



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:28 PM UTC

PDB ID : 7V7U / pdb_00007v7u
EMDB ID : EMD-31782
Title : Cryo-EM structure of SARS-CoV-2 S-Delta variant (B.1.617.2), two RBD-up conformation 2
Authors : Yang, T.J.; Yu, P.Y.; Chang, Y.C.; Hsu, S.T.D.
Deposited on : 2021-08-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

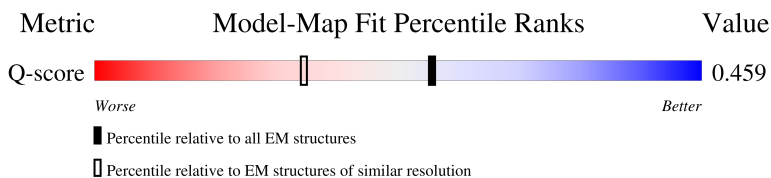
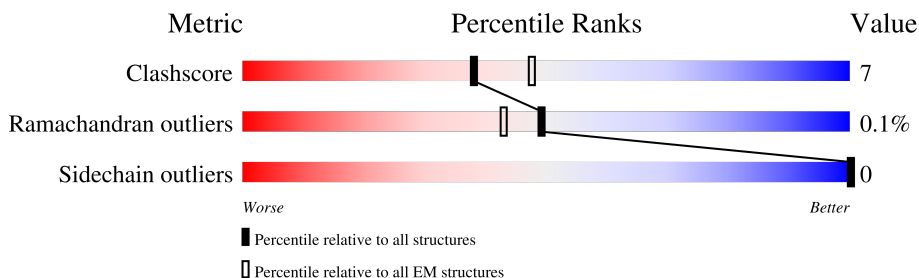
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.00 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.



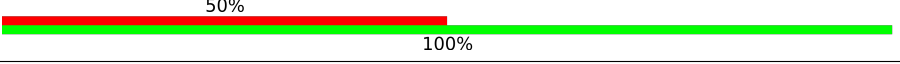
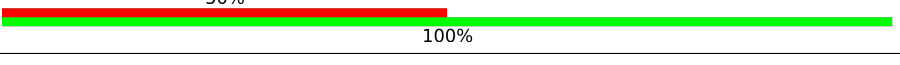
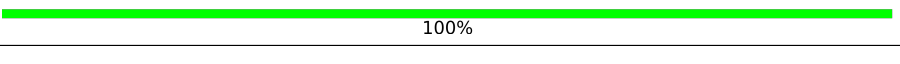
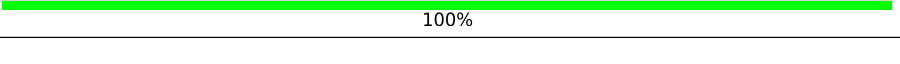
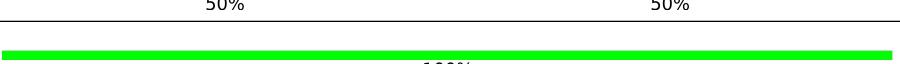
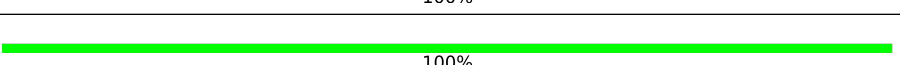
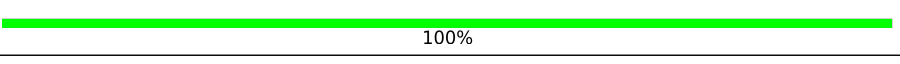
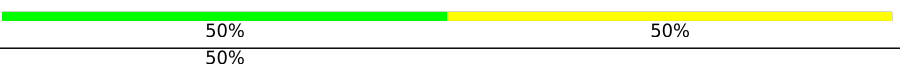
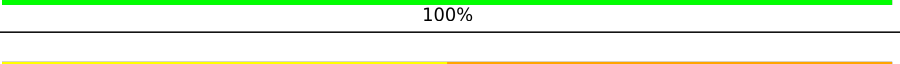
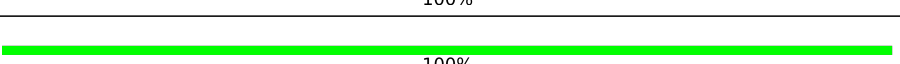
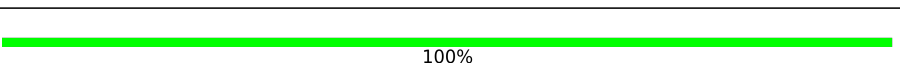
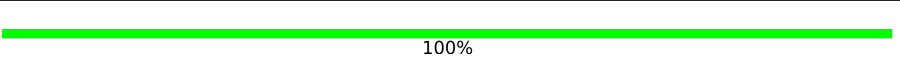
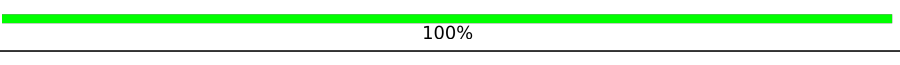
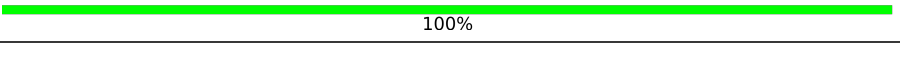
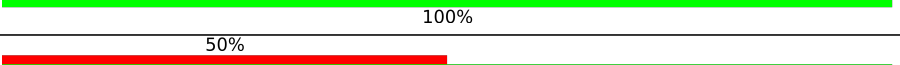
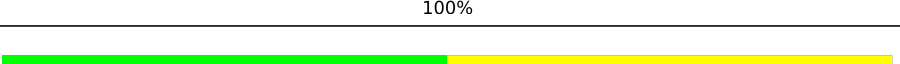
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1281	
1	B	1281	
1	C	1281	
2	D	2	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	d	2	 100%
2	e	2	 100%
2	f	2	 100%
2	g	2	 50%50%
2	h	2	 100%
2	i	2	 100%
2	j	2	 100%
2	k	2	 100%
2	l	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25283 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	1027	Total	C	N	O	S	0	0
			8016	5113	1340	1527	36		
1	B	1033	Total	C	N	O	S	0	0
			8077	5156	1351	1534	36		
1	C	1028	Total	C	N	O	S	0	0
			8028	5122	1341	1529	36		

There are 270 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	156	GLY	GLU	variant	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	450	ARG	LEU	variant	UNP P0DTC2
A	476	LYS	THR	variant	UNP P0DTC2
A	612	GLY	ASP	variant	UNP P0DTC2
A	679	ARG	PRO	engineered mutation	UNP P0DTC2
A	680	GLY	ARG	engineered mutation	UNP P0DTC2
A	681	SER	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	948	ASN	ASP	variant	UNP P0DTC2
A	984	PRO	LYS	engineered mutation	UNP P0DTC2
A	985	PRO	VAL	engineered mutation	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	PHE	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	TYR	-	expression tag	UNP P0DTC2
A	1214	ILE	-	expression tag	UNP P0DTC2
A	1215	PRO	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ALA	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	ARG	-	expression tag	UNP P0DTC2
A	1220	ASP	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	GLN	-	expression tag	UNP P0DTC2
A	1223	ALA	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	VAL	-	expression tag	UNP P0DTC2
A	1226	ARG	-	expression tag	UNP P0DTC2
A	1227	LYS	-	expression tag	UNP P0DTC2
A	1228	ASP	-	expression tag	UNP P0DTC2
A	1229	GLY	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	TRP	-	expression tag	UNP P0DTC2
A	1232	VAL	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	SER	-	expression tag	UNP P0DTC2
A	1236	THR	-	expression tag	UNP P0DTC2
A	1237	PHE	-	expression tag	UNP P0DTC2
A	1238	LEU	-	expression tag	UNP P0DTC2
A	1239	LYS	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLN	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	ASN	-	expression tag	UNP P0DTC2
A	1244	SER	-	expression tag	UNP P0DTC2
A	1245	ALA	-	expression tag	UNP P0DTC2
A	1246	ASP	-	expression tag	UNP P0DTC2
A	1247	ILE	-	expression tag	UNP P0DTC2
A	1248	GLN	-	expression tag	UNP P0DTC2
A	1249	HIS	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	ARG	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	LEU	-	expression tag	UNP P0DTC2
A	1255	GLU	-	expression tag	UNP P0DTC2
A	1256	SER	-	expression tag	UNP P0DTC2
A	1257	ARG	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	PRO	-	expression tag	UNP P0DTC2
A	1260	PHE	-	expression tag	UNP P0DTC2
A	1261	GLU	-	expression tag	UNP P0DTC2
A	1262	GLN	-	expression tag	UNP P0DTC2
A	1263	LYS	-	expression tag	UNP P0DTC2
A	1264	LEU	-	expression tag	UNP P0DTC2
A	1265	ILE	-	expression tag	UNP P0DTC2
A	1266	SER	-	expression tag	UNP P0DTC2
A	1267	GLU	-	expression tag	UNP P0DTC2
A	1268	GLU	-	expression tag	UNP P0DTC2
A	1269	ASP	-	expression tag	UNP P0DTC2
A	1270	LEU	-	expression tag	UNP P0DTC2
A	1271	ASN	-	expression tag	UNP P0DTC2
A	1272	MET	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	THR	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2
A	1278	HIS	-	expression tag	UNP P0DTC2
A	1279	HIS	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
B	19	ARG	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	156	GLY	GLU	variant	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	450	ARG	LEU	variant	UNP P0DTC2
B	476	LYS	THR	variant	UNP P0DTC2
B	612	GLY	ASP	variant	UNP P0DTC2
B	679	ARG	PRO	engineered mutation	UNP P0DTC2
B	680	GLY	ARG	engineered mutation	UNP P0DTC2
B	681	SER	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	948	ASN	ASP	variant	UNP P0DTC2
B	984	PRO	LYS	engineered mutation	UNP P0DTC2
B	985	PRO	VAL	engineered mutation	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	PHE	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	TYR	-	expression tag	UNP P0DTC2
B	1214	ILE	-	expression tag	UNP P0DTC2
B	1215	PRO	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ALA	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	ARG	-	expression tag	UNP P0DTC2
B	1220	ASP	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	GLN	-	expression tag	UNP P0DTC2
B	1223	ALA	-	expression tag	UNP P0DTC2
B	1224	TYR	-	expression tag	UNP P0DTC2
B	1225	VAL	-	expression tag	UNP P0DTC2
B	1226	ARG	-	expression tag	UNP P0DTC2
B	1227	LYS	-	expression tag	UNP P0DTC2
B	1228	ASP	-	expression tag	UNP P0DTC2
B	1229	GLY	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	TRP	-	expression tag	UNP P0DTC2
B	1232	VAL	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	SER	-	expression tag	UNP P0DTC2
B	1236	THR	-	expression tag	UNP P0DTC2
B	1237	PHE	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	LYS	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	GLN	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	ASN	-	expression tag	UNP P0DTC2
B	1244	SER	-	expression tag	UNP P0DTC2
B	1245	ALA	-	expression tag	UNP P0DTC2
B	1246	ASP	-	expression tag	UNP P0DTC2
B	1247	ILE	-	expression tag	UNP P0DTC2
B	1248	GLN	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1252	ARG	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	LEU	-	expression tag	UNP P0DTC2
B	1255	GLU	-	expression tag	UNP P0DTC2
B	1256	SER	-	expression tag	UNP P0DTC2
B	1257	ARG	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	PRO	-	expression tag	UNP P0DTC2
B	1260	PHE	-	expression tag	UNP P0DTC2
B	1261	GLU	-	expression tag	UNP P0DTC2
B	1262	GLN	-	expression tag	UNP P0DTC2
B	1263	LYS	-	expression tag	UNP P0DTC2
B	1264	LEU	-	expression tag	UNP P0DTC2
B	1265	ILE	-	expression tag	UNP P0DTC2
B	1266	SER	-	expression tag	UNP P0DTC2
B	1267	GLU	-	expression tag	UNP P0DTC2
B	1268	GLU	-	expression tag	UNP P0DTC2
B	1269	ASP	-	expression tag	UNP P0DTC2
B	1270	LEU	-	expression tag	UNP P0DTC2
B	1271	ASN	-	expression tag	UNP P0DTC2
B	1272	MET	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	THR	-	expression tag	UNP P0DTC2
B	1275	GLY	-	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
B	1281	HIS	-	expression tag	UNP P0DTC2
C	19	ARG	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	156	GLY	GLU	variant	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	450	ARG	LEU	variant	UNP P0DTC2
C	476	LYS	THR	variant	UNP P0DTC2
C	612	GLY	ASP	variant	UNP P0DTC2
C	679	ARG	PRO	engineered mutation	UNP P0DTC2
C	680	GLY	ARG	engineered mutation	UNP P0DTC2
C	681	SER	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	948	ASN	ASP	variant	UNP P0DTC2
C	984	PRO	LYS	engineered mutation	UNP P0DTC2
C	985	PRO	VAL	engineered mutation	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	PHE	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	TYR	-	expression tag	UNP P0DTC2
C	1214	ILE	-	expression tag	UNP P0DTC2
C	1215	PRO	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ALA	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	ARG	-	expression tag	UNP P0DTC2
C	1220	ASP	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	GLN	-	expression tag	UNP P0DTC2
C	1223	ALA	-	expression tag	UNP P0DTC2
C	1224	TYR	-	expression tag	UNP P0DTC2
C	1225	VAL	-	expression tag	UNP P0DTC2
C	1226	ARG	-	expression tag	UNP P0DTC2
C	1227	LYS	-	expression tag	UNP P0DTC2
C	1228	ASP	-	expression tag	UNP P0DTC2
C	1229	GLY	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	TRP	-	expression tag	UNP P0DTC2
C	1232	VAL	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	SER	-	expression tag	UNP P0DTC2
C	1236	THR	-	expression tag	UNP P0DTC2
C	1237	PHE	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	LYS	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	GLN	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	ASN	-	expression tag	UNP P0DTC2
C	1244	SER	-	expression tag	UNP P0DTC2
C	1245	ALA	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1246	ASP	-	expression tag	UNP P0DTC2
C	1247	ILE	-	expression tag	UNP P0DTC2
C	1248	GLN	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	GLY	-	expression tag	UNP P0DTC2
C	1252	ARG	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	LEU	-	expression tag	UNP P0DTC2
C	1255	GLU	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	ARG	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	PRO	-	expression tag	UNP P0DTC2
C	1260	PHE	-	expression tag	UNP P0DTC2
C	1261	GLU	-	expression tag	UNP P0DTC2
C	1262	GLN	-	expression tag	UNP P0DTC2
C	1263	LYS	-	expression tag	UNP P0DTC2
C	1264	LEU	-	expression tag	UNP P0DTC2
C	1265	ILE	-	expression tag	UNP P0DTC2
C	1266	SER	-	expression tag	UNP P0DTC2
C	1267	GLU	-	expression tag	UNP P0DTC2
C	1268	GLU	-	expression tag	UNP P0DTC2
C	1269	ASP	-	expression tag	UNP P0DTC2
C	1270	LEU	-	expression tag	UNP P0DTC2
C	1271	ASN	-	expression tag	UNP P0DTC2
C	1272	MET	-	expression tag	UNP P0DTC2
C	1273	HIS	-	expression tag	UNP P0DTC2
C	1274	THR	-	expression tag	UNP P0DTC2
C	1275	GLY	-	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
C	1281	HIS	-	expression tag	UNP P0DTC2

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



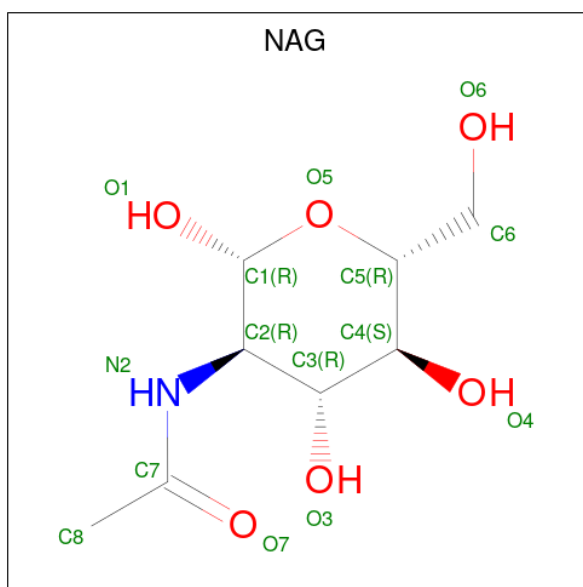
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16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

Continued on next page...

Continued from previous page...

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

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



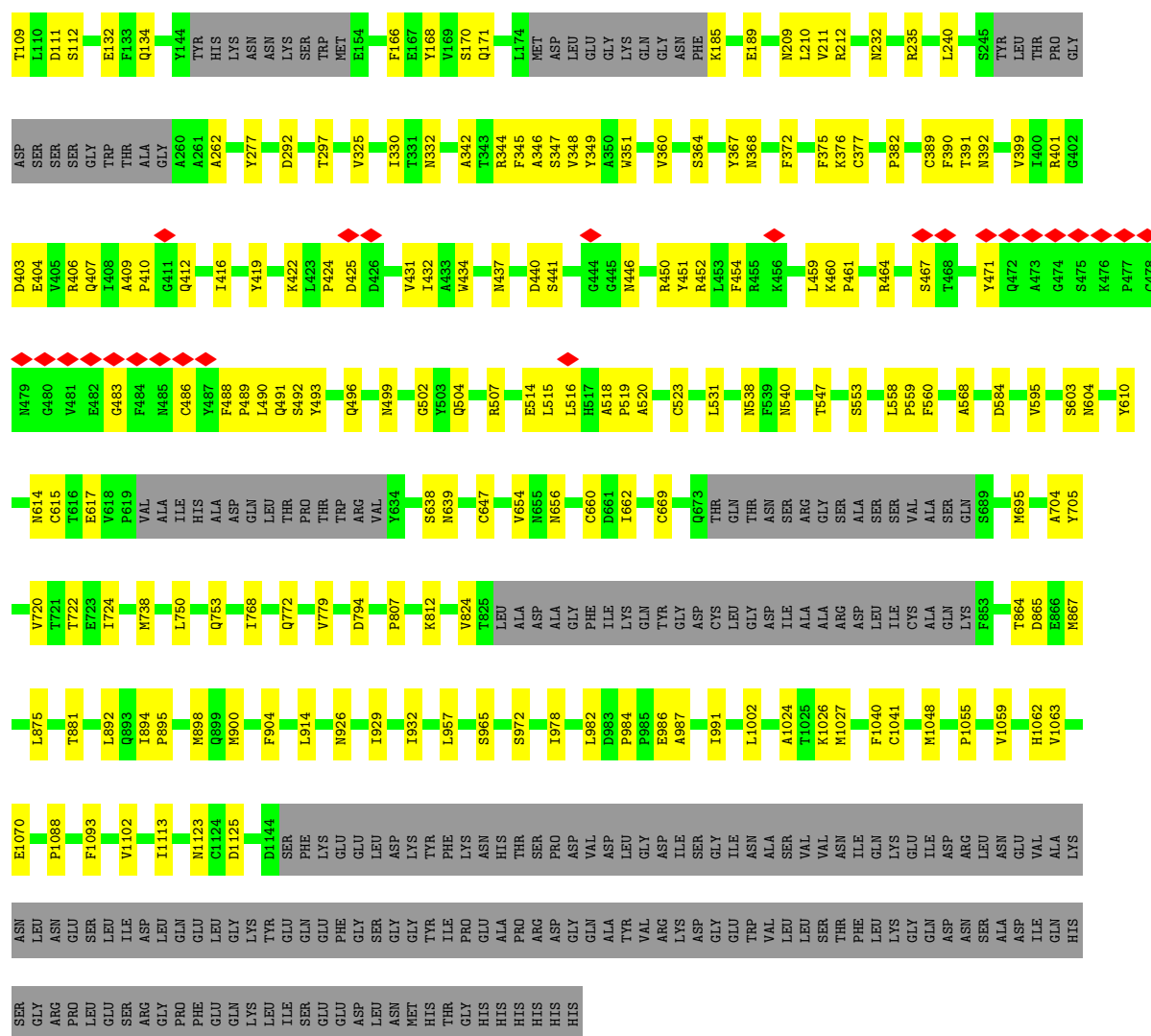
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3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

- Molecule 1: Spike glycoprotein

[illegible]

- Molecule 1: Spike glycoprotein

MET	PHE	VAL	PHE	LEU	LEU	VAL	LEU	LEU	PRO	PRO	VAL	SER	SER	GLY	R19	T20	L24	T29	N30	S31	F32	D40	S46	S60	N61	V62	T63	N64	F65	H66	ALA	ILE	ILE	HIS	VAL	SER	GLY	THR	ASN	GLY	THR	LYS	ARG	PHE	ASP	N81	Y91	N99	I100	I101	R102	I108
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------



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

Chain D:  50%



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

Chain E:  100%



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



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



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



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



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



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



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





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

Chain M: 

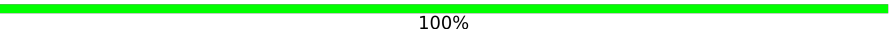


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



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

Chain O: 



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

Chain P: 

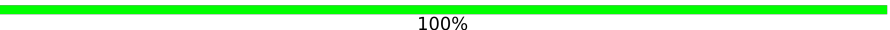


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 



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

Chain R: 



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

Chain S:  50% 50%

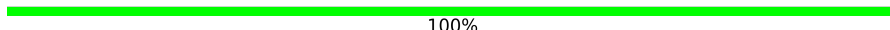


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 100%

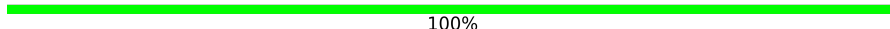


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

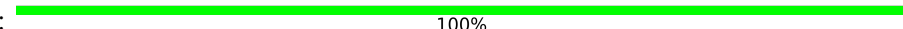


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



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

Chain W:  100%



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

Chain X:  50% 50%



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

Chain Y:  100%



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

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  50% 100%



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

Chain c:  50% 50%



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

Chain d:  100%



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

Chain e:  100%



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

Chain f:  100%



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

Chain g:  50% 50%



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

Chain h:  100%

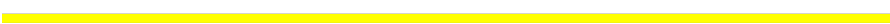


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  100%



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

Chain j:  100%



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

Chain k:  100%



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

Chain 1:

100%

MOL
MOL2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136969	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.953	Depositor
Minimum map value	-1.324	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.25	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	0.19	0/8197	0.37	2/11155 (0.0%)
1	B	0.20	0/8261	0.34	0/11242
1	C	0.20	0/8210	0.32	0/11173
All	All	0.20	0/24668	0.34	2/33570 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	982	LEU	CA-C-N	13.71	139.04	120.67
1	A	982	LEU	C-N-CA	13.71	139.04	120.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8016	0	7819	125	0
1	B	8077	0	7882	121	0
1	C	8028	0	7828	126	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	2	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	S	28	0	25	2	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	W	28	0	25	0	0
2	X	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	1	0
2	d	28	0	25	0	0
2	e	28	0	25	0	0
2	f	28	0	25	0	0
2	g	28	0	25	1	0
2	h	28	0	25	0	0
2	i	28	0	25	0	0
2	j	28	0	25	1	0
2	k	28	0	25	0	0
2	l	28	0	25	0	0
3	A	56	0	52	1	0
3	B	70	0	65	1	0
3	C	56	0	52	0	0
All	All	25283	0	24573	368	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 7.

All (368) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:PHE:O	1:A:262:ALA:HA	1.64	0.98
1:A:553:SER:HB3	1:A:584:ASP:HB2	1.65	0.79
1:C:65:PHE:O	1:C:262:ALA:HA	1.88	0.73
1:A:390:PHE:HD2	1:A:515:LEU:HB2	1.56	0.71
1:C:64:TRP:HE1	1:C:262:ALA:HB1	1.55	0.70
1:C:538:ASN:HB3	1:C:547:THR:HG22	1.73	0.70
1:B:969:GLY:HA3	1:B:993:ARG:HH21	1.57	0.69
1:A:326:ARG:HH21	1:A:578:GLN:HB2	1.58	0.69
1:B:139:PRO:HB3	1:B:157:VAL:HB	1.74	0.68
1:A:565:ARG:HD3	1:A:569:ASP:HA	1.75	0.68
1:A:356:ILE:HB	1:A:393:VAL:HB	1.75	0.67
1:B:415:LYS:NZ	1:B:453:LEU:O	2.29	0.66
1:C:391:THR:HA	1:C:520:ALA:HA	1.76	0.66
1:B:126:VAL:HG13	1:B:172:PRO:HA	1.77	0.66
1:B:317:ARG:NH2	1:C:738:MET:SD	2.70	0.65
1:C:377:CYS:HB2	1:C:382:PRO:HG3	1.79	0.65
1:C:553:SER:HB3	1:C:584:ASP:HB2	1.78	0.65
1:A:108:THR:O	1:A:235:ARG:NH1	2.30	0.65
1:B:46:SER:HA	1:B:277:TYR:O	1.96	0.65
1:B:18:LEU:HG	1:B:244:ARG:HH12	1.61	0.64
1:B:81:ASN:O	1:B:237:GLN:NE2	2.28	0.64
1:A:982:LEU:HD13	1:A:986:GLU:HG2	1.79	0.64
1:B:1127:VAL:HB	1:B:1130:ILE:HD11	1.80	0.64
1:B:212:ARG:NH1	1:B:264:TYR:OH	2.31	0.64
1:A:391:THR:HA	1:A:520:ALA:HA	1.80	0.63
1:A:390:PHE:HA	1:A:515:LEU:HD13	1.80	0.63
1:C:450:ARG:HG2	1:C:492:SER:HA	1.80	0.63
1:B:565:ARG:HD3	1:B:569:ASP:HA	1.81	0.62
1:A:355:ARG:HH22	1:A:392:ASN:HD22	1.46	0.62
1:C:722:THR:HG23	1:C:932:ILE:HD11	1.82	0.62
1:A:409:ALA:HB3	1:A:412:GLN:HG3	1.80	0.62
1:B:64:TRP:HE1	1:B:262:ALA:HB1	1.64	0.61
1:B:95:THR:OG1	1:B:97:LYS:NZ	2.33	0.61
1:A:325:VAL:HG12	1:A:540:ASN:HD21	1.65	0.61
1:A:333:LEU:HD23	1:A:360:VAL:HG13	1.82	0.61
1:A:875:LEU:HD13	1:A:1027:MET:HE2	1.83	0.60
1:C:349:TYR:OH	1:C:450:ARG:NH1	2.34	0.60
1:A:977:ASP:OD2	1:A:981:ARG:NH2	2.35	0.60
1:C:440:ASP:O	1:C:446:ASN:ND2	2.34	0.60
1:C:1026:LYS:NZ	1:C:1040:PHE:O	2.34	0.60
1:A:124:THR:OG1	1:A:125:ASN:OD1	2.19	0.60
1:C:212:ARG:O	1:C:212:ARG:NH1	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:SER:OG	1:A:639:ASN:OD1	2.20	0.59
1:B:99:ASN:O	1:B:102:ARG:NH2	2.33	0.58
1:B:27:ALA:HB3	1:B:64:TRP:HE3	1.68	0.58
1:B:344:ARG:NH2	1:B:449:TYR:OH	2.37	0.58
1:C:325:VAL:HG12	1:C:540:ASN:HB3	1.86	0.58
1:A:727:VAL:HG22	1:A:1057:GLY:HA2	1.86	0.57
1:B:65:PHE:O	1:B:262:ALA:HA	2.04	0.57
2:J:1:NAG:H3	2:J:1:NAG:H83	1.86	0.57
1:A:424:PRO:HB3	1:A:461:PRO:HB3	1.85	0.57
1:C:46:SER:HA	1:C:277:TYR:O	2.04	0.57
1:B:100:ILE:HG22	1:B:240:LEU:HD12	1.86	0.57
1:A:210:LEU:HD23	1:A:212:ARG:H	1.70	0.57
1:A:340:PHE:HB2	3:A:2002:NAG:H82	1.87	0.57
1:A:99:ASN:OD1	1:A:102:ARG:NH2	2.38	0.57
1:A:112:SER:HA	1:A:132:GLU:HB3	1.86	0.57
1:C:401:ARG:HB2	1:C:404:GLU:HG3	1.87	0.57
1:C:984:PRO:O	1:C:987:ALA:N	2.37	0.57
1:A:380:VAL:HG21	1:A:388:LEU:HD11	1.86	0.57
1:C:603:SER:OG	1:C:604:ASN:N	2.38	0.56
1:B:391:THR:HB	1:B:520:ALA:HA	1.87	0.56
1:B:168:TYR:HE1	1:B:170:SER:HB2	1.70	0.56
1:A:452:ARG:NH2	1:A:467:SER:O	2.34	0.56
1:A:483:GLY:H	1:A:486:CYS:HB2	1.71	0.56
1:C:112:SER:N	1:C:134:GLN:OE1	2.37	0.56
1:A:983:ASP:OD2	1:A:985:PRO:HD2	2.06	0.56
1:A:639:ASN:HD21	1:A:652:GLU:HG3	1.70	0.56
1:C:351:TRP:O	1:C:464:ARG:NH2	2.30	0.56
1:C:807:PRO:O	1:C:812:LYS:NZ	2.39	0.56
1:C:99:ASN:O	1:C:102:ARG:NH2	2.30	0.55
2:Q:2:NAG:H83	2:Q:2:NAG:H3	1.89	0.55
1:A:46:SER:HA	1:A:277:TYR:O	2.06	0.55
2:S:2:NAG:H83	2:S:2:NAG:H3	1.87	0.55
2:g:1:NAG:H3	2:g:1:NAG:H83	1.88	0.55
1:B:616:THR:OG1	1:B:617:GLU:OE1	2.21	0.55
1:B:1046:HIS:HA	1:B:1064:THR:HG22	1.88	0.55
1:B:326:ARG:NH2	1:B:578:GLN:OE1	2.40	0.55
1:B:1085:ALA:HB2	1:B:1124:CYS:HB3	1.87	0.55
1:C:452:ARG:NH2	1:C:467:SER:O	2.36	0.55
1:A:31:SER:HB3	1:A:60:SER:H	1.72	0.54
1:A:112:SER:N	1:A:134:GLN:OE1	2.38	0.54
1:A:354:LYS:HB3	1:A:395:ALA:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:PHE:HD1	1:C:432:ILE:HG12	1.72	0.54
1:C:704:ALA:HB2	2:j:2:NAG:H5	1.88	0.54
1:C:99:ASN:OD1	1:C:102:ARG:NH2	2.40	0.54
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.25	0.54
1:B:128:ILE:HB	1:B:168:TYR:HB3	1.90	0.54
1:A:807:PRO:O	1:A:812:LYS:NZ	2.41	0.54
1:C:516:LEU:HD23	1:C:518:ALA:H	1.71	0.54
1:B:455:ARG:NH1	1:B:458:ASN:O	2.40	0.54
1:A:903:ARG:NH1	1:A:1047:LEU:O	2.38	0.53
1:A:603:SER:OG	1:A:604:ASN:N	2.42	0.53
1:B:470:ILE:HD13	1:B:482:GLU:HG3	1.89	0.53
1:A:704:ALA:HB2	2:M:2:NAG:H62	1.91	0.53
1:B:97:LYS:HE3	1:B:185:LYS:HD2	1.89	0.53
1:B:740:ILE:HD11	1:B:751:LEU:HD22	1.91	0.53
1:A:768:ILE:HD11	1:A:1010:LEU:HD23	1.91	0.53
1:B:657:SER:HB3	1:B:696:SER:HB2	1.91	0.53
1:C:367:TYR:HE1	1:C:382:PRO:HB2	1.73	0.53
1:A:638:SER:OG	1:A:639:ASN:N	2.39	0.53
1:C:410:PRO:HB3	1:C:425:ASP:HA	1.91	0.53
1:C:638:SER:OG	1:C:639:ASN:N	2.41	0.53
1:C:965:SER:O	1:C:965:SER:OG	2.25	0.53
1:A:322:GLU:H	1:A:537:VAL:HG12	1.73	0.52
1:B:1091:GLY:HA3	1:B:1103:THR:O	2.09	0.52
1:C:409:ALA:HB3	1:C:412:GLN:HG3	1.89	0.52
1:C:875:LEU:HD13	1:C:1027:MET:HE2	1.91	0.52
1:B:894:ILE:HD12	1:B:895:PRO:HD2	1.91	0.52
1:B:739:TYR:CE1	1:B:964:LEU:HD21	2.44	0.52
1:A:19:ARG:HG3	1:A:20:THR:HG23	1.91	0.52
1:B:391:THR:HG22	1:B:514:GLU:OE2	2.10	0.52
1:B:904:PHE:HE1	1:B:1047:LEU:HD11	1.74	0.52
1:C:929:ILE:O	1:C:932:ILE:HG22	2.10	0.52
1:B:97:LYS:HG3	1:B:185:LYS:N	2.25	0.52
1:C:112:SER:HA	1:C:132:GLU:HB3	1.91	0.52
1:C:347:SER:OG	1:C:450:ARG:O	2.27	0.52
1:C:232:ASN:HB3	2:c:1:NAG:HN2	1.74	0.52
1:A:401:ARG:HB2	1:A:404:GLU:HG3	1.92	0.52
1:C:894:ILE:HD12	1:C:895:PRO:HD2	1.91	0.52
1:C:972:SER:HB3	1:C:978:ILE:HD11	1.90	0.52
1:C:31:SER:HB3	1:C:60:SER:H	1.74	0.51
1:C:406:ARG:NH1	1:C:407:GLN:HG2	2.25	0.51
1:B:325:VAL:HG23	1:B:540:ASN:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:TYR:HB2	1:A:647:CYS:SG	2.50	0.51
1:A:865:ASP:OD1	1:A:866:GLU:N	2.43	0.51
1:B:476:LYS:NZ	1:B:482:GLU:O	2.41	0.51
1:C:348:VAL:HG21	1:C:416:ILE:HD12	1.91	0.51
1:C:794:ASP:OD1	1:C:794:ASP:N	2.43	0.51
1:B:227:LEU:HB3	1:B:229:ILE:HG12	1.92	0.51
1:B:987:ALA:O	1:B:991:ILE:HG12	2.10	0.51
1:C:617:GLU:O	1:C:617:GLU:HG2	2.10	0.51
1:B:285:ASP:OD1	1:B:286:ALA:N	2.44	0.51
1:A:576:ASP:OD1	1:A:576:ASP:N	2.44	0.51
1:B:97:LYS:HE3	1:B:185:LYS:HA	1.92	0.51
1:A:347:SER:OG	1:A:450:ARG:O	2.28	0.50
1:C:108:THR:O	1:C:235:ARG:NH1	2.44	0.50
1:C:376:LYS:HG3	1:C:431:VAL:HB	1.94	0.50
1:A:894:ILE:HD12	1:A:895:PRO:HD2	1.93	0.50
1:B:720:VAL:HG22	1:B:1063:VAL:HG22	1.92	0.50
1:C:342:ALA:HB3	1:C:345:PHE:HE1	1.75	0.50
1:B:602:THR:HA	3:B:2004:NAG:H82	1.94	0.50
1:A:166:PHE:HE1	1:A:168:TYR:HB2	1.77	0.50
1:A:198:TYR:HE1	1:C:519:PRO:HG2	1.77	0.49
1:A:446:ASN:HB3	1:A:495:PHE:HB2	1.95	0.49
1:B:473:ALA:N	1:B:485:ASN:O	2.38	0.49
1:A:125:ASN:HD22	1:A:169:VAL:HG13	1.77	0.49
1:B:1075:THR:HG22	1:C:898:MET:HE1	1.94	0.49
1:A:1051:PRO:O	1:A:1052:GLN:NE2	2.31	0.49
1:C:451:TYR:CZ	1:C:491:GLN:HB2	2.47	0.49
1:B:199:PHE:HD2	1:B:201:ILE:HD11	1.77	0.49
1:C:654:VAL:HG12	1:C:656:ASN:H	1.78	0.49
1:A:892:LEU:HD22	1:C:1070:GLU:HG2	1.95	0.48
1:B:640:VAL:HG22	1:B:649:ILE:HG12	1.94	0.48
1:A:768:ILE:O	1:A:772:GLN:HG2	2.13	0.48
1:B:106:PHE:HB2	1:B:117:LEU:HB2	1.94	0.48
1:B:727:VAL:HG22	1:B:1057:GLY:HA2	1.96	0.48
1:A:99:ASN:O	1:A:102:ARG:NH2	2.28	0.48
1:A:377:CYS:HB2	1:A:382:PRO:HG3	1.95	0.48
1:A:689:SER:OG	1:A:690:ILE:N	2.47	0.48
1:A:350:ALA:HA	1:A:464:ARG:HD3	1.94	0.48
1:B:372:PHE:HD1	1:B:434:TRP:CD1	2.32	0.48
1:B:515:LEU:H	1:B:517:HIS:CE1	2.30	0.48
1:B:88:ASP:OD1	1:B:89:GLY:N	2.47	0.47
1:B:212:ARG:HD3	1:B:213:ASP:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:PHE:HD2	1:C:489:PRO:HA	1.79	0.47
1:B:515:LEU:H	1:B:517:HIS:HE1	1.62	0.47
1:B:775:ASN:O	1:B:779:VAL:HG23	2.15	0.47
1:C:166:PHE:HE1	1:C:168:TYR:HB2	1.79	0.47
1:C:372:PHE:HA	1:C:434:TRP:HB3	1.95	0.47
1:C:391:THR:HG22	1:C:514:GLU:O	2.13	0.47
1:C:210:LEU:HD23	1:C:212:ARG:H	1.79	0.47
1:A:375:PHE:HE2	1:A:382:PRO:HB3	1.78	0.47
1:C:364:SER:O	1:C:368:ASN:ND2	2.47	0.47
1:A:129:LYS:NZ	1:A:167:GLU:OE2	2.48	0.47
1:A:431:VAL:HG22	1:A:510:VAL:HG22	1.97	0.47
1:B:340:PHE:HB2	2:S:1:NAG:H82	1.96	0.47
1:B:424:PRO:HG2	1:B:427:PHE:HB2	1.96	0.47
1:C:900:MET:HE1	1:C:1048:MET:SD	2.54	0.47
1:A:986:GLU:N	1:A:986:GLU:OE1	2.46	0.47
1:C:424:PRO:HD3	1:C:461:PRO:HB3	1.96	0.47
1:C:558:LEU:HG	1:C:559:PRO:HD2	1.97	0.47
1:A:617:GLU:HG2	1:A:617:GLU:O	2.15	0.47
1:C:297:THR:OG1	1:C:595:VAL:HG21	2.15	0.47
1:C:531:LEU:H	1:C:531:LEU:HD23	1.80	0.47
1:B:724:ILE:HG12	1:B:1059:VAL:HG22	1.97	0.47
1:B:210:LEU:HD23	1:B:211:VAL:N	2.30	0.47
1:A:227:LEU:HB3	1:A:229:ILE:HG12	1.96	0.47
1:A:794:ASP:OD1	1:A:794:ASP:N	2.47	0.47
1:A:405:VAL:HG23	1:A:406:ARG:HD3	1.97	0.46
1:C:496:GLN:H	1:C:499:ASN:ND2	2.13	0.46
1:A:342:ALA:O	1:A:507:ARG:NH1	2.44	0.46
1:B:401:ARG:HD3	1:B:493:TYR:CD1	2.51	0.46
1:C:403:ASP:N	1:C:502:GLY:O	2.47	0.46
1:C:437:ASN:HB2	1:C:504:GLN:HB3	1.96	0.46
1:C:1041:CYS:HB2	1:C:1062:HIS:CE1	2.50	0.46
1:B:112:SER:N	1:B:134:GLN:OE1	2.40	0.46
1:C:437:ASN:O	1:C:441:SER:OG	2.24	0.46
1:A:40:ASP:OD1	1:A:40:ASP:N	2.49	0.46
1:A:499:ASN:HD22	1:A:503:TYR:HD2	1.64	0.46
1:B:25:PRO:HD2	1:B:66:HIS:HB3	1.97	0.46
1:B:102:ARG:HG3	1:B:141:LEU:HD22	1.97	0.46
1:B:652:GLU:HB2	1:B:691:ILE:HG22	1.97	0.46
1:C:720:VAL:HG22	1:C:1063:VAL:HG22	1.97	0.46
1:A:751:LEU:HD21	1:A:757:PHE:HZ	1.80	0.46
1:A:815:PHE:HE2	1:A:933:GLN:HE21	1.62	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:TRP:CD1	1:C:351:TRP:H	2.33	0.46
1:C:864:THR:HG22	1:C:867:MET:HE3	1.98	0.46
1:B:558:LEU:HB2	1:B:561:GLN:HG2	1.98	0.46
1:C:40:ASP:N	1:C:40:ASP:OD1	2.47	0.46
1:C:488:PHE:CE2	1:C:490:LEU:HB2	2.51	0.46
1:A:427:PHE:HE1	1:A:512:SER:HB2	1.80	0.46
1:B:30:ASN:HB3	1:B:32:PHE:CZ	2.51	0.46
1:C:824:VAL:HG13	1:C:1055:PRO:HG2	1.97	0.46
1:B:48:LEU:HD21	1:B:304:PHE:HD1	1.80	0.45
1:C:982:LEU:HD13	1:C:986:GLU:HB2	1.98	0.45
1:B:46:SER:CA	1:B:277:TYR:O	2.64	0.45
1:C:987:ALA:O	1:C:991:ILE:HG12	2.16	0.45
1:A:424:PRO:HG2	1:A:427:PHE:HB2	1.99	0.45
1:C:558:LEU:HD23	1:C:560:PHE:CE1	2.52	0.45
1:B:314:SER:OG	1:B:315:ASN:N	2.49	0.45
1:C:390:PHE:HD1	1:C:515:LEU:HB2	1.80	0.45
1:C:401:ARG:HG3	1:C:493:TYR:HE1	1.80	0.45
1:A:904:PHE:CD2	1:A:914:LEU:HB2	2.51	0.45
1:B:584:ASP:OD1	1:B:584:ASP:N	2.50	0.45
1:A:516:LEU:HD23	1:A:517:HIS:N	2.32	0.45
1:C:724:ILE:HG12	1:C:1059:VAL:HG22	1.99	0.45
1:B:1037:ARG:H	1:B:1037:ARG:HG2	1.58	0.45
1:B:399:VAL:HG22	1:B:507:ARG:HG2	1.99	0.45
1:A:202:TYR:CD1	1:A:223:PRO:HA	2.53	0.44
1:A:325:VAL:H	1:A:529:THR:HG22	1.82	0.44
1:A:348:VAL:HG21	1:A:416:ILE:HD12	1.99	0.44
1:B:118:LEU:HD21	1:B:120:VAL:HG23	1.98	0.44
1:C:1123:ASN:ND2	1:C:1125:ASP:OD2	2.49	0.44
1:B:1102:VAL:HG13	1:B:1113:ILE:HG12	1.99	0.44
1:C:168:TYR:HE1	1:C:170:SER:HB2	1.80	0.44
1:A:987:ALA:O	1:A:991:ILE:HG12	2.18	0.44
1:A:1041:CYS:HB2	1:A:1062:HIS:CE1	2.52	0.44
1:B:316:PHE:HZ	1:B:613:VAL:HG11	1.82	0.44
1:C:483:GLY:H	1:C:486:CYS:HB2	1.82	0.44
1:A:342:ALA:HB3	1:A:345:PHE:HE1	1.83	0.44
1:B:325:VAL:O	1:B:326:ARG:HD2	2.17	0.44
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.87	0.44
1:A:790:PRO:HG3	1:C:705:TYR:HB3	1.99	0.44
1:B:711:ALA:HB3	1:C:892:LEU:HB3	2.00	0.44
1:C:29:THR:HG23	1:C:62:VAL:HG13	1.99	0.44
1:C:91:TYR:OH	1:C:189:GLU:OE2	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:HD13	1:C:240:LEU:HG	1.99	0.44
1:C:390:PHE:HA	1:C:515:LEU:HD13	2.00	0.44
1:C:662:ILE:O	1:C:669:CYS:HB2	2.18	0.44
1:B:971:ILE:HD12	1:B:981:ARG:HH21	1.82	0.44
1:C:292:ASP:OD1	1:C:292:ASP:N	2.51	0.44
1:A:566:ASP:OD1	1:A:567:ILE:N	2.47	0.44
1:B:199:PHE:HB3	1:B:227:LEU:HB2	1.99	0.44
1:A:399:VAL:HG22	1:A:507:ARG:HG2	2.00	0.43
1:C:984:PRO:HA	1:C:987:ALA:HB3	2.00	0.43
1:B:127:VAL:HG22	1:B:129:LYS:HE3	1.99	0.43
1:A:327:PHE:O	1:A:578:GLN:NE2	2.51	0.43
1:A:865:ASP:OD1	1:A:865:ASP:C	2.61	0.43
1:A:1099:HIS:ND1	2:N:1:NAG:H5	2.33	0.43
1:C:132:GLU:N	1:C:132:GLU:OE1	2.51	0.43
1:C:170:SER:OG	1:C:171:GLN:N	2.52	0.43
1:B:459:LEU:HD22	1:B:463:GLU:OE2	2.18	0.43
1:A:89:GLY:HA3	1:A:268:LEU:HD12	2.00	0.43
1:A:639:ASN:OD1	1:A:639:ASN:N	2.49	0.43
1:B:36:VAL:HG21	1:B:218:PHE:HE1	1.83	0.43
1:B:986:GLU:O	1:B:990:GLN:HG2	2.19	0.43
1:C:452:ARG:HA	1:C:490:LEU:HD23	2.01	0.43
1:B:631:TRP:O	1:B:635:SER:N	2.41	0.43
1:B:983:ASP:OD1	1:B:983:ASP:N	2.51	0.43
1:C:46:SER:CA	1:C:277:TYR:O	2.66	0.43
1:A:410:PRO:HG3	1:A:427:PHE:HD2	1.83	0.43
1:A:125:ASN:HD21	2:D:1:NAG:H61	1.84	0.43
1:B:197:GLY:HA2	1:B:230:GLY:HA2	2.01	0.43
1:B:450:ARG:HA	1:B:492:SER:HA	2.01	0.43
1:A:576:ASP:OD2	1:A:579:THR:HB	2.18	0.43
1:A:1002:LEU:HD12	1:A:1002:LEU:HA	1.87	0.43
1:B:1139:LEU:O	1:B:1142:GLU:HG3	2.17	0.43
1:C:419:TYR:HA	1:C:459:LEU:HD23	2.01	0.43
1:A:375:PHE:CD1	1:A:432:ILE:HG12	2.54	0.42
1:A:746:GLU:H	1:A:746:GLU:CD	2.27	0.42
1:A:962:LYS:HE2	1:C:568:ALA:HA	2.01	0.42
1:B:131:CYS:HB2	1:B:133:PHE:CZ	2.54	0.42
1:B:452:ARG:HG3	1:B:489:PRO:HB2	2.01	0.42
1:C:722:THR:CG2	1:C:932:ILE:HD11	2.49	0.42
1:A:170:SER:OG	1:A:171:GLN:N	2.51	0.42
1:A:389:CYS:HB3	1:A:523:CYS:HB3	1.17	0.42
1:B:169:VAL:HG11	2:P:2:NAG:H82	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:NH1	1:B:531:LEU:HD23	2.33	0.42
1:B:435:ASN:HB2	1:B:506:TYR:CZ	2.54	0.42
1:A:212:ARG:C	1:A:212:ARG:HH11	2.27	0.42
1:A:449:TYR:HB3	1:A:493:TYR:HD2	1.83	0.42
1:B:226:ASP:OD1	1:B:227:LEU:N	2.52	0.42
1:B:1071:LYS:HE2	1:B:1071:LYS:HB3	1.90	0.42
1:A:121:ASN:ND2	1:A:173:PHE:H	2.17	0.42
1:A:568:ALA:HA	1:B:962:LYS:HE2	2.00	0.42
1:A:999:LEU:HD23	1:A:999:LEU:HA	1.90	0.42
1:A:1026:LYS:NZ	1:A:1040:PHE:O	2.40	0.42
1:B:194:ASN:HB2	1:B:199:PHE:CD1	2.55	0.42
1:B:809:LYS:NZ	1:B:818:ASP:OD2	2.44	0.42
1:C:558:LEU:HD23	1:C:560:PHE:HE1	1.83	0.42
2:M:1:NAG:O3	2:M:2:NAG:N2	2.53	0.42
1:A:343:THR:O	1:A:507:ARG:NH2	2.50	0.42
1:A:356:ILE:HG22	1:A:522:VAL:HG21	2.01	0.42
1:B:617:GLU:OE1	1:B:617:GLU:N	2.53	0.42
1:B:804:LEU:HD23	1:B:804:LEU:HA	1.90	0.42
1:C:344:ARG:CZ	1:C:346:ALA:HA	2.49	0.42
1:B:164:CYS:HB3	1:B:167:GLU:OE1	2.20	0.42
1:B:474:GLY:N	1:B:485:ASN:HB3	2.34	0.42
1:B:984:PRO:HG2	1:B:985:PRO:HD3	2.01	0.42
1:A:64:TRP:HE1	1:A:262:ALA:HB1	1.85	0.42
1:A:1088:PRO:HD3	1:A:1093:PHE:CE2	2.54	0.42
1:B:372:PHE:HA	1:B:434:TRP:HB3	2.02	0.42
1:C:614:ASN:OD1	1:C:615:CYS:N	2.53	0.42
1:C:389:CYS:HB3	1:C:523:CYS:HB3	1.13	0.42
1:C:926:ASN:O	1:C:929:ILE:HG22	2.20	0.42
1:A:659:GLU:O	1:A:693:TYR:OH	2.29	0.41
1:B:96:GLU:HB3	1:B:188:ARG:HH11	1.84	0.41
1:B:121:ASN:HD21	1:B:174:LEU:H	1.68	0.41
1:B:632:ARG:HA	1:B:635:SER:HB3	2.01	0.41
1:C:399:VAL:HG22	1:C:507:ARG:HG2	2.02	0.41
1:C:957:LEU:HD23	1:C:957:LEU:HA	1.85	0.41
1:C:1002:LEU:HD12	1:C:1002:LEU:HA	1.85	0.41
1:A:121:ASN:HD22	1:A:173:PHE:H	1.68	0.41
1:B:195:ILE:HG22	1:B:196:ASP:OD1	2.21	0.41
1:C:610:TYR:HB2	1:C:647:CYS:SG	2.60	0.41
1:B:188:ARG:HB3	1:B:190:PHE:HE1	1.84	0.41
1:C:454:PHE:HB3	1:C:471:TYR:CD2	2.56	0.41
1:C:750:LEU:O	1:C:753:GLN:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:MET:HE2	1:A:898:MET:HB3	1.83	0.41
1:C:865:ASP:OD1	1:C:865:ASP:N	2.52	0.41
1:A:95:THR:O	1:A:95:THR:HG23	2.21	0.41
1:B:102:ARG:HA	1:B:102:ARG:HD3	1.77	0.41
1:C:422:LYS:HB3	1:C:460:LYS:O	2.20	0.41
1:A:129:LYS:HG2	1:A:167:GLU:HG3	2.03	0.41
1:A:188:ARG:HB3	1:A:190:PHE:HE1	1.86	0.41
1:A:352:ASN:HB2	1:A:397:SER:OG	2.21	0.41
1:A:736:CYS:HB3	1:A:758:CYS:HB2	1.90	0.41
1:A:1016:ILE:HD13	1:A:1016:ILE:HA	1.96	0.41
1:B:703:VAL:HG13	1:C:881:THR:HG21	2.03	0.41
1:B:774:LYS:HD3	1:B:778:GLU:OE2	2.20	0.41
1:B:1136:TYR:OH	1:B:1141:PRO:HG3	2.21	0.41
1:C:1102:VAL:HG13	1:C:1113:ILE:HG12	2.02	0.41
1:A:419:TYR:O	1:A:452:ARG:HD2	2.21	0.41
1:A:663:PRO:HA	1:A:669:CYS:HB3	2.02	0.41
1:C:185:LYS:HE3	1:C:209:ASN:HA	2.02	0.41
1:C:392:ASN:OD1	1:C:514:GLU:HB3	2.21	0.41
1:A:338:GLU:OE2	1:A:354:LYS:NZ	2.46	0.40
1:A:442:LYS:O	1:A:497:PRO:HD3	2.20	0.40
1:A:1143:LEU:HD23	1:A:1143:LEU:HA	1.90	0.40
1:B:292:ASP:OD1	1:B:292:ASP:N	2.54	0.40
1:B:794:ASP:N	1:B:794:ASP:OD1	2.54	0.40
1:B:1080:CYS:SG	1:B:1130:ILE:HG21	2.61	0.40
1:B:1091:GLY:CA	1:B:1103:THR:O	2.69	0.40
1:C:332:ASN:O	1:C:360:VAL:HG12	2.21	0.40
1:C:779:VAL:HG22	1:C:1024:ALA:HB2	2.03	0.40
1:C:904:PHE:CD2	1:C:914:LEU:HB2	2.56	0.40
1:A:351:TRP:HB3	1:A:398:PHE:HB3	2.02	0.40
1:B:804:LEU:HD23	1:B:876:LEU:HD23	2.02	0.40
1:C:168:TYR:CE1	1:C:170:SER:HB2	2.56	0.40
1:C:660:CYS:HB2	1:C:695:MET:HG2	2.03	0.40
1:B:291:LEU:HD12	1:B:291:LEU:HA	1.91	0.40
1:C:30:ASN:HB3	1:C:32:PHE:CE2	2.57	0.40
1:C:1088:PRO:HD3	1:C:1093:PHE:CE2	2.57	0.40
1:B:1047:LEU:HD23	1:B:1047:LEU:HA	1.87	0.40
1:C:210:LEU:HD23	1:C:211:VAL:N	2.37	0.40
1:C:768:ILE:O	1:C:772:GLN:HG2	2.21	0.40
1:A:392:ASN:OD1	1:A:514:GLU:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1011/1281 (79%)	970 (96%)	40 (4%)	1 (0%)	48	80
1	B	1017/1281 (79%)	963 (95%)	54 (5%)	0	100	100
1	C	1012/1281 (79%)	959 (95%)	52 (5%)	1 (0%)	48	80
All	All	3040/3843 (79%)	2892 (95%)	146 (5%)	2 (0%)	49	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ILE
1	C	330	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	898/1113 (81%)	898 (100%)	0	100	100
1	B	904/1113 (81%)	904 (100%)	0	100	100
1	C	899/1113 (81%)	899 (100%)	0	100	100
All	All	2701/3339 (81%)	2701 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	81	ASN
1	A	171	GLN
1	A	437	ASN
1	A	491	GLN
1	A	653	HIS
1	A	990	GLN
1	B	121	ASN
1	B	952	GLN
1	C	315	ASN
1	C	332	ASN
1	C	437	ASN
1	C	446	ASN
1	C	491	GLN
1	C	760	GLN
1	C	899	GLN
1	C	990	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

70 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	2,1	14,14,15	0.44	0	17,19,21	0.75	1 (5%)
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2,1	14,14,15	0.40	0	17,19,21	0.38	0
2	NAG	E	2	2	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	F	1	2,1	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	F	2	2	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	G	1	2,1	14,14,15	0.21	0	17,19,21	0.50	0
2	NAG	G	2	2	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	H	1	2,1	14,14,15	0.22	0	17,19,21	0.39	0
2	NAG	H	2	2	14,14,15	0.17	0	17,19,21	0.45	0
2	NAG	I	1	2,1	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.22	0	17,19,21	0.40	0
2	NAG	J	1	2,1	14,14,15	0.45	0	17,19,21	1.33	2 (11%)
2	NAG	J	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	K	1	2,1	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.49	0
2	NAG	L	1	2,1	14,14,15	0.22	0	17,19,21	0.47	0
2	NAG	L	2	2	14,14,15	0.19	0	17,19,21	0.44	0
2	NAG	M	1	2,1	14,14,15	0.45	0	17,19,21	0.93	1 (5%)
2	NAG	M	2	2	14,14,15	0.17	0	17,19,21	0.57	0
2	NAG	N	1	2,1	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	N	2	2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	O	1	2,1	14,14,15	0.18	0	17,19,21	0.48	0
2	NAG	O	2	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	P	1	2,1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	P	2	2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	Q	1	2,1	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	Q	2	2	14,14,15	0.50	0	17,19,21	1.34	2 (11%)
2	NAG	R	1	2,1	14,14,15	0.19	0	17,19,21	0.55	0
2	NAG	R	2	2	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	S	1	2,1	14,14,15	0.26	0	17,19,21	0.41	0
2	NAG	S	2	2	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
2	NAG	T	1	2,1	14,14,15	0.21	0	17,19,21	0.51	0
2	NAG	T	2	2	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	U	1	2,1	14,14,15	0.36	0	17,19,21	0.39	0
2	NAG	U	2	2	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	V	1	2,1	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	V	2	2	14,14,15	0.19	0	17,19,21	0.49	0
2	NAG	W	1	2,1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	W	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	X	1	2,1	14,14,15	0.69	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	X	2	2	14,14,15	0.18	0	17,19,21	0.57	0
2	NAG	Y	1	2,1	14,14,15	0.19	0	17,19,21	0.46	0
2	NAG	Y	2	2	14,14,15	0.20	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Z	1	2,1	14,14,15	0.17	0	17,19,21	0.46	0
2	NAG	Z	2	2	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	a	1	2,1	14,14,15	0.32	0	17,19,21	0.60	0
2	NAG	a	2	2	14,14,15	0.18	0	17,19,21	0.47	0
2	NAG	b	1	2,1	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	b	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	c	1	2,1	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	c	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	d	1	2,1	14,14,15	0.30	0	17,19,21	0.49	0
2	NAG	d	2	2	14,14,15	0.25	0	17,19,21	0.42	0
2	NAG	e	1	2,1	14,14,15	0.34	0	17,19,21	0.43	0
2	NAG	e	2	2	14,14,15	0.19	0	17,19,21	0.47	0
2	NAG	f	1	2,1	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	f	2	2	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	g	1	2,1	14,14,15	0.42	0	17,19,21	1.31	2 (11%)
2	NAG	g	2	2	14,14,15	0.19	0	17,19,21	0.49	0
2	NAG	h	1	2,1	14,14,15	0.25	0	17,19,21	0.47	0
2	NAG	h	2	2	14,14,15	0.19	0	17,19,21	0.49	0
2	NAG	i	1	2,1	14,14,15	0.27	0	17,19,21	0.49	0
2	NAG	i	2	2	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	j	1	2,1	14,14,15	0.57	0	17,19,21	1.03	1 (5%)
2	NAG	j	2	2	14,14,15	0.22	0	17,19,21	0.54	0
2	NAG	k	1	2,1	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	k	2	2	14,14,15	0.17	0	17,19,21	0.43	0
2	NAG	l	1	2,1	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	l	2	2	14,14,15	0.19	0	17,19,21	0.43	0

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Z	2	2	-	1/6/23/26	0/1/1/1
2	NAG	a	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	a	2	2	-	0/6/23/26	0/1/1/1
2	NAG	b	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	NAG	c	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	c	2	2	-	2/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	4/6/23/26	0/1/1/1
2	NAG	e	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	f	2	2	-	2/6/23/26	0/1/1/1
2	NAG	g	1	2,1	-	6/6/23/26	0/1/1/1
2	NAG	g	2	2	-	0/6/23/26	0/1/1/1
2	NAG	h	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	h	2	2	-	0/6/23/26	0/1/1/1
2	NAG	i	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	i	2	2	-	0/6/23/26	0/1/1/1
2	NAG	j	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	j	2	2	-	2/6/23/26	0/1/1/1
2	NAG	k	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	k	2	2	-	2/6/23/26	0/1/1/1
2	NAG	l	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	l	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1	NAG	O5-C1	2.20	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	C2-N2-C7	4.57	129.03	122.90
2	S	2	NAG	C2-N2-C7	4.55	129.00	122.90
2	g	1	NAG	C2-N2-C7	4.53	128.97	122.90
2	Q	2	NAG	C2-N2-C7	4.51	128.94	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	1	NAG	C1-O5-C5	3.07	116.29	112.19
2	X	1	NAG	C1-O5-C5	3.05	116.28	112.19
2	M	1	NAG	C1-O5-C5	2.62	115.70	112.19
2	D	1	NAG	C1-O5-C5	2.21	115.14	112.19
2	Q	2	NAG	C1-C2-N2	2.18	113.86	110.43
2	S	2	NAG	C1-C2-N2	2.13	113.79	110.43
2	J	1	NAG	C1-C2-N2	2.12	113.78	110.43
2	g	1	NAG	C1-C2-N2	2.12	113.77	110.43

There are no chirality outliers.

All (128) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	k	2	NAG	C4-C5-C6-O6
2	j	2	NAG	O5-C5-C6-O6
2	b	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	e	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	g	1	NAG	O5-C5-C6-O6
2	k	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	X	1	NAG	O5-C5-C6-O6
2	j	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	b	2	NAG	C4-C5-C6-O6
2	g	1	NAG	C4-C5-C6-O6
2	e	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	c	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	S	2	NAG	C8-C7-N2-C2
2	S	2	NAG	O7-C7-N2-C2
2	T	2	NAG	C8-C7-N2-C2
2	T	2	NAG	O7-C7-N2-C2
2	U	1	NAG	C8-C7-N2-C2
2	U	1	NAG	O7-C7-N2-C2
2	b	1	NAG	C8-C7-N2-C2
2	b	1	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
2	e	1	NAG	C8-C7-N2-C2
2	e	1	NAG	O7-C7-N2-C2
2	g	1	NAG	C8-C7-N2-C2
2	g	1	NAG	O7-C7-N2-C2
2	l	2	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	X	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	Q	1	NAG	C4-C5-C6-O6
2	l	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	c	2	NAG	O5-C5-C6-O6
2	a	1	NAG	C4-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	S	1	NAG	O5-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
2	Z	1	NAG	C4-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	f	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C1-C2-N2-C7
2	M	1	NAG	C1-C2-N2-C7
2	R	1	NAG	C1-C2-N2-C7
2	X	1	NAG	C1-C2-N2-C7
2	T	1	NAG	C4-C5-C6-O6
2	f	1	NAG	O5-C5-C6-O6
2	l	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C3-C2-N2-C7
2	R	1	NAG	C3-C2-N2-C7
2	X	1	NAG	C3-C2-N2-C7
2	d	1	NAG	C3-C2-N2-C7
2	j	1	NAG	C3-C2-N2-C7
2	H	2	NAG	O5-C5-C6-O6
2	l	1	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C1-C2-N2-C7
2	Q	2	NAG	C1-C2-N2-C7
2	S	2	NAG	C1-C2-N2-C7
2	W	2	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

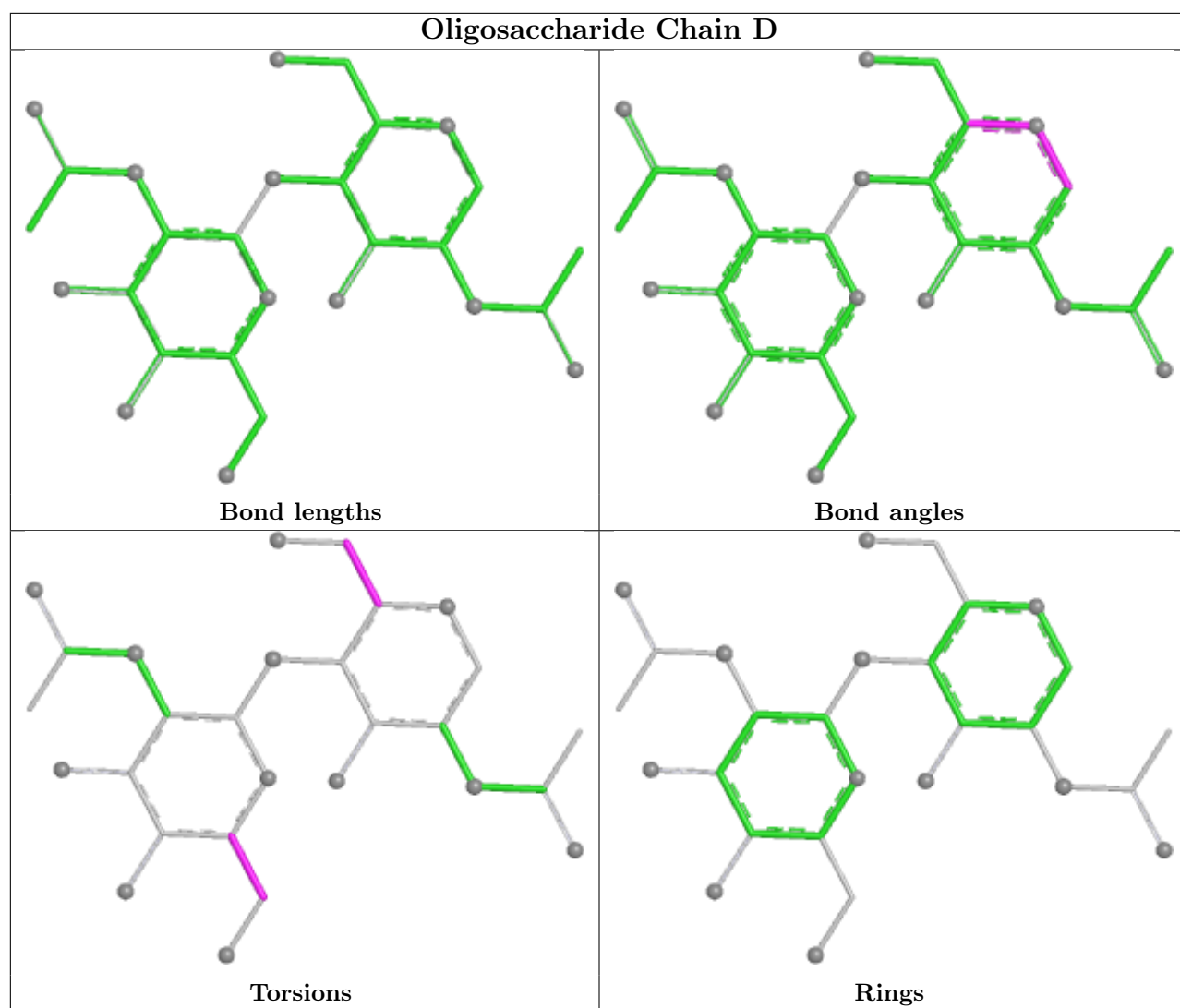
Mol	Chain	Res	Type	Atoms
2	d	1	NAG	C1-C2-N2-C7
2	g	1	NAG	C1-C2-N2-C7
2	j	1	NAG	C1-C2-N2-C7
2	L	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C3-C2-N2-C7
2	M	1	NAG	C3-C2-N2-C7
2	Q	2	NAG	C3-C2-N2-C7
2	S	2	NAG	C3-C2-N2-C7
2	g	1	NAG	C3-C2-N2-C7
2	b	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6

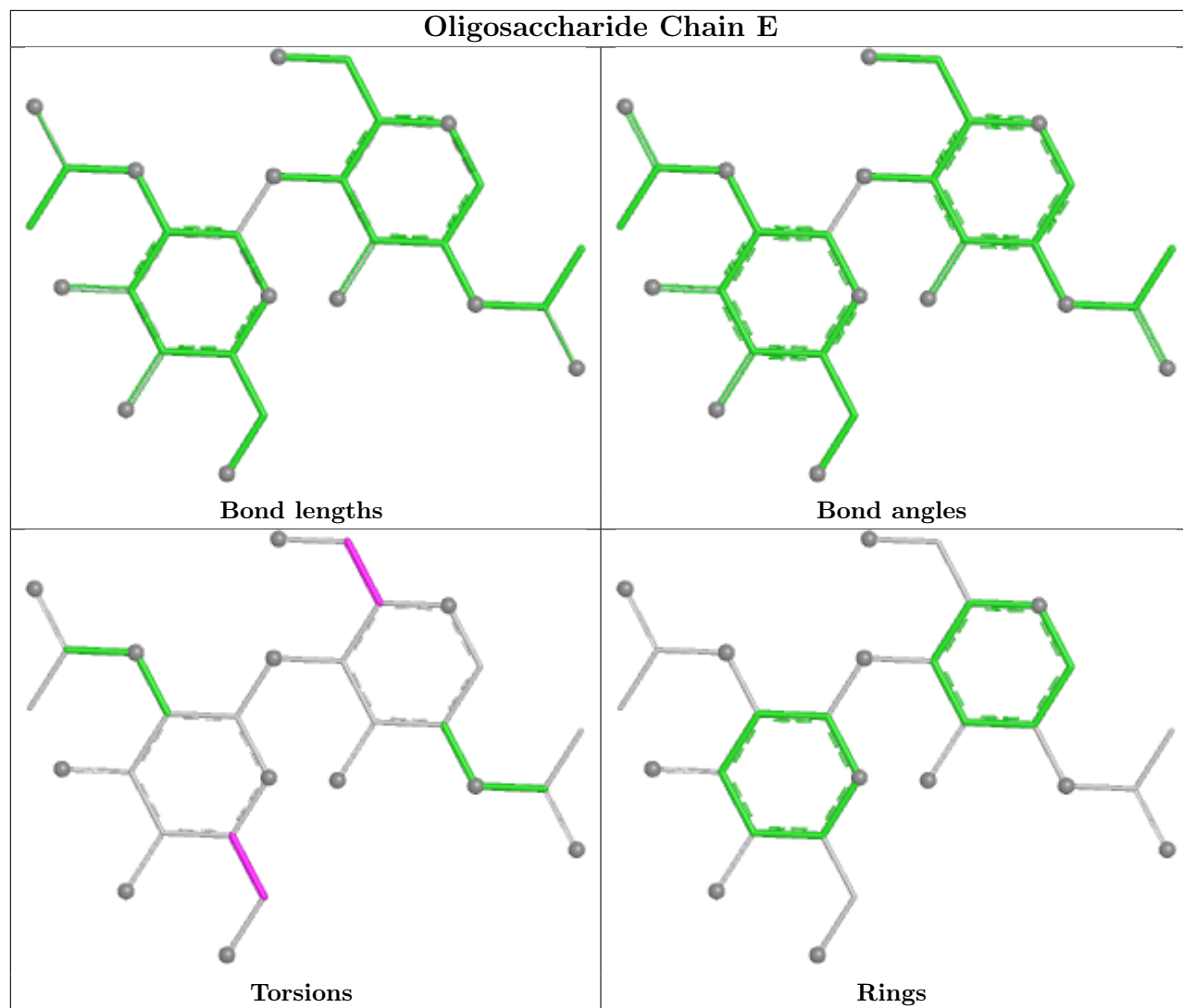
There are no ring outliers.

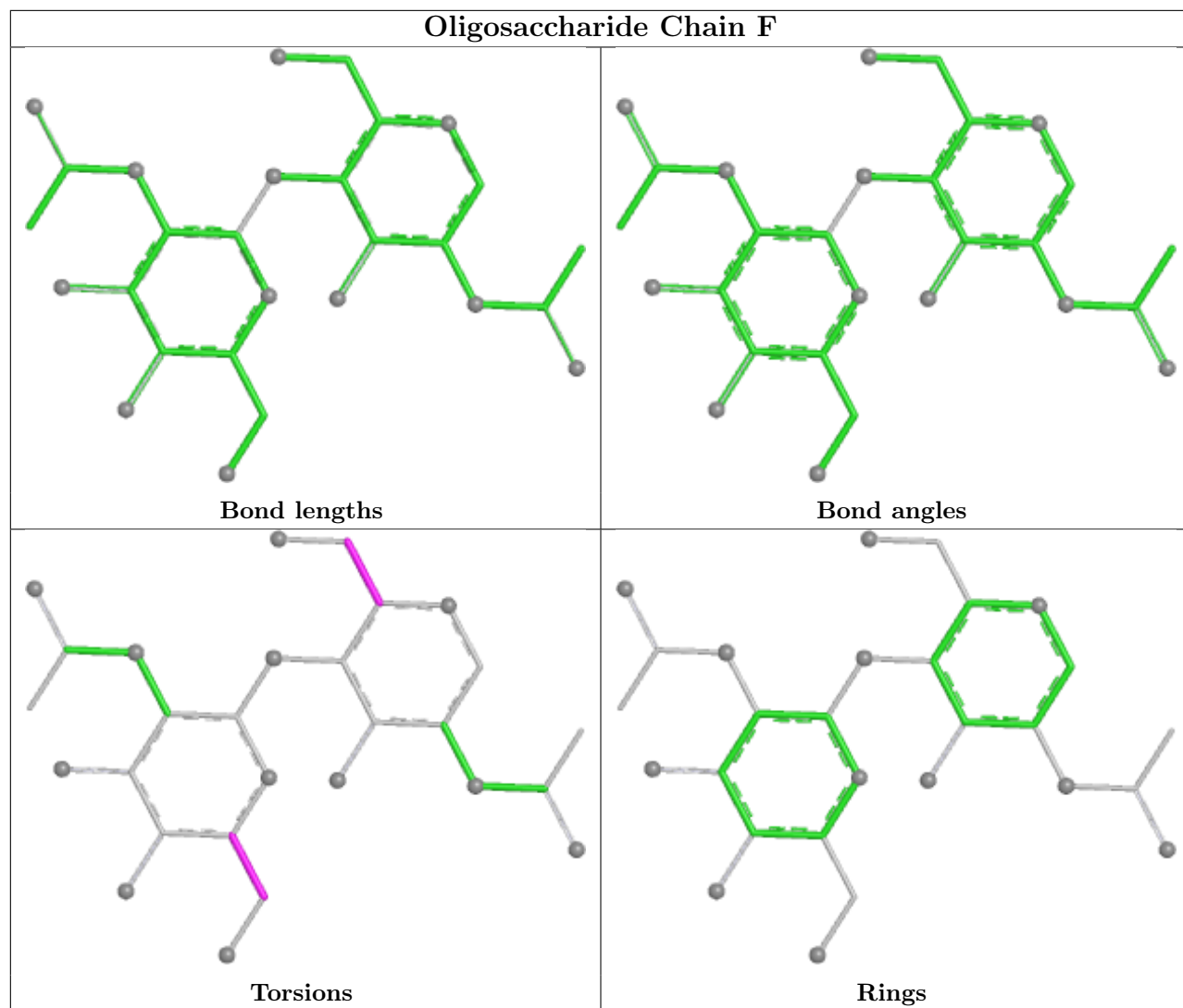
12 monomers are involved in 12 short contacts:

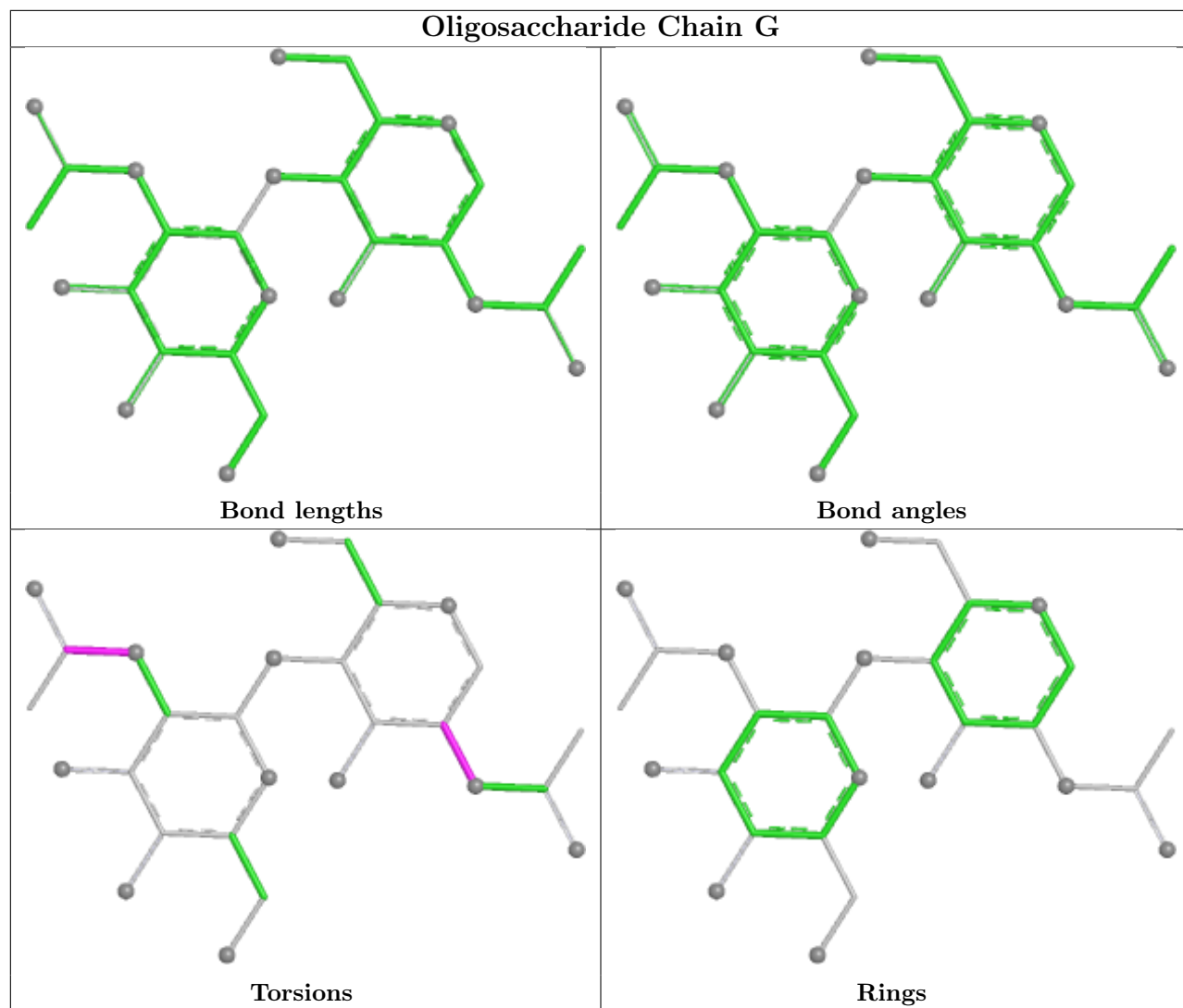
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	S	2	NAG	1	0
2	c	1	NAG	1	0
2	M	2	NAG	2	0
2	g	1	NAG	1	0
2	M	1	NAG	1	0
2	P	2	NAG	1	0
2	N	1	NAG	1	0
2	Q	2	NAG	1	0
2	S	1	NAG	1	0
2	J	1	NAG	1	0
2	j	2	NAG	1	0

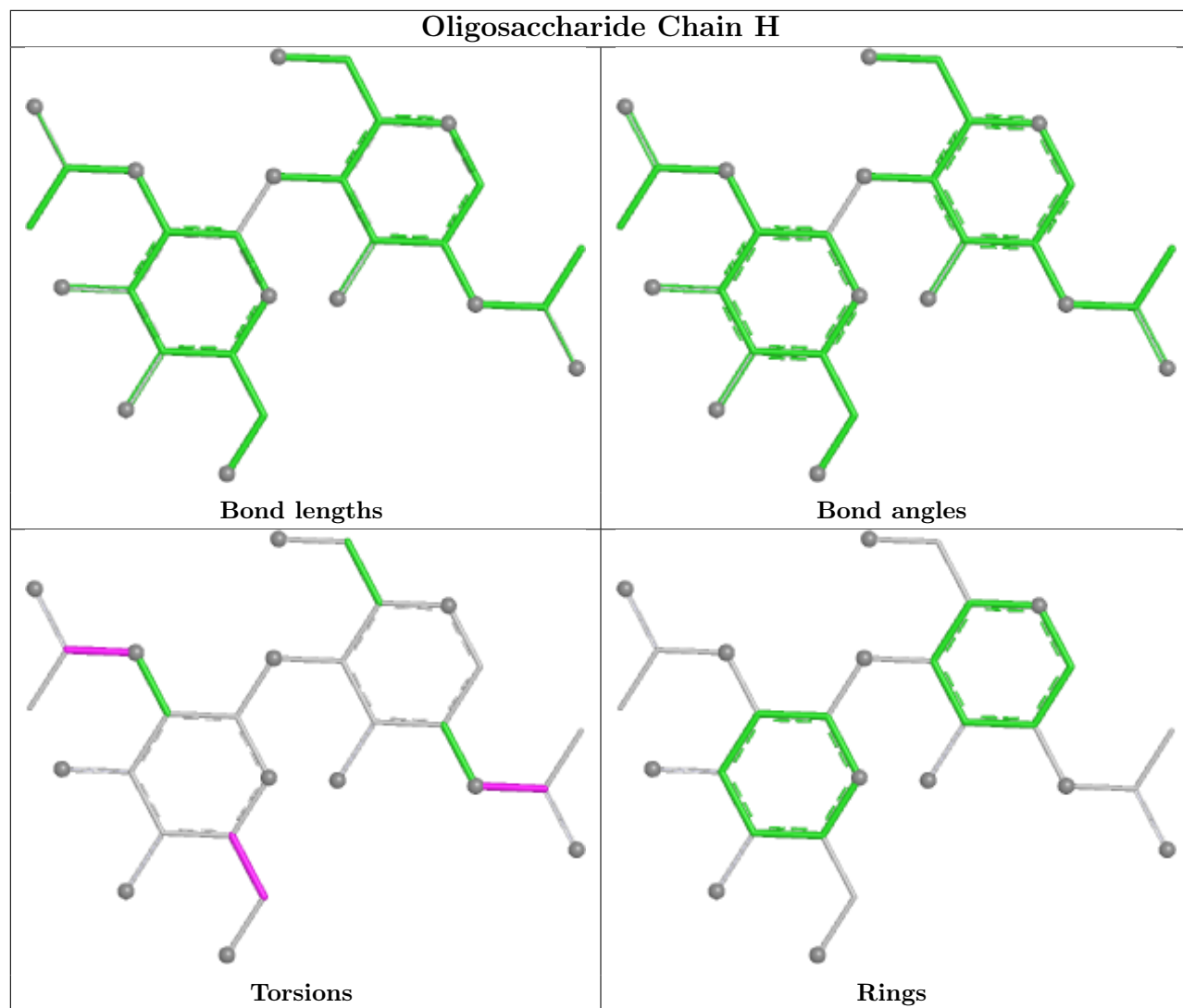
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

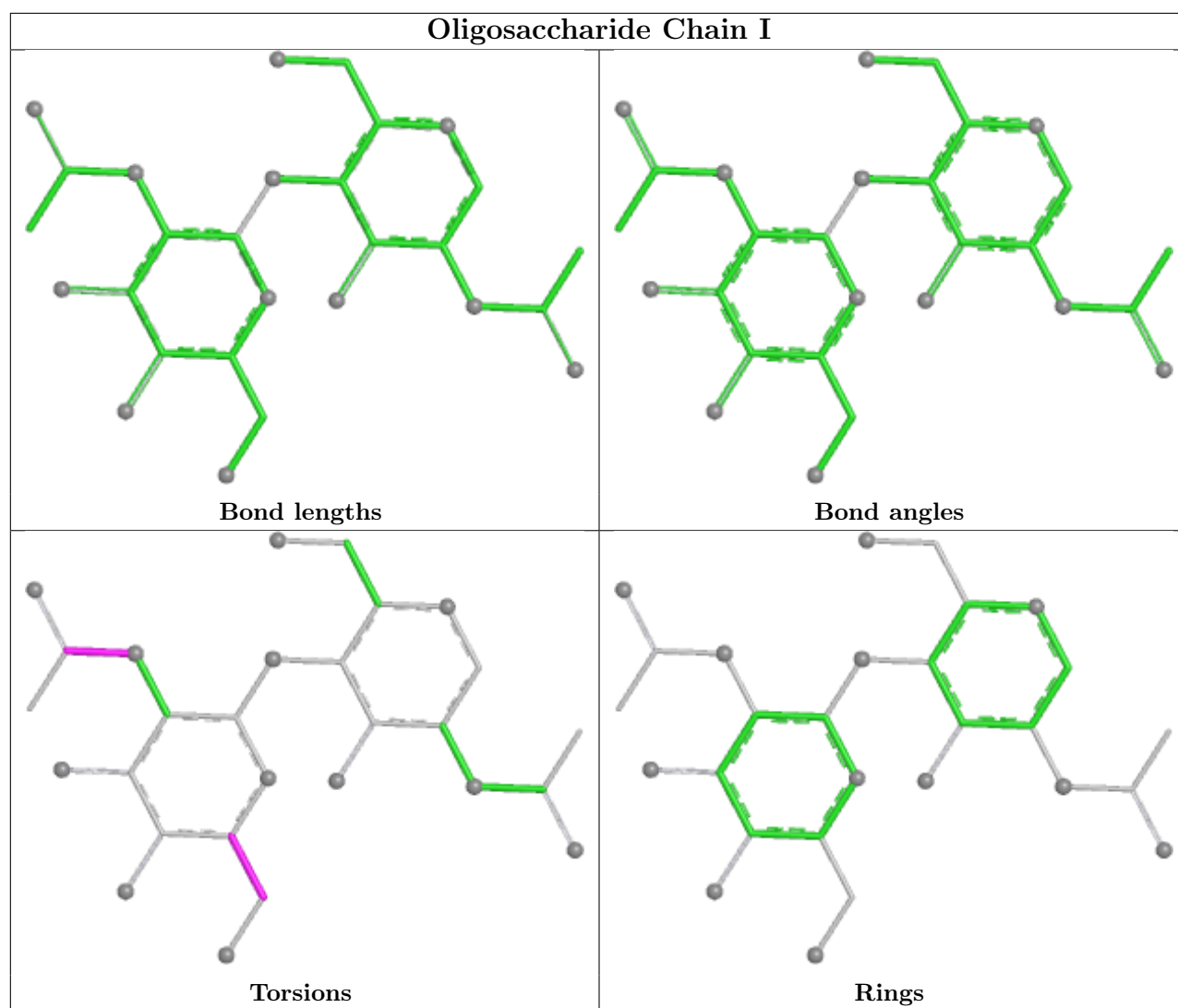


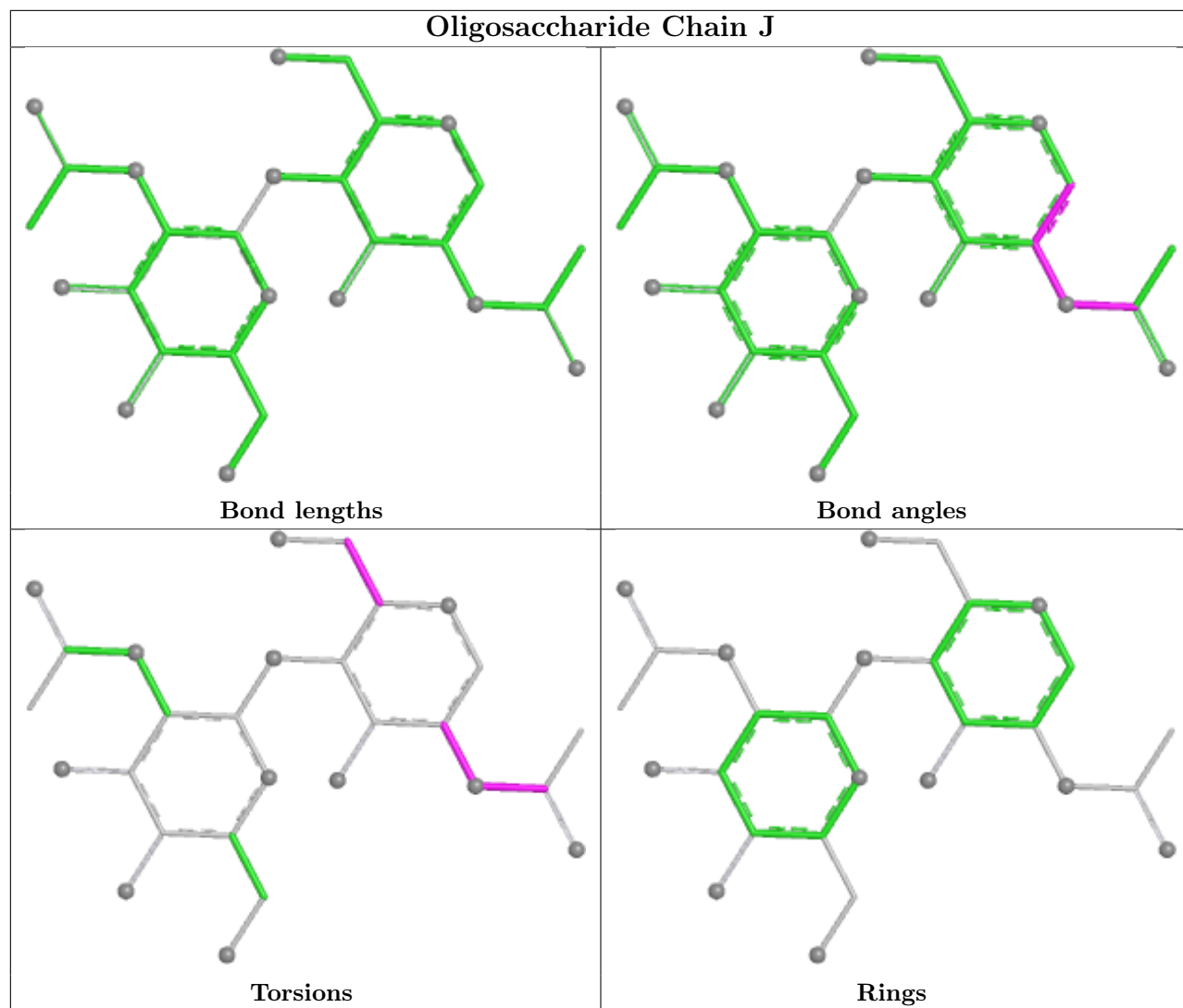


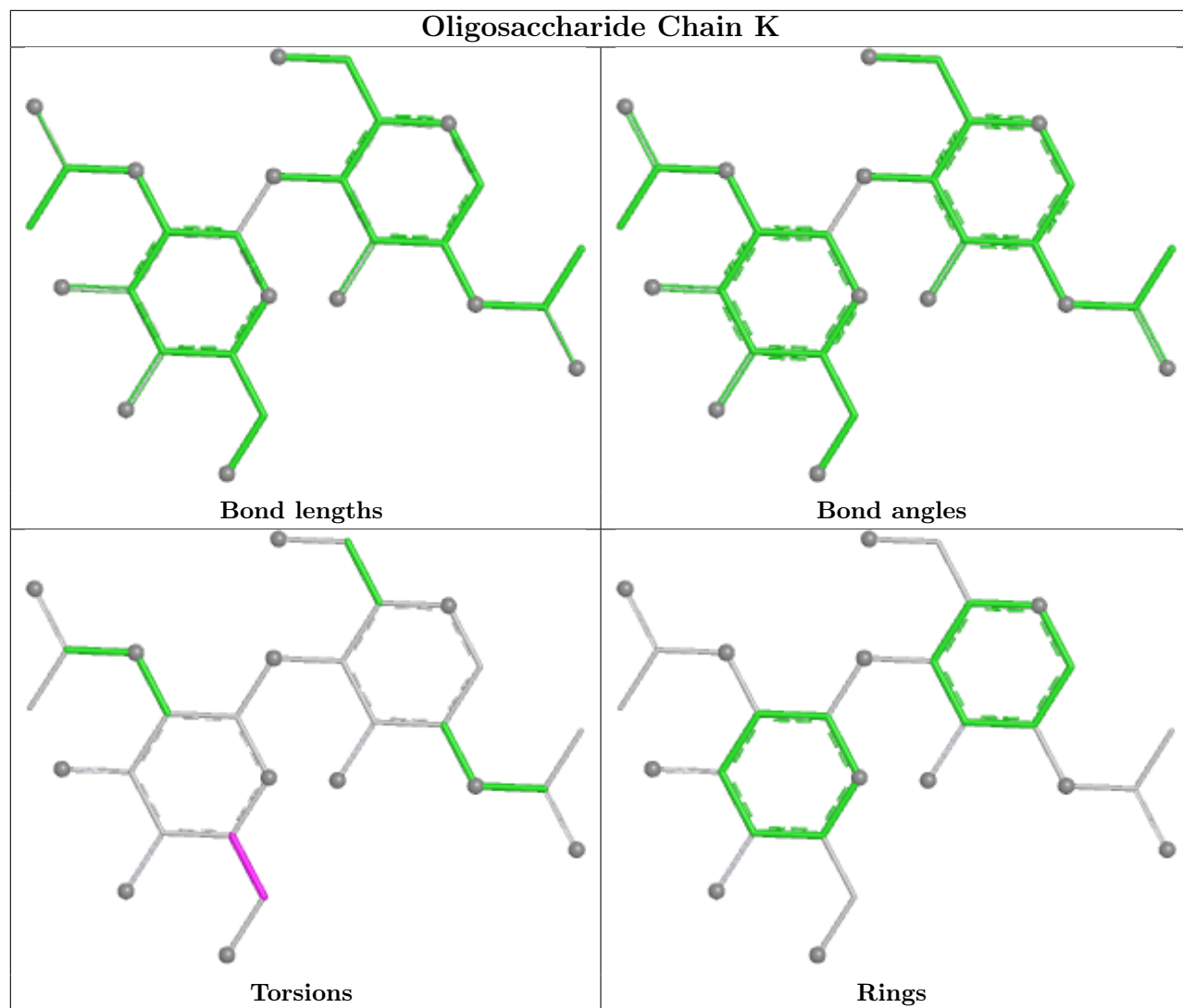


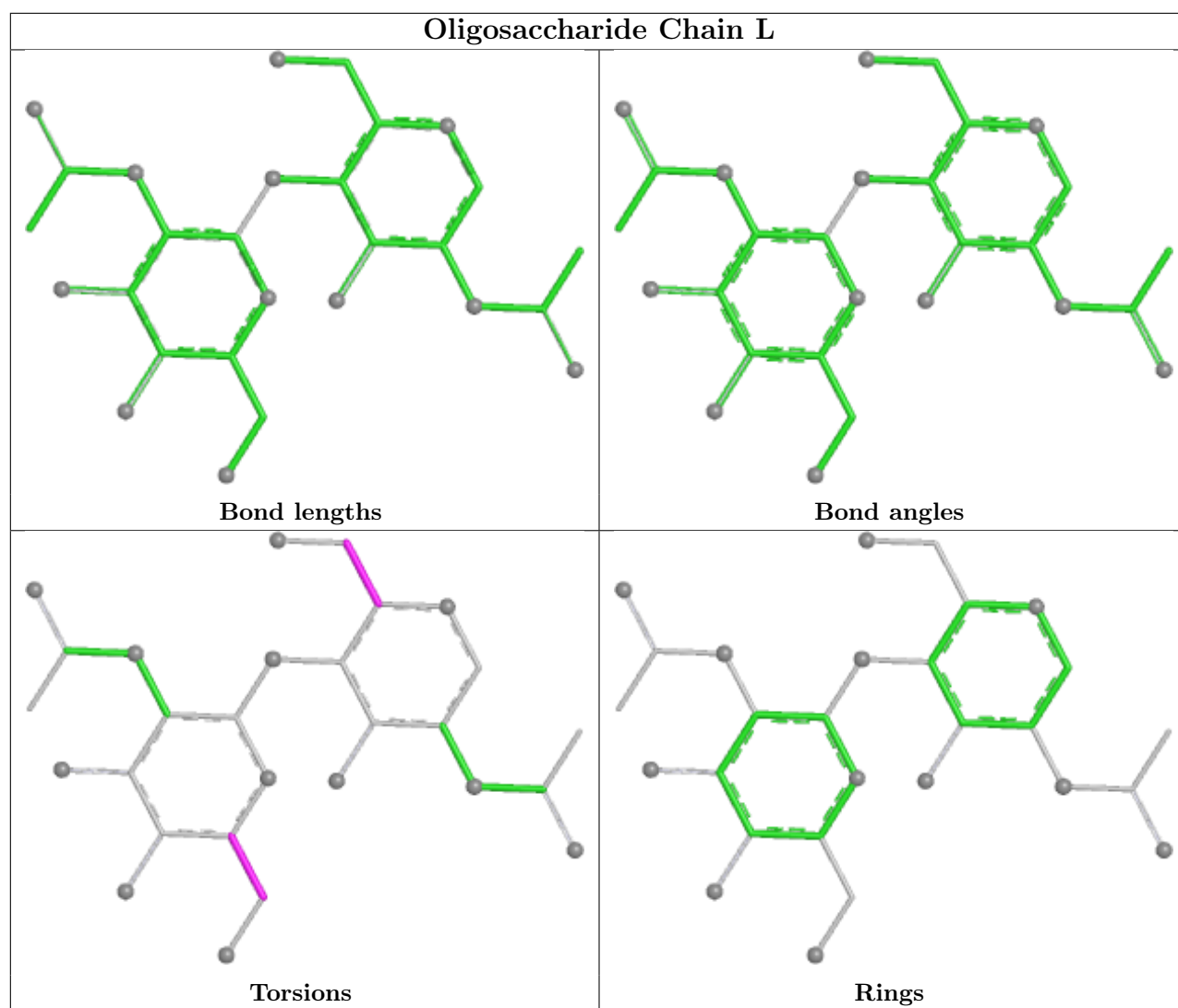


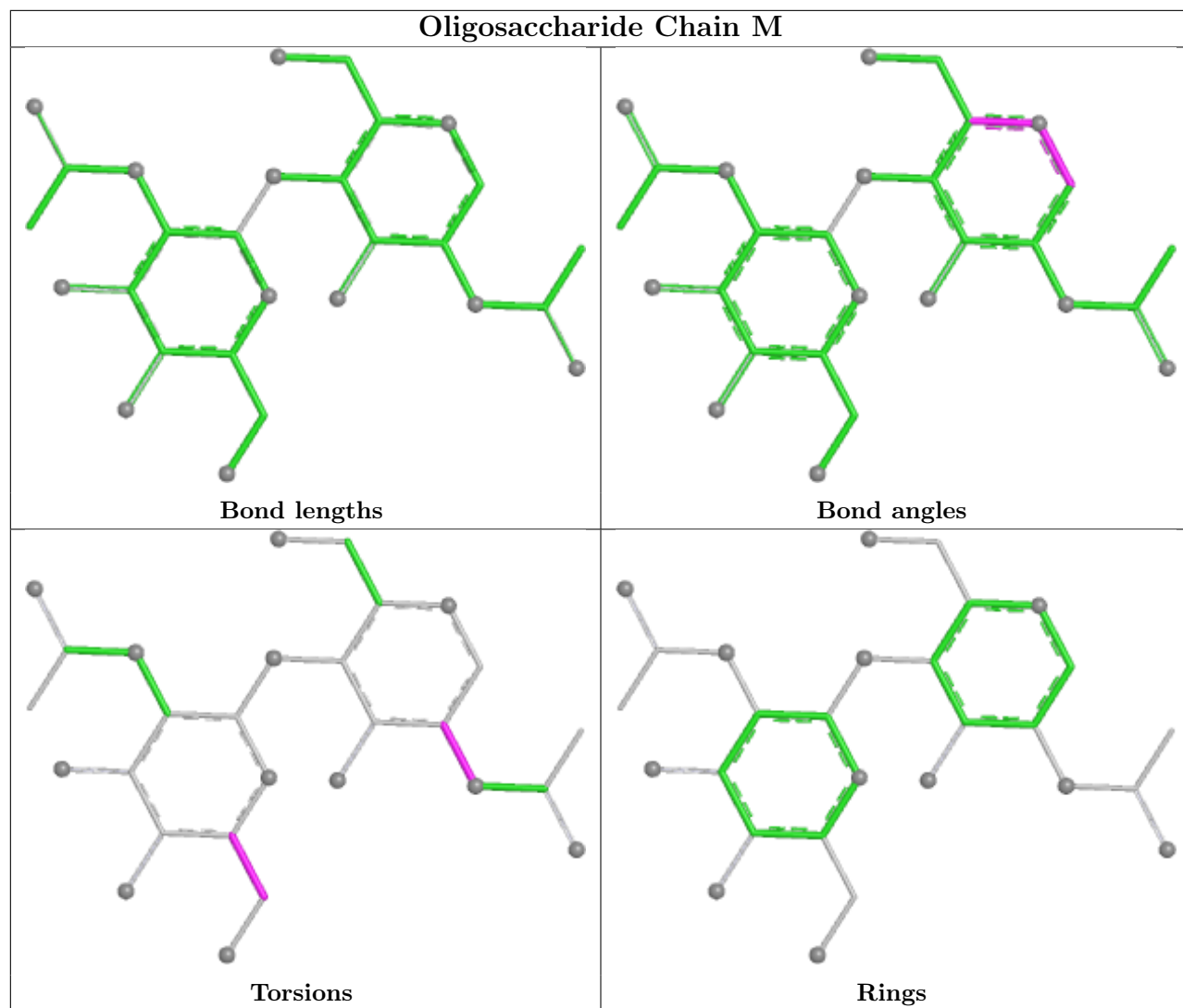


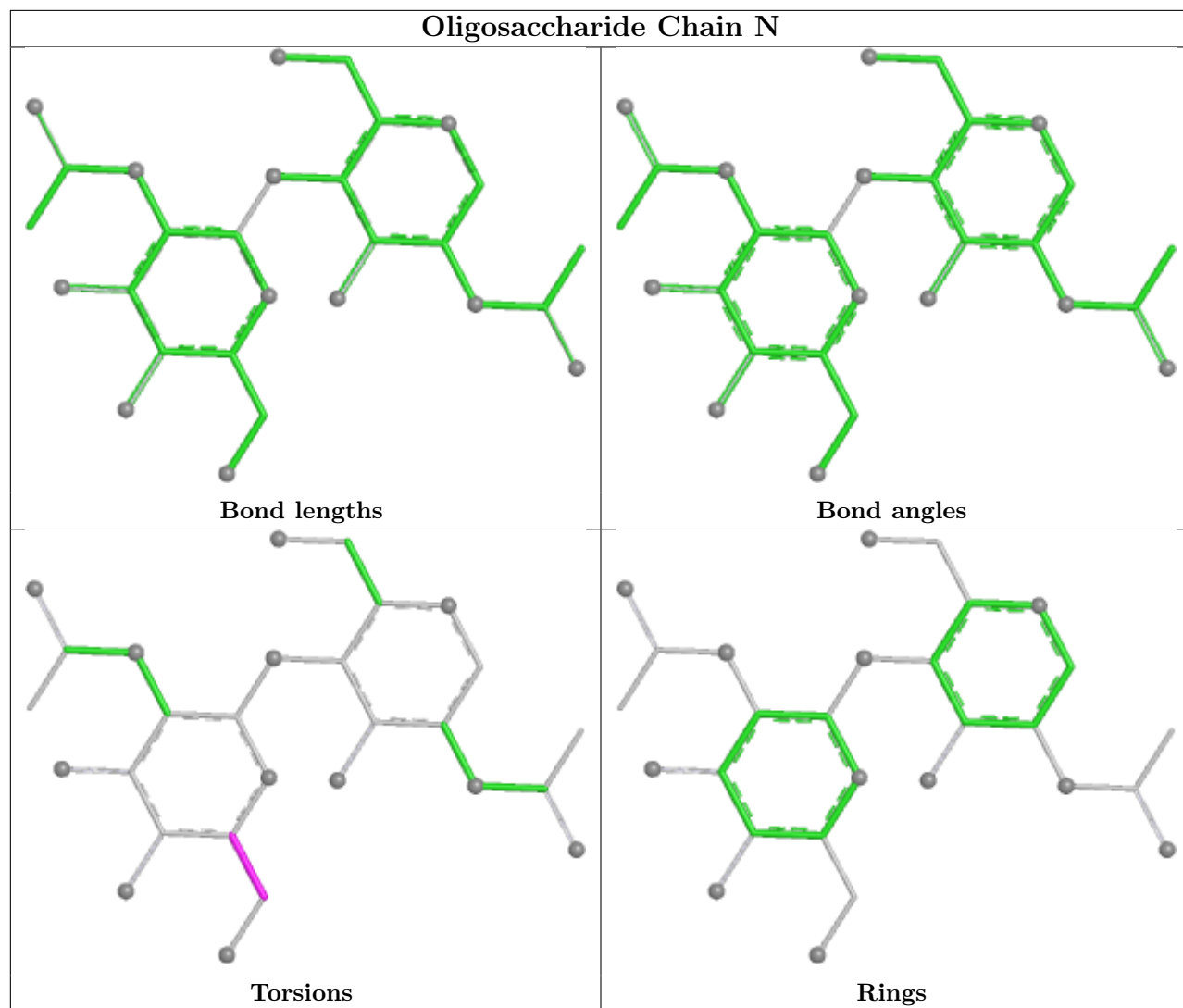


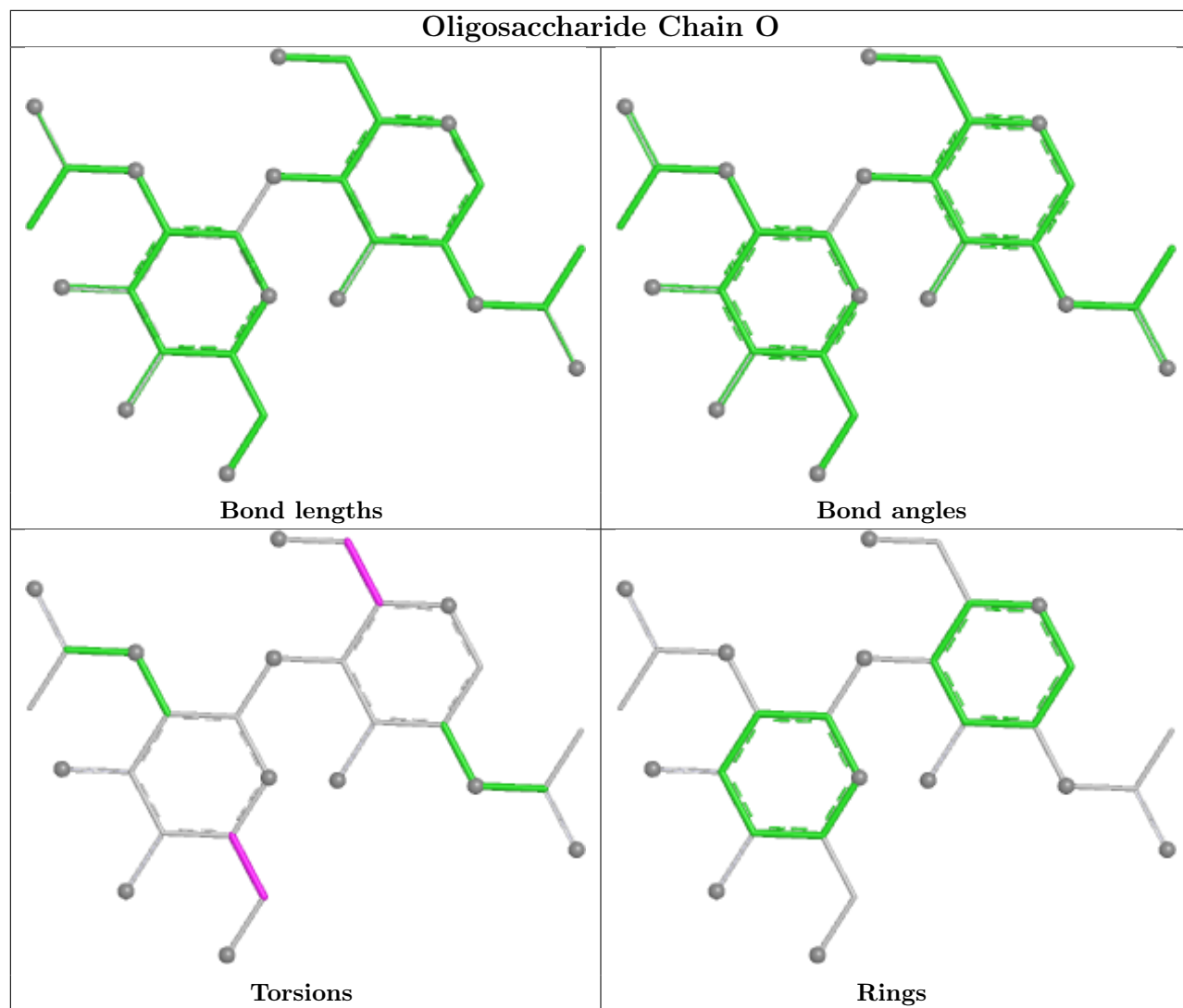


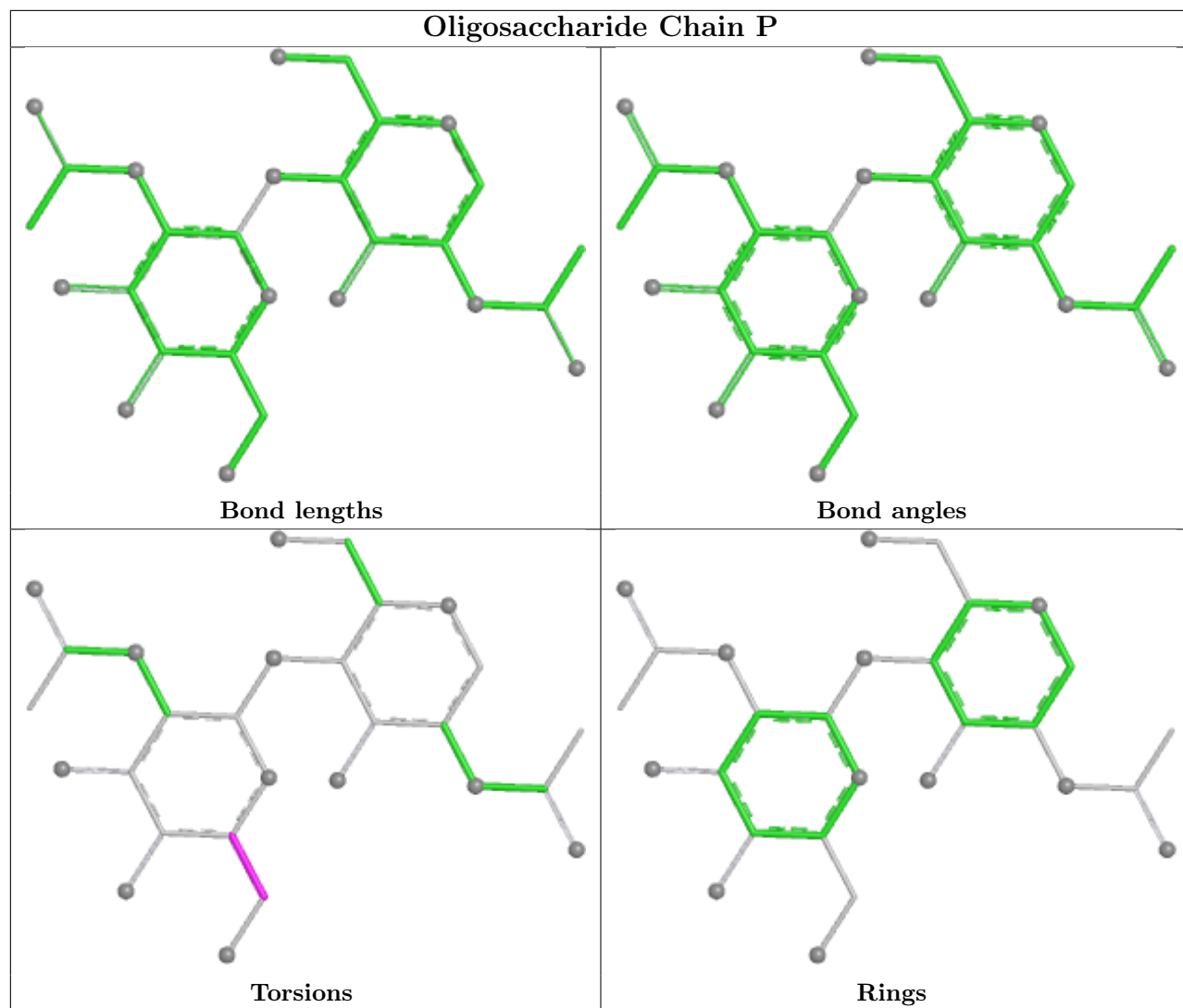


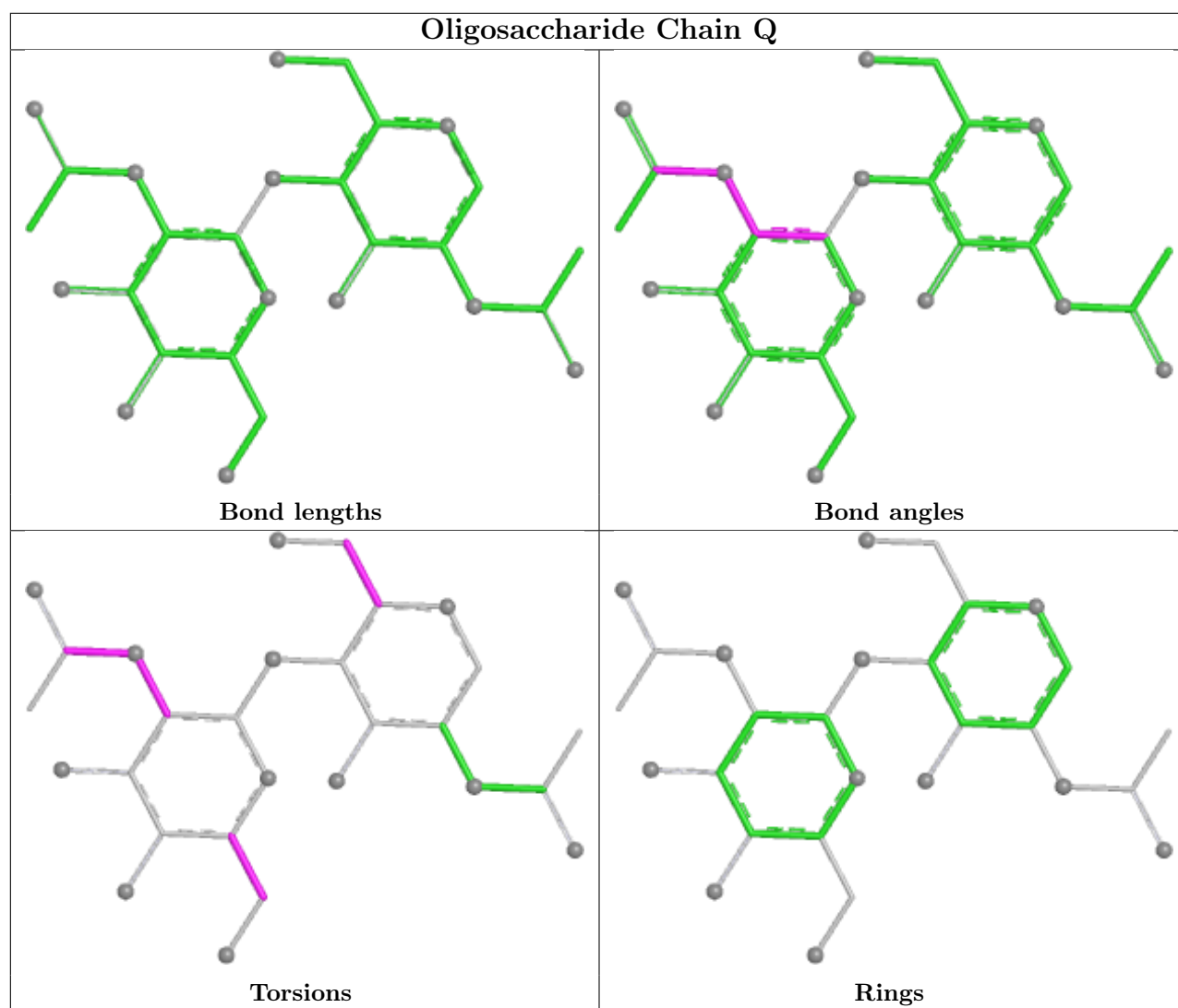


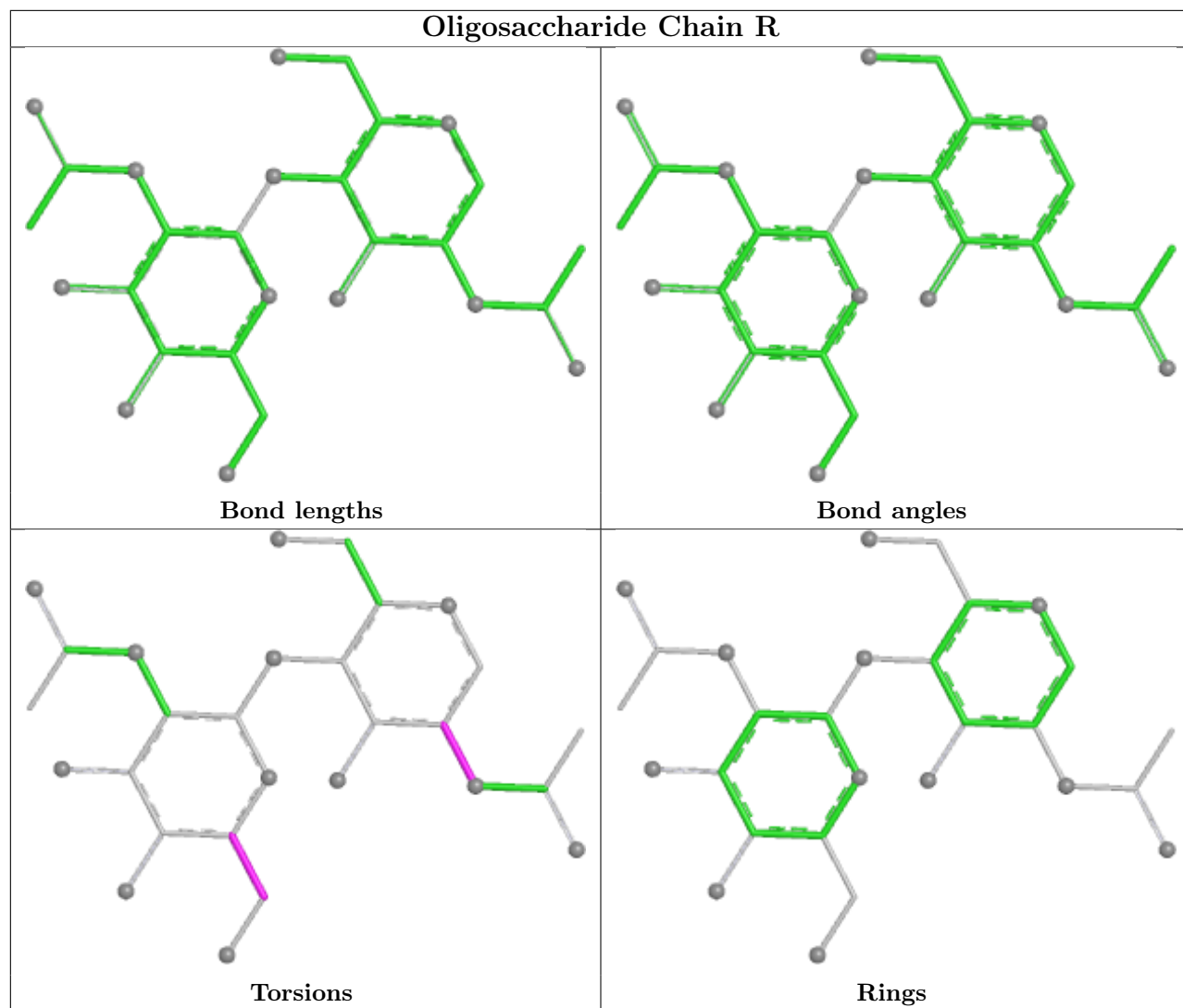


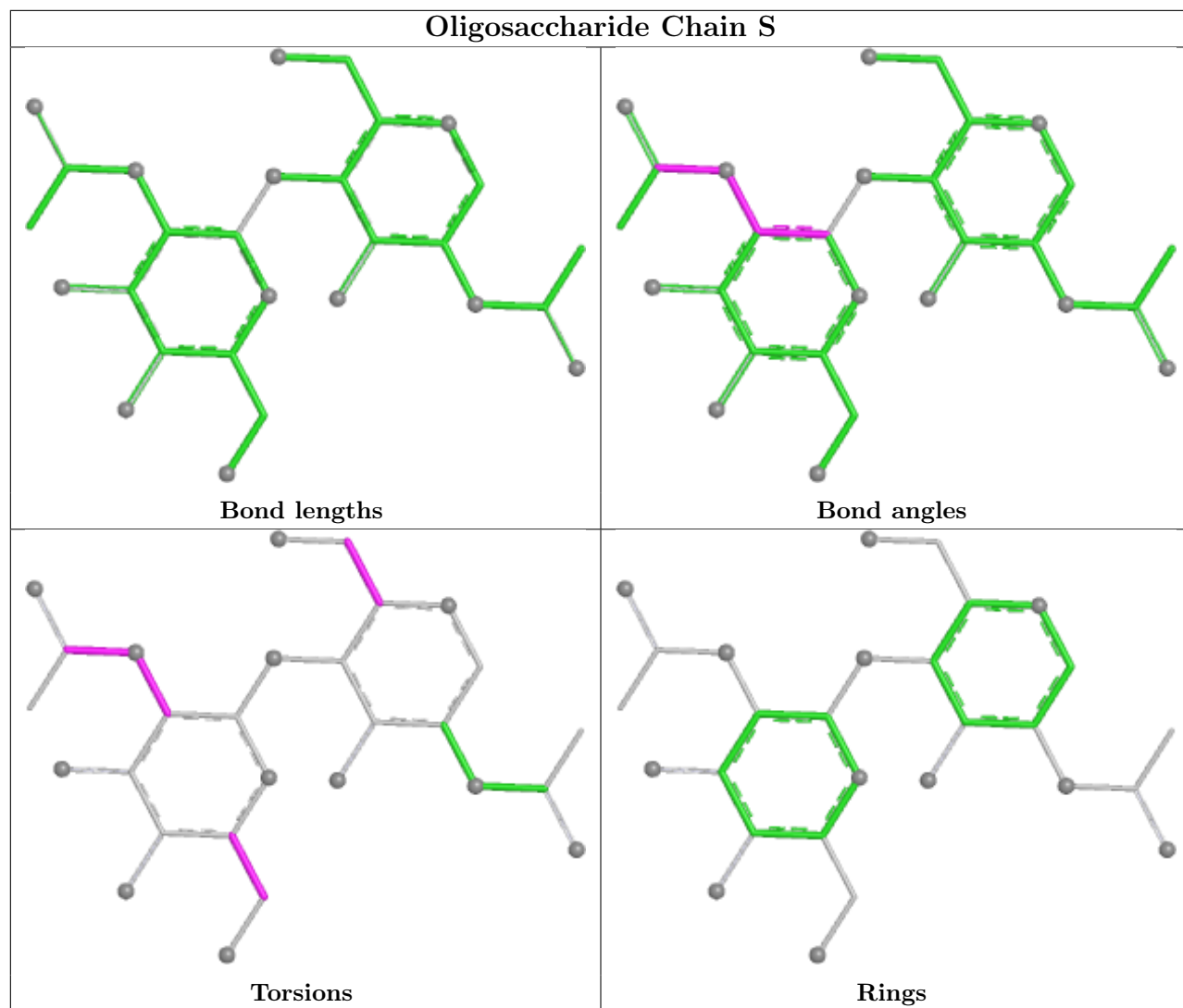


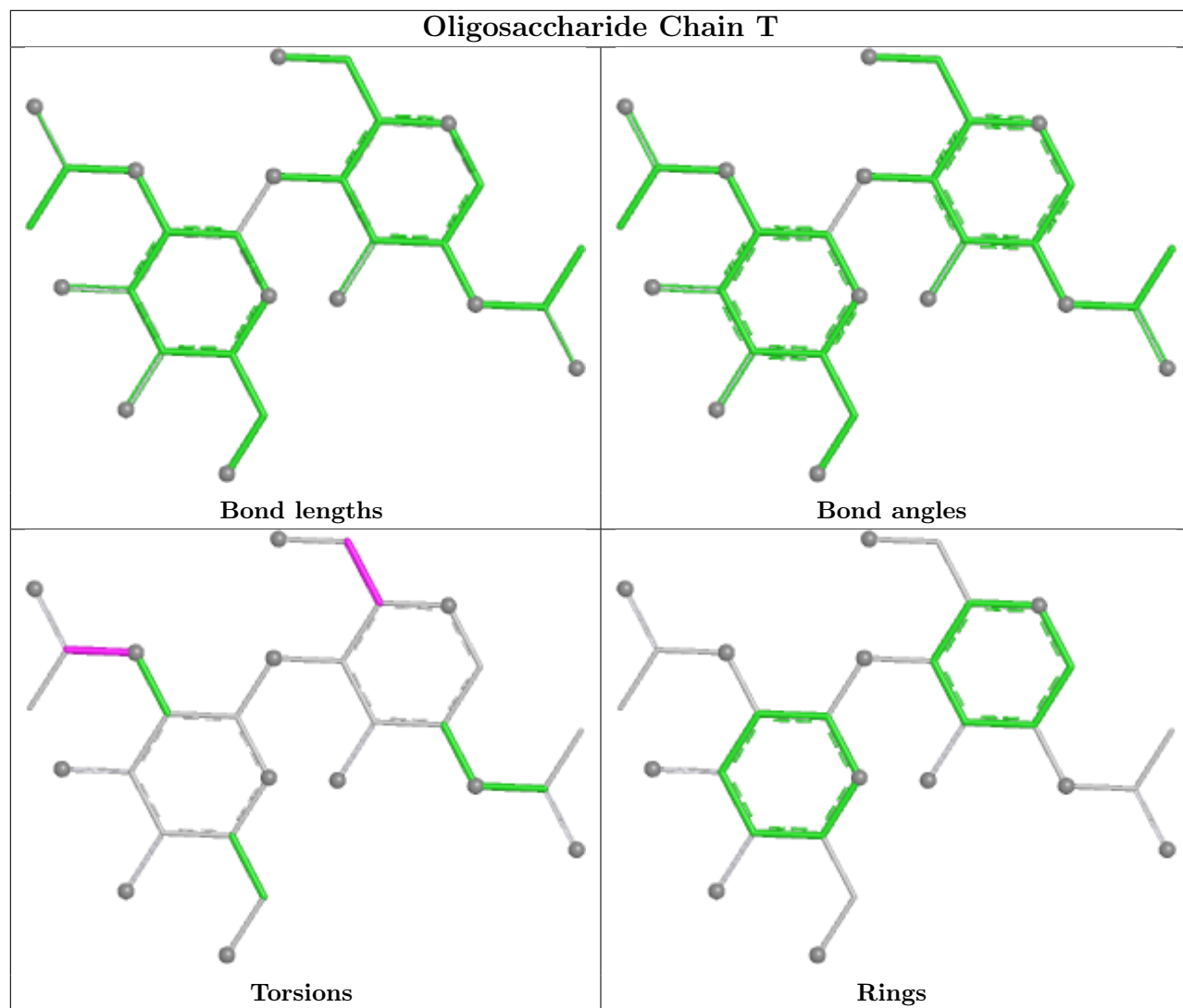


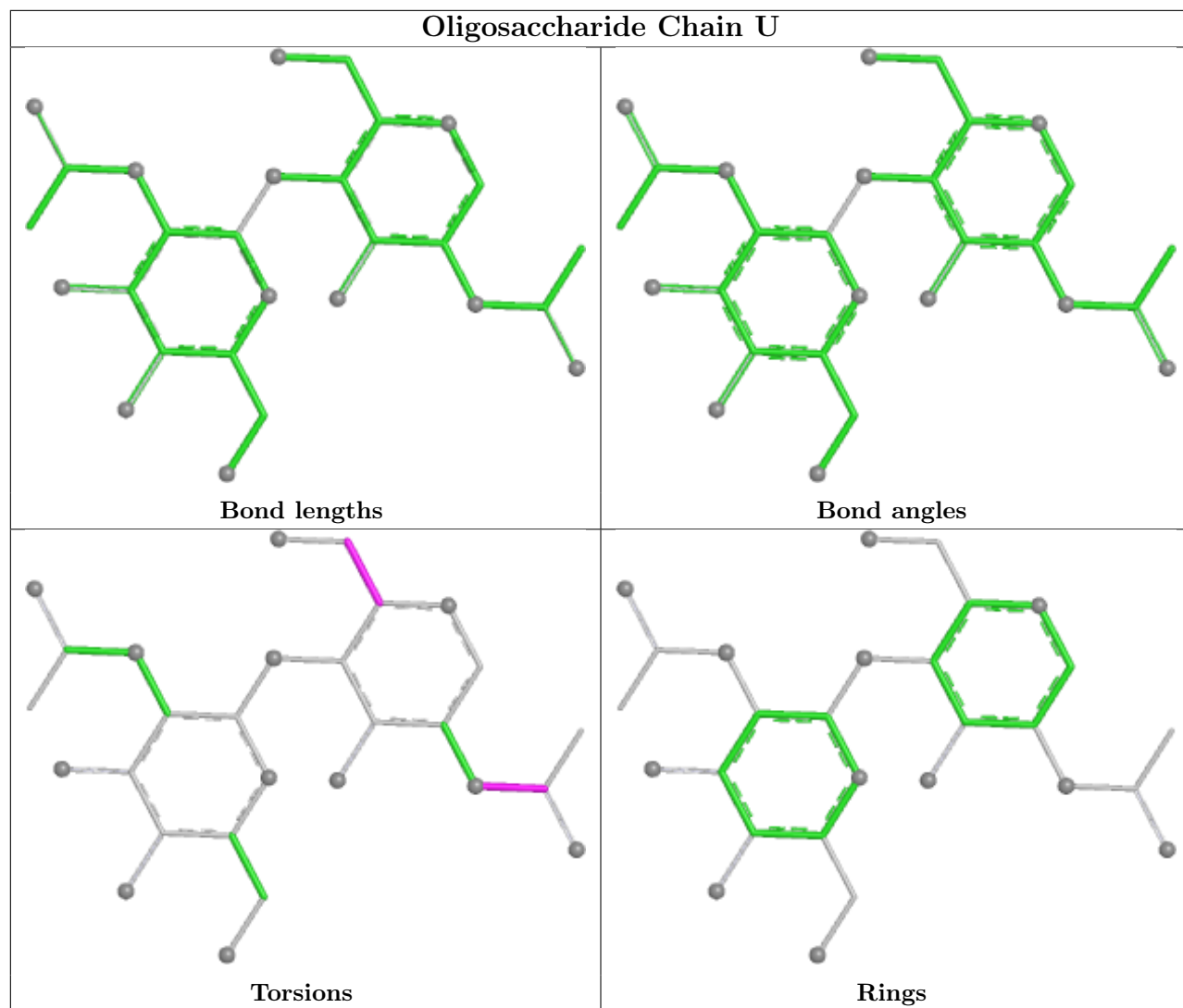


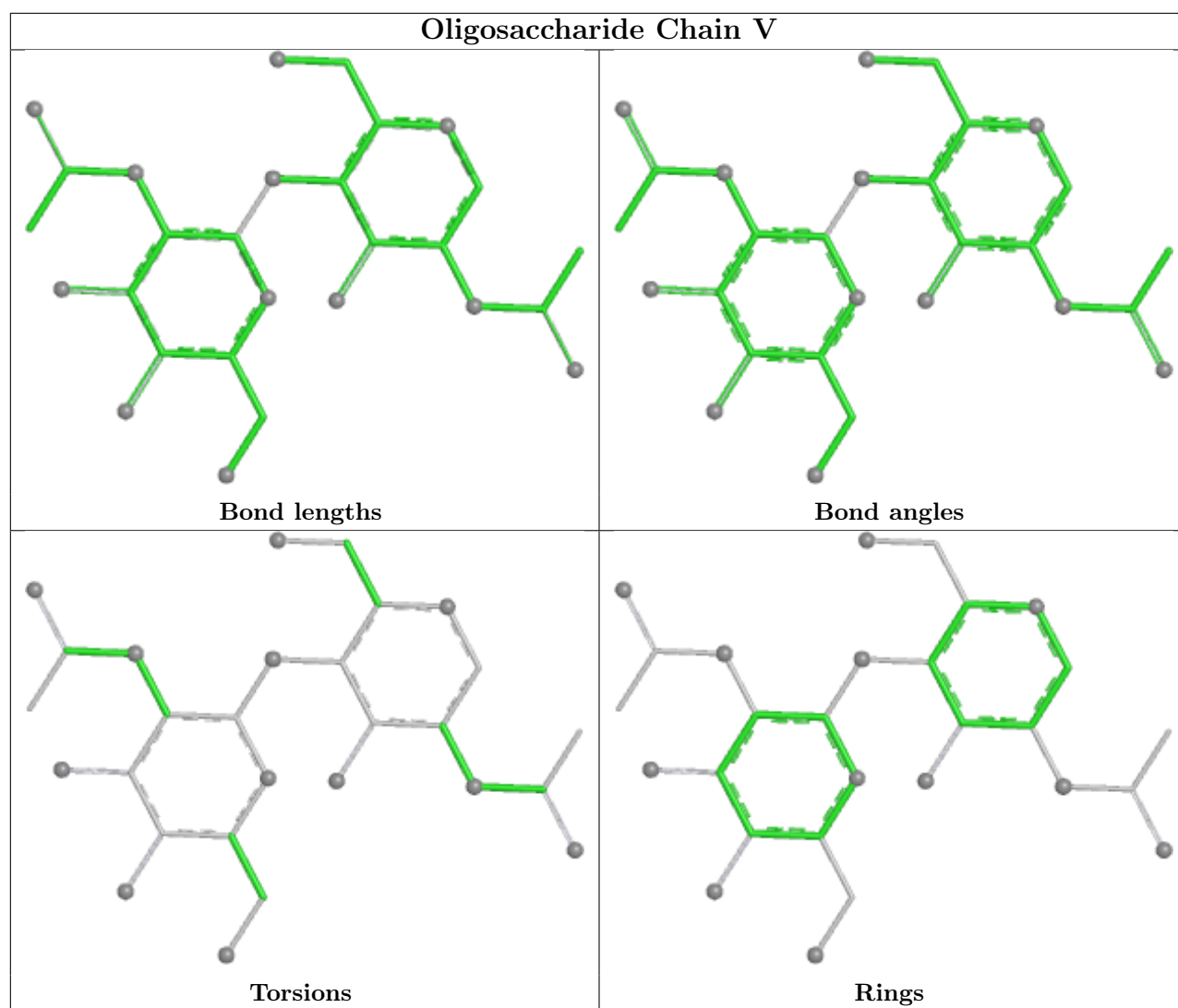


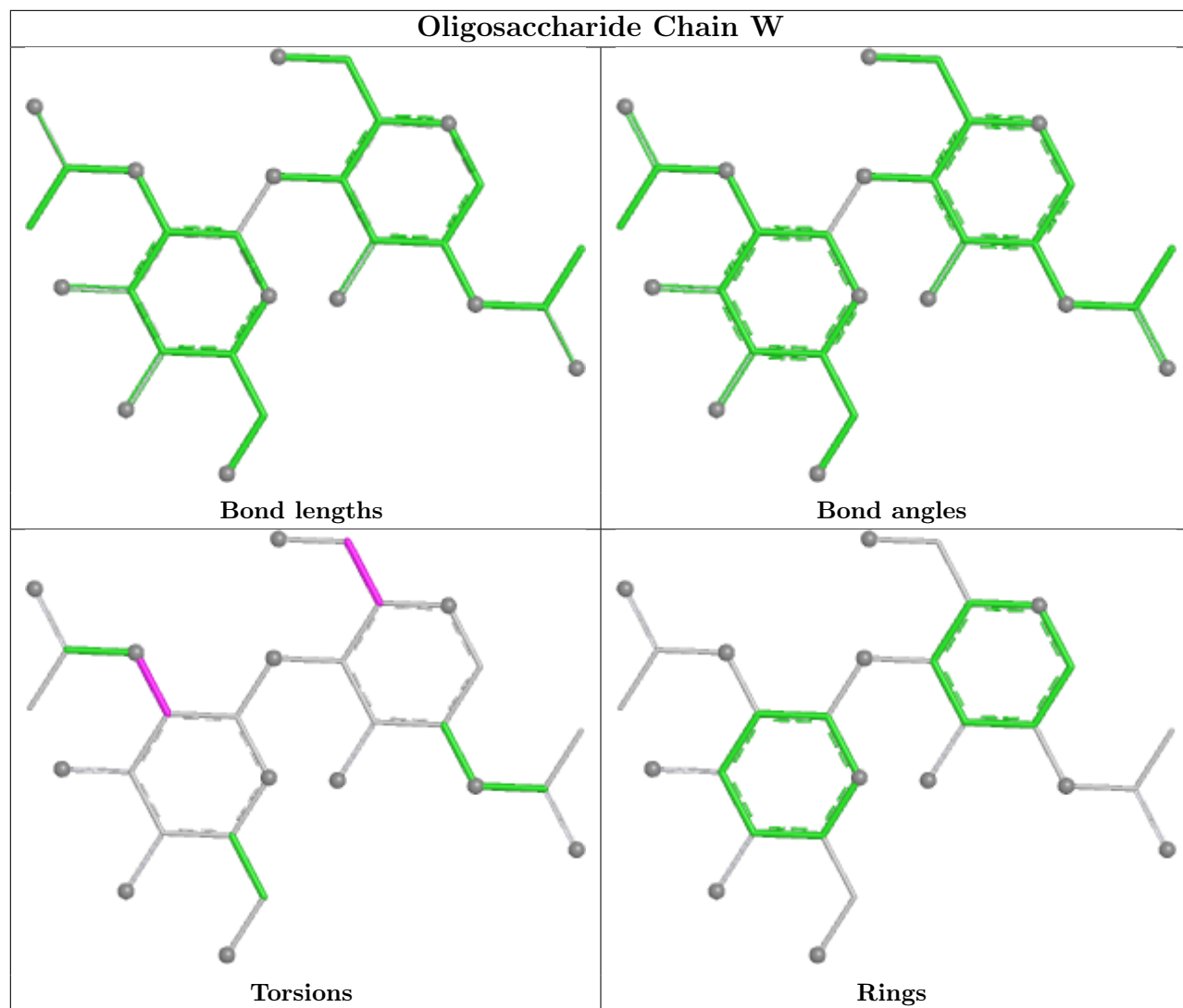


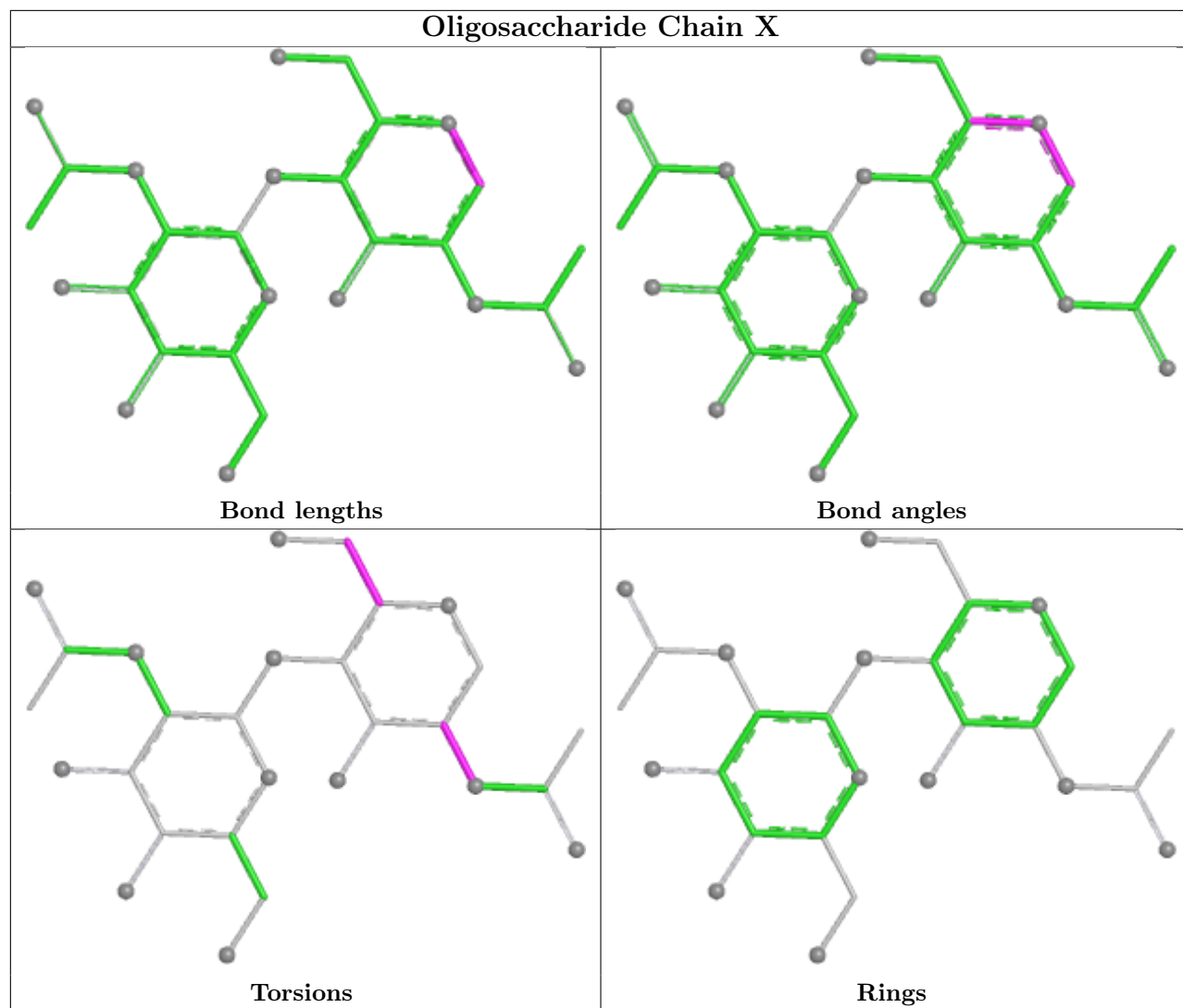


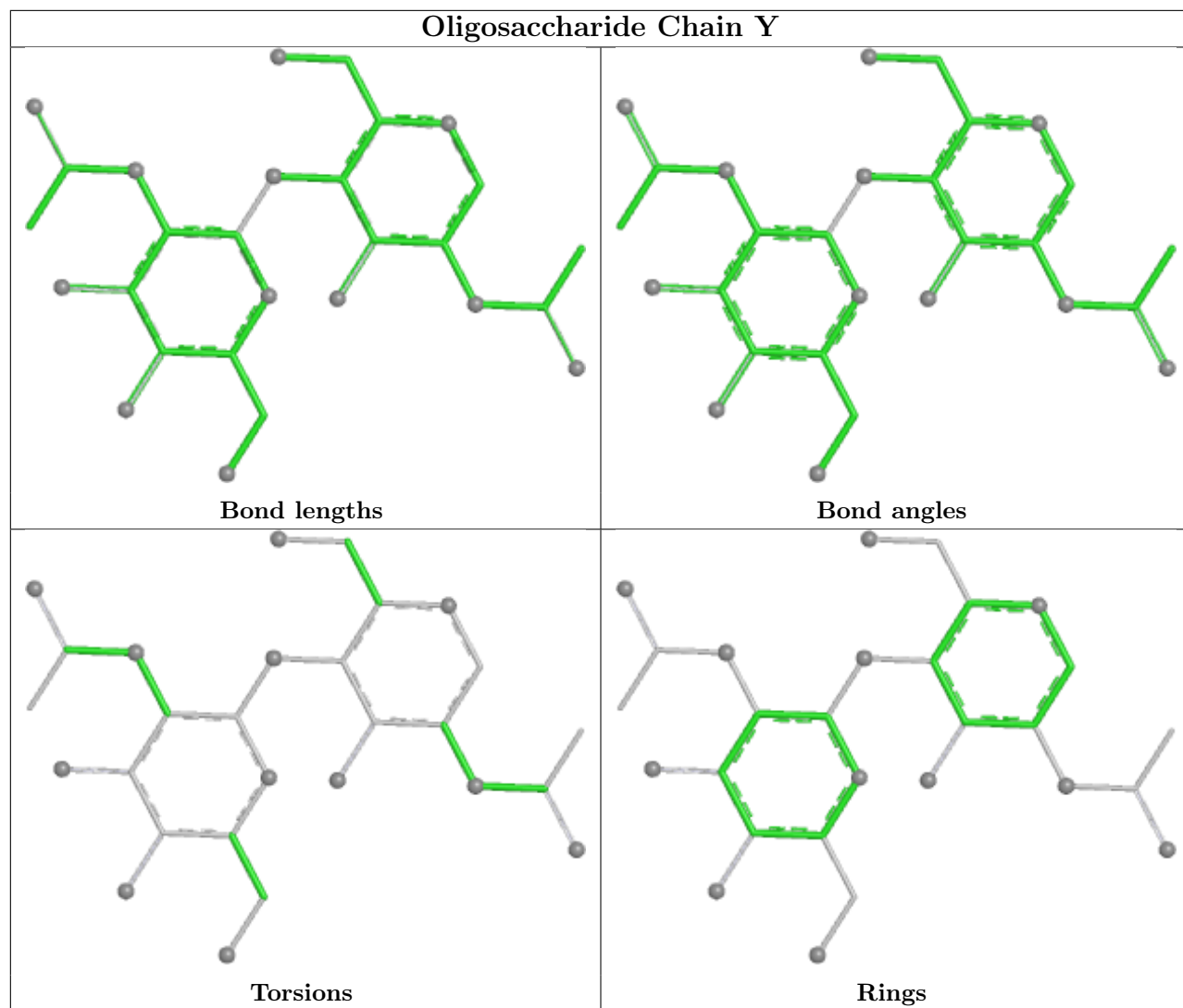


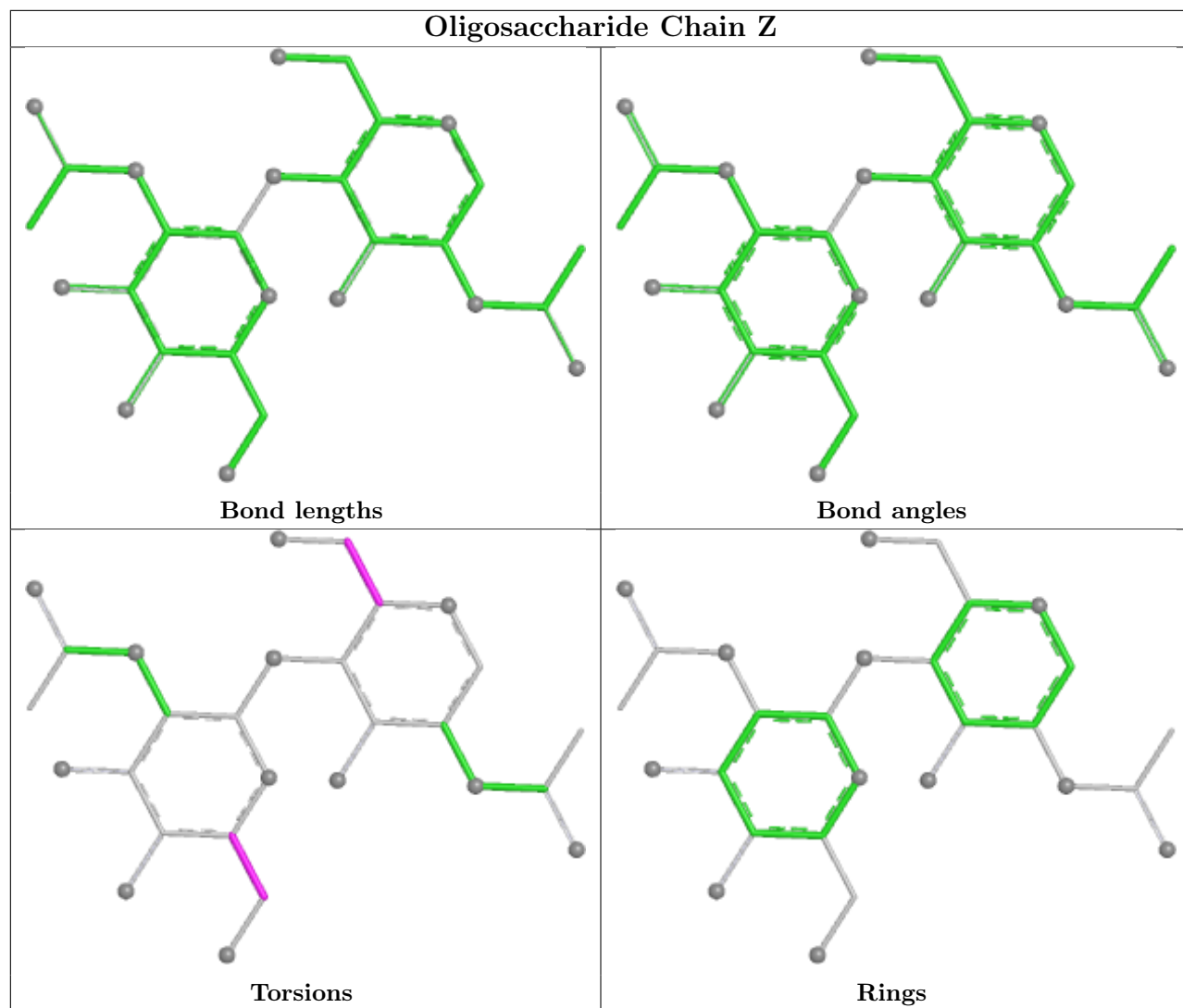


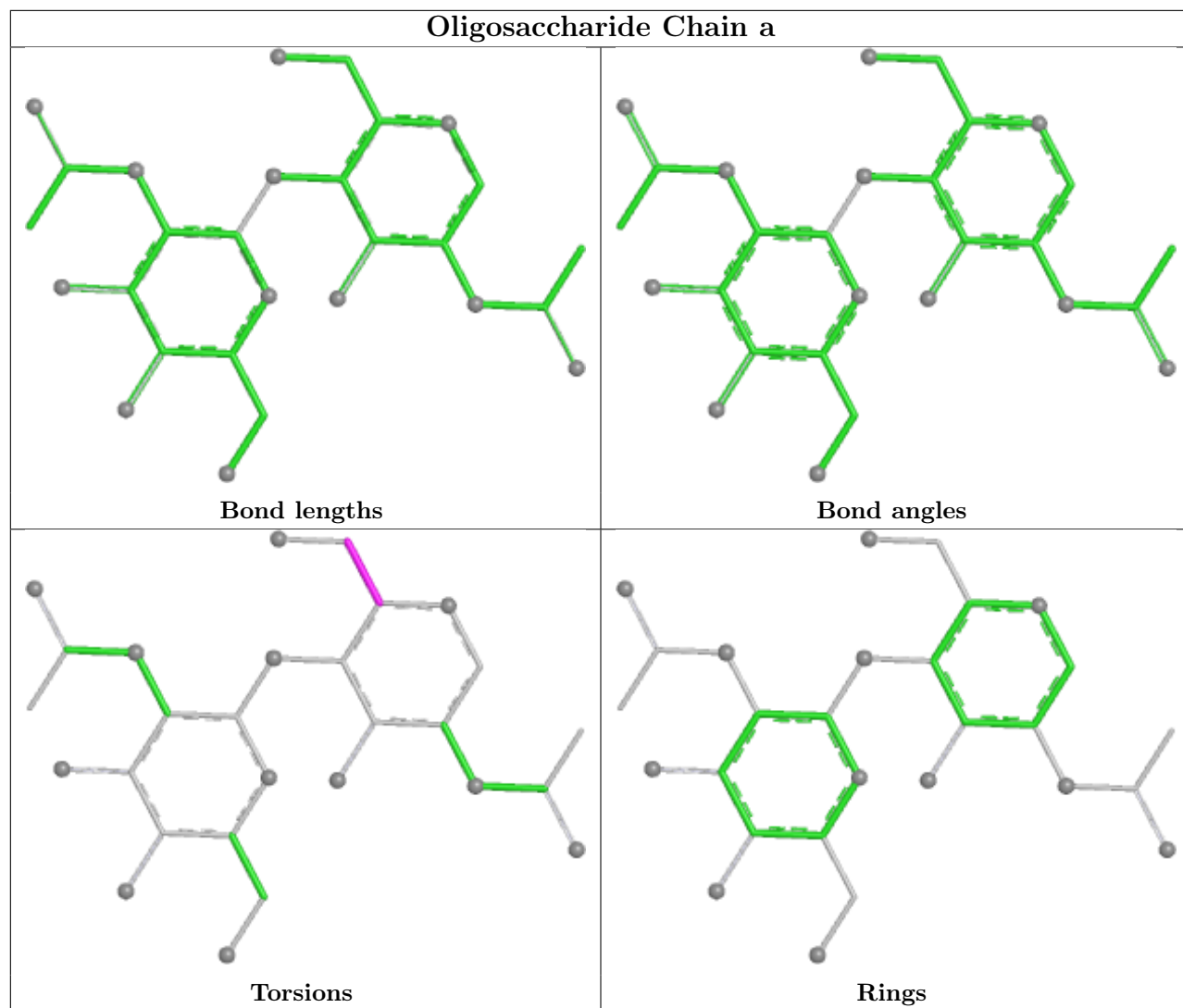


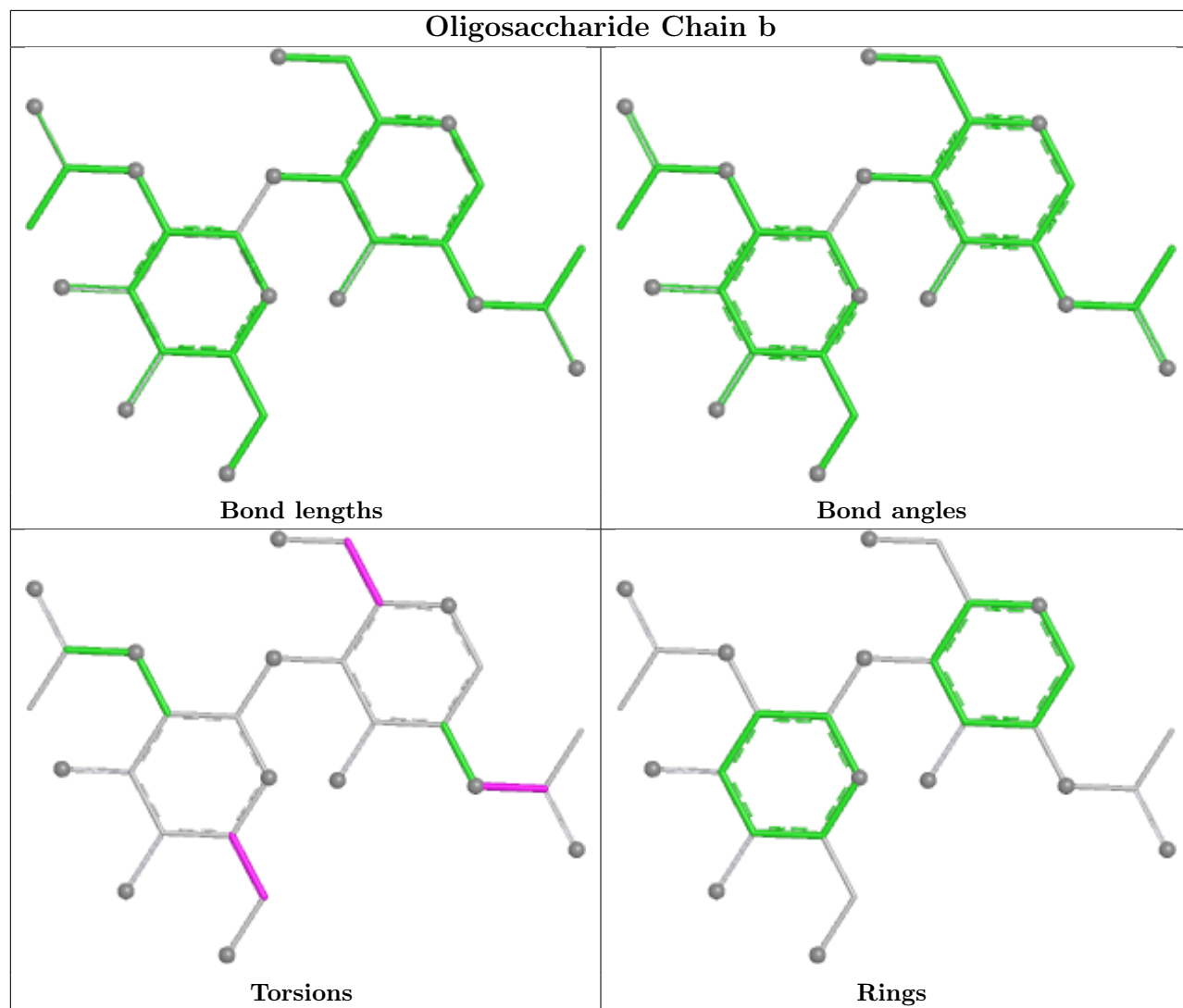


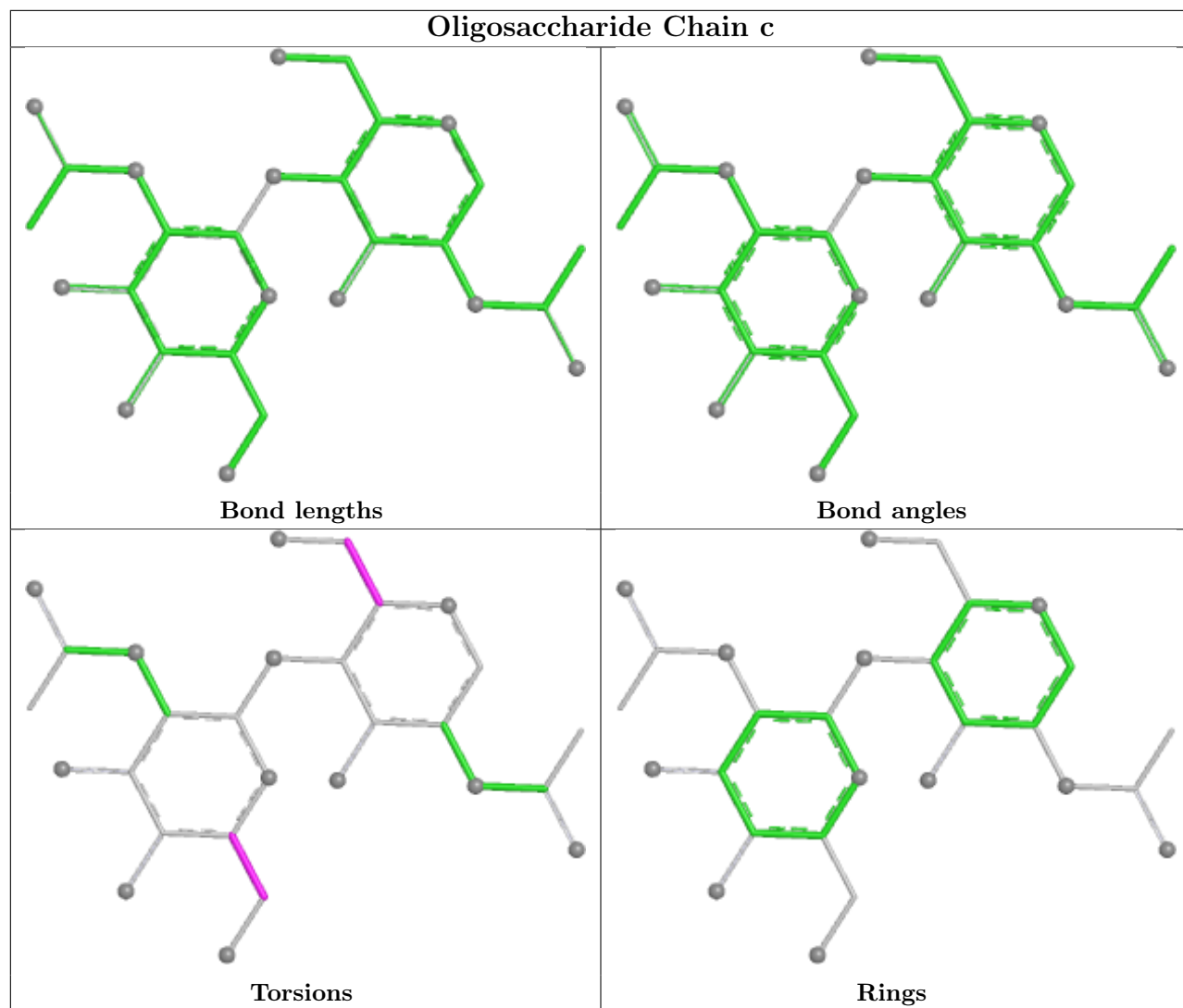


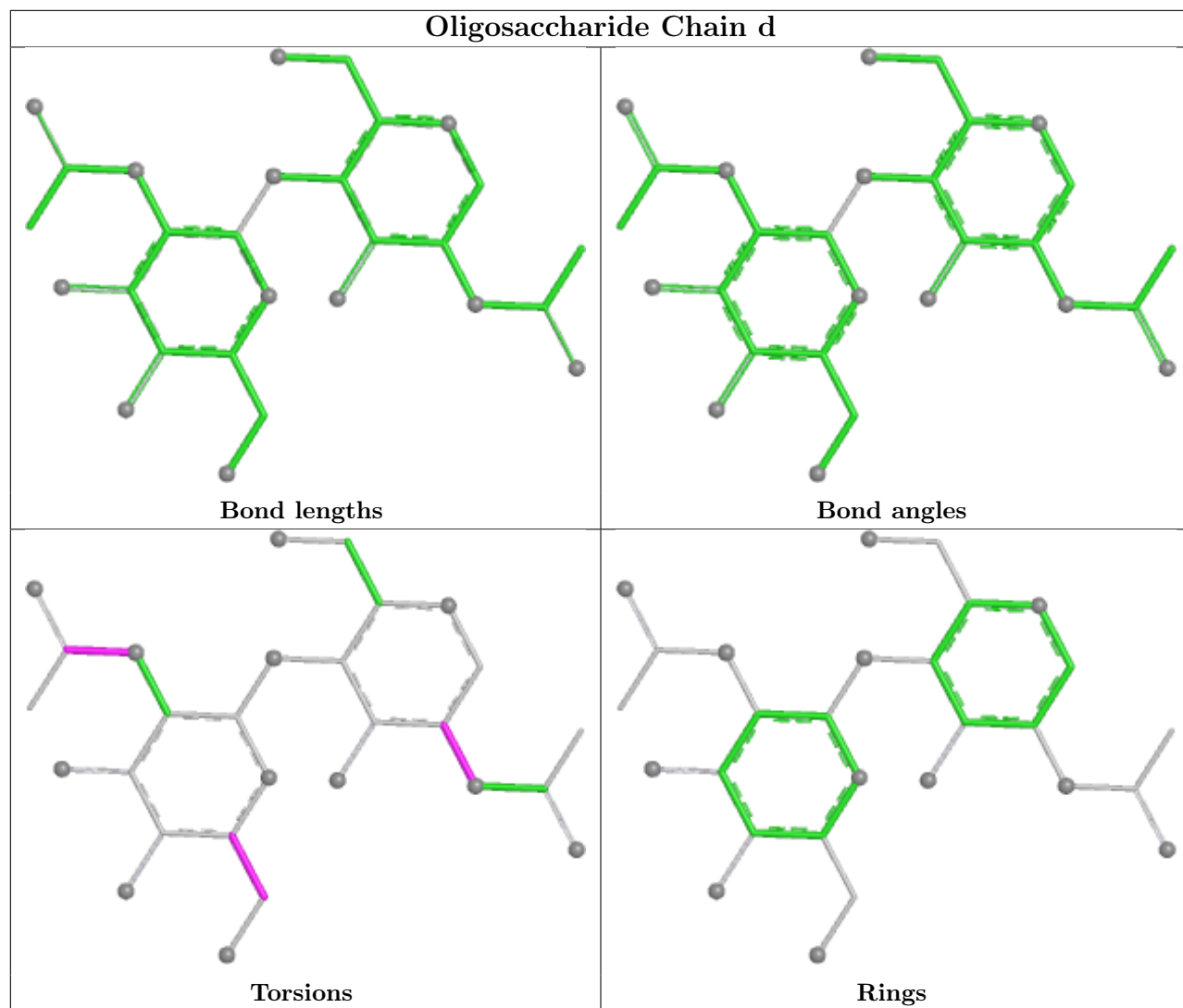


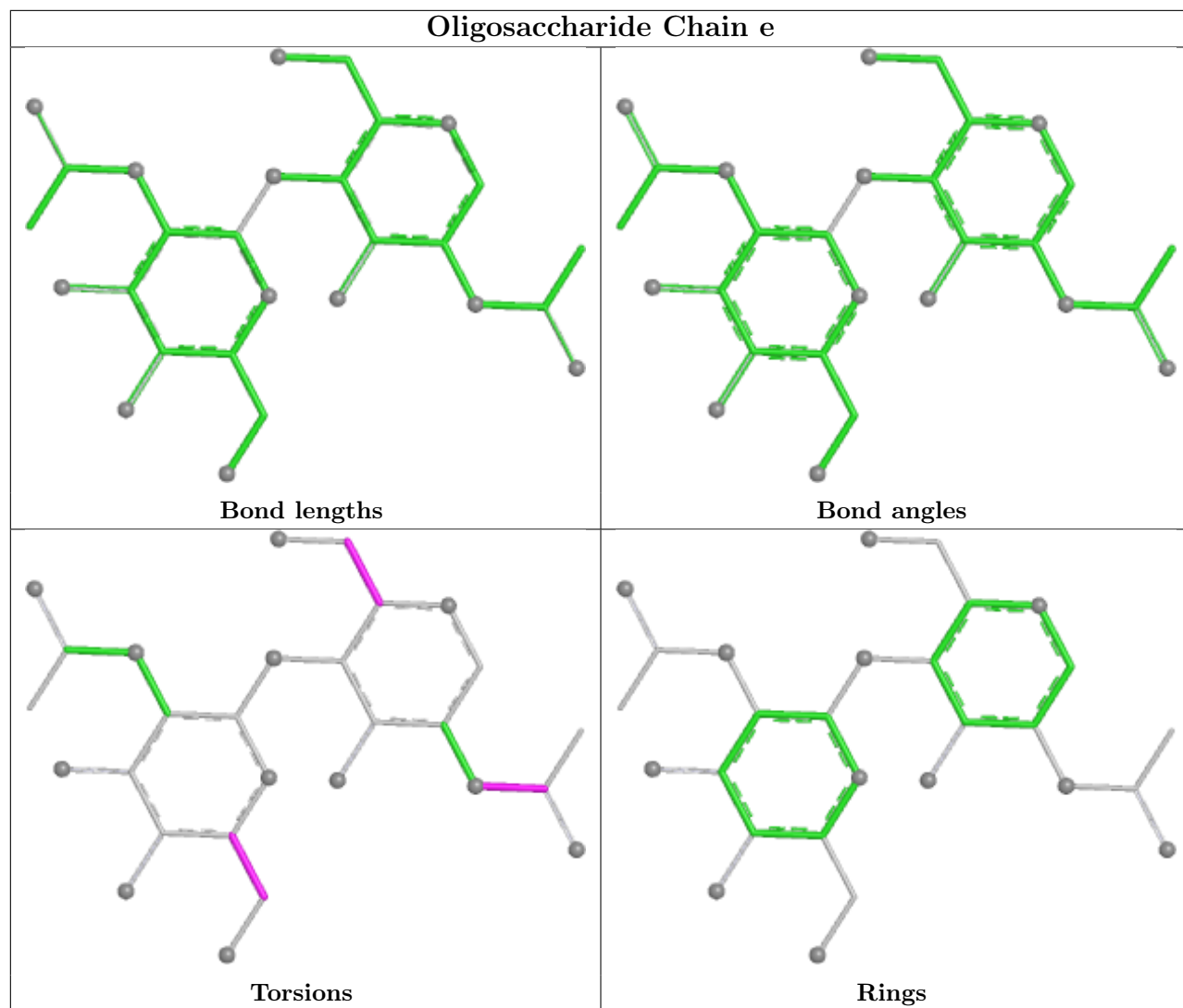


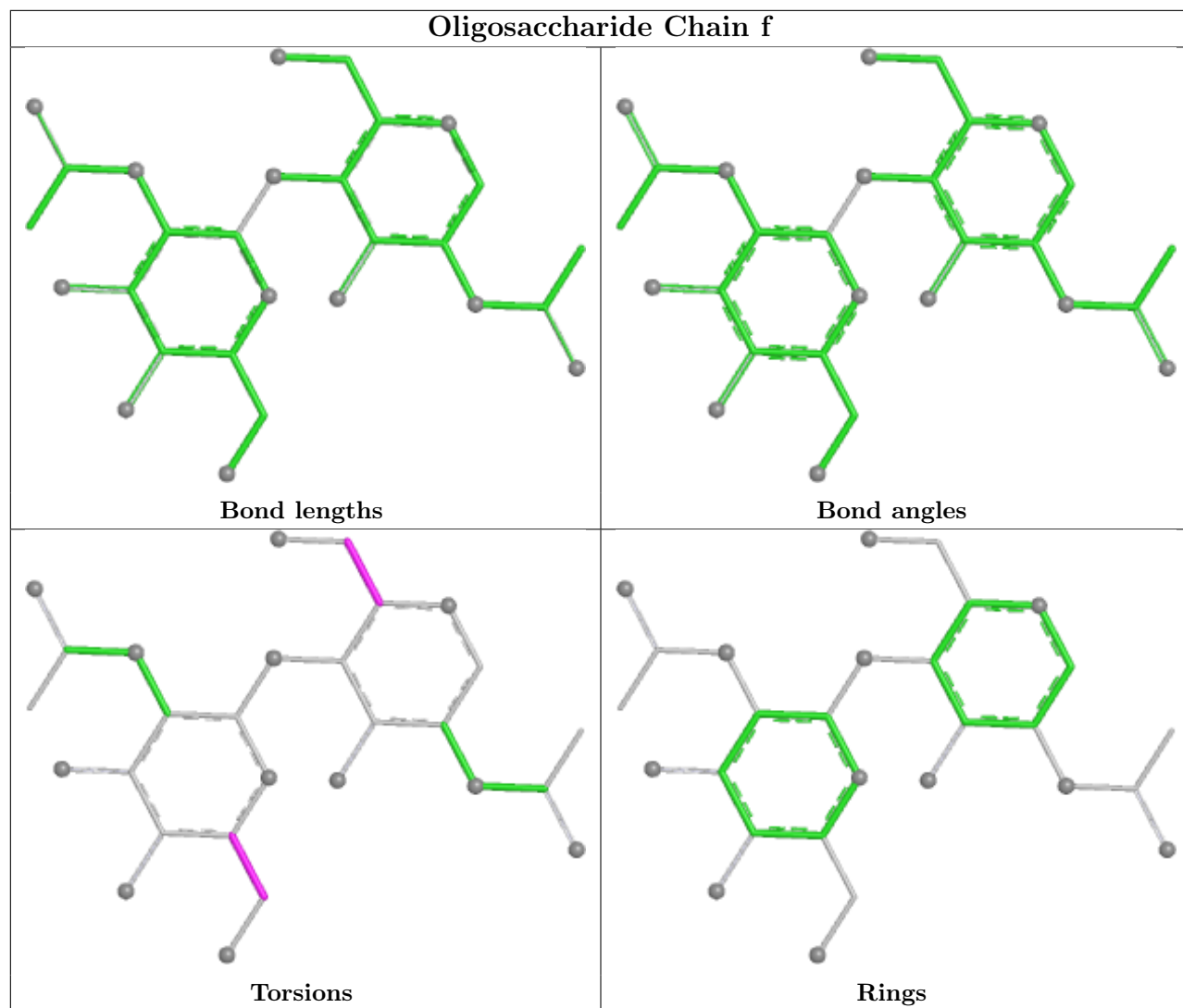


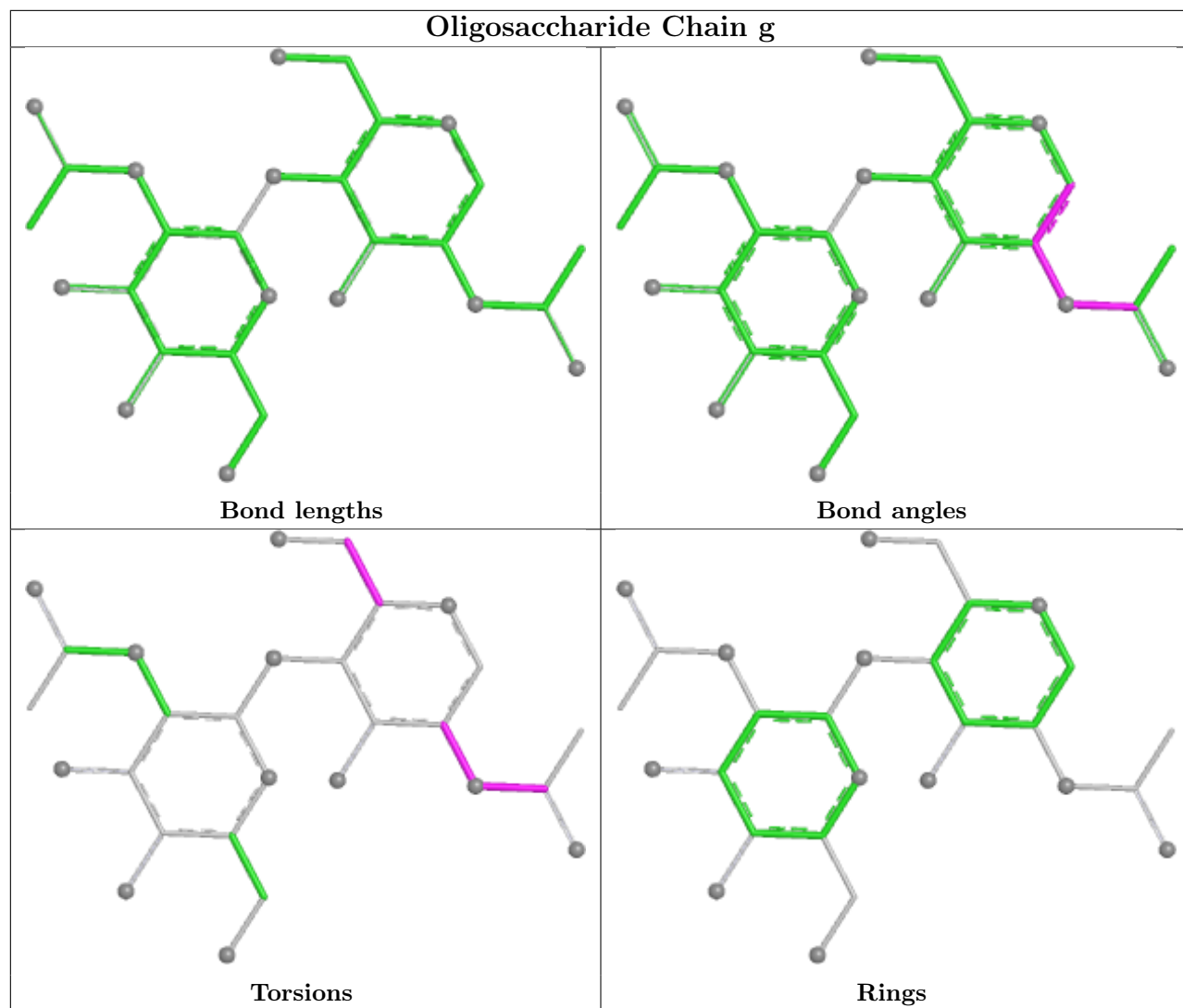


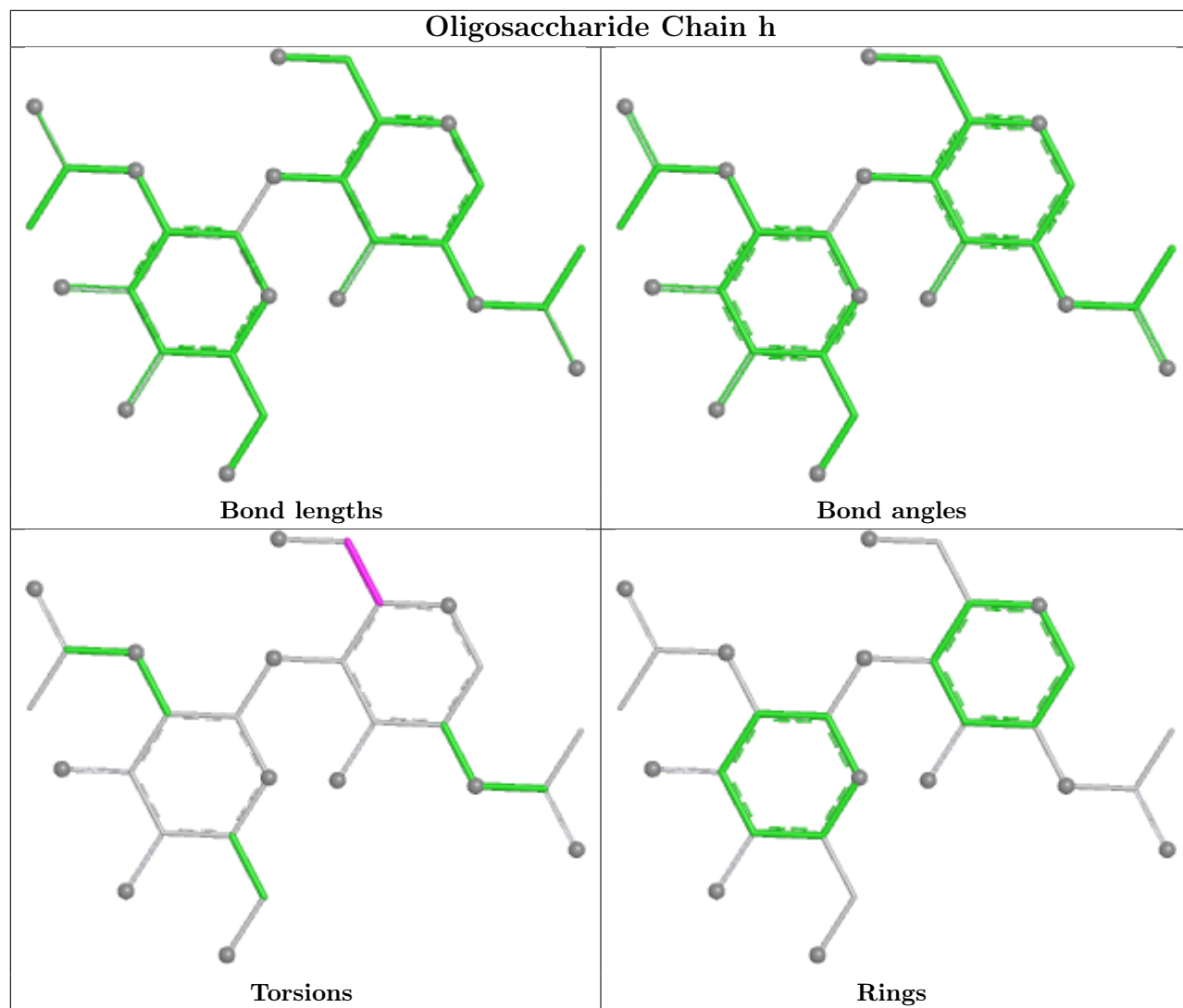


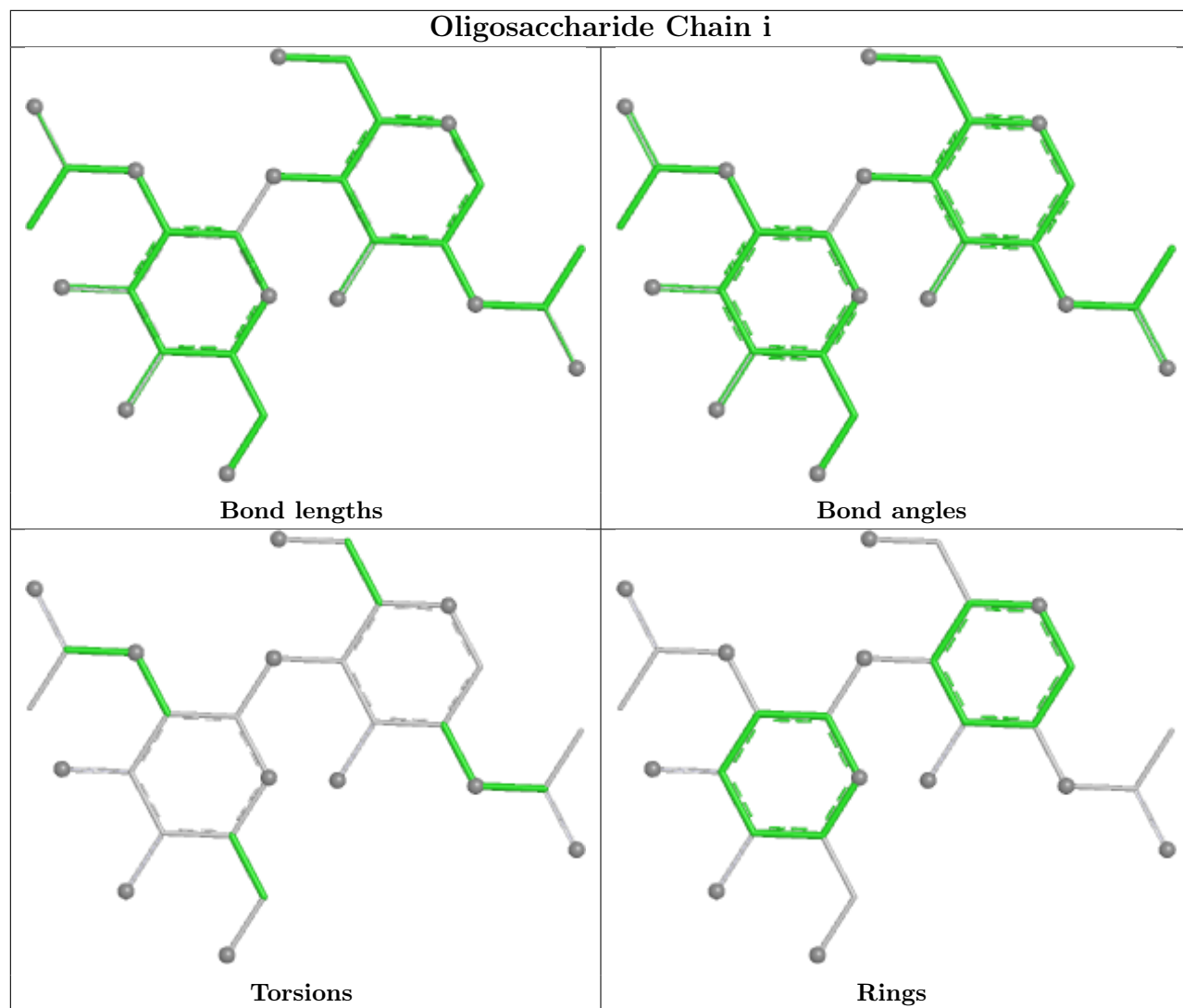


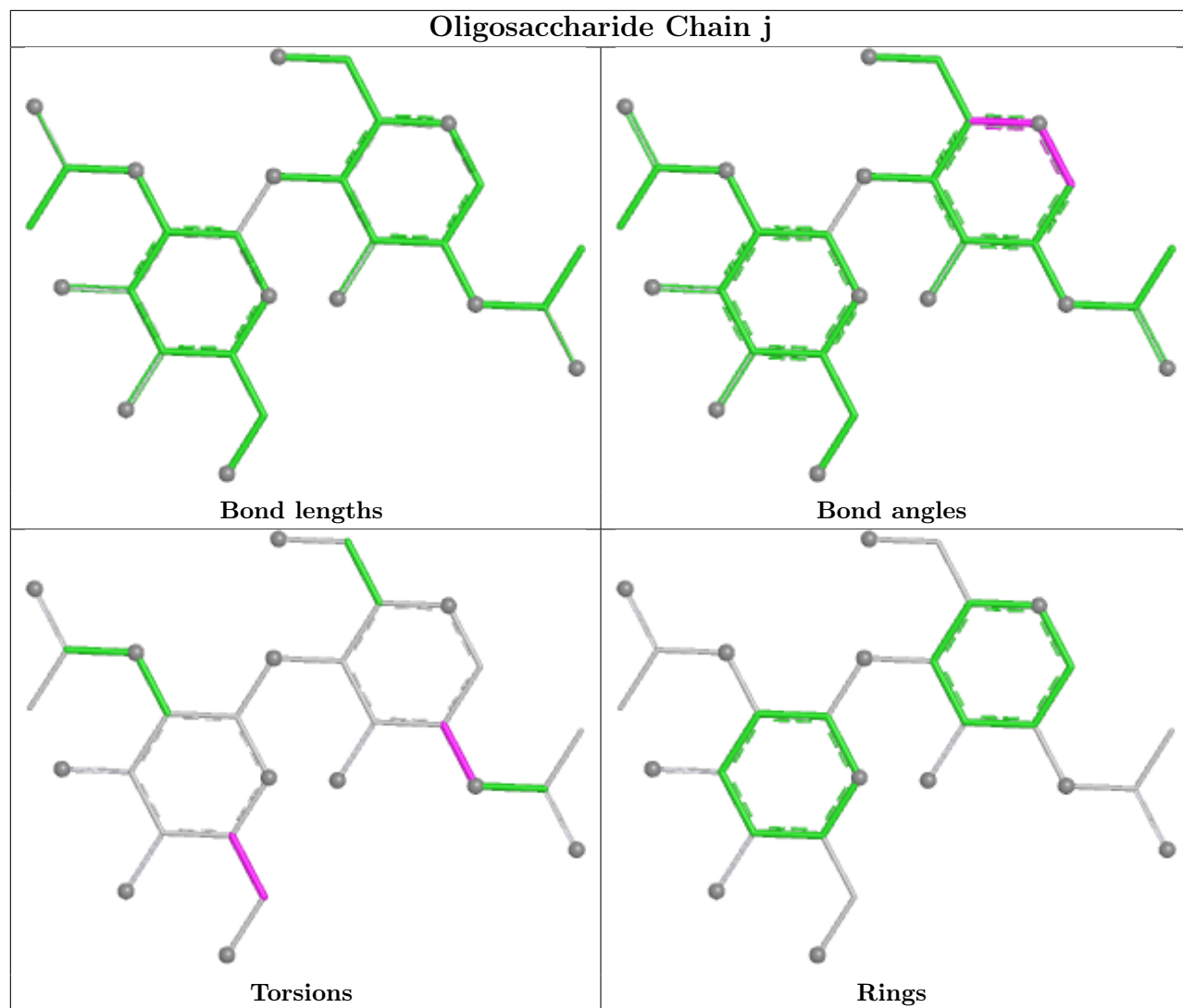


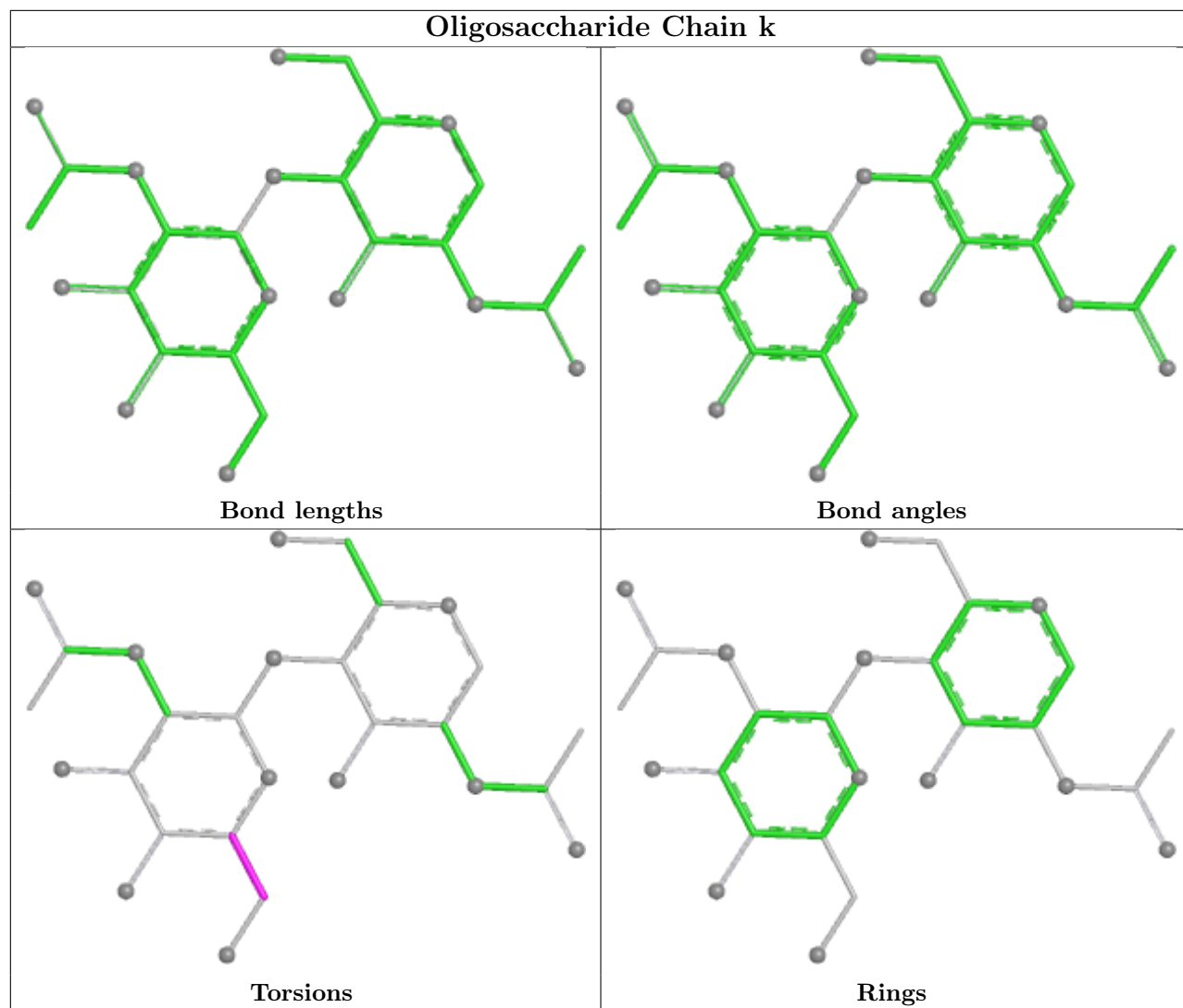


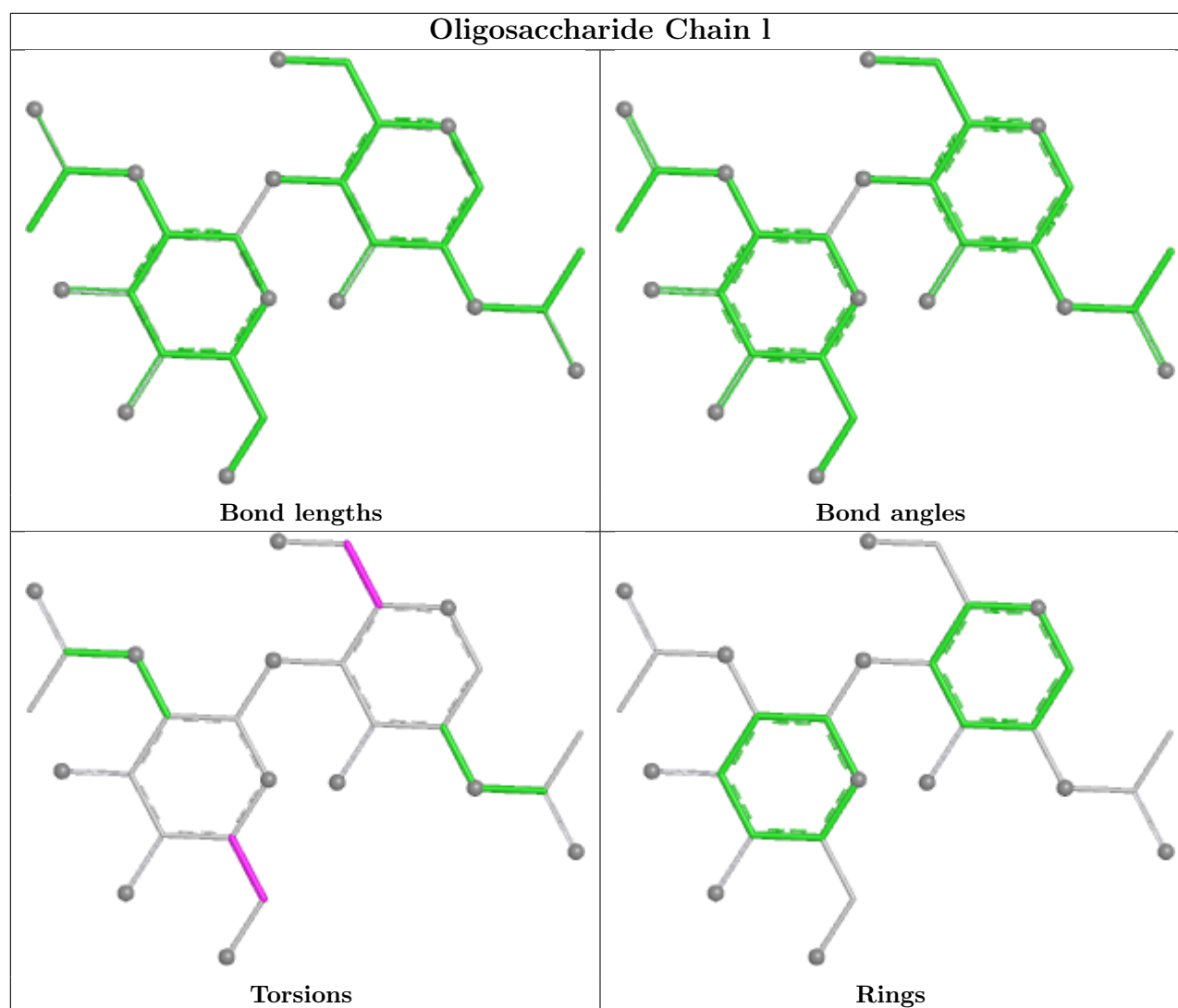












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NAG	B	2003	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	2003	1	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	C	2002	1	14,14,15	0.17	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	2002	1	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	B	2001	1	14,14,15	0.32	0	17,19,21	0.38	0
3	NAG	C	2004	1	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	B	2005	1	14,14,15	0.24	0	17,19,21	0.53	0
3	NAG	A	2004	1	14,14,15	0.27	0	17,19,21	0.52	0
3	NAG	C	2003	1	14,14,15	0.25	0	17,19,21	0.41	0
3	NAG	C	2001	1	14,14,15	0.23	0	17,19,21	0.39	0
3	NAG	A	2001	1	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	A	2002	1	14,14,15	0.18	0	17,19,21	0.44	0
3	NAG	B	2004	1	14,14,15	0.22	0	17,19,21	0.41	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2004	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

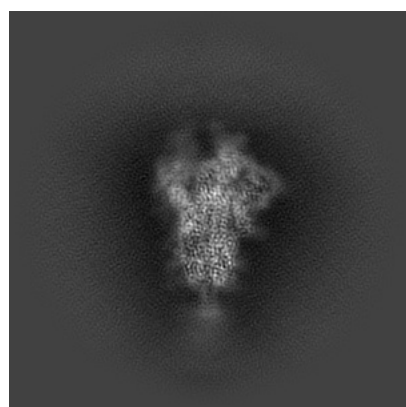
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31782. These allow visual inspection of the internal detail of the map and identification of artifacts.

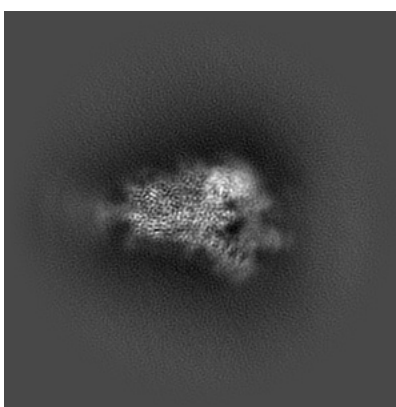
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

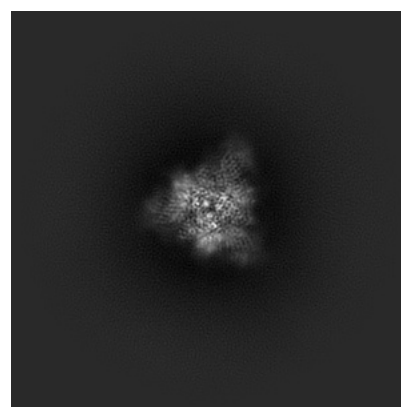
6.1.1 Primary map



X



Y

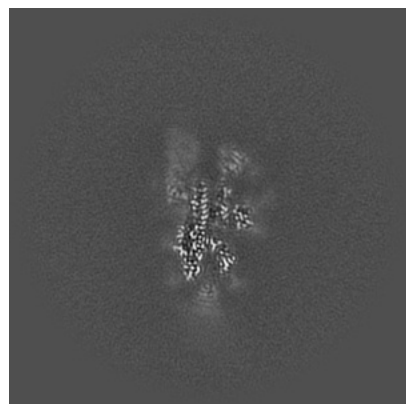


Z

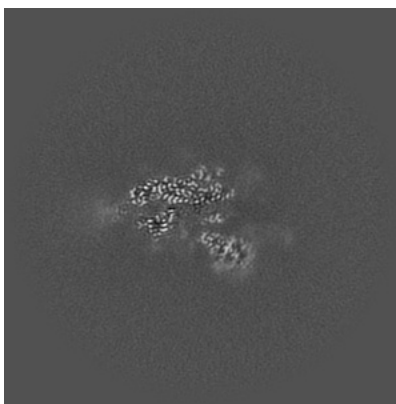
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

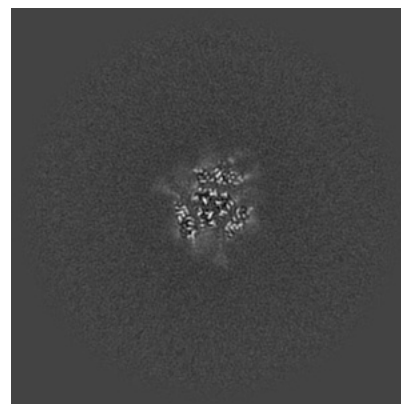
6.2.1 Primary map



X Index: 192



Y Index: 192

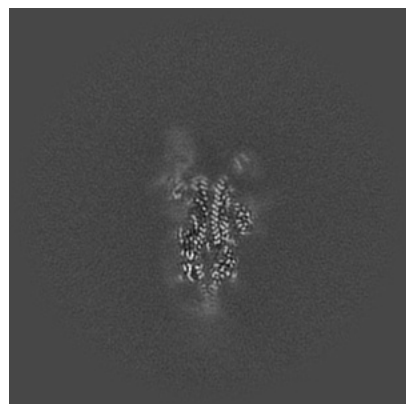


Z Index: 192

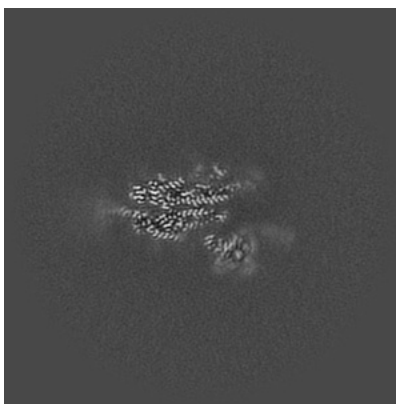
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

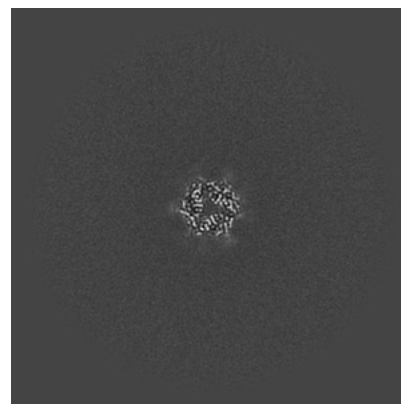
6.3.1 Primary map



X Index: 187



Y Index: 196

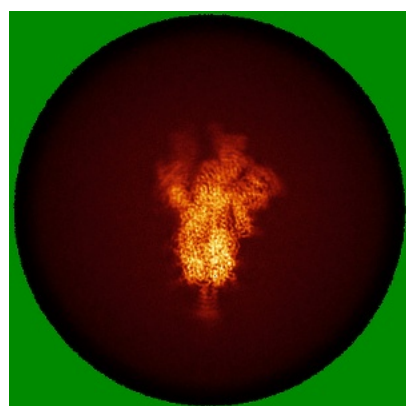


Z Index: 144

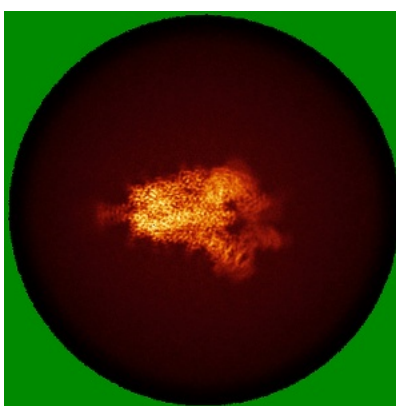
The images above show the largest variance slices of the map in three orthogonal directions.

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

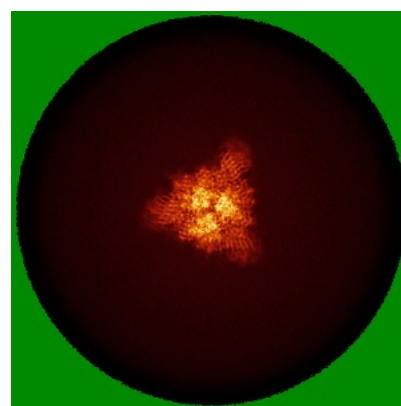
6.4.1 Primary map



X



Y

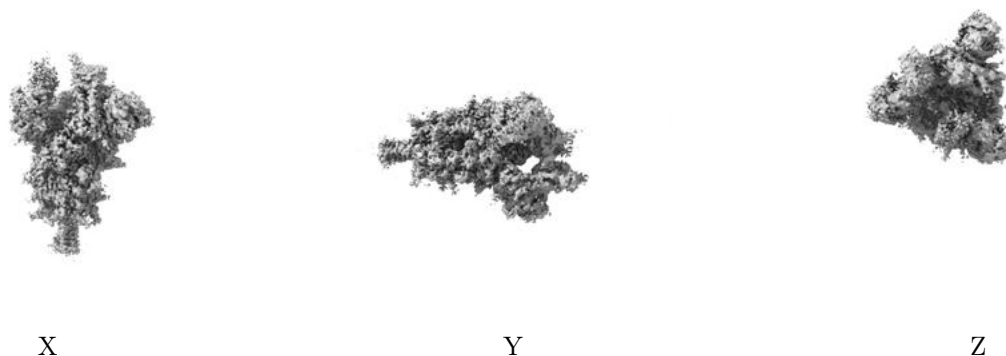


Z

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



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

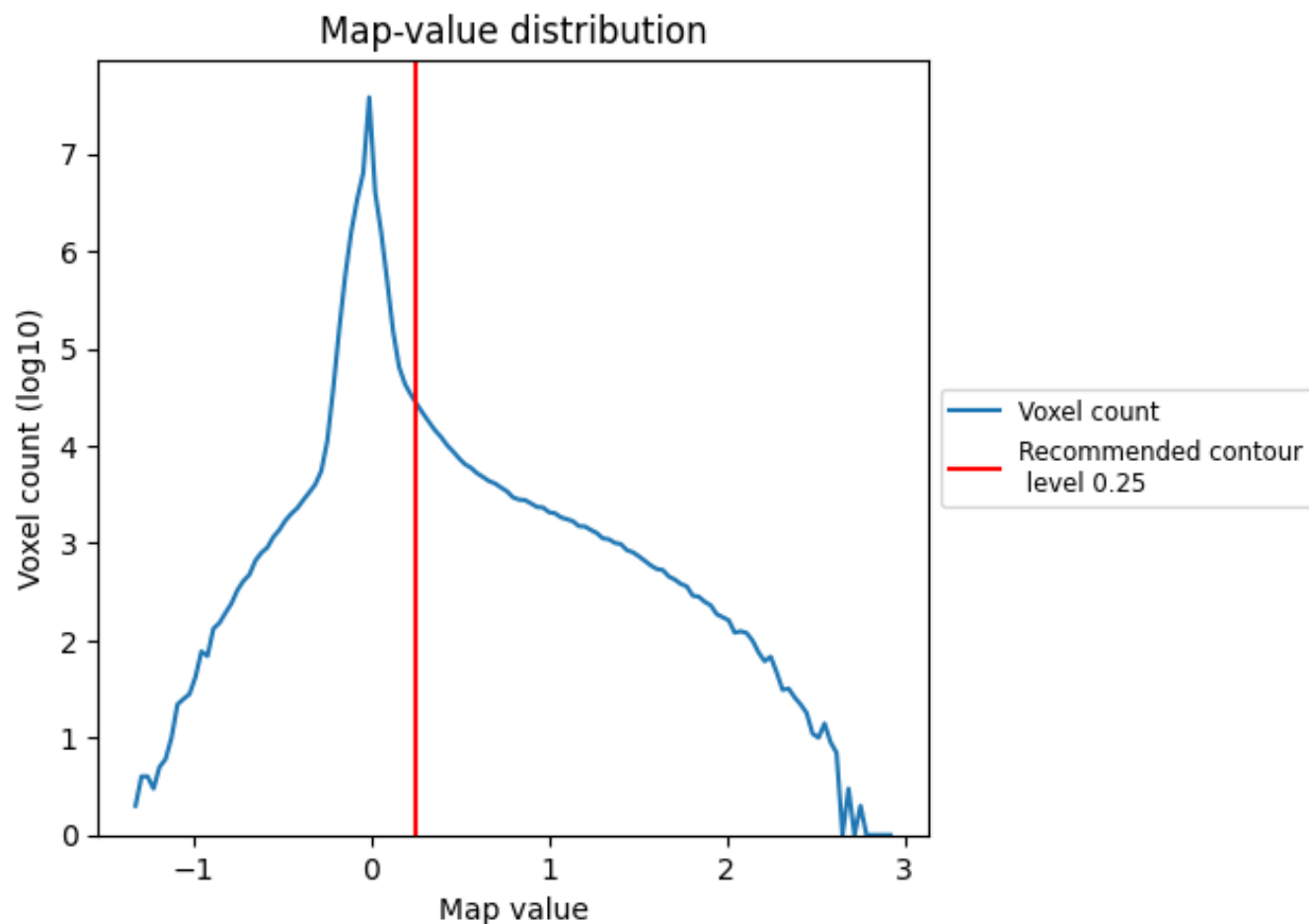
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

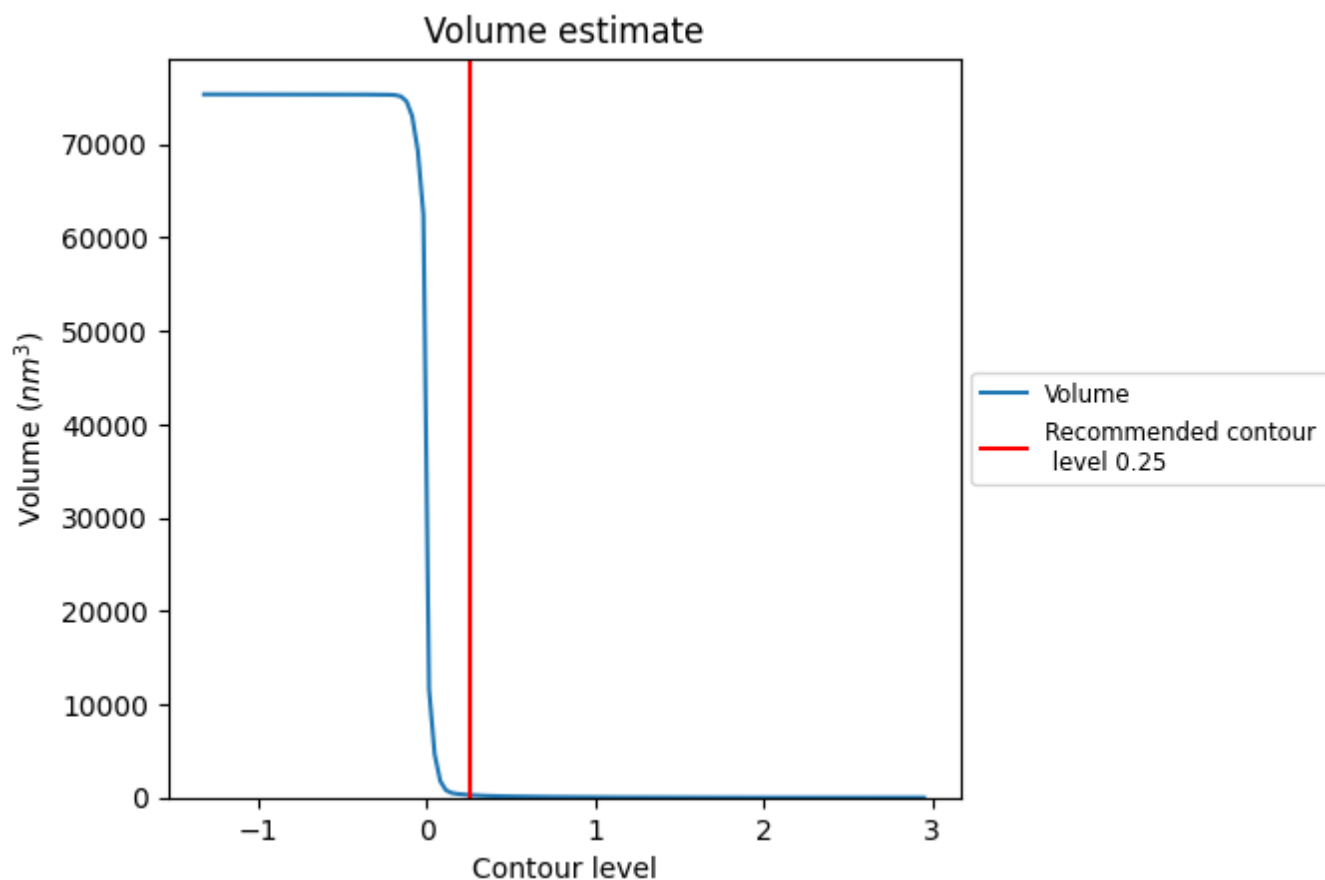
This section contains the results of statistical analysis of the map.

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.

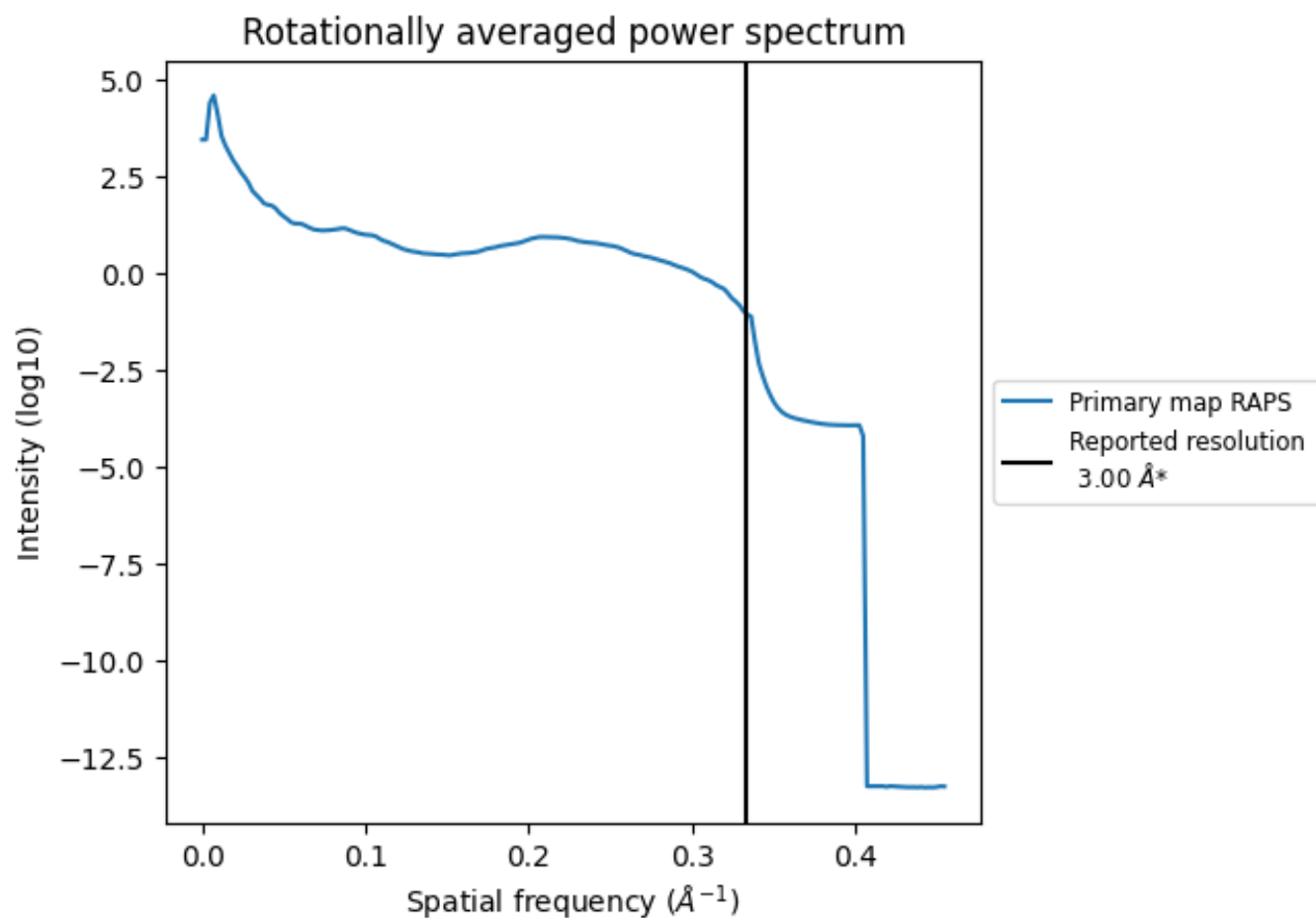
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm^3 ; this corresponds to an approximate mass of 250 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 0.333 Å⁻¹

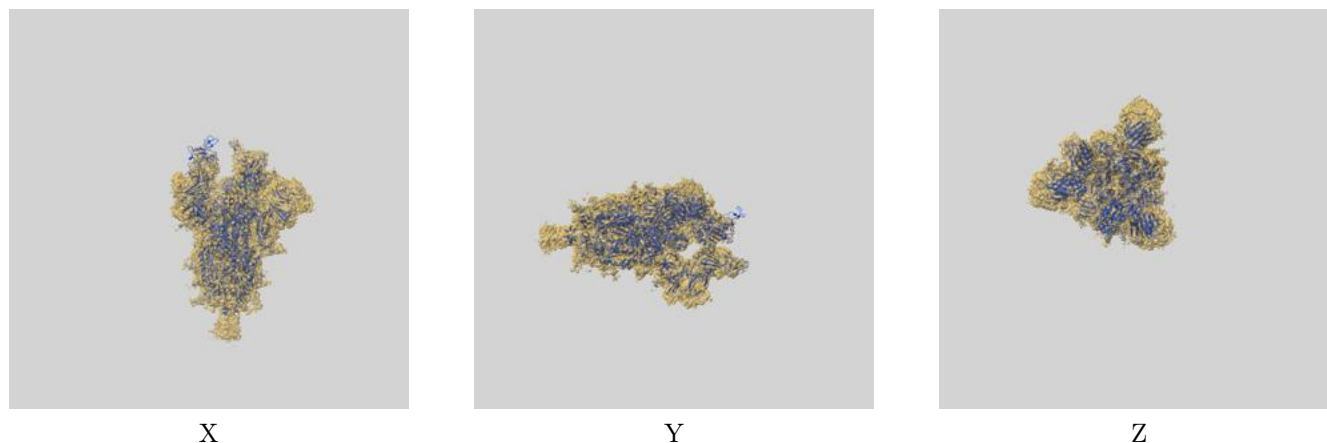
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

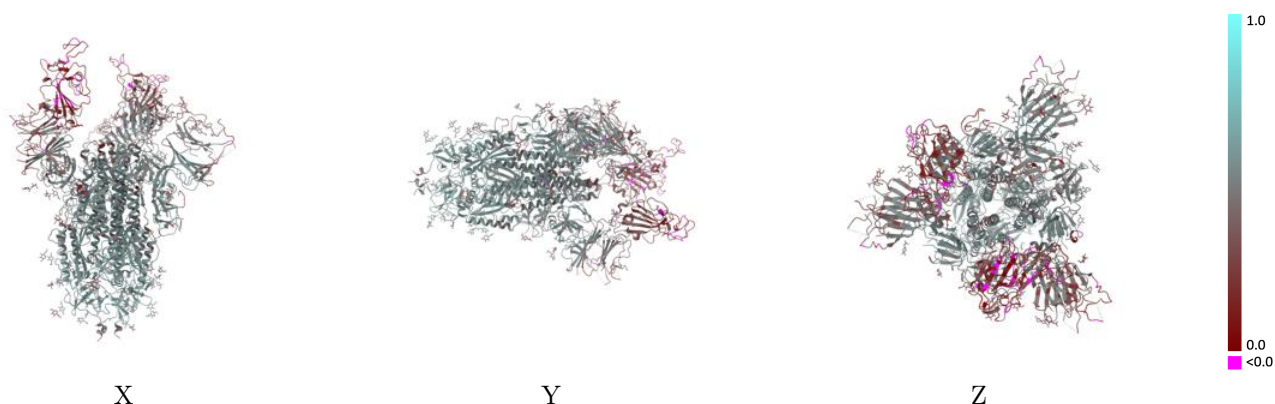
This section contains information regarding the fit between EMDB map EMD-31782 and PDB model 7V7U. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



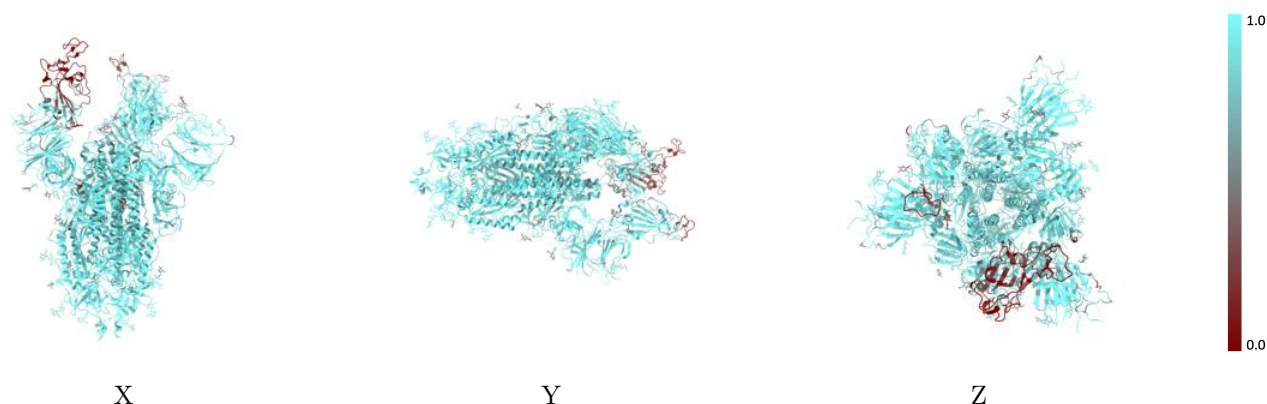
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



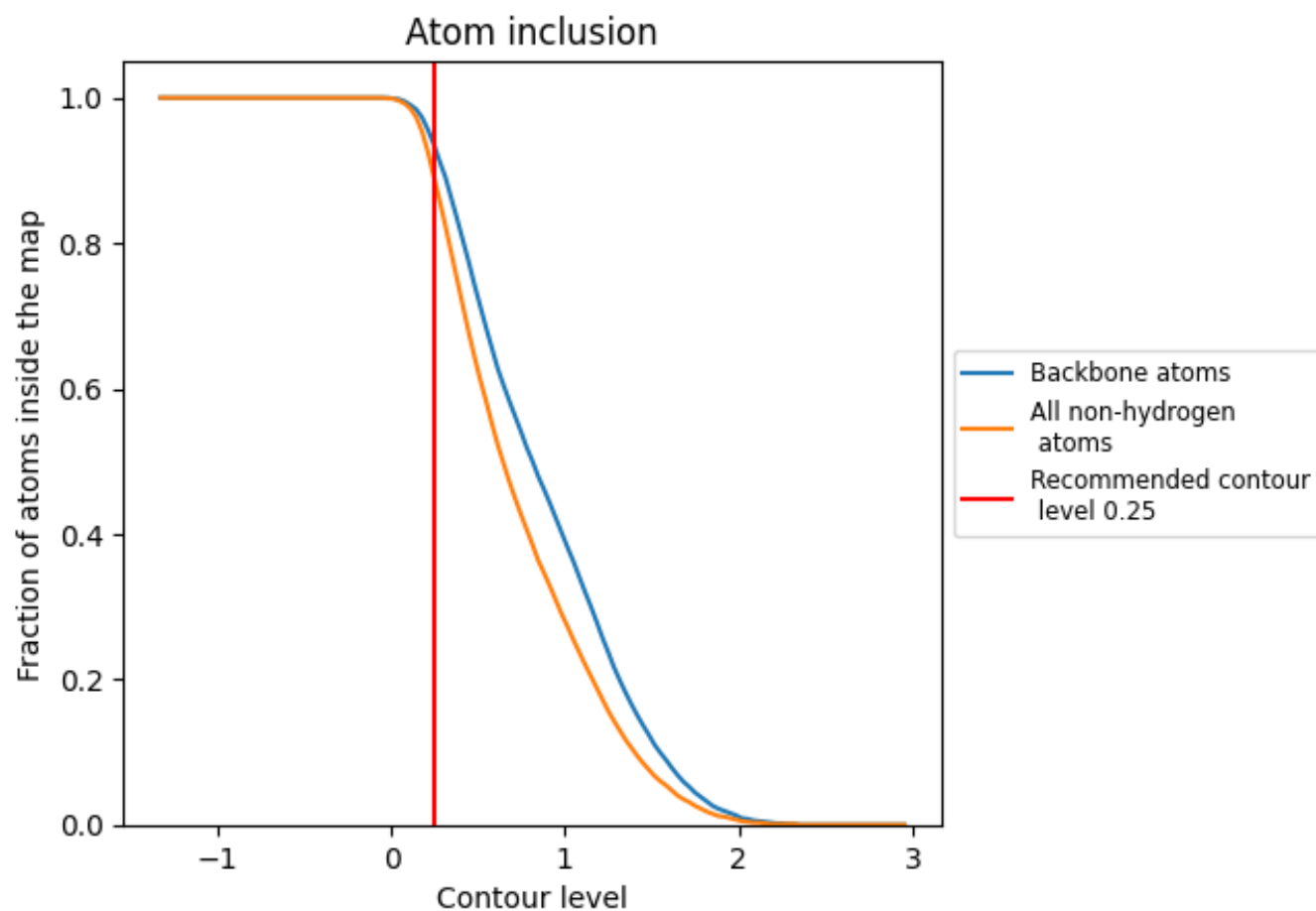
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.8890	 0.4590
A	 0.8290	 0.4410
B	 0.9340	 0.4800
C	 0.9180	 0.4640
D	 0.8930	 0.3520
E	 0.3210	 0.1530
F	 0.2860	 0.2320
G	 0.6430	 0.4020
H	 0.7860	 0.3290
I	 0.7140	 0.3810
J	 0.8210	 0.4220
K	 1.0000	 0.4780
L	 0.9290	 0.4600
M	 0.6430	 0.3680
N	 0.9640	 0.5190
O	 0.8930	 0.4320
P	 0.7500	 0.3380
Q	 0.5000	 0.1520
R	 0.6430	 0.3580
S	 0.9290	 0.3690
T	 0.5000	 0.3920
U	 0.9640	 0.4720
V	 1.0000	 0.4800
W	 0.9290	 0.4970
X	 0.7500	 0.2290
Y	 0.9640	 0.5210
Z	 0.8930	 0.4760
a	 0.9640	 0.3170
b	 0.4290	 0.2740
c	 0.7140	 0.3840
d	 0.6790	 0.3710
e	 0.8930	 0.4060
f	 0.7140	 0.4120
g	 0.7860	 0.4210
h	 1.0000	 0.5270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.9290	 0.4500
j	 0.7140	 0.3550
k	 1.0000	 0.5080
l	 0.9640	 0.5020