



## wwPDB EM Validation Summary Report ⓘ

Jan 15, 2022 – 08:31 am GMT

PDB ID : 7Q6E  
EMDB ID : EMD-13857  
Title : Beta049 fab in complex with SARS-CoV2 beta-Spike glycoprotein, The Beta mAb response underscores the antigenic distance to other SARS-CoV-2 variants  
Authors : Duyvesteyn, H.M.E.; Ren, J.; Stuart, D.I.  
Deposited on : 2021-11-07  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

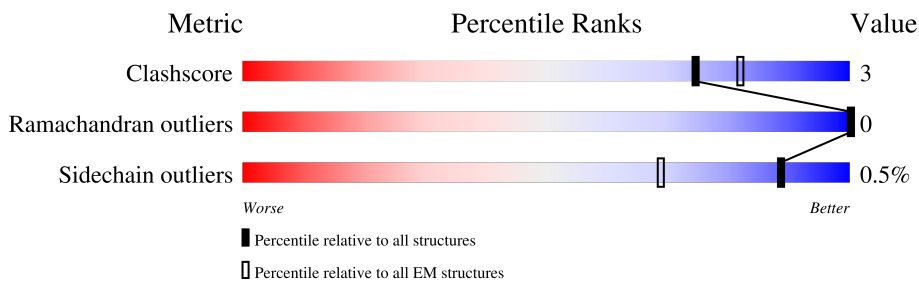
EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.24

# 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 2.70 Å.

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



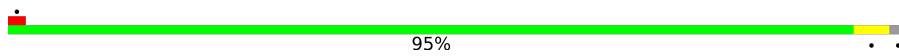



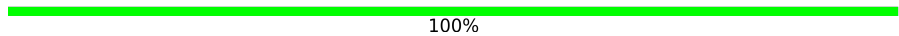
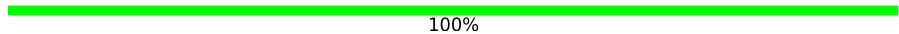
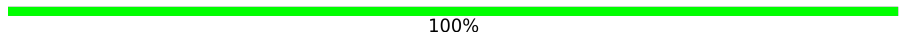
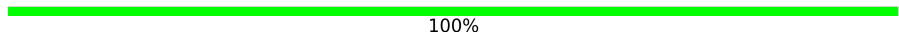
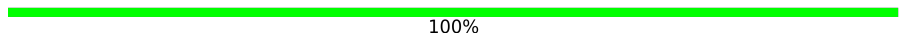
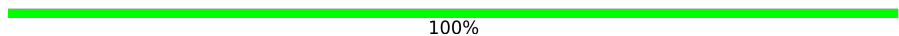
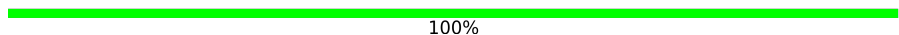
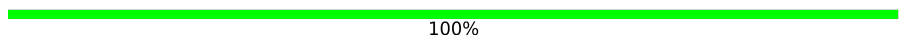
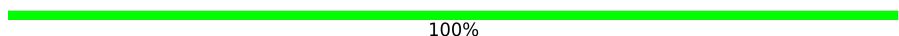
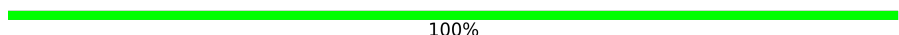
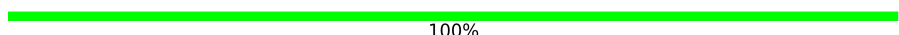
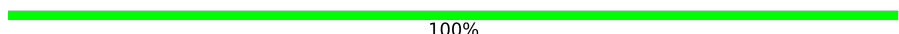
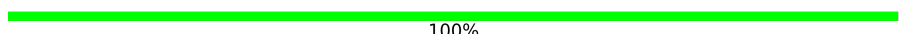

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1285	
1	B	1285	
1	C	1285	
2	F	216	
2	K	216	
2	L	216	
3	E	223	
3	H	223	

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Mol	Chain	Length	Quality of chain
3	J	223	 95%
4	D	7	 43% 57%
4	V	7	 57% 14% 29%
5	G	2	 50% 50%
5	I	2	 100%
5	M	2	 100%
5	N	2	 100%
5	O	2	 100%
5	Q	2	 100%
5	R	2	 100%
5	S	2	 100%
5	T	2	 100%
5	U	2	 100%
5	W	2	 100%
5	X	2	 100%
5	Y	2	 100%
5	Z	2	 100%
6	P	6	 50% 50%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 34341 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1013	7903	5048	1313	1507	35	0	0
1	B	1008	7871	5031	1308	1497	35	0	0
1	C	1001	7811	4992	1297	1487	35	0	0

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	243	ILE	ARG	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	481	LYS	GLU	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	698	VAL	ALA	variant	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1203	TYR	-	expression tag	UNP P0DTC2
A	1204	GLU	-	expression tag	UNP P0DTC2
A	1205	GLN	-	expression tag	UNP P0DTC2
A	1206	GLY	-	expression tag	UNP P0DTC2
A	1207	SER	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	TYR	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	SER	-	expression tag	UNP P0DTC2
A	1257	ALA	-	expression tag	UNP P0DTC2
A	1258	TRP	-	expression tag	UNP P0DTC2
A	1259	SER	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	PRO	-	expression tag	UNP P0DTC2
A	1262	GLN	-	expression tag	UNP P0DTC2
A	1263	PHE	-	expression tag	UNP P0DTC2
A	1264	GLU	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	SER	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	SER	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	ALA	-	expression tag	UNP P0DTC2
A	1278	TRP	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	PRO	-	expression tag	UNP P0DTC2
A	1282	GLN	-	expression tag	UNP P0DTC2
A	1283	PHE	-	expression tag	UNP P0DTC2
A	1284	GLU	-	expression tag	UNP P0DTC2
A	1285	LYS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	243	ILE	ARG	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	LYS	GLU	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	698	VAL	ALA	variant	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1203	TYR	-	expression tag	UNP P0DTC2
B	1204	GLU	-	expression tag	UNP P0DTC2
B	1205	GLN	-	expression tag	UNP P0DTC2
B	1206	GLY	-	expression tag	UNP P0DTC2
B	1207	SER	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	TYR	-	expression tag	UNP P0DTC2
B	1210	ILE	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ALA	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	ASP	-	expression tag	UNP P0DTC2
B	1217	GLY	-	expression tag	UNP P0DTC2
B	1218	GLN	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	TYR	-	expression tag	UNP P0DTC2
B	1221	VAL	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	LYS	-	expression tag	UNP P0DTC2
B	1224	ASP	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	GLU	-	expression tag	UNP P0DTC2
B	1227	TRP	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	LEU	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	SER	-	expression tag	UNP P0DTC2
B	1232	THR	-	expression tag	UNP P0DTC2
B	1233	PHE	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1236	ARG	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	PRO	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	GLY	-	expression tag	UNP P0DTC2
B	1256	SER	-	expression tag	UNP P0DTC2
B	1257	ALA	-	expression tag	UNP P0DTC2
B	1258	TRP	-	expression tag	UNP P0DTC2
B	1259	SER	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	PRO	-	expression tag	UNP P0DTC2
B	1262	GLN	-	expression tag	UNP P0DTC2
B	1263	PHE	-	expression tag	UNP P0DTC2
B	1264	GLU	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	SER	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	SER	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1278	TRP	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
B	1281	PRO	-	expression tag	UNP P0DTC2
B	1282	GLN	-	expression tag	UNP P0DTC2
B	1283	PHE	-	expression tag	UNP P0DTC2
B	1284	GLU	-	expression tag	UNP P0DTC2
B	1285	LYS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	243	ILE	ARG	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	481	LYS	GLU	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	698	VAL	ALA	variant	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1203	TYR	-	expression tag	UNP P0DTC2
C	1204	GLU	-	expression tag	UNP P0DTC2
C	1205	GLN	-	expression tag	UNP P0DTC2
C	1206	GLY	-	expression tag	UNP P0DTC2
C	1207	SER	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	TYR	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ALA	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	ASP	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	GLN	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1220	TYR	-	expression tag	UNP P0DTC2
C	1221	VAL	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	LYS	-	expression tag	UNP P0DTC2
C	1224	ASP	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	TRP	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	LEU	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	SER	-	expression tag	UNP P0DTC2
C	1232	THR	-	expression tag	UNP P0DTC2
C	1233	PHE	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	PRO	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	GLY	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	ALA	-	expression tag	UNP P0DTC2
C	1258	TRP	-	expression tag	UNP P0DTC2
C	1259	SER	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1262	GLN	-	expression tag	UNP P0DTC2
C	1263	PHE	-	expression tag	UNP P0DTC2
C	1264	GLU	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	SER	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	SER	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	ALA	-	expression tag	UNP P0DTC2
C	1278	TRP	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	PRO	-	expression tag	UNP P0DTC2
C	1282	GLN	-	expression tag	UNP P0DTC2
C	1283	PHE	-	expression tag	UNP P0DTC2
C	1284	GLU	-	expression tag	UNP P0DTC2
C	1285	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Beta-49 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	216	Total	C	N	O	S	0	0
			1652	1031	283	332	6		
2	F	216	Total	C	N	O	S	0	0
			1652	1031	283	332	6		
2	K	216	Total	C	N	O	S	0	0
			1652	1031	283	332	6		

- Molecule 3 is a protein called Beta-49 heavy chain.

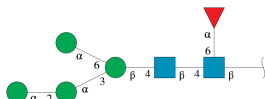
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	219	Total	C	N	O	S	0	0
			1603	1015	264	317	7		
3	E	219	Total	C	N	O	S	0	0
			1603	1015	264	317	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	219	1603	1015	264	317	7	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	7	82	46	2	34	0	0
4	V	7	82	46	2	34	0	0

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



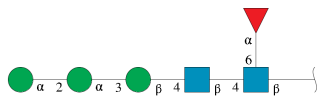
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	2	28	16	2	10	0	0
5	I	2	28	16	2	10	0	0
5	M	2	28	16	2	10	0	0
5	N	2	28	16	2	10	0	0
5	O	2	28	16	2	10	0	0
5	Q	2	28	16	2	10	0	0
5	R	2	28	16	2	10	0	0
5	S	2	28	16	2	10	0	0

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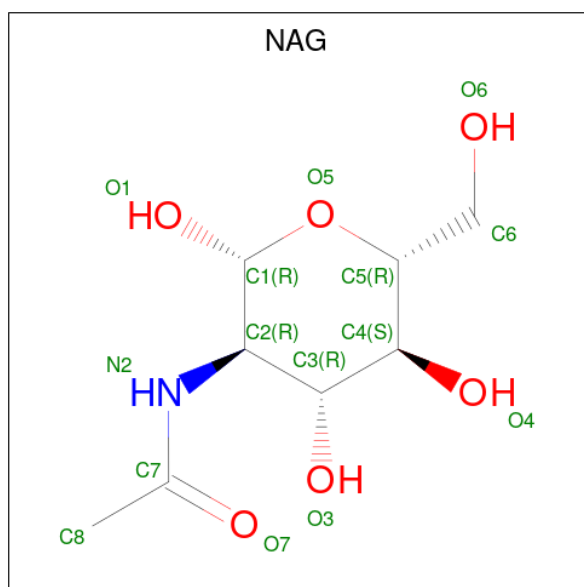
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	T	2	28	16	2	10	0	0
5	U	2	28	16	2	10	0	0
5	W	2	28	16	2	10	0	0
5	X	2	28	16	2	10	0	0
5	Y	2	28	16	2	10	0	0
5	Z	2	28	16	2	10	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	P	6	71	40	2	29	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	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	A	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0
7	B	1	126	72	9	45	0

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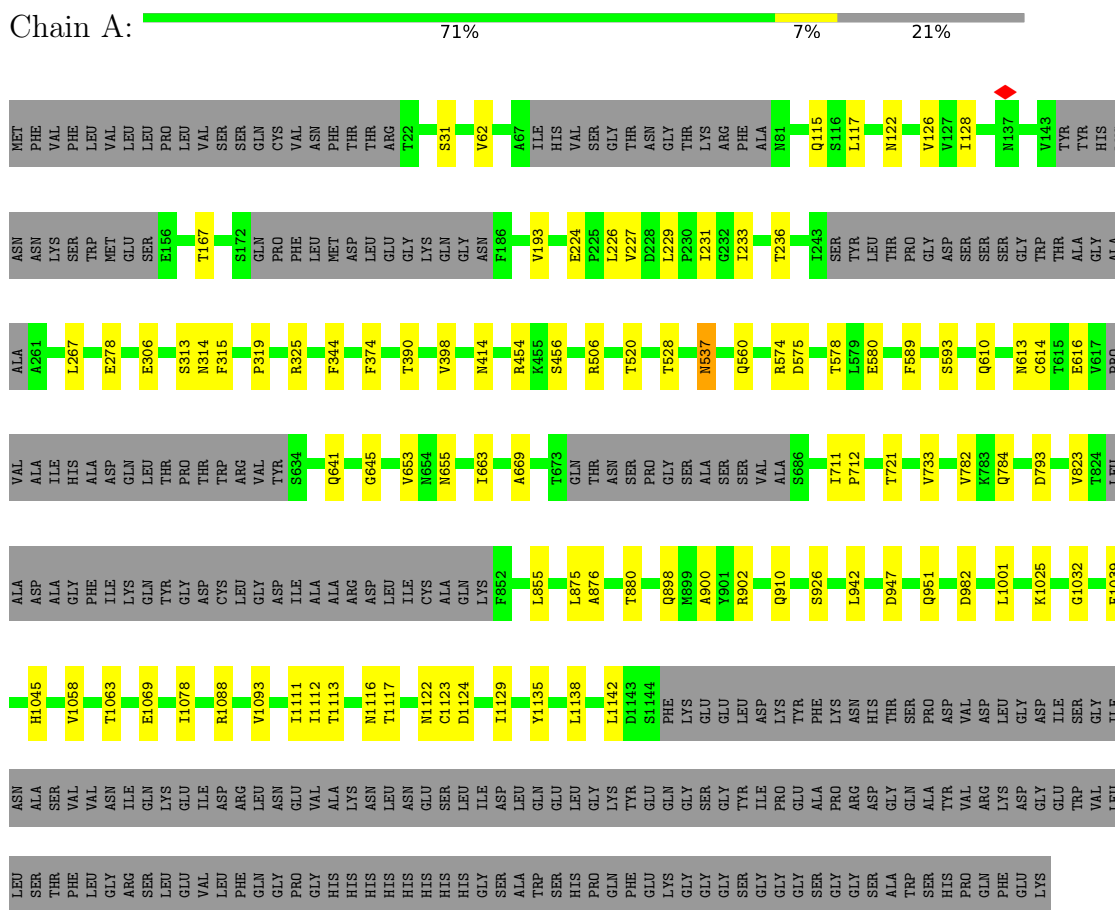
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	B	1	Total 126	C 72	N 9	O 45	0
7	B	1	Total 126	C 72	N 9	O 45	0
7	B	1	Total 126	C 72	N 9	O 45	0
7	B	1	Total 126	C 72	N 9	O 45	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0
7	C	1	Total 112	C 64	N 8	O 40	0

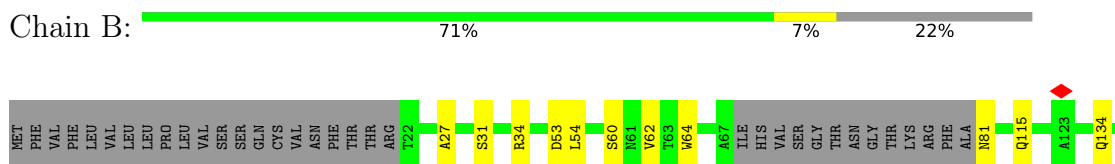
### 3 Residue-property plots i

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

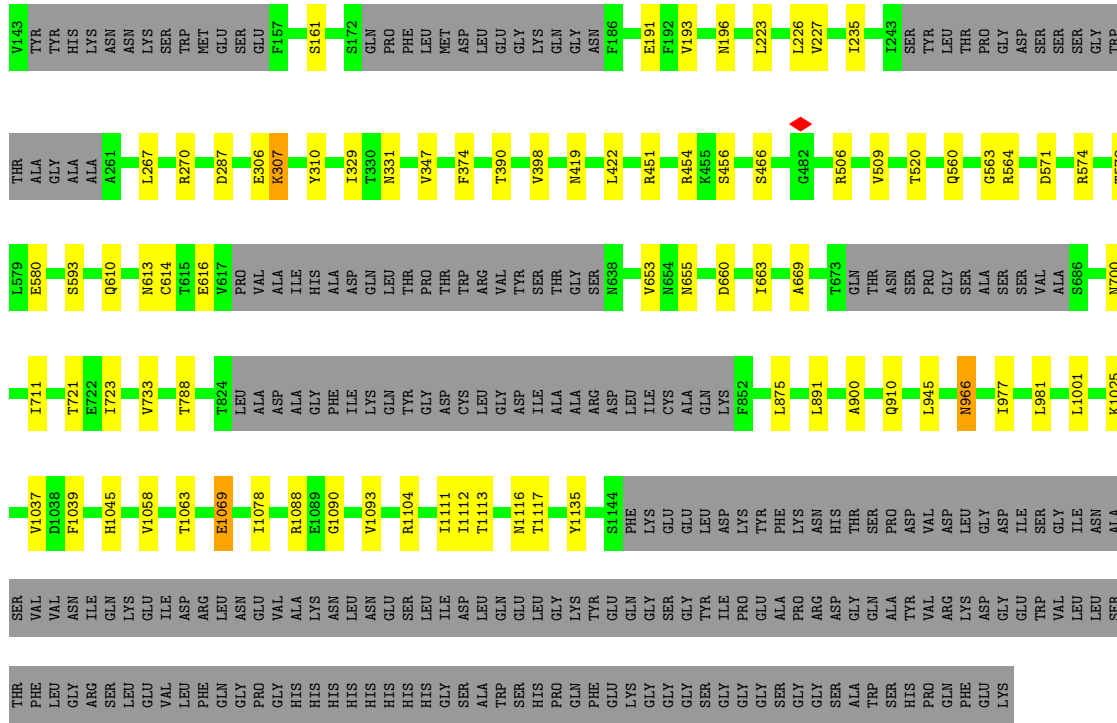
- Molecule 1: Spike glycoprotein



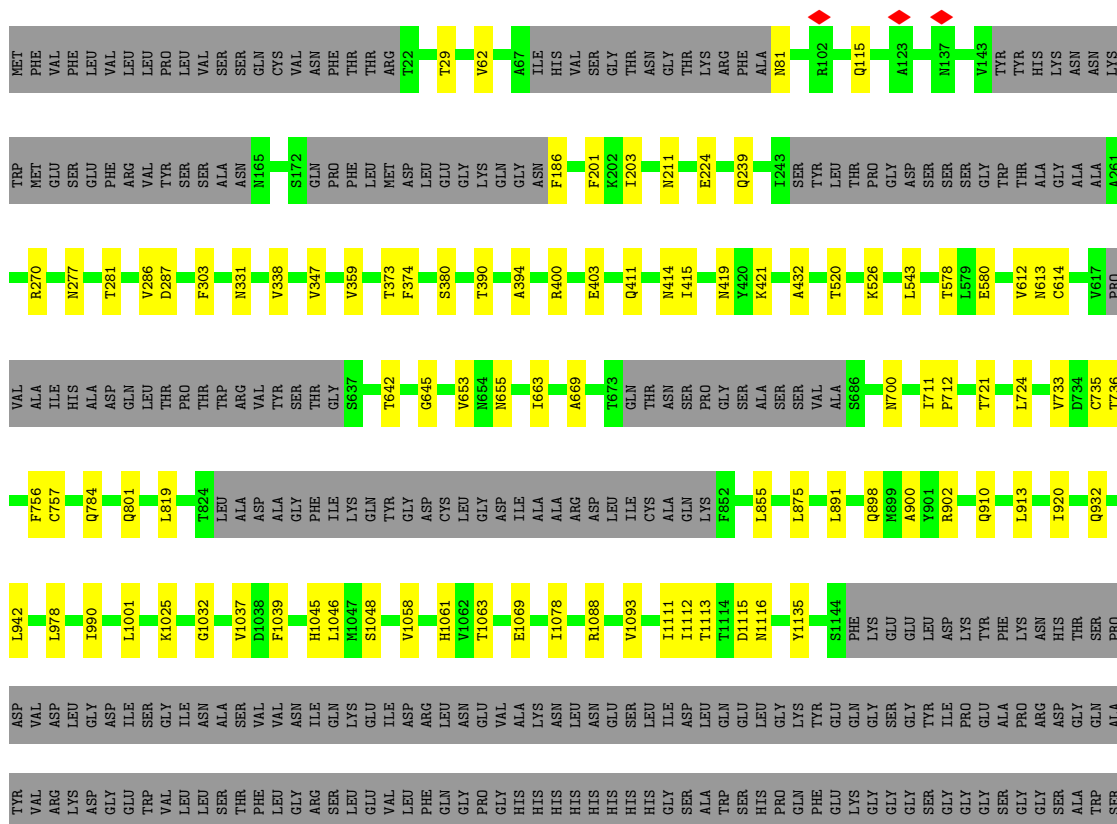
- Molecule 1: Spike glycoprotein







● Molecule 1: Spike glycoprotein



HIS  
PRO  
GLN  
PHE  
GLU  
LYS

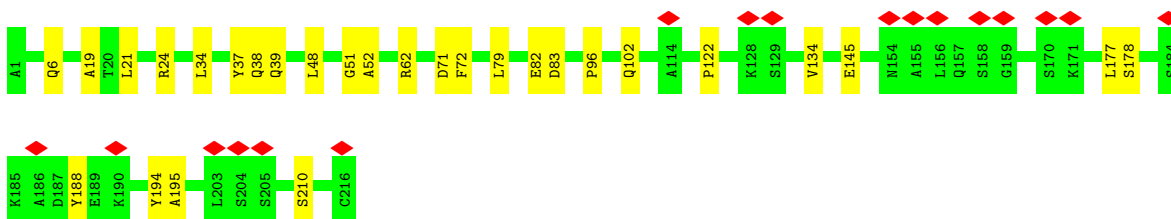
- Molecule 2: Beta-49 light chain

Chain L: 91% 9%



- Molecule 2: Beta-49 light chain

Chain F: 8% 87% 13%



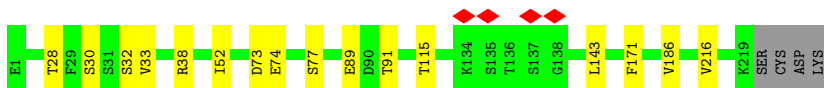
- Molecule 2: Beta-49 light chain

Chain K: 93% 7%



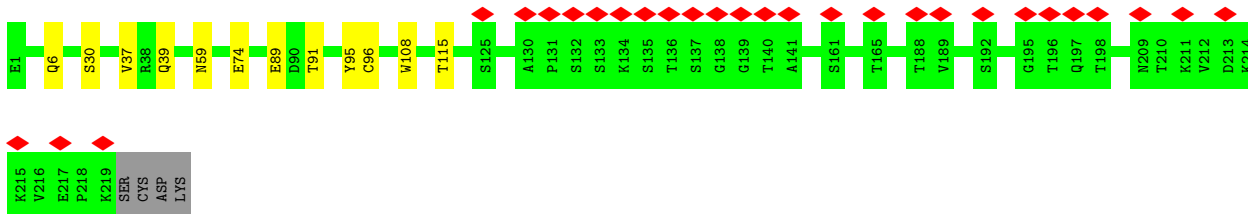
- Molecule 3: Beta-49 heavy chain

Chain H: 91% 7%



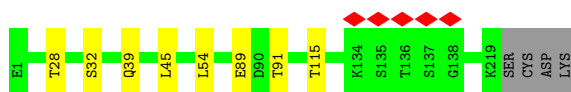
- Molecule 3: Beta-49 heavy chain

Chain E: 13% 93% 5%



- Molecule 3: Beta-49 heavy chain

Chain J:  95%



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  43% 57%



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  57% 14% 29%



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

Chain G:  50% 50%



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

Chain I:  100%



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

Chain M:  100%



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

Chain N:  100%

NAG1  
NAG2

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

Chain O:  100%

NAG1  
NAG2

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

Chain Q:  100%

NAG1  
NAG2

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

Chain R:  100%

NAG1  
NAG2

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

Chain S:  100%

NAG1  
NAG2

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

Chain T:  100%

NAG1  
NAG2

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

Chain U:  100%

NAG1  
NAG2

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

Chain W:  100%

MAG1  
MAG2

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

Chain X:  100%

MAG1  
MAG2

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

Chain Y:  100%

MAG1  
MAG2

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

Chain Z:  100%

MAG1  
MAG2

- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5  
FUC6

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	222689	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 ( $e^-/\text{\AA}^2$ )	38.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.325	Depositor
Minimum map value	-1.517	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.0718	Depositor
Map size ( $\text{\AA}$ )	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	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, MAN, FUC, BMA

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	0.27	0/8083	0.47	0/11001
1	B	0.26	0/8051	0.47	0/10958
1	C	0.27	0/7989	0.47	0/10874
2	F	0.25	0/1689	0.48	0/2293
2	K	0.26	0/1689	0.49	0/2293
2	L	0.26	0/1689	0.49	0/2293
3	E	0.25	0/1640	0.46	0/2237
3	H	0.26	0/1640	0.47	0/2237
3	J	0.25	0/1640	0.46	0/2237
All	All	0.26	0/34110	0.47	0/46423

There are no bond length outliers.

There are no bond angle outliers.

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	7903	0	7701	61	0
1	B	7871	0	7675	51	0
1	C	7811	0	7621	53	0
2	F	1652	0	1601	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1652	0	1601	9	0
2	L	1652	0	1601	11	0
3	E	1603	0	1583	8	0
3	H	1603	0	1583	8	0
3	J	1603	0	1583	5	0
4	D	82	0	70	1	0
4	V	82	0	70	1	0
5	G	28	0	25	1	0
5	I	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	W	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
6	P	71	0	61	1	0
7	A	126	0	117	0	0
7	B	126	0	117	0	0
7	C	112	0	104	0	0
All	All	34341	0	33438	214	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 3.

The worst 5 of 214 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:1088:ARG:NH1	1:A:1117:THR:O	2.13	0.81
1:A:193:VAL:HG13	1:A:267:LEU:HD11	1.67	0.76
2:K:38:GLN:HB2	2:K:48:LEU:HD11	1.69	0.74
2:F:37:TYR:HH	3:E:108:TRP:HE1	1.36	0.74
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.70	0.74

There are no symmetry-related clashes.



## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	997/1285 (78%)	965 (97%)	32 (3%)	0	100	100
1	B	992/1285 (77%)	960 (97%)	32 (3%)	0	100	100
1	C	985/1285 (77%)	954 (97%)	31 (3%)	0	100	100
2	F	214/216 (99%)	212 (99%)	2 (1%)	0	100	100
2	K	214/216 (99%)	206 (96%)	8 (4%)	0	100	100
2	L	214/216 (99%)	208 (97%)	6 (3%)	0	100	100
3	E	217/223 (97%)	215 (99%)	2 (1%)	0	100	100
3	H	217/223 (97%)	214 (99%)	3 (1%)	0	100	100
3	J	217/223 (97%)	217 (100%)	0	0	100	100
All	All	4267/5172 (82%)	4151 (97%)	116 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	886/1109 (80%)	881 (99%)	5 (1%)	86	95
1	B	882/1109 (80%)	875 (99%)	7 (1%)	81	93
1	C	876/1109 (79%)	872 (100%)	4 (0%)	88	96
2	F	185/186 (100%)	185 (100%)	0	100	100
2	K	185/186 (100%)	184 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	185/186 (100%)	185 (100%)	0	100	100
3	E	180/187 (96%)	180 (100%)	0	100	100
3	H	180/187 (96%)	180 (100%)	0	100	100
3	J	180/187 (96%)	180 (100%)	0	100	100
All	All	3739/4446 (84%)	3722 (100%)	17 (0%)	89	96

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	612	VAL
2	K	34	LEU
1	B	564	ARG
1	B	788	THR
1	B	875	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	115	GLN
1	A	537	ASN
2	L	139	ASN
2	K	126	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](#)

48 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	D	1	1,4	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.40	0
4	BMA	D	3	4	11,11,12	0.57	0	15,15,17	0.91	0
4	MAN	D	4	4	11,11,12	0.65	0	15,15,17	0.94	1 (6%)
4	MAN	D	5	4	11,11,12	0.95	1 (9%)	15,15,17	1.49	4 (26%)
4	MAN	D	6	4	11,11,12	0.60	0	15,15,17	1.00	2 (13%)
4	FUC	D	7	4	10,10,11	0.63	0	14,14,16	0.76	0
5	NAG	G	1	1,5	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	I	1	1,5	14,14,15	0.24	0	17,19,21	0.41	0
5	NAG	I	2	5	14,14,15	0.18	0	17,19,21	0.40	0
5	NAG	M	1	1,5	14,14,15	0.21	0	17,19,21	0.46	0
5	NAG	M	2	5	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	N	1	1,5	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	N	2	5	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	O	1	1,5	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	O	2	5	14,14,15	0.22	0	17,19,21	0.42	0
6	NAG	P	1	1,6	14,14,15	0.26	0	17,19,21	0.48	0
6	NAG	P	2	6	14,14,15	0.21	0	17,19,21	0.39	0
6	BMA	P	3	6	11,11,12	0.64	0	15,15,17	0.74	0
6	MAN	P	4	6	11,11,12	0.64	0	15,15,17	1.06	2 (13%)
6	MAN	P	5	6	11,11,12	1.38	2 (18%)	15,15,17	2.13	4 (26%)
6	FUC	P	6	6	10,10,11	0.70	0	14,14,16	0.76	0
5	NAG	Q	1	1,5	14,14,15	0.19	0	17,19,21	0.41	0
5	NAG	Q	2	5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	R	1	1,5	14,14,15	0.20	0	17,19,21	0.49	0
5	NAG	R	2	5	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	S	1	1,5	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	S	2	5	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	T	1	1,5	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	T	2	5	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	U	1	1,5	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	U	2	5	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	V	1	1,4	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	V	2	4	14,14,15	0.20	0	17,19,21	0.39	0
4	BMA	V	3	4	11,11,12	0.48	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MAN	V	4	4	11,11,12	1.36	1 (9%)	15,15,17	1.25	1 (6%)
4	MAN	V	5	4	11,11,12	0.77	0	15,15,17	0.91	1 (6%)
4	MAN	V	6	4	11,11,12	0.60	0	15,15,17	1.02	2 (13%)
4	FUC	V	7	4	10,10,11	0.59	0	14,14,16	0.80	0
5	NAG	W	1	1,5	14,14,15	0.18	0	17,19,21	0.45	0
5	NAG	W	2	5	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	X	1	1,5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	X	2	5	14,14,15	0.18	0	17,19,21	0.44	0
5	NAG	Y	1	1,5	14,14,15	0.31	0	17,19,21	0.46	0
5	NAG	Y	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	Z	1	1,5	14,14,15	0.21	0	17,19,21	0.42	0
5	NAG	Z	2	5	14,14,15	0.21	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
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	0/2/19/22	0/1/1/1
4	FUC	D	7	4	-	-	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	2/6/23/26	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
6	MAN	P	4	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	P	5	6	-	0/2/19/22	0/1/1/1
6	FUC	P	6	6	-	-	0/1/1/1
5	NAG	Q	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	NAG	R	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	NAG	S	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	0/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
4	MAN	V	4	4	-	0/2/19/22	0/1/1/1
4	MAN	V	5	4	-	0/2/19/22	0/1/1/1
4	MAN	V	6	4	-	0/2/19/22	0/1/1/1
4	FUC	V	7	4	-	-	0/1/1/1
5	NAG	W	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	0/6/23/26	0/1/1/1
5	NAG	X	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Y	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	5	MAN	C1-C2	3.91	1.61	1.52
4	V	4	MAN	C2-C3	3.38	1.57	1.52
4	D	5	MAN	C1-C2	3.02	1.59	1.52
6	P	5	MAN	O5-C1	2.13	1.47	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	5	MAN	C1-O5-C5	5.47	119.60	112.19
6	P	5	MAN	C1-C2-C3	3.84	114.38	109.67
6	P	5	MAN	O5-C1-C2	3.48	116.14	110.77
4	D	5	MAN	C1-O5-C5	3.45	116.86	112.19
4	V	4	MAN	C1-C2-C3	2.93	113.26	109.67

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

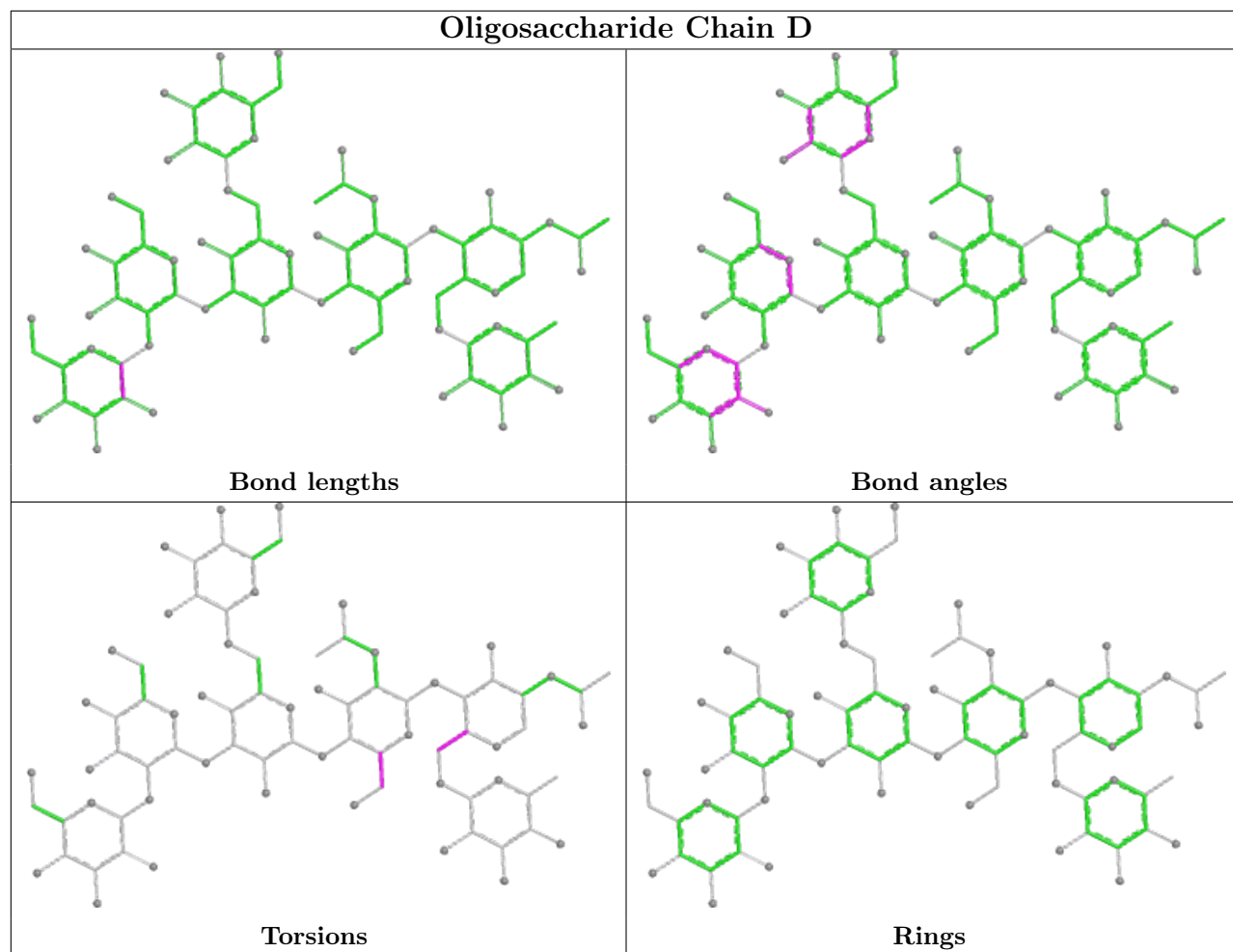
Mol	Chain	Res	Type	Atoms
5	M	2	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	Q	2	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6

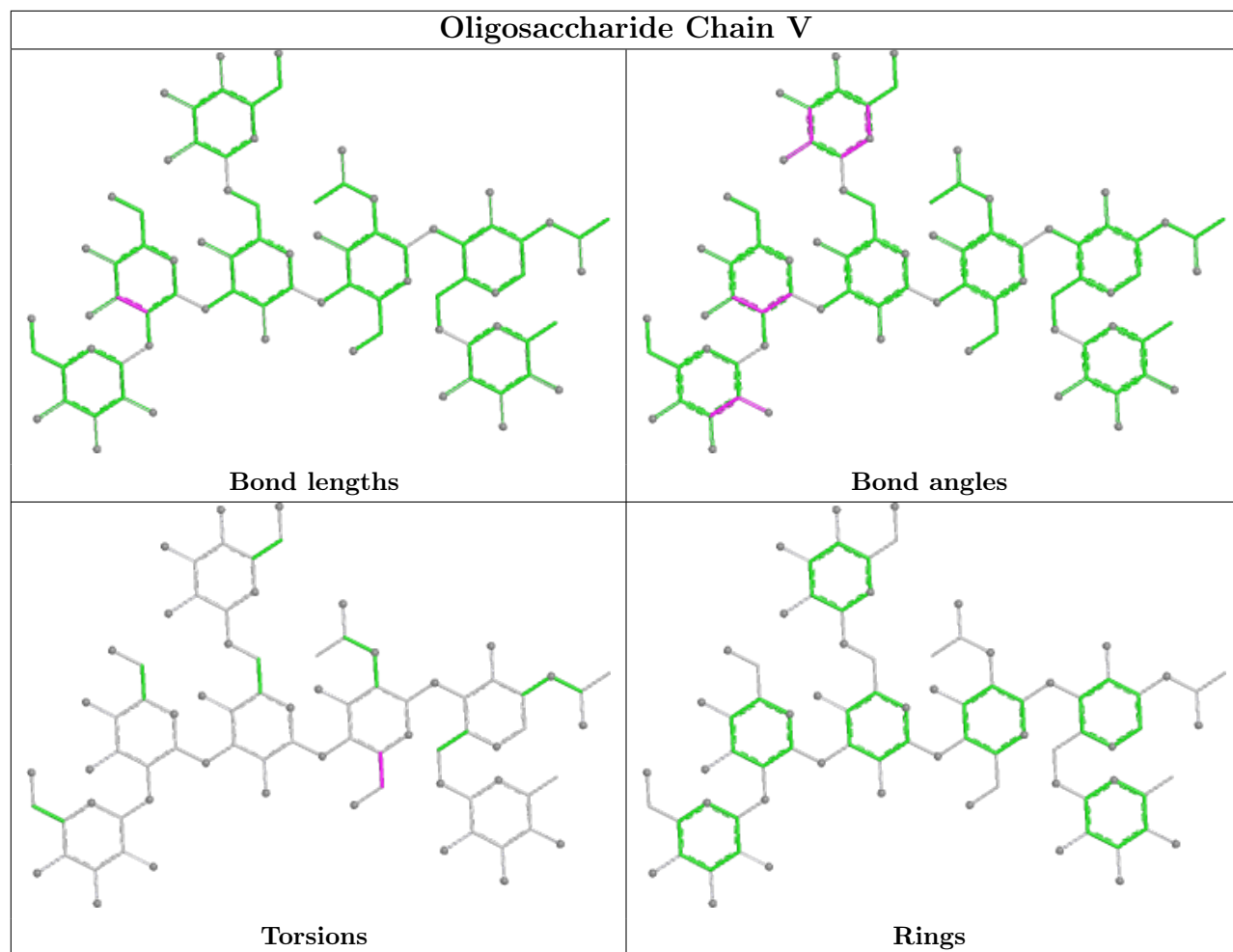
There are no ring outliers.

5 monomers are involved in 4 short contacts:

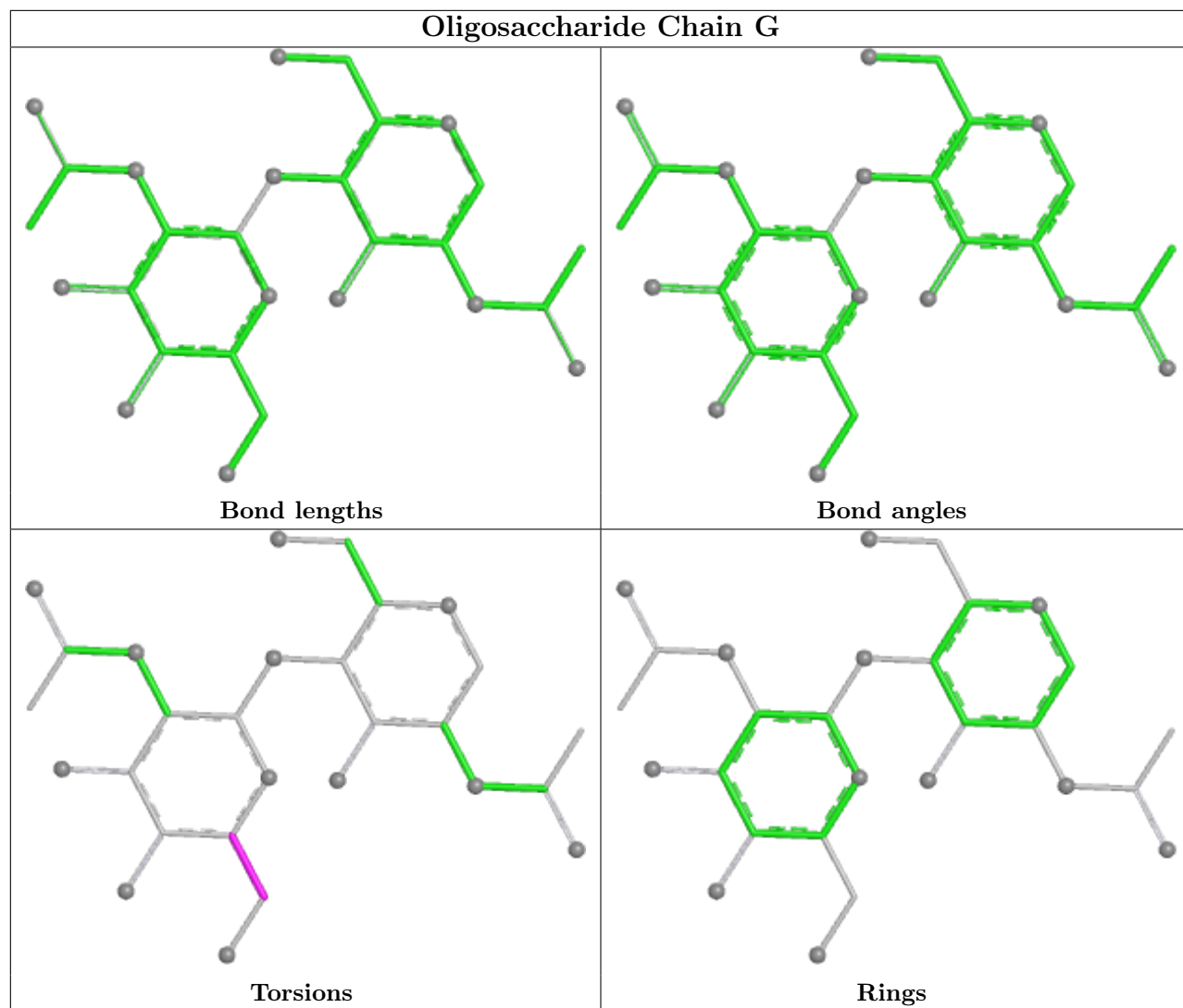
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
5	G	1	NAG	1	0
6	P	1	NAG	1	0
4	V	4	MAN	1	0
4	V	5	MAN	1	0

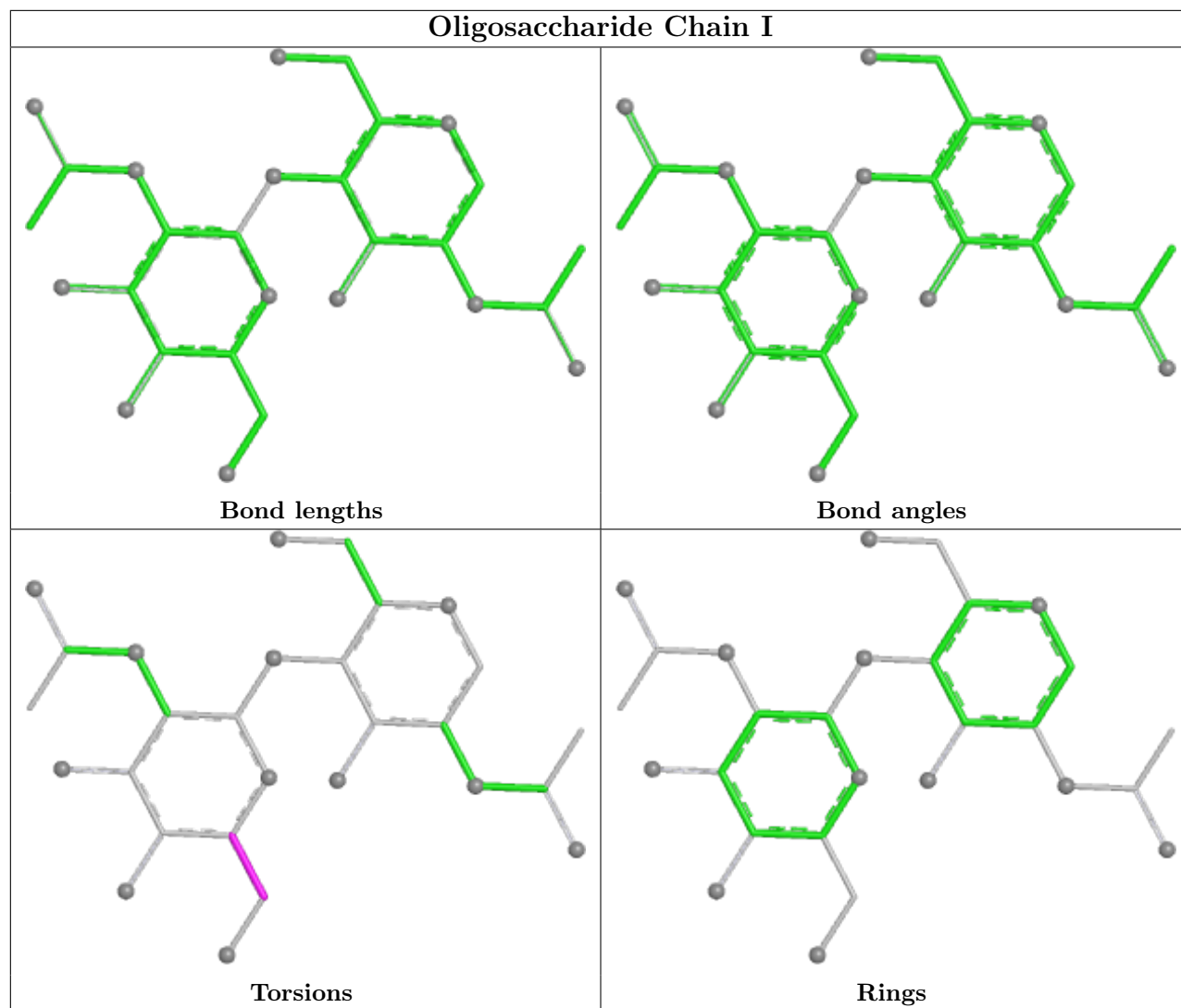
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

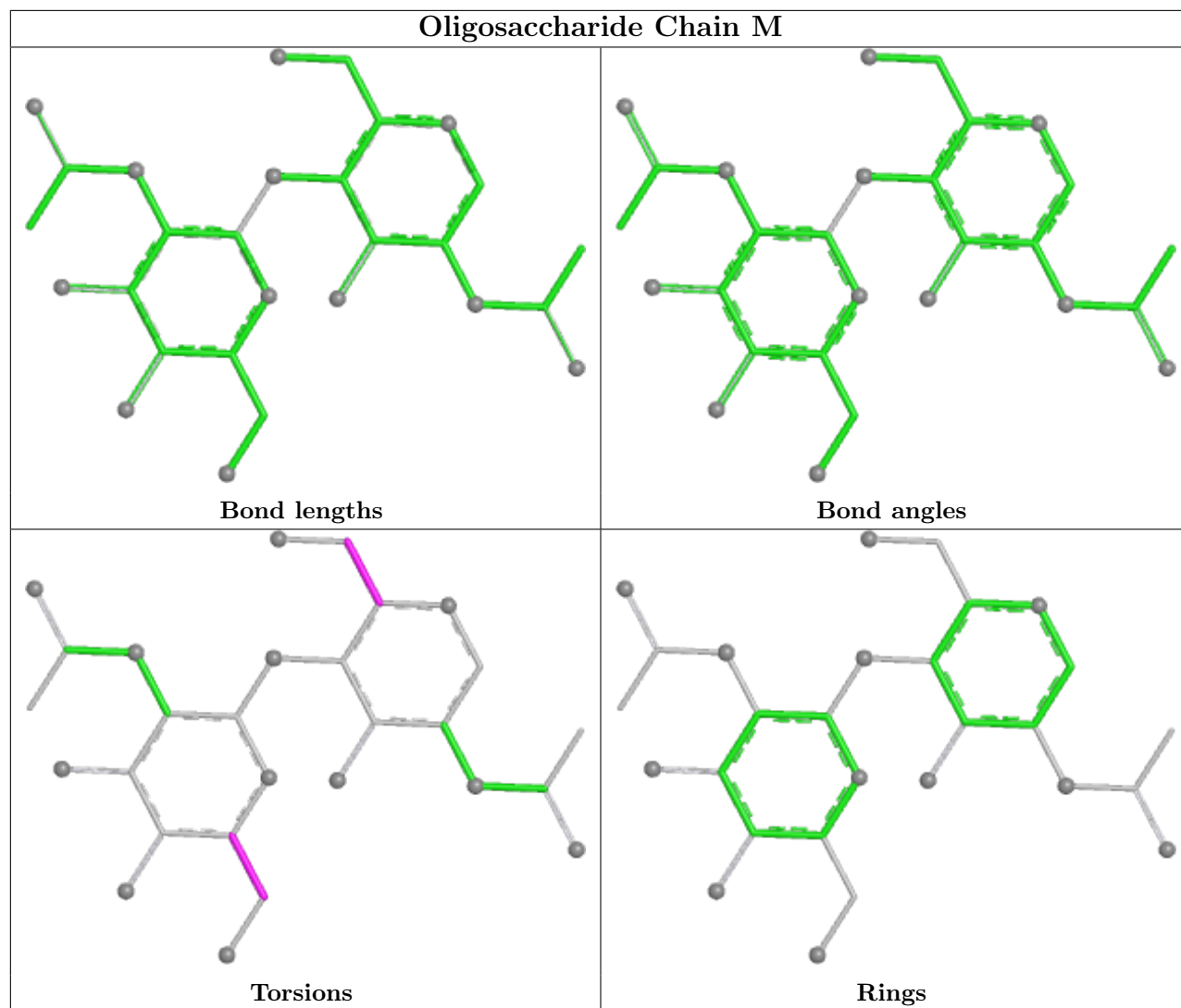


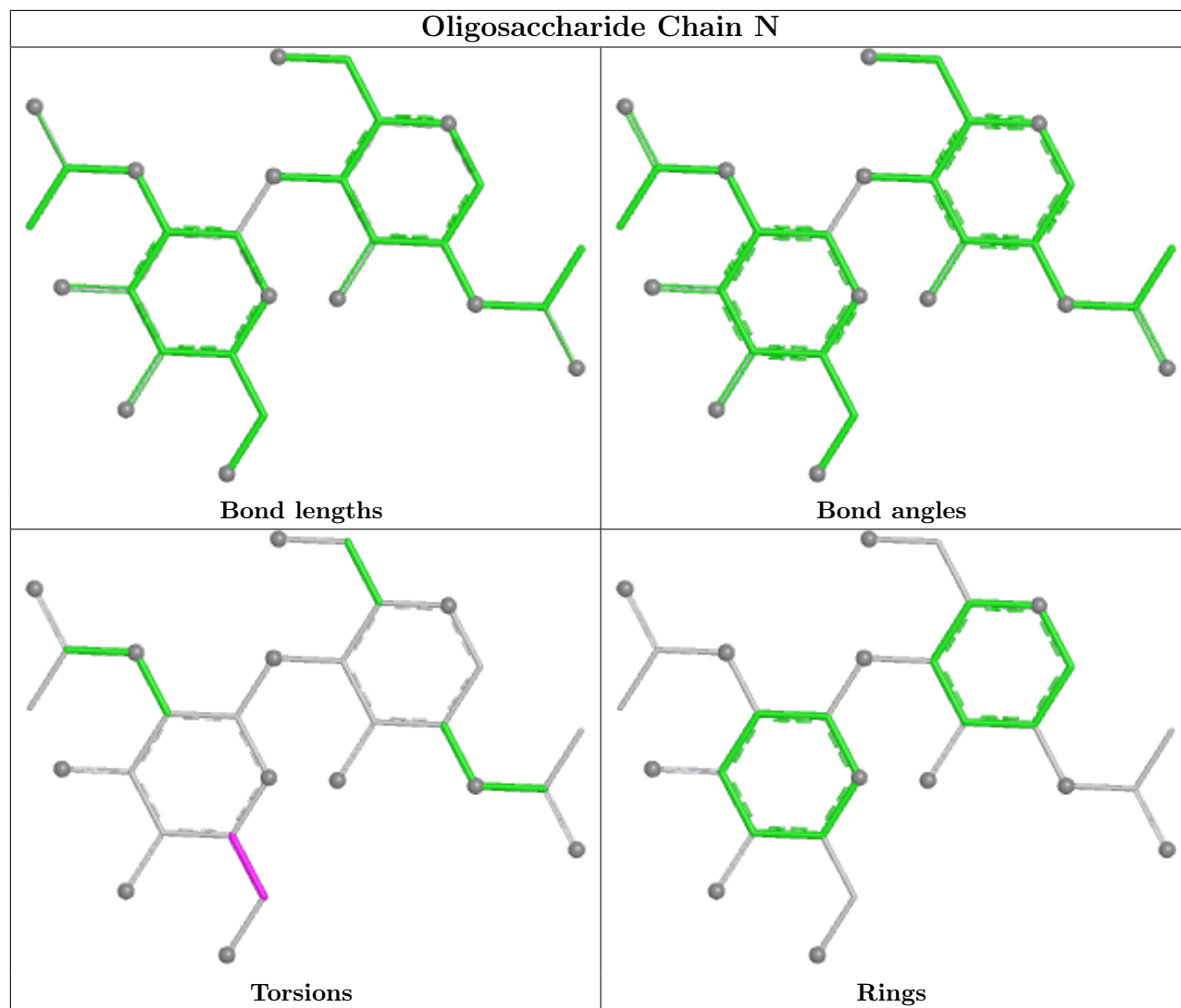


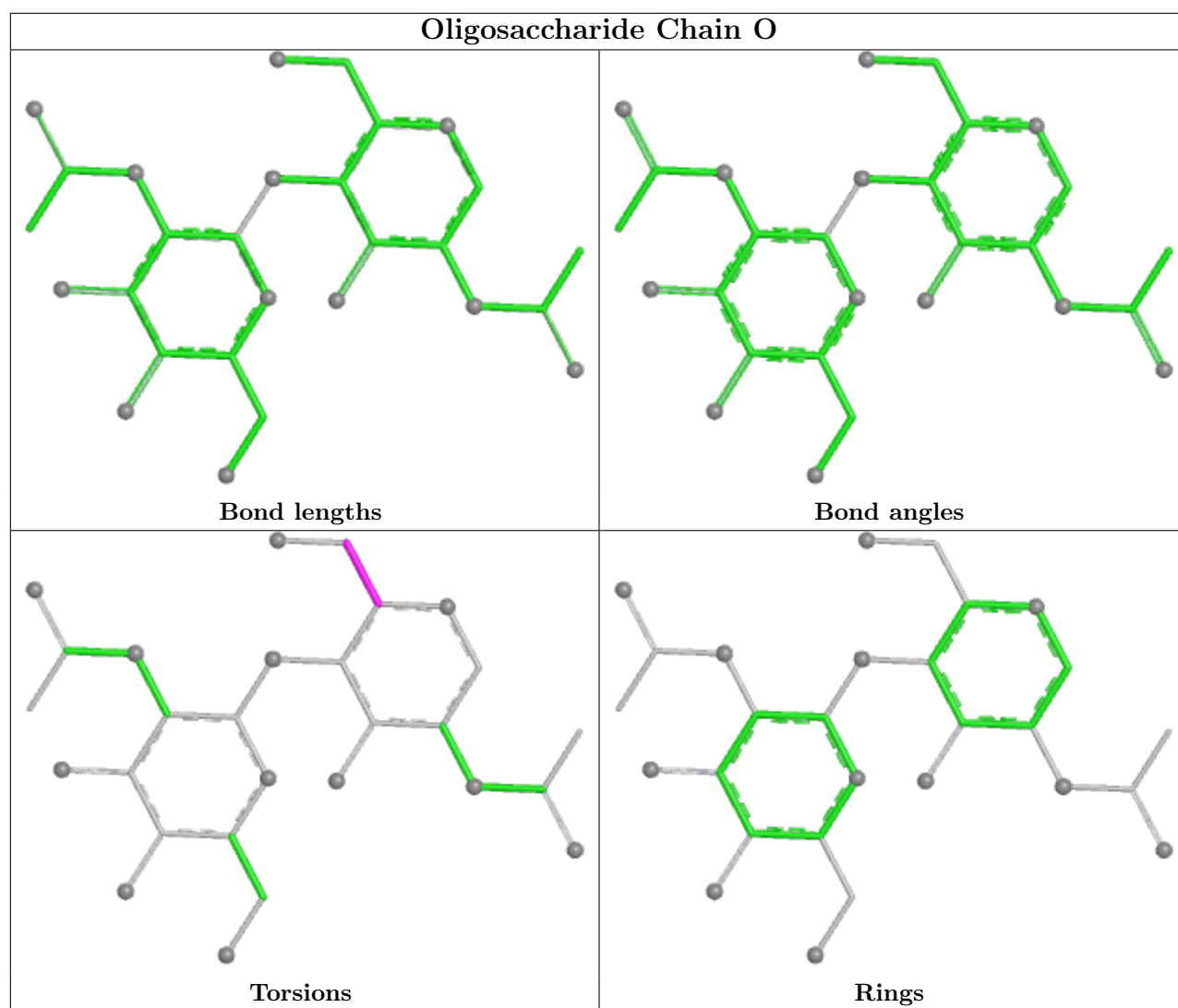


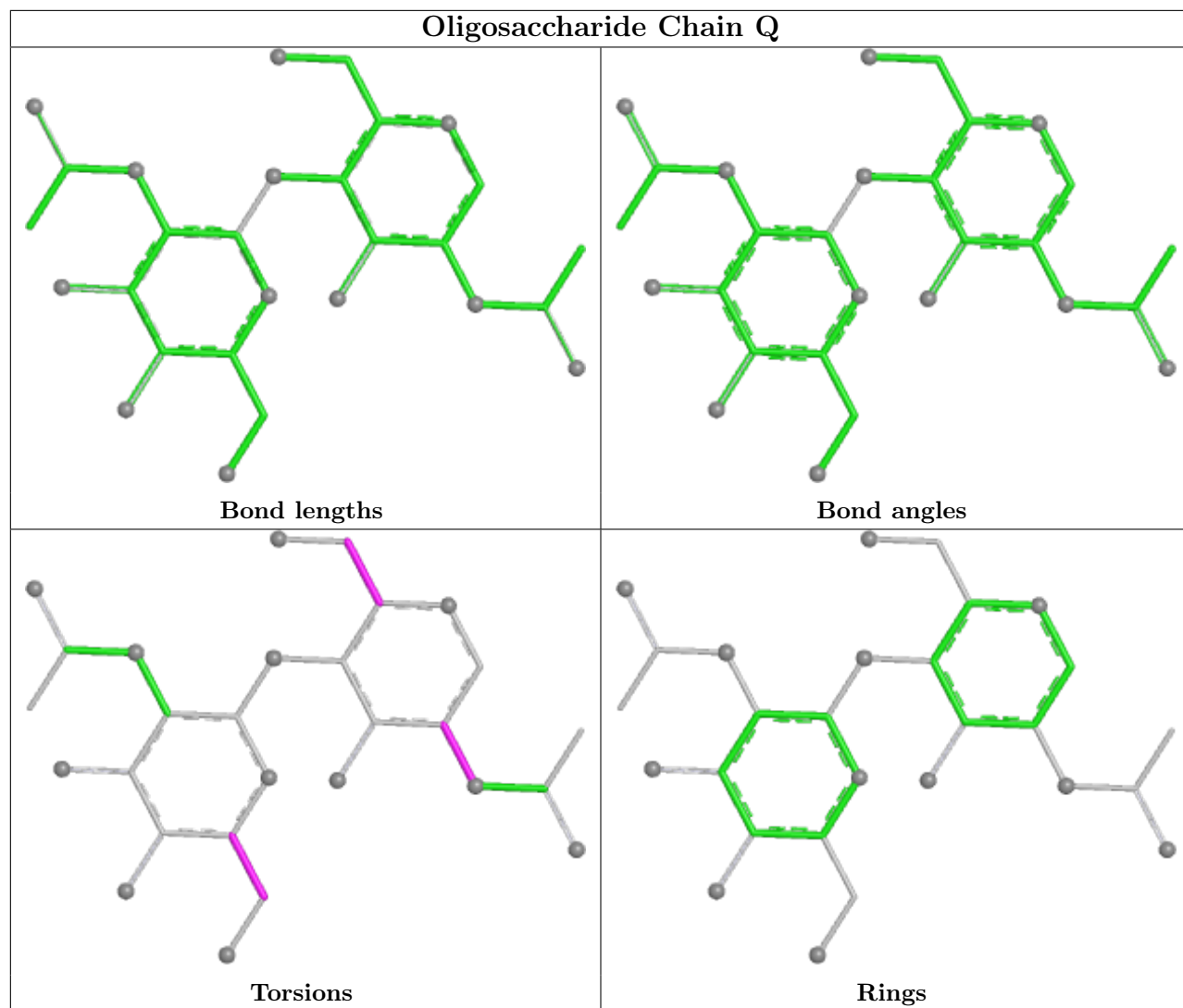


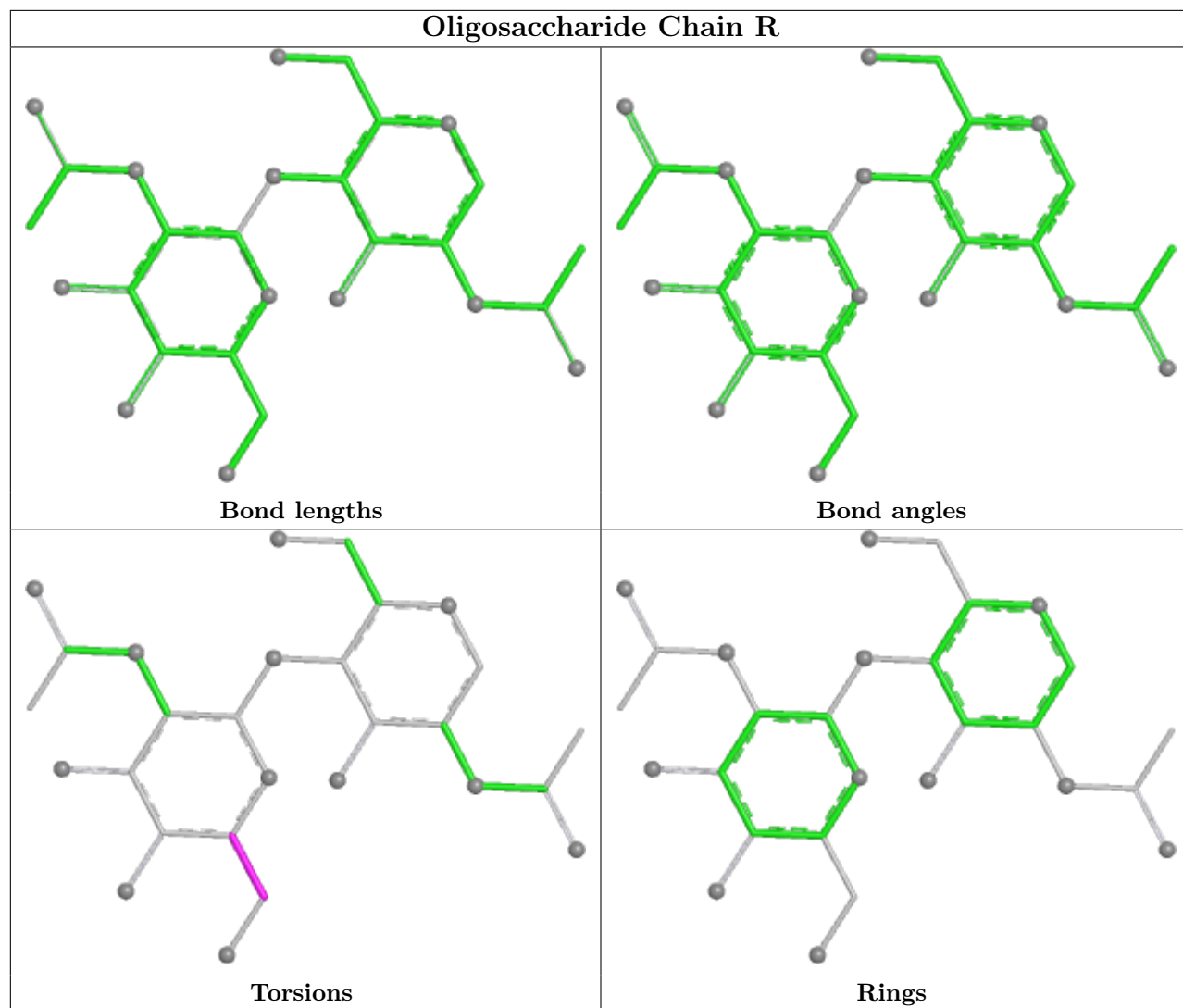


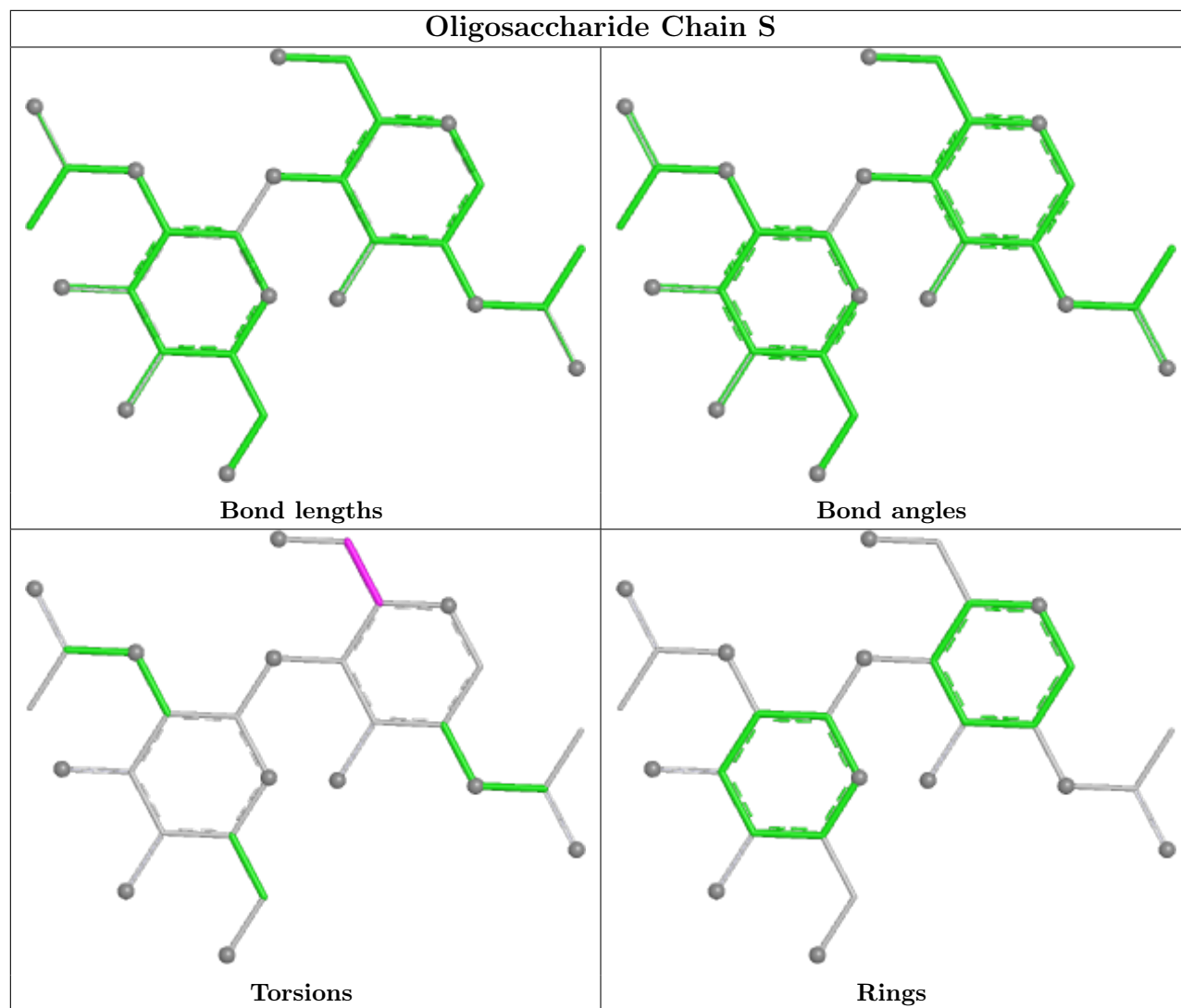




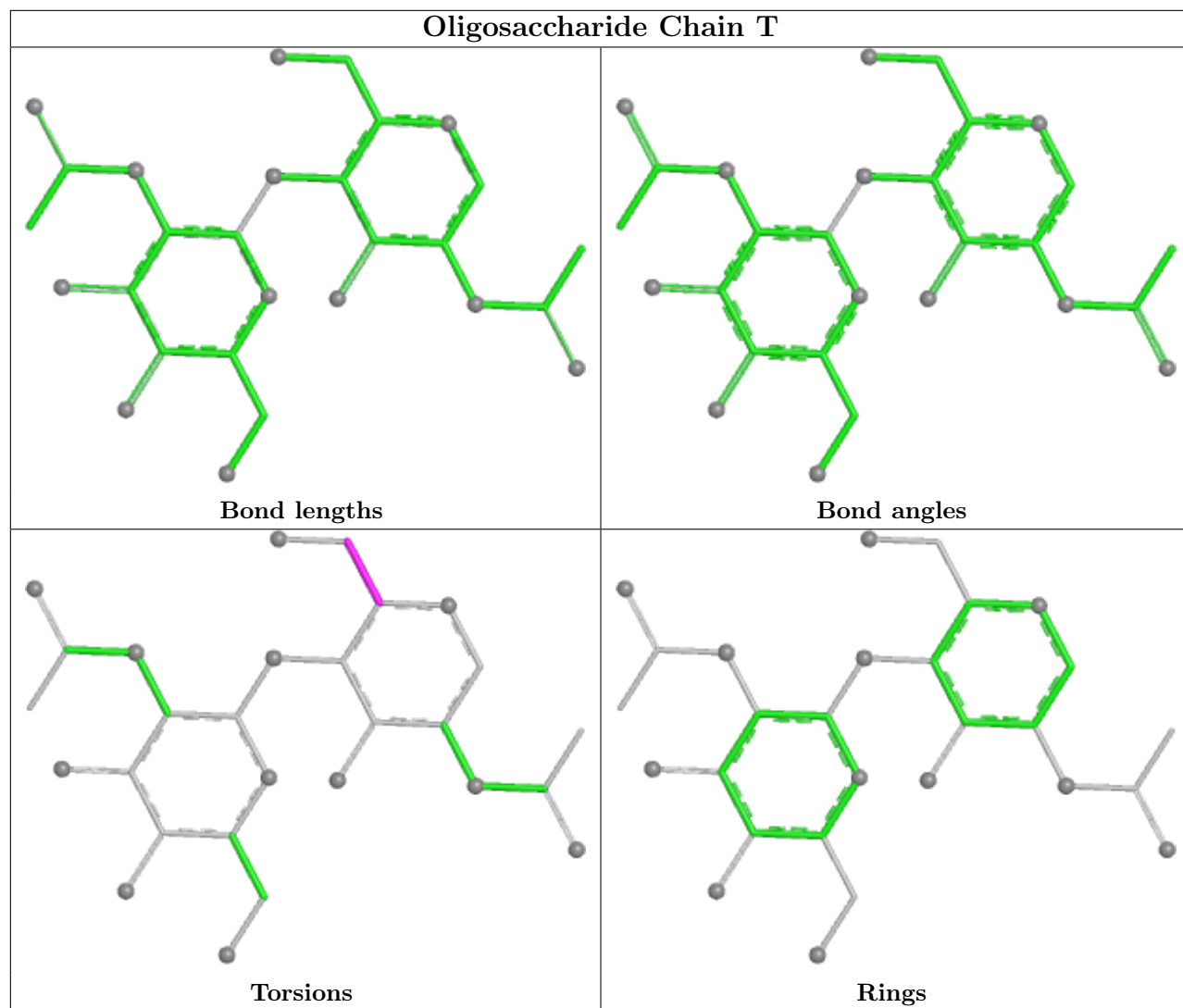


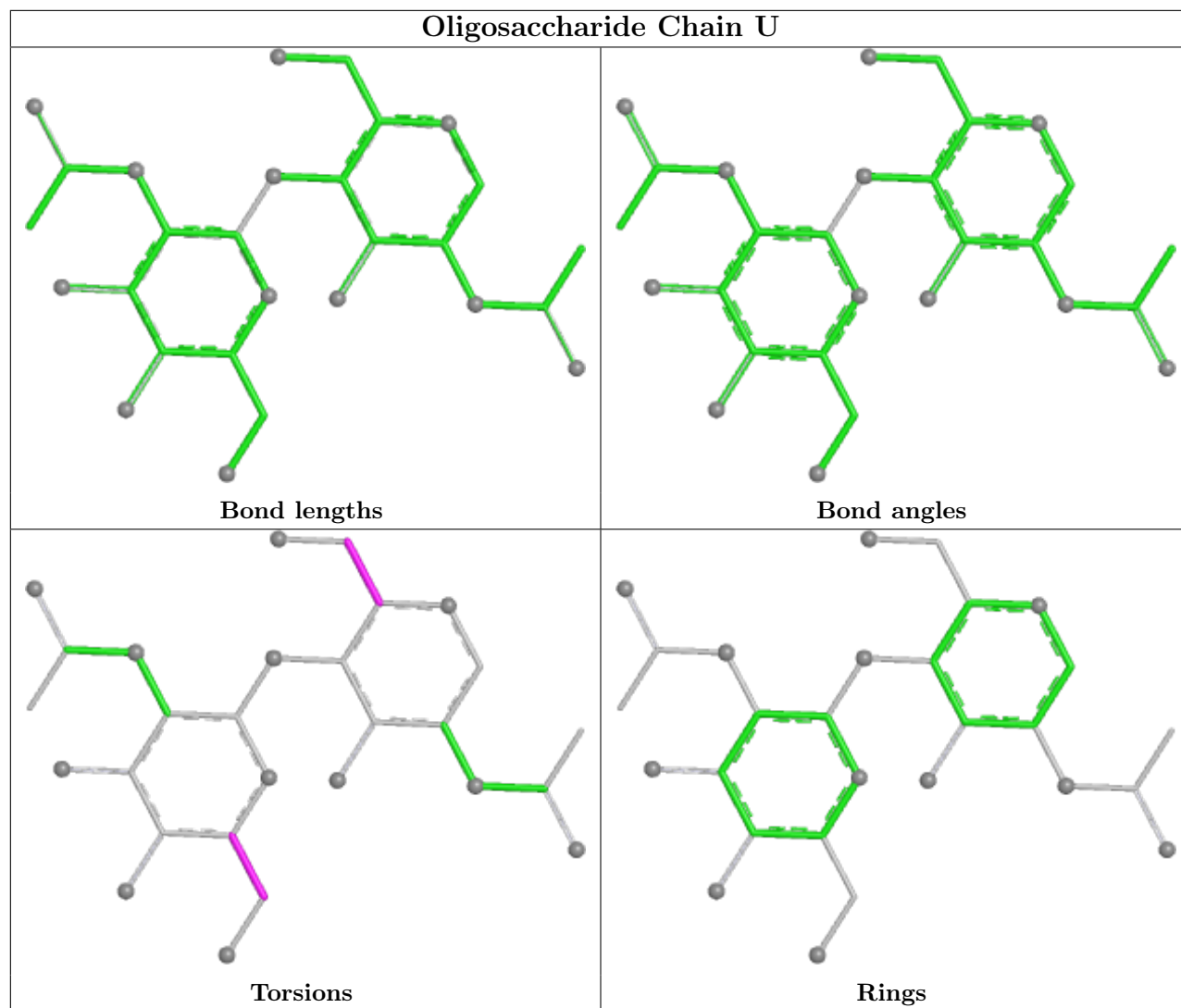


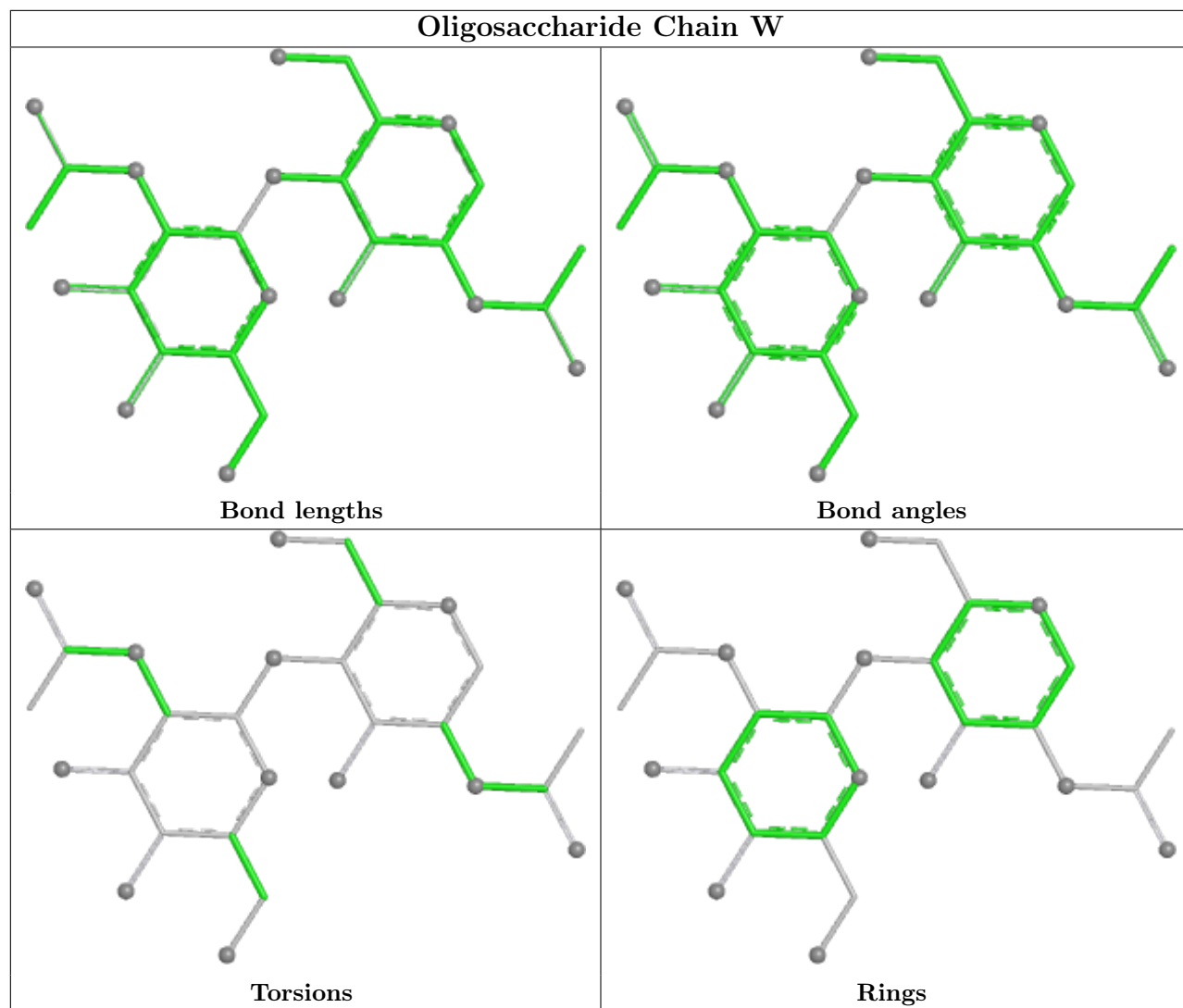


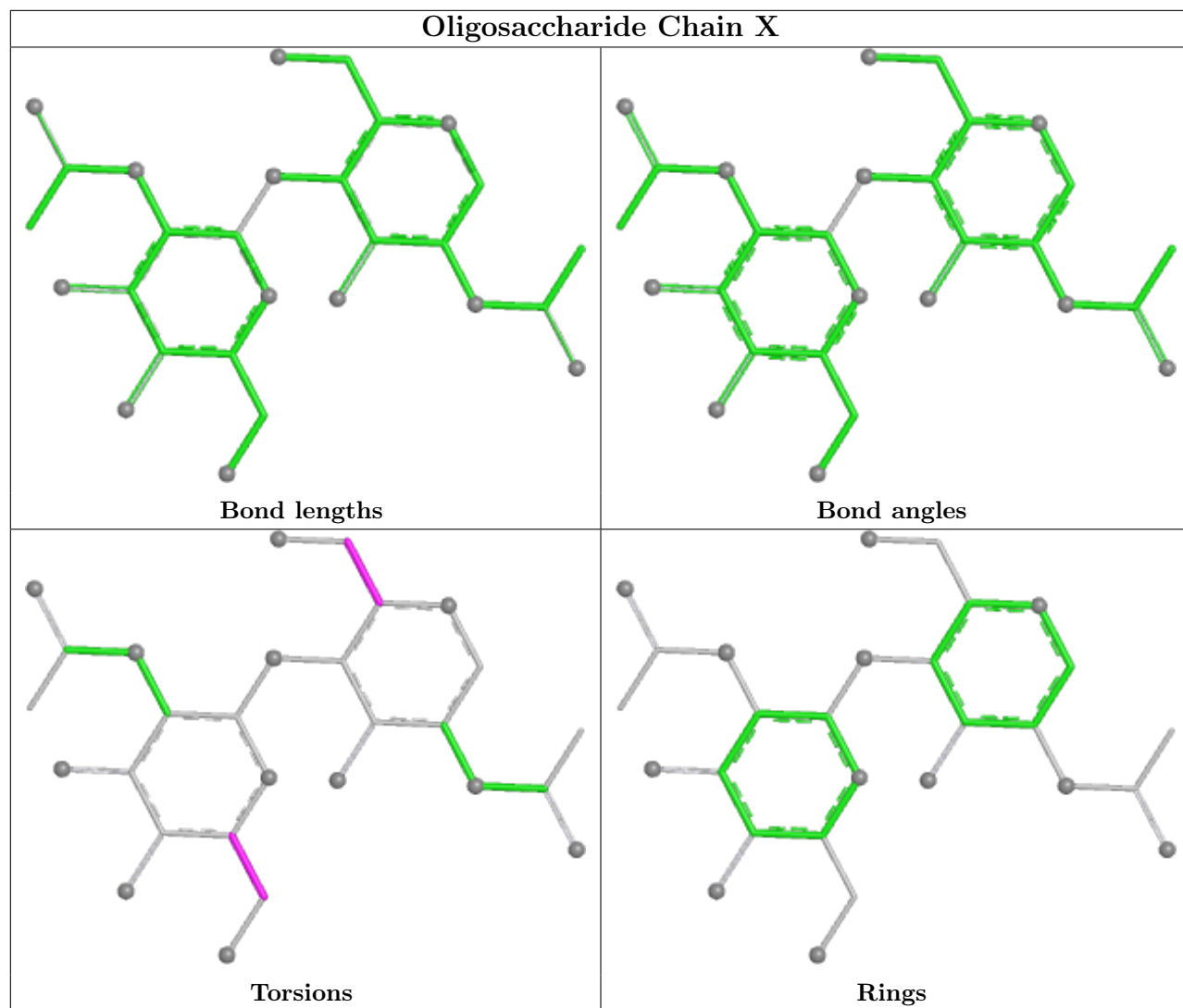


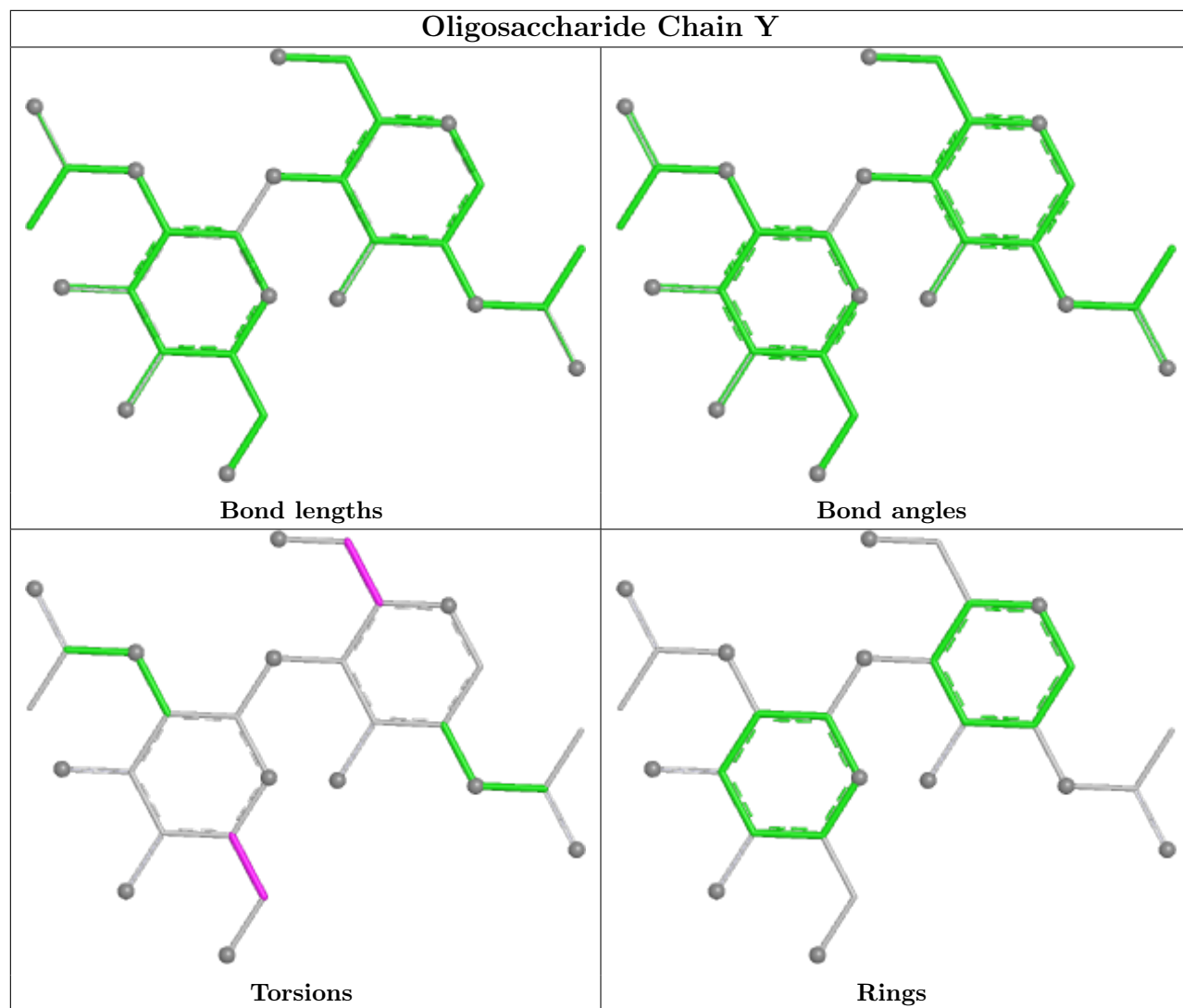


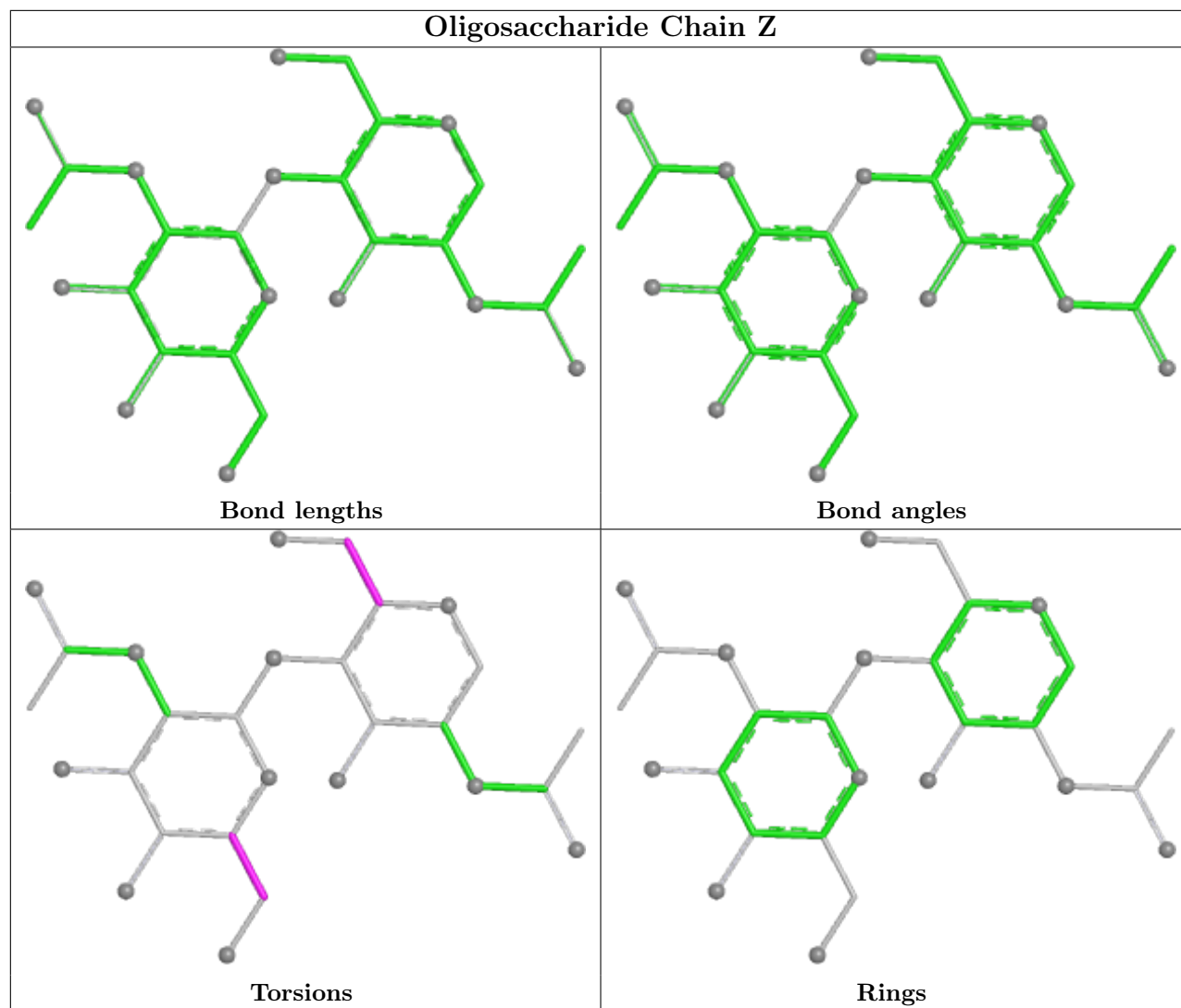


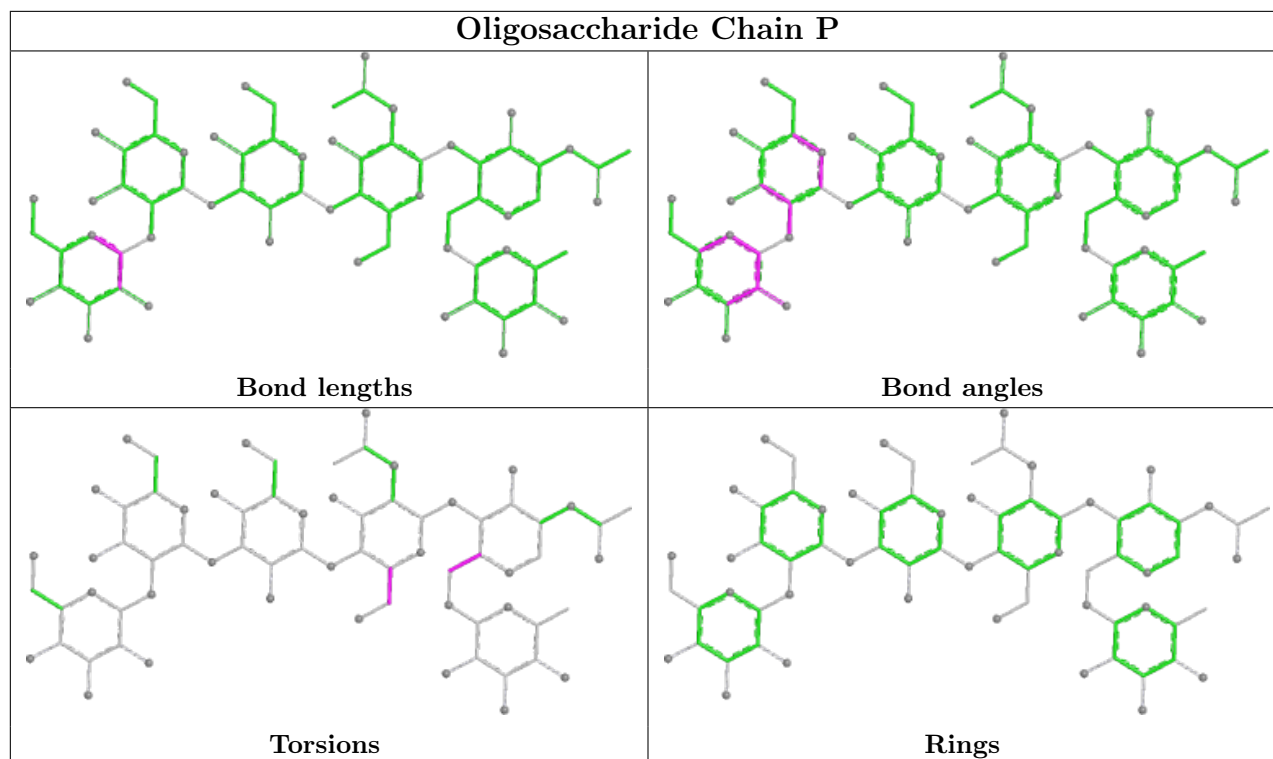












## 5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.44	0
7	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.41	0
7	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.39	0
7	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.39	0
7	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.37	0
7	NAG	A	1305	1	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.39	0
7	NAG	B	1305	1	14,14,15	0.19	0	17,19,21	0.45	0
7	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.47	0
7	NAG	A	1306	1	14,14,15	0.19	0	17,19,21	0.42	0
7	NAG	A	1307	1	14,14,15	0.31	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.38	0
7	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.44	0
7	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.44	0
7	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.42	0
7	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.49	0
7	NAG	B	1307	1	14,14,15	0.19	0	17,19,21	0.40	0
7	NAG	C	1307	1	14,14,15	0.23	0	17,19,21	0.51	0
7	NAG	C	1306	1	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.40	0
7	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.40	0
7	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.46	0
7	NAG	B	1308	1	14,14,15	0.26	0	17,19,21	0.53	0
7	NAG	B	1303	1	14,14,15	0.22	0	17,19,21	0.45	0
7	NAG	B	1309	1	14,14,15	0.20	0	17,19,21	0.42	0
7	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.40	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
7	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1307	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1305	NAG	O5-C5-C6-O6
7	C	1304	NAG	O5-C5-C6-O6
7	A	1304	NAG	O5-C5-C6-O6
7	B	1302	NAG	O5-C5-C6-O6
7	C	1301	NAG	O5-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.

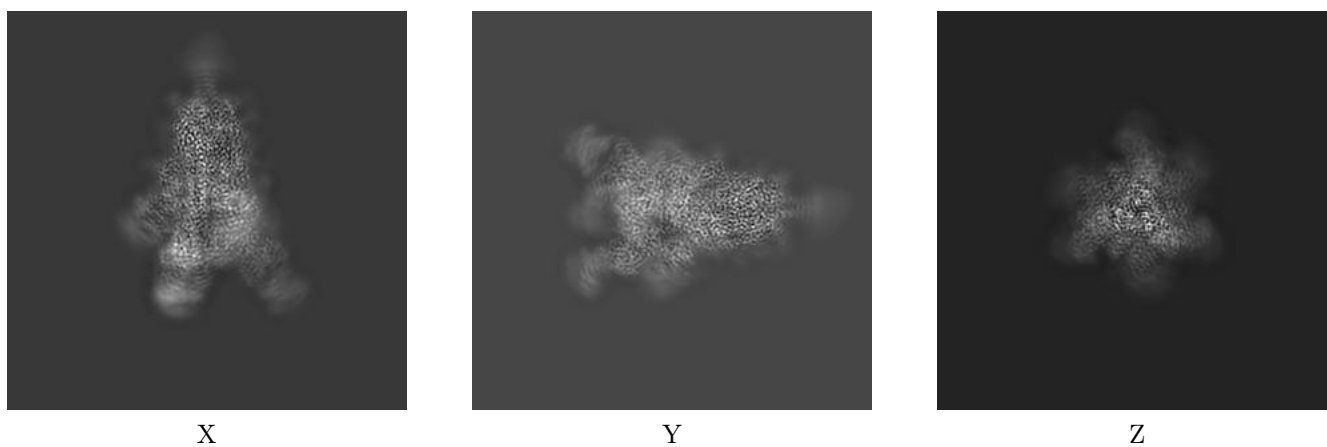
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13857. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

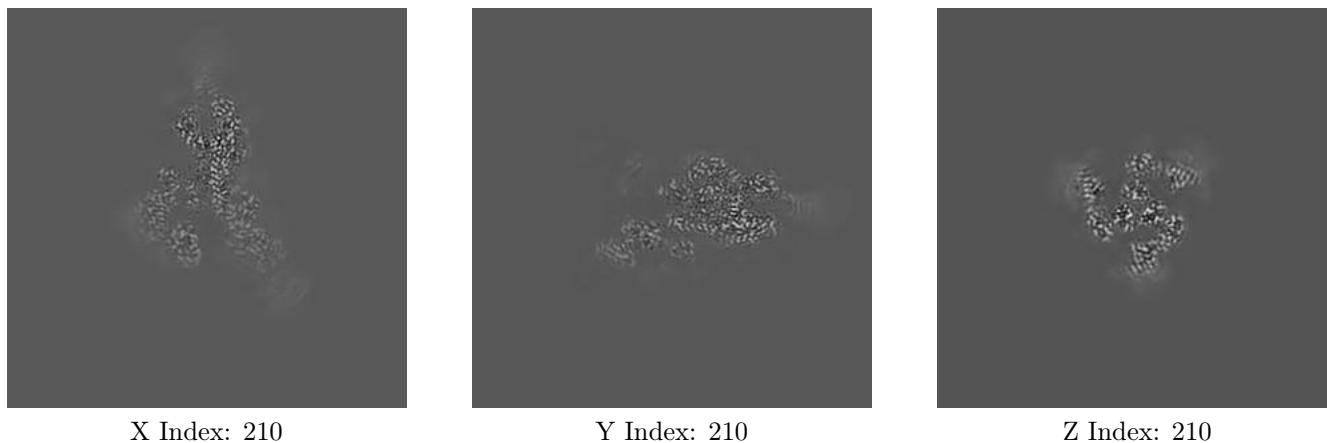
#### 6.1.1 Primary map



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

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

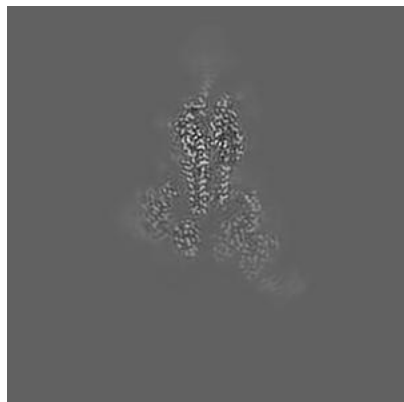
#### 6.2.1 Primary map



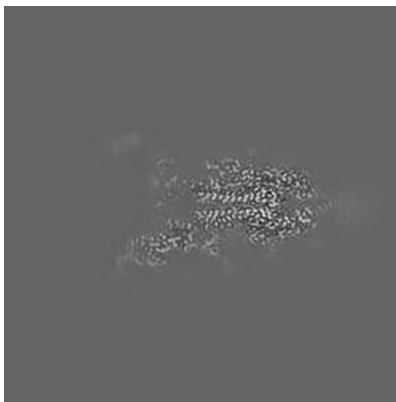
The images above show central slices of the map in three orthogonal directions.

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

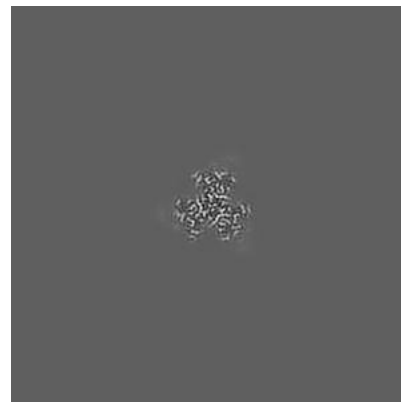
### 6.3.1 Primary map



X Index: 220



Y Index: 203



Z Index: 277

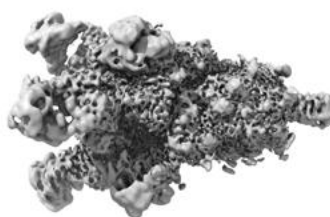
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

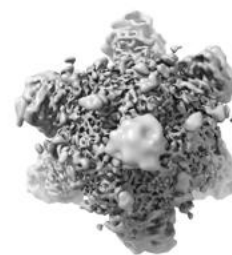
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0718. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

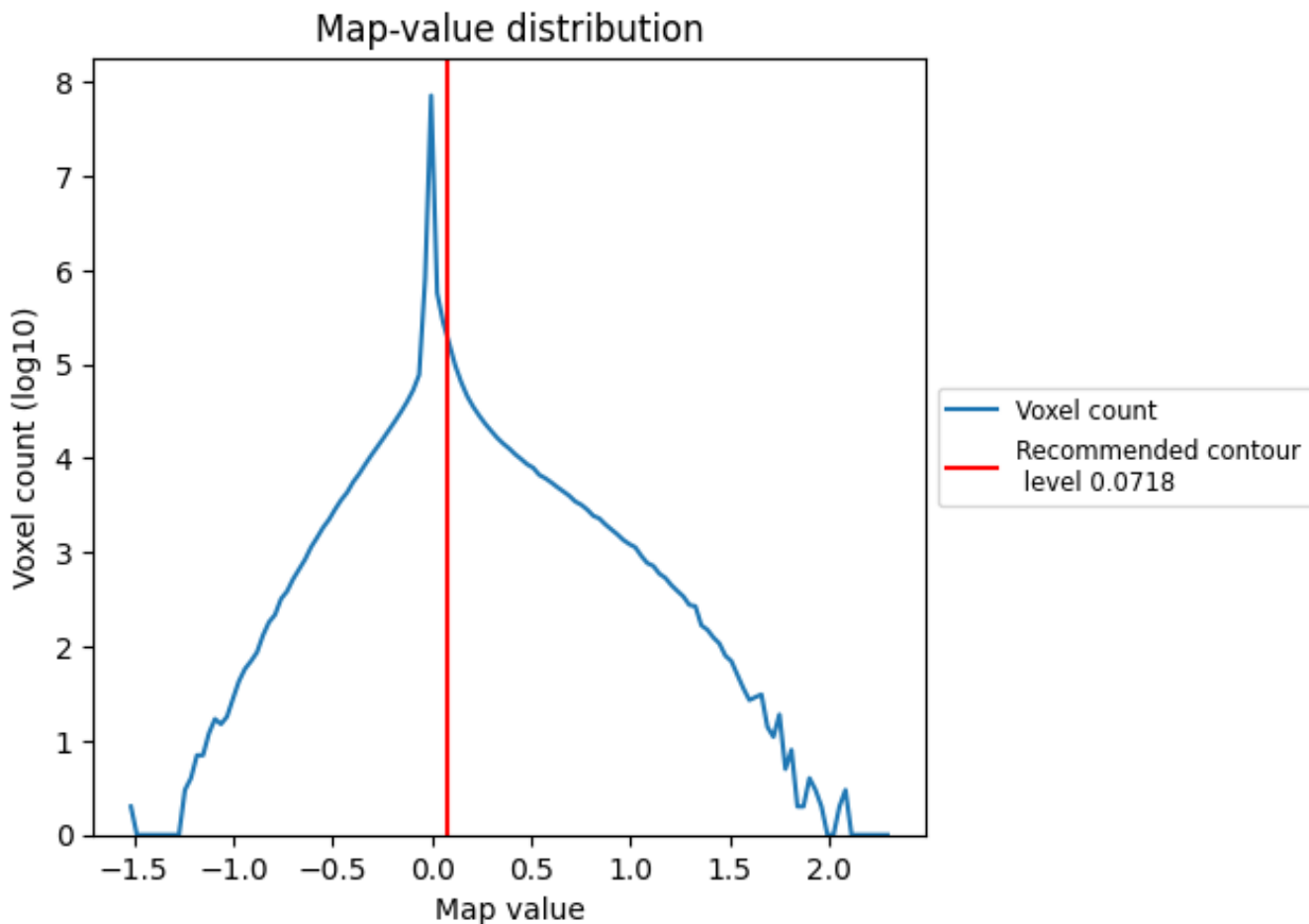
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

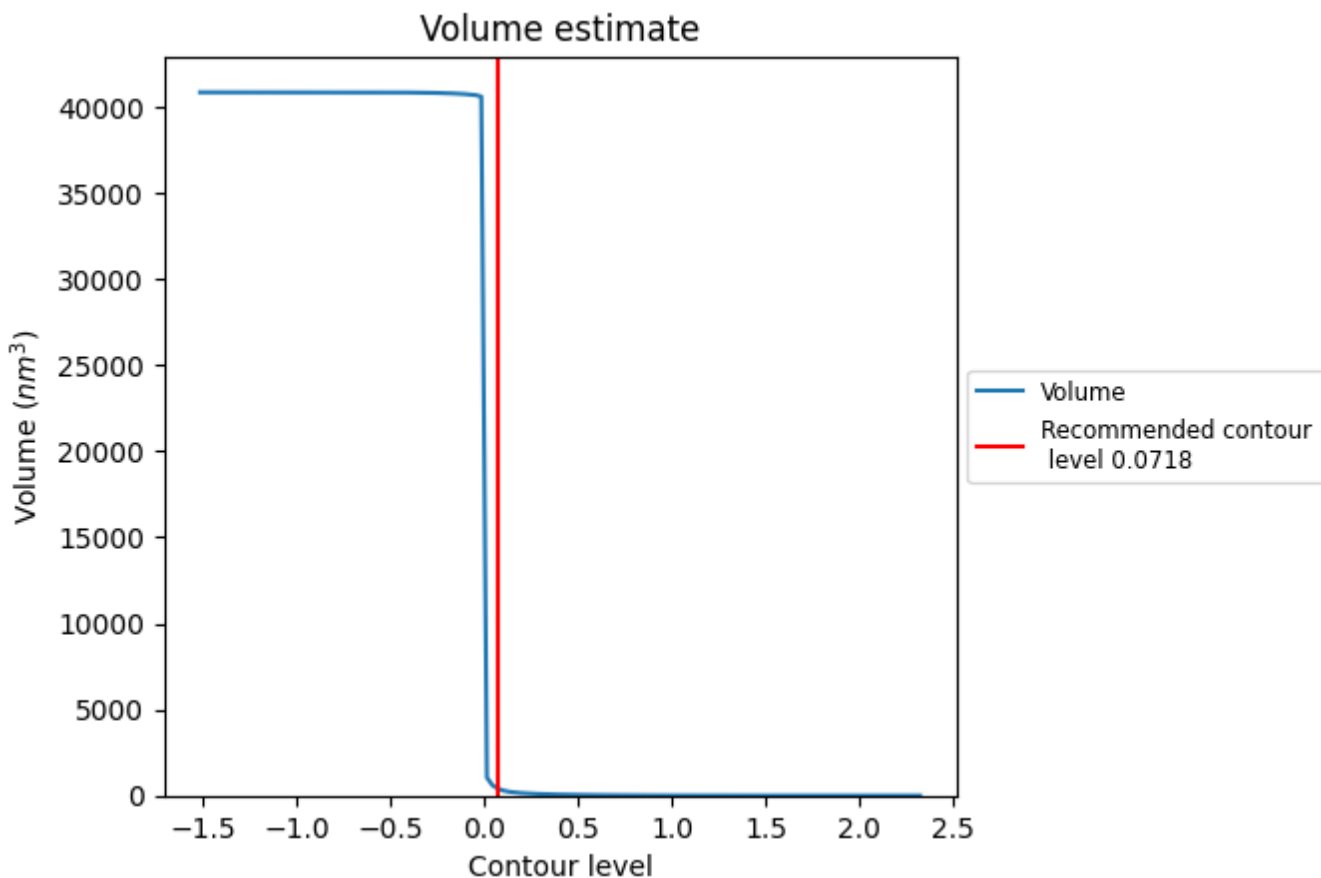
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

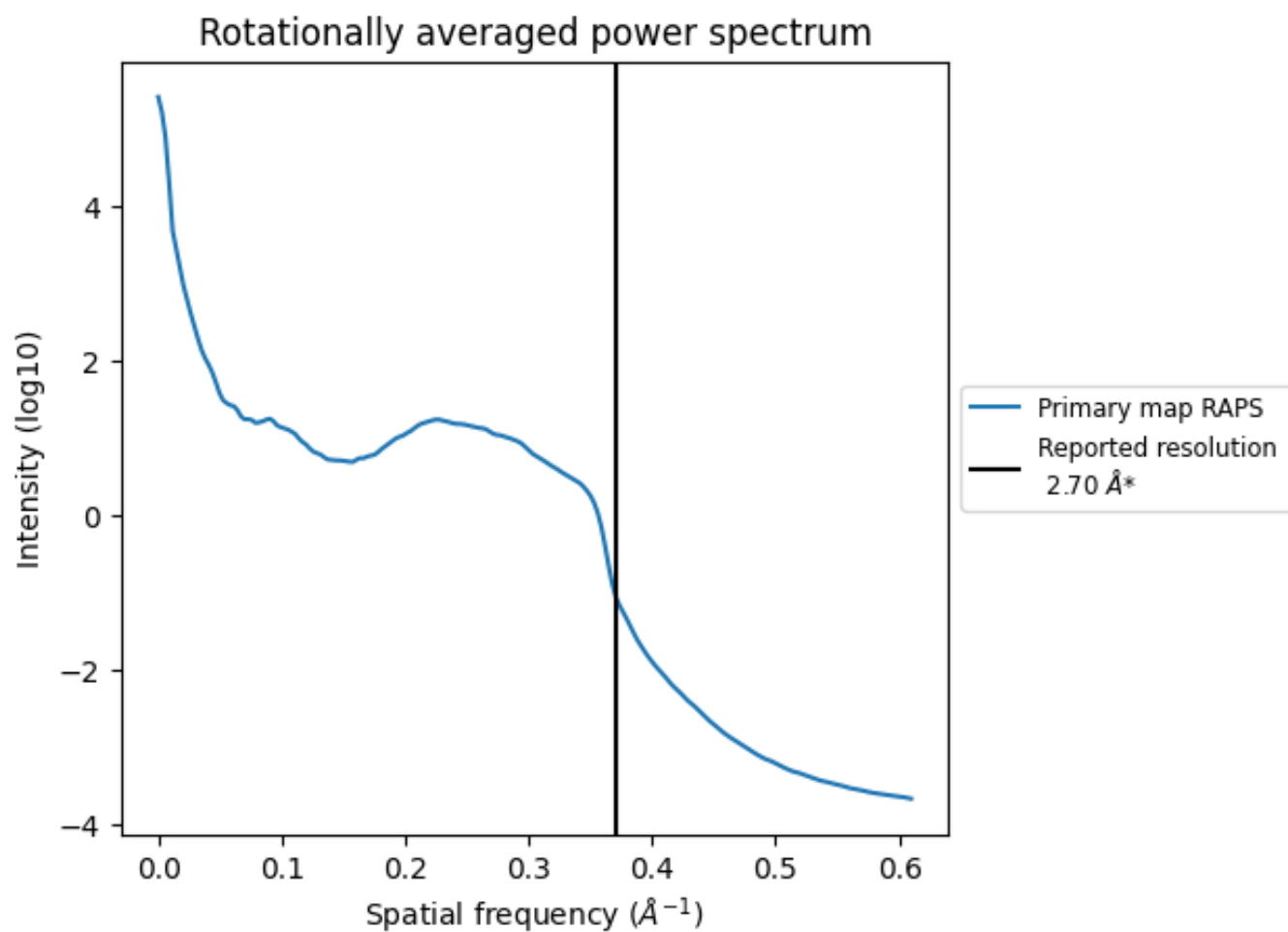
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 411 nm<sup>3</sup>; this corresponds to an approximate mass of 371 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.370 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation

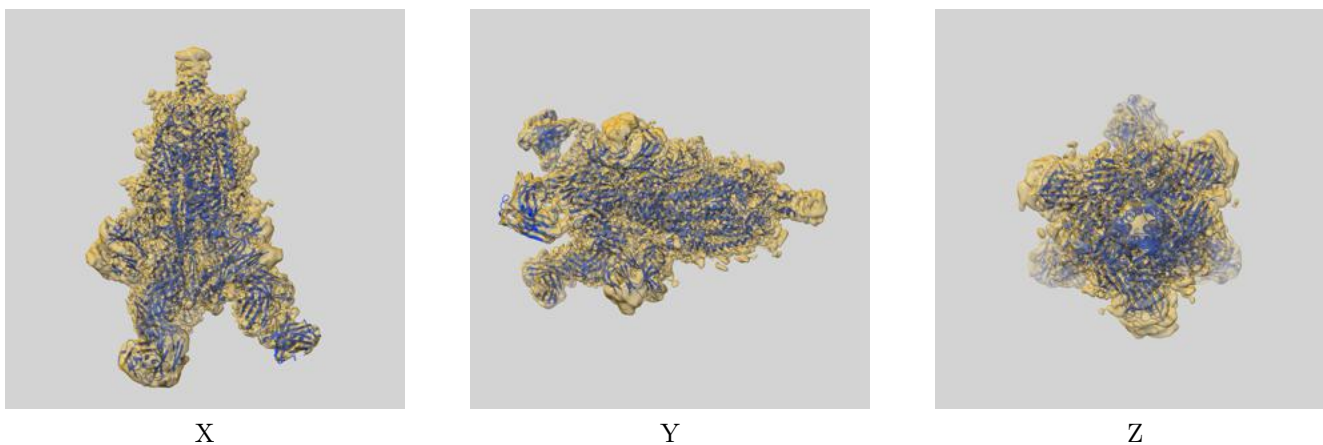
This section was not generated. No FSC curve or half-maps provided.



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

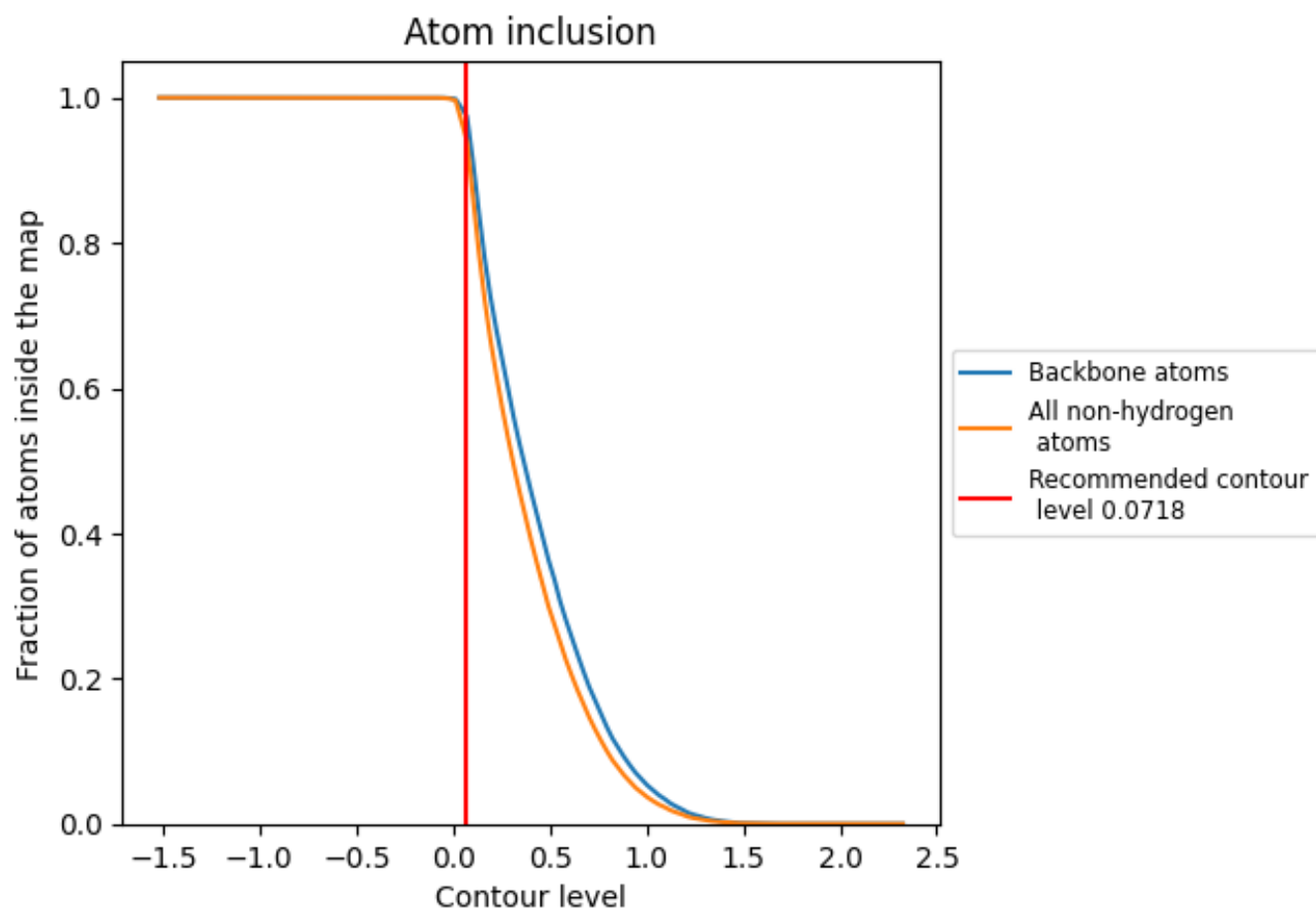
This section contains information regarding the fit between EMDB map EMD-13857 and PDB model 7Q6E. Per-residue inclusion information can be found in section 3 on page 16.

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



The images above show the 3D surface view of the map at the recommended contour level 0.0718 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 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.