



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2025 – 05:00 PM EDT

PDB ID : 9BJ3
EMDB ID : EMD-44628
Title : Structure of the SARS-CoV-2 S 6P trimer complex with the human neutralizing antibody Fab fragment, C1596
Authors : Rubio, A.A.; Abernathy, M.E.; Barnes, C.O.
Deposited on : 2024-04-24
Resolution : 3.04 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

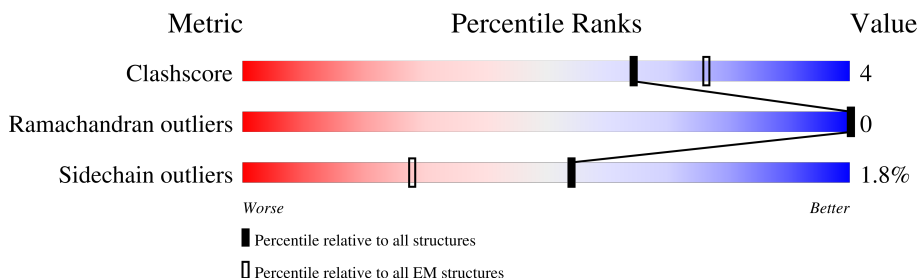
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 Å.

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



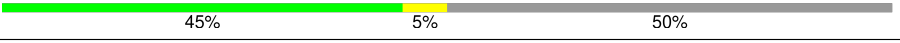




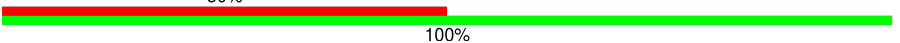


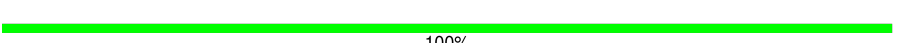




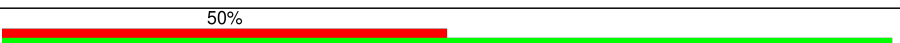
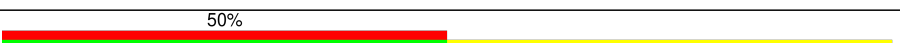

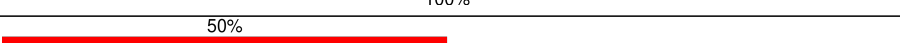
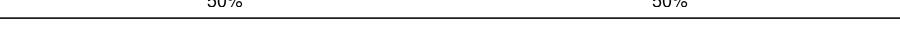

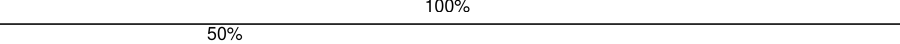
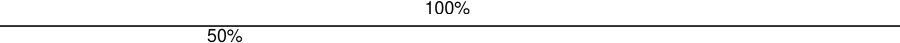
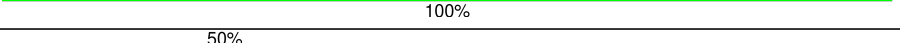
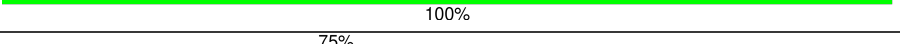


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1271	<div> <div>5%</div> <div>72%</div> <div>10%</div> <div>18%</div> </div>
1	B	1271	<div> <div>5%</div> <div>73%</div> <div>8%</div> <div>18%</div> </div>
1	S	1271	<div> <div>6%</div> <div>73%</div> <div>8%</div> <div>18%</div> </div>
2	C	240	<div> <div>50%</div> <div>47%</div> </div>
2	E	240	<div> <div>48%</div> <div>5%</div> <div>47%</div> </div>
2	H	240	<div> <div>48%</div> <div>5%</div> <div>47%</div> </div>
3	D	215	<div> <div>45%</div> <div>5%</div> <div>50%</div> </div>
3	F	215	<div> <div>46%</div> <div>5%</div> <div>50%</div> </div>



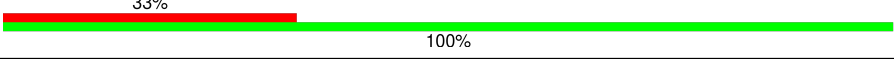
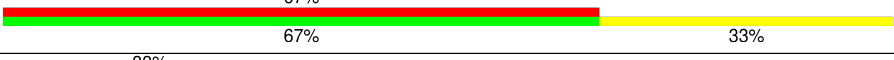
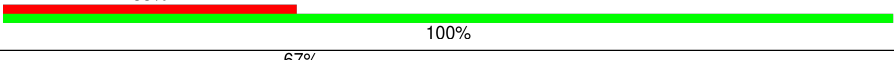

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Mol	Chain	Length	Quality of chain
3	L	215	
4	G	2	
4	J	2	
4	K	2	
4	M	2	
4	N	2	
4	Q	2	
4	R	2	
4	T	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	b	2	
4	c	2	
4	d	2	
4	f	2	
4	g	2	
4	h	2	
4	i	2	
4	l	2	
4	m	2	
5	I	4	
5	U	4	
5	e	4	

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Mol	Chain	Length	Quality of chain
6	O	3	
6	P	3	
6	Z	3	
6	a	3	
6	j	3	
6	k	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30621 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	1037	Total	C	N	O	S	0	0
			8022	5115	1341	1531	35		
1	B	1037	Total	C	N	O	S	0	0
			8022	5115	1341	1531	35		
1	S	1037	Total	C	N	O	S	0	0
			8022	5115	1341	1531	35		

There are 213 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	ILE	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	LEU	-	expression tag	UNP P0DTC2
A	1262	ASN	-	expression tag	UNP P0DTC2
A	1263	ASP	-	expression tag	UNP P0DTC2
A	1264	ILE	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	ALA	-	expression tag	UNP P0DTC2
A	1268	GLN	-	expression tag	UNP P0DTC2
A	1269	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	ILE	-	expression tag	UNP P0DTC2
A	1271	GLU	-	expression tag	UNP P0DTC2
A	1272	TRP	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	GLU	-	expression tag	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	LEU	-	expression tag	UNP P0DTC2
B	1262	ASN	-	expression tag	UNP P0DTC2
B	1263	ASP	-	expression tag	UNP P0DTC2
B	1264	ILE	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	ALA	-	expression tag	UNP P0DTC2
B	1268	GLN	-	expression tag	UNP P0DTC2
B	1269	LYS	-	expression tag	UNP P0DTC2
B	1270	ILE	-	expression tag	UNP P0DTC2
B	1271	GLU	-	expression tag	UNP P0DTC2
B	1272	TRP	-	expression tag	UNP P0DTC2
B	1273	HIS	-	expression tag	UNP P0DTC2
B	1274	GLU	-	expression tag	UNP P0DTC2
S	?	-	ARG	deletion	UNP P0DTC2
S	?	-	ARG	deletion	UNP P0DTC2
S	?	-	ALA	deletion	UNP P0DTC2
S	685	ALA	ARG	conflict	UNP P0DTC2
S	817	PRO	PHE	engineered mutation	UNP P0DTC2
S	892	PRO	ALA	engineered mutation	UNP P0DTC2
S	899	PRO	ALA	engineered mutation	UNP P0DTC2
S	942	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	986	PRO	LYS	engineered mutation	UNP P0DTC2
S	987	PRO	VAL	engineered mutation	UNP P0DTC2
S	1214	SER	-	expression tag	UNP P0DTC2
S	1215	GLY	-	expression tag	UNP P0DTC2
S	1216	ARG	-	expression tag	UNP P0DTC2
S	1217	LEU	-	expression tag	UNP P0DTC2
S	1218	VAL	-	expression tag	UNP P0DTC2
S	1219	PRO	-	expression tag	UNP P0DTC2
S	1220	ARG	-	expression tag	UNP P0DTC2
S	1221	GLY	-	expression tag	UNP P0DTC2
S	1222	SER	-	expression tag	UNP P0DTC2
S	1223	PRO	-	expression tag	UNP P0DTC2
S	1224	GLY	-	expression tag	UNP P0DTC2
S	1225	SER	-	expression tag	UNP P0DTC2
S	1226	GLY	-	expression tag	UNP P0DTC2
S	1227	TYR	-	expression tag	UNP P0DTC2
S	1228	ILE	-	expression tag	UNP P0DTC2
S	1229	PRO	-	expression tag	UNP P0DTC2
S	1230	GLU	-	expression tag	UNP P0DTC2
S	1231	ALA	-	expression tag	UNP P0DTC2
S	1232	PRO	-	expression tag	UNP P0DTC2
S	1233	ARG	-	expression tag	UNP P0DTC2
S	1234	ASP	-	expression tag	UNP P0DTC2
S	1235	GLY	-	expression tag	UNP P0DTC2
S	1236	GLN	-	expression tag	UNP P0DTC2
S	1237	ALA	-	expression tag	UNP P0DTC2
S	1238	TYR	-	expression tag	UNP P0DTC2
S	1239	VAL	-	expression tag	UNP P0DTC2
S	1240	ARG	-	expression tag	UNP P0DTC2
S	1241	LYS	-	expression tag	UNP P0DTC2
S	1242	ASP	-	expression tag	UNP P0DTC2
S	1243	GLY	-	expression tag	UNP P0DTC2
S	1244	GLU	-	expression tag	UNP P0DTC2
S	1245	TRP	-	expression tag	UNP P0DTC2
S	1246	VAL	-	expression tag	UNP P0DTC2
S	1247	LEU	-	expression tag	UNP P0DTC2
S	1248	LEU	-	expression tag	UNP P0DTC2
S	1249	SER	-	expression tag	UNP P0DTC2
S	1250	THR	-	expression tag	UNP P0DTC2
S	1251	PHE	-	expression tag	UNP P0DTC2
S	1252	LEU	-	expression tag	UNP P0DTC2
S	1253	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1254	HIS	-	expression tag	UNP P0DTC2
S	1255	HIS	-	expression tag	UNP P0DTC2
S	1256	HIS	-	expression tag	UNP P0DTC2
S	1257	HIS	-	expression tag	UNP P0DTC2
S	1258	HIS	-	expression tag	UNP P0DTC2
S	1259	HIS	-	expression tag	UNP P0DTC2
S	1260	GLY	-	expression tag	UNP P0DTC2
S	1261	LEU	-	expression tag	UNP P0DTC2
S	1262	ASN	-	expression tag	UNP P0DTC2
S	1263	ASP	-	expression tag	UNP P0DTC2
S	1264	ILE	-	expression tag	UNP P0DTC2
S	1265	PHE	-	expression tag	UNP P0DTC2
S	1266	GLU	-	expression tag	UNP P0DTC2
S	1267	ALA	-	expression tag	UNP P0DTC2
S	1268	GLN	-	expression tag	UNP P0DTC2
S	1269	LYS	-	expression tag	UNP P0DTC2
S	1270	ILE	-	expression tag	UNP P0DTC2
S	1271	GLU	-	expression tag	UNP P0DTC2
S	1272	TRP	-	expression tag	UNP P0DTC2
S	1273	HIS	-	expression tag	UNP P0DTC2
S	1274	GLU	-	expression tag	UNP P0DTC2

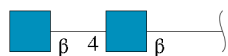
- Molecule 2 is a protein called C1596 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	128	Total	C	N	O	S	0	0
			970	616	163	186	5		
2	E	128	Total	C	N	O	S	0	0
			970	616	163	186	5		
2	H	128	Total	C	N	O	S	0	0
			970	616	163	186	5		

- Molecule 3 is a protein called C1596 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	108	Total	C	N	O	S	0	0
			807	509	137	159	2		
3	F	108	Total	C	N	O	S	0	0
			807	509	137	159	2		
3	L	108	Total	C	N	O	S	0	0
			807	509	137	159	2		

- Molecule 4 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
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		

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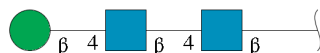
Mol	Chain	Residues	Atoms				AltConf	Trace
4	i	2	Total	C	N	O	0	0
			28	16	2	10		
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	4	Total	C	N	O	0	0
			50	28	2	20		
5	U	4	Total	C	N	O	0	0
			50	28	2	20		
5	e	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	3	Total	C	N	O	0	0
			39	22	2	15		
6	P	3	Total	C	N	O	0	0
			39	22	2	15		
6	Z	3	Total	C	N	O	0	0
			39	22	2	15		
6	a	3	Total	C	N	O	0	0
			39	22	2	15		
6	j	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	k	3	39	22	2	15	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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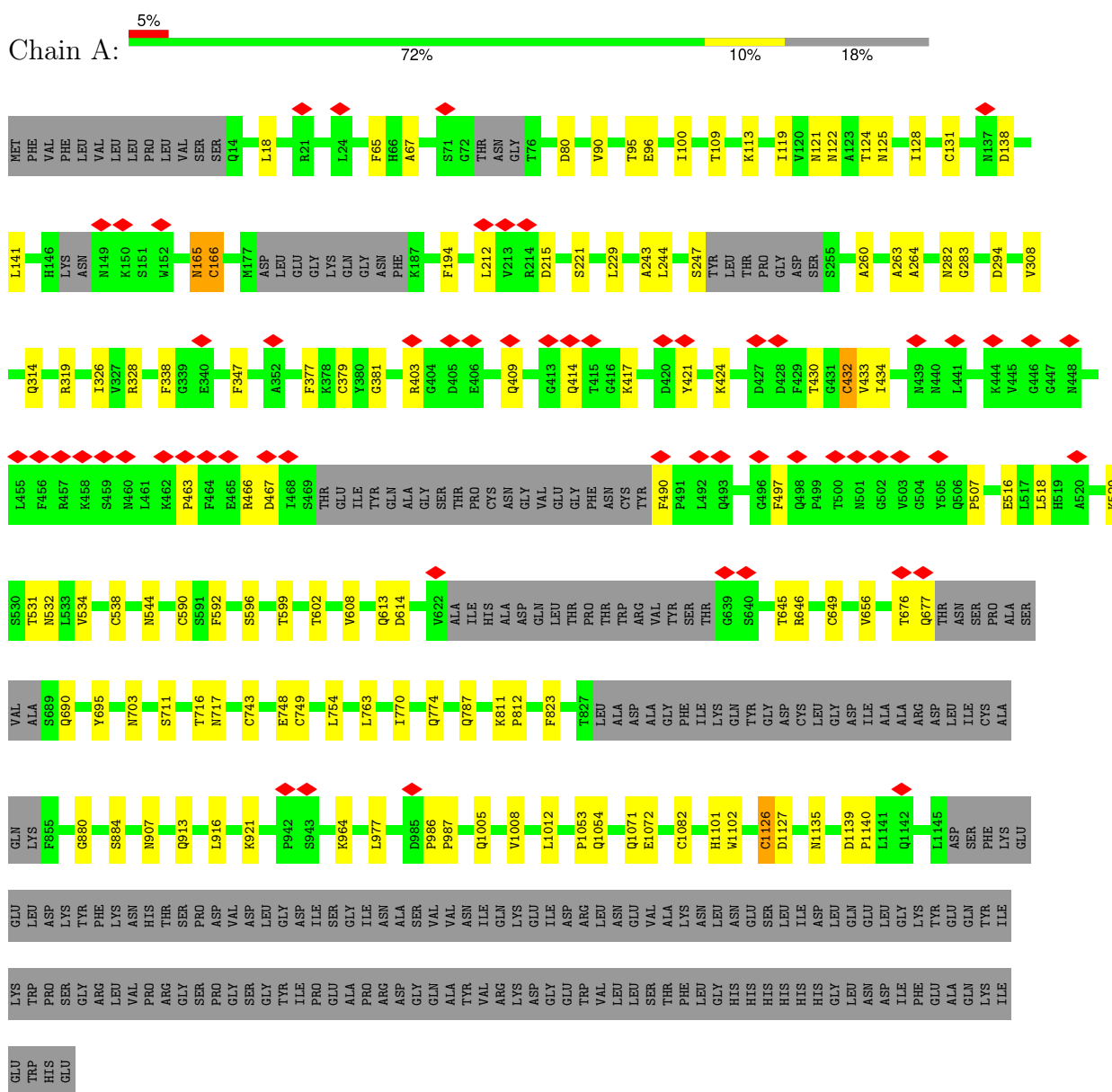
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Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	S	1	Total	C	N	O	0
			14	8	1	5	
7	S	1	Total	C	N	O	0
			14	8	1	5	
7	S	1	Total	C	N	O	0
			14	8	1	5	
7	S	1	Total	C	N	O	0
			14	8	1	5	
7	S	1	Total	C	N	O	0
			14	8	1	5	

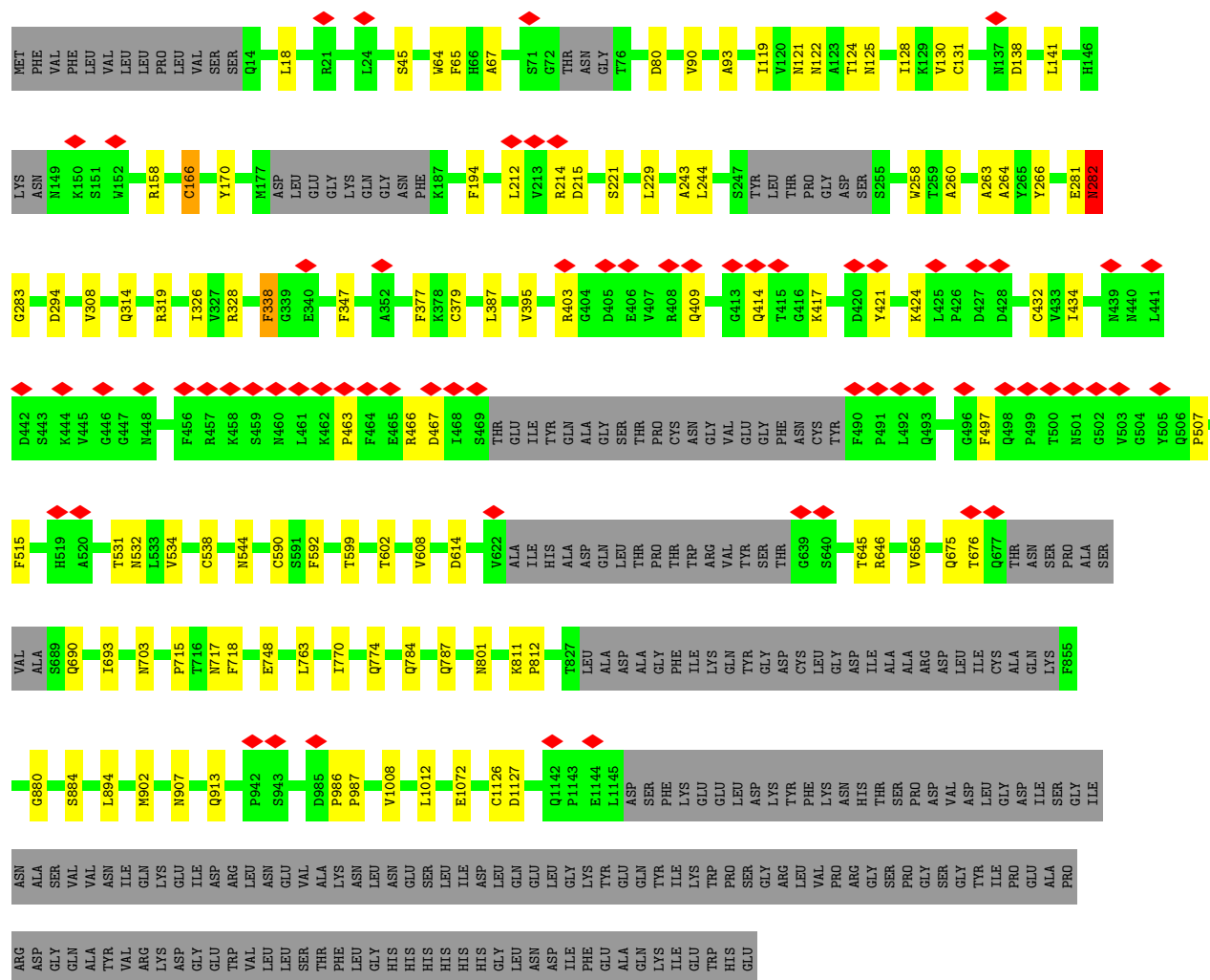
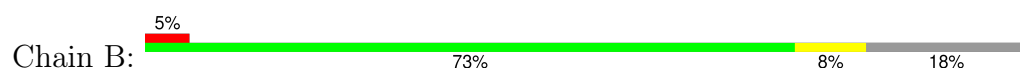
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

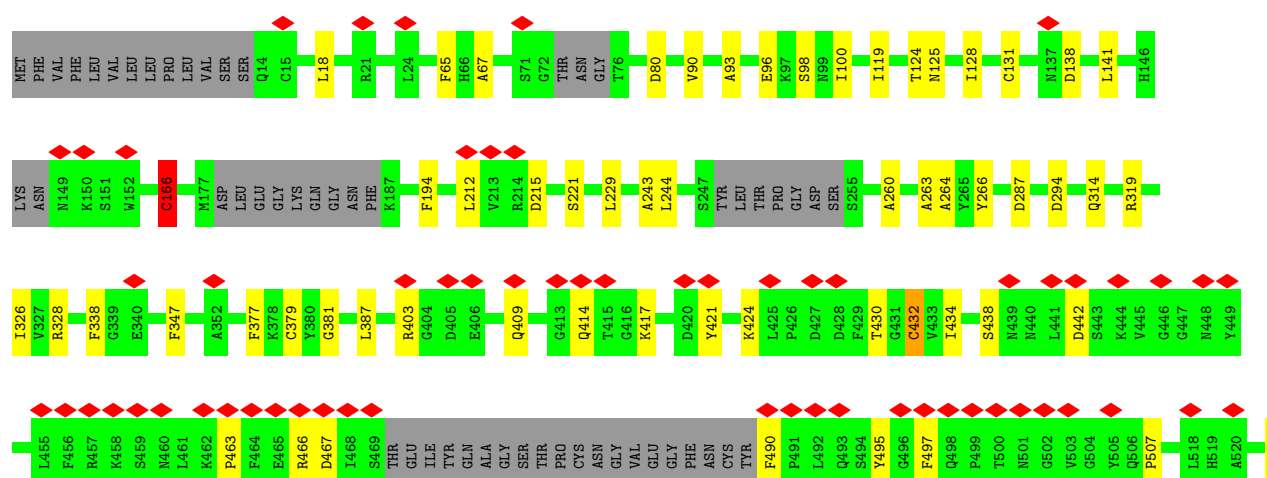
- Molecule 1: Spike glycoprotein

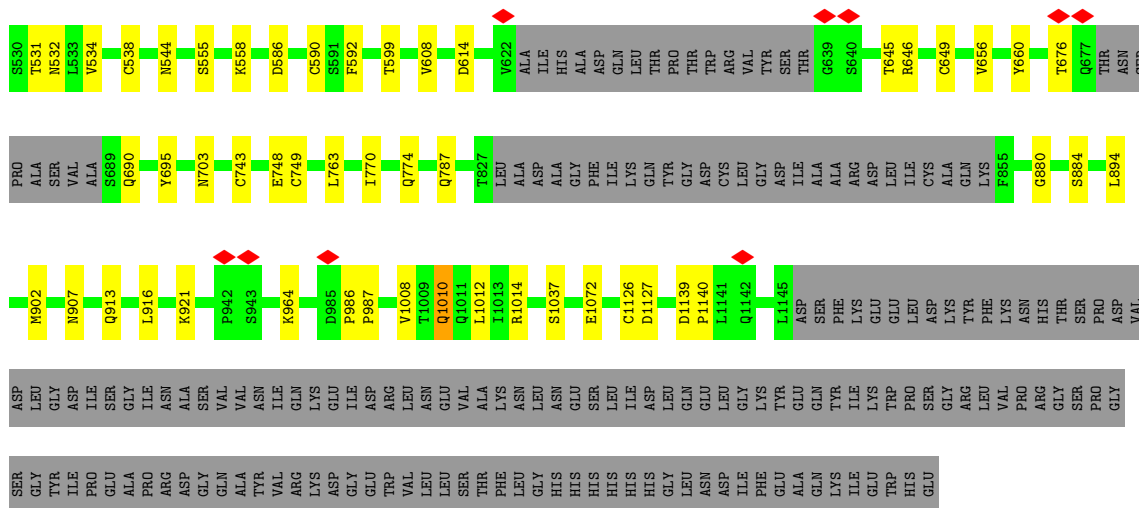


- Molecule 1: Spike glycoprotein

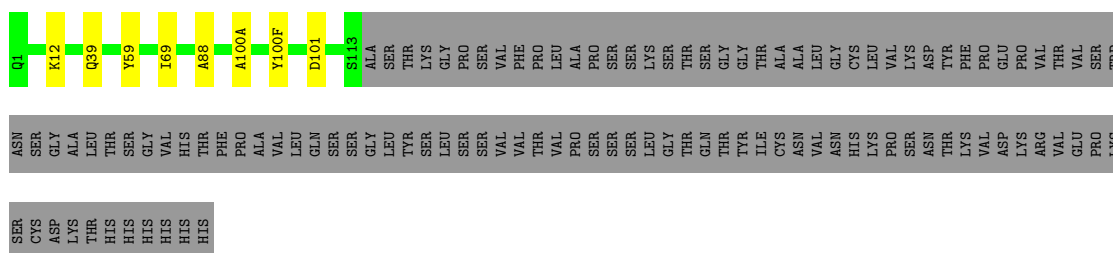


• Molecule 1: Spike glycoprotein

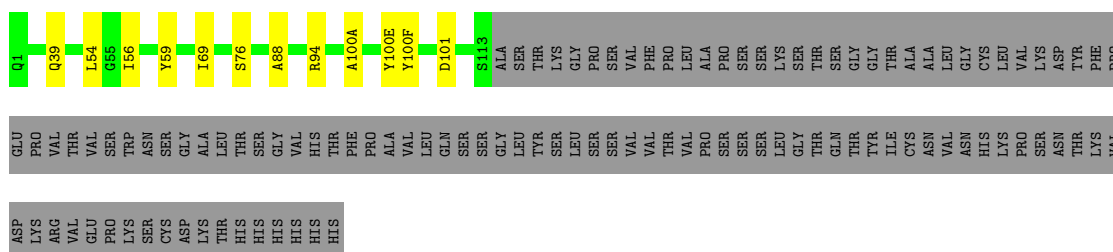




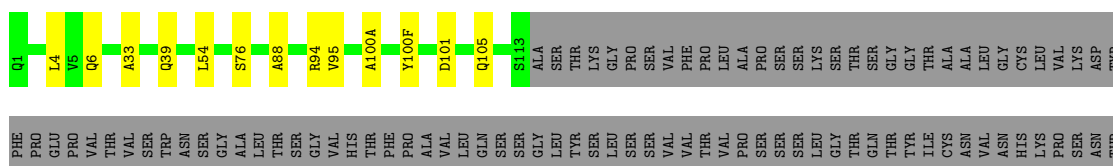
- Molecule 2: C1596 Fab Heavy Chain



- Molecule 2: C1596 Fab Heavy Chain



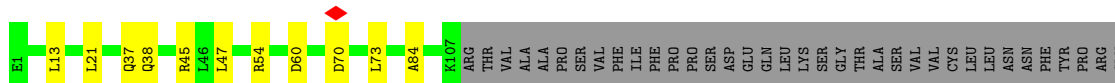
- Molecule 2: C1596 Fab Heavy Chain



LYS
VAL
ASP
LYS
ARG
VAL
GLU
PRO
SER
CYS
LYS
ASP
LYS
THR
HIS
HIS
HIS
HIS
HIS

• Molecule 3: C1596 Light Chain

Chain D: 

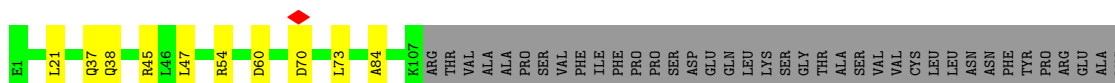


ALA
LYS
VAL
GLN
TRP
LYS
TRP
PHE
ASN
ARG
GLY
GLU
CYS

PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

• Molecule 3: C1596 Light Chain

Chain F: 

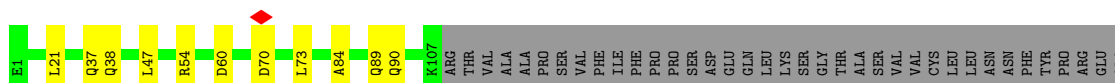


VAL
GLN
TRP
LYS
VAL
ASP
ASN
ALA
LEU
GLN
SER
GLY
ASN
SER
GLN
SER
VAL
THR
GLU
GLN
ASP
SER
LYS
ASP
SER
THR
TYR
ALA
SER
SER
LEU
SER
SER
PHE
THR
THR
THR
LEU
SER
LYS
ALA
GLN
TYR
LYS
GLY
HIS
LYS
VAL
SER
VAL
ALA
CYS
GLU
VAL
THR
HIS
ASN
GLN
PHE
TYR
SER
PRO
SER
PRO
ALA
LYS

THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

• Molecule 3: C1596 Light Chain

Chain L: 



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

VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

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

Chain G: 

MAG1
MAG2

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



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



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



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



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



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



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

Chain T:  100%



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

Chain V:  100%
50% 50%



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

Chain W:  50%
50% 50%



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

Chain X:  50%
100%



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

Chain Y:  50%
100%



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

Chain b:  50%
100%



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



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



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



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



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



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



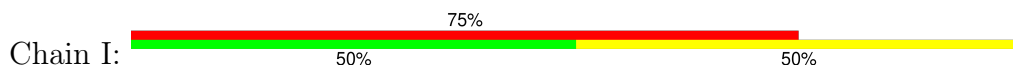
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



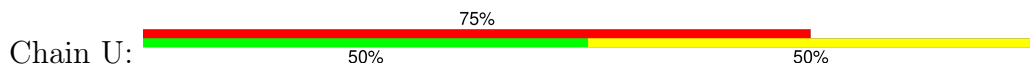
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



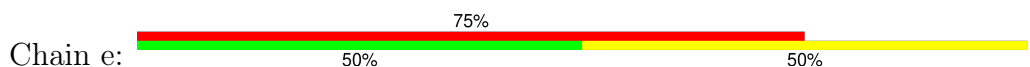
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j: 



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	362680	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.371	Depositor
Minimum map value	-0.894	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.139	Depositor
Map size (Å)	368.1072, 368.1072, 368.1072	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8521, 0.8521, 0.8521	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.26	0/8203	0.51	2/11176 (0.0%)
1	B	0.26	0/8203	0.51	3/11176 (0.0%)
1	S	0.25	0/8203	0.49	2/11176 (0.0%)
2	C	0.25	0/993	0.49	0/1350
2	E	0.25	0/993	0.49	0/1350
2	H	0.25	0/993	0.49	0/1350
3	D	0.25	0/825	0.51	0/1121
3	F	0.25	0/825	0.51	0/1121
3	L	0.25	0/825	0.51	0/1121
All	All	0.25	0/30063	0.50	7/40941 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	S	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	CYS	CA-CB-SG	7.74	127.94	114.00
1	B	282	ASN	CB-CA-C	5.81	122.01	110.40
1	S	166	CYS	CA-CB-SG	5.67	124.21	114.00
1	S	614	ASP	CB-CG-OD1	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	CYS	CA-CB-SG	5.08	123.14	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	432	CYS	Peptide
1	B	282	ASN	Peptide
1	B	432	CYS	Peptide
1	S	432	CYS	Peptide

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	8022	0	7772	71	0
1	B	8022	0	7773	61	0
1	S	8022	0	7773	61	0
2	C	970	0	948	5	0
2	E	970	0	948	8	0
2	H	970	0	948	8	0
3	D	807	0	792	4	0
3	F	807	0	792	4	0
3	L	807	0	792	5	0
4	G	28	0	25	1	0
4	J	28	0	25	1	0
4	K	28	0	25	1	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	Q	28	0	25	1	0
4	R	28	0	25	0	0
4	T	28	0	25	0	0
4	V	28	0	25	2	0
4	W	28	0	25	1	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	b	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	c	28	0	25	0	0
4	d	28	0	25	0	0
4	f	28	0	25	0	0
4	g	28	0	25	0	0
4	h	28	0	25	0	0
4	i	28	0	25	0	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
5	I	50	0	43	1	0
5	U	50	0	43	0	0
5	e	50	0	43	0	0
6	O	39	0	34	1	0
6	P	39	0	34	0	0
6	Z	39	0	34	0	0
6	a	39	0	34	0	0
6	j	39	0	34	0	0
6	k	39	0	34	0	0
7	A	84	0	78	0	0
7	B	84	0	78	0	0
7	S	84	0	78	0	0
All	All	30621	0	29630	229	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 4.

The worst 5 of 229 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:379:CYS:HA	1:A:432:CYS:HB3	1.62	0.81
1:B:531:THR:HG22	1:B:532:ASN:H	1.50	0.77
1:S:379:CYS:HA	1:S:432:CYS:HB3	1.67	0.77
1:S:131:CYS:HA	1:S:166:CYS:HB2	1.67	0.76
1:S:531:THR:HG22	1:S:532:ASN:H	1.48	0.76

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	1019/1271 (80%)	954 (94%)	65 (6%)	0	100	100
1	B	1019/1271 (80%)	951 (93%)	68 (7%)	0	100	100
1	S	1019/1271 (80%)	954 (94%)	65 (6%)	0	100	100
2	C	126/240 (52%)	117 (93%)	9 (7%)	0	100	100
2	E	126/240 (52%)	118 (94%)	8 (6%)	0	100	100
2	H	126/240 (52%)	117 (93%)	9 (7%)	0	100	100
3	D	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
3	F	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
3	L	106/215 (49%)	103 (97%)	3 (3%)	0	100	100
All	All	3753/5178 (72%)	3520 (94%)	233 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	892/1109 (80%)	874 (98%)	18 (2%)	50	75
1	B	892/1109 (80%)	879 (98%)	13 (2%)	60	80
1	S	892/1109 (80%)	873 (98%)	19 (2%)	48	74
2	C	101/199 (51%)	101 (100%)	0	100	100
2	E	101/199 (51%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	101/199 (51%)	100 (99%)	1 (1%)	73	87
3	D	88/186 (47%)	85 (97%)	3 (3%)	32	63
3	F	88/186 (47%)	86 (98%)	2 (2%)	45	72
3	L	88/186 (47%)	87 (99%)	1 (1%)	70	85
All	All	3243/4482 (72%)	3186 (98%)	57 (2%)	54	77

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	902	MET
1	S	1126	CYS
3	F	70	ASP
1	S	1037	SER
1	S	649	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	914	ASN
1	S	125	ASN
1	B	949	GLN
2	H	6	GLN
1	S	448	ASN

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 ⓘ

72 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	$\# Z > 2$
4	NAG	G	1	4,1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	G	2	4	14,14,15	0.36	0	17,19,21	0.44	0
5	NAG	I	1	1,5	14,14,15	0.51	0	17,19,21	0.69	0
5	NAG	I	2	5	14,14,15	0.27	0	17,19,21	0.44	0
5	BMA	I	3	5	11,11,12	0.63	0	15,15,17	0.97	0
5	MAN	I	4	5	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
4	NAG	J	1	4,1	14,14,15	0.55	0	17,19,21	0.66	1 (5%)
4	NAG	J	2	4	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	K	1	4,1	14,14,15	0.39	0	17,19,21	0.49	0
4	NAG	K	2	4	14,14,15	0.48	0	17,19,21	1.35	2 (11%)
4	NAG	M	1	4,1	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	M	2	4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	N	1	4,1	14,14,15	0.33	0	17,19,21	0.46	0
4	NAG	N	2	4	14,14,15	0.33	0	17,19,21	0.49	0
6	NAG	O	1	6,1	14,14,15	0.43	0	17,19,21	0.65	0
6	NAG	O	2	6	14,14,15	0.30	0	17,19,21	0.42	0
6	BMA	O	3	6	11,11,12	0.55	0	15,15,17	0.86	1 (6%)
6	NAG	P	1	6,1	14,14,15	0.35	0	17,19,21	0.92	1 (5%)
6	NAG	P	2	6	14,14,15	0.47	0	17,19,21	0.93	0
6	BMA	P	3	6	11,11,12	0.56	0	15,15,17	0.98	1 (6%)
4	NAG	Q	1	4,1	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	Q	2	4	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	R	1	4,1	14,14,15	0.48	0	17,19,21	0.65	0
4	NAG	R	2	4	14,14,15	0.55	0	17,19,21	0.48	0
4	NAG	T	1	4,1	14,14,15	0.31	0	17,19,21	0.63	0
4	NAG	T	2	4	14,14,15	0.35	0	17,19,21	0.43	0
5	NAG	U	1	1,5	14,14,15	0.27	0	17,19,21	0.69	0
5	NAG	U	2	5	14,14,15	0.27	0	17,19,21	0.52	0
5	BMA	U	3	5	11,11,12	0.74	0	15,15,17	1.06	1 (6%)
5	MAN	U	4	5	11,11,12	0.66	0	15,15,17	0.92	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.50	0	17,19,21	0.92	1 (5%)
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	W	1	4,1	14,14,15	0.33	0	17,19,21	0.50	0
4	NAG	W	2	4	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
4	NAG	X	1	4,1	14,14,15	0.26	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	X	2	4	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	Y	1	4,1	14,14,15	0.42	0	17,19,21	0.47	0
4	NAG	Y	2	4	14,14,15	0.21	0	17,19,21	0.49	0
6	NAG	Z	1	6,1	14,14,15	0.25	0	17,19,21	0.45	0
6	NAG	Z	2	6	14,14,15	0.26	0	17,19,21	0.41	0
6	BMA	Z	3	6	11,11,12	0.52	0	15,15,17	0.80	0
6	NAG	a	1	6,1	14,14,15	0.42	0	17,19,21	0.56	0
6	NAG	a	2	6	14,14,15	0.21	0	17,19,21	0.62	0
6	BMA	a	3	6	11,11,12	0.43	0	15,15,17	0.94	1 (6%)
4	NAG	b	1	4,1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	b	2	4	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	c	1	4,1	14,14,15	0.34	0	17,19,21	0.67	1 (5%)
4	NAG	c	2	4	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	d	1	4,1	14,14,15	0.41	0	17,19,21	0.62	0
4	NAG	d	2	4	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	e	1	1,5	14,14,15	0.31	0	17,19,21	0.59	0
5	NAG	e	2	5	14,14,15	0.26	0	17,19,21	0.43	0
5	BMA	e	3	5	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
5	MAN	e	4	5	11,11,12	0.64	0	15,15,17	0.91	2 (13%)
4	NAG	f	1	4,1	14,14,15	0.61	0	17,19,21	0.74	1 (5%)
4	NAG	f	2	4	14,14,15	0.41	0	17,19,21	0.43	0
4	NAG	g	1	4,1	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	g	2	4	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
4	NAG	h	1	4,1	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	h	2	4	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	i	1	4,1	14,14,15	0.32	0	17,19,21	0.43	0
4	NAG	i	2	4	14,14,15	0.23	0	17,19,21	0.44	0
6	NAG	j	1	6,1	14,14,15	0.27	0	17,19,21	0.48	0
6	NAG	j	2	6	14,14,15	0.25	0	17,19,21	0.42	0
6	BMA	j	3	6	11,11,12	0.54	0	15,15,17	0.76	0
6	NAG	k	1	6,1	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	k	2	6	14,14,15	0.24	0	17,19,21	0.61	0
6	BMA	k	3	6	11,11,12	0.49	0	15,15,17	0.90	1 (6%)
4	NAG	l	1	4,1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	l	2	4	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	m	1	4,1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	m	2	4	14,14,15	0.23	0	17,19,21	0.44	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	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
4	NAG	J	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	5/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
6	NAG	O	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	BMA	P	3	6	-	0/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	1/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
5	MAN	U	4	5	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	V	2	4	-	1/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	5/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Y	2	4	-	4/6/23/26	0/1/1/1
6	NAG	Z	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	NAG	a	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	BMA	a	3	6	-	0/2/19/22	0/1/1/1
4	NAG	b	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	2/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	1/6/23/26	0/1/1/1
5	NAG	e	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
5	BMA	e	3	5	-	2/2/19/22	0/1/1/1
5	MAN	e	4	5	-	0/2/19/22	0/1/1/1
4	NAG	f	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	g	2	4	-	5/6/23/26	0/1/1/1
4	NAG	h	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	h	2	4	-	0/6/23/26	0/1/1/1
4	NAG	i	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	i	2	4	-	4/6/23/26	0/1/1/1
6	NAG	j	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
6	BMA	j	3	6	-	0/2/19/22	0/1/1/1
6	NAG	k	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	k	2	6	-	2/6/23/26	0/1/1/1
6	BMA	k	3	6	-	2/2/19/22	0/1/1/1
4	NAG	l	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	l	2	4	-	0/6/23/26	0/1/1/1
4	NAG	m	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2	NAG	C2-N2-C7	4.61	129.08	122.90
4	g	2	NAG	C2-N2-C7	4.56	129.01	122.90
4	W	2	NAG	C2-N2-C7	4.55	129.00	122.90
4	V	1	NAG	C1-O5-C5	3.15	116.41	112.19
4	f	1	NAG	C1-O5-C5	2.52	115.57	112.19

There are no chirality outliers.

5 of 110 torsion outliers are listed below:

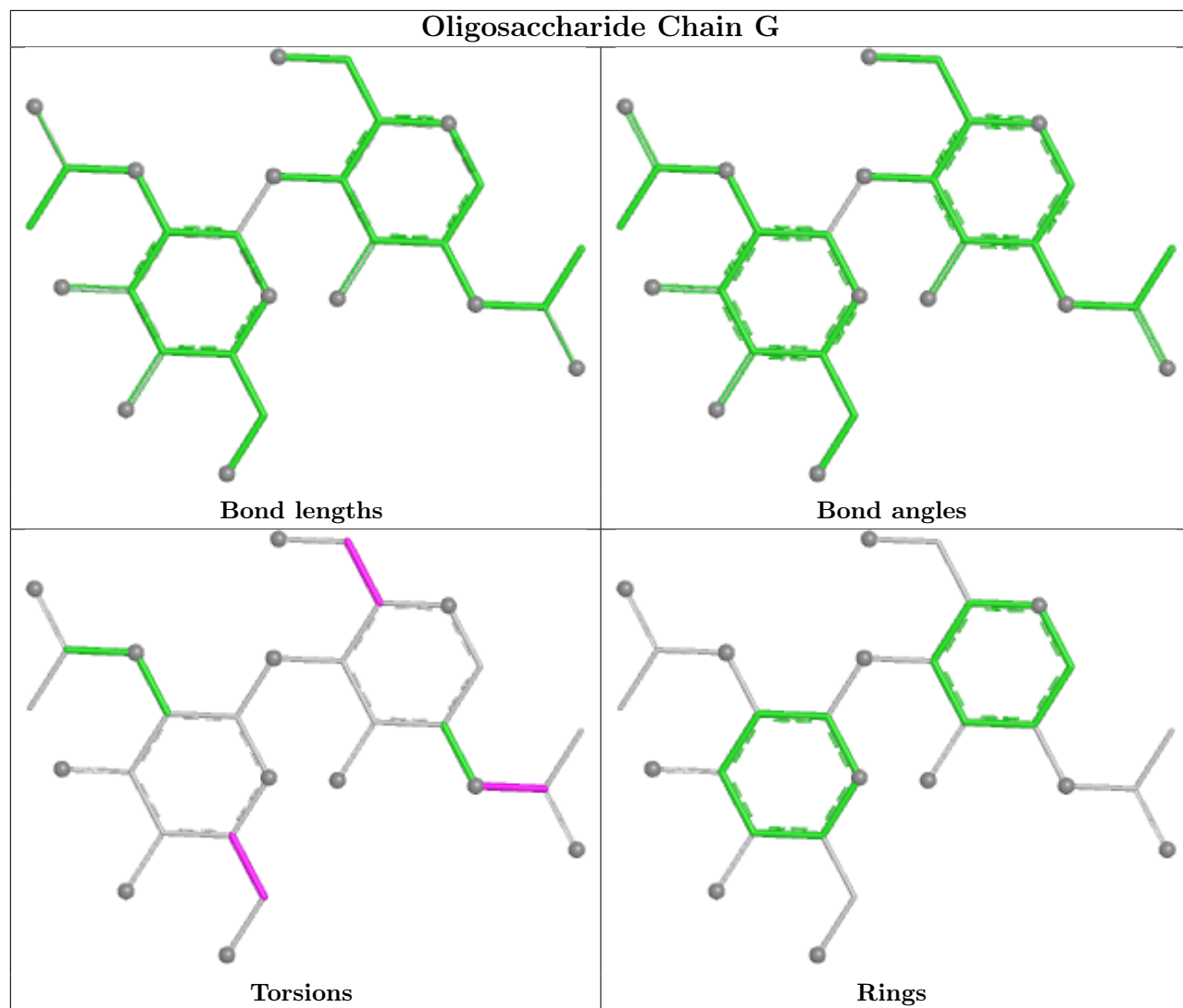
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C1-C2-N2-C7
4	R	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6

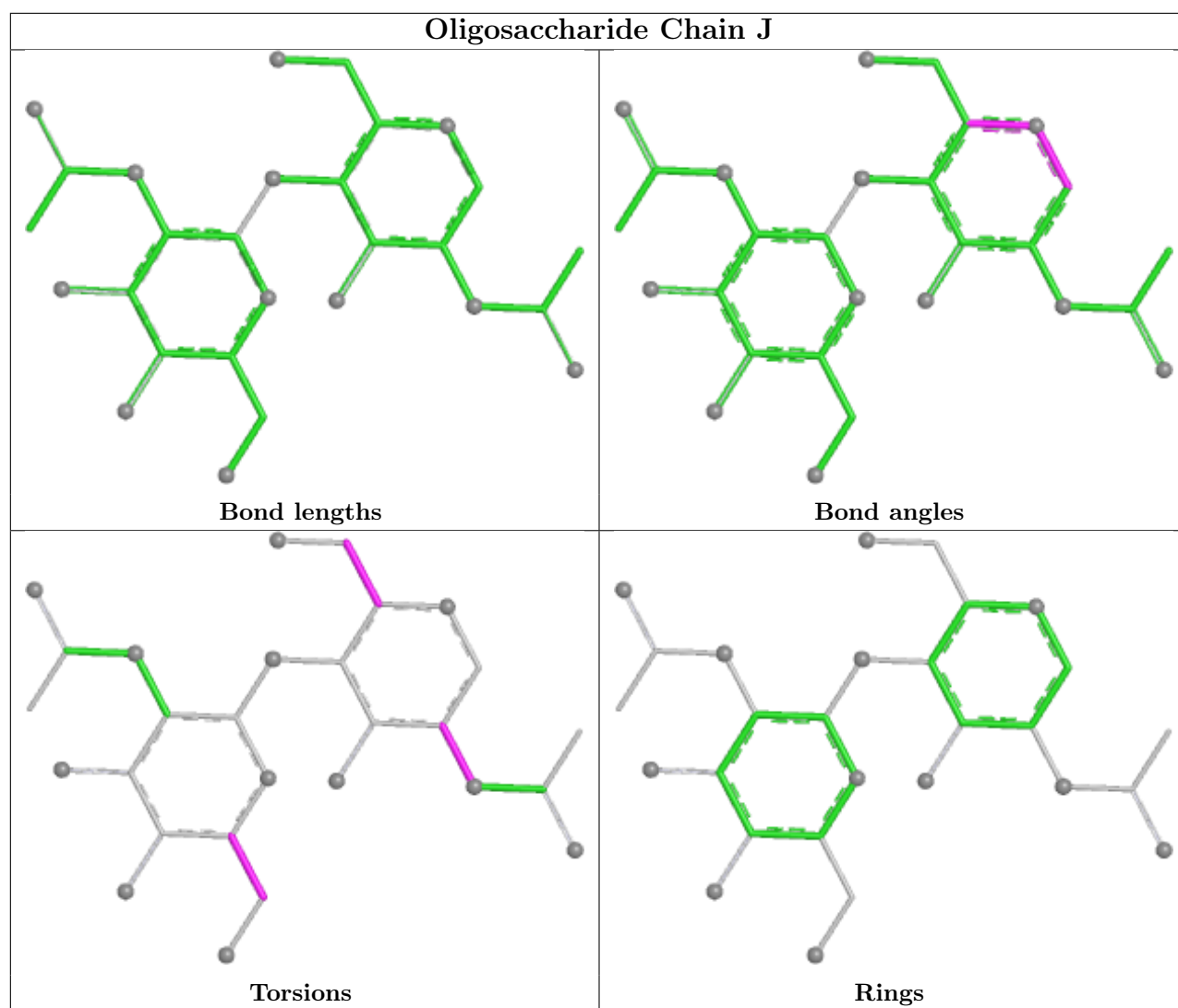
There are no ring outliers.

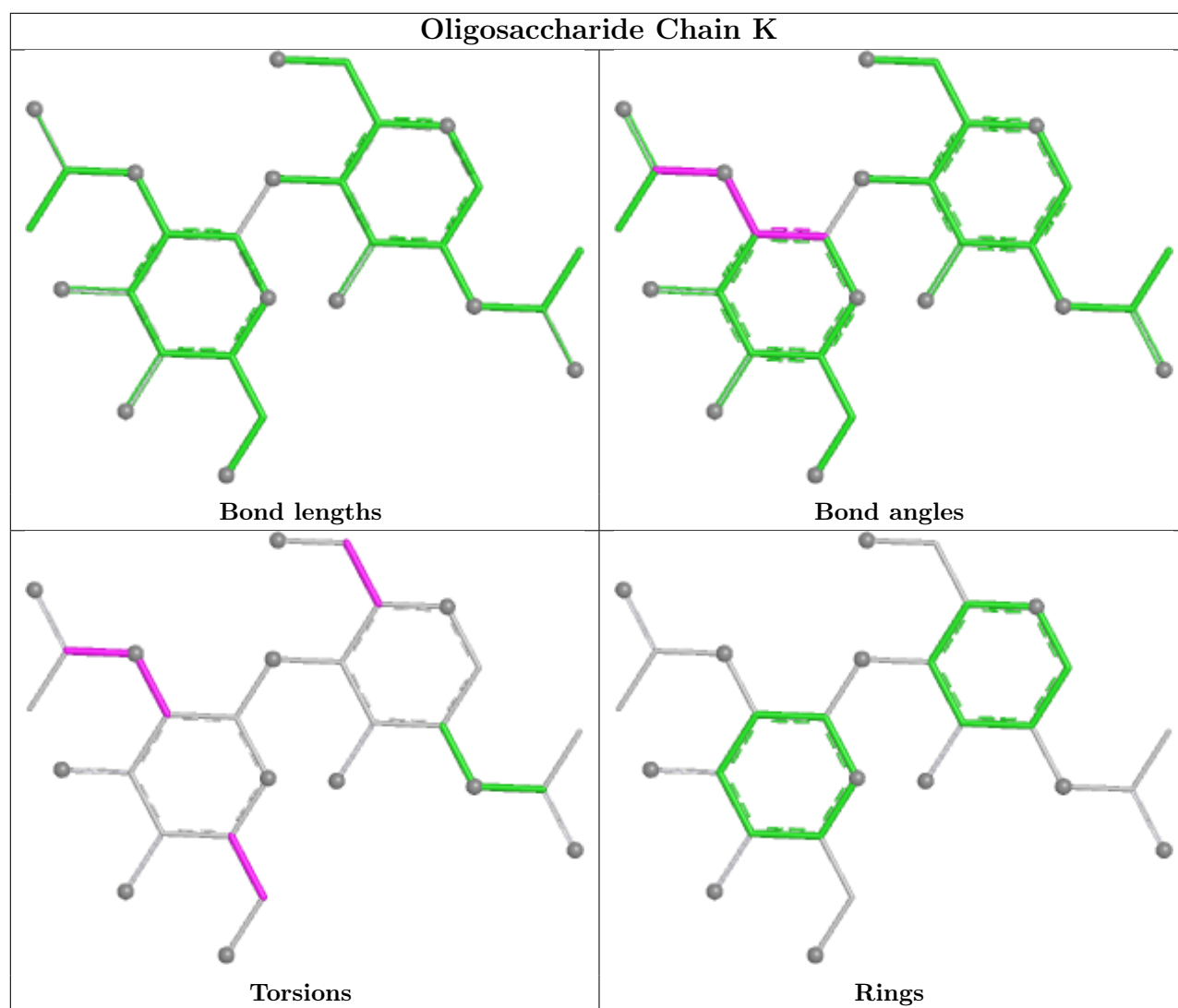
10 monomers are involved in 9 short contacts:

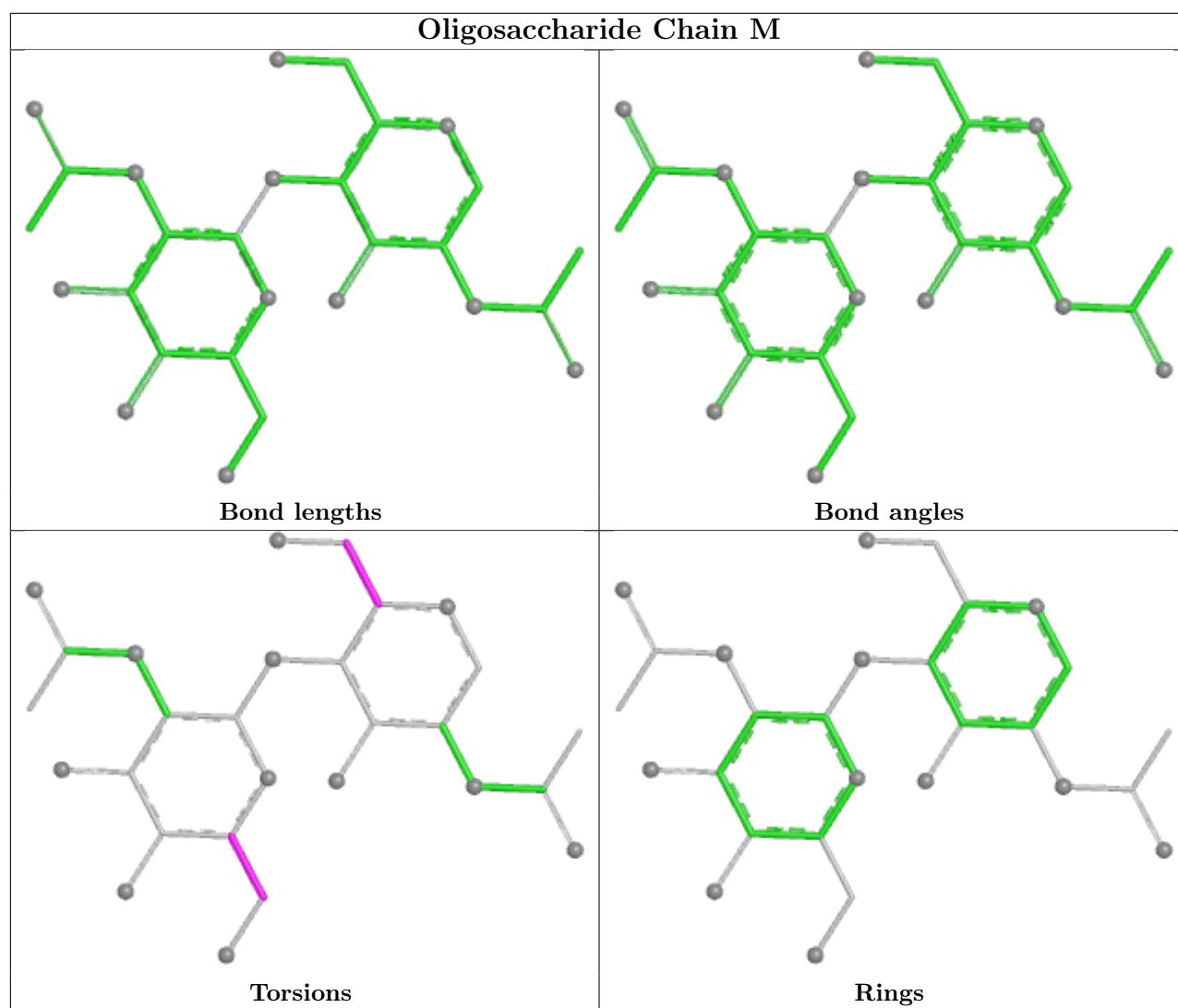
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1	NAG	1	0
4	W	2	NAG	1	0
4	K	2	NAG	1	0
5	I	3	BMA	1	0
4	V	1	NAG	2	0
6	O	1	NAG	1	0
4	V	2	NAG	1	0
4	J	1	NAG	1	0
4	J	2	NAG	1	0
4	G	2	NAG	1	0

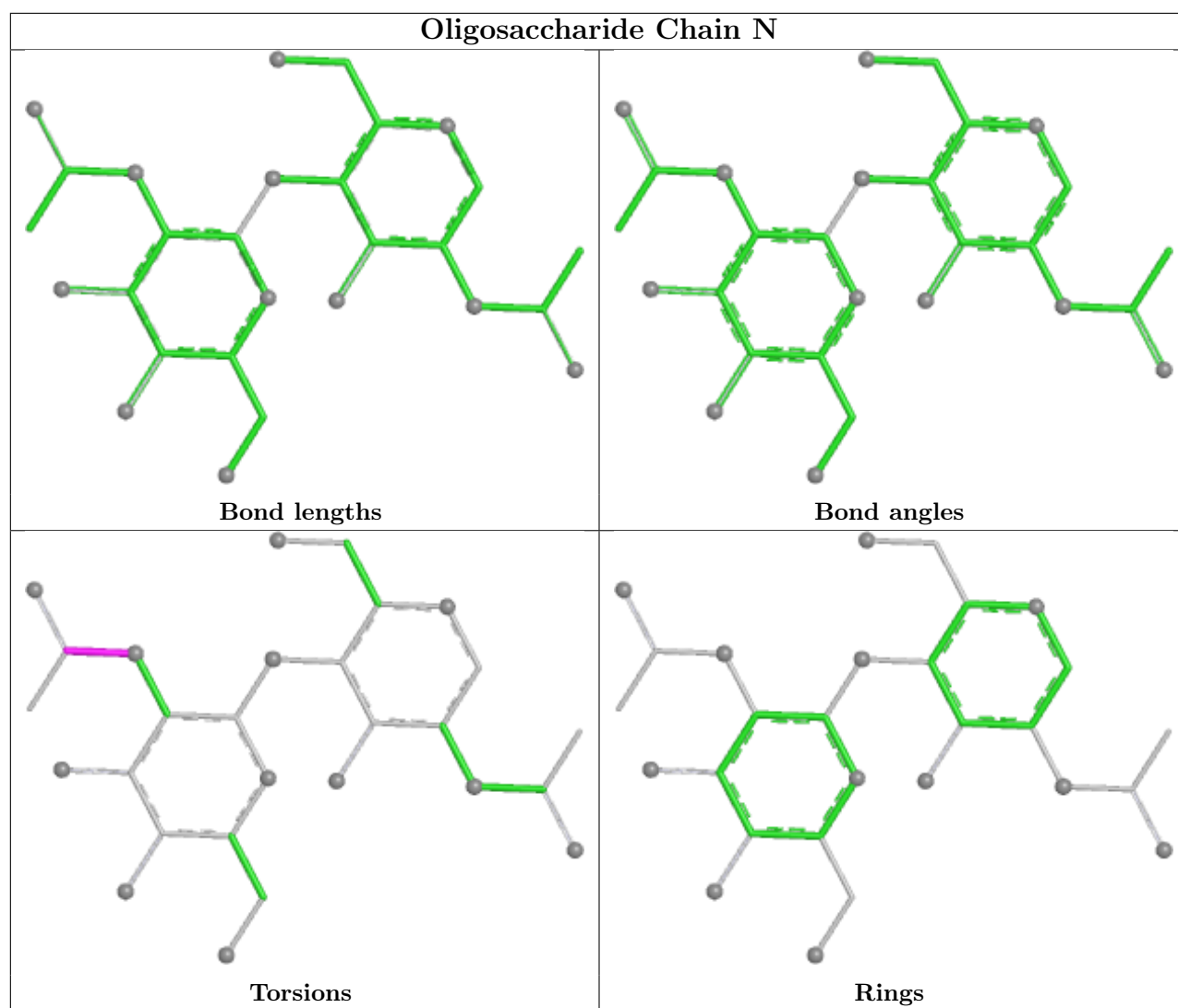
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

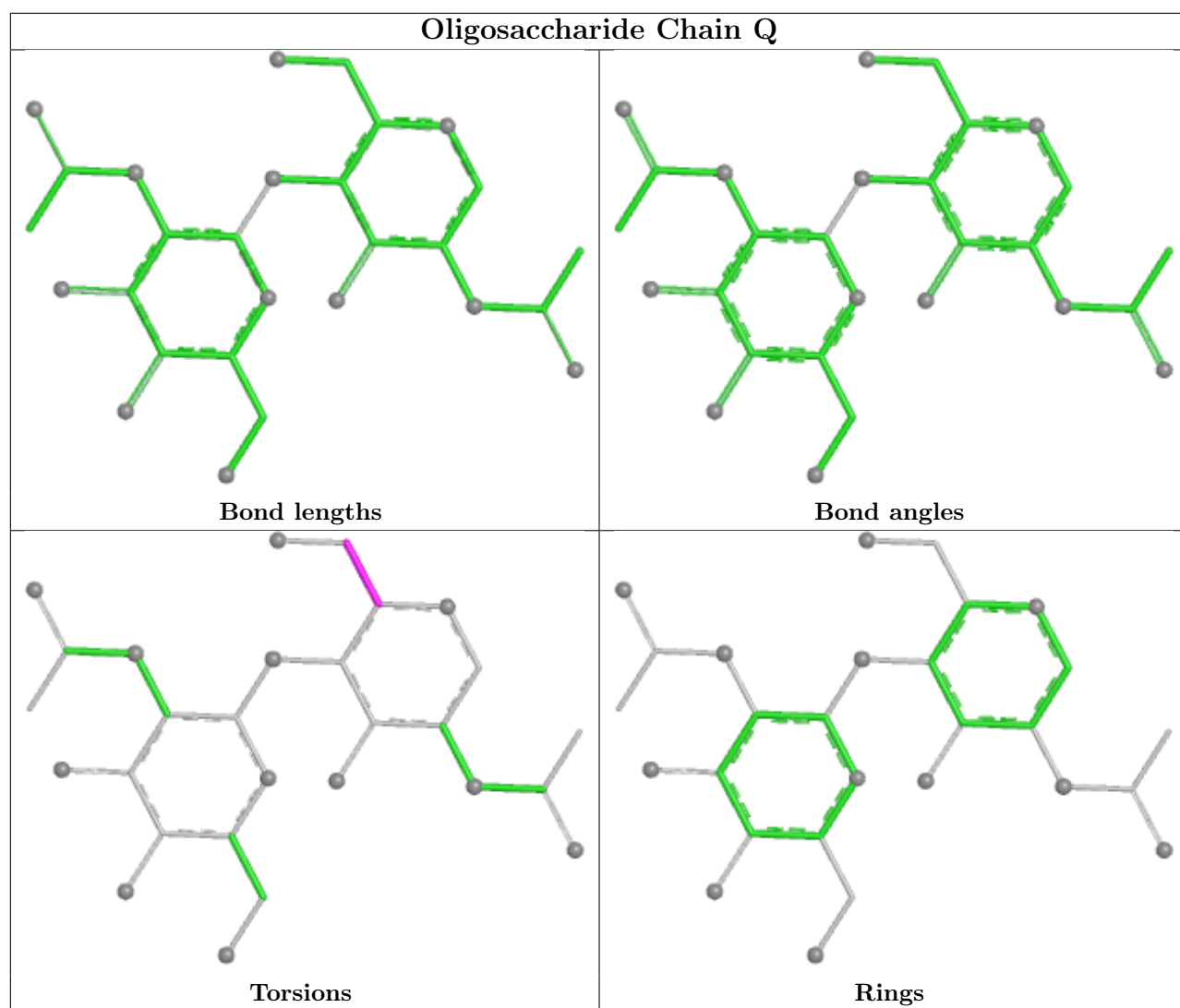


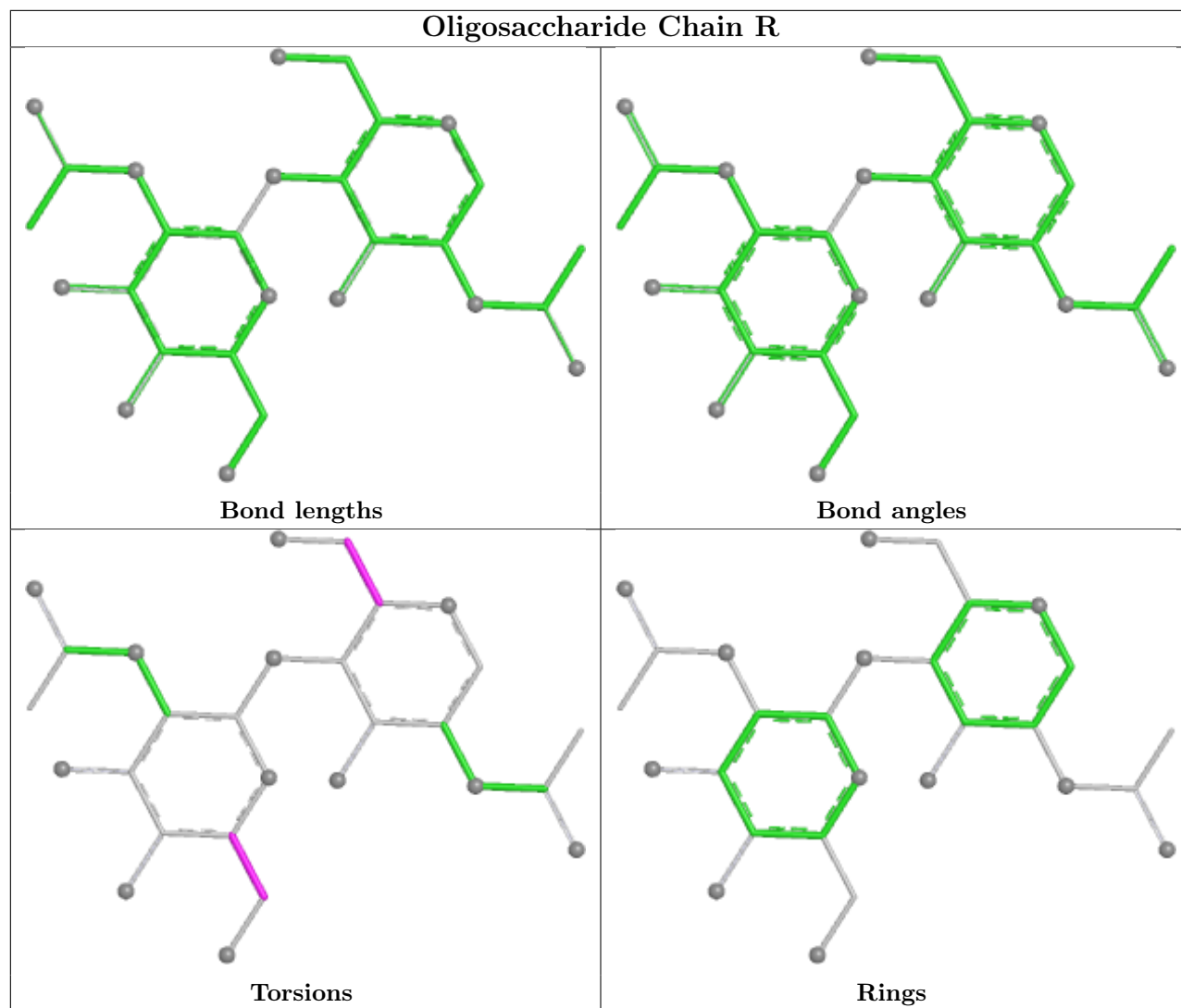


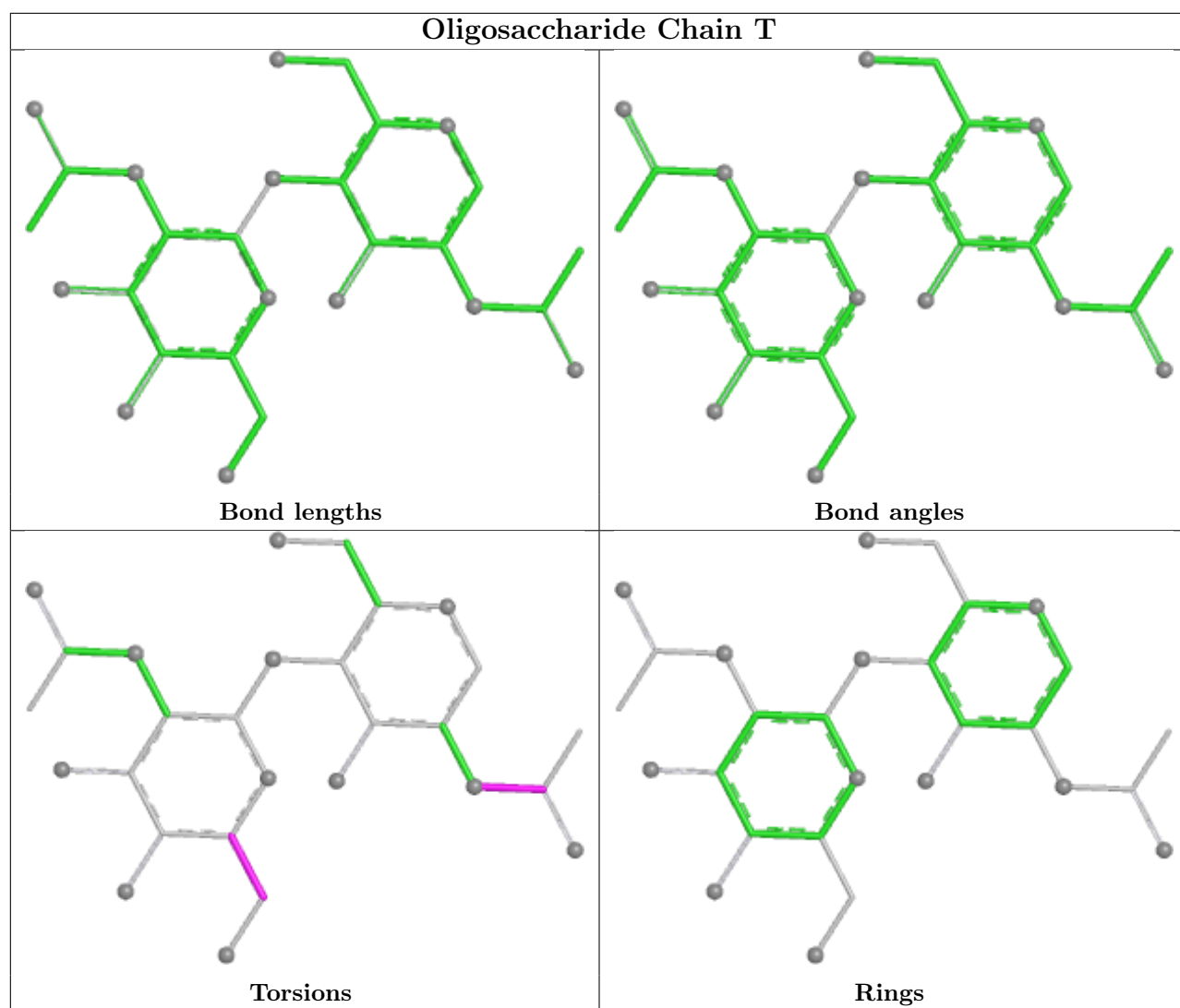


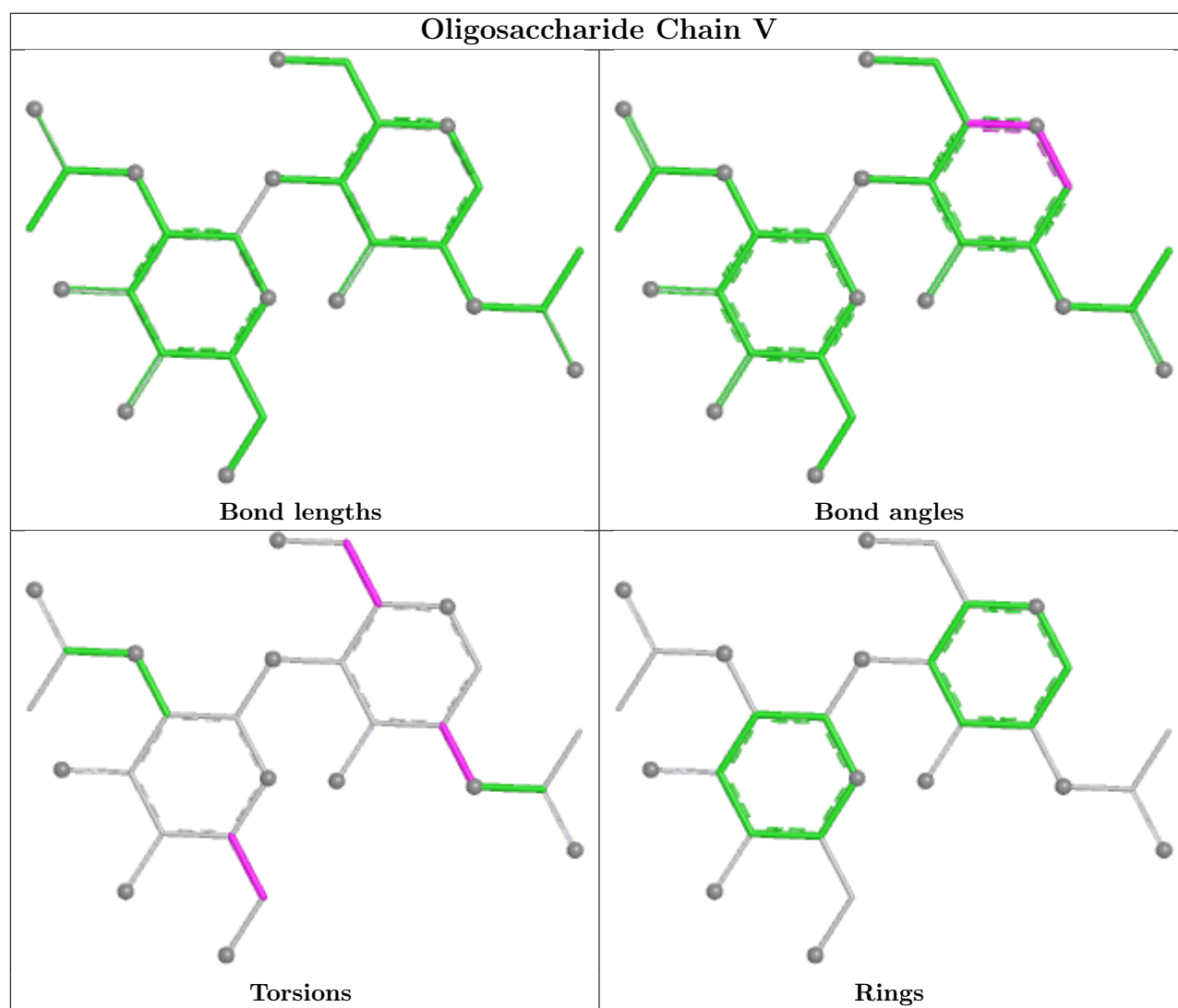


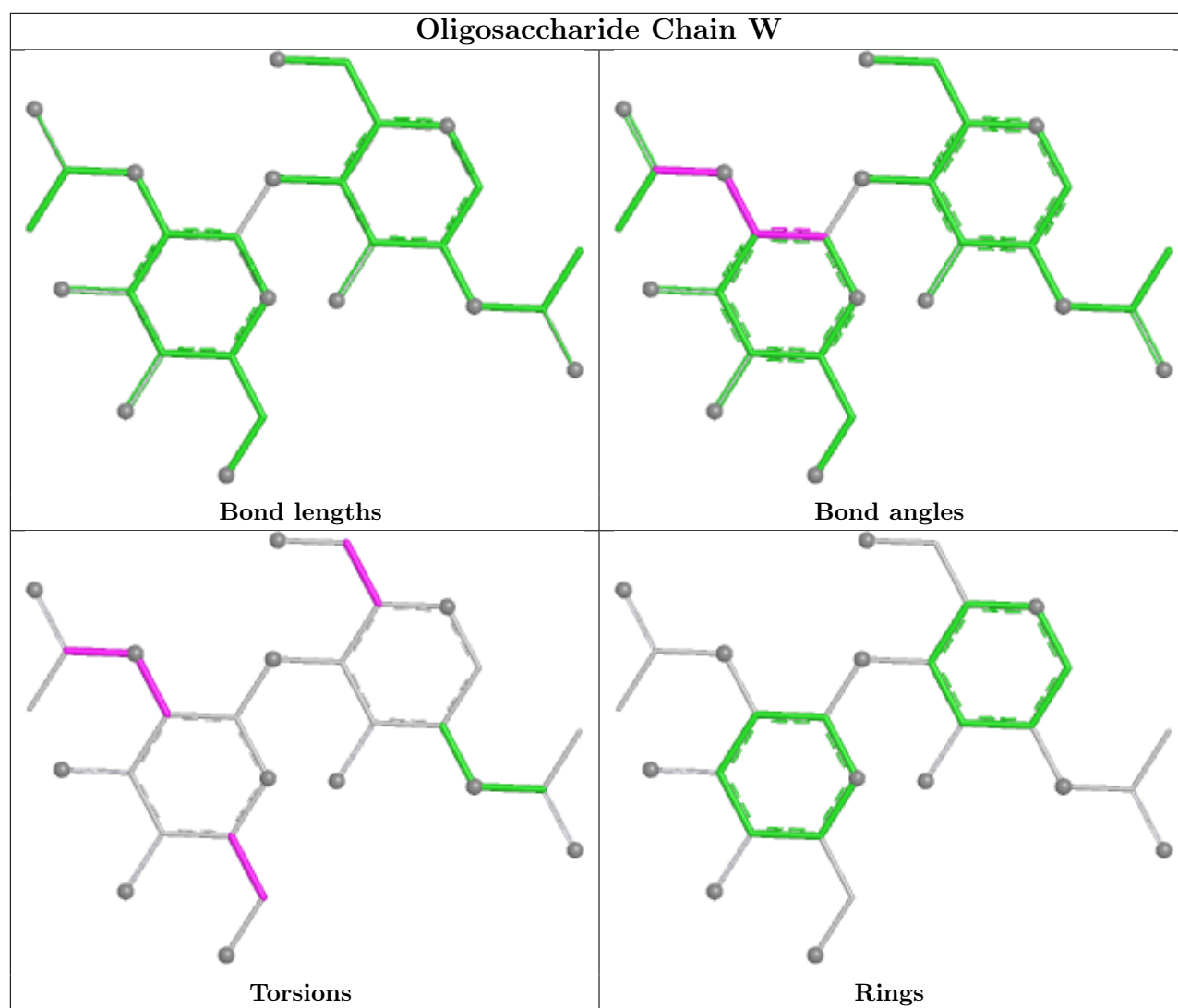


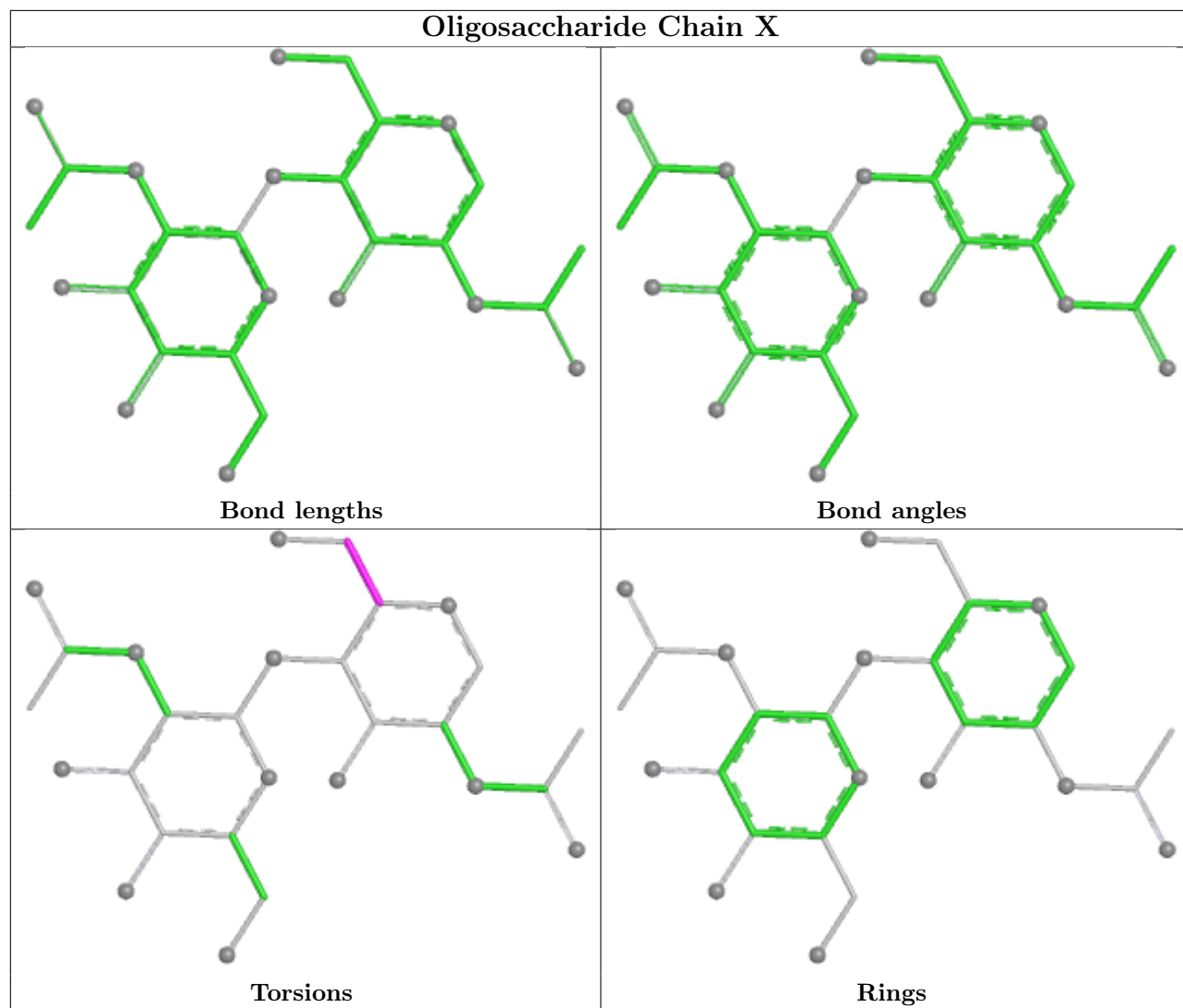


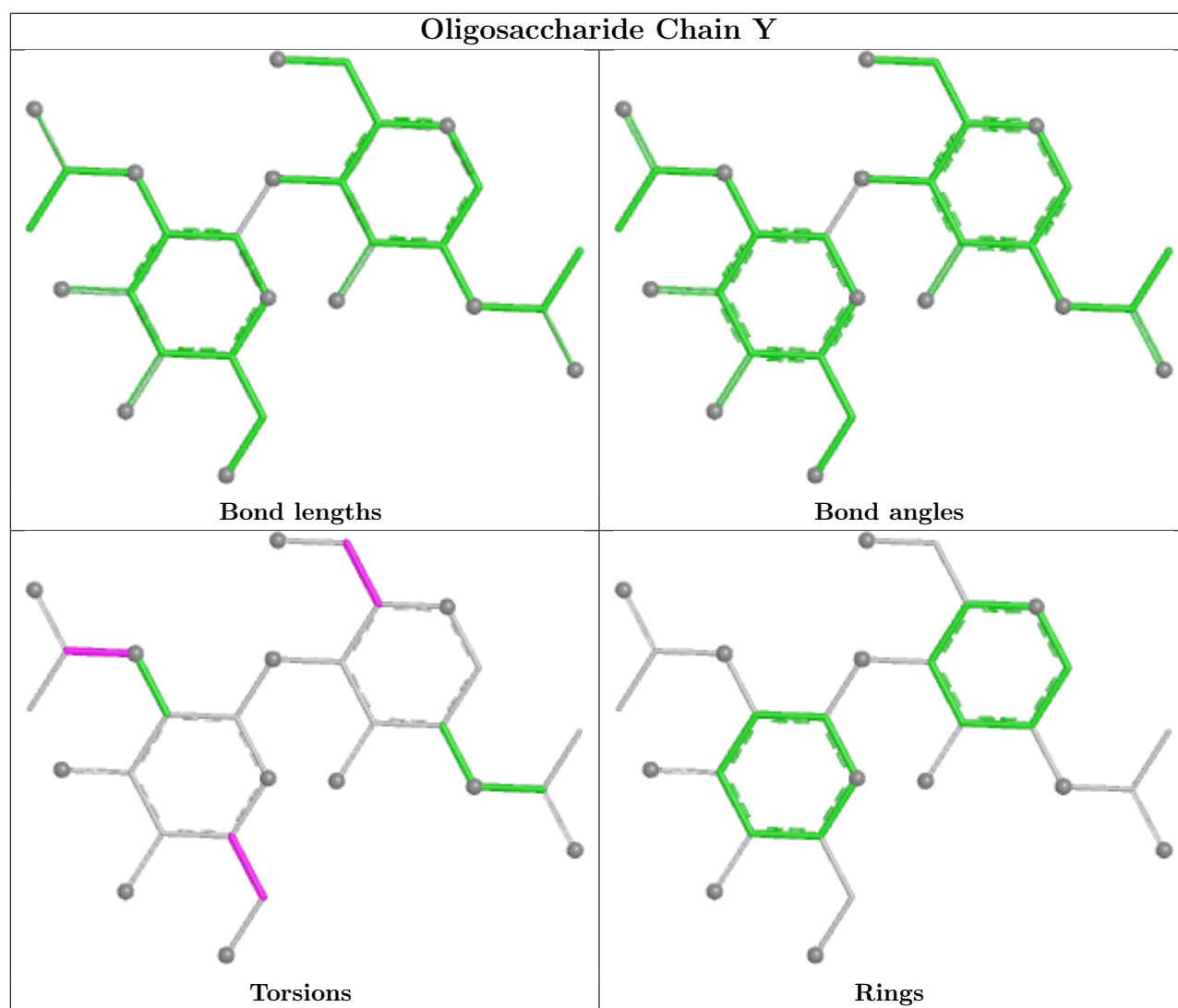


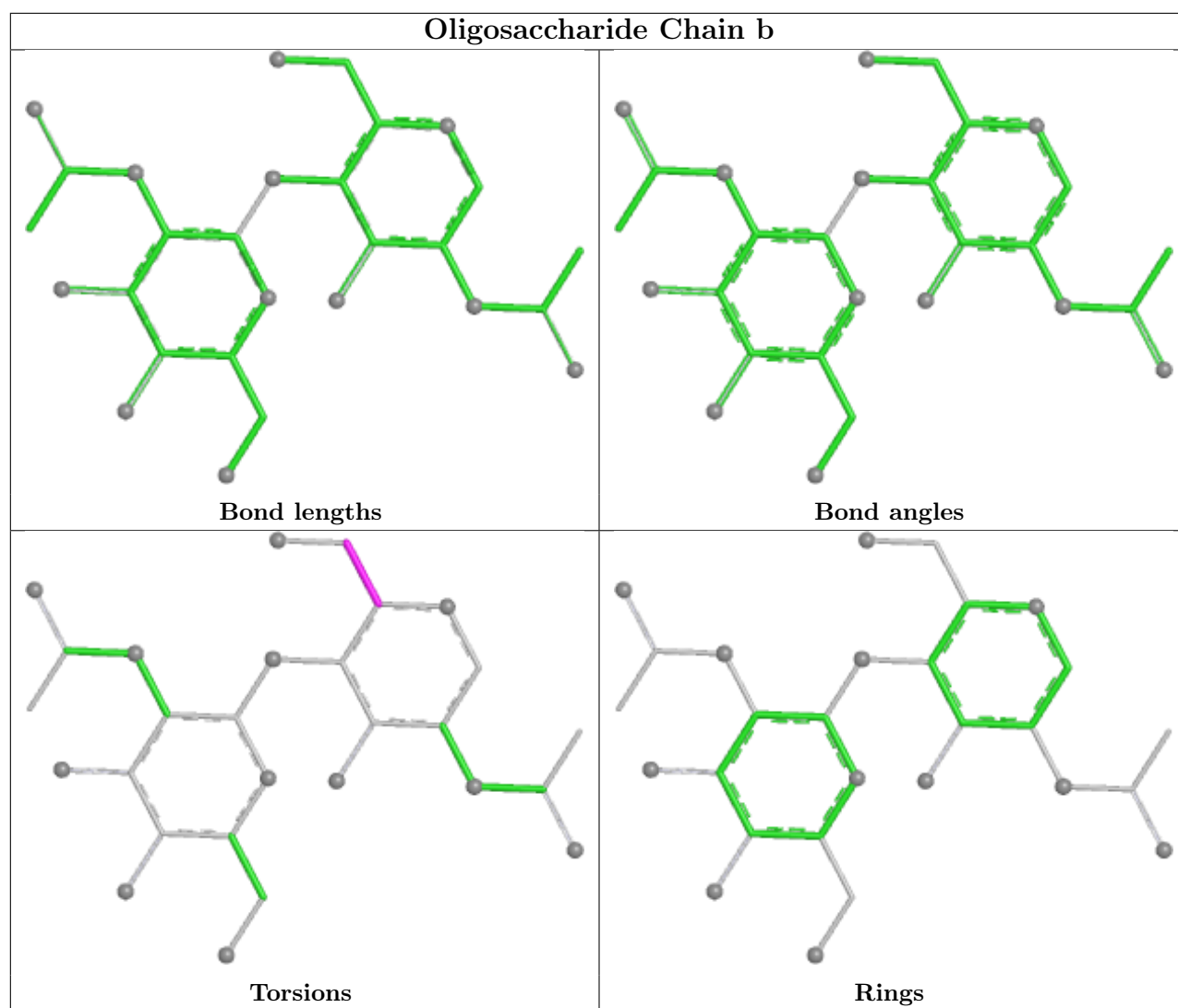


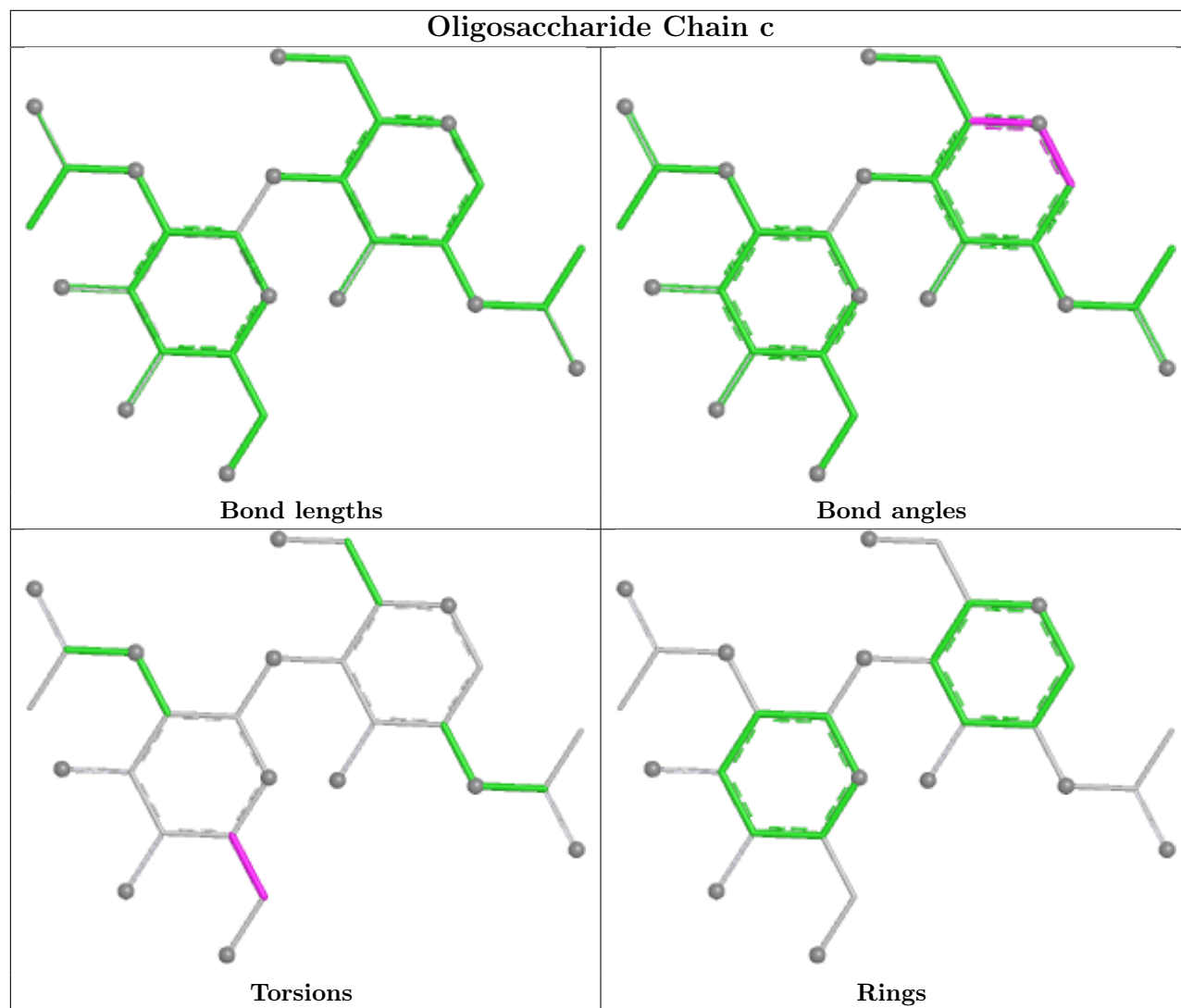


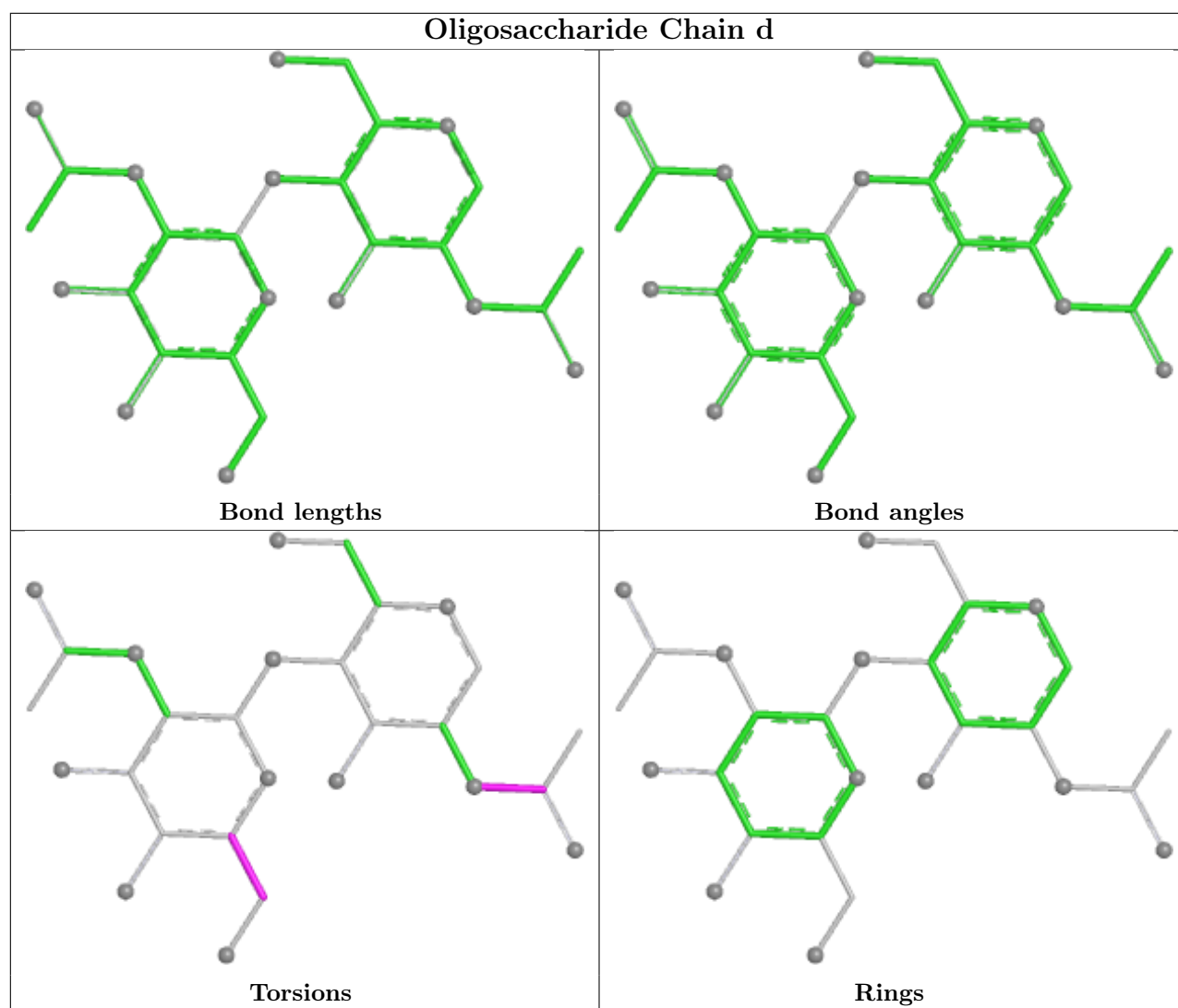


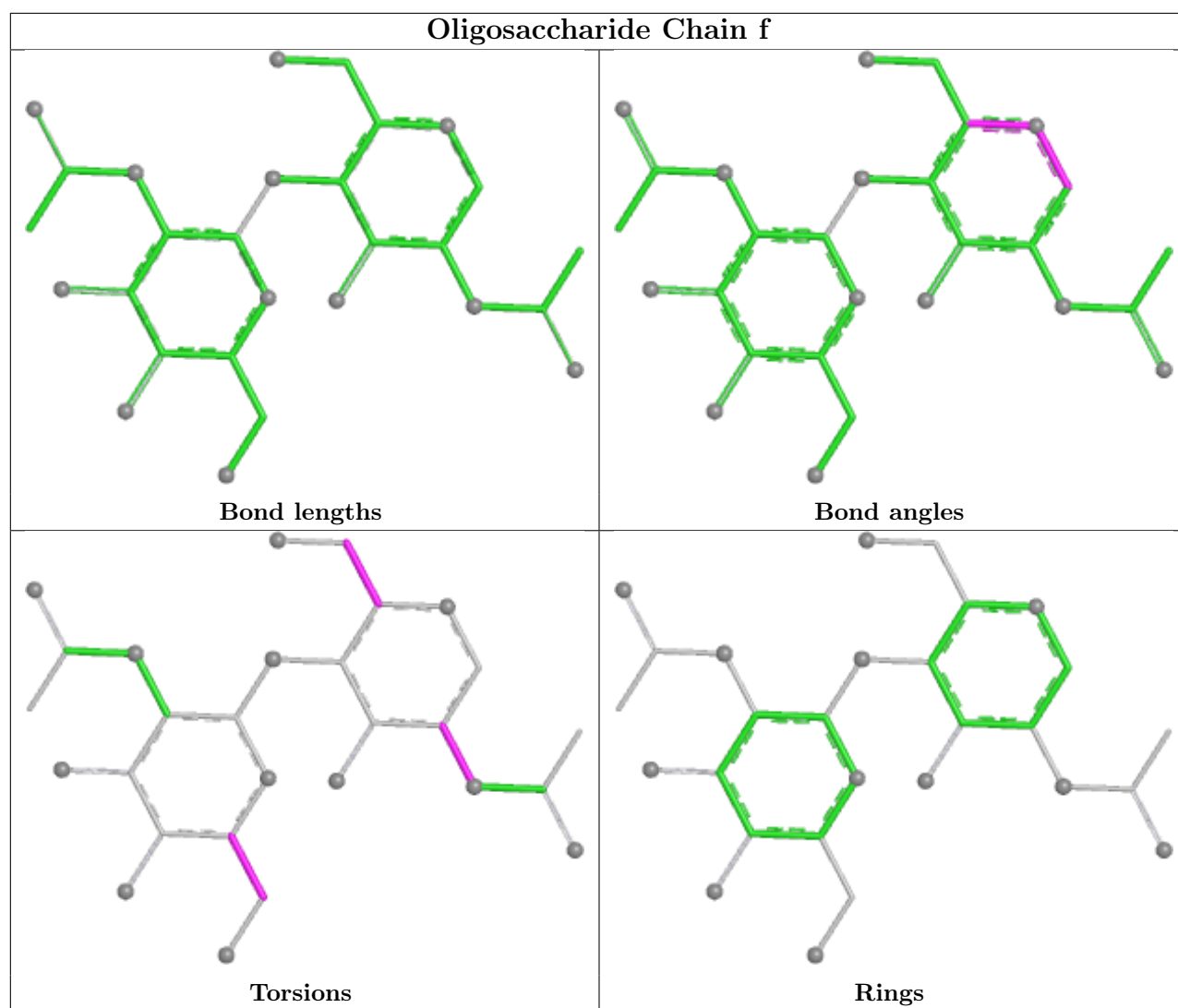


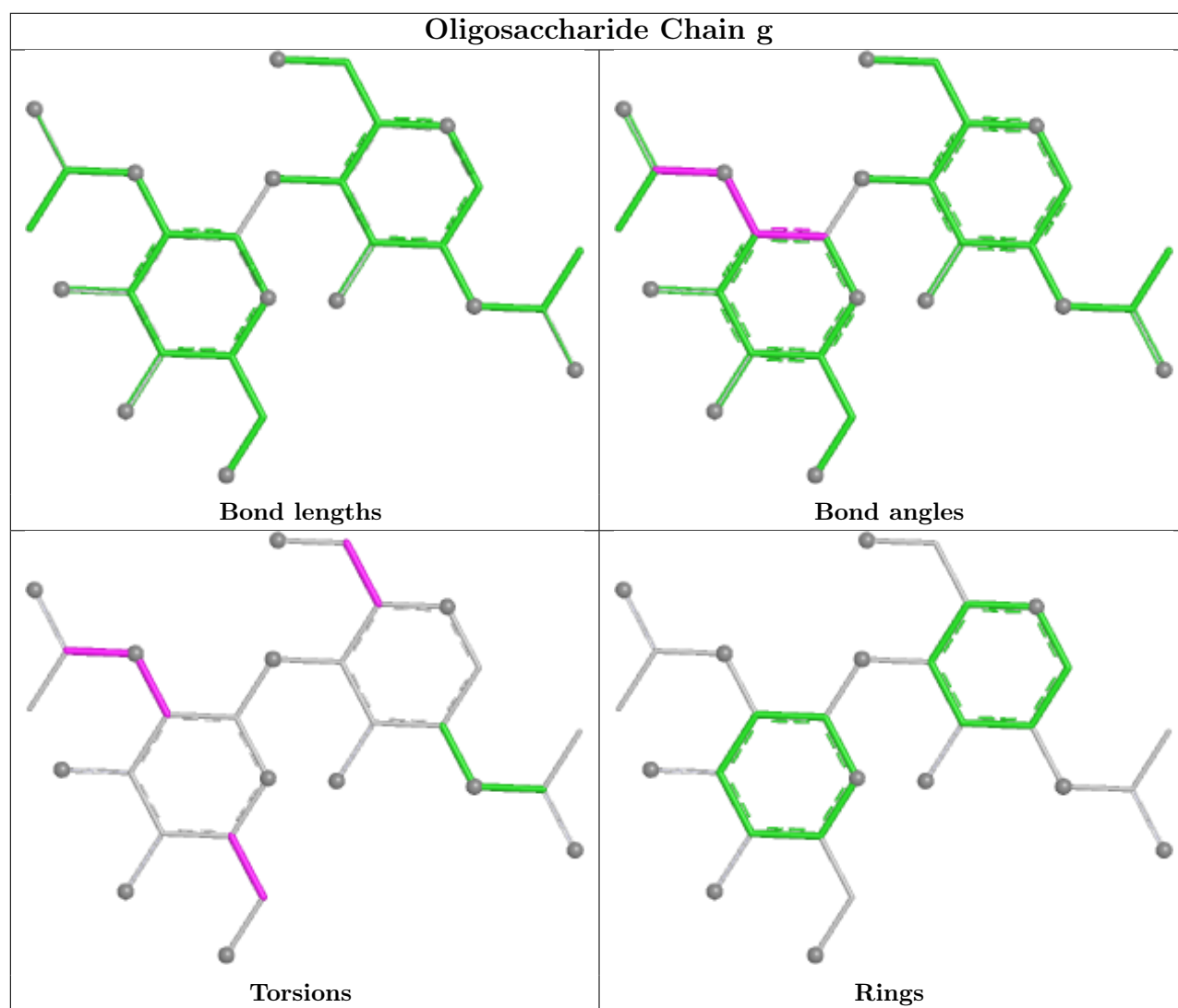


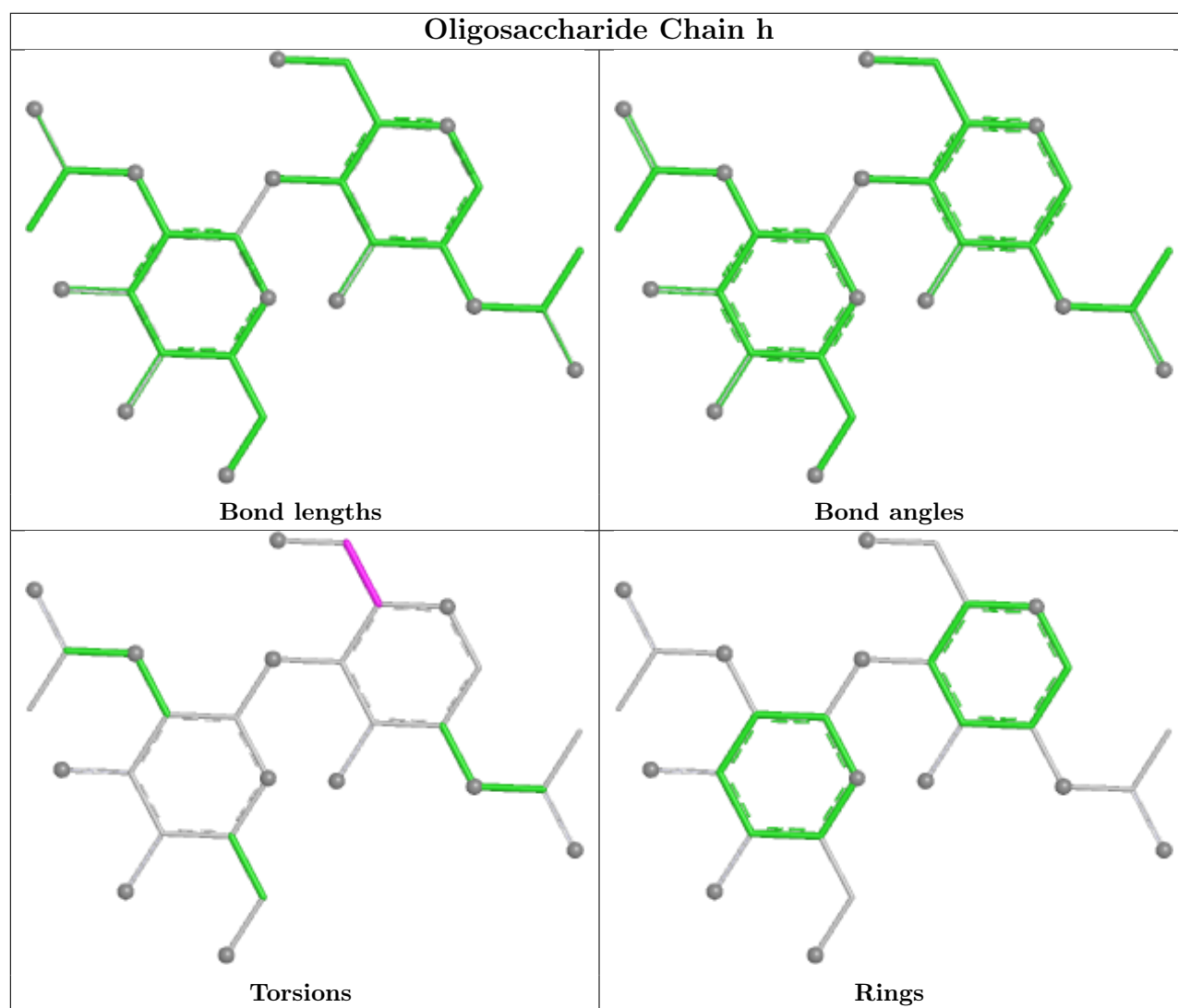


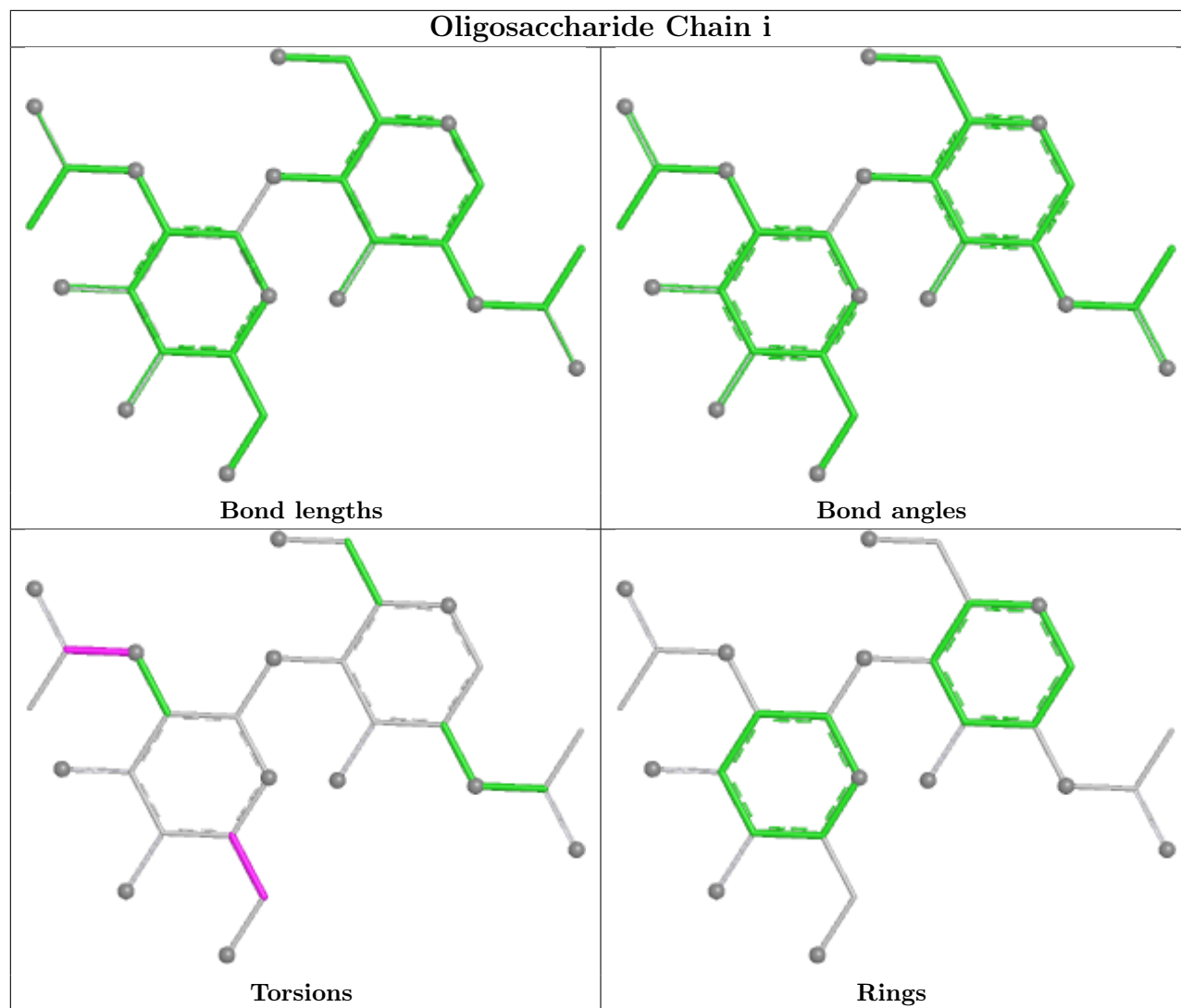


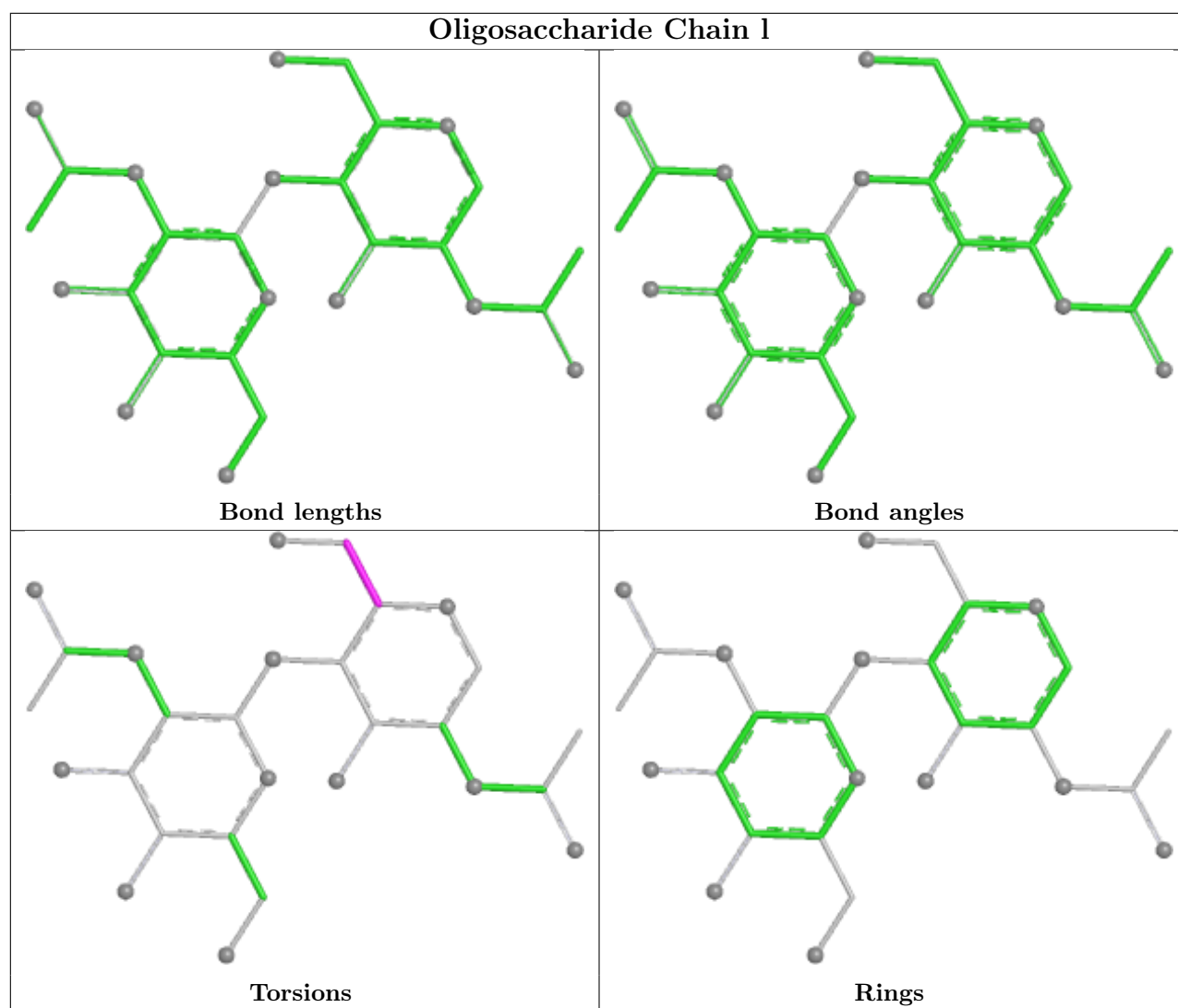


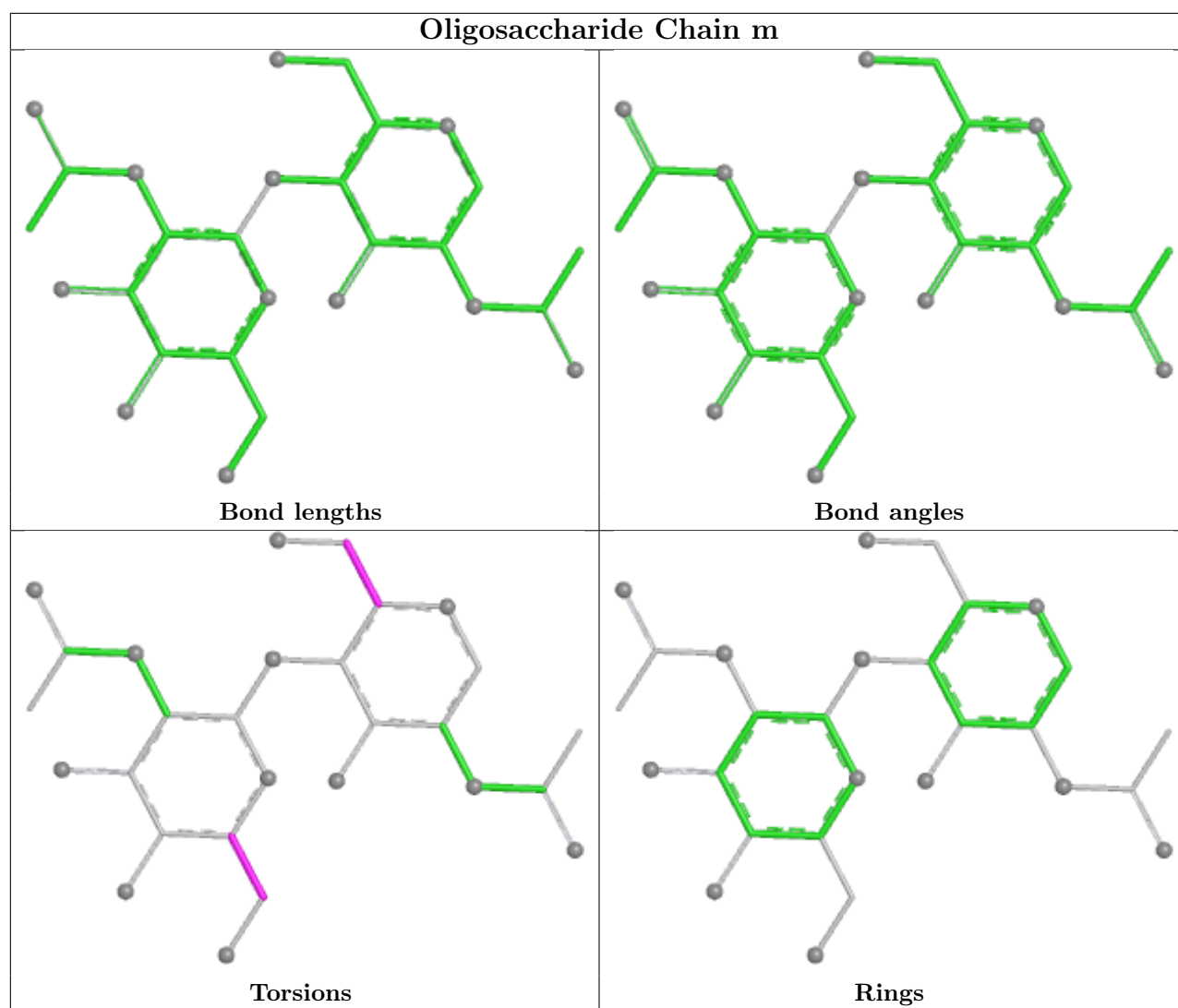


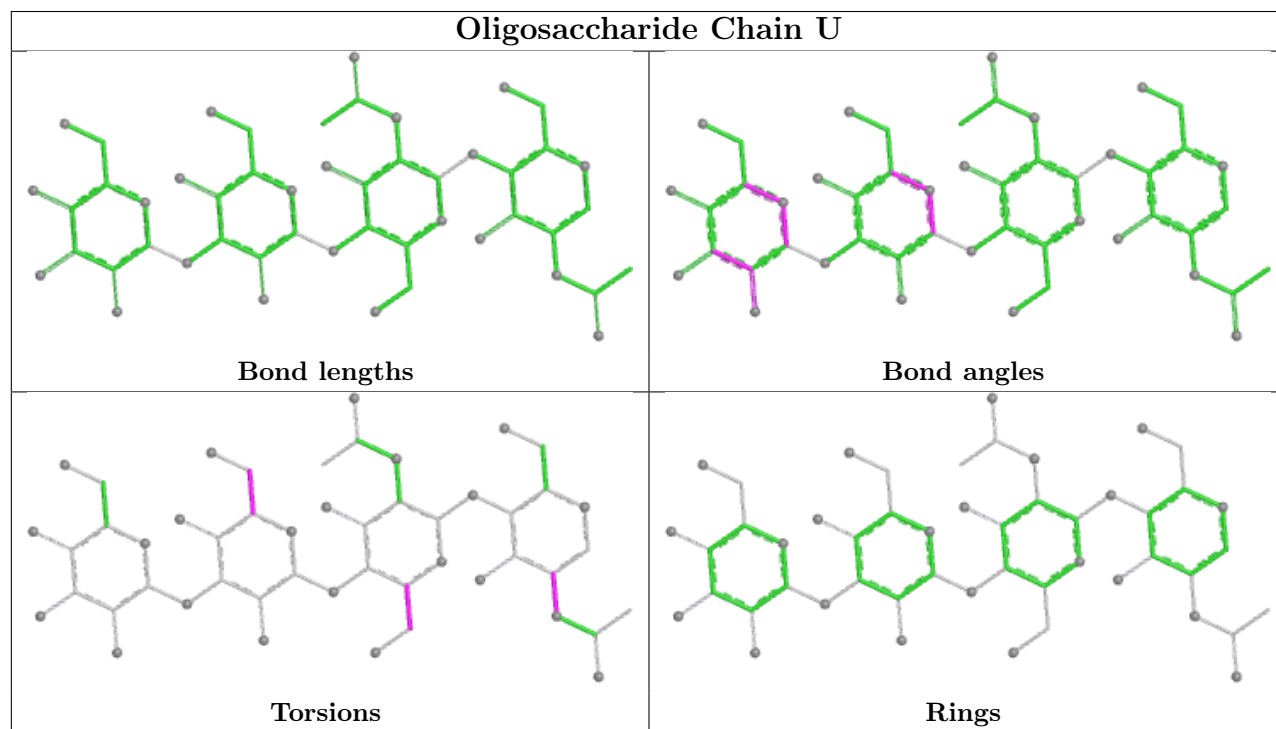
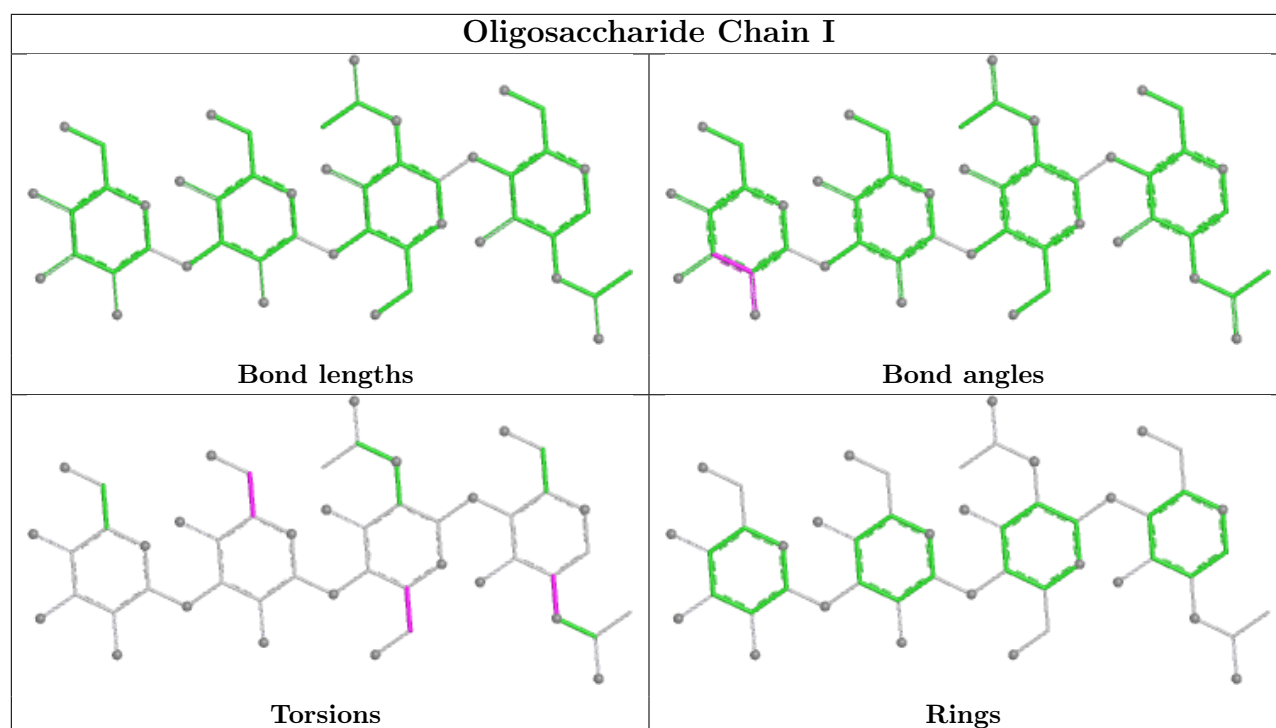


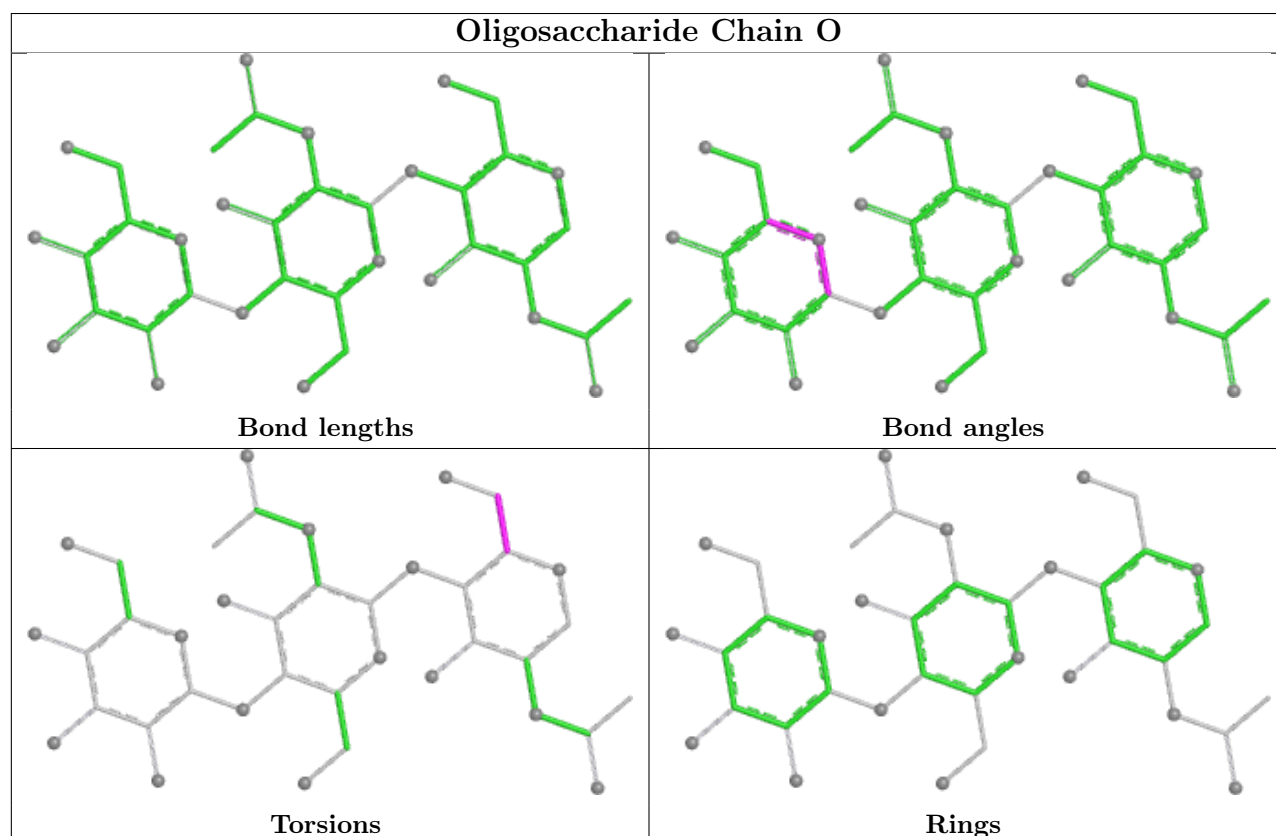
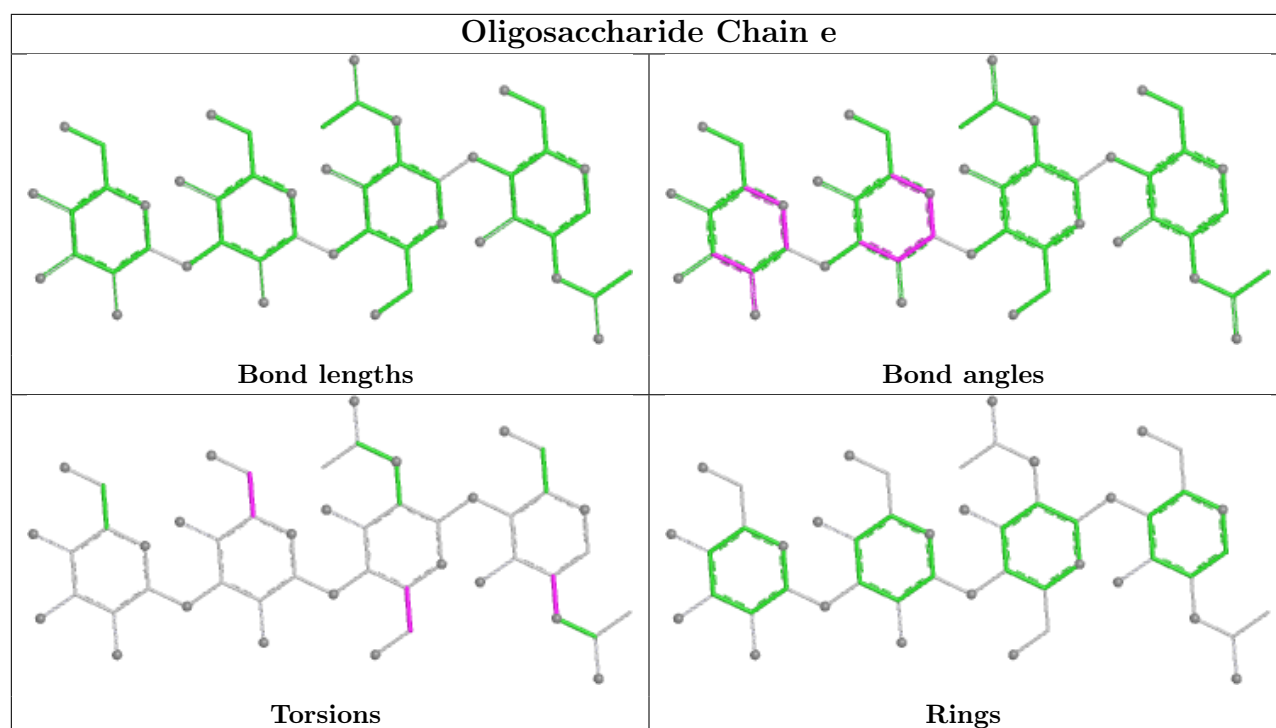


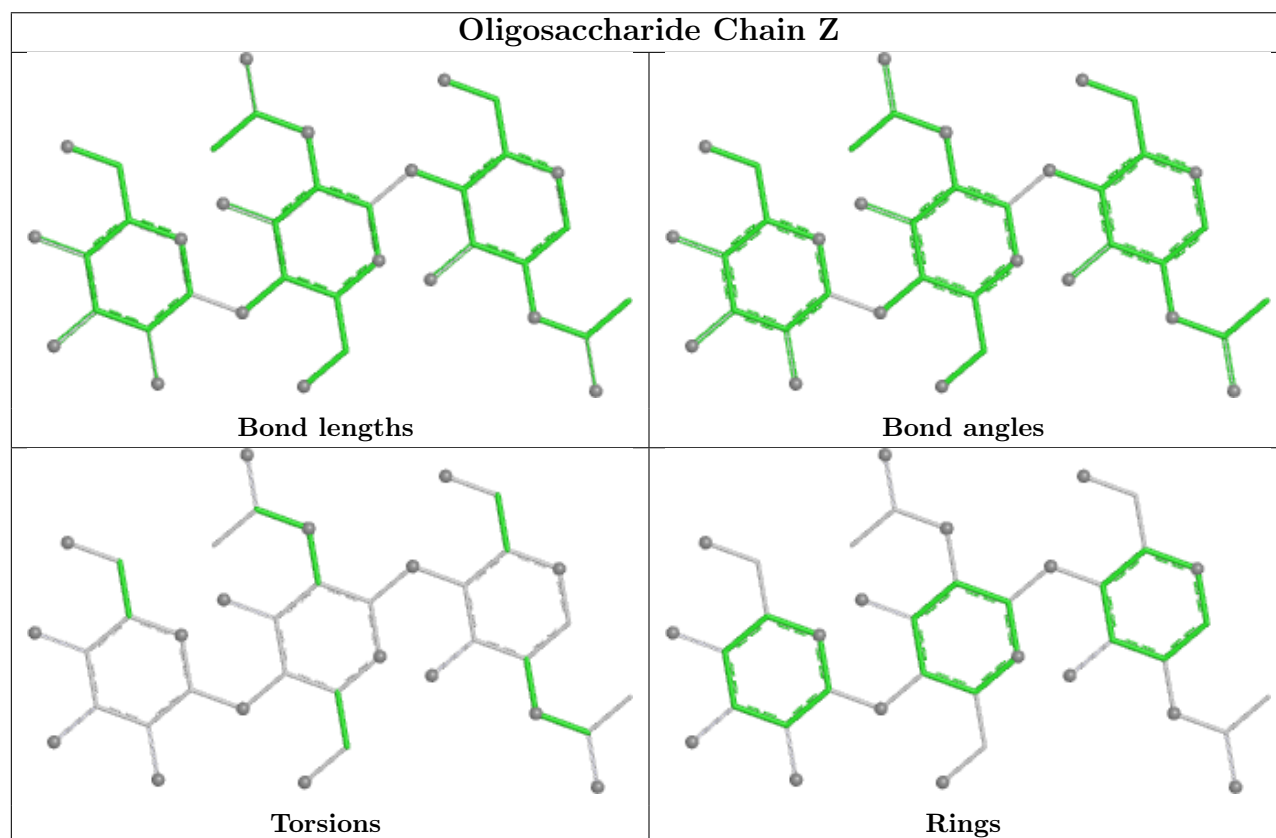
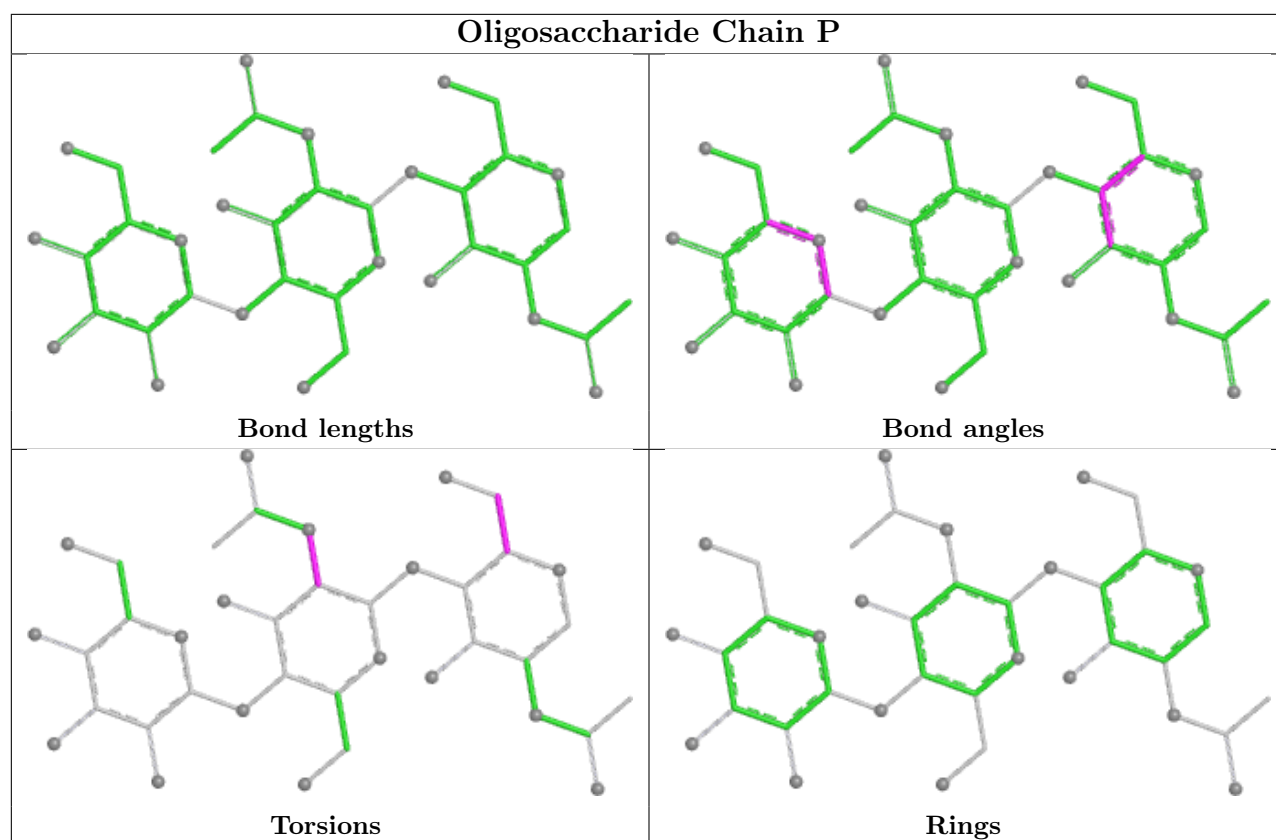


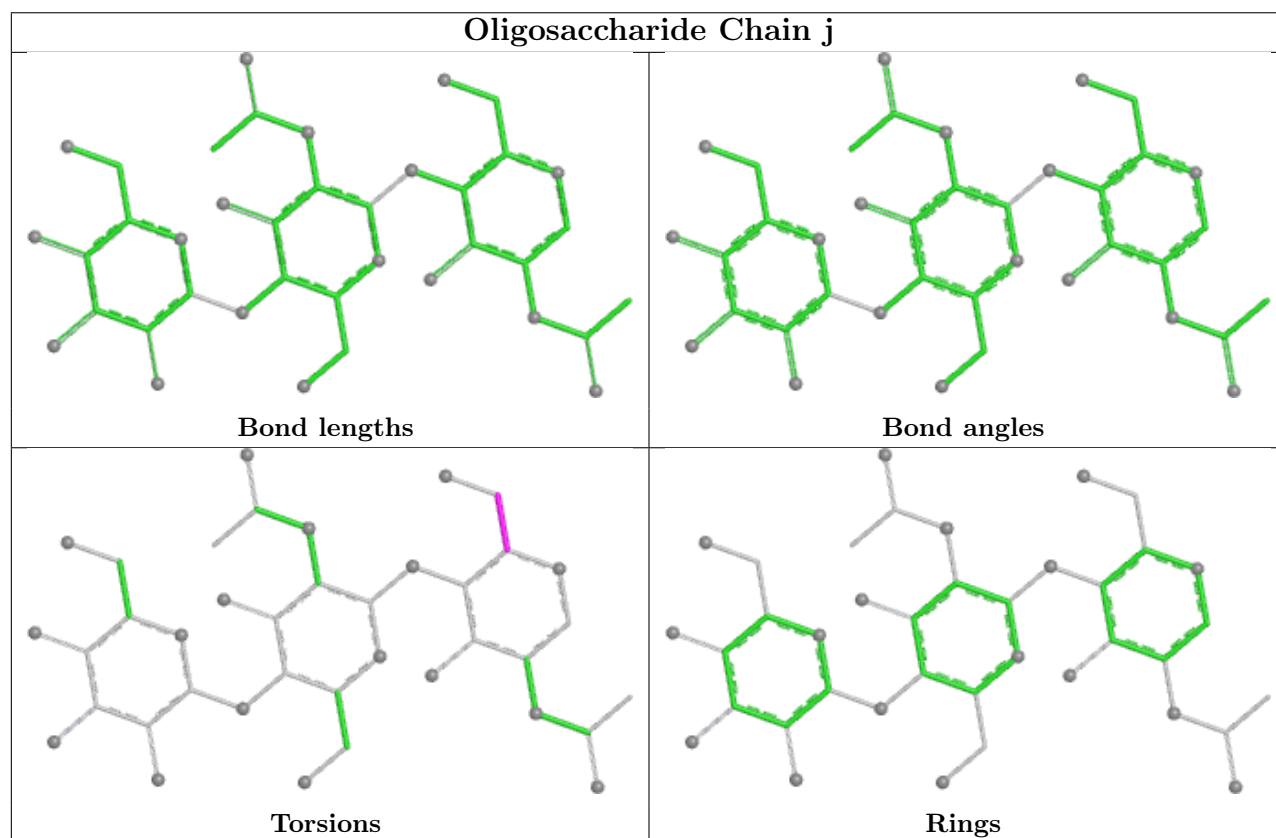
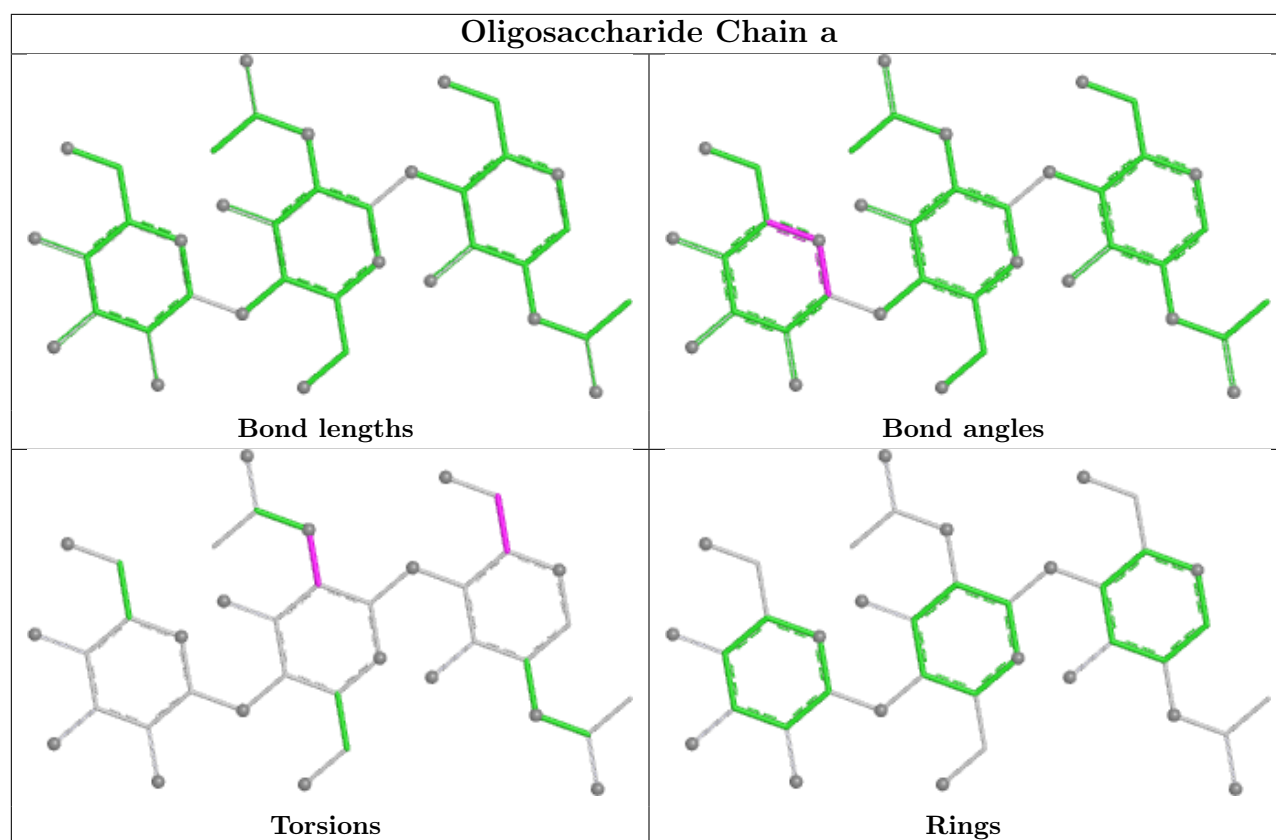


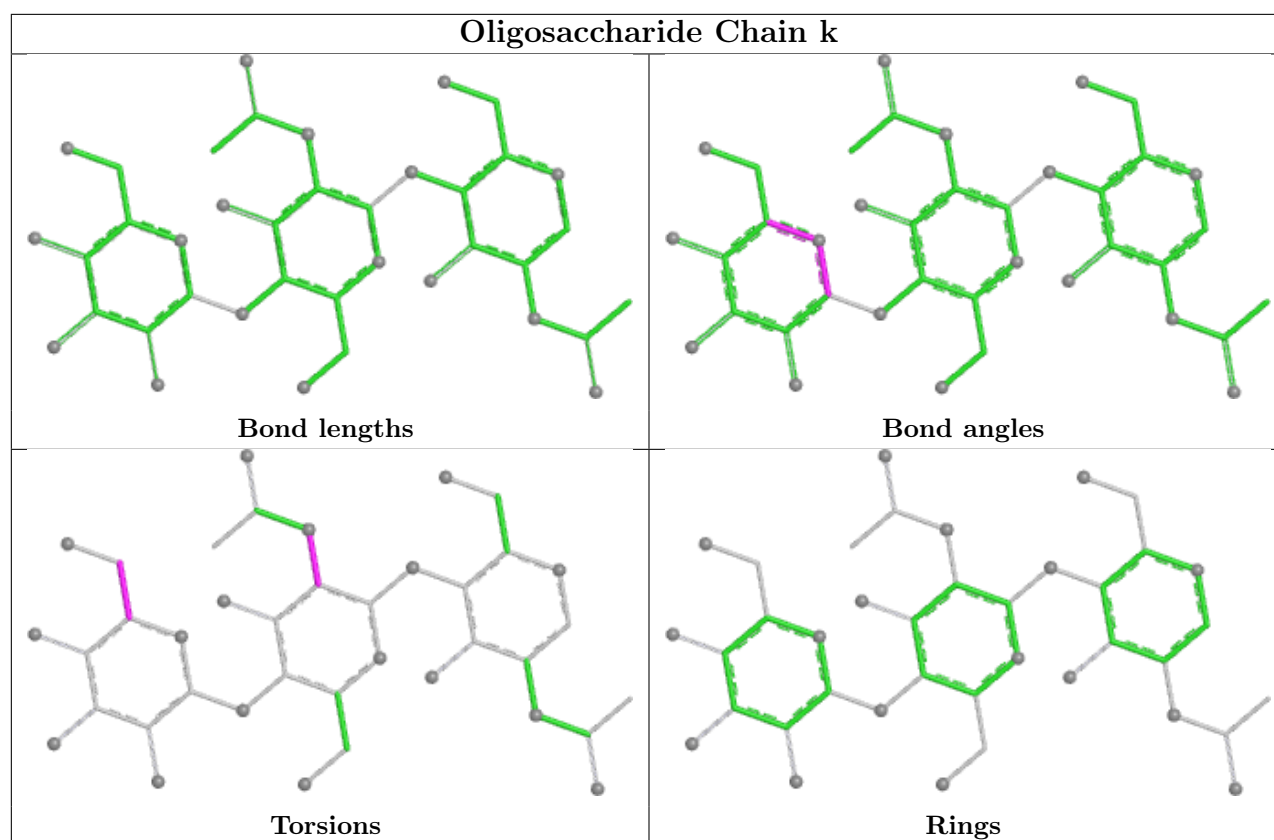












5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
7	NAG	A	1302	1	14,14,15	0.19	0	17,19,21	0.48	0
7	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.52	0
7	NAG	A	1301	1	14,14,15	0.17	0	17,19,21	0.50	0
7	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.53	0
7	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.67	1 (5%)
7	NAG	S	1303	1	14,14,15	0.21	0	17,19,21	0.53	0
7	NAG	A	1304	1	14,14,15	0.31	0	17,19,21	0.51	0
7	NAG	S	1304	1	14,14,15	0.30	0	17,19,21	0.53	0
7	NAG	B	1301	1	14,14,15	0.60	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1305	1	14,14,15	0.42	0	17,19,21	0.75	0
7	NAG	B	1306	1	14,14,15	0.91	1 (7%)	17,19,21	1.17	1 (5%)
7	NAG	S	1301	1	14,14,15	0.24	0	17,19,21	0.46	0
7	NAG	S	1305	1	14,14,15	0.25	0	17,19,21	0.54	0
7	NAG	S	1302	1	14,14,15	0.23	0	17,19,21	0.52	0
7	NAG	A	1303	1	14,14,15	0.20	0	17,19,21	0.55	0
7	NAG	S	1306	1	14,14,15	0.88	1 (7%)	17,19,21	1.15	1 (5%)
7	NAG	A	1305	1	14,14,15	0.53	0	17,19,21	0.79	0
7	NAG	A	1306	1	14,14,15	0.90	1 (7%)	17,19,21	1.18	1 (5%)

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
7	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	S	1303	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	S	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1306	1	-	4/6/23/26	0/1/1/1
7	NAG	S	1301	1	-	4/6/23/26	0/1/1/1
7	NAG	S	1305	1	-	3/6/23/26	0/1/1/1
7	NAG	S	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
7	NAG	S	1306	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1306	NAG	O5-C1	2.95	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1306	NAG	O5-C1	2.94	1.48	1.43
7	S	1306	NAG	O5-C1	2.82	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1306	NAG	C1-O5-C5	4.39	118.07	112.19
7	B	1306	NAG	C1-O5-C5	4.34	118.00	112.19
7	S	1306	NAG	C1-O5-C5	4.23	117.86	112.19
7	B	1302	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1305	NAG	C1-C2-N2-C7
7	S	1301	NAG	O5-C5-C6-O6
7	A	1303	NAG	C4-C5-C6-O6
7	A	1301	NAG	O5-C5-C6-O6
7	B	1302	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

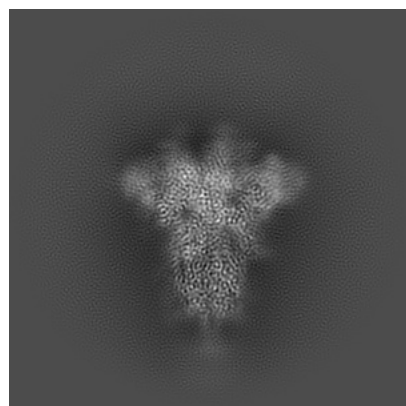
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44628. These allow visual inspection of the internal detail of the map and identification of artifacts.

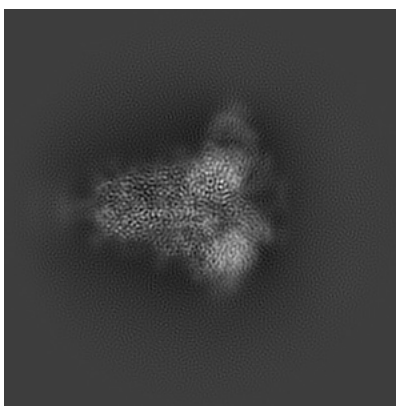
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

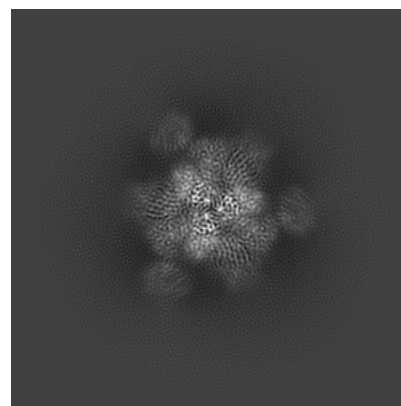
6.1.1 Primary map



X

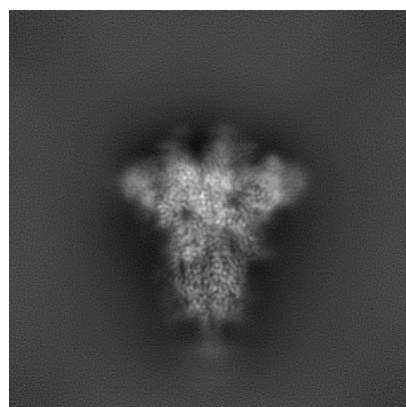


Y

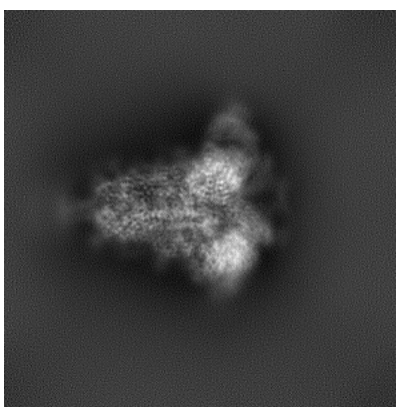


Z

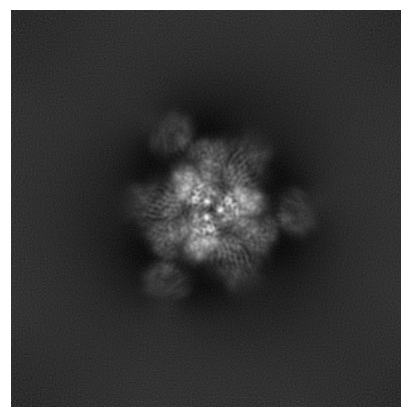
6.1.2 Raw map



X



Y

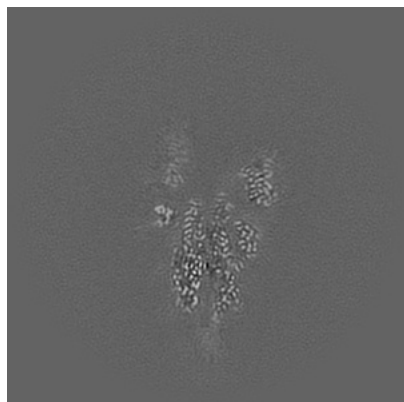


Z

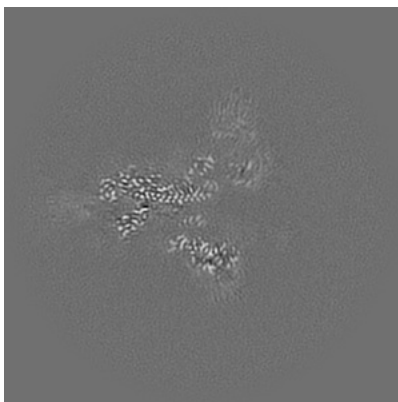
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

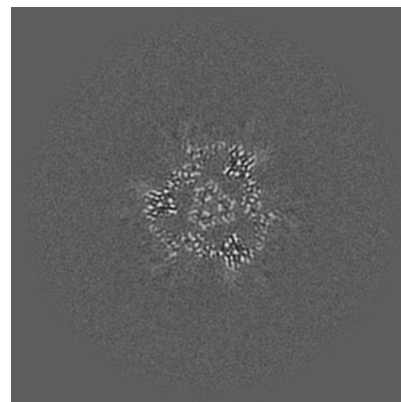
6.2.1 Primary map



X Index: 216

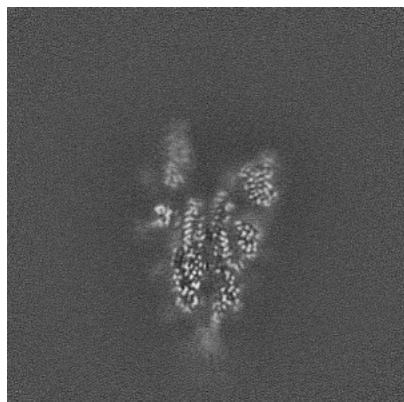


Y Index: 216

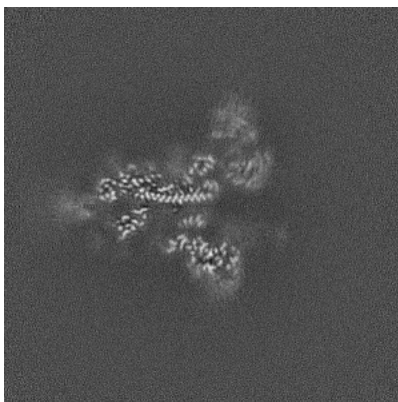


Z Index: 216

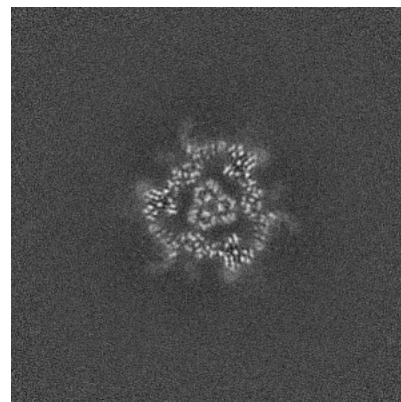
6.2.2 Raw map



X Index: 216



Y Index: 216

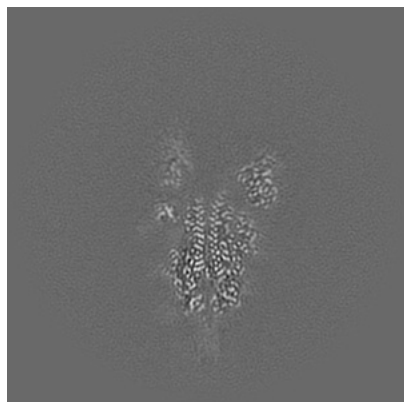


Z Index: 216

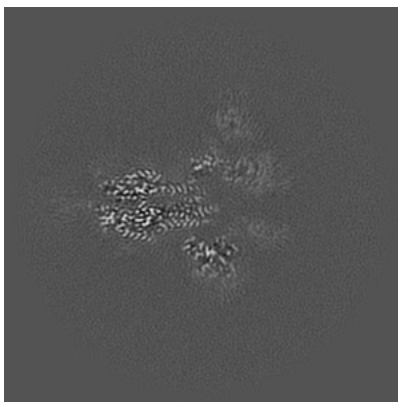
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

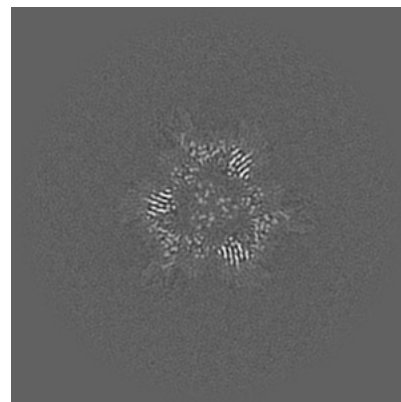
6.3.1 Primary map



X Index: 211

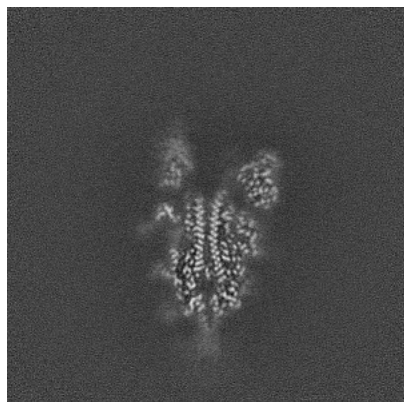


Y Index: 228

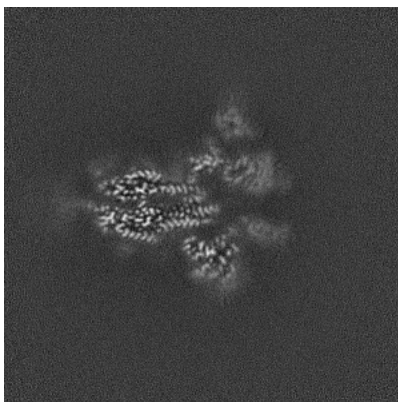


Z Index: 219

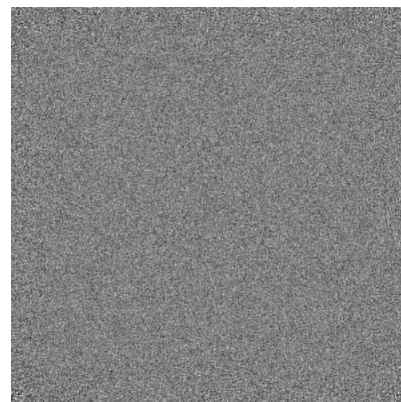
6.3.2 Raw map



X Index: 211



Y Index: 228

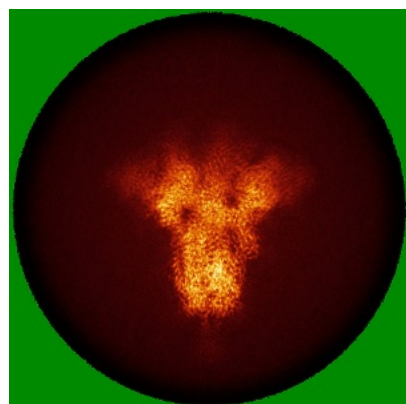


Z Index: 431

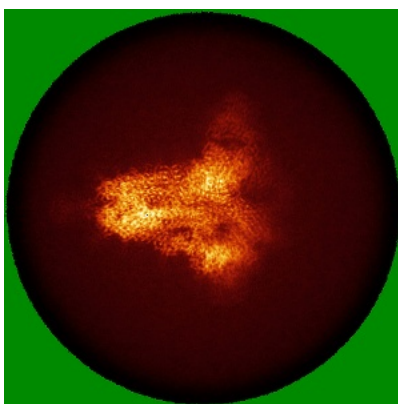
The images above show the largest variance slices of the map in three orthogonal directions.

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

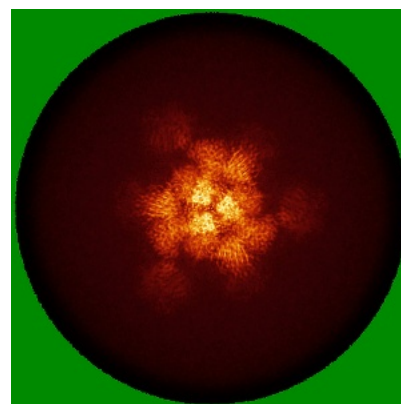
6.4.1 Primary map



X

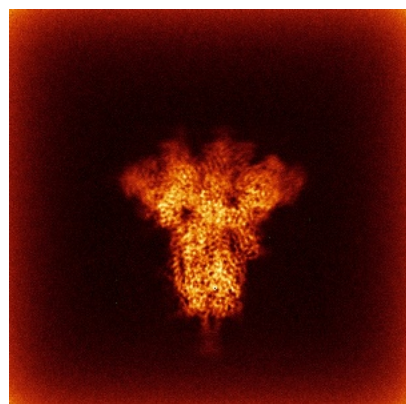


Y

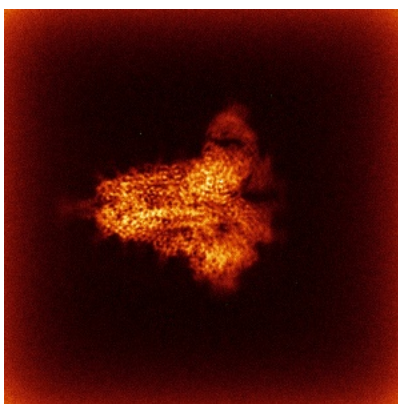


Z

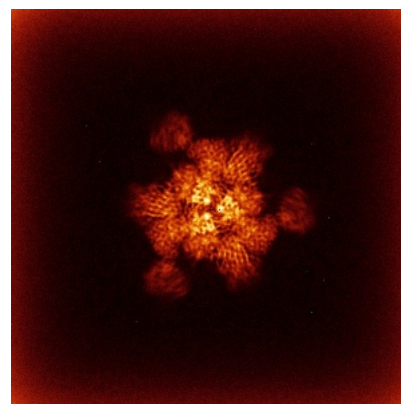
6.4.2 Raw map



X



Y

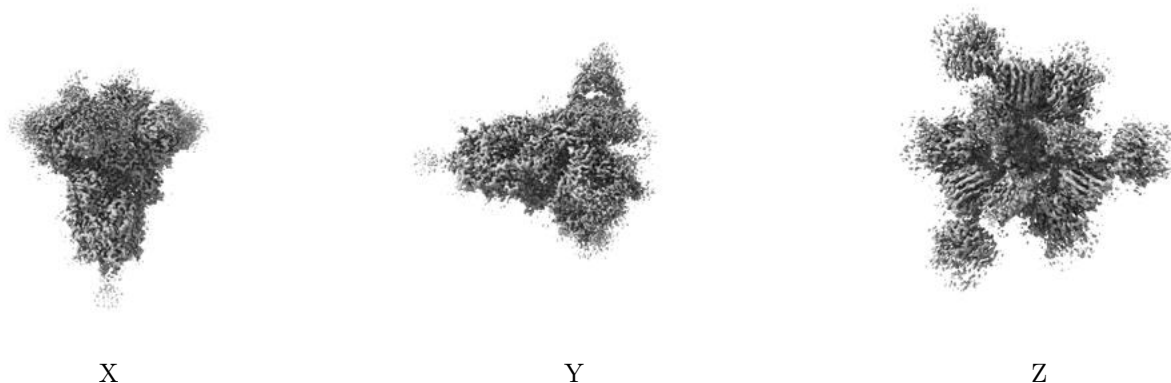


Z

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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

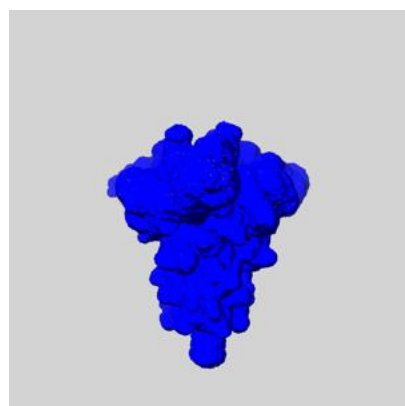
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

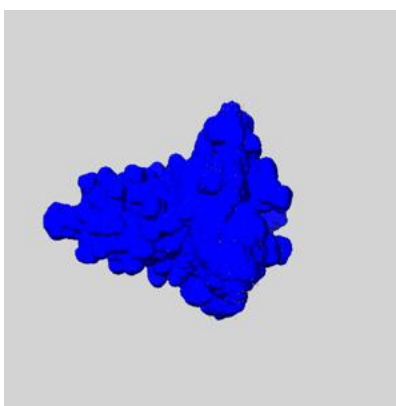
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

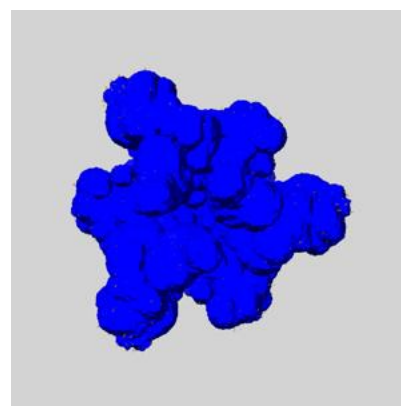
6.6.1 emd_44628_msk_1.map [i](#)



X



Y

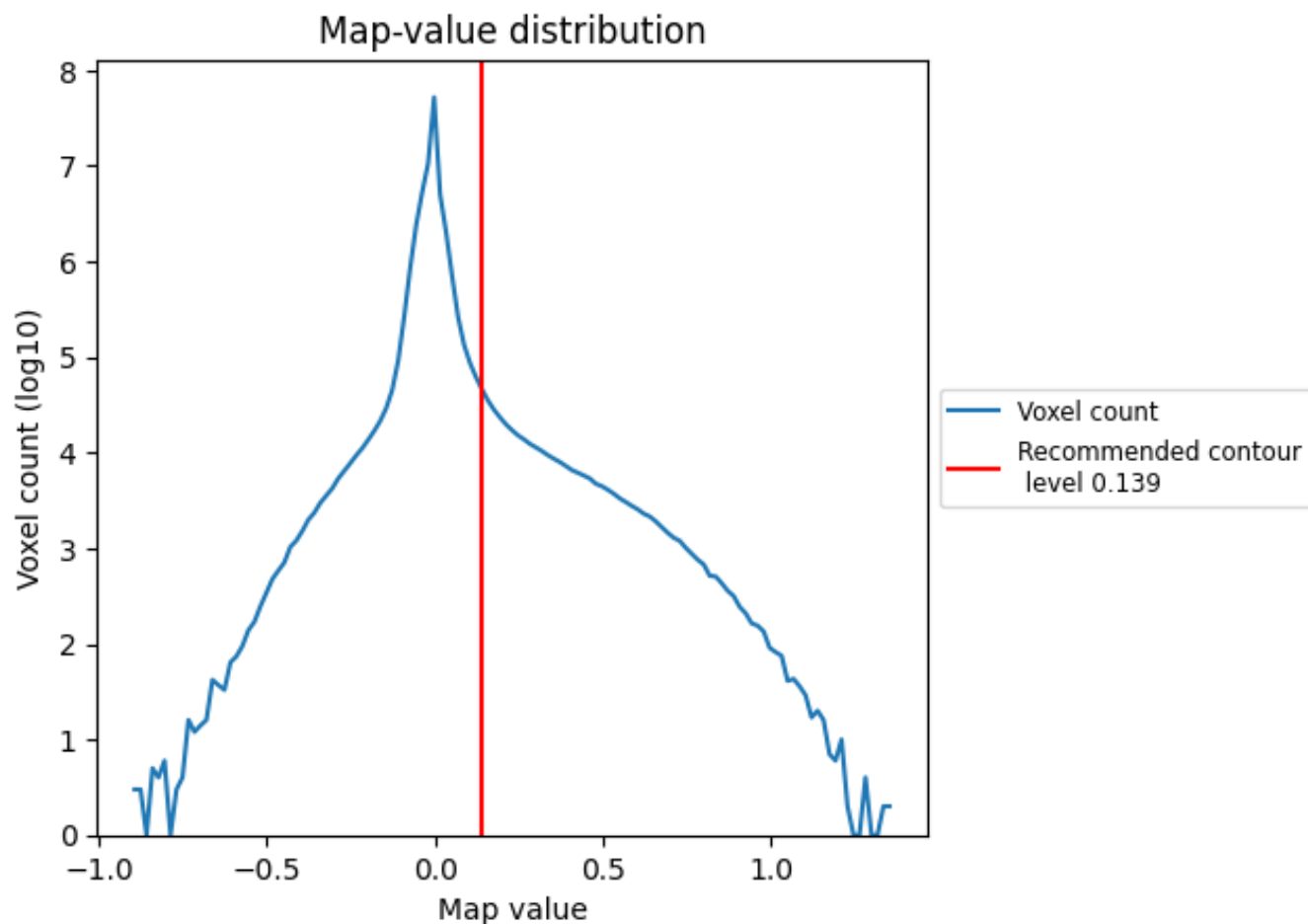


Z

7 Map analysis [i](#)

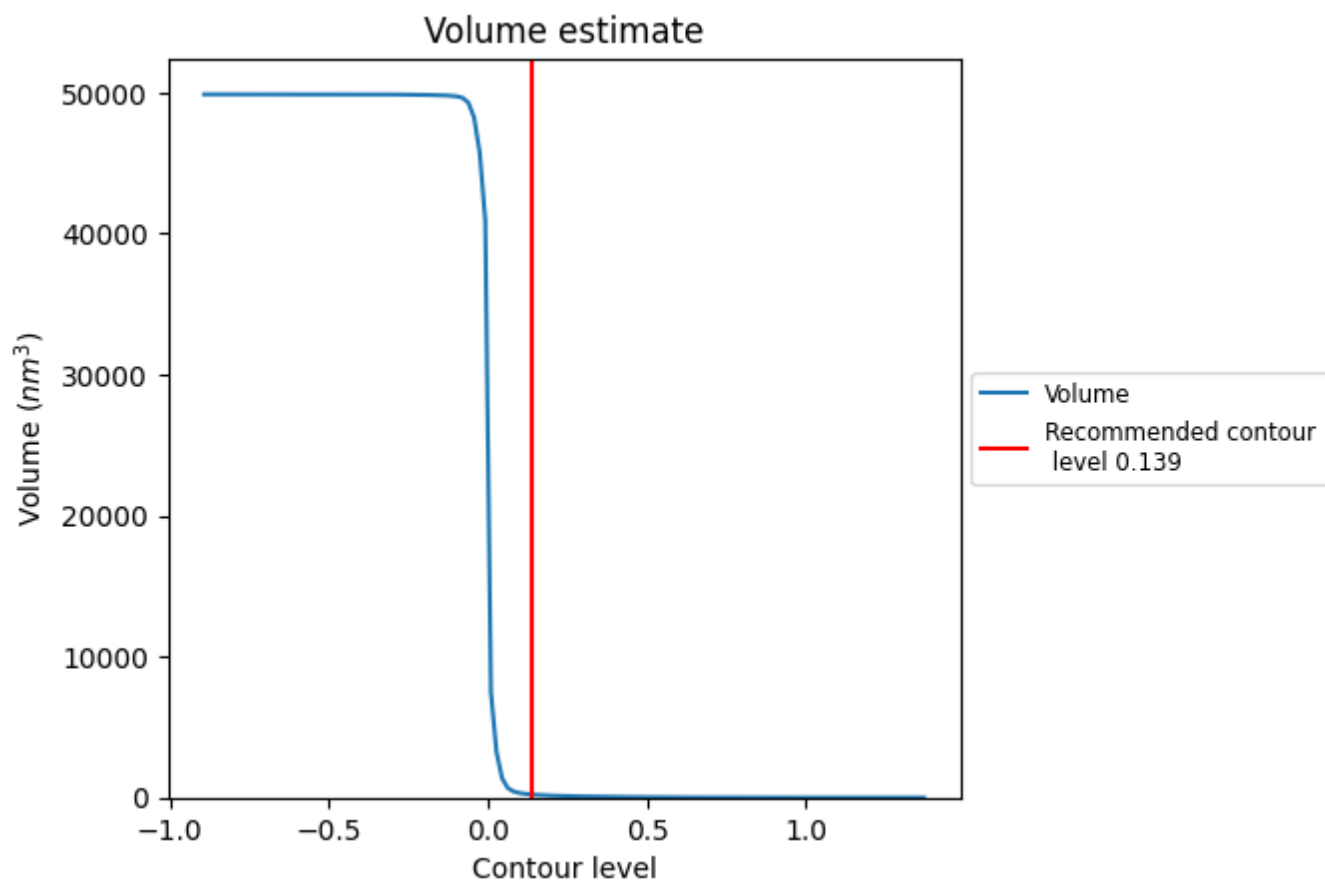
This section contains the results of statistical analysis of the map.

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.

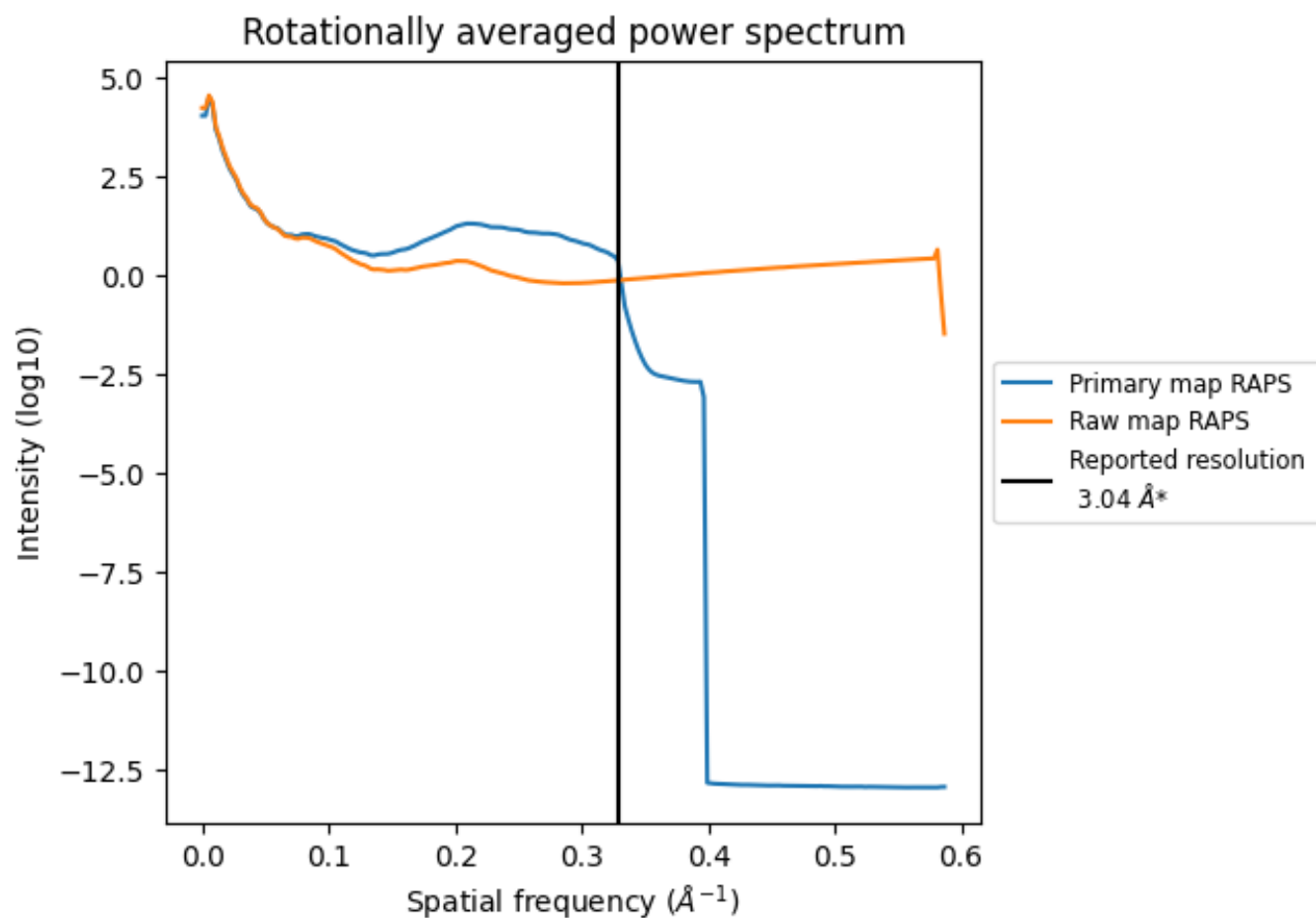
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm^3 ; this corresponds to an approximate mass of 192 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 ⓘ

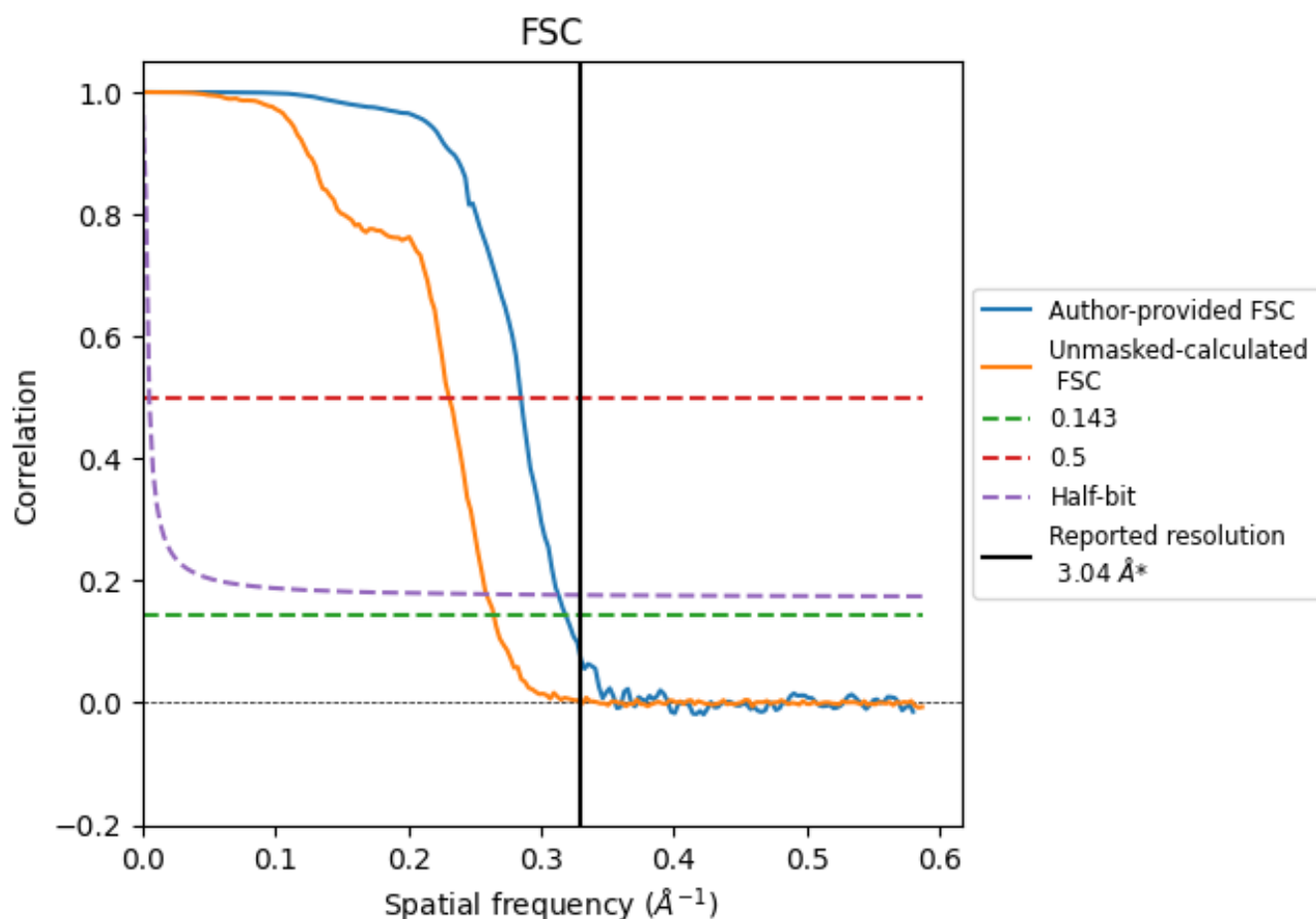


*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.329 Å⁻¹

8.2 Resolution estimates [i](#)

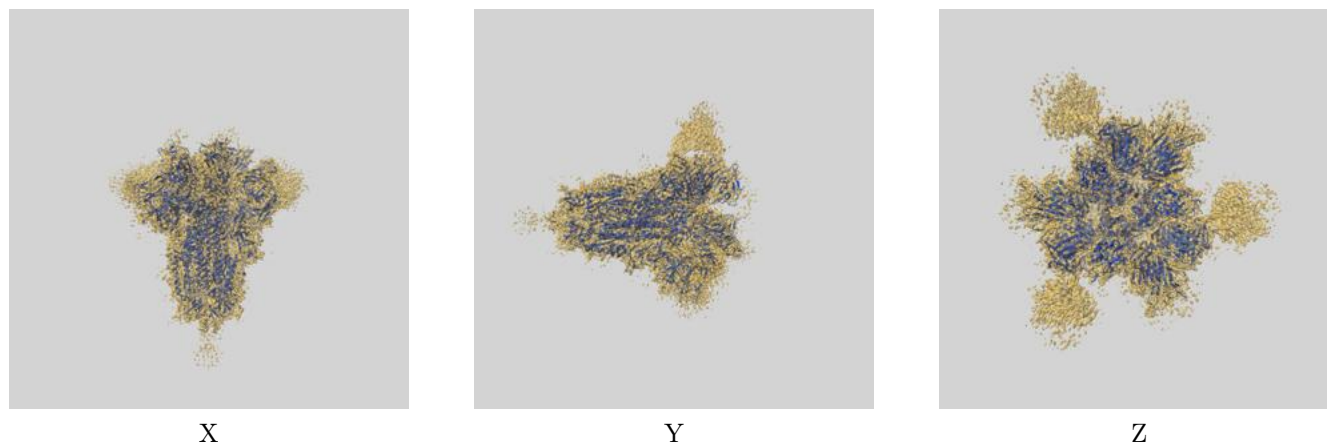
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.14	3.51	3.19
Unmasked-calculated*	3.78	4.33	3.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 3.04 by more than 10 %

9 Map-model fit [i](#)

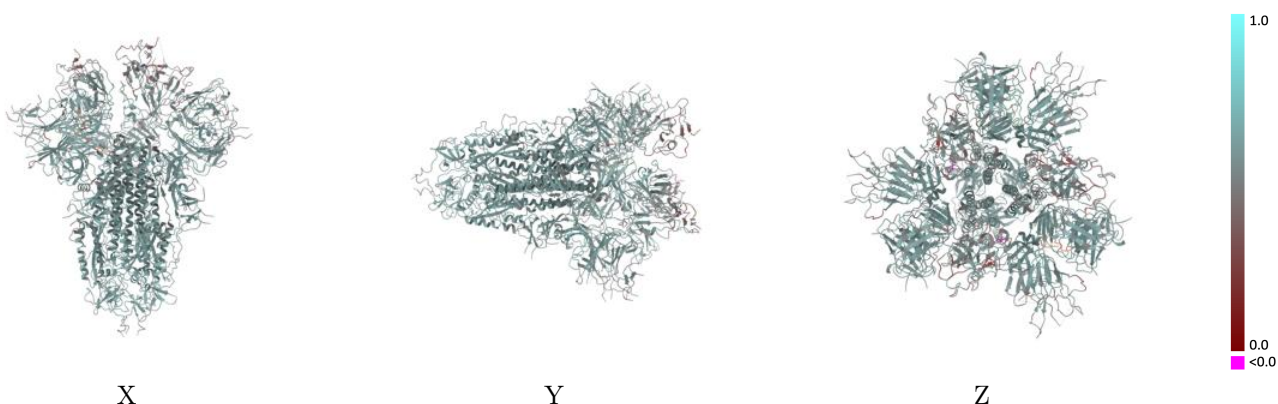
This section contains information regarding the fit between EMDB map EMD-44628 and PDB model 9BJ3. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



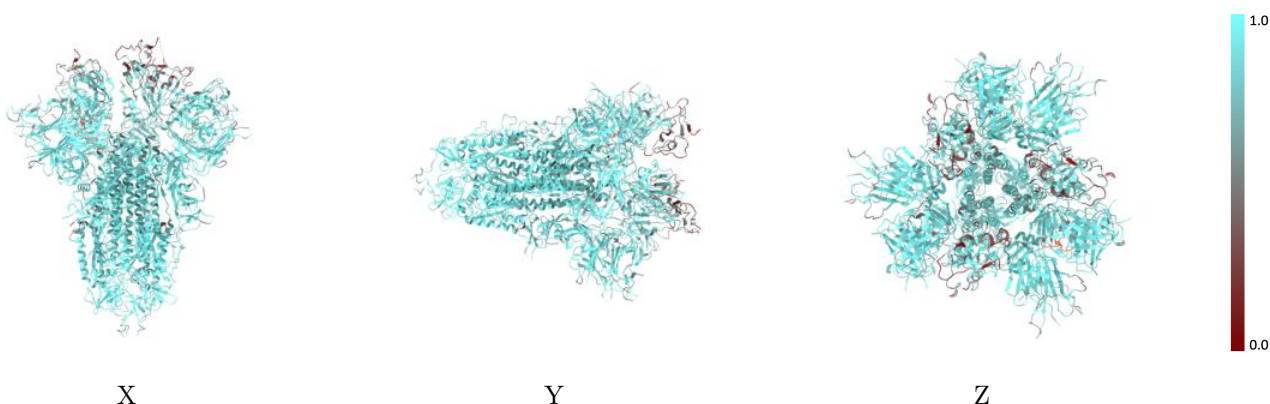
The images above show the 3D surface view of the map at the recommended contour level 0.139 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



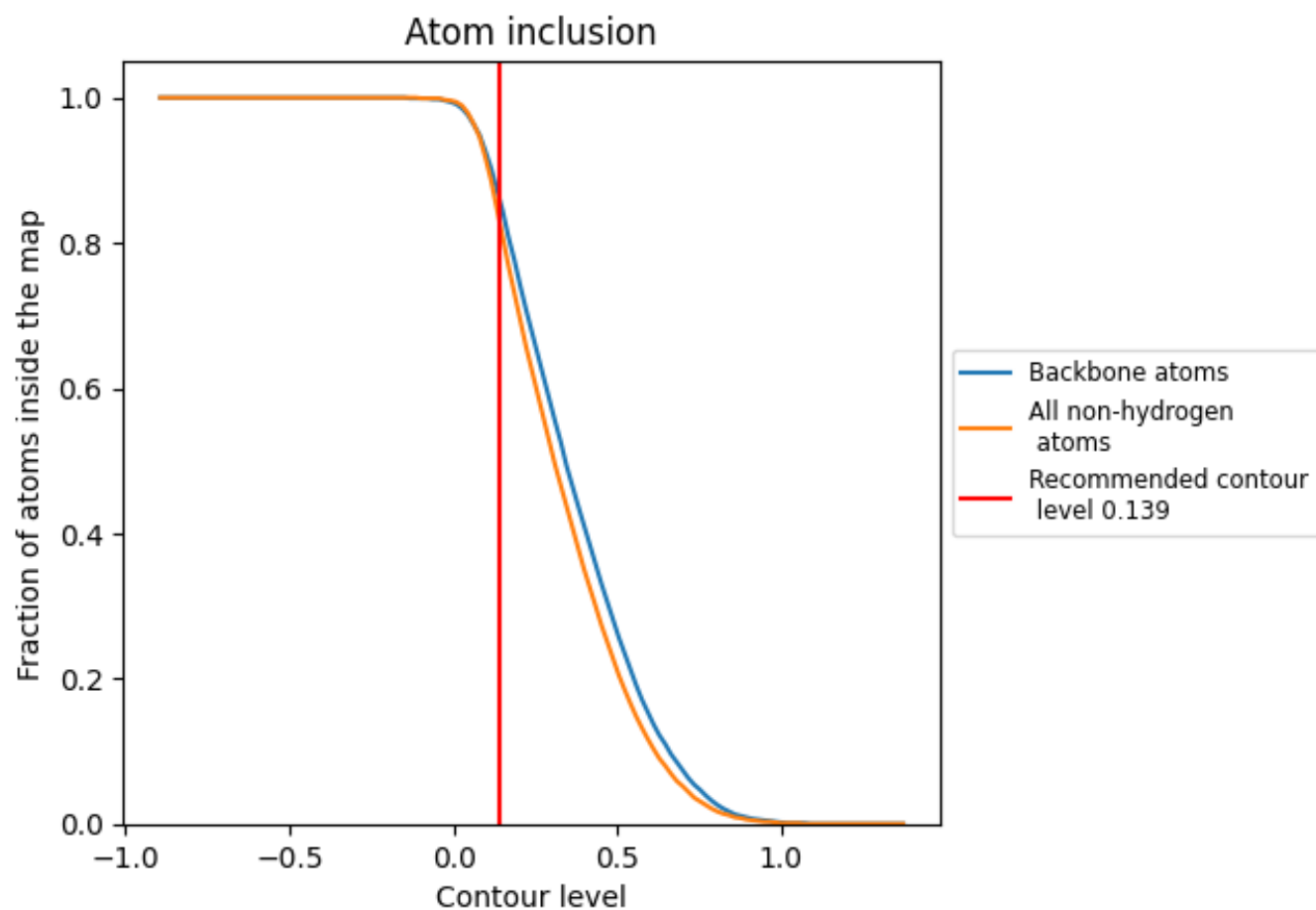
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.139).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 83% 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 (0.139) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.5560
A	 0.8380	 0.5570
B	 0.8370	 0.5560
C	 0.9060	 0.5790
D	 0.8520	 0.5730
E	 0.9090	 0.5800
F	 0.8580	 0.5720
G	 0.7140	 0.4990
H	 0.9080	 0.5800
I	 0.2000	 0.3590
J	 0.2500	 0.3380
K	 0.6790	 0.5300
L	 0.8580	 0.5750
M	 0.3930	 0.4330
N	 0.3930	 0.3920
O	 0.5130	 0.4440
P	 0.4360	 0.3510
Q	 0.6430	 0.4660
R	 0.4290	 0.3880
S	 0.8400	 0.5570
T	 0.6430	 0.5140
U	 0.3000	 0.3760
V	 0.1790	 0.3060
W	 0.6430	 0.5150
X	 0.4290	 0.3980
Y	 0.4290	 0.3800
Z	 0.5380	 0.4550
a	 0.4360	 0.3660
b	 0.6430	 0.4700
c	 0.5000	 0.3430
d	 0.7140	 0.5200
e	 0.2200	 0.3840
f	 0.2860	 0.3480
g	 0.6790	 0.5310
h	 0.4290	 0.3790



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Chain	Atom inclusion	Q-score
i	 0.3930	 0.4010
j	 0.5130	 0.4500
k	 0.4620	 0.3360
l	 0.5710	 0.4810
m	 0.5000	 0.3750