



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:55 PM EST

PDB ID : 7MJM
EMDB ID : EMD-23878
Title : Cryo-EM structure of the SARS-CoV-2 N501Y mutant spike protein ectodomain bound to human ACE2 ectodomain
Authors : Zhu, X.; Mannar, D.; Srivastava, S.S.; Berezuk, A.M.; Demers, J.P.; Saville, J.W.; Leopold, K.; Li, W.; Dimitrov, D.S.; Tuttle, K.S.; Zhou, S.; Chittori, S.; Subramaniam, S.
Deposited on : 2021-04-20
Resolution : 2.83 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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 ≥ 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	1288	
1	B	1288	
1	C	1288	
2	D	606	
2	E	606	
3	F	2	
3	G	2	
3	H	2	

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Mol	Chain	Length	Quality of chain
3	I	2	 50% 100%
3	J	2	 50% 50%
3	K	2	 100%
3	L	2	 50% 50% 50%
3	M	2	 100%
3	N	2	 50% 50%
3	O	2	 50% 100%
3	P	2	 50% 50%
3	Q	2	 100%
3	R	2	 50% 50% 50%
3	S	2	 100%
3	T	2	 50% 50%
3	U	2	 100%
3	V	2	 50% 50%
3	W	2	 100%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 35096 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	1040	8140	5200	1355	1548	37	0	0
1	B	1040	8140	5200	1355	1548	37	0	0
1	C	1040	8140	5200	1355	1548	37	0	0

There are 270 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	TYR	ASN	engineered mutation	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	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	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	501	TYR	ASN	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	501	TYR	ASN	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

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

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
D	622	HIS	-	expression tag	UNP Q9BYF1
D	623	HIS	-	expression tag	UNP Q9BYF1
E	616	HIS	-	expression tag	UNP Q9BYF1
E	617	HIS	-	expression tag	UNP Q9BYF1
E	618	HIS	-	expression tag	UNP Q9BYF1
E	619	HIS	-	expression tag	UNP Q9BYF1
E	620	HIS	-	expression tag	UNP Q9BYF1
E	621	HIS	-	expression tag	UNP Q9BYF1
E	622	HIS	-	expression tag	UNP Q9BYF1
E	623	HIS	-	expression tag	UNP Q9BYF1

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



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

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	A	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0

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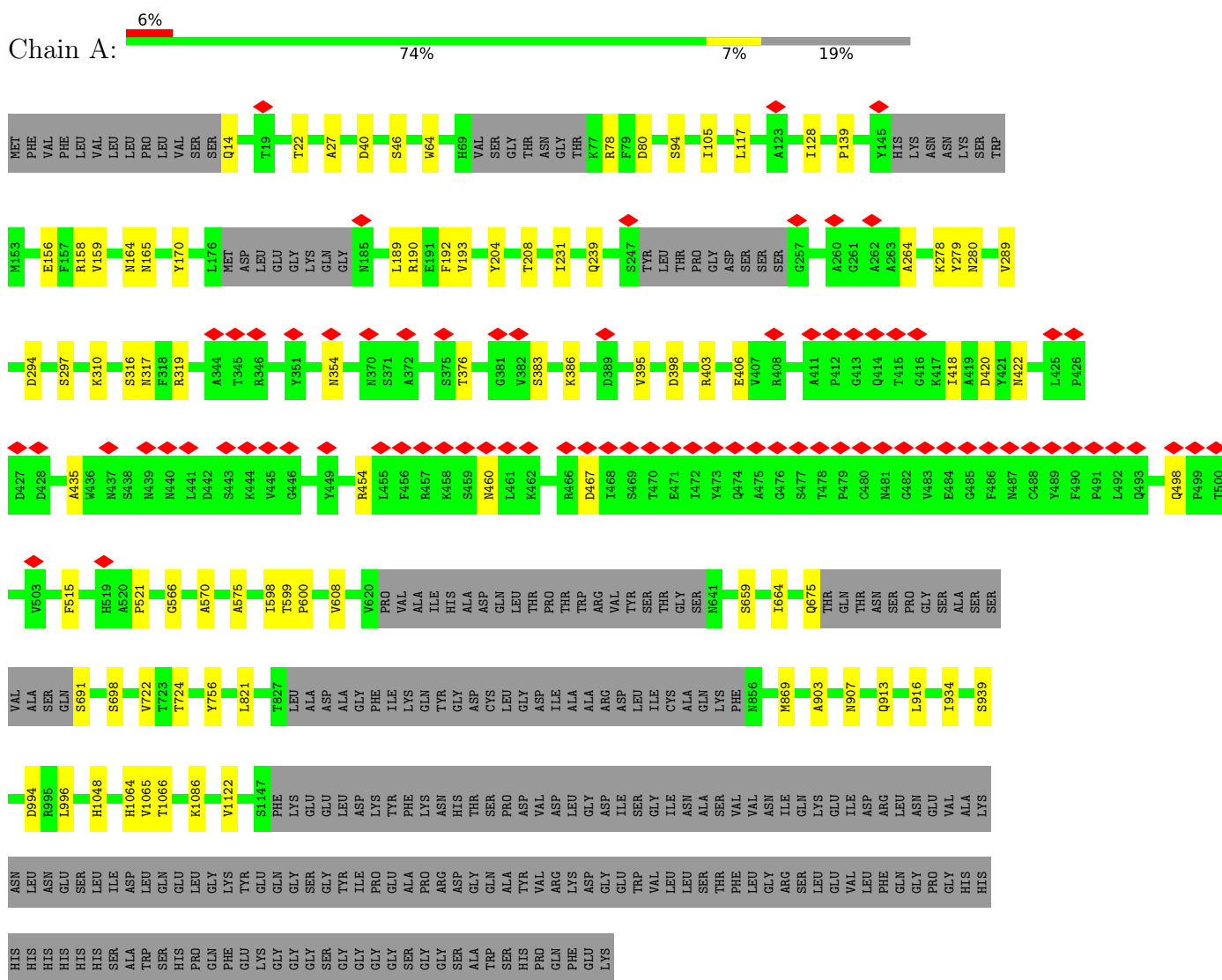
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	112	64	8	40	0
4	B	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	C	1	112	64	8	40	0
4	D	1	56	32	4	20	0
4	D	1	56	32	4	20	0
4	D	1	56	32	4	20	0
4	D	1	56	32	4	20	0
4	E	1	56	32	4	20	0
4	E	1	56	32	4	20	0
4	E	1	56	32	4	20	0
4	E	1	56	32	4	20	0

3 Residue-property plots [i](#)

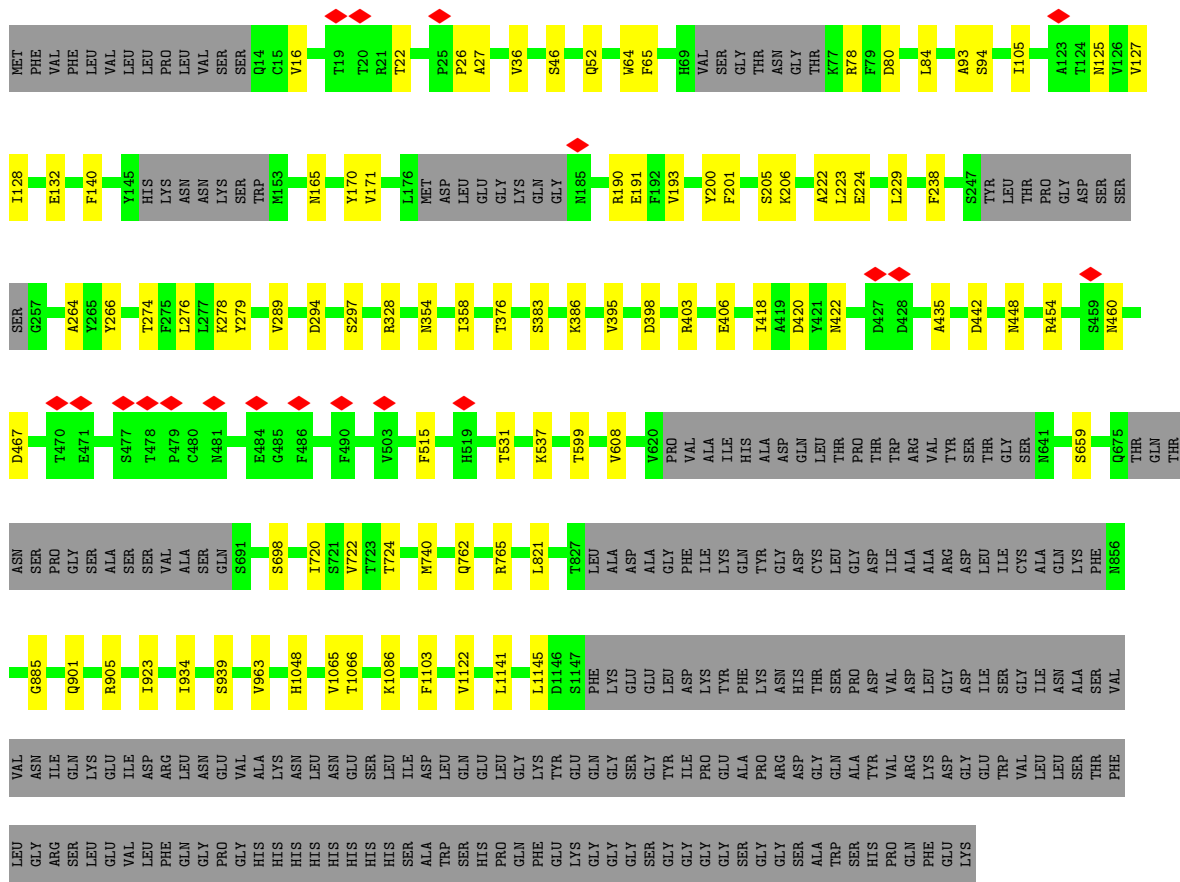
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

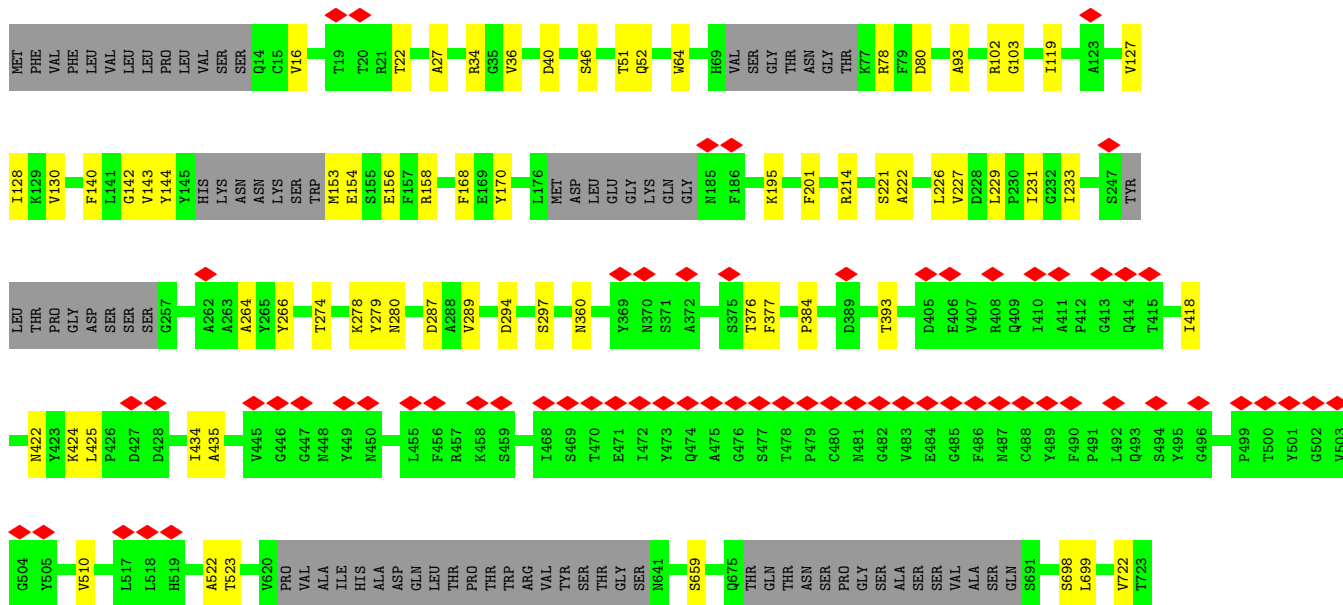
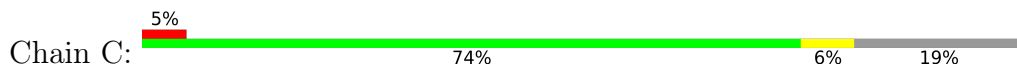


• Molecule 1: Spike glycoprotein



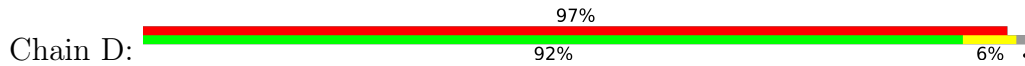


• Molecule 1: Spike glycoprotein

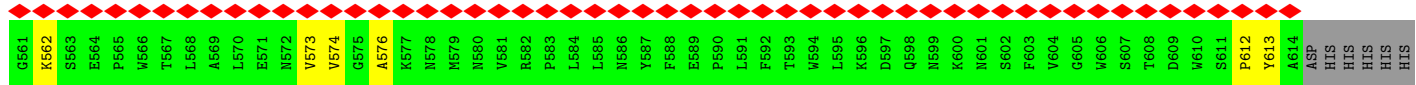


IT24	L821	T827	LEU	ALA	ASP	LYS	ASP	ALA	ASP	GLY	ASP	ILE	ALA	GLU	ALA	SER	ARG	ASP	ASP	ILE	LEU	ASN	LYS	PHE	N856	L916	L923	L934	S939	D985	F986	A989	H1048	V1065	T1066	K1086	V1122	P1143	D1146		
S1147	PHE	LYS	GLU	LEU	ASP	LYS	TYR	ALA	PHE	GLY	PRO	LYS	ASN	ILE	GLU	ALA	TRP	VAL	ASP	LEU	GLY	ASP	ILE	PHE	N856	L916	L923	L934	S939	D985	F986	A989	H1048	V1065	T1066	K1086	V1122	P1143	D1146		
GLU	GLN	GLY	SER	GLY	TYR	ILE	PRO	ALA	TYR	ALA	PRO	LYS	ASN	ILE	GLU	ALA	TRP	VAL	ASP	LEU	GLY	ASP	ILE	PHE	N856	L916	L923	L934	S939	D985	F986	A989	H1048	V1065	T1066	K1086	V1122	P1143	D1146		
LYS	GLY	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

● Molecule 2: Processed angiotensin-converting enzyme 2

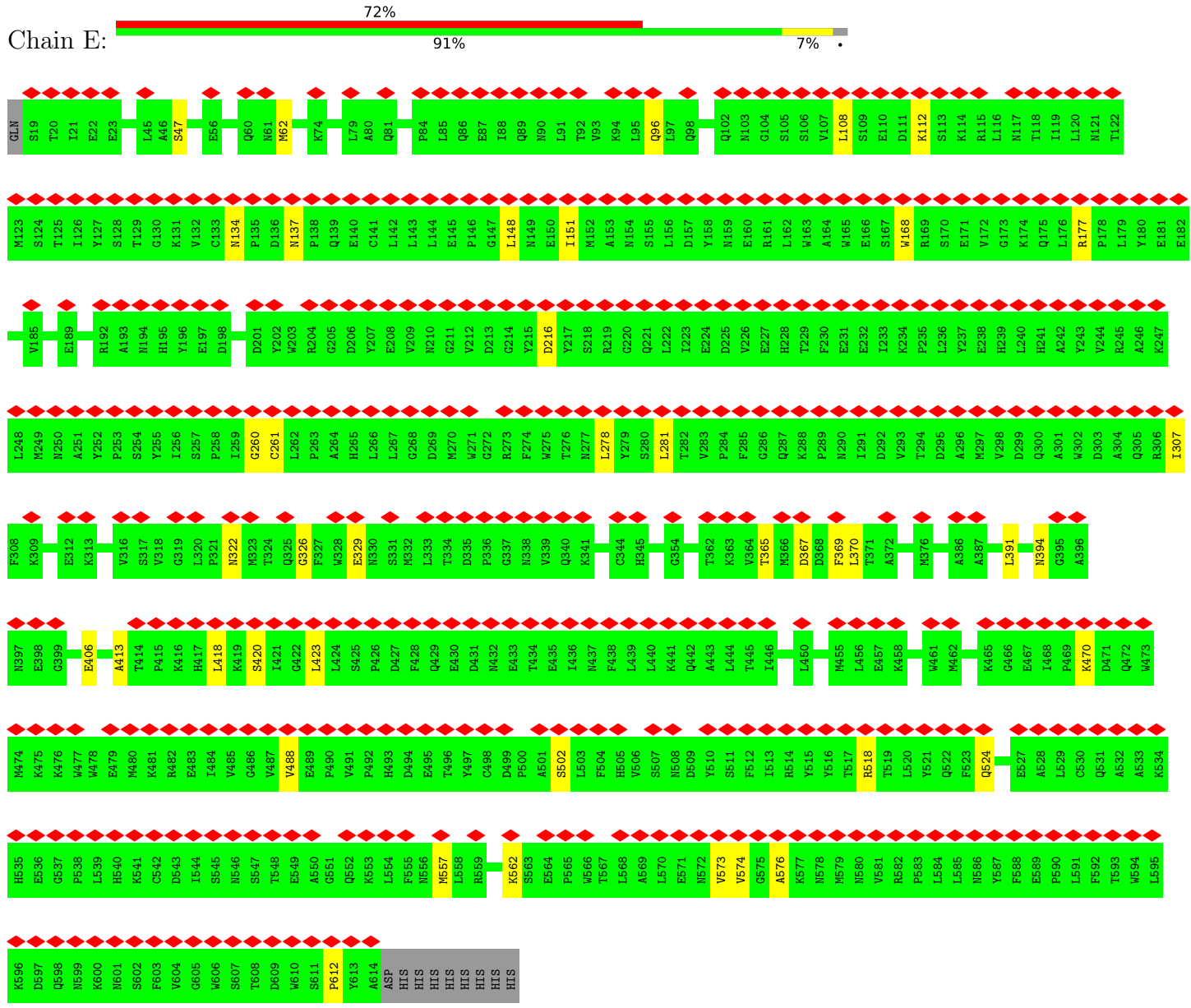


GLN	S19	T20	I21	E22	E23	Q24	K26	T27	F28	L29	D30	K31	F32	N33	H34	E35	A36	E37	D38	L39	Q42	S43	S44	L45	A46	S47	M48	N49	Y50	N51	F52	N53	I54	T55	E56	E57	N58	V59	Q60	N61	H62	N63	H64	A65	G66	D67	H68	N69	S70	A71	F72	L73	K74	E75	Q76	S77	T78		
L79	A80	Q81	M82	H83	P84	L85	Q86	E87	L88	Q89	N90	D91	T92	N93	K94	L95	Q96	L97	Q98	A99	L100	Q101	Q102	M103	G104	S105	S106	L107	N108	S109	E110	D111	K112	S113	K114	R115	L116	M117	T118	I119	L120	M121	T122	N123	S124	T125	I126	L127	N128	T129	G130	K131	V132	C133	N134	P135	D136	M137	P138
Q139	E140	C141	L142	P143	L144	E145	P146	L147	L148	M149	E150	I151	M152	A153	M154	S155	L156	D157	Y158	M159	E160	R161	L162	W163	A164	W165	E166	S167	R168	S169	F170	E171	V172	G173	K174	Q175	L176	R177	P178	L179	Y180	E181	E182	Y183	Y184	V185	L186	K187	N188	E189	M190	A191	E192	A193	N194	H195	Y196	E197	D198
Y199	G200	D201	Y202	W203	R204	G205	D206	Y207	E208	V209	N210	G211	V212	D213	G214	Y215	D216	Y217	S218	R219	G220	Q221	L222	I223	E224	D225	V226	E227	H228	T229	F230	E231	E232	I233	K234	P235	L236	Y237	E238	H239	L240	H241	A242	Y243	V244	R245	A246	K247	L248	M249	N250	A251	E252	P253	S254	Y255	L256	S257	P258
I259	G260	C261	L262	P263	A264	L266	L267	G268	D269	M270	W271	G272	R273	F274	W275	T276	W277	L278	Y279	S280	L281	T282	V283	P284	F285	G286	Q287	K288	P289	N290	I291	D292	V293	T294	D295	A296	M297	V298	D299	Q300	A301	W302	D303	A304	Q305	R306	I307	F308	K309	E310	A311	E312	K313	F314	F315	V316	S317	V318	
G319	L320	P321	M322	M323	T324	Q325	G326	F327	M328	E329	M330	S331	M332	L333	T334	D335	P336	G337	M338	V339	Q340	K341	A342	V343	C344	H345	P346	S347	A348	W349	D350	A413	T414	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426	D427	F428	Q429	E430	D431	N432	E433	T434	E435	I436	M437	G377	H378	I379
Q380	Y381	D382	M383	A384	Y385	A386	A387	Q388	P389	L392	R393	N394	G395	A396	N397	E398	G399	F400	H401	E402	A403	V404	G405	E406	I407	M408	S409	L410	S411	A412	A413	T414	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426	D427	F428	Q429	E430	D431	N432	E433	T434	E435	I436	M437	G377	H378	I379	
K441	Q442	A443	L444	T445	I446	V447	G448	T449	L450	P451	F452	L453	Y454	M455	L456	E457	K458	W459	R460	W461	M462	V463	F464	K465	G466	E467	I468	P469	K470	D471	Q472	W473	M474	K475	K476	W477	W478	E479	M480	K481	R482	E483	I484	V485	G486	V487	V488	E489	P490	V491	P492	H493	L494	E495	F496	T497	M498	D499	P500
A501	S502	L503	F504	H505	V506	S507	N508	D509	Y510	S511	F512	I513	R514	Y515	Y516	T517	R518	T519	L520	Y521	Q522	F523	Q524	F525	Q526	E527	A528	L529	C530	Q531	A532	A533	K534	H535	E536	G537	P538	L539	H540	K541	C542	D543	I544	S545	N546	S547	T548	E549	A550	G551	Q552	K553	L554	F555	N556	M557	L558	R559	L560



HIS
HIS
HIS

- Molecule 2: Processed angiotensin-converting enzyme 2



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





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

Chain G:  100%



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

Chain H:  50% 50%



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

Chain I:  50% 100%



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

Chain J:  50% 50%



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

Chain K:  100%



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

Chain L:  50% 50% 50%



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

Chain M:  100%



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

Chain N:  50% 50%



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

Chain O:  50% 100%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  50% 50%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain U:  100%



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

Chain V:  50% 50%



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

Chain W:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194473	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.312	Depositor
Minimum map value	-0.419	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.153	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/8330	0.55	0/11341
1	B	0.29	0/8330	0.54	0/11341
1	C	0.28	0/8330	0.55	0/11341
2	D	0.28	0/4999	0.53	0/6792
2	E	0.28	0/4999	0.53	0/6792
All	All	0.28	0/34988	0.54	0/47607

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	8140	0	7927	51	0
1	B	8140	0	7927	56	0
1	C	8140	0	7927	50	0
2	D	4862	0	4637	21	0
2	E	4862	0	4637	23	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
4	A	112	0	104	1	0
4	B	112	0	104	1	0
4	C	112	0	104	2	0
4	D	56	0	52	1	0
4	E	56	0	52	1	0
All	All	35096	0	33921	196	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 196 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:SER:HA	1:B:279:TYR:O	1.93	0.69
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.79	0.64
1:A:105:ILE:HB	1:A:239:GLN:HB2	1.79	0.63
1:B:901:GLN:HE21	1:B:905:ARG:HH21	1.47	0.62
1:C:51:THR:O	1:C:274:THR:HA	1.99	0.62

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	1024/1288 (80%)	997 (97%)	27 (3%)	0	100	100
1	B	1024/1288 (80%)	990 (97%)	34 (3%)	0	100	100
1	C	1024/1288 (80%)	992 (97%)	32 (3%)	0	100	100
2	D	594/606 (98%)	584 (98%)	10 (2%)	0	100	100
2	E	594/606 (98%)	584 (98%)	10 (2%)	0	100	100
All	All	4260/5076 (84%)	4147 (97%)	113 (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	912/1116 (82%)	912 (100%)	0	100	100
1	B	912/1116 (82%)	912 (100%)	0	100	100
1	C	912/1116 (82%)	912 (100%)	0	100	100
2	D	526/536 (98%)	526 (100%)	0	100	100
2	E	526/536 (98%)	526 (100%)	0	100	100
All	All	3788/4420 (86%)	3788 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	901	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](#)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	F	1	1,3	14,14,15	1.00	2 (14%)	17,19,21	0.58	0
3	NAG	F	2	3	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	G	1	1,3	14,14,15	0.35	0	17,19,21	0.67	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	H	1	1,3	14,14,15	0.71	1 (7%)	17,19,21	1.09	1 (5%)
3	NAG	H	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	I	1	1,3	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	I	2	3	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	J	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.55	0
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	K	1	1,3	14,14,15	0.26	0	17,19,21	0.63	0
3	NAG	K	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	L	1	1,3	14,14,15	0.83	1 (7%)	17,19,21	0.57	0
3	NAG	L	2	3	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	M	1	1,3	14,14,15	0.31	0	17,19,21	0.65	0
3	NAG	M	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	N	1	1,3	14,14,15	0.72	1 (7%)	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	O	1	1,3	14,14,15	0.35	0	17,19,21	0.45	0
3	NAG	O	2	3	14,14,15	0.32	0	17,19,21	0.55	0
3	NAG	P	1	1,3	14,14,15	0.94	1 (7%)	17,19,21	0.60	0
3	NAG	P	2	3	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	Q	1	1,3	14,14,15	0.27	0	17,19,21	0.61	0
3	NAG	Q	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	R	1	1,3	14,14,15	0.97	1 (7%)	17,19,21	0.77	1 (5%)
3	NAG	R	2	3	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	S	1	1,3	14,14,15	0.36	0	17,19,21	0.68	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.50	0
3	NAG	T	1	1,3	14,14,15	0.73	1 (7%)	17,19,21	1.10	1 (5%)
3	NAG	T	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	U	1	1,3	14,14,15	0.34	0	17,19,21	0.45	0
3	NAG	U	2	3	14,14,15	0.33	0	17,19,21	0.54	0
3	NAG	V	1	1,3	14,14,15	0.76	1 (7%)	17,19,21	0.57	0
3	NAG	V	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	NAG	W	1	1,3	14,14,15	0.27	0	17,19,21	0.60	0
3	NAG	W	2	3	14,14,15	0.23	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	3.31	1.49	1.43
3	P	1	NAG	O5-C1	3.02	1.48	1.43
3	F	1	NAG	C1-C2	3.01	1.56	1.52
3	L	1	NAG	C1-C2	2.46	1.56	1.52
3	V	1	NAG	O5-C1	2.44	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C2-N2-C7	3.21	127.47	122.90
3	H	1	NAG	C2-N2-C7	3.19	127.45	122.90
3	T	1	NAG	C2-N2-C7	3.17	127.42	122.90
3	R	1	NAG	C4-C3-C2	-2.04	108.03	111.02

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

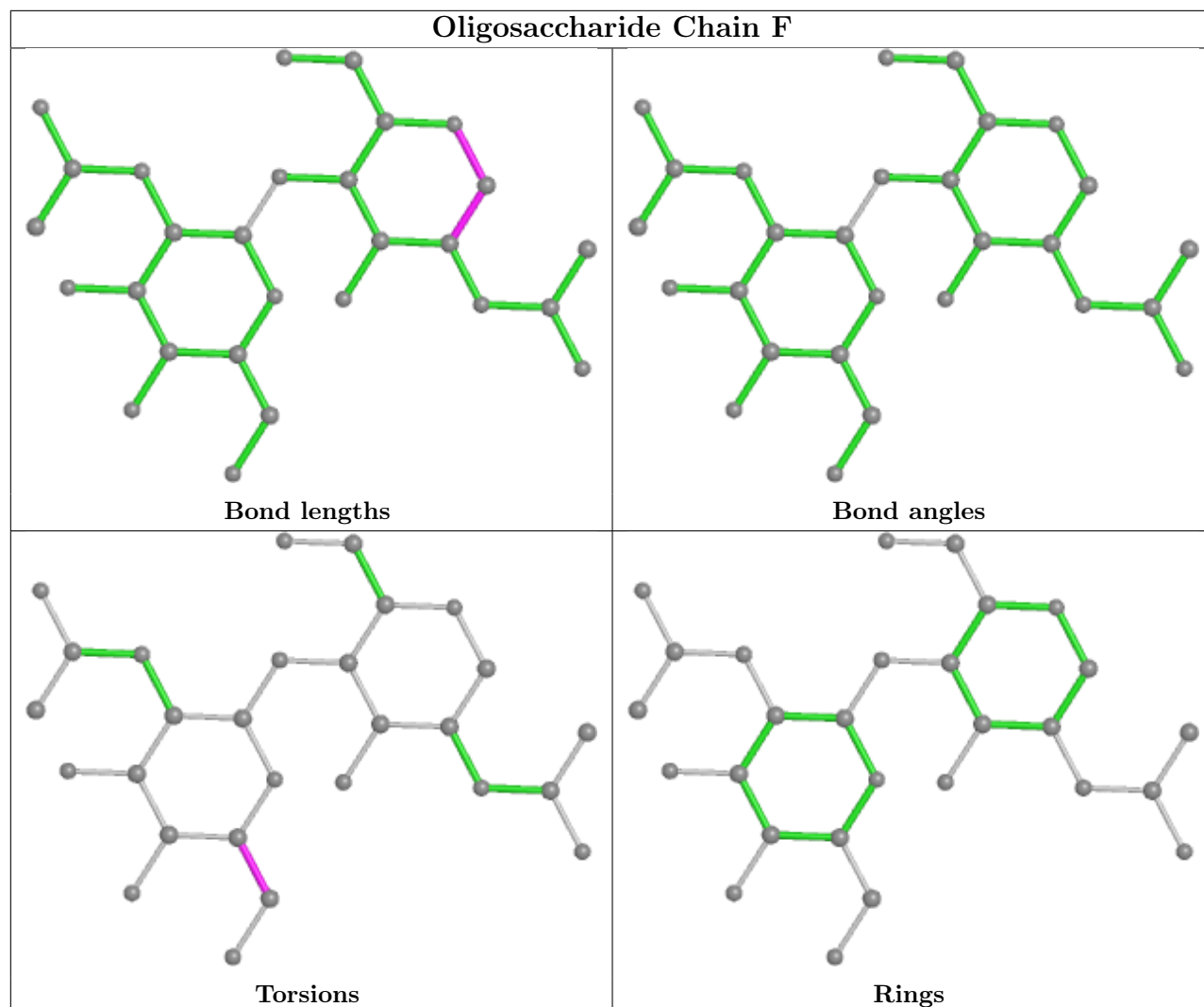
Mol	Chain	Res	Type	Atoms
3	O	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6

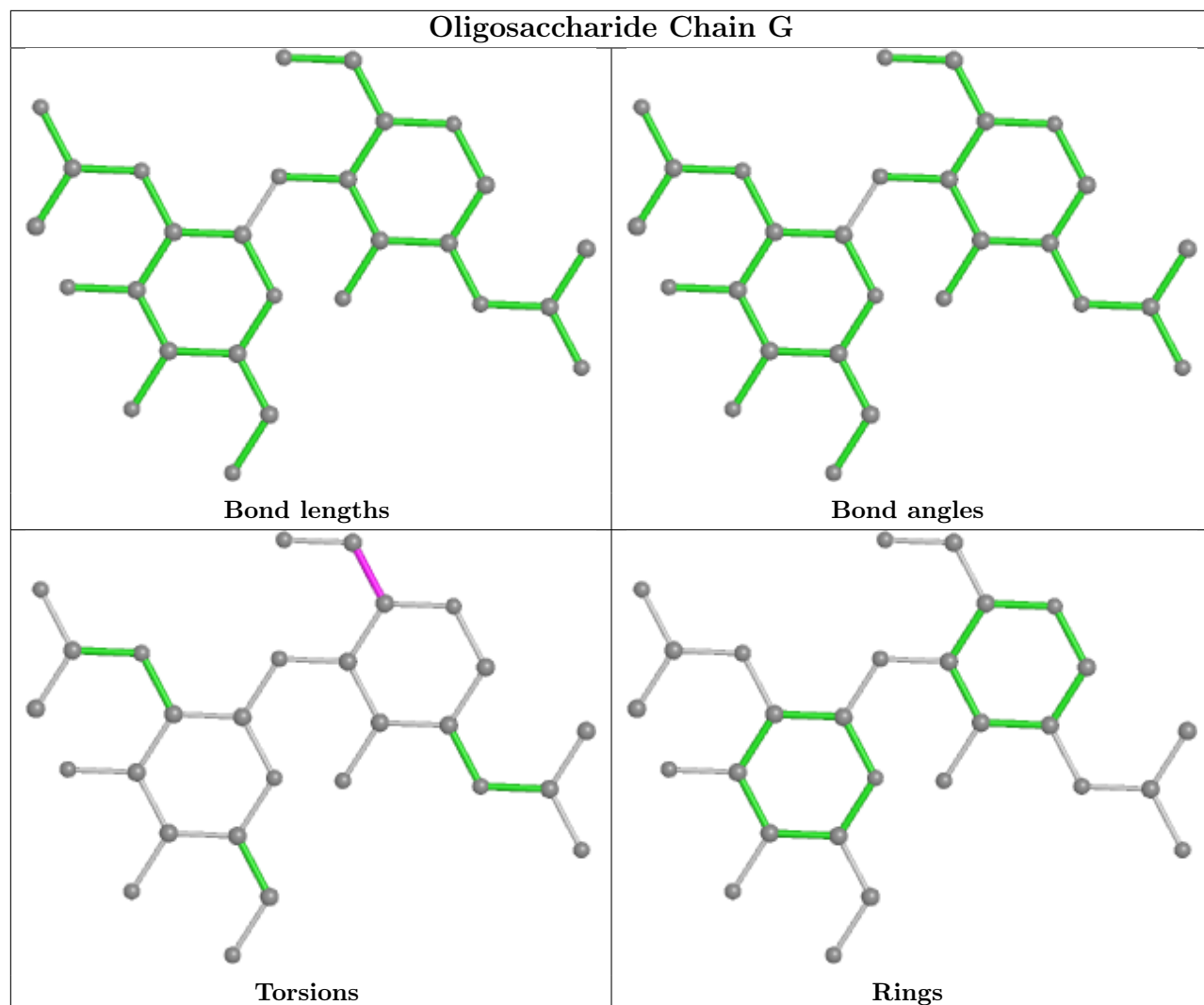
There are no ring outliers.

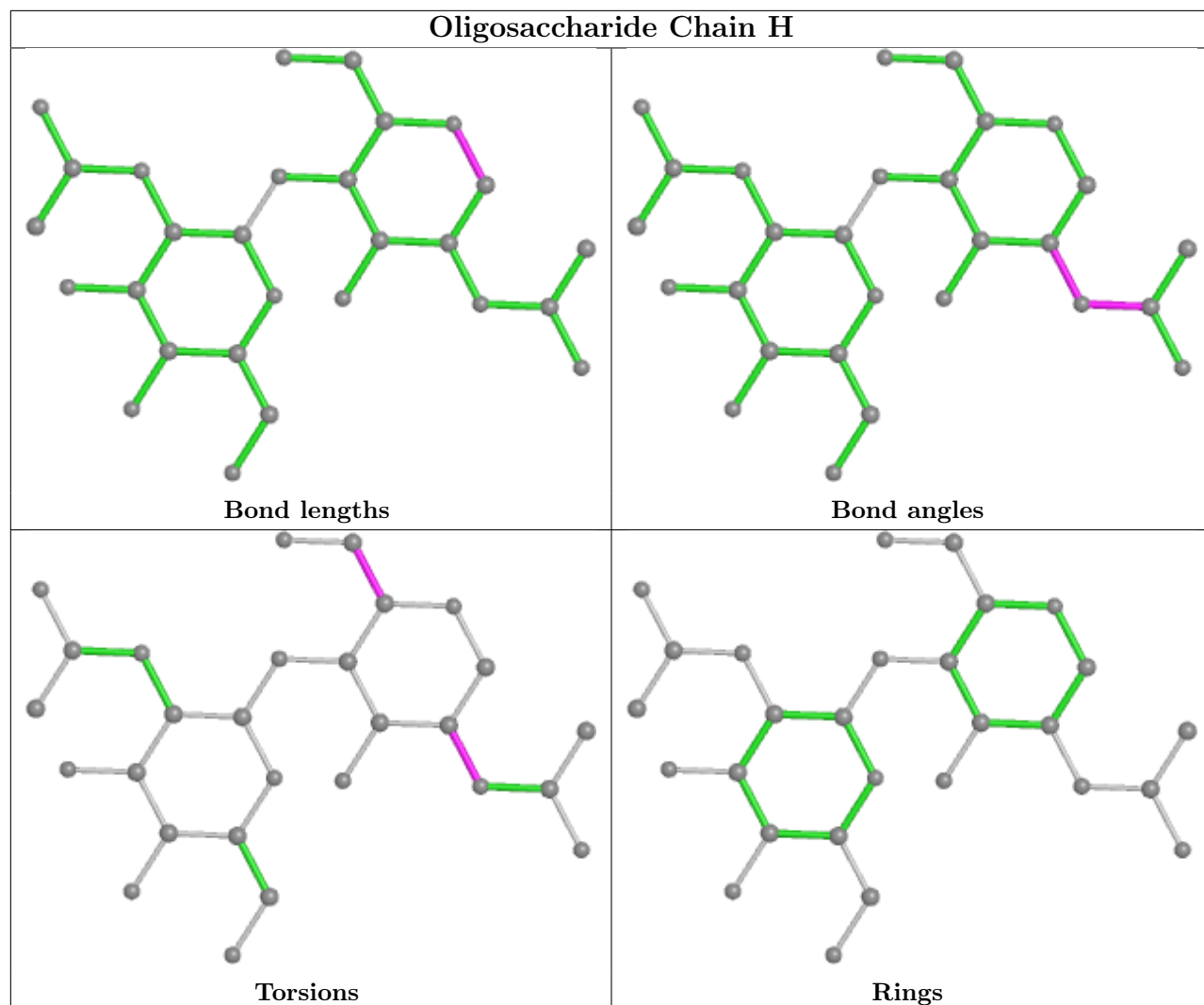
1 monomer is involved in 1 short contact:

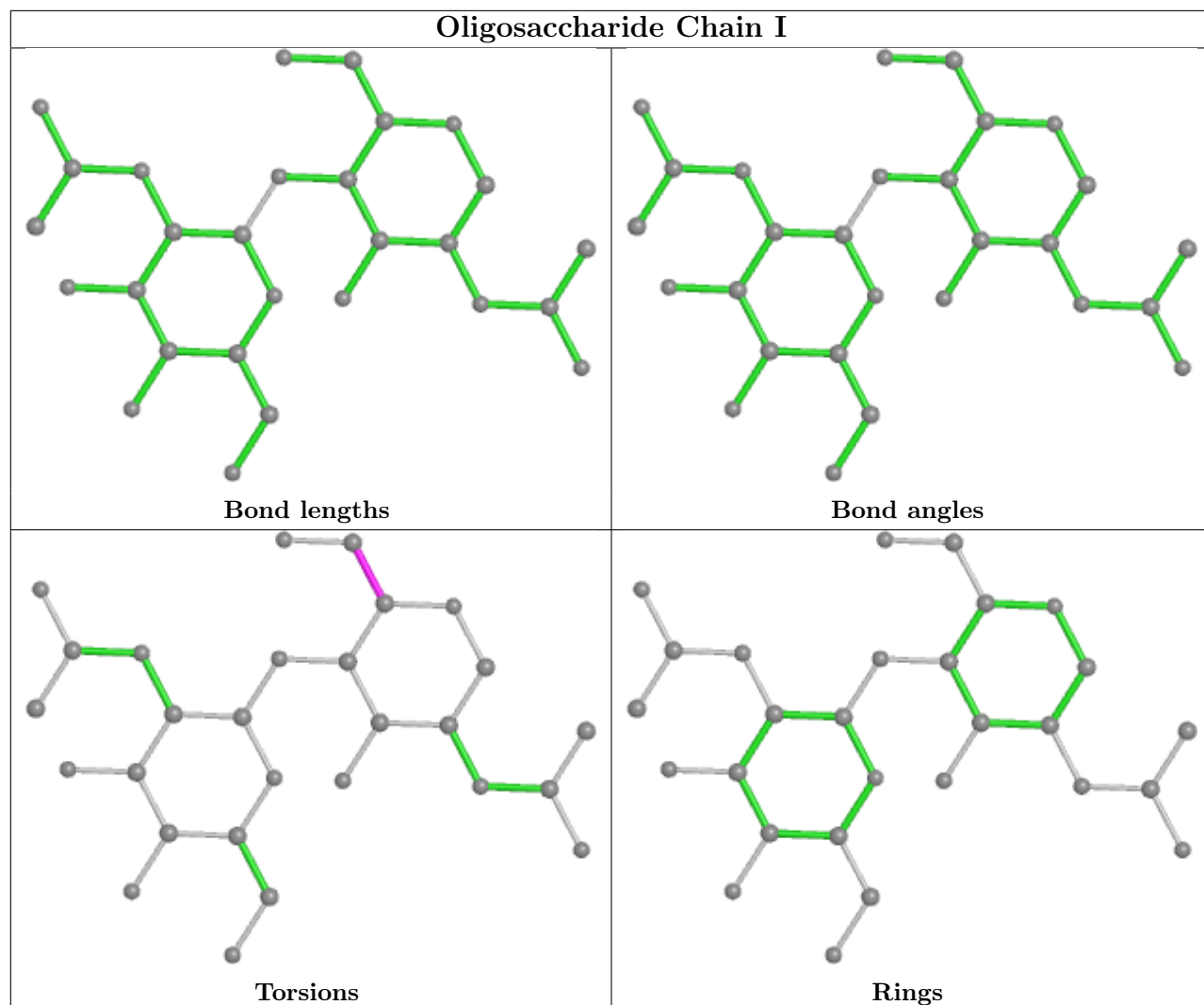
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0

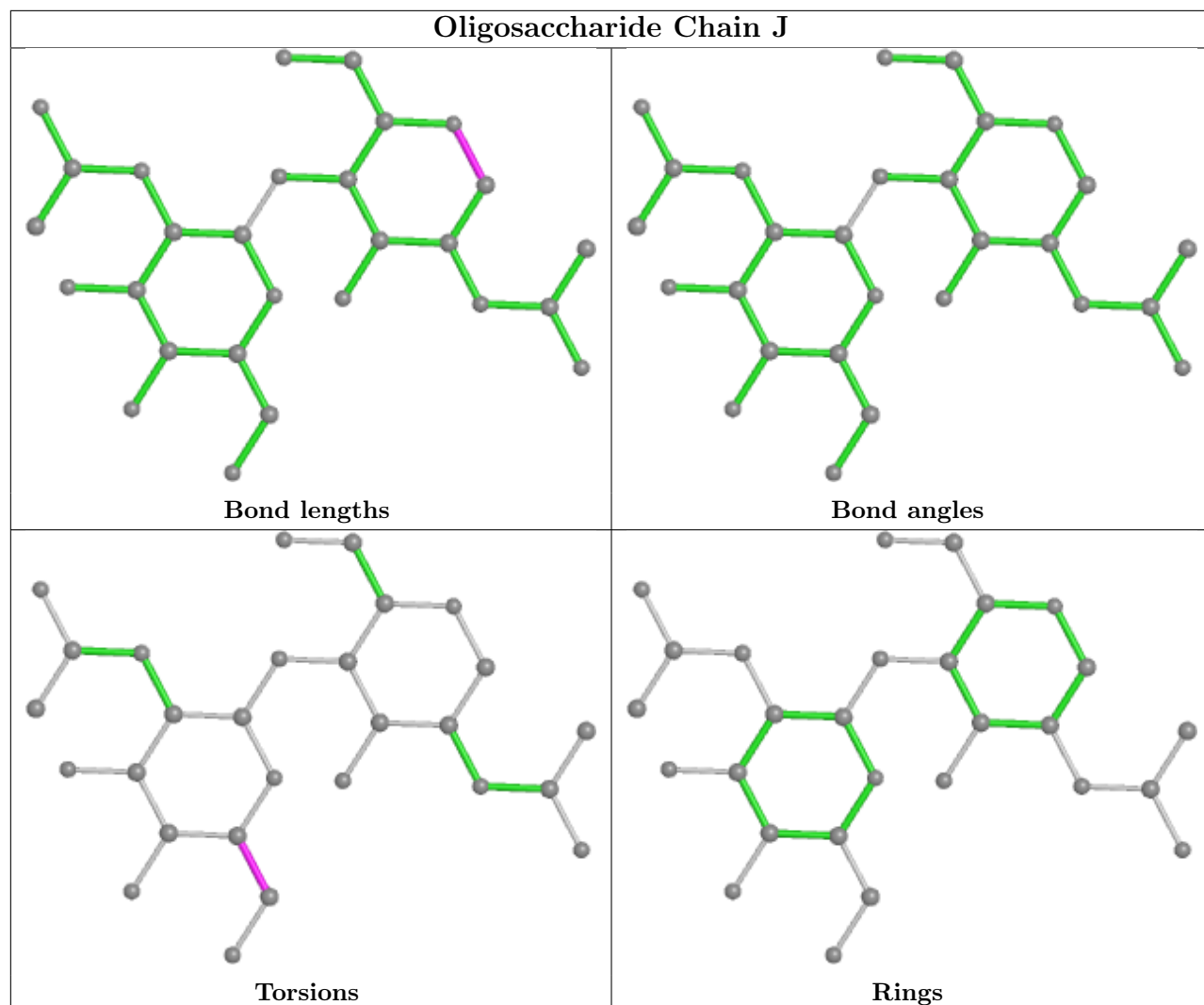
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

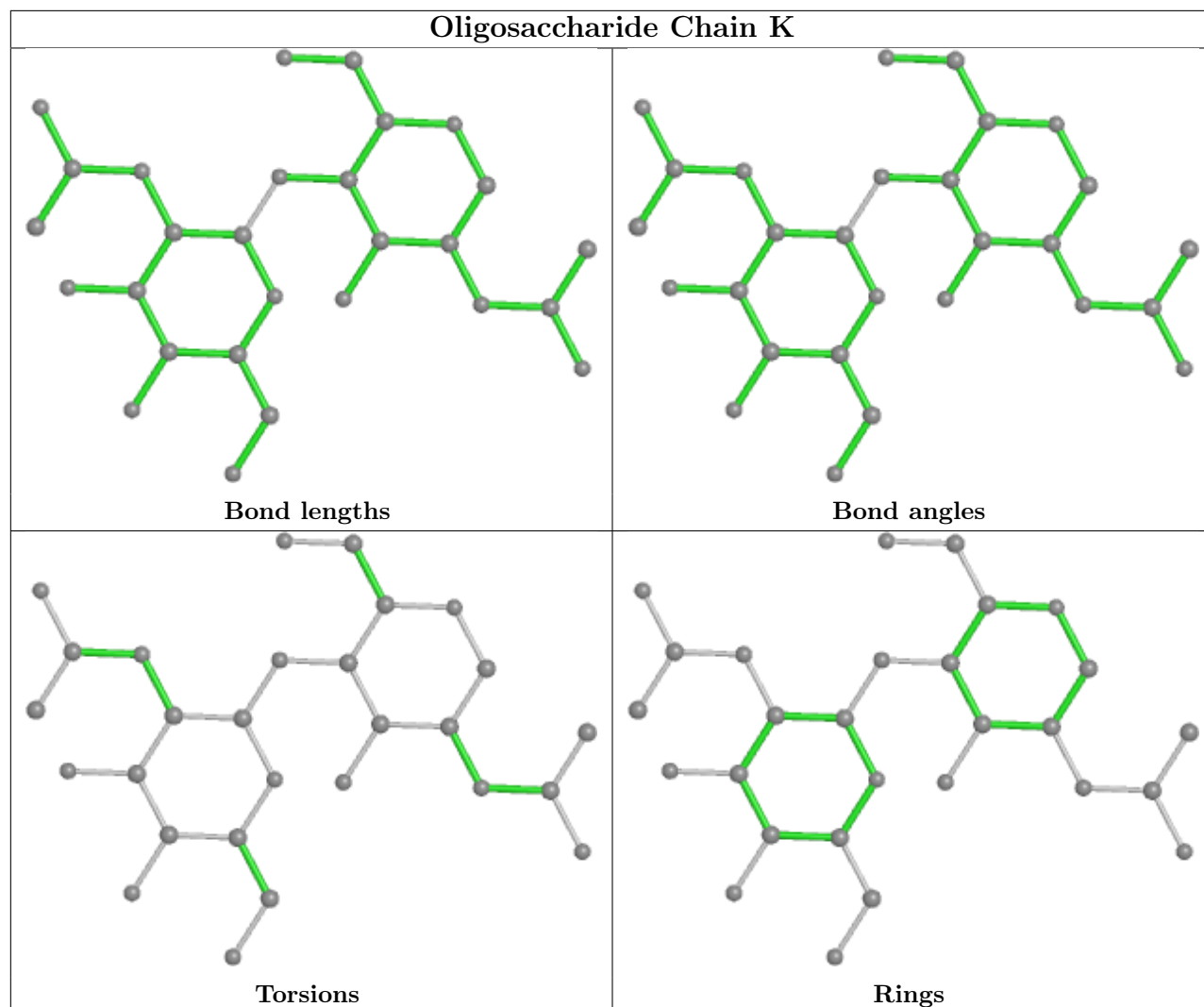


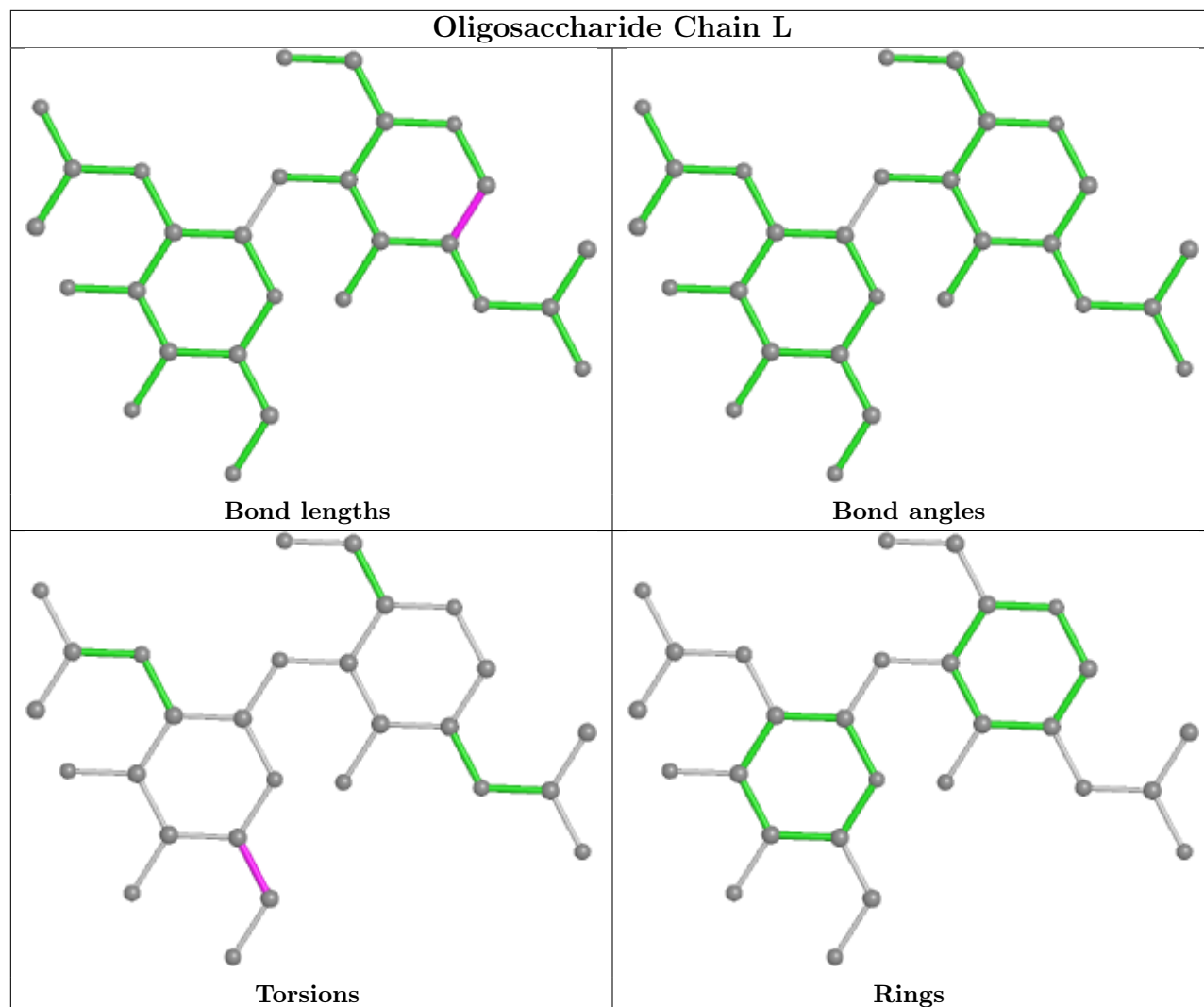


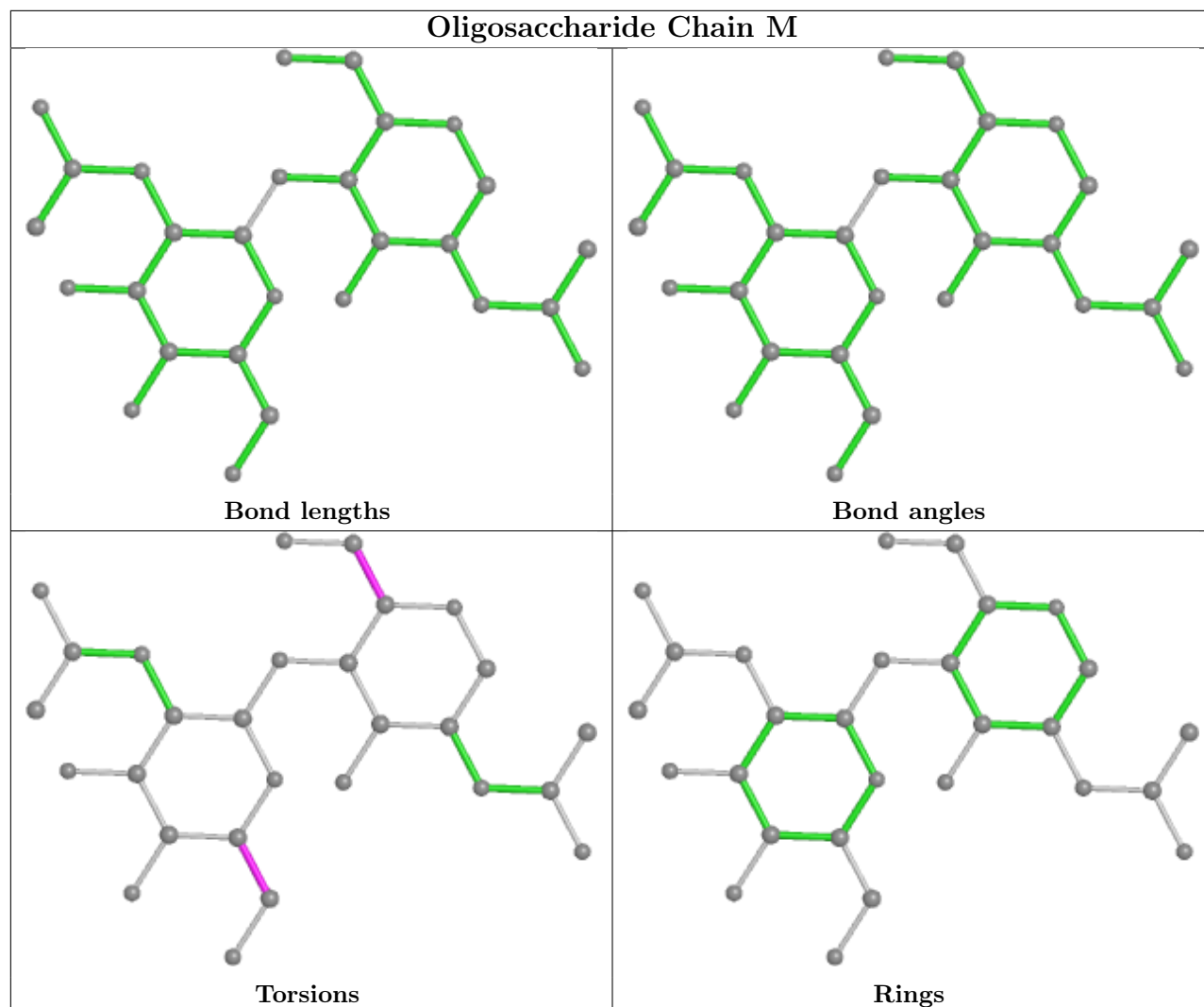


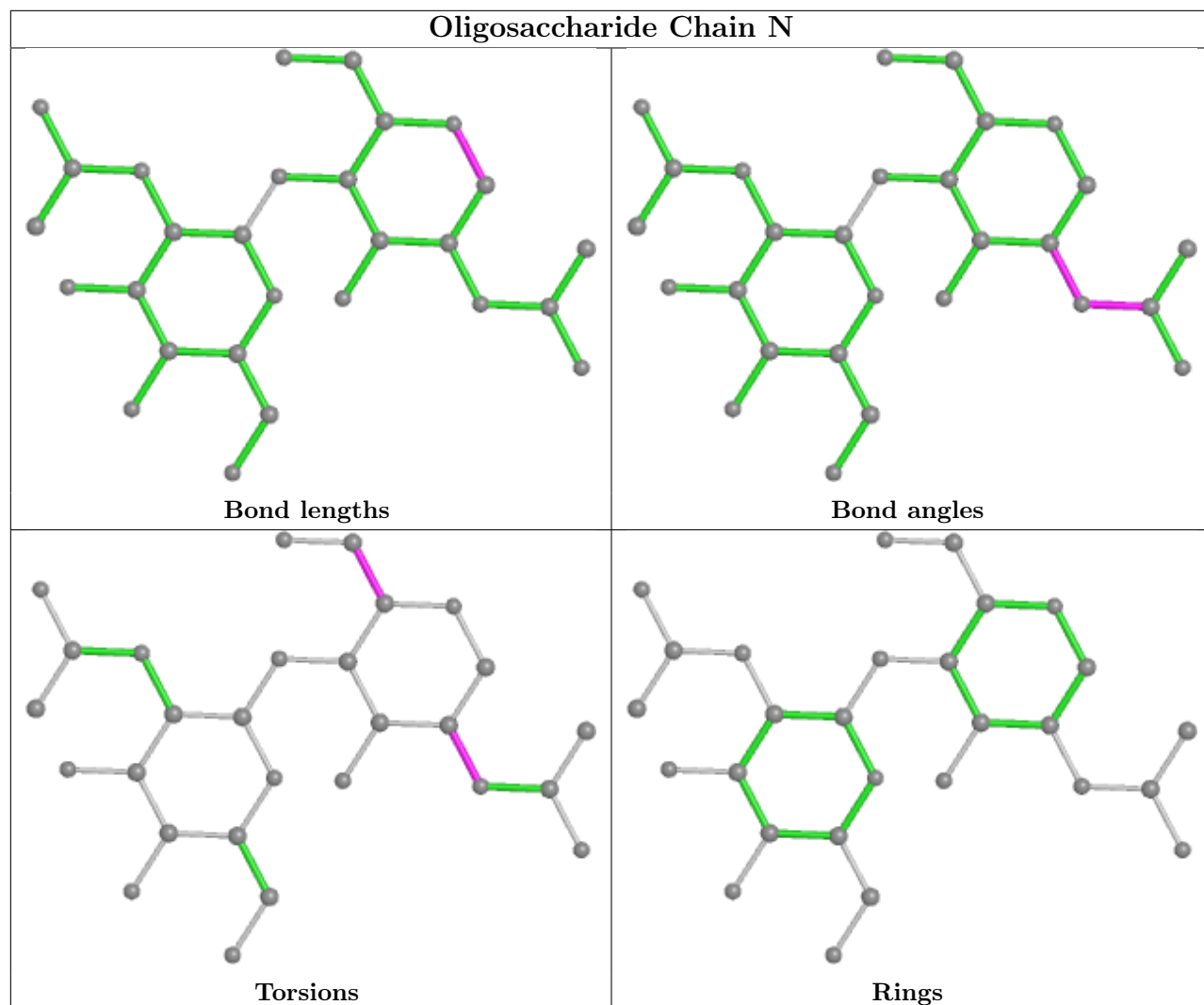


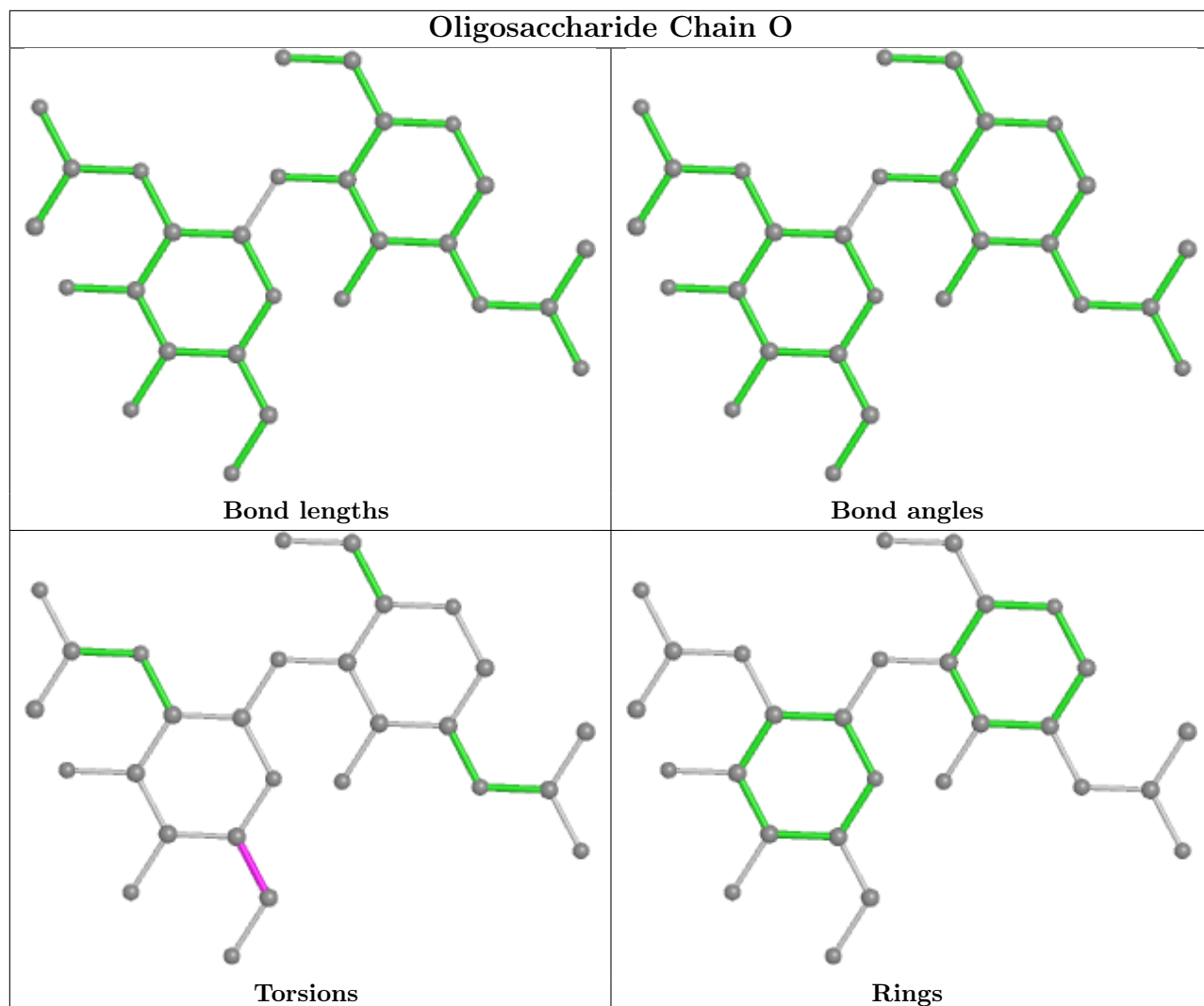


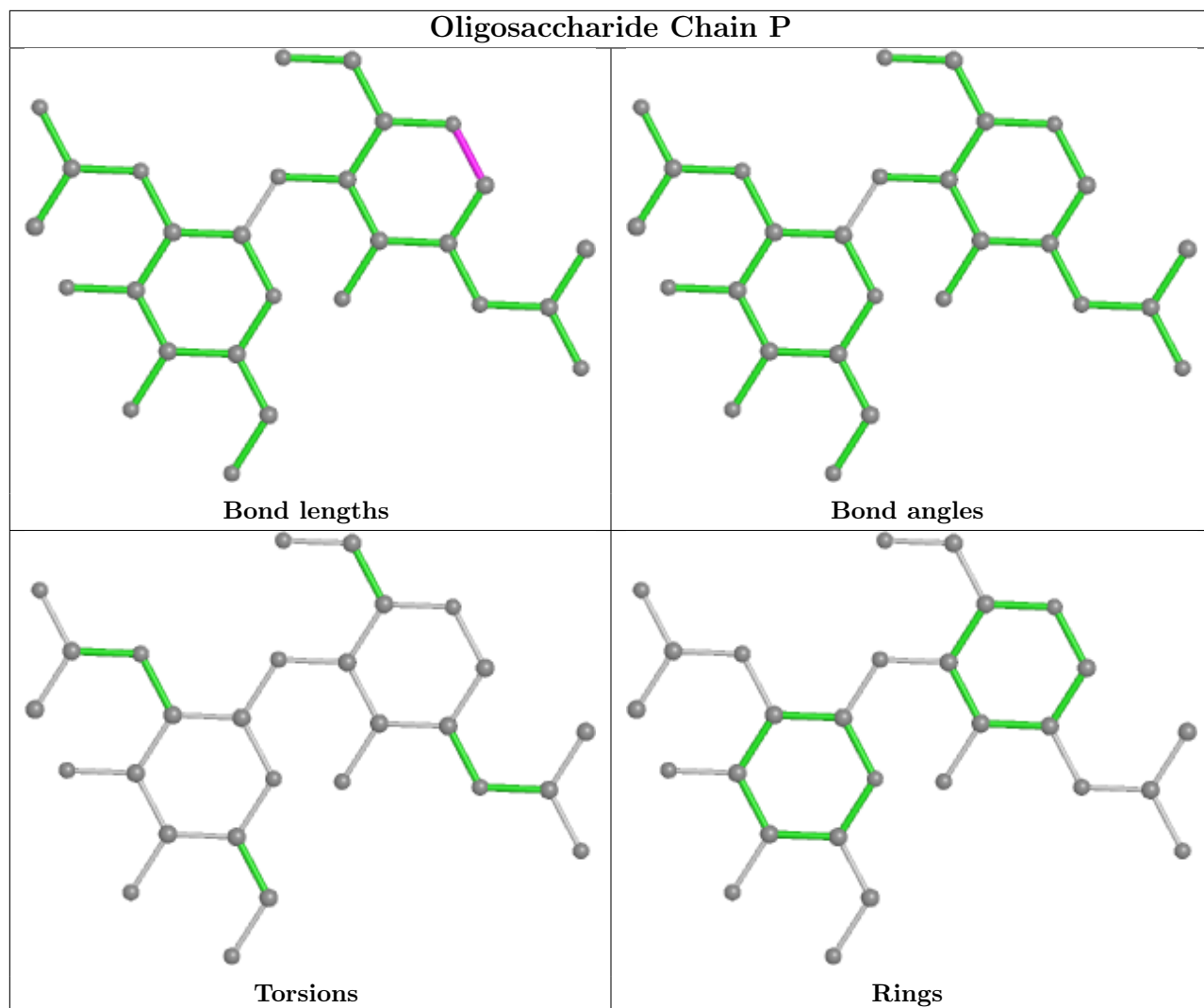


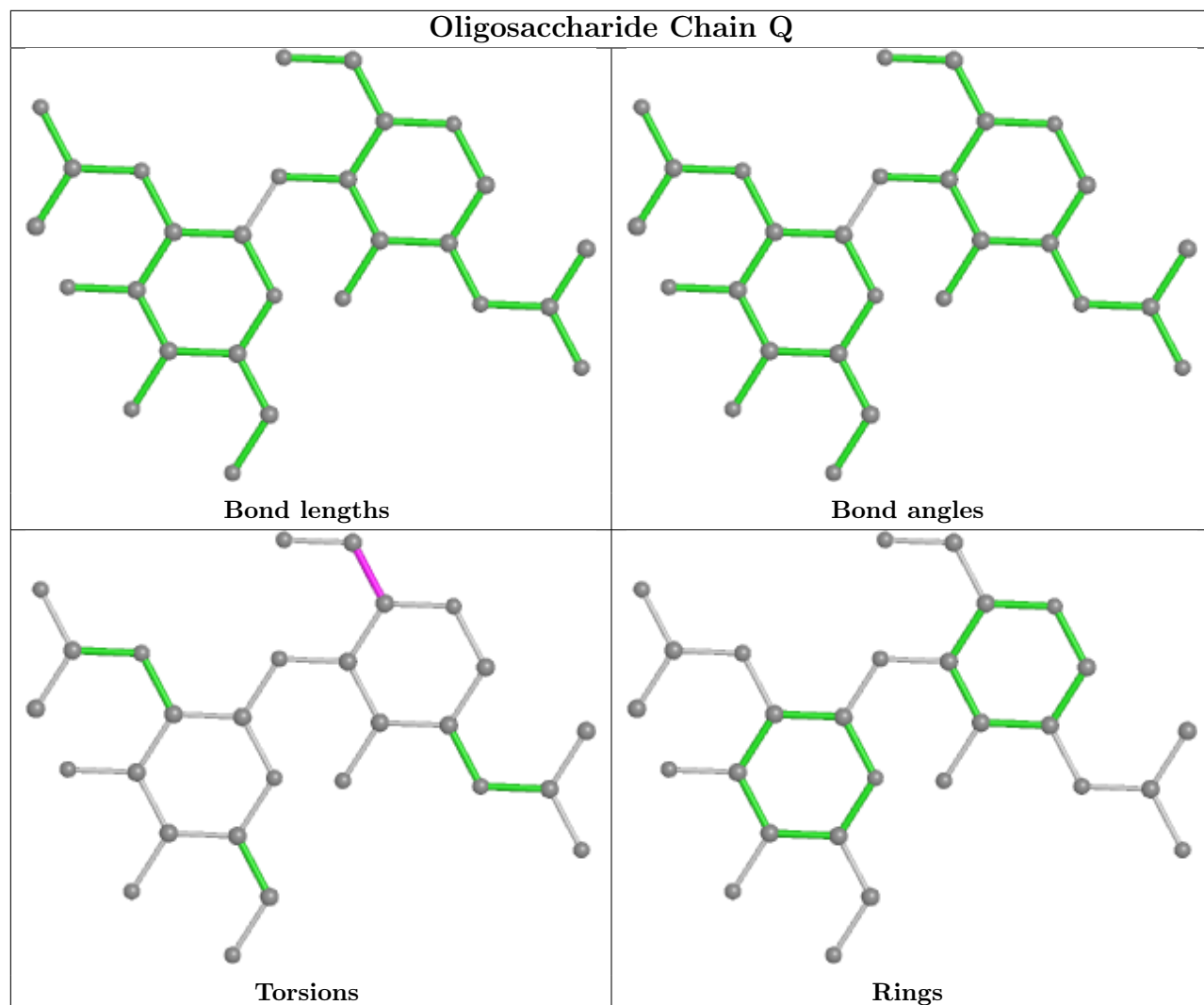


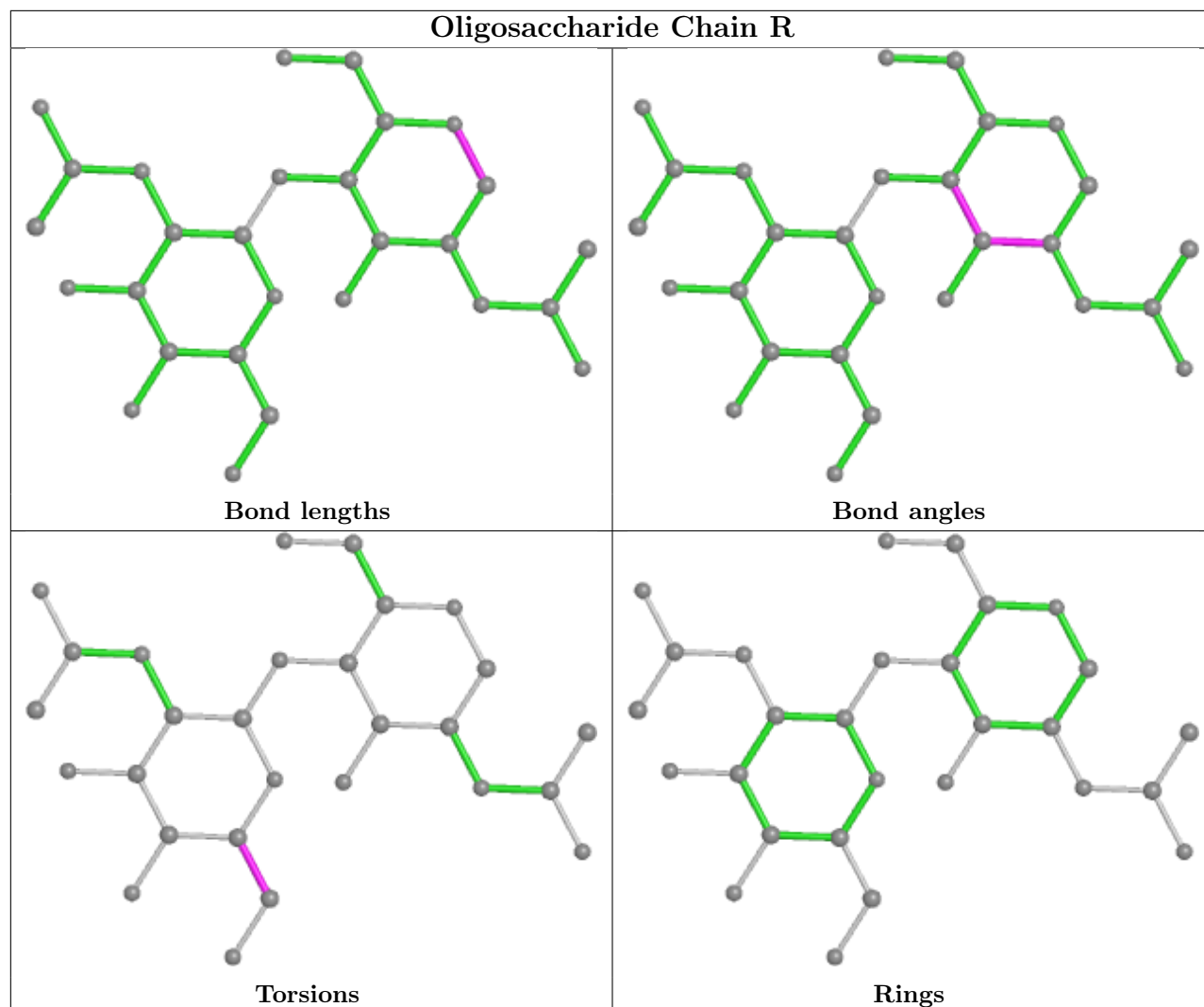


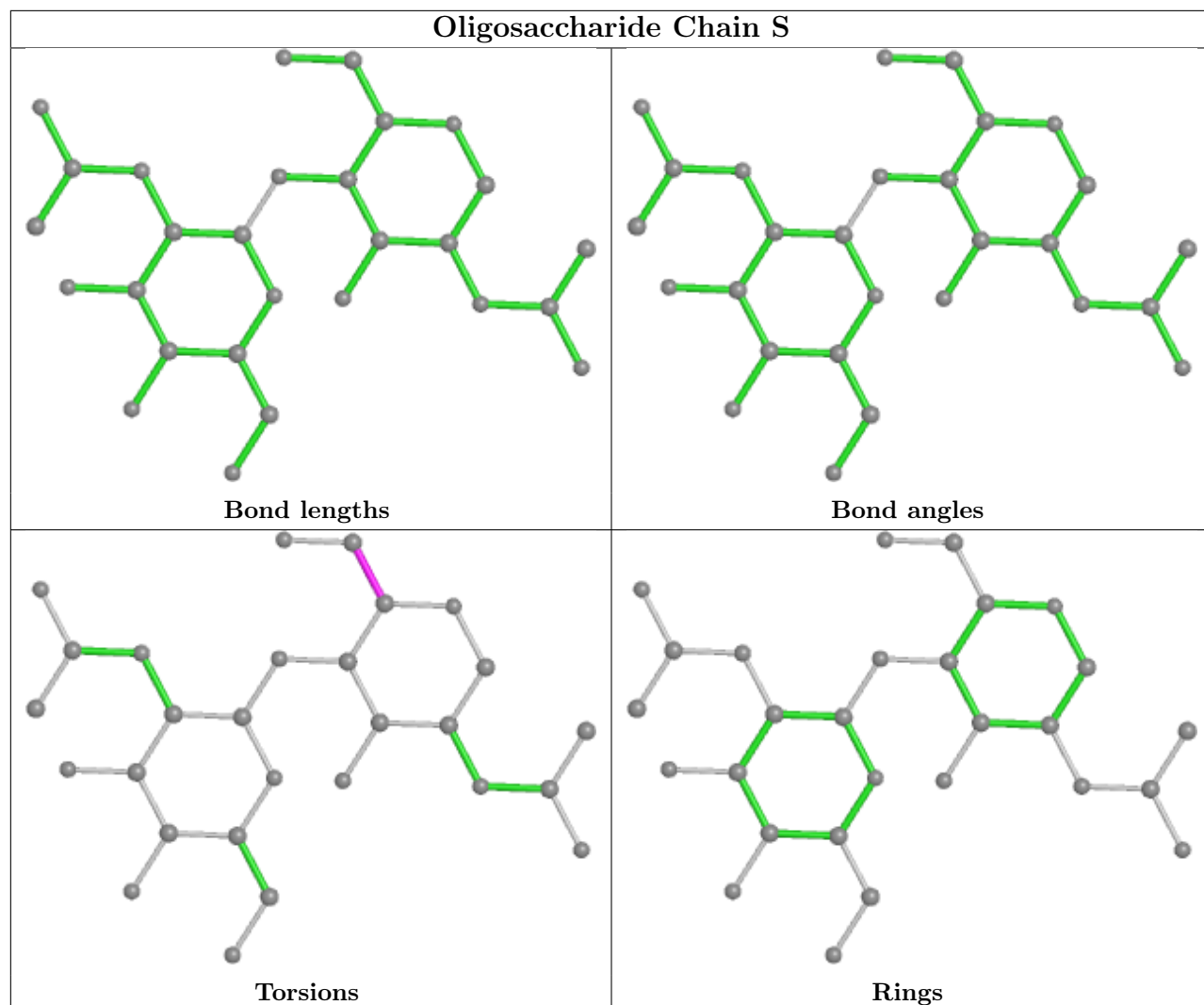


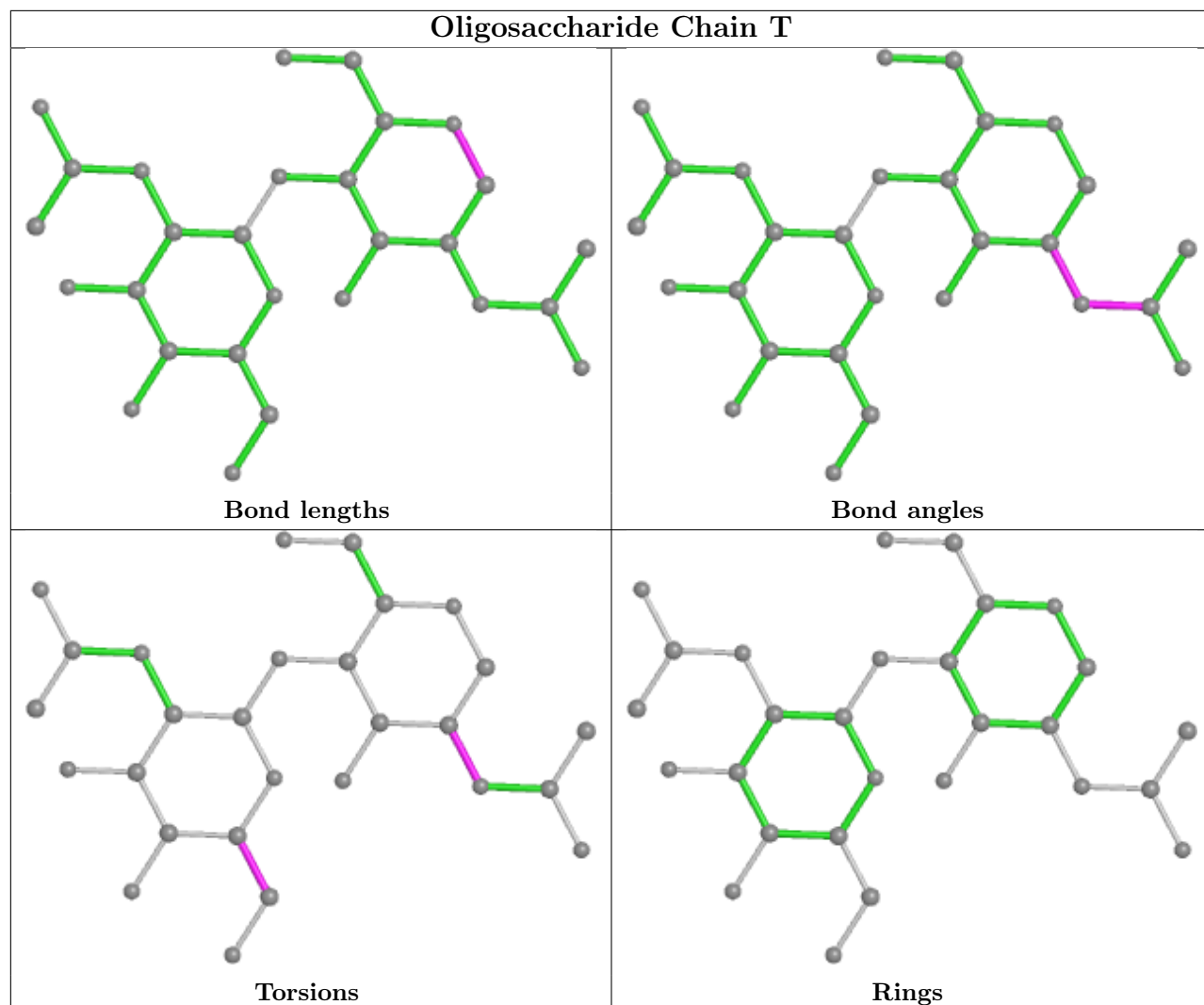


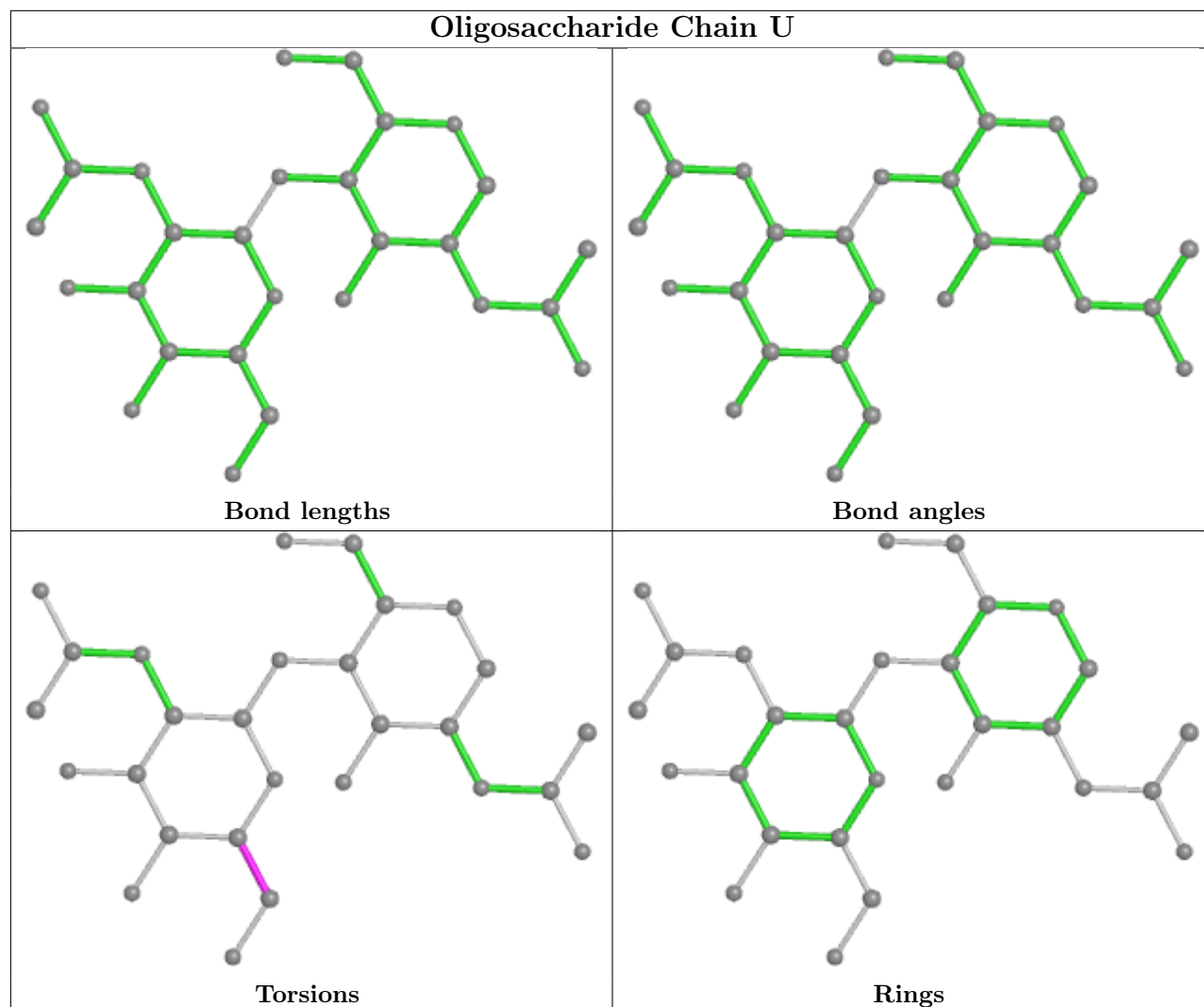


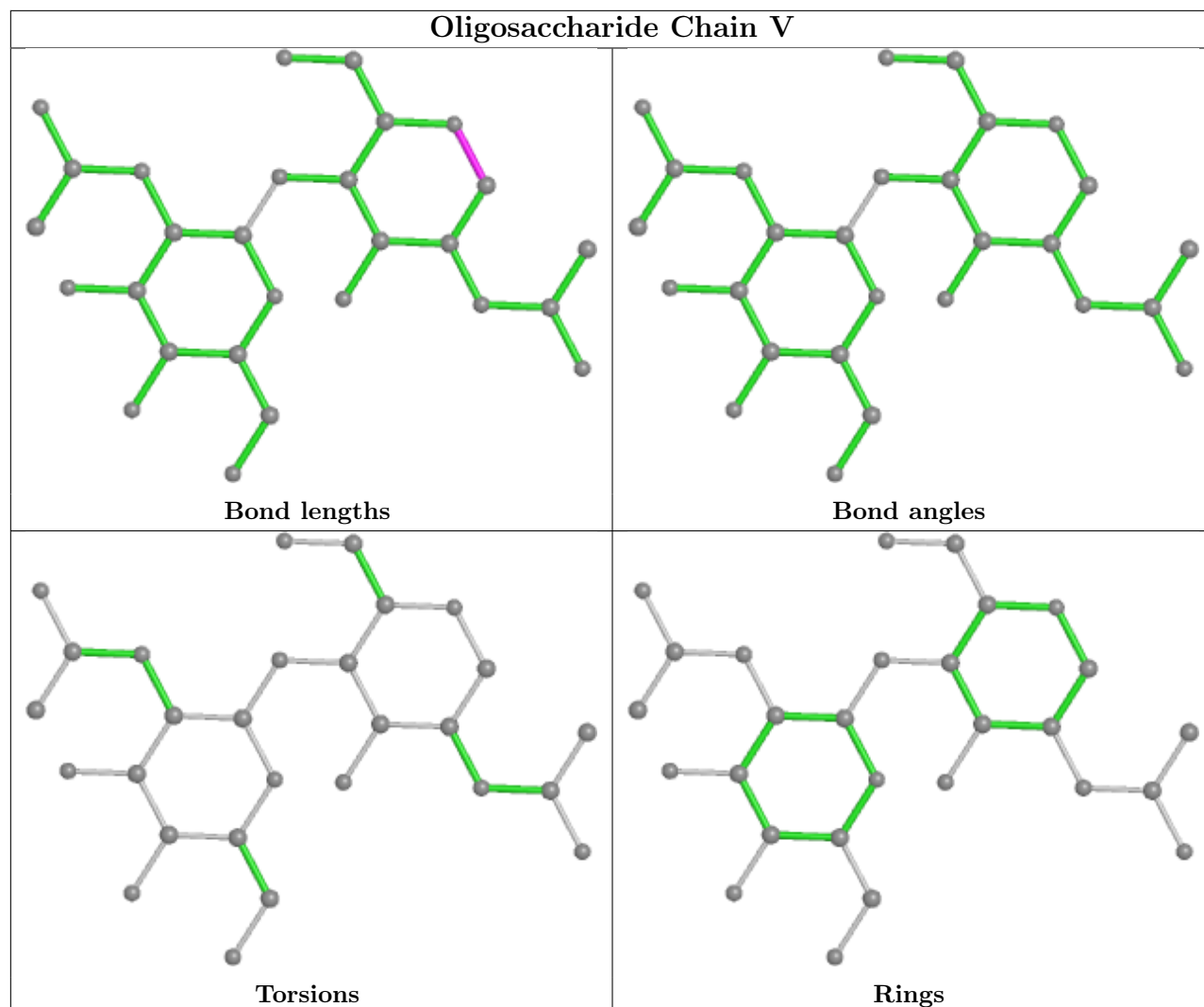


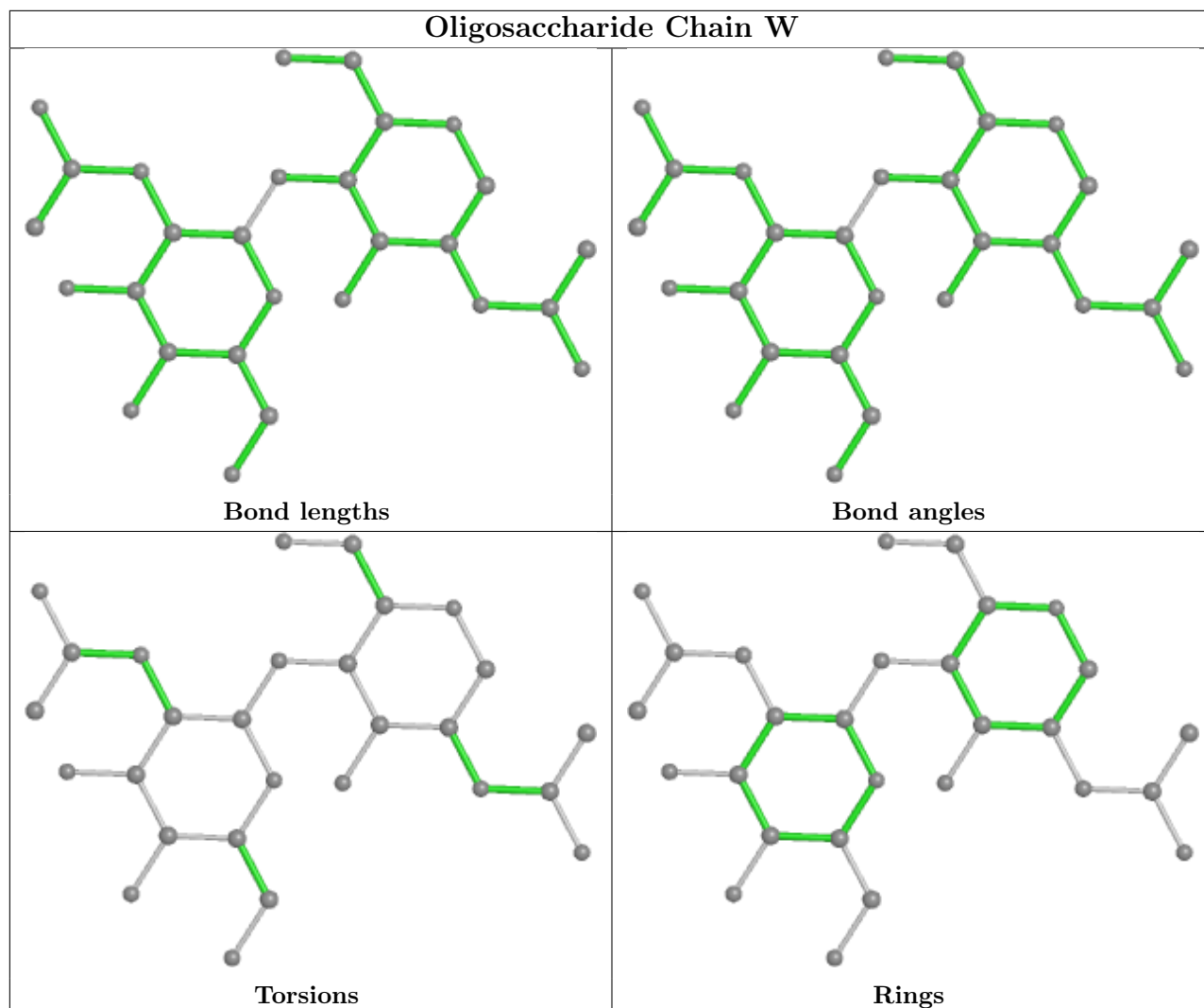












5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	E	703	2	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.48	0
4	NAG	E	701	2	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	E	704	2	14,14,15	0.24	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	B	1307	1	14,14,15	0.76	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	C	1303	1	14,14,15	0.69	0	17,19,21	0.49	0
4	NAG	D	704	2	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	D	701	2	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	1304	1	14,14,15	0.48	0	17,19,21	0.47	0
4	NAG	B	1305	1	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	A	1304	1	14,14,15	0.81	1 (7%)	17,19,21	0.55	0
4	NAG	B	1304	1	14,14,15	0.53	0	17,19,21	0.52	0
4	NAG	A	1306	1	14,14,15	0.62	0	17,19,21	0.96	1 (5%)
4	NAG	D	702	2	14,14,15	0.54	0	17,19,21	0.44	0
4	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	A	1307	1	14,14,15	0.72	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	A	1303	1	14,14,15	0.66	0	17,19,21	0.50	0
4	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	C	1307	1	14,14,15	0.26	0	17,19,21	0.38	0
4	NAG	B	1303	1	14,14,15	0.61	0	17,19,21	0.43	0
4	NAG	D	703	2	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	E	702	2	14,14,15	0.55	0	17,19,21	0.46	0
4	NAG	B	1308	1	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	B	1306	1	14,14,15	0.43	0	17,19,21	0.99	1 (5%)
4	NAG	B	1302	1	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	C	1306	1	14,14,15	0.59	0	17,19,21	0.53	0
4	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.47	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	E	703	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	E	701	2	-	2/6/23/26	0/1/1/1
4	NAG	E	704	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	D	704	2	-	0/6/23/26	0/1/1/1
4	NAG	D	701	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	D	702	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	D	703	2	-	2/6/23/26	0/1/1/1
4	NAG	E	702	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1304	NAG	C1-C2	2.57	1.56	1.52
4	B	1307	NAG	C1-C2	2.48	1.56	1.52
4	A	1307	NAG	C1-C2	2.34	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1306	NAG	C2-N2-C7	3.10	127.31	122.90
4	A	1307	NAG	C2-N2-C7	2.91	127.05	122.90
4	B	1307	NAG	C2-N2-C7	2.86	126.97	122.90
4	A	1306	NAG	C2-N2-C7	2.80	126.89	122.90

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	701	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	E	701	NAG	C4-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	704	NAG	1	0
4	D	704	NAG	1	0
4	C	1305	NAG	1	0
4	C	1302	NAG	1	0
4	A	1305	NAG	1	0
4	B	1302	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

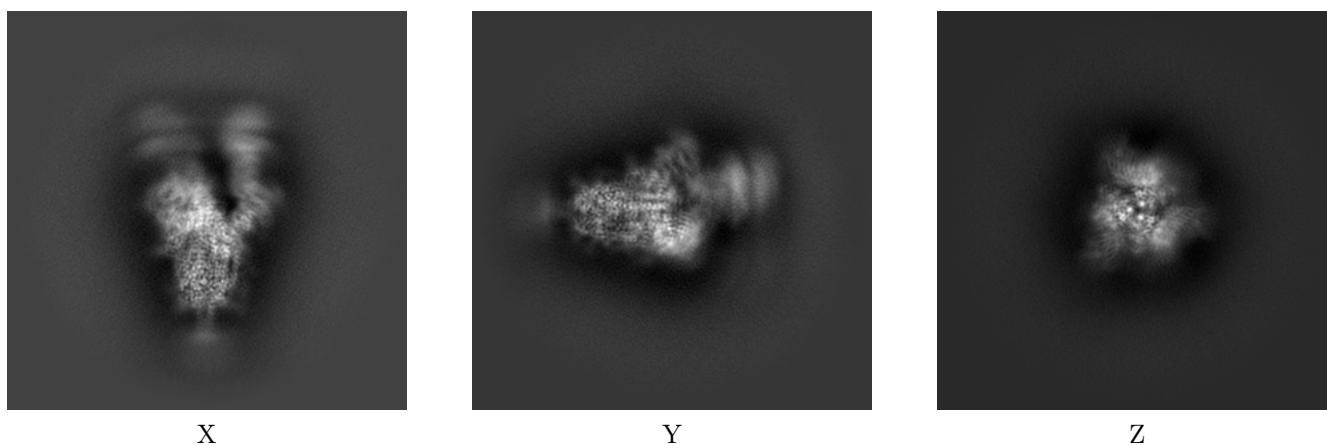
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23878. 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](#)

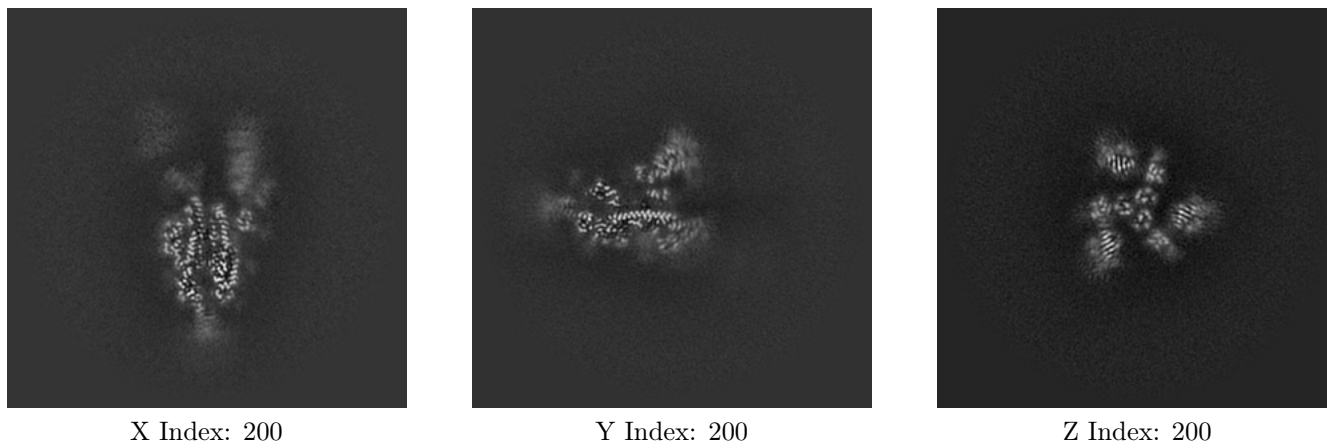
6.1.1 Primary map



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

6.2 Central slices [i](#)

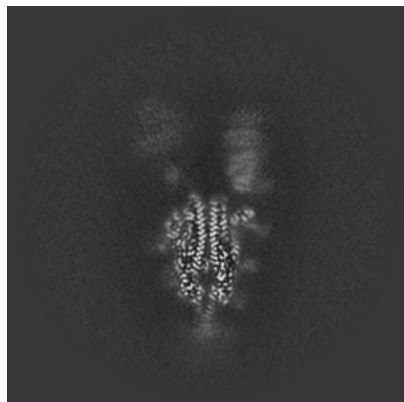
6.2.1 Primary map



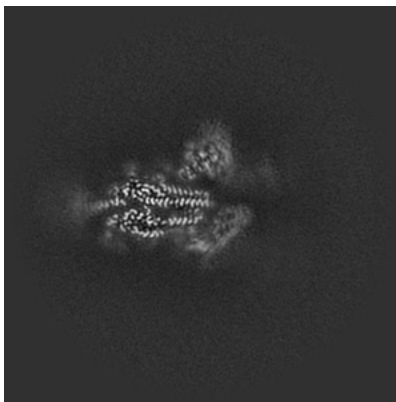
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

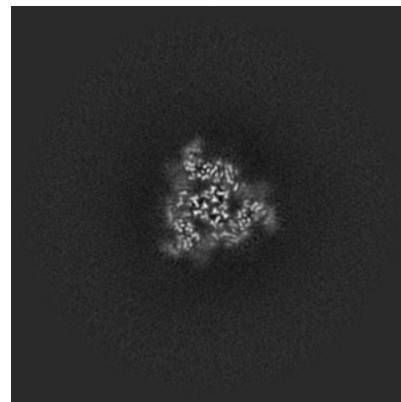
6.3.1 Primary map



X Index: 204



Y Index: 192



Z Index: 186

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

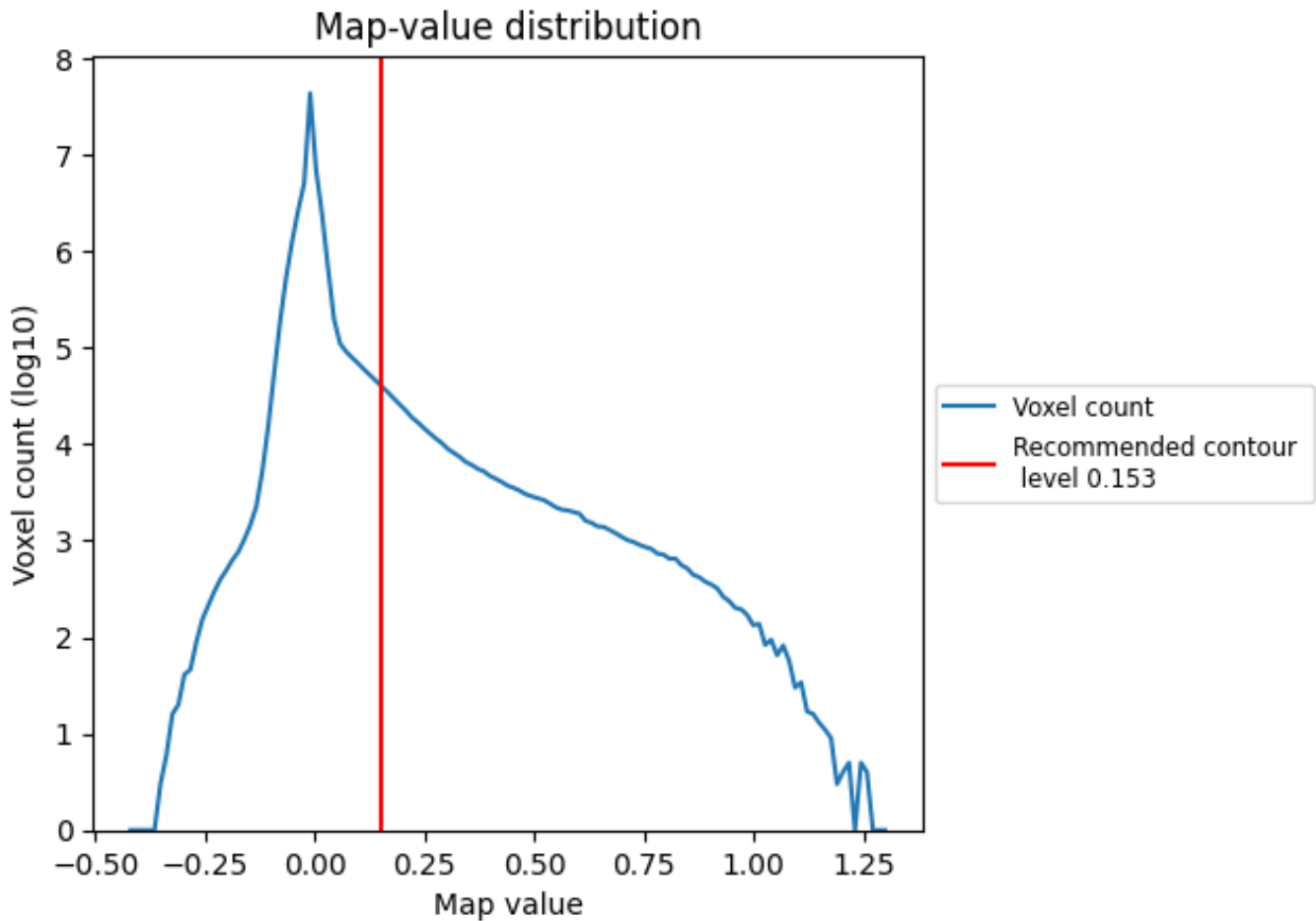
6.5 Mask visualisation

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

7 Map analysis [i](#)

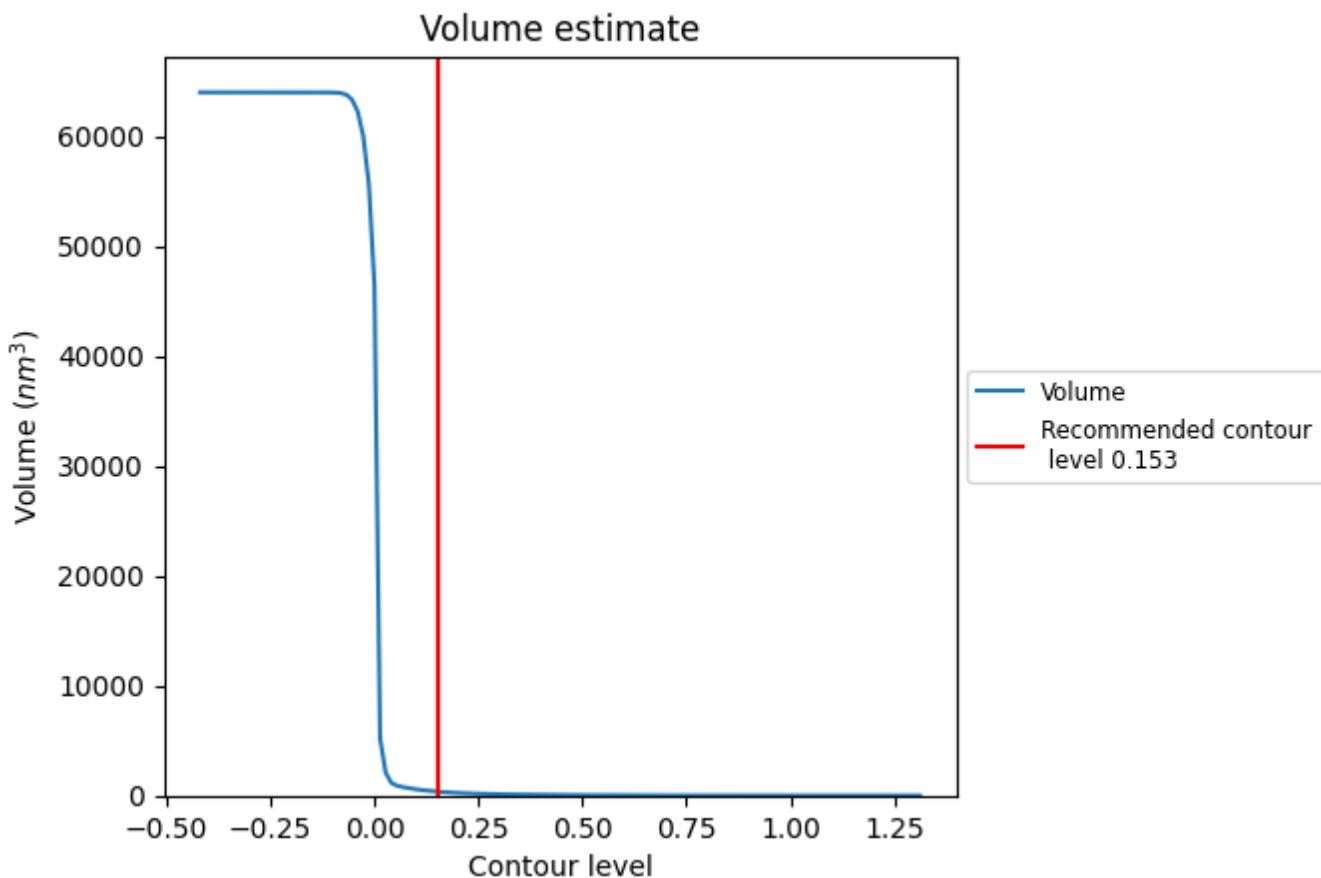
This section contains the results of statistical analysis of the map.

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.

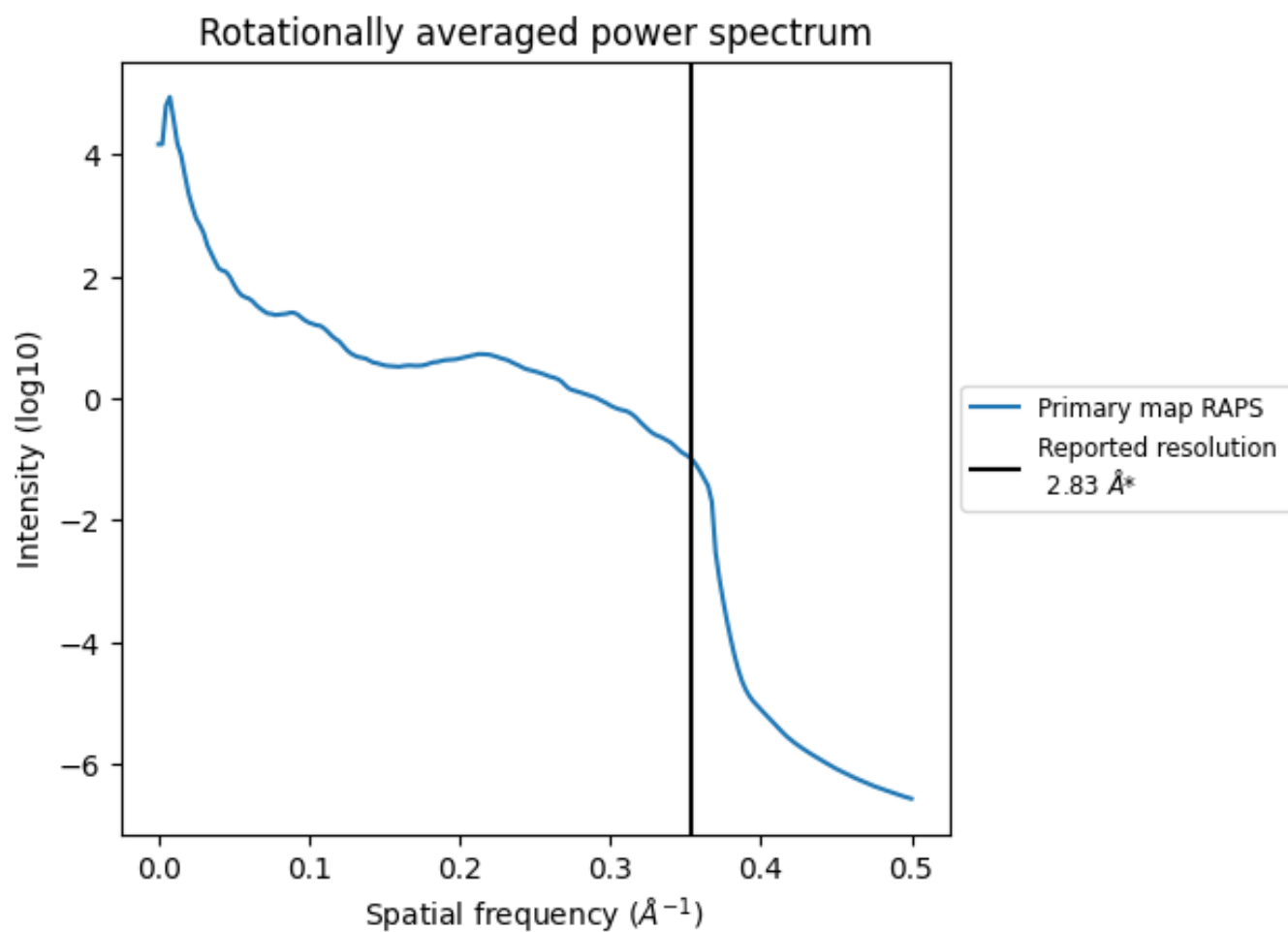
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 354 nm³; this corresponds to an approximate mass of 320 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

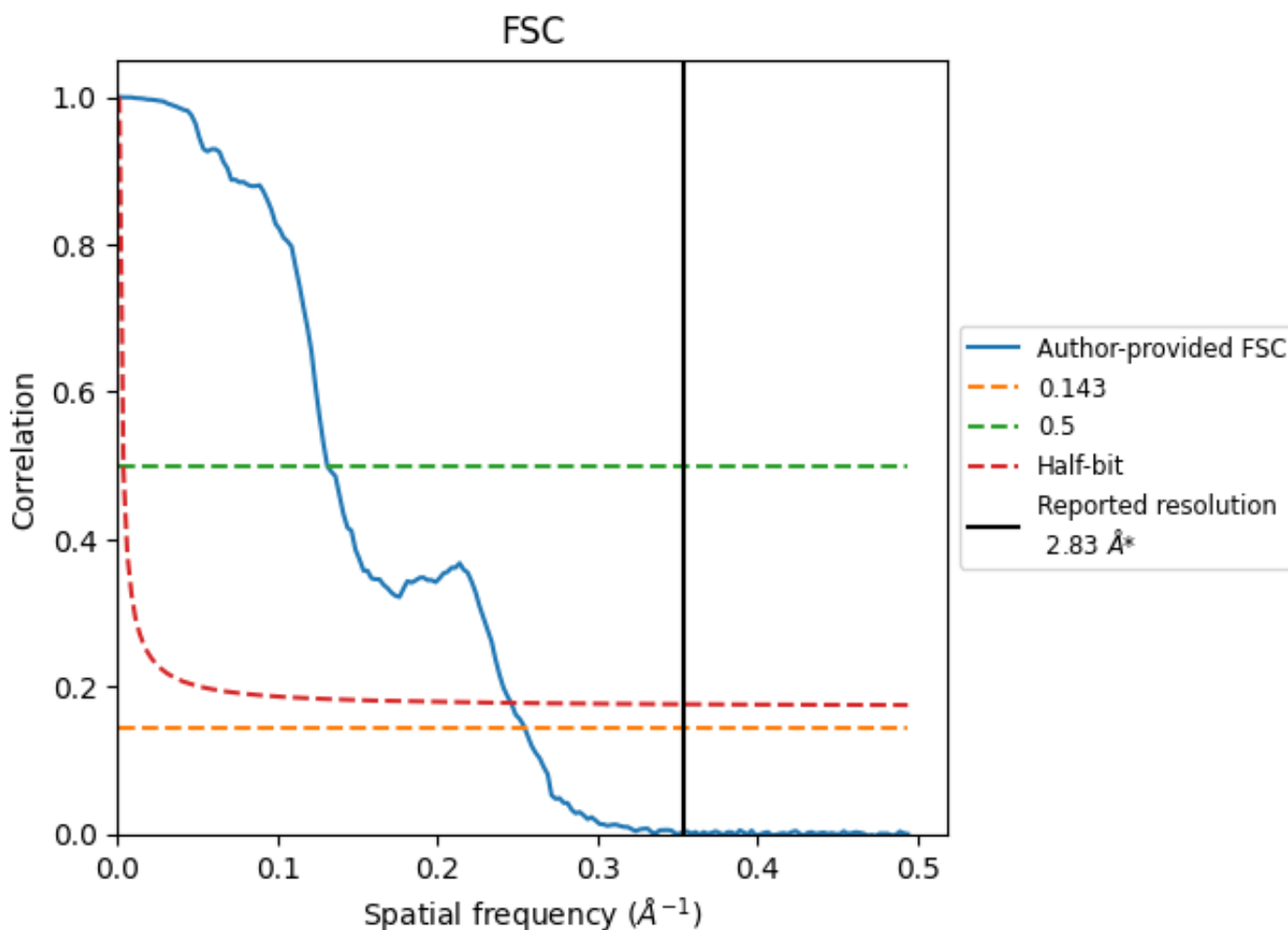


*Reported resolution corresponds to spatial frequency of 0.353\AA^{-1}

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 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

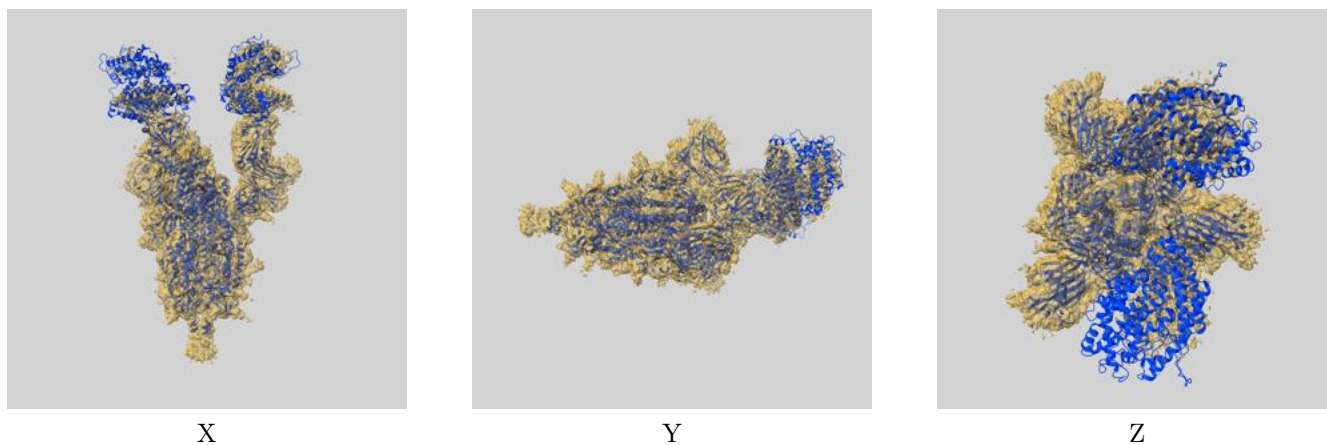
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	3.93	7.63	4.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

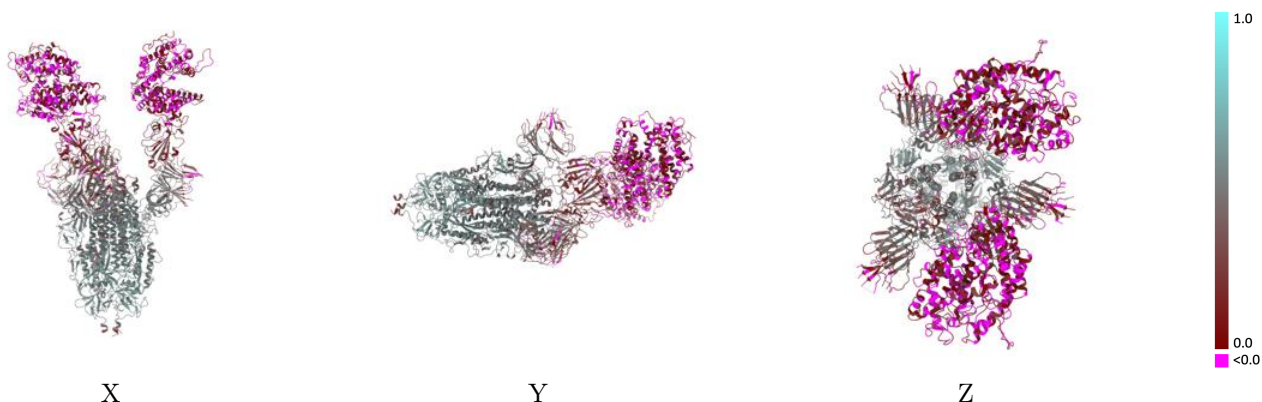
This section contains information regarding the fit between EMDB map EMD-23878 and PDB model 7MJM. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



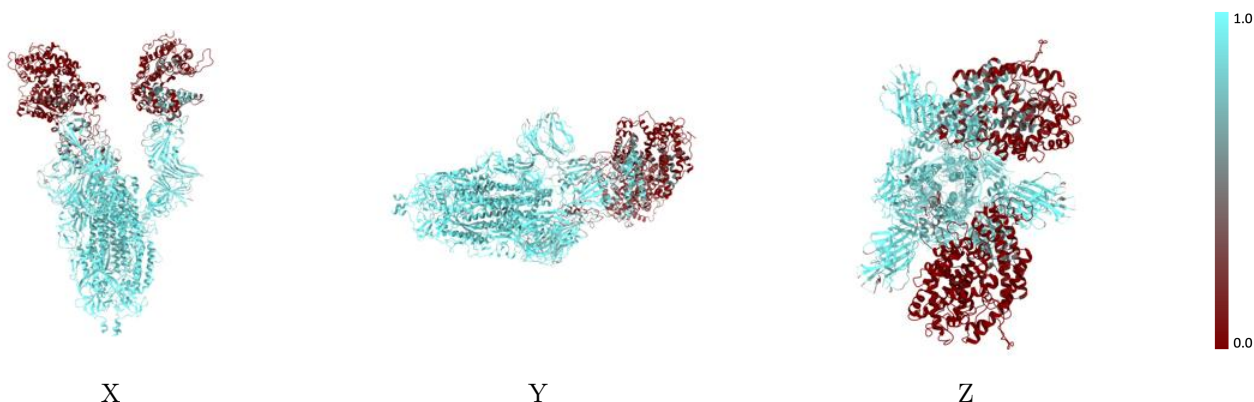
The images above show the 3D surface view of the map at the recommended contour level 0.153 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



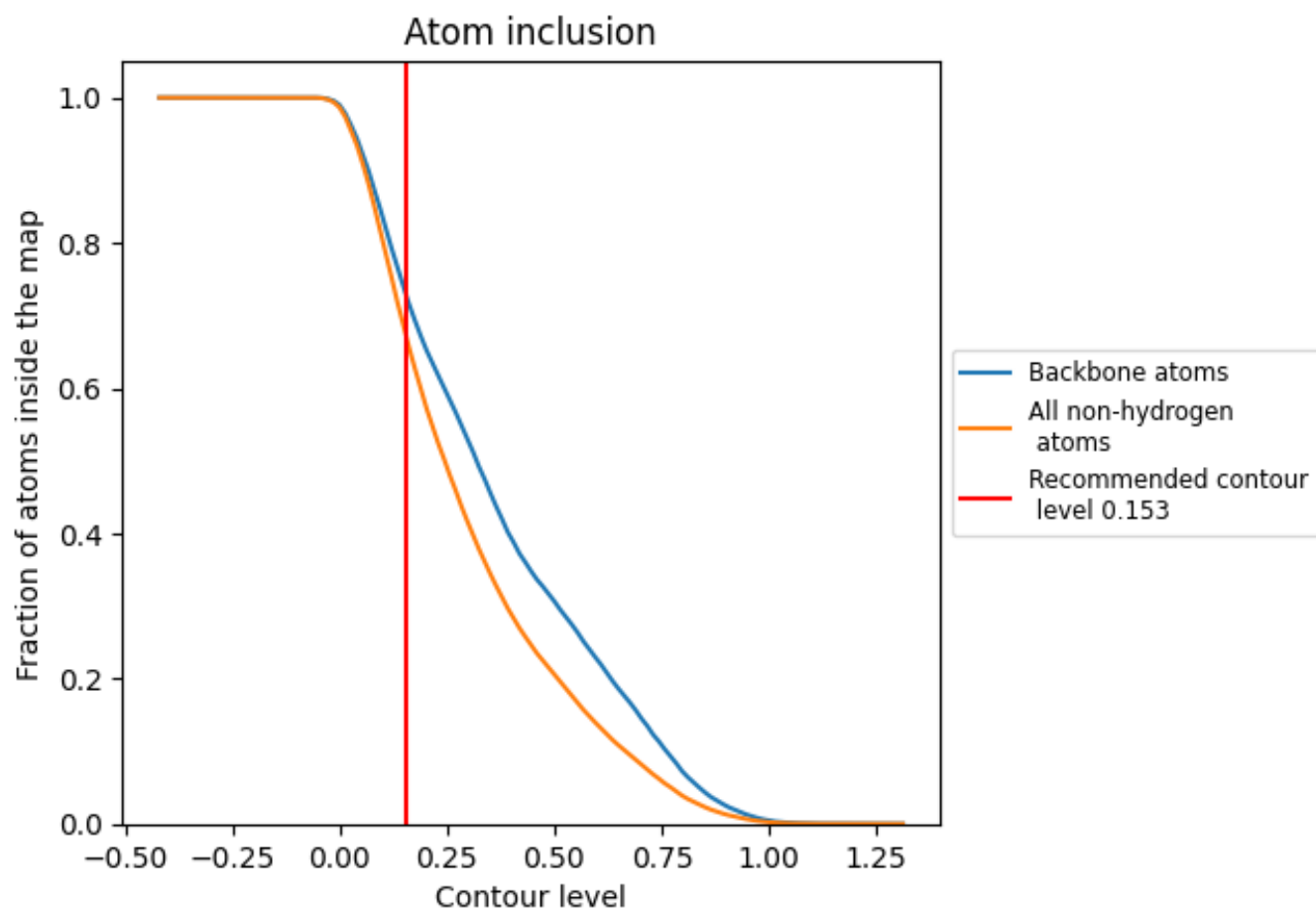
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.153).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 68% 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 (0.153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6761	 0.2990
A	 0.8580	 0.3860
B	 0.9201	 0.4030
C	 0.8790	 0.4220
D	 0.0333	 0.0260
E	 0.2559	 0.0370
F	 0.2143	 0.1960
G	 0.8929	 0.4680
H	 0.8571	 0.3930
I	 0.5357	 0.4470
J	 0.8929	 0.4300
K	 0.8929	 0.4550
L	 0.3214	 0.2550
M	 1.0000	 0.5070
N	 0.8929	 0.4310
O	 0.5714	 0.4540
P	 0.8571	 0.4010
Q	 0.7500	 0.4350
R	 0.4286	 0.1420
S	 0.8929	 0.4880
T	 0.8929	 0.4380
U	 0.5714	 0.4250
V	 0.8571	 0.4290
W	 0.8214	 0.4130

