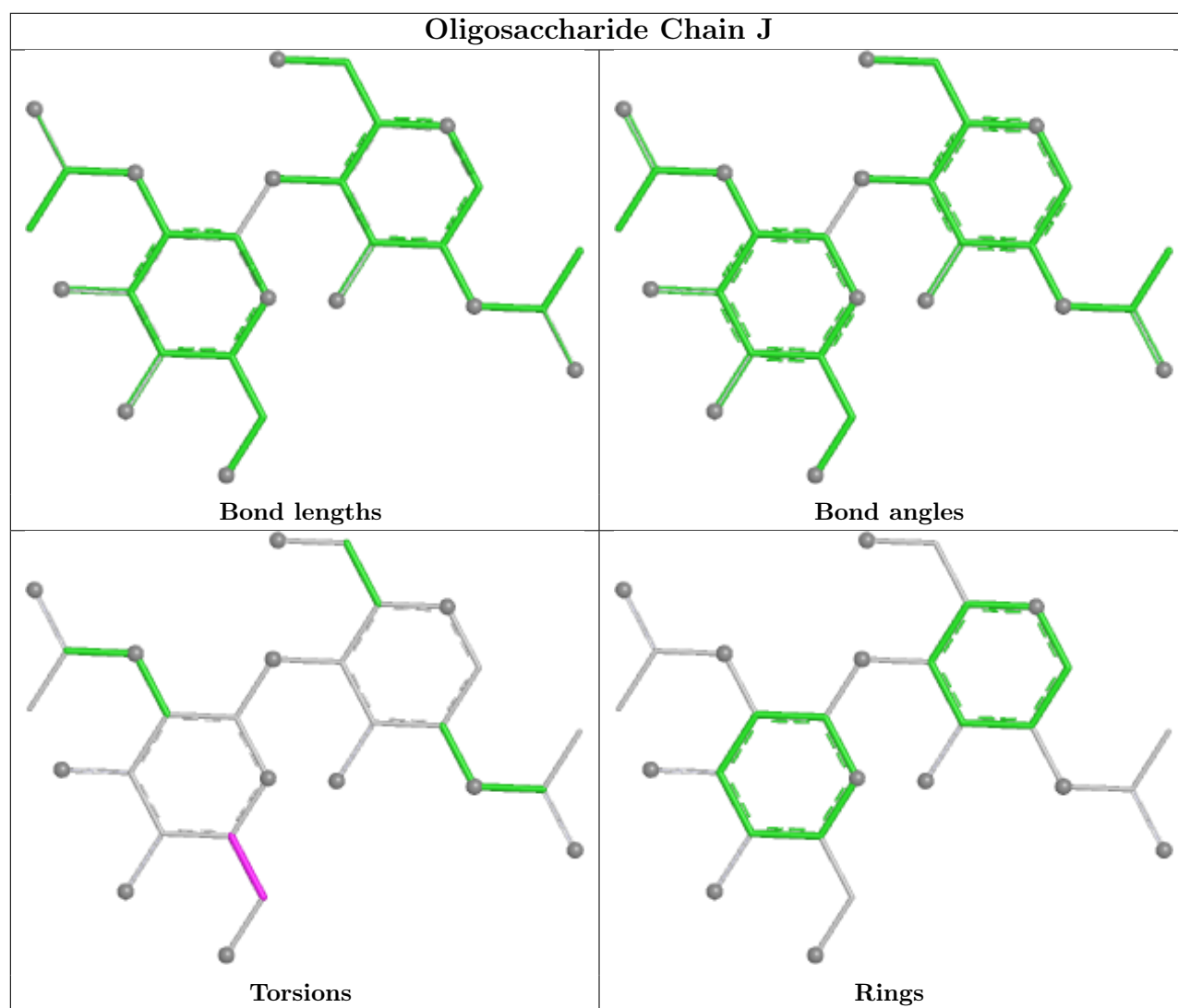
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

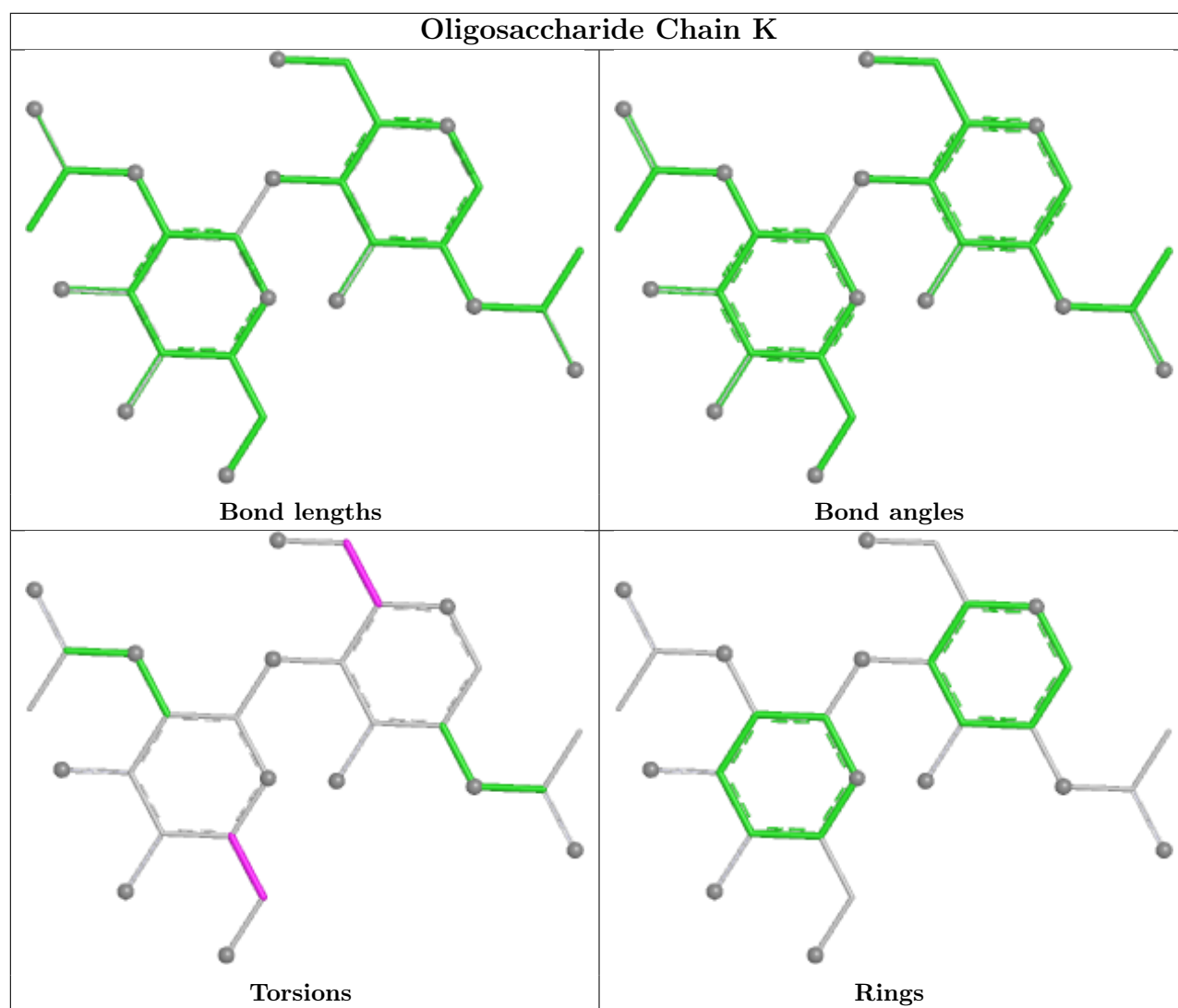


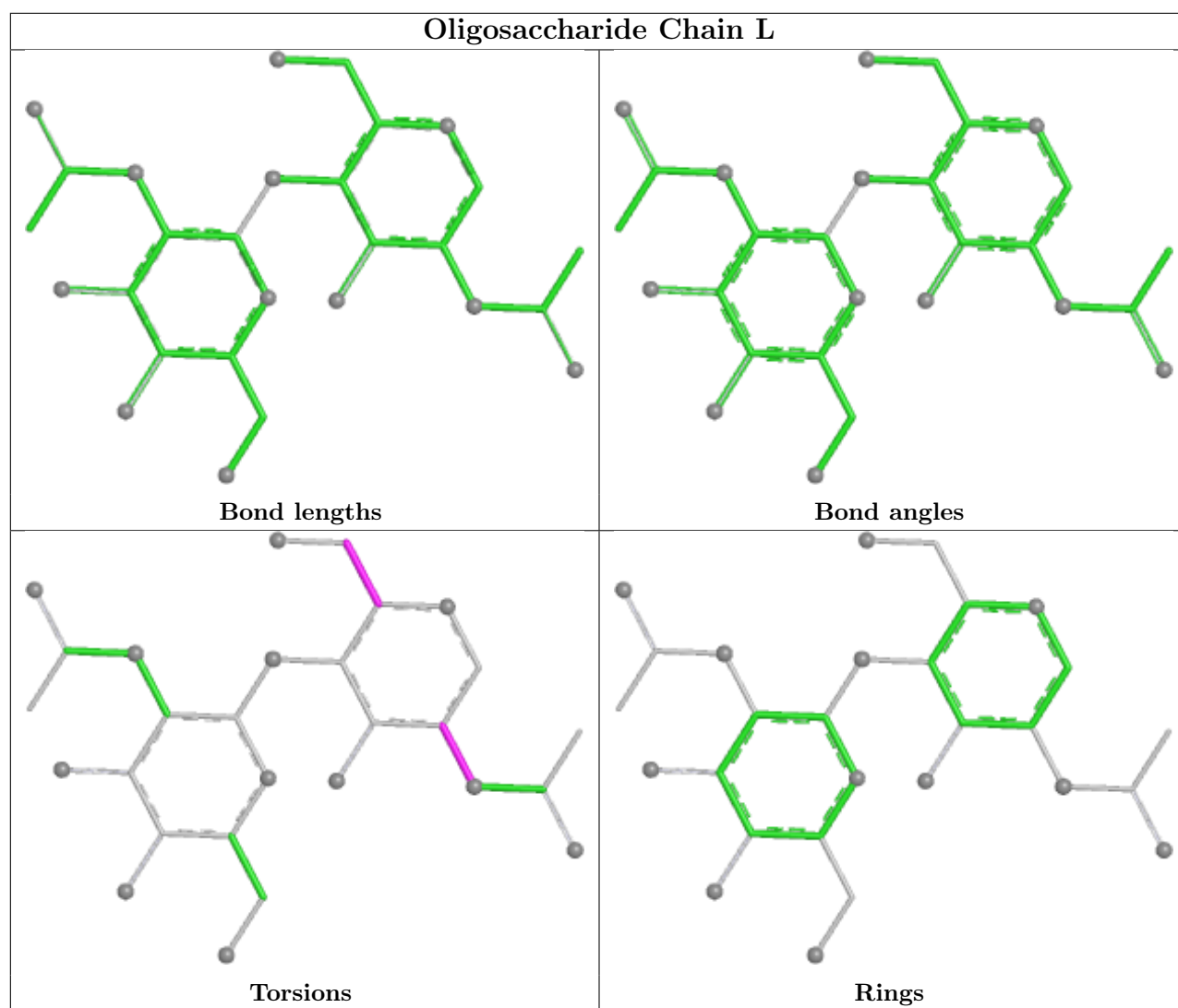


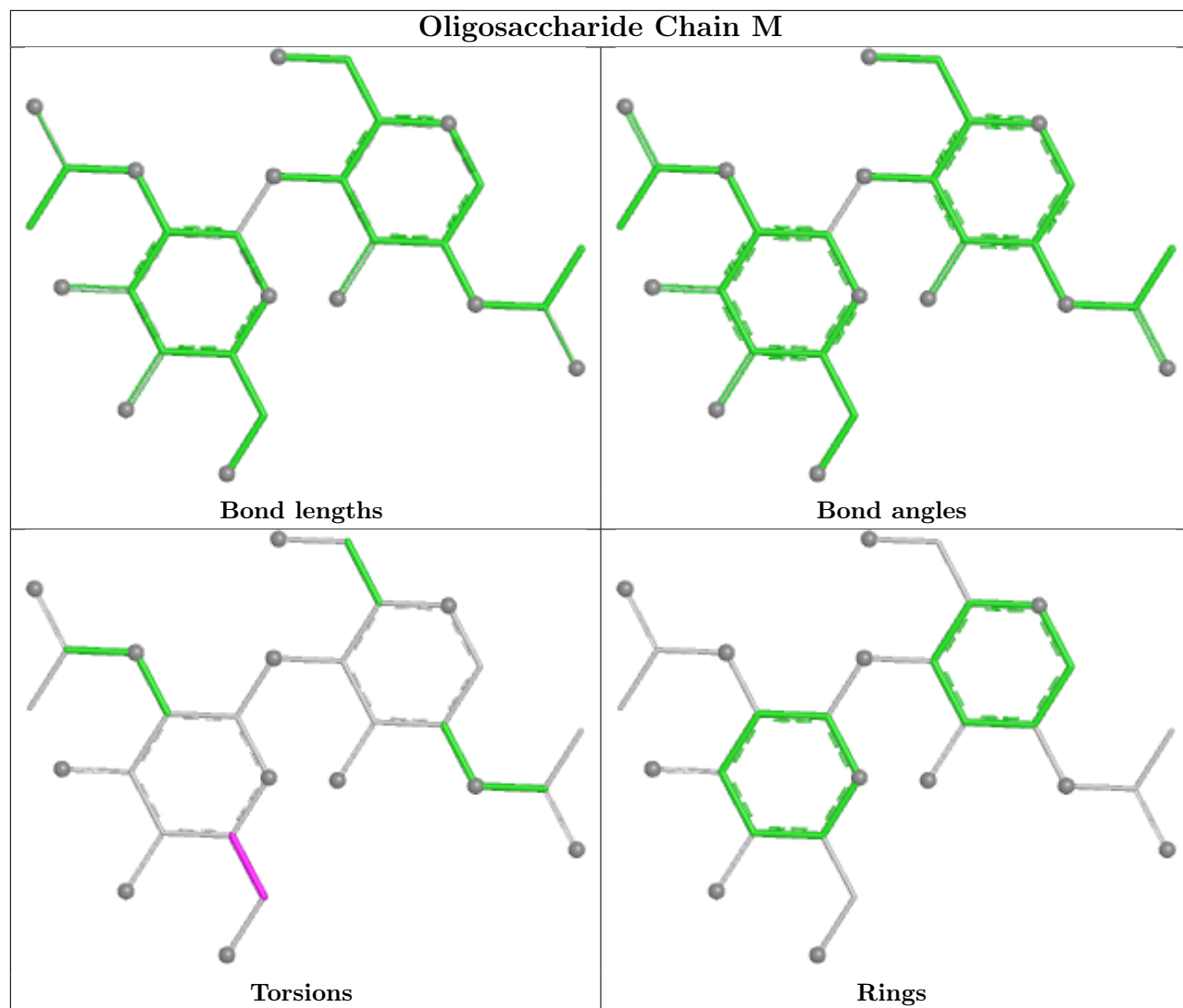


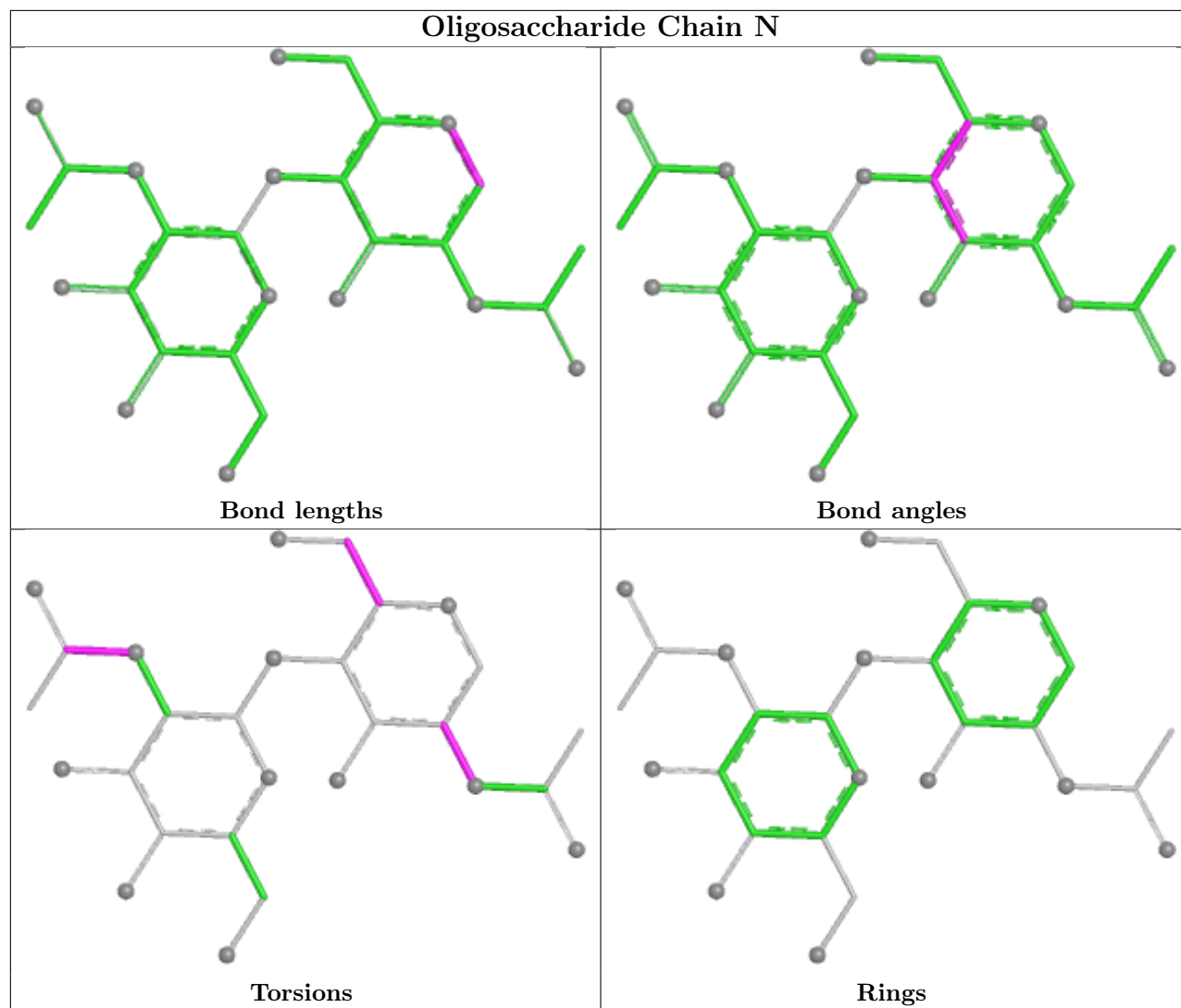


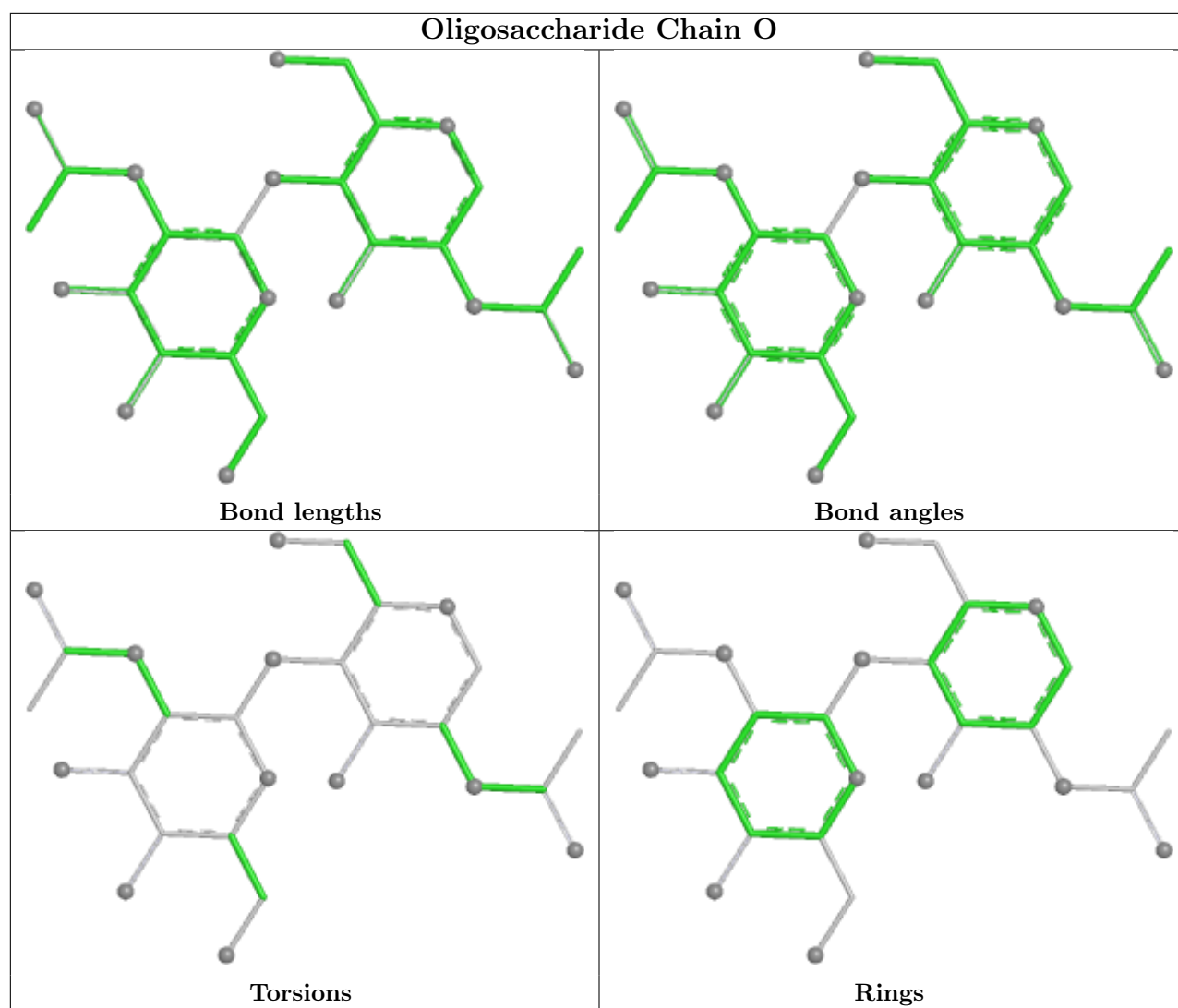


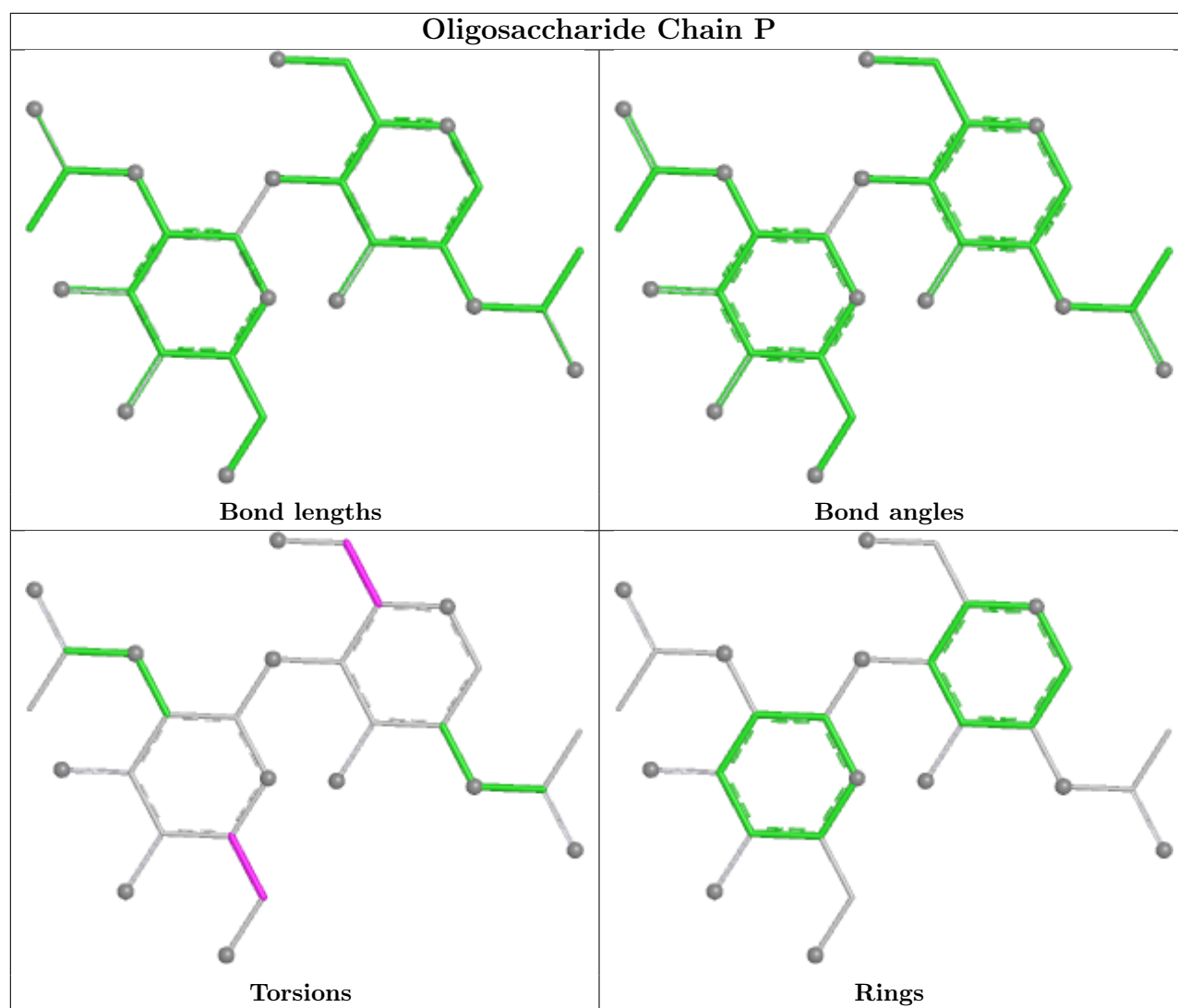


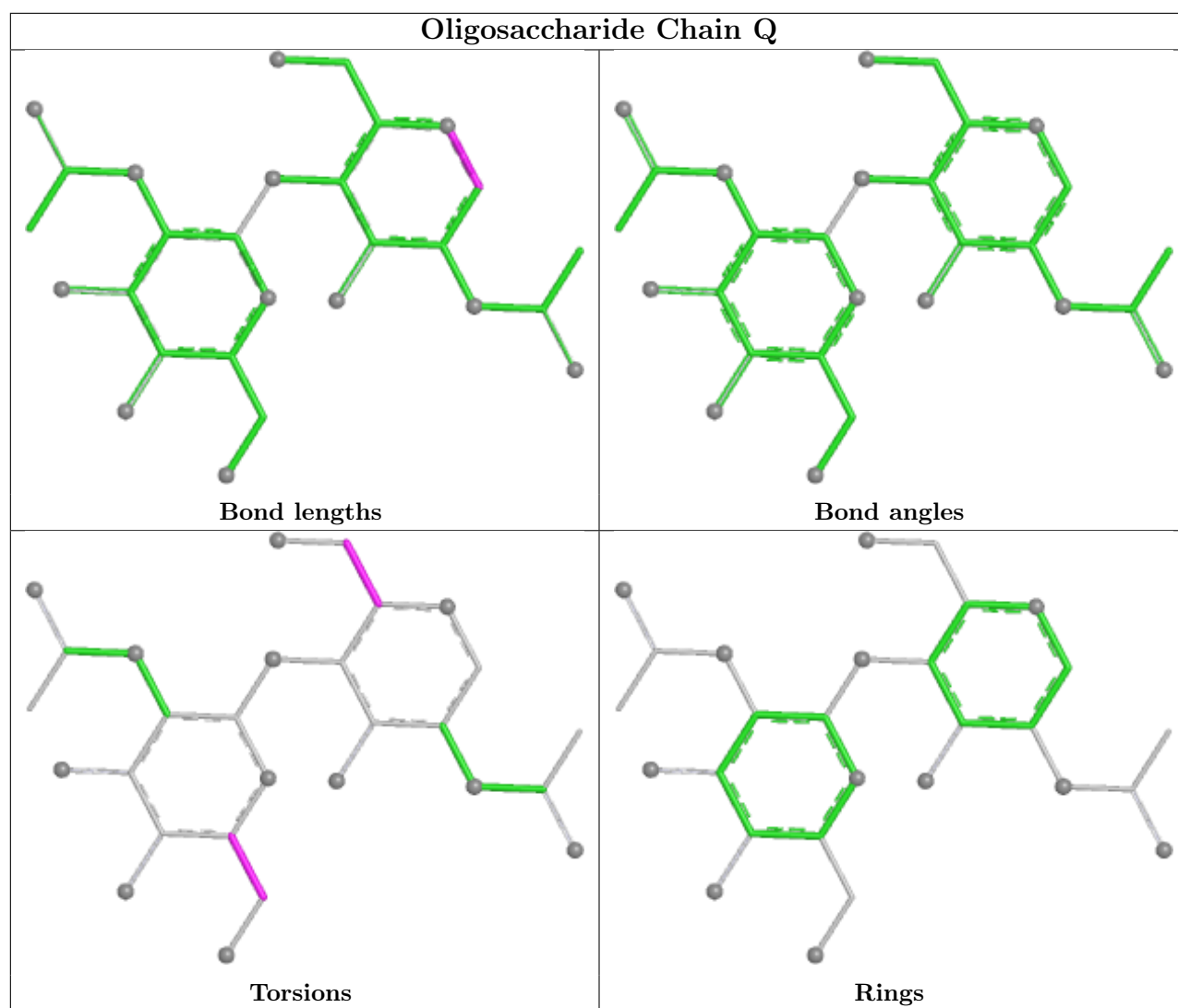


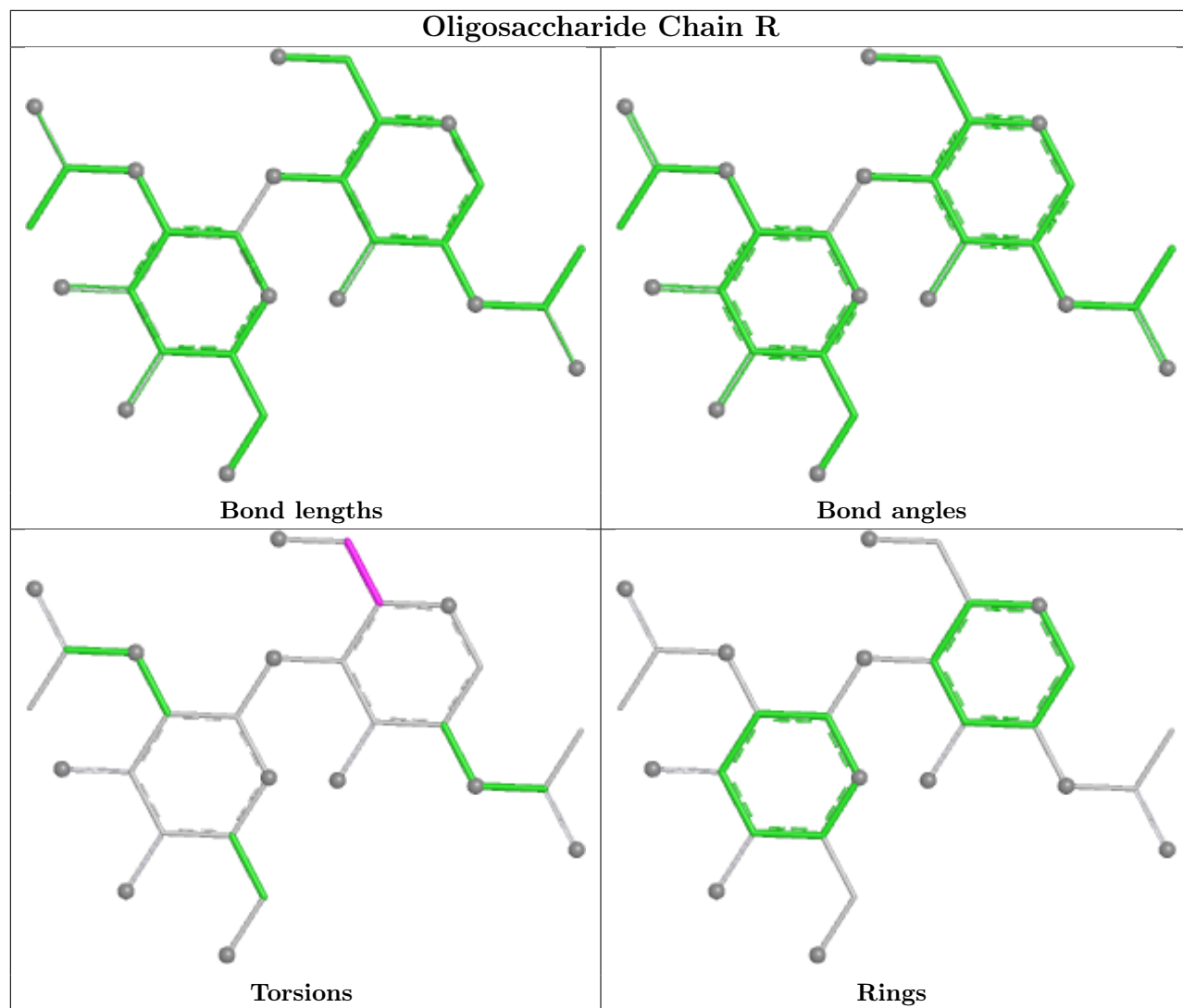


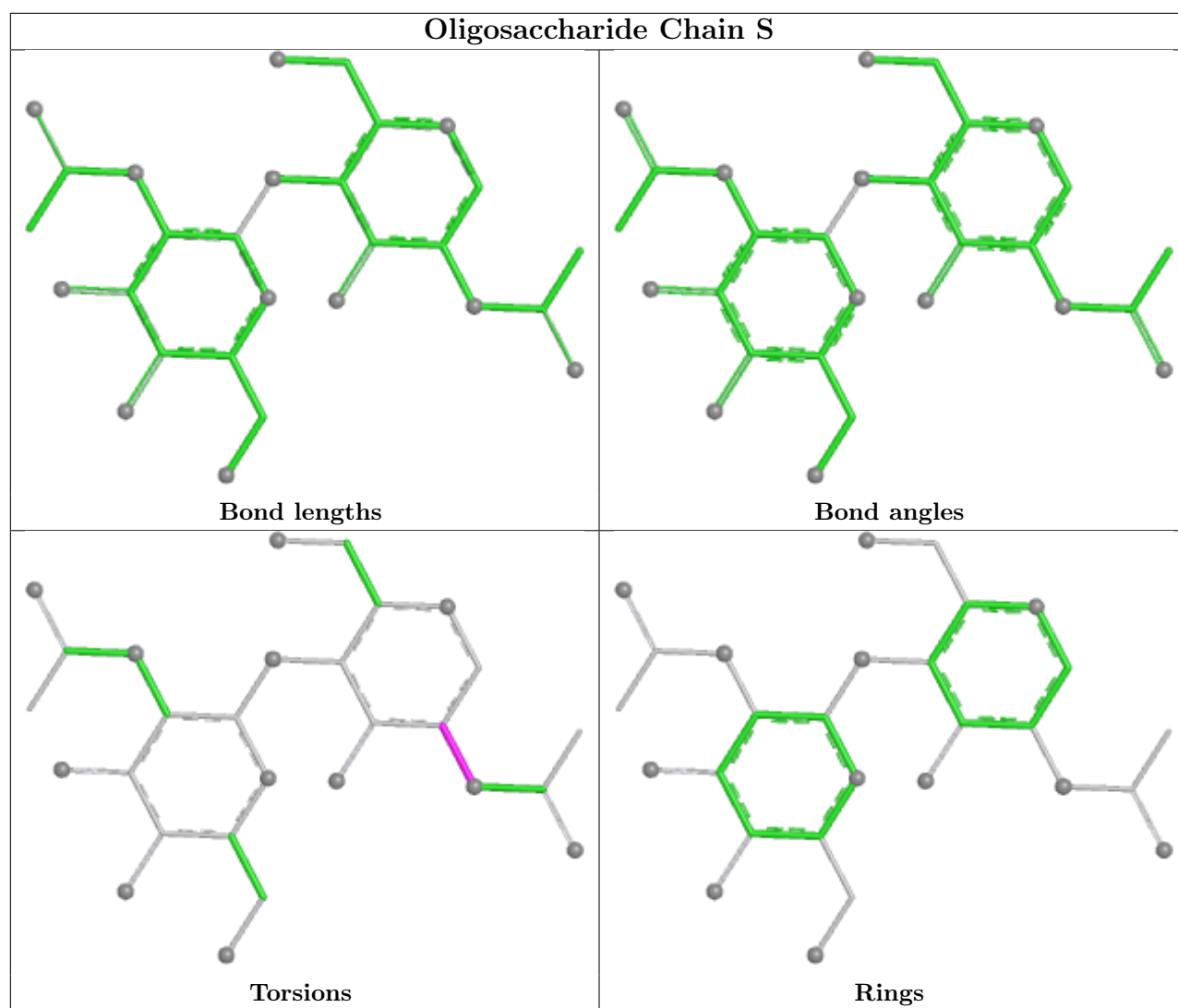


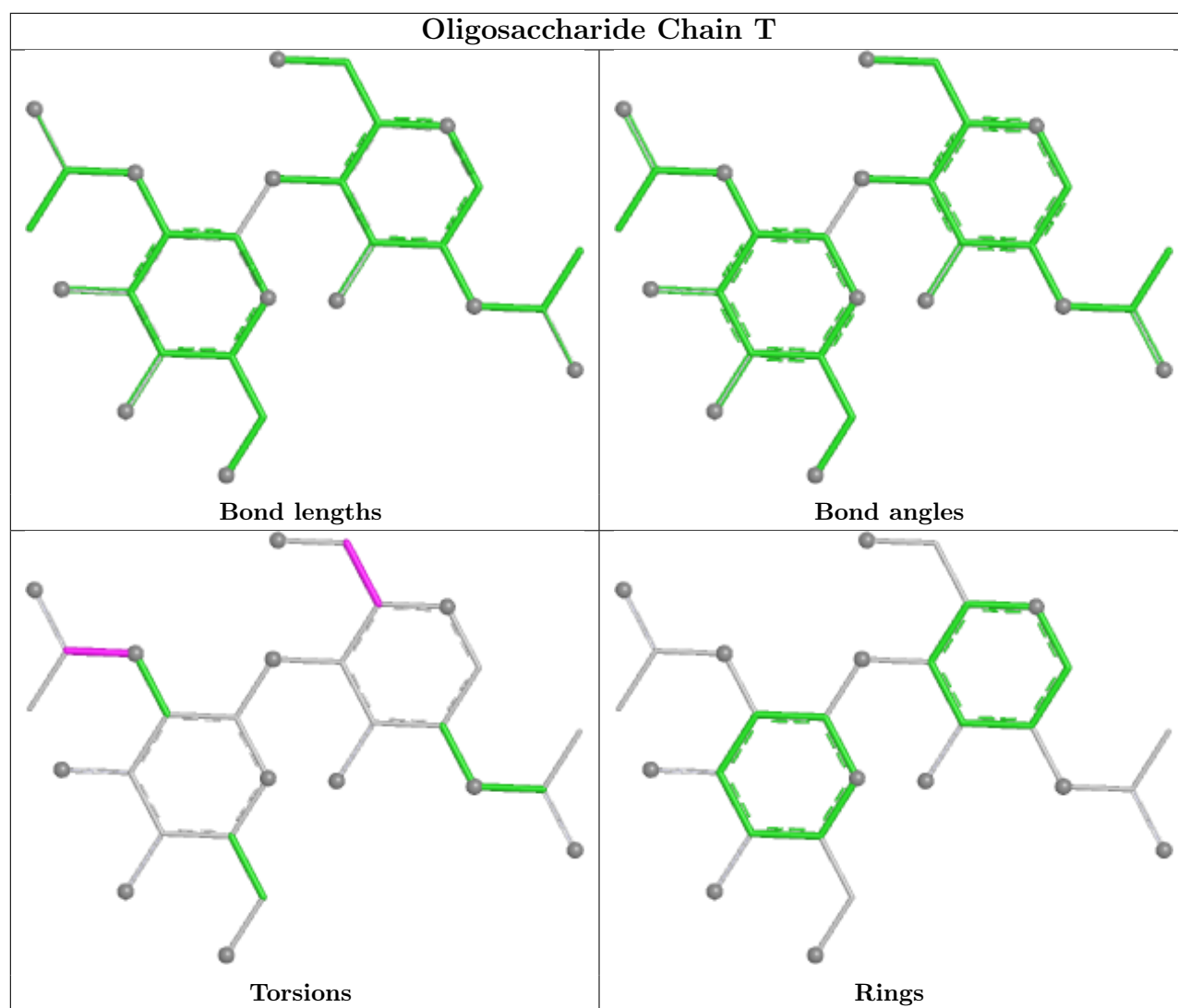


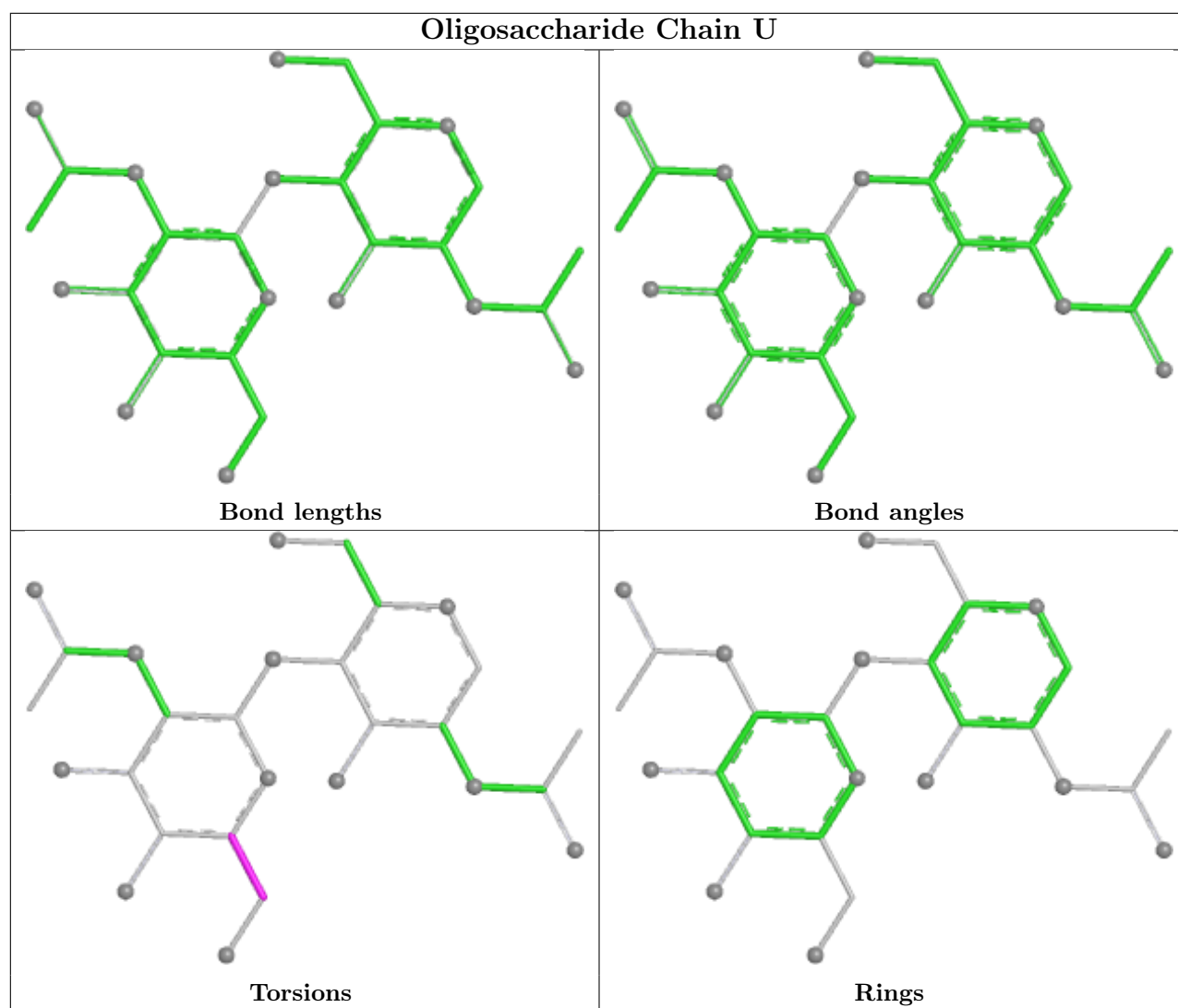


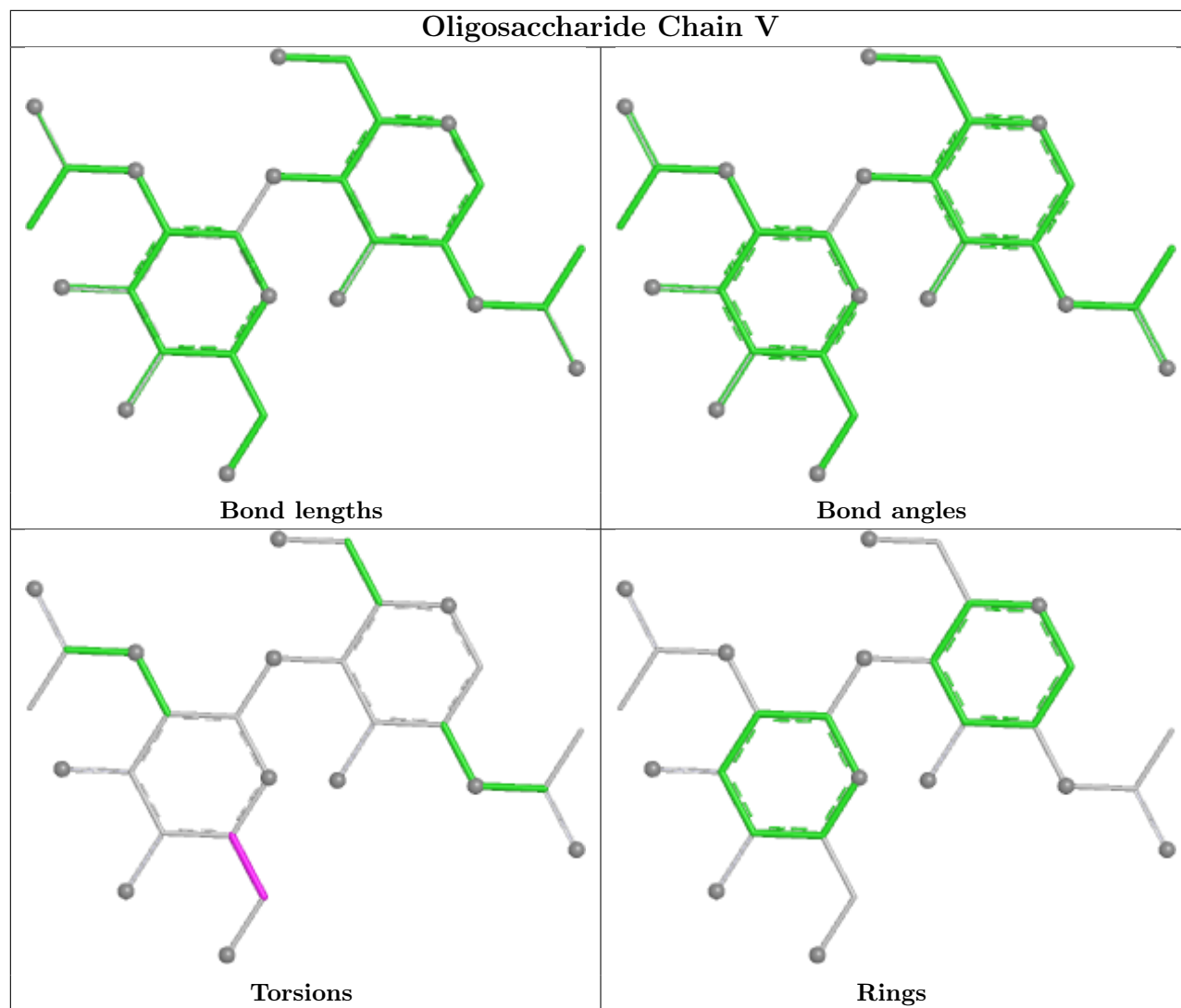


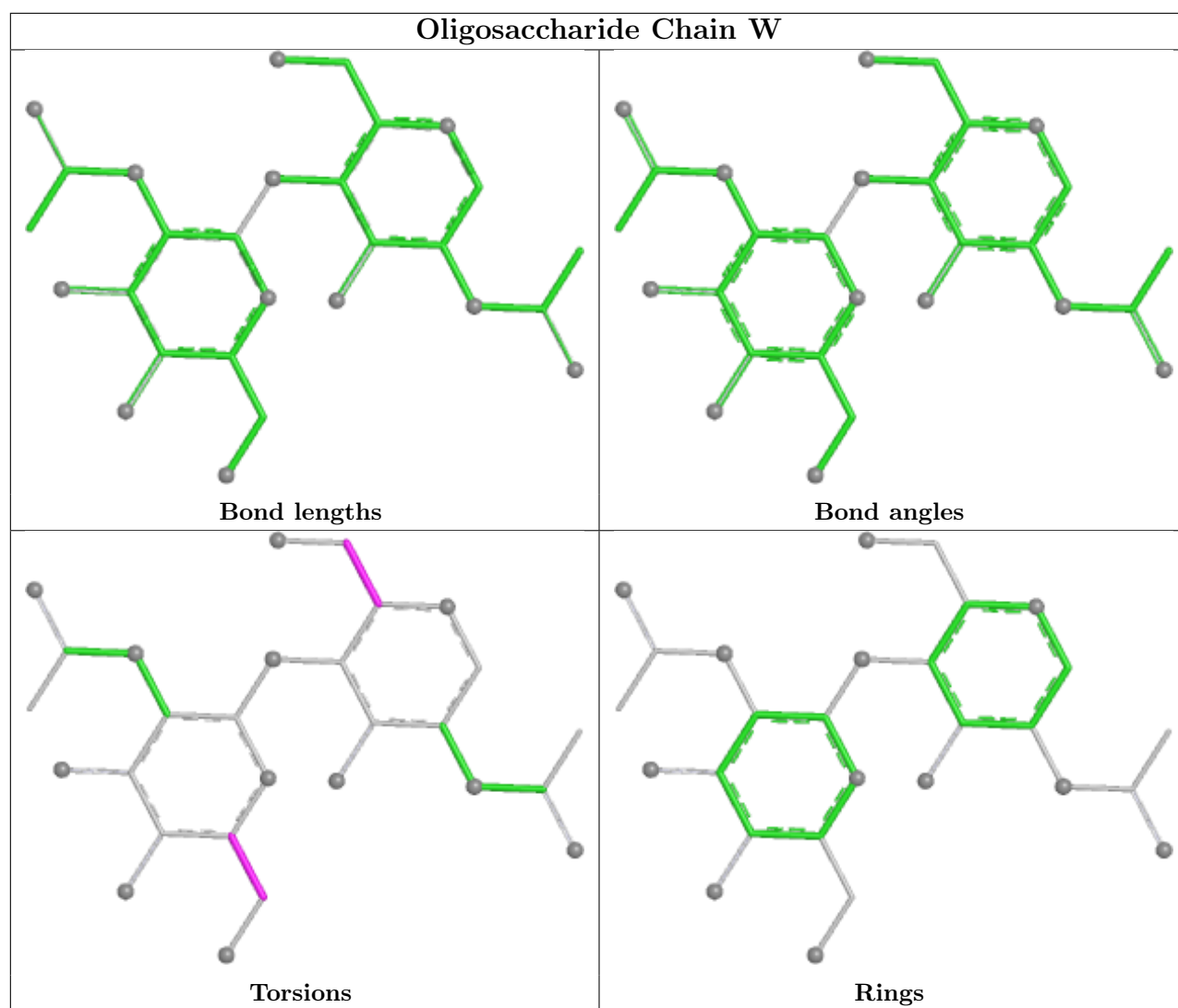


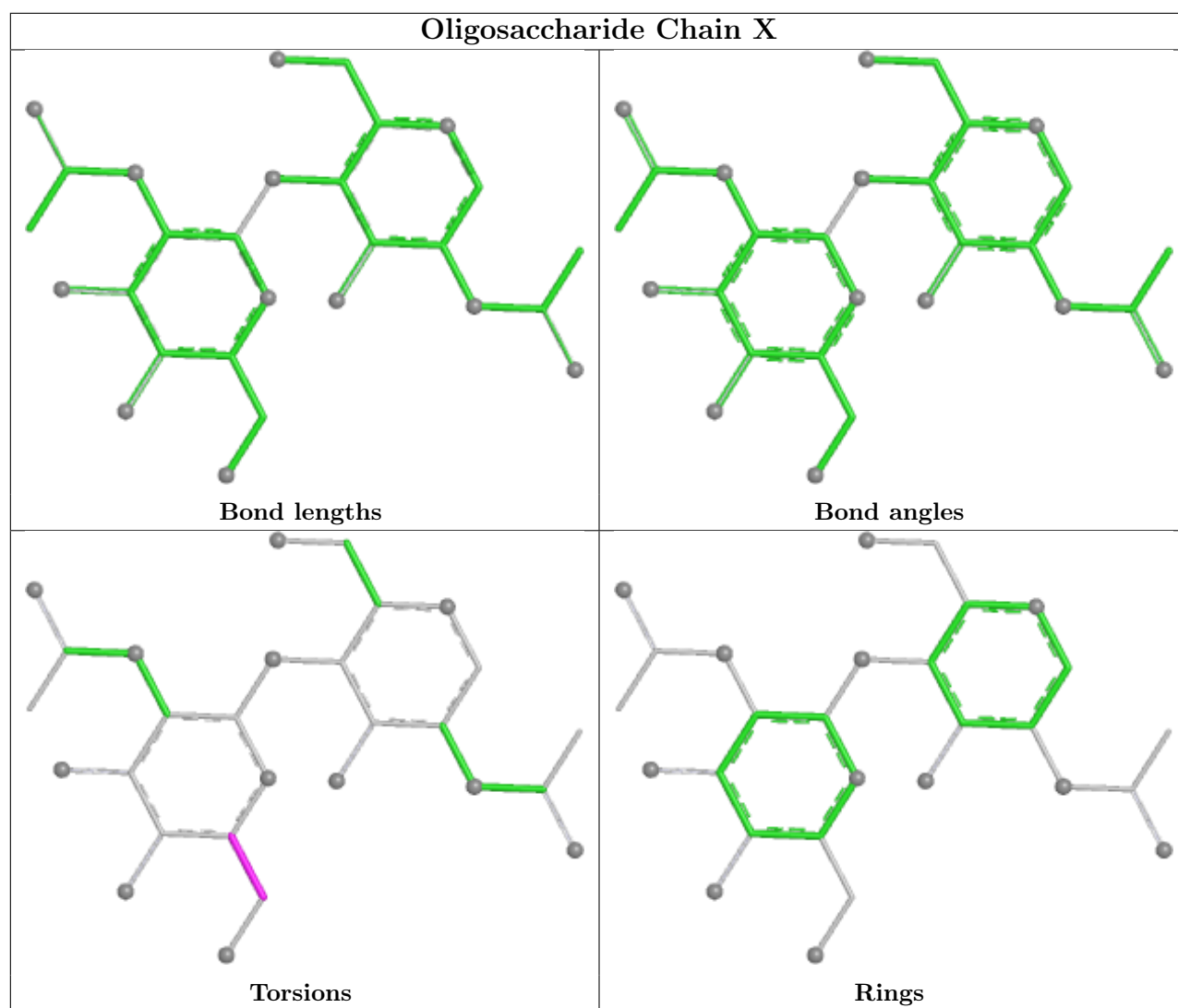


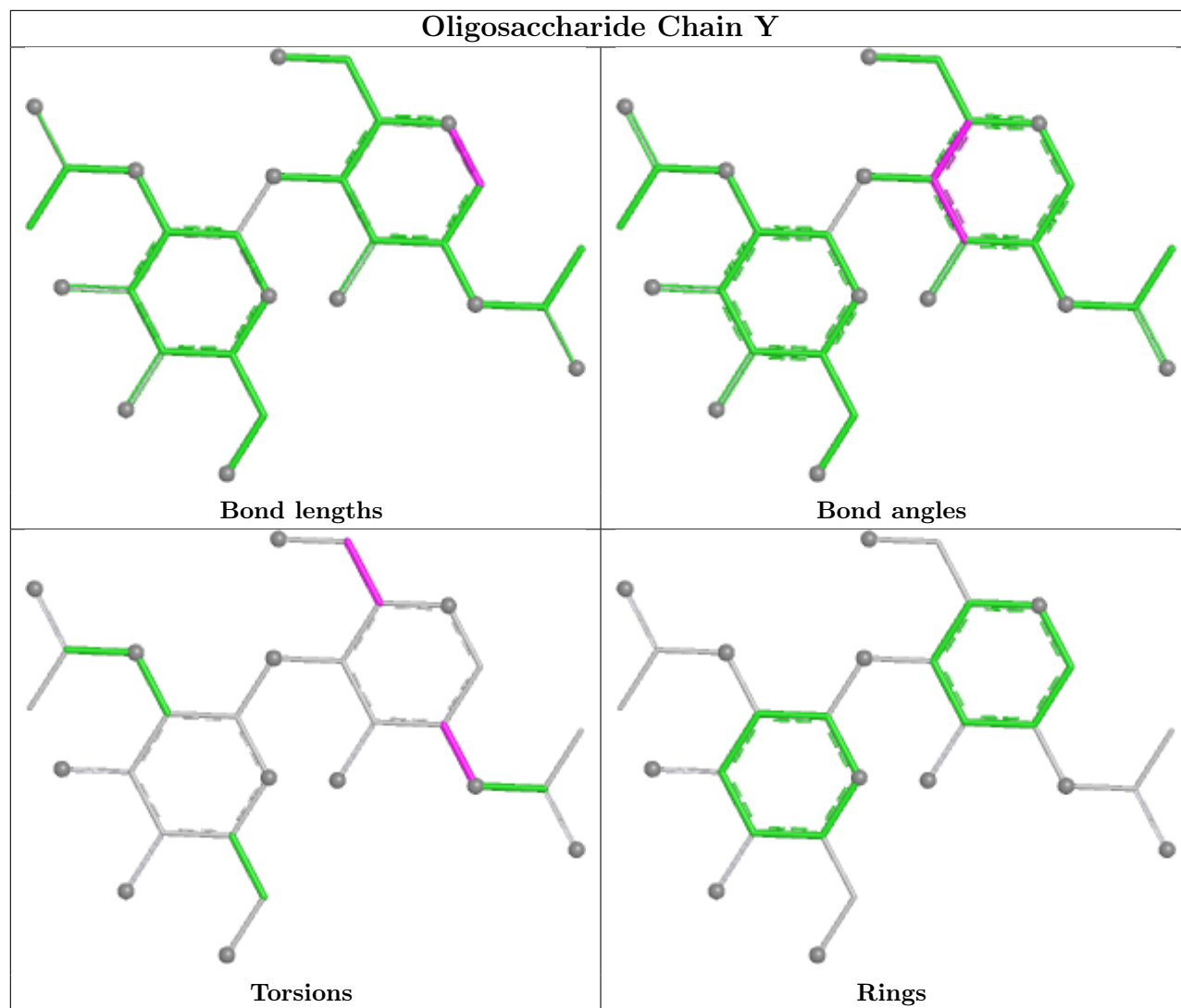


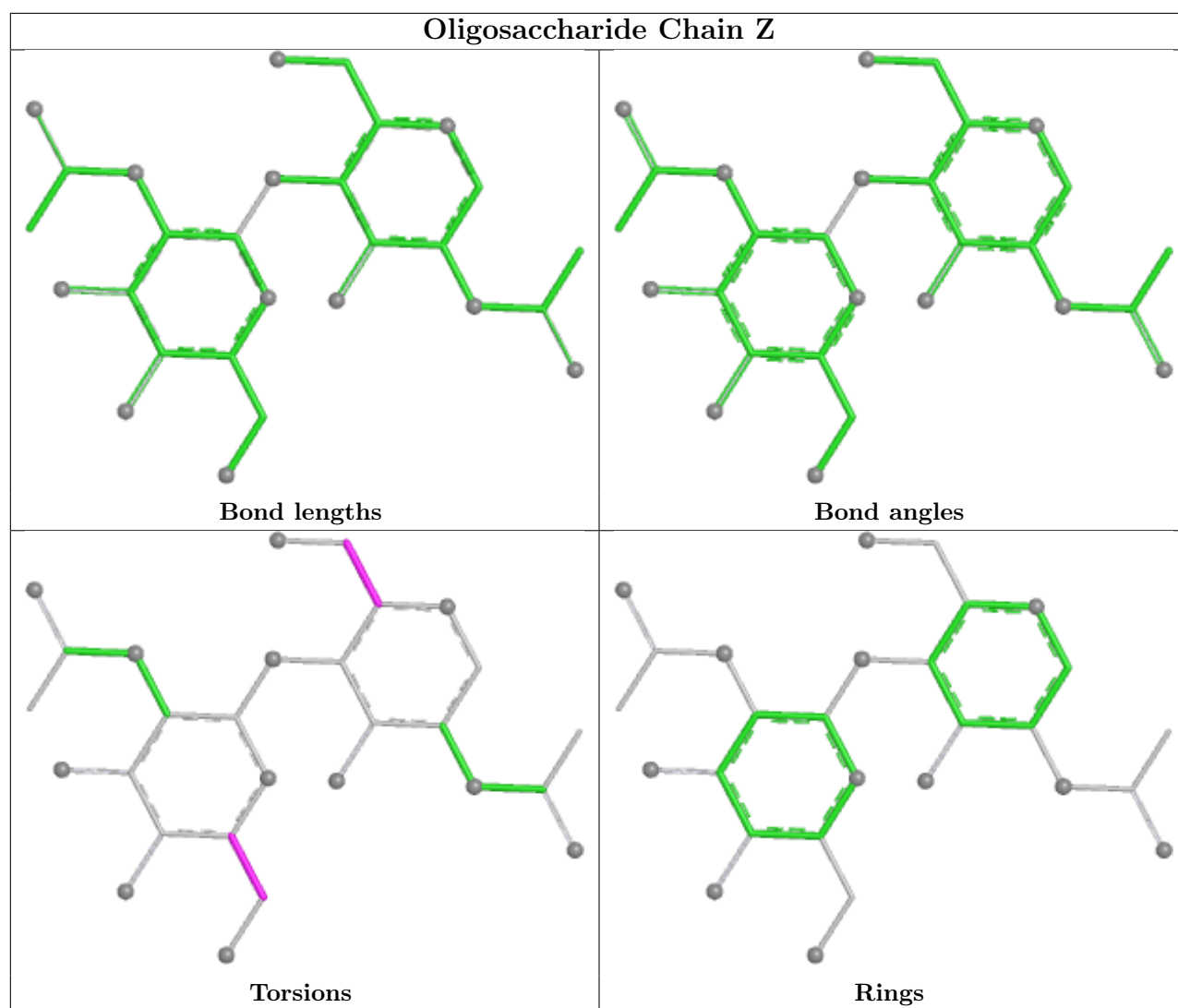


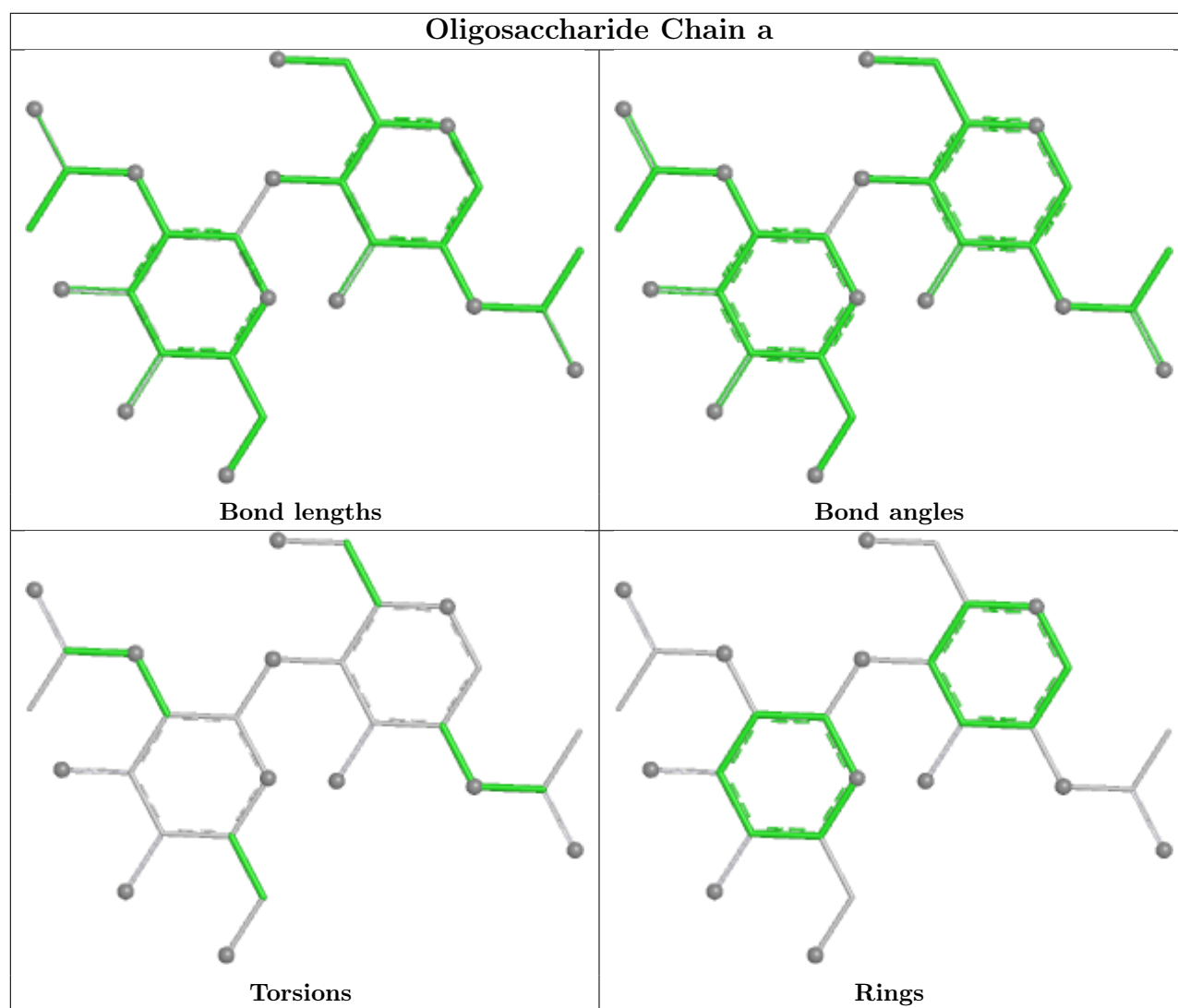


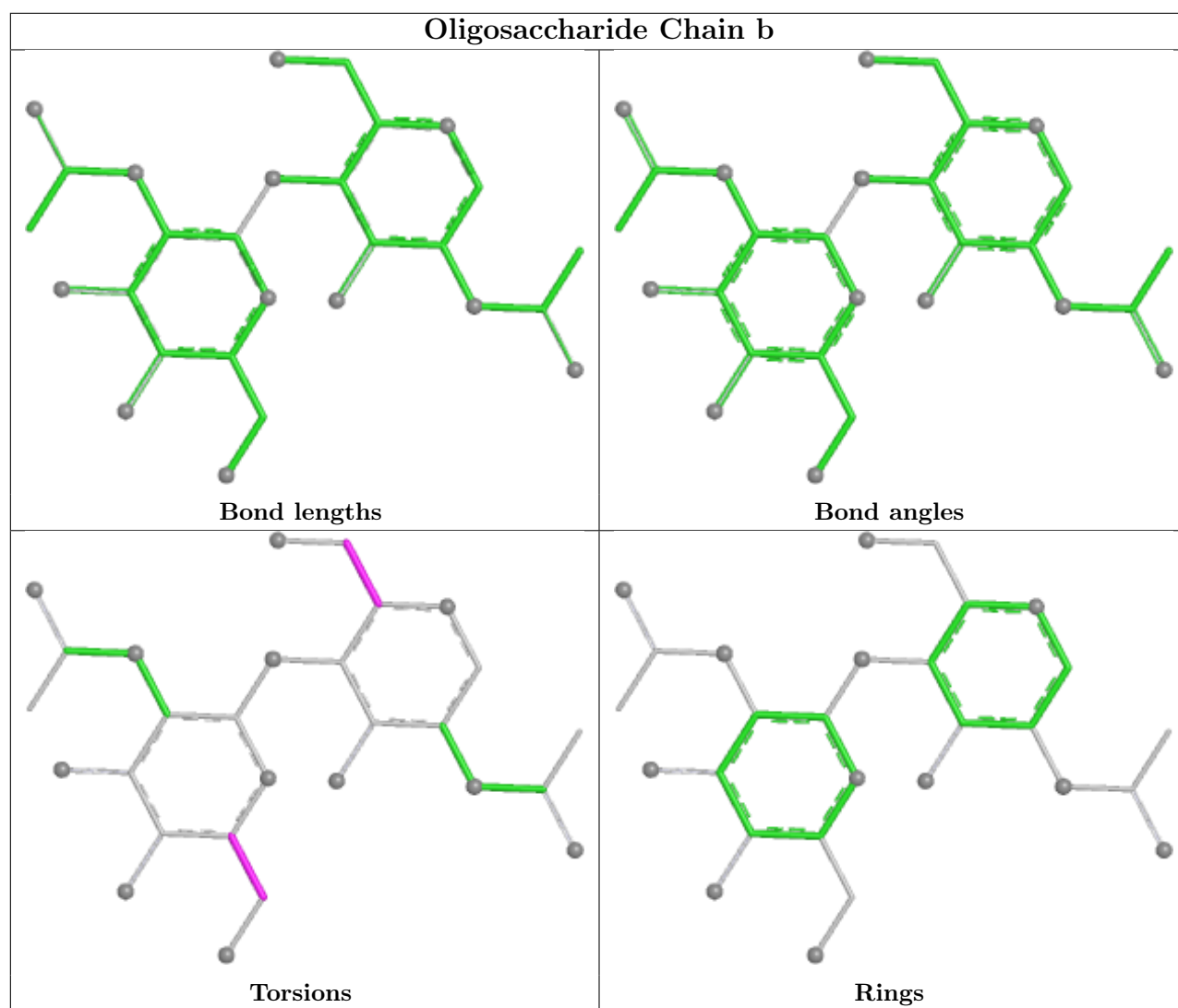


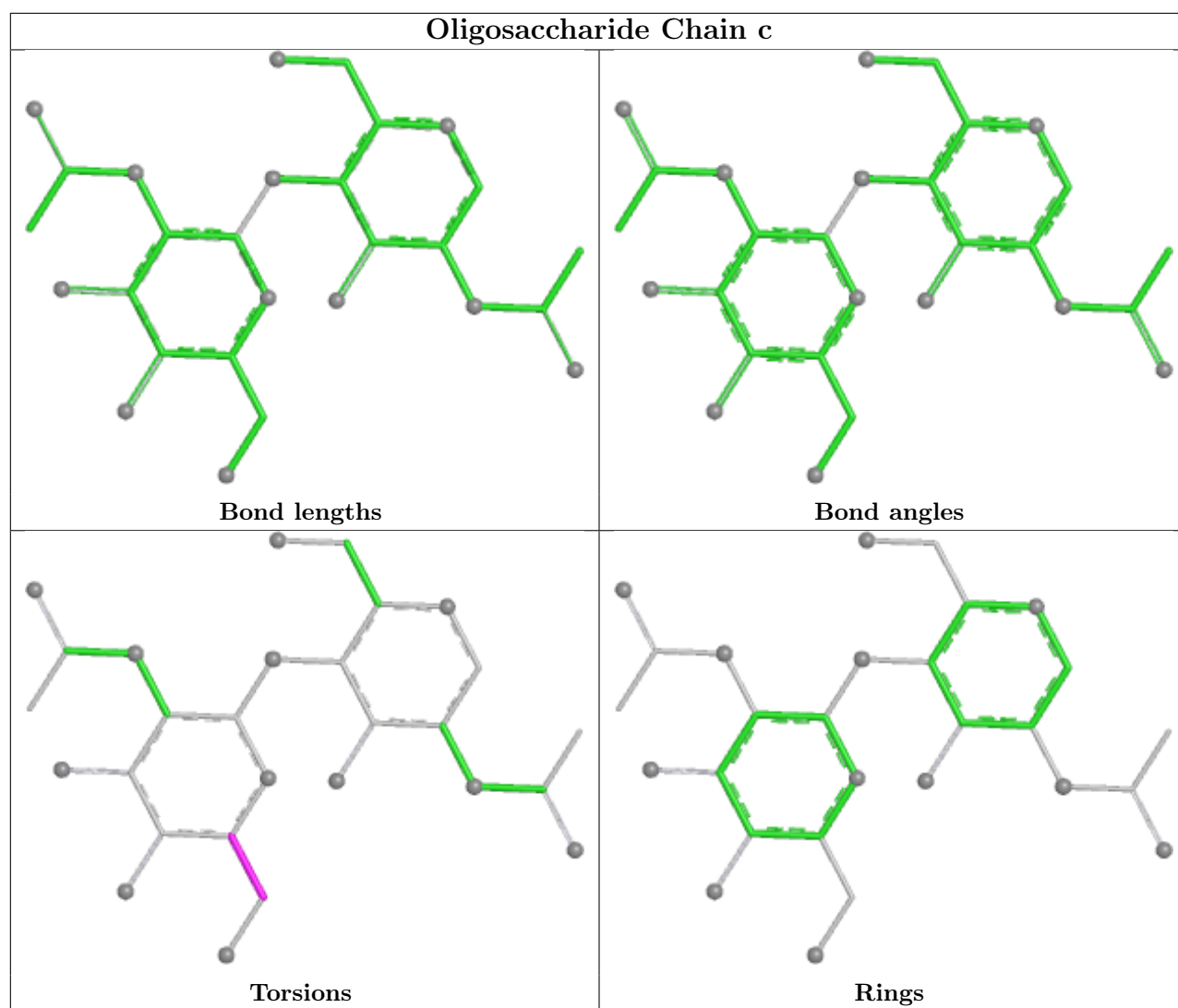


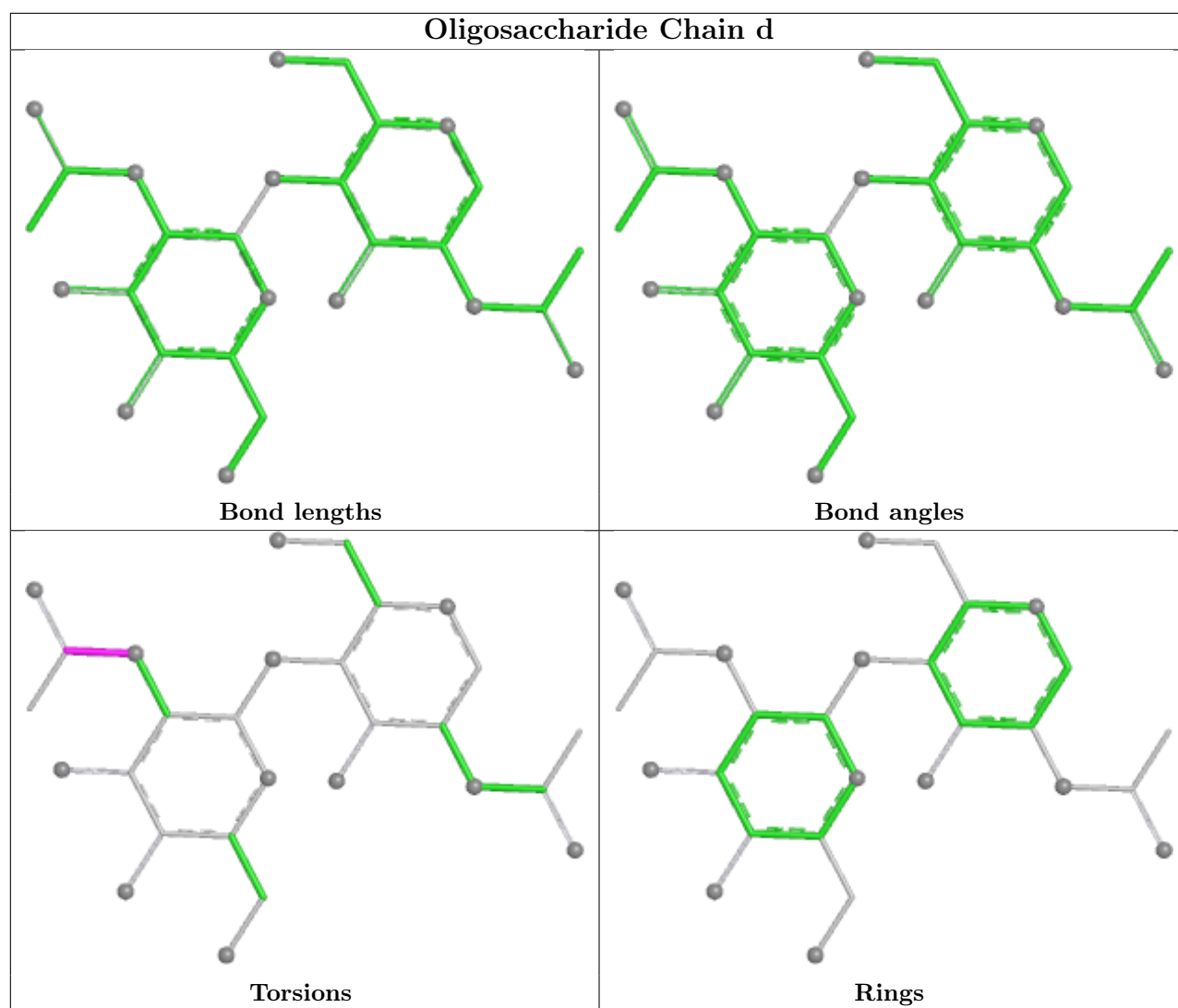


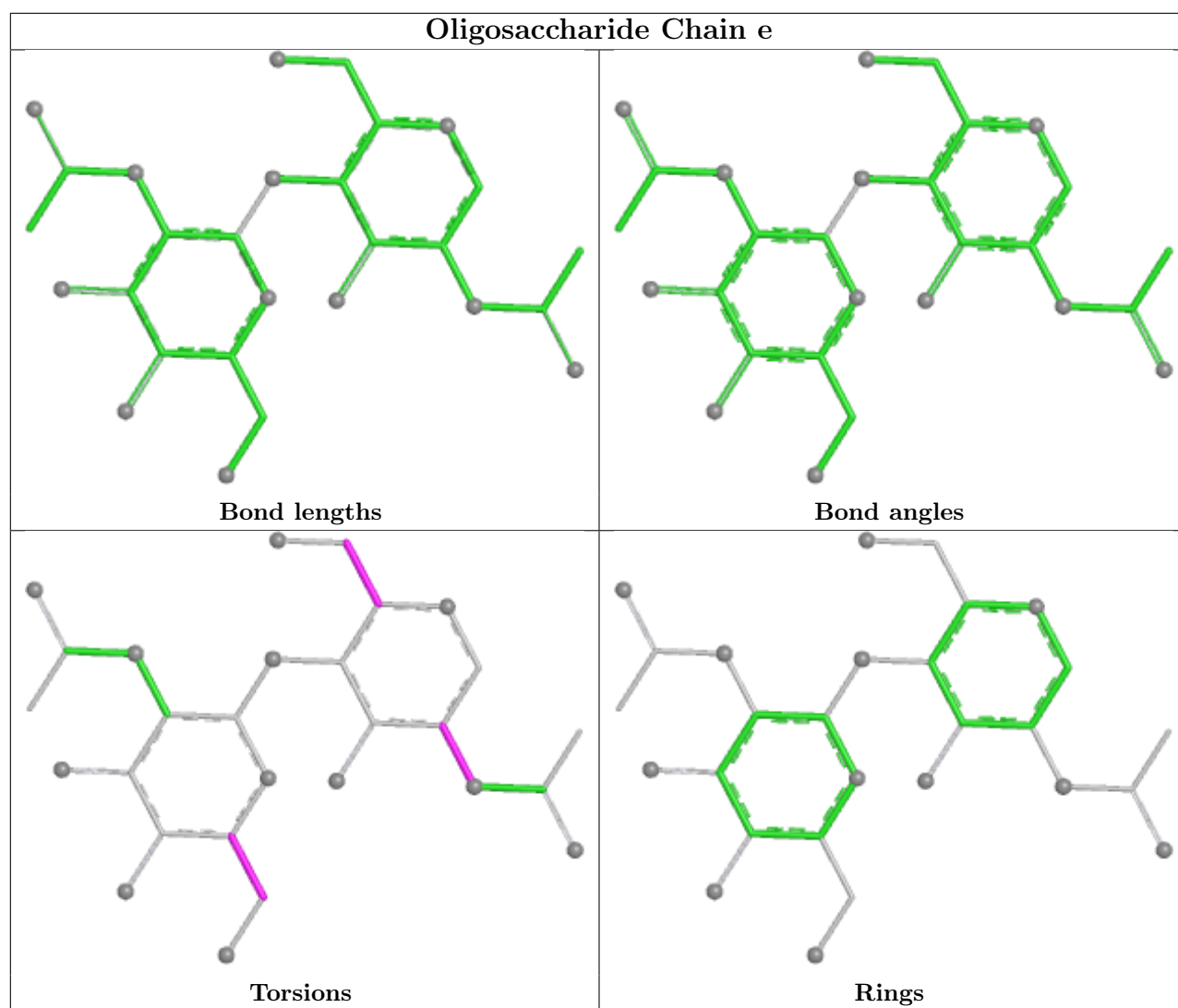


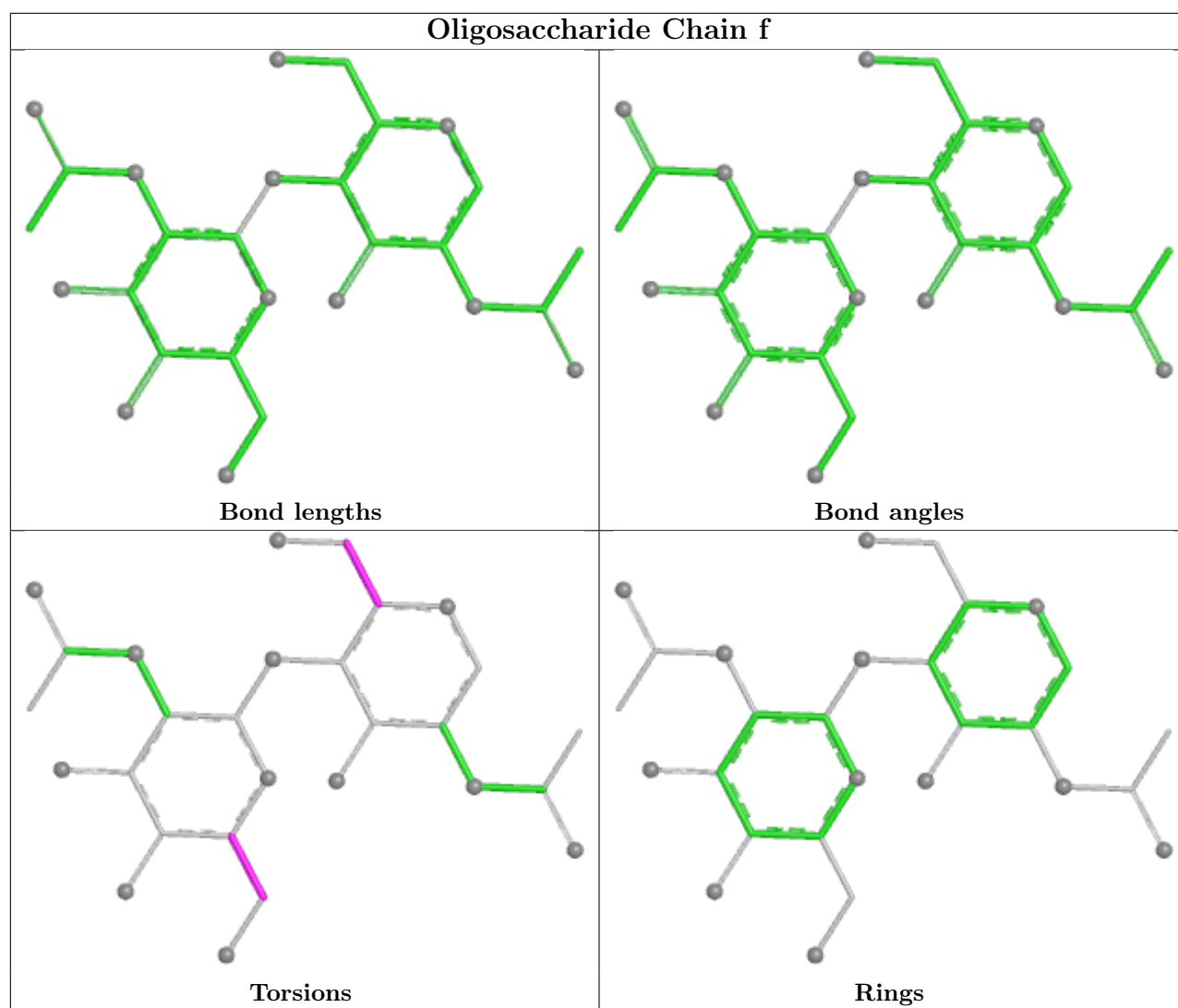


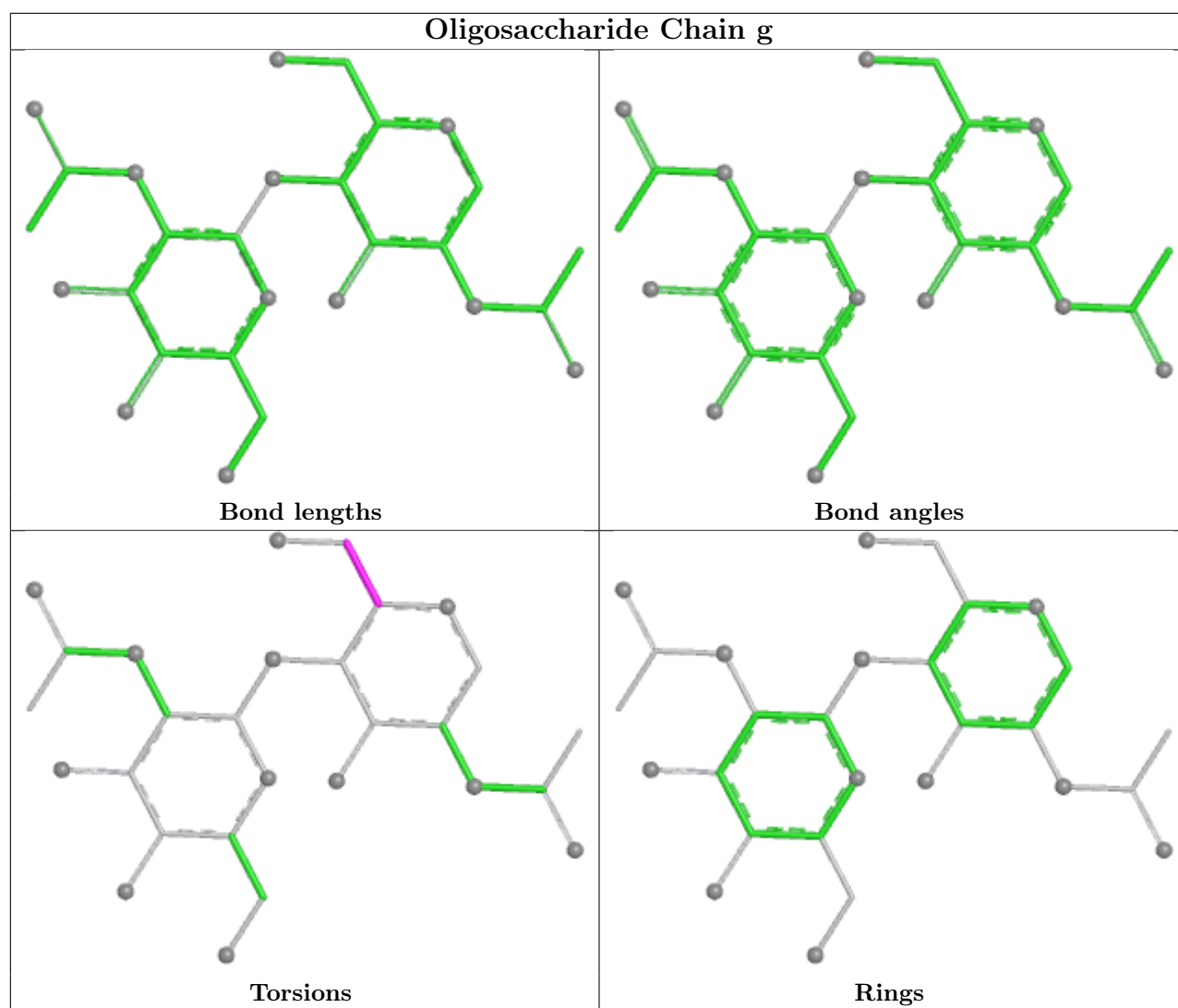


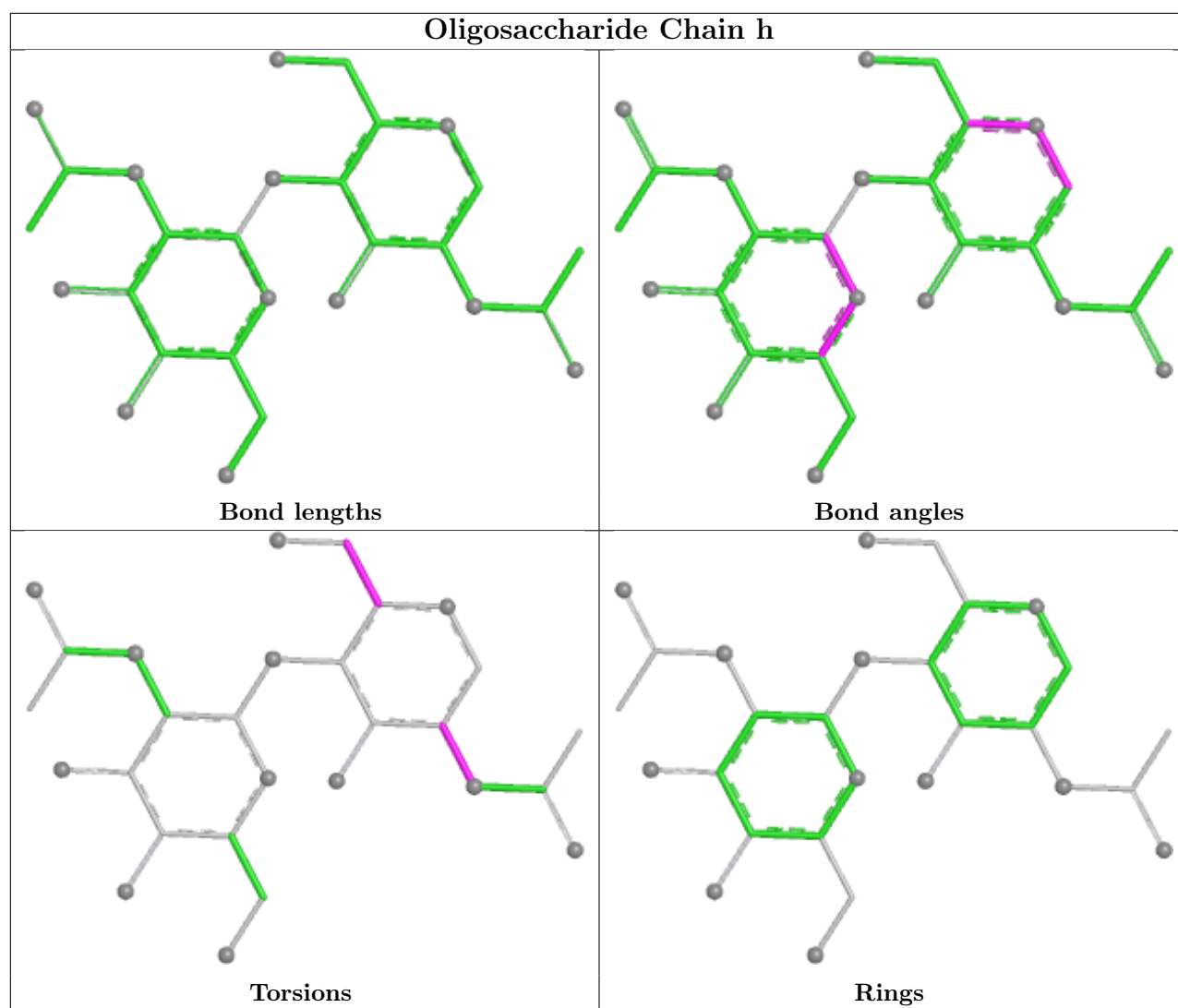


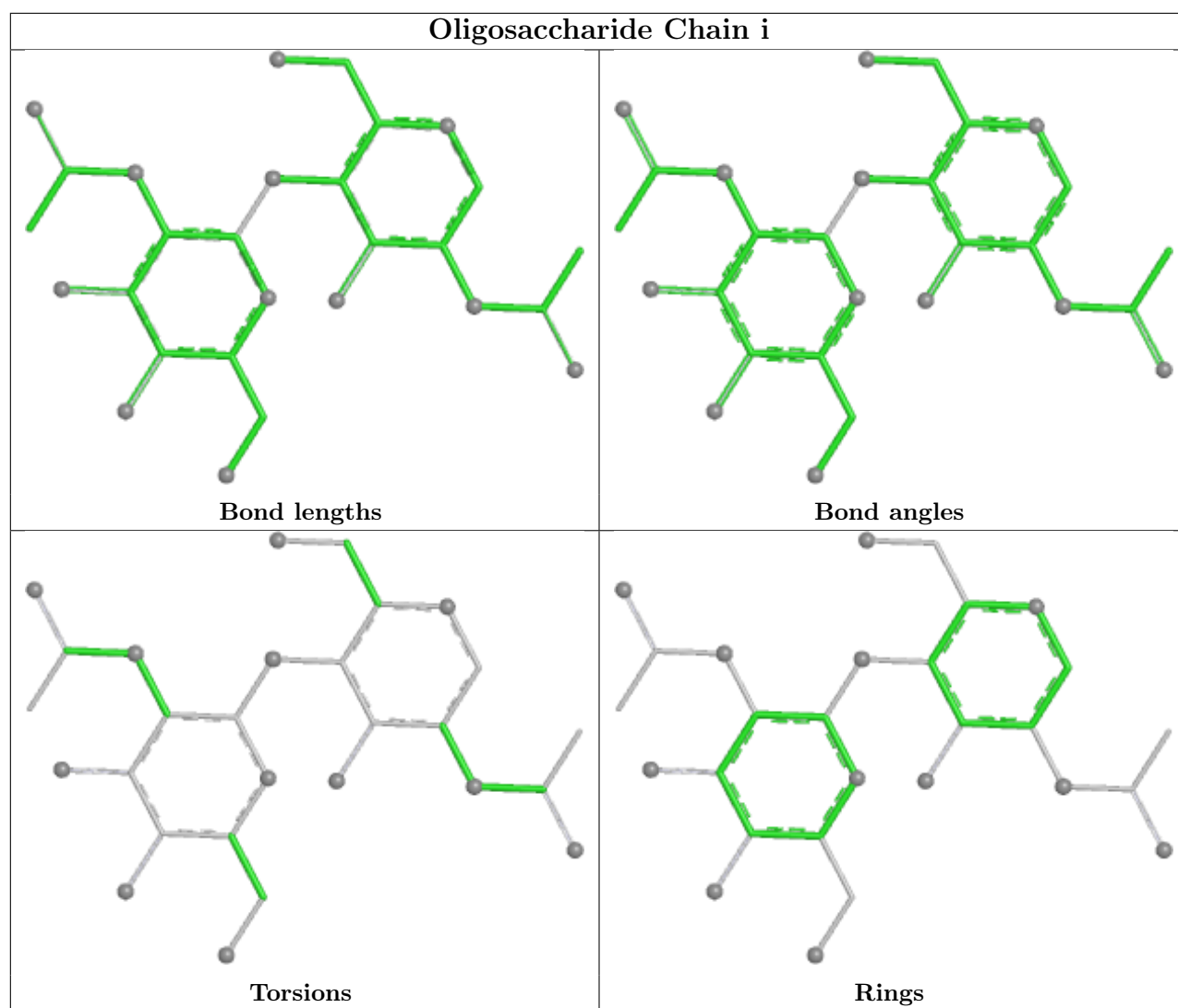


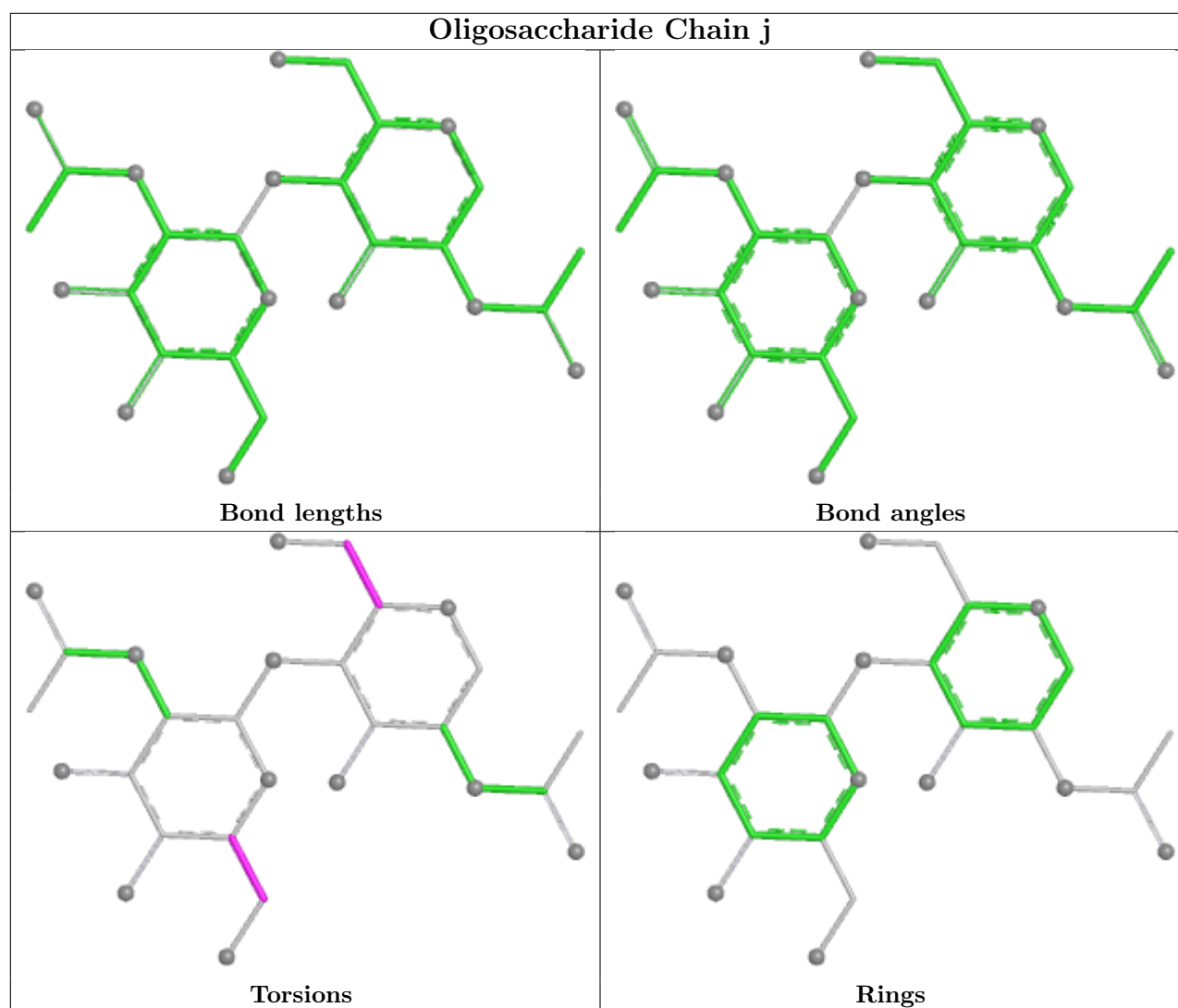












5.6 Ligand geometry [i](#)

13 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	B	2004	1	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	C	2004	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	C	2005	1	14,14,15	0.32	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2002	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	A	2001	1	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	C	2002	1	14,14,15	0.23	0	17,19,21	0.72	1 (5%)
4	NAG	B	2003	1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	C	2001	1	14,14,15	0.46	0	17,19,21	0.52	0
4	NAG	C	2003	1	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	A	2004	1	14,14,15	0.39	0	17,19,21	1.34	2 (11%)
4	NAG	A	2003	1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	B	2002	1	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	B	2001	1	14,14,15	0.24	0	17,19,21	0.36	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	B	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	6/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2004	NAG	C2-N2-C7	4.58	129.04	122.90
4	C	2002	NAG	C1-O5-C5	2.53	115.57	112.19
4	A	2004	NAG	C1-C2-N2	2.18	113.86	110.43

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2002	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	A	2002	NAG	O5-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	A	2002	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2004	NAG	1	0
4	A	2001	NAG	2	0
4	C	2001	NAG	2	0
4	A	2004	NAG	1	0
4	B	2002	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

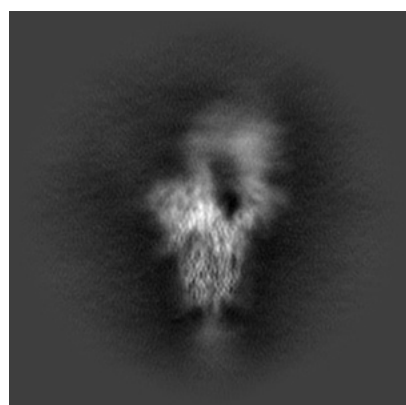
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31790. These allow visual inspection of the internal detail of the map and identification of artifacts.

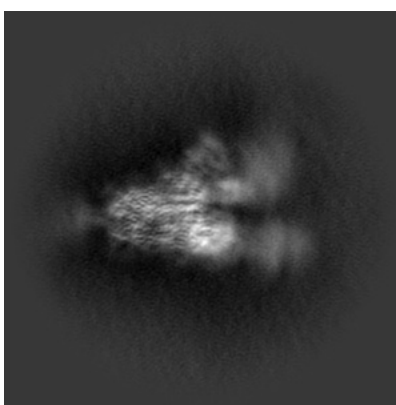
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

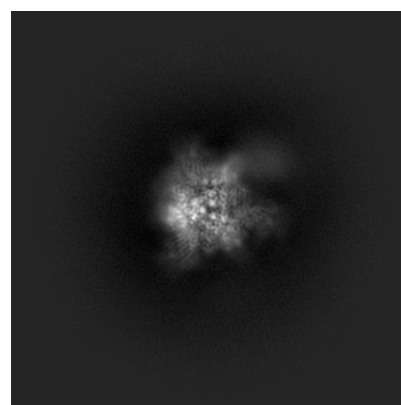
6.1.1 Primary map



X



Y

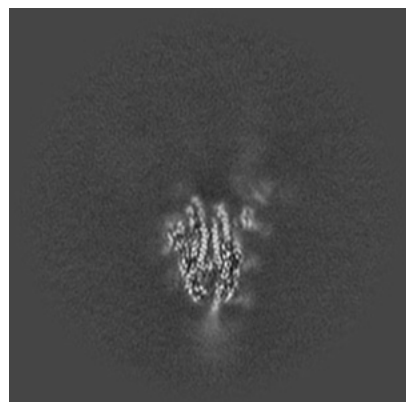


Z

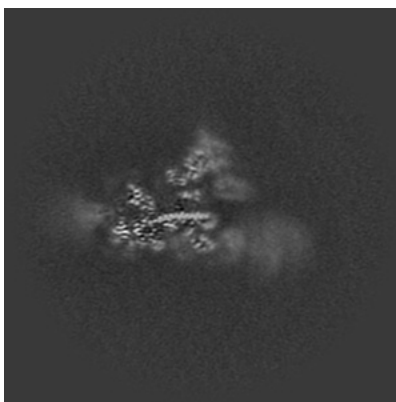
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

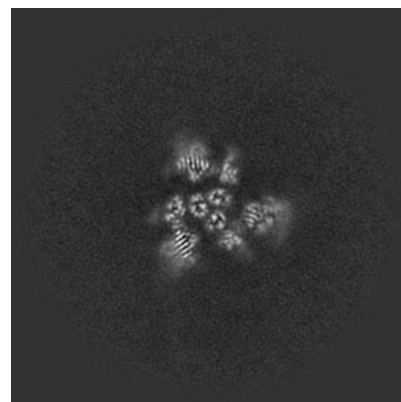
6.2.1 Primary map



X Index: 192



Y Index: 192

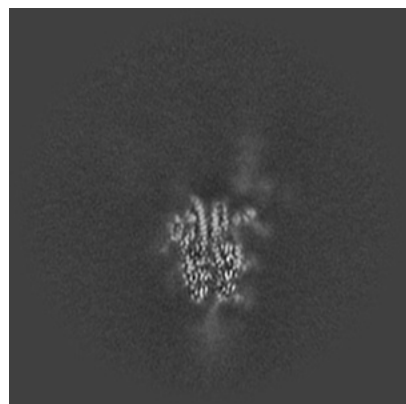


Z Index: 192

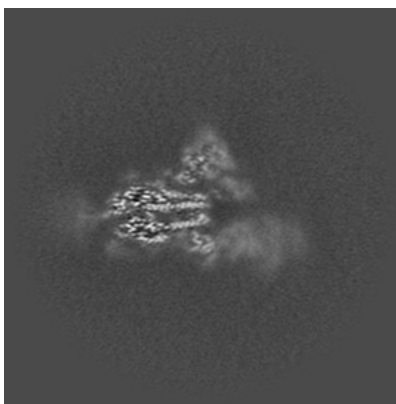
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

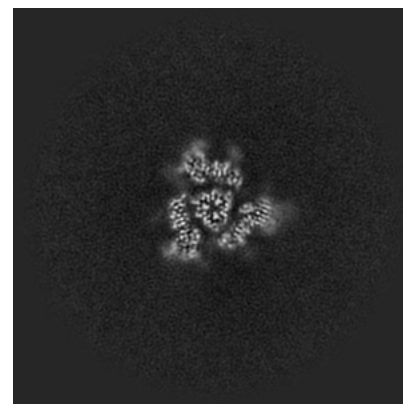
6.3.1 Primary map



X Index: 195



Y Index: 185



Z Index: 186

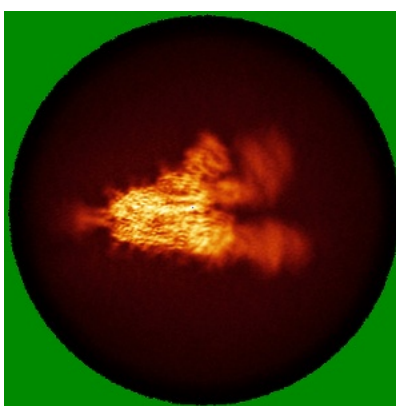
The images above show the largest variance slices of the map in three orthogonal directions.

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

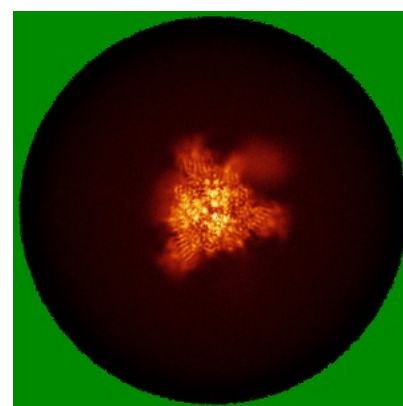
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

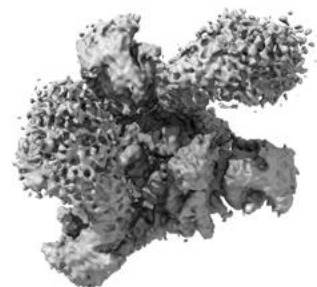
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

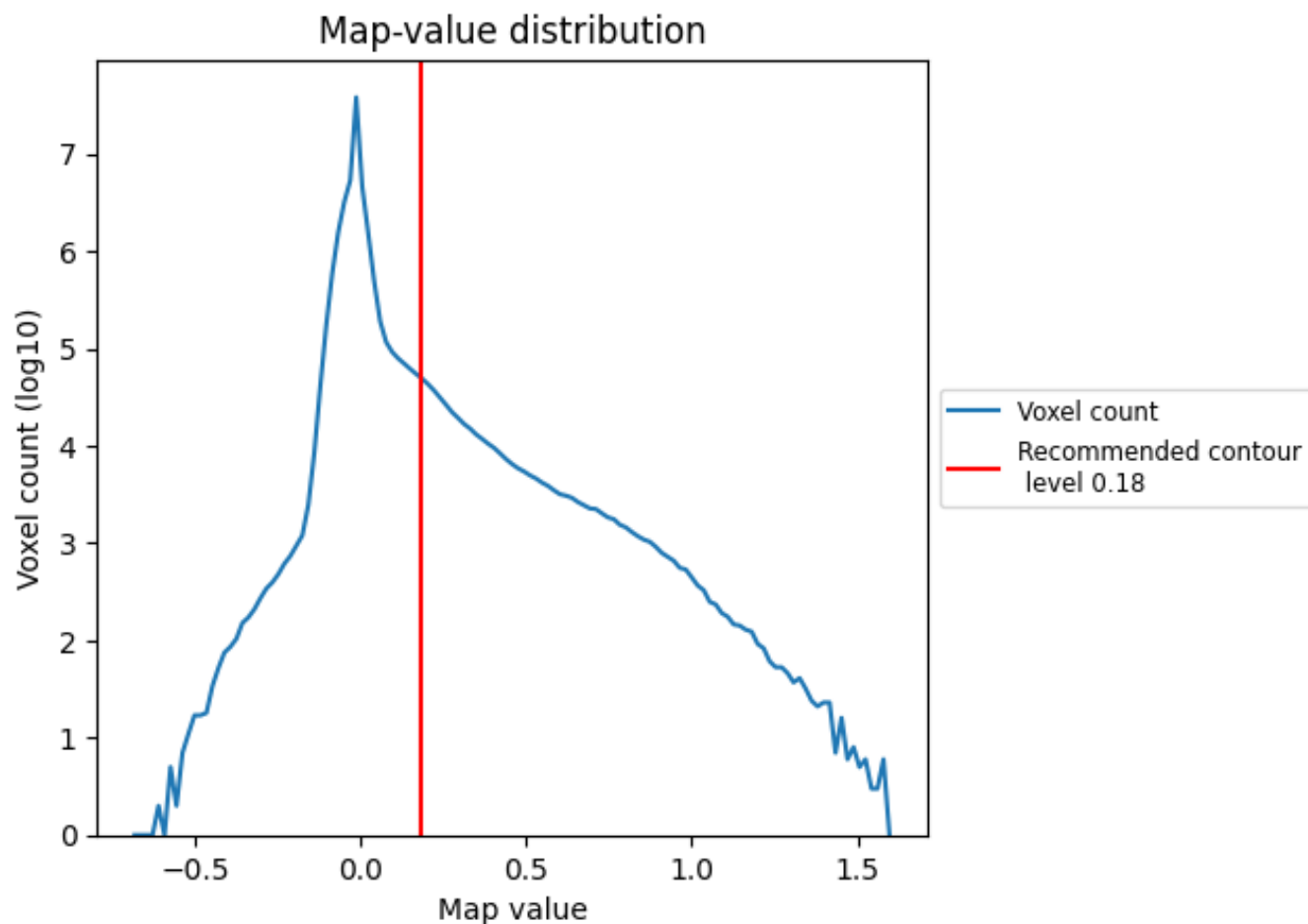
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

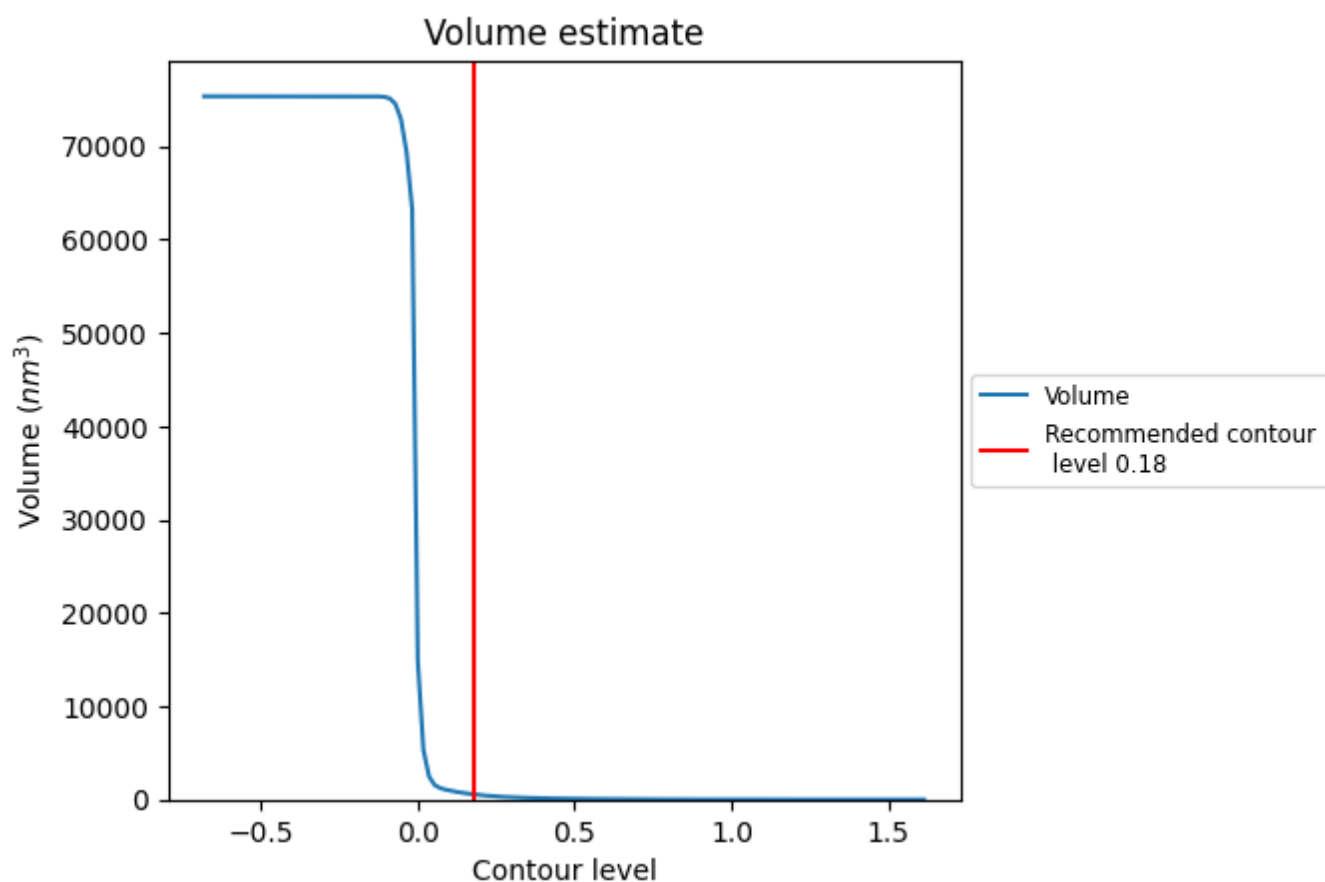
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

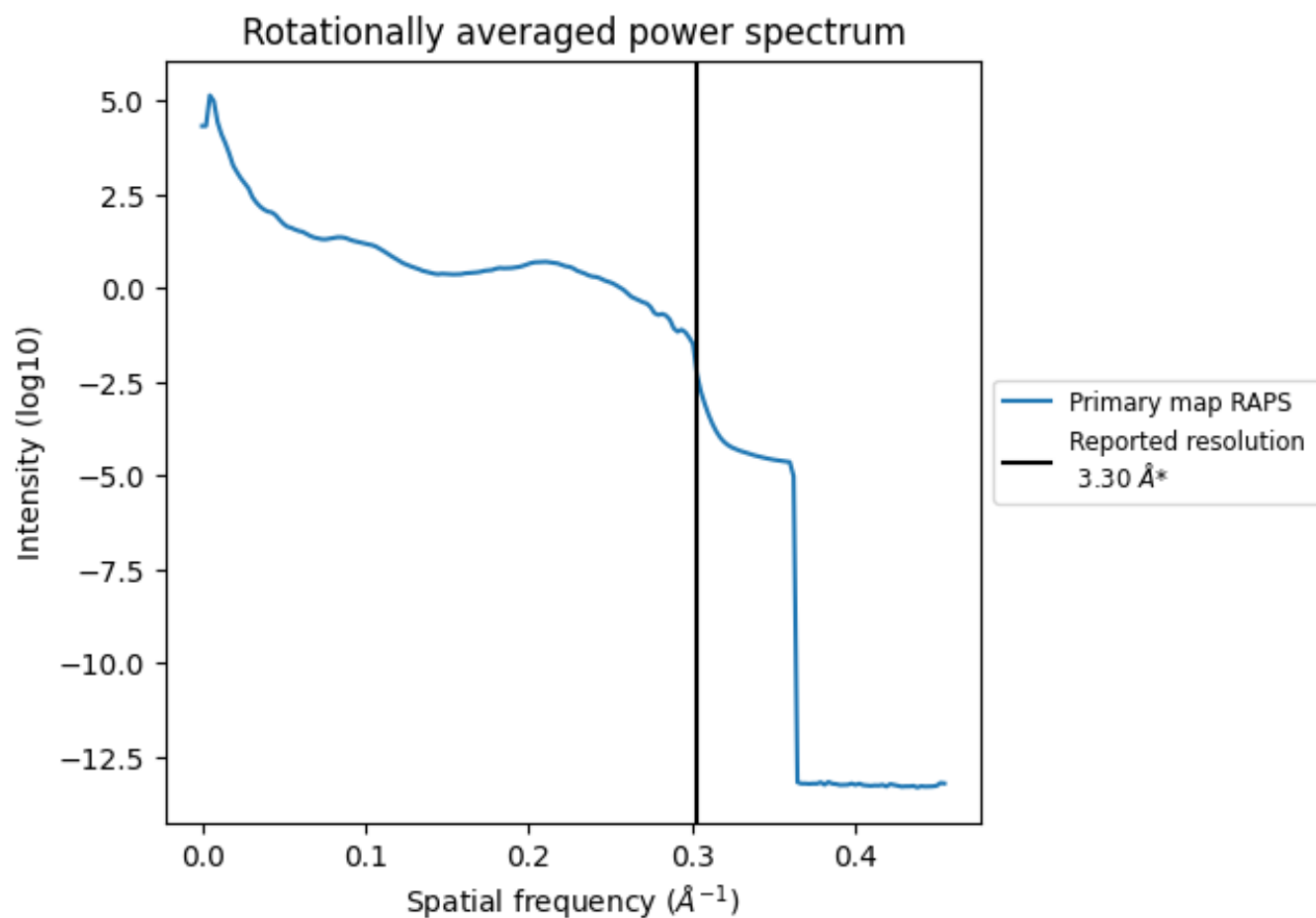
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 554 nm^3 ; this corresponds to an approximate mass of 501 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

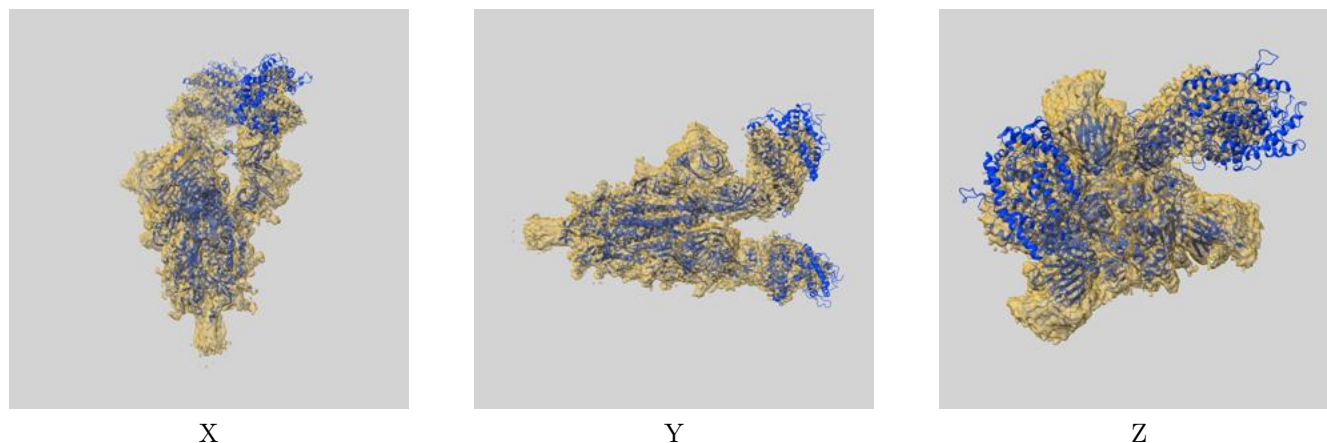
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

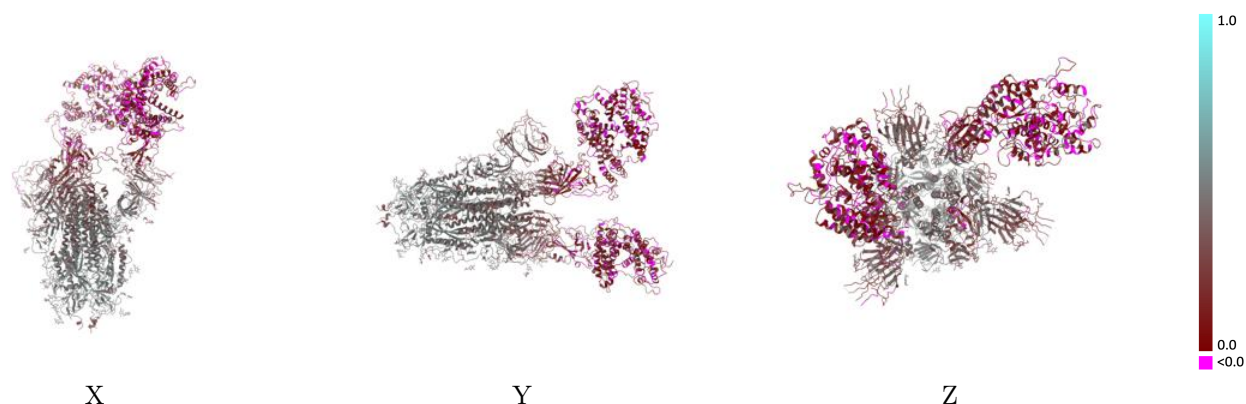
This section contains information regarding the fit between EMDB map EMD-31790 and PDB model 7V85. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



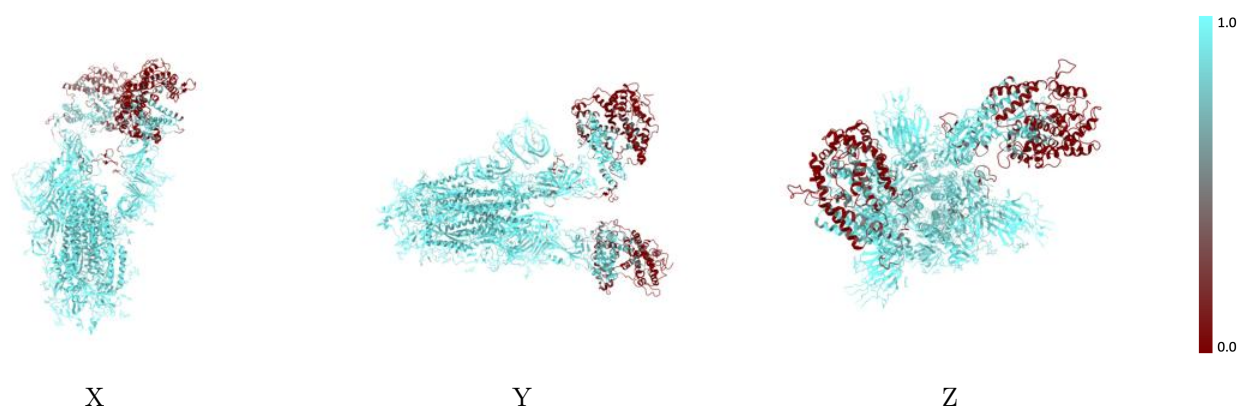
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



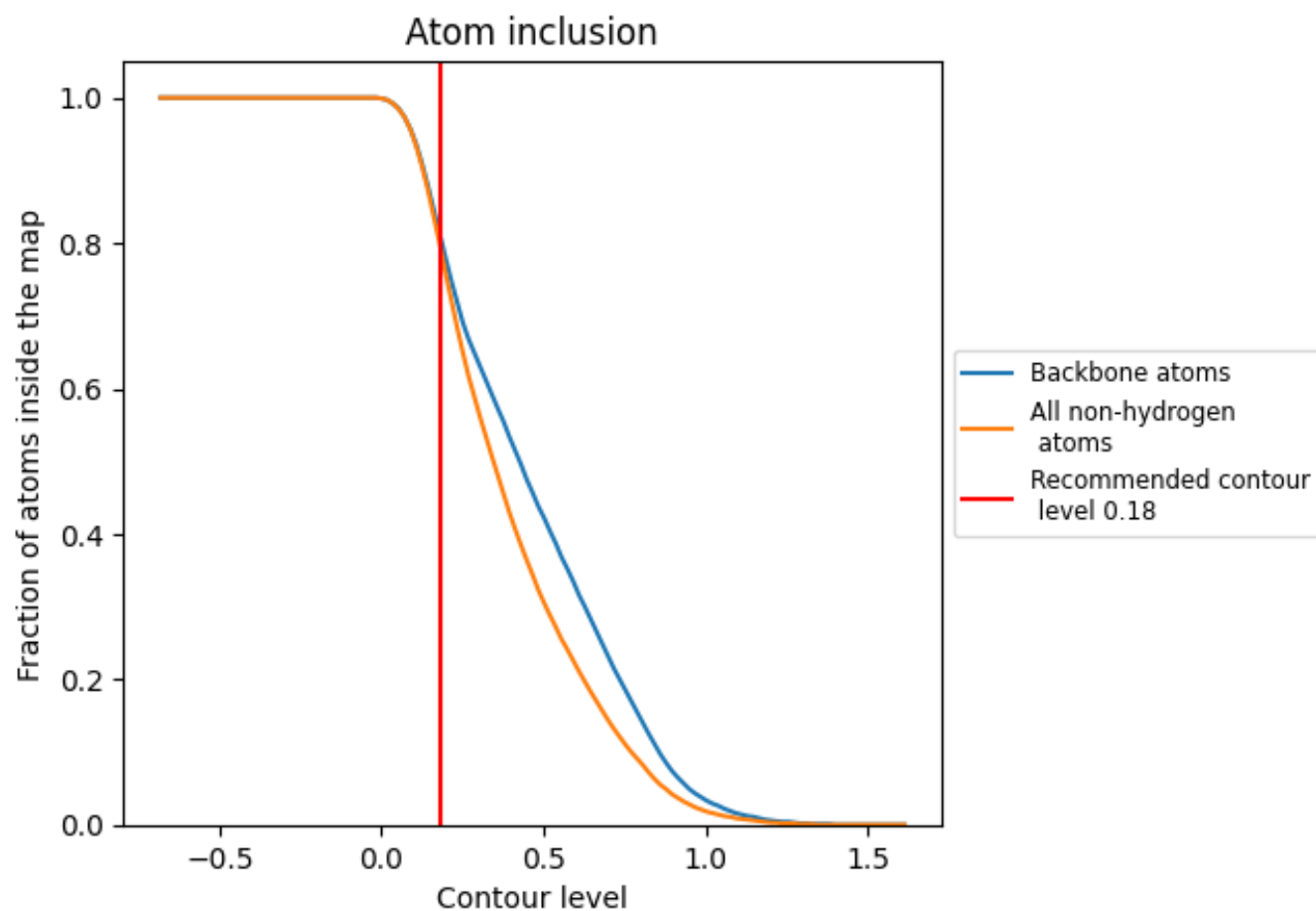
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.3030
A	 0.9610	 0.3670
B	 0.9750	 0.3730
C	 0.9490	 0.3890
D	 0.8570	 0.3360
E	 0.7140	 0.3090
F	 0.3250	 0.1070
G	 0.8930	 0.3110
H	 0.4330	 0.1170
I	 1.0000	 0.3870
J	 0.9290	 0.3060
K	 0.9640	 0.4400
L	 1.0000	 0.5030
M	 1.0000	 0.4410
N	 0.7860	 0.3410
O	 0.9640	 0.4470
P	 0.9640	 0.4730
Q	 0.9290	 0.4150
R	 0.4290	 0.2540
S	 0.8930	 0.2350
T	 0.9640	 0.3540
U	 1.0000	 0.4270
V	 0.8570	 0.4000
W	 1.0000	 0.4800
X	 1.0000	 0.4500
Y	 0.7860	 0.2960
Z	 1.0000	 0.4220
a	 0.9640	 0.4460
b	 0.9290	 0.2990
c	 0.8930	 0.4010
d	 0.9290	 0.3420
e	 0.8210	 0.3730
f	 1.0000	 0.4730
g	 0.9640	 0.4310
h	 0.8570	 0.3840



Continued on next page...

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Chain	Atom inclusion	Q-score
i	 0.9640	 0.4460
j	 1.0000	 0.4720