



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 06:55 PM EST

PDB ID : 7T9K
EMDB ID : EMD-25760
Title : Cryo-EM structure of SARS-CoV-2 Omicron spike protein in complex with human ACE2
Authors : Zhu, X.; Mannar, D.; Saville, J.W.; Srivastava, S.S.; Berezuk, A.M.; Tuttle, K.S.; Subramaniam, S.
Deposited on : 2021-12-19
Resolution : 2.45 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) : 2.31.3

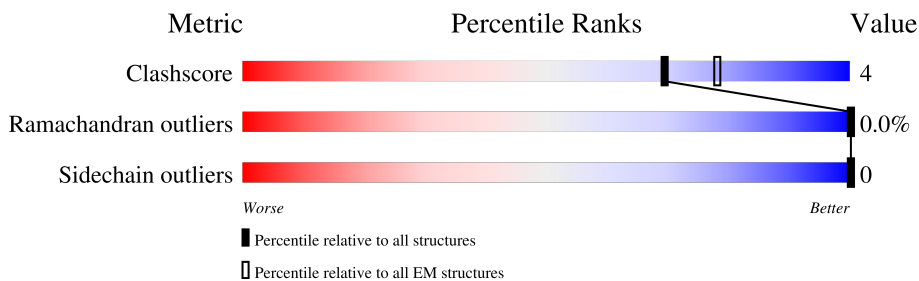
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.45 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.



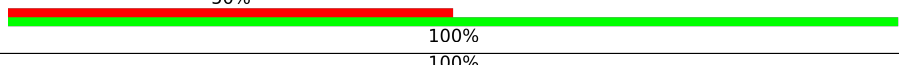
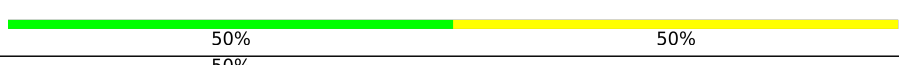
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1285	
1	B	1285	
1	C	1285	
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	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33398 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	1032	8101	5189	1349	1526	37	0	0
1	B	1032	8101	5189	1349	1526	37	0	0
1	C	833	6502	4158	1078	1237	29	0	0

There are 387 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	conflict	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	ASP	TYR	conflict	UNP P0DTC2
A	210A	ILE	-	insertion	UNP P0DTC2
A	210B	VAL	-	insertion	UNP P0DTC2
A	210C	ARG	ASN	conflict	UNP P0DTC2
A	210D	GLU	LEU	conflict	UNP P0DTC2
A	210E	PRO	VAL	conflict	UNP P0DTC2
A	210F	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	547	LYS	THR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	856	LYS	ASN	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	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	981	PHE	LEU	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
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	conflict	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	ASP	TYR	conflict	UNP P0DTC2
B	210A	ILE	-	insertion	UNP P0DTC2
B	210B	VAL	-	insertion	UNP P0DTC2
B	210C	ARG	ASN	conflict	UNP P0DTC2
B	210D	GLU	LEU	conflict	UNP P0DTC2
B	210E	PRO	VAL	conflict	UNP P0DTC2
B	210F	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	conflict	UNP P0DTC2
B	371	LEU	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	547	LYS	THR	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	856	LYS	ASN	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	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	981	PHE	LEU	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	conflict	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	ASP	TYR	conflict	UNP P0DTC2
C	210A	ILE	-	insertion	UNP P0DTC2
C	210B	VAL	-	insertion	UNP P0DTC2
C	210C	ARG	ASN	conflict	UNP P0DTC2
C	210D	GLU	LEU	conflict	UNP P0DTC2
C	210E	PRO	VAL	conflict	UNP P0DTC2
C	210F	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	conflict	UNP P0DTC2
C	371	LEU	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	conflict	UNP P0DTC2
C	493	ARG	GLN	conflict	UNP P0DTC2
C	496	SER	GLY	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	547	LYS	THR	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	856	LYS	ASN	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	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	981	PHE	LEU	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	595	4857	3108	804	916	29	0	0
2	E	595	4857	3108	804	916	29	0	0

There are 16 discrepancies between the modelled and reference sequences:

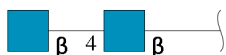
Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
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.



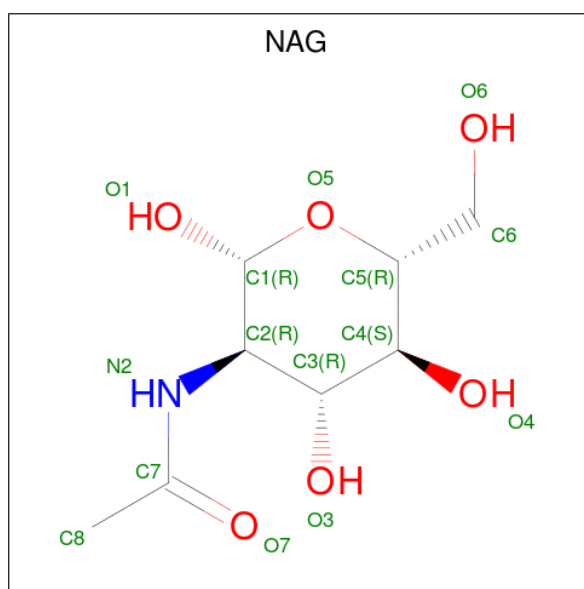
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C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

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

- 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	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0
4	A	1	Total 112	C 64	N 8	O 40	0

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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	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
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	C	1	84	48	6	30	0
4	C	1	84	48	6	30	0
4	C	1	84	48	6	30	0
4	C	1	84	48	6	30	0
4	C	1	84	48	6	30	0
4	C	1	84	48	6	30	0
4	C	1	84	48	6	30	0
4	D	1	84	48	6	30	0
4	D	1	84	48	6	30	0

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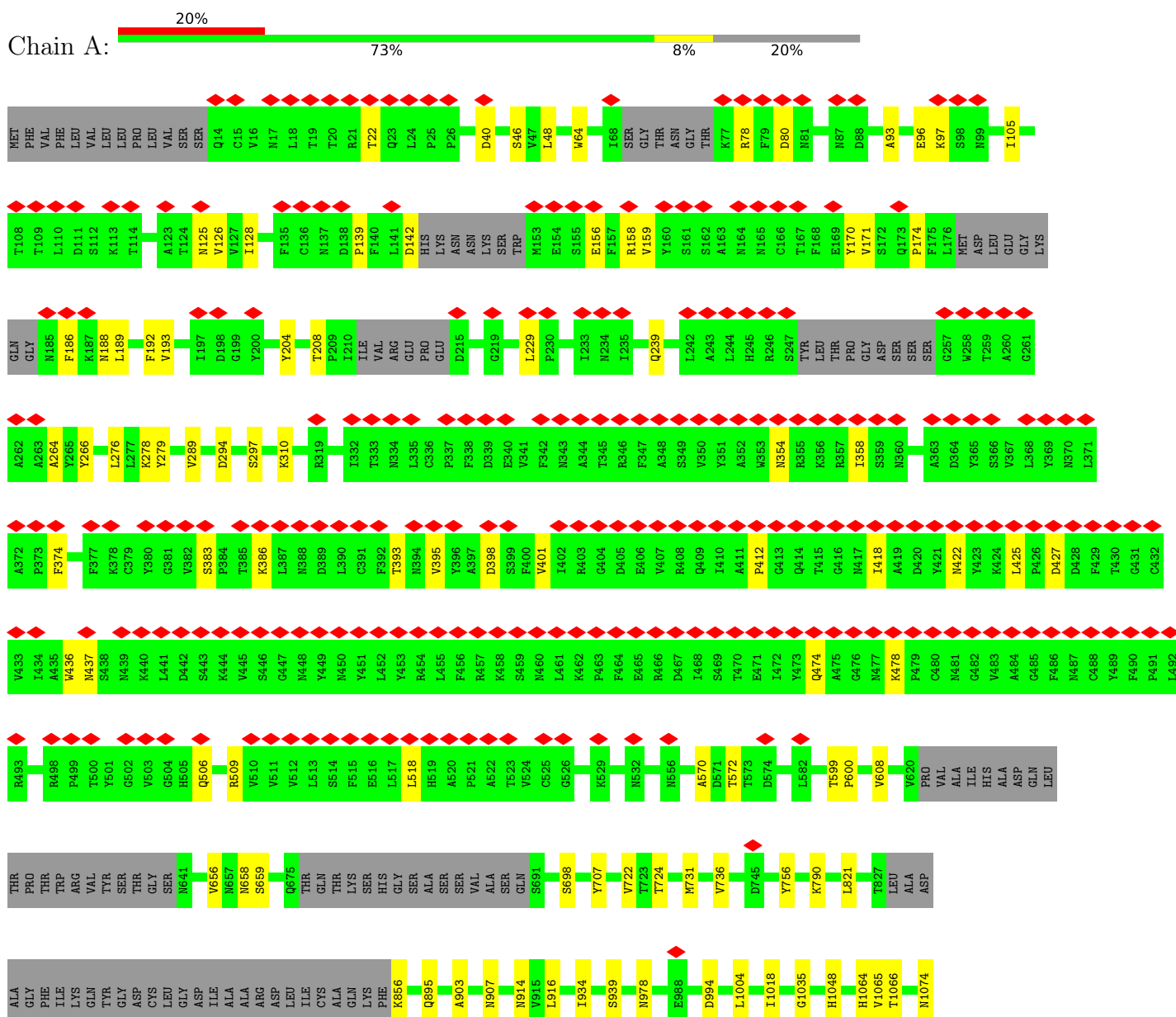
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	D	1	Total 84	48	6	30	0
4	D	1	Total 84	48	6	30	0
4	D	1	Total 84	48	6	30	0
4	D	1	Total 84	48	6	30	0
4	E	1	Total 84	48	6	30	0
4	E	1	Total 84	48	6	30	0
4	E	1	Total 84	48	6	30	0
4	E	1	Total 84	48	6	30	0
4	E	1	Total 84	48	6	30	0
4	E	1	Total 84	48	6	30	0

3 Residue-property plots

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

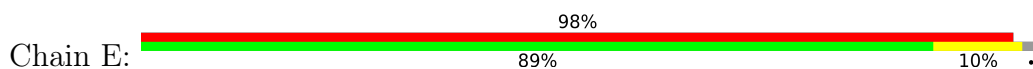
• Molecule 1: Spike glycoprotein



GLN	S19	T20	I21	E22	E23	Q24	A25	K26	T27	F28	L29	D30	K31	F32	N33	H34	E35	A36	E37	D38	L39	F40	Y41	Q42	S43	L44	A45	A46	S47	W48	N49	Y50	N51	T52	N53	I54	T55	E56	E57	N58	V59	Q60	N61	H62	N63	N64	A65	G66	D67	K68	M69	S70	A71	F72	L73	K74	E75	Q76	S77	
T78	L79	A80	Q81	H82	Y83	P84	L85	Q86	E87	I88	Q89	N90	L91	T92	V93	K94	L95	L96	L97	Q98	A99	L100	Q101	L102	N103	G104	S105	S106	V107	L108	S109	E110	D111	K112	S113	L114	L115	L116	N117	T118	I119	L120	N121	T122	N123	S124	T125	I126	K127	M128	T129	G130	K131	V132	C133	M134	P135	D136	M137	
F138	Q139	E140	C141	L142	L143	L144	E145	P146	L147	L148	M149	E150	L151	M152	A153	M154	S155	L156	D157	Y158	M159	E160	R161	L162	M163	A164	W165	E166	W167	W168	R169	S170	E171	V172	G173	K174	Q175	L176	R177	P178	L179	Y180	E181	E182	Y183	V184	W185	L186	M187	M188	E189	M190	L191	R192	A193	M194	Y195	E196	E197	
D198	Y199	G200	D201	W202	W203	A204	G205	D206	Y207	E208	V209	M210	G211	W212	D213	G214	Y215	D216	Y217	S218	R219	G220	Q221	L222	L223	E224	D225	W226	E227	H228	T229	F230	E231	E232	T233	K234	P235	L236	Y237	E238	H239	L240	H241	A242	Y243	V244	R245	A246	L247	L248	M249	K250	A251	Y252	P253	Y254	I255	I256	S257	
P258	L259	G260	C261	L262	P263	A264	H265	L266	L267	G268	D269	M270	W271	G272	R273	F274	W275	T276	N277	L278	Y279	S280	L281	T282	V283	P284	F285	G286	E287	K288	P289	N290	L291	D292	V293	T294	D295	A296	M297	V298	D299	Q300	A301	W302	D303	A304	Q305	R306	L307	F308	K309	E310	A311	E312	K313	F314	F315	V316	S317	
V318	G319	L320	P321	M322	M323	L324	Q325	G326	F327	W328	E329	N330	S331	N332	L333	T334	D335	P336	G337	N338	V339	Q340	K341	A342	V343	C344	H345	P346	T347	A348	V349	D350	L351	G352	K353	G354	D355	F356	R357	L358	L359	M360	C361	T362	K363	V364	T365	M366	D367	F368	F369	L370	T371	A372	H373	H374	E375	M376	G377	
H378	I379	Q380	Y381	D382	M383	A384	Y385	A386	A387	Q388	P389	F390	L391	L392	R393	M394	G395	A396	N397	E398	G399	F400	H401	E402	A403	V404	G405	E406	I407	M408	A409	L410	S411	A412	A413	T414	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426	D427	F428	Q429	E430	D431	M432	E433	T434	E435	I436	N437	
F438	L439	L440	K441	Q442	A443	L444	T445	I446	V447	G448	T449	L450	K451	F452	T453	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	Y479	M480	K481	R482	E483	I484	W485	G486	V487	V488	E489	P490	V491	F492	H493	D494	E495	T496	Y497	
C498	D499	P500	A501	S502	L503	F504	H505	V506	S507	N508	D509	Y510	S511	F512	L513	R514	Y515	Y516	T517	R518	T519	L520	Y521	F522	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	V487	T548	E549	A550	G551	Q552	K553	L554	M555	M556	M557
L558	R559	L560	G561	K562	S563	E564	P565	W566	T567	L568	A569	L570	E571	N572	V573	V574	G575	A576	K577	N578	M579	N580	V581	R582	P583	L584	L585	M586	F587	E588	E589	P590	L591	F592	T593	W594	L595	K596	D597	Q598	K600	N601	S602	F603	V604	G605	W606	S607	T608	D609	W610	S611	P612	Y613	ALA	ASP	HIS	HIS		

HIS
HIS
HIS
HIS
HIS

● Molecule 2: Processed angiotensin-converting enzyme 2



GLN	S19	T20	I21	E22	E23	Q24	A25	K26	T27	F28	L29	D30	K31	F32	N33	H34	E35	A36	E37	D38	L39	F40	Y41	Q42	S43	L44	L45	A46	S47	W48	N49	Y50	N51	T52	N53	I54	T55	E56	E57	N58	V59	Q60	N61	H62	N63	N64	A65	G66	D67	K68	M69	S70	A71	F72	L73	K74	E75	Q76	S77
T78	L79	A80	Q81	H82	Y83	P84	L85	Q86	E87	I88	Q89	N90	L91	T92	V93	K94	L95	L96	L97	Q98	A99	L100	Q101	L102	N103	G104	S105	S106	V107	L108	S109	E110	D111	K112	S113	L114	L115	L116	N117	T118	I119	L120	N121	T122	N123	S124	T125	I126	K127	M128	T129	G130	K131	V132	C133	M134	P135	D136	M137

P138	P139	Q139	E140	C141	L142	L143	L144	E145	P146	G147	L148	N149	E150	I151	M152	A153	N154	S155	L156	D157	Y158	N159	E160	R161	L162	W163	A164	W165	E166	S167	W168	R169	S170	E171	V172	G173	K174	Q175	L176	R177	P178	L179	Y180	E181	E182	Y183	V184	V185	L186	K187	N188	E189	M190	A191	R192	A193	N194	Y195	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	W226	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	Y252	P253	S254	Y255	I256	S257	
P258	I259	G260	C261	P262	P263	A264	H265	L266	L267	G268	D269	M270	W271	G272	R273	F274	W275	T276	N277	L278	Y279	S280	L281	T282	W283	P284	F285	G286	Q287	K288	P289	N290	I291	D292	V293	T294	D295	A296	M297	V298	D299	Q300	A301	W302	S303	A304	Q305	R306	I307	F308	K309	E310	A311	E312	K313	F314	F315	V316	S317	
V318	G319	L320	P321	M322	M323	T324	Q325	G326	F327	W328	E329	N330	S331	M332	L333	T334	D335	P336	G337	N338	V339	Q340	K341	A342	V343	C344	H345	P346	T347	A348	W349	D350	L351	G352	K353	G354	D355	F356	R357	I358	L359	M360	C361	T362	K363	V364	T365	M366	D367	D368	F369	L370	T371	A372	H373	H374	E375	M376	G377	
H378	I379	Q380	Y381	D382	M383	A384	Y385	A386	A387	Q388	P389	F390	L391	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	M432	E433	T434	E435	I436	N437	
F438	L439	L440	K441	Q442	A443	L444	T445	I446	V447	G448	T449	L450	P451	F452	T453	Y454	M455	L456	E457	K458	M459	R460	M461	M462	V463	F464	K465	G466	E467	I468	P469	K470	D471	Q472	N473	M474	K475	K476	N477	W478	E479	M480	K481	R482	E483	I484	V485	G486	V487	V488	E489	P490	V491	F492	H493	D494	E495	T496	Y497	
C498	D499	F500	A501	S502	L503	F504	H505	V506	S507	M508	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	C541	C542	D543	I544	S545	N546	S547	T548	E549	A550	V551	Q552	K553	L554	F555	N556	M557	
L558	R559	L560	G561	K562	S563	E564	P565	W566	T567	L568	A569	L570	E571	N572	V573	W574	G575	A576	K577	N578	M579	N580	V581	R582	P583	L584	L585	N586	Y587	F588	E589	P590	L591	F592	T593	W594	L595	K596	D597	Q598	N599	K600	N601	S602	F603	V604	G605	W606	S607	T608	D609	W610	S611	P612	Y613	ALA	ASP	HIS	HIS	HIS

HIS
HIS
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HIS
HIS

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



MAG1
MAG2

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



MAG1
MAG2

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

Chain H: 



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

Chain I: 



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

Chain J: 



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

Chain K: 



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

Chain L: 



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

Chain M: 



- 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% 100%



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

Chain Q:  50% 50% 50%



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

Chain R:  100% 100%



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

Chain S:  50% 50%



- 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:  50% 100%



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

Chain V:  50% 100%



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

Chain W:  50% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	272266	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.148	Depositor
Minimum map value	-0.416	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.152	Depositor
Map size (\AA)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.29	0/8292	0.55	0/11281
1	B	0.30	0/8292	0.56	1/11281 (0.0%)
1	C	0.30	0/6644	0.56	0/9036
2	D	0.29	0/4994	0.54	0/6785
2	E	0.29	0/4994	0.54	0/6785
All	All	0.30	0/33216	0.55	1/45168 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	517	LEU	CA-CB-CG	5.26	127.40	115.30

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	8101	0	7925	62	0
1	B	8101	0	7925	70	0
1	C	6502	0	6386	61	0
2	D	4857	0	4630	31	0
2	E	4857	0	4630	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
4	A	112	0	104	0	0
4	B	112	0	104	1	0
4	C	84	0	78	1	0
4	D	84	0	78	0	0
4	E	84	0	78	0	0
All	All	33398	0	32388	242	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 242 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:C:142:ASP:HB2	1:C:156:GLU:HB3	1.74	0.69
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.77	0.65
1:B:856:LYS:HD3	1:B:966:LEU:HD12	1.78	0.65
1:B:46:SER:HA	1:B:279:TYR:O	1.97	0.65
1:B:156:GLU:OE2	1:B:158:ARG:NH1	2.32	0.63

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	1014/1285 (79%)	993 (98%)	21 (2%)	0	100	100
1	B	1014/1285 (79%)	992 (98%)	21 (2%)	1 (0%)	51	64
1	C	813/1285 (63%)	801 (98%)	12 (2%)	0	100	100
2	D	593/606 (98%)	577 (97%)	16 (3%)	0	100	100
2	E	593/606 (98%)	577 (97%)	16 (3%)	0	100	100
All	All	4027/5067 (80%)	3940 (98%)	86 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	337	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	907/1116 (81%)	907 (100%)	0	100	100
1	B	907/1116 (81%)	907 (100%)	0	100	100
1	C	733/1116 (66%)	733 (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	3599/4420 (81%)	3599 (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	C	1011	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	0.72	0	17,19,21	0.65	1 (5%)
3	NAG	F	2	3	14,14,15	0.33	0	17,19,21	0.40	0
3	NAG	G	1	1,3	14,14,15	0.31	0	17,19,21	0.61	1 (5%)
3	NAG	G	2	3	14,14,15	0.34	0	17,19,21	0.48	0
3	NAG	H	1	1,3	14,14,15	0.48	0	17,19,21	1.10	2 (11%)
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	I	1	1,3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	J	1	1,3	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	J	2	3	14,14,15	0.36	0	17,19,21	0.39	0
3	NAG	K	1	1,3	14,14,15	0.28	0	17,19,21	0.57	0
3	NAG	K	2	3	14,14,15	0.37	0	17,19,21	0.53	0
3	NAG	L	1	1,3	14,14,15	0.58	0	17,19,21	0.61	0
3	NAG	L	2	3	14,14,15	0.43	0	17,19,21	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	M	1	1,3	14,14,15	0.32	0	17,19,21	0.64	1 (5%)
3	NAG	M	2	3	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	N	1	1,3	14,14,15	0.44	0	17,19,21	1.03	2 (11%)
3	NAG	N	2	3	14,14,15	0.35	0	17,19,21	0.48	0
3	NAG	O	1	1,3	14,14,15	0.21	0	17,19,21	0.54	0
3	NAG	O	2	3	14,14,15	0.31	0	17,19,21	0.42	0
3	NAG	P	1	1,3	14,14,15	0.32	0	17,19,21	0.51	0
3	NAG	P	2	3	14,14,15	0.34	0	17,19,21	0.39	0
3	NAG	Q	1	1,3	14,14,15	0.40	0	17,19,21	0.65	1 (5%)
3	NAG	Q	2	3	14,14,15	0.45	0	17,19,21	0.45	0
3	NAG	R	1	1,3	14,14,15	0.54	0	17,19,21	0.58	0
3	NAG	R	2	3	14,14,15	0.39	0	17,19,21	0.50	0
3	NAG	S	1	1,3	14,14,15	0.29	0	17,19,21	0.61	1 (5%)
3	NAG	S	2	3	14,14,15	0.38	0	17,19,21	0.45	0
3	NAG	T	1	1,3	14,14,15	0.39	0	17,19,21	1.05	2 (11%)
3	NAG	T	2	3	14,14,15	0.40	0	17,19,21	0.58	0
3	NAG	U	1	1,3	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	U	2	3	14,14,15	0.33	0	17,19,21	0.44	0
3	NAG	V	1	1,3	14,14,15	0.27	0	17,19,21	0.56	0
3	NAG	V	2	3	14,14,15	0.35	0	17,19,21	0.42	0
3	NAG	W	1	1,3	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	W	2	3	14,14,15	0.42	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	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	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	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C2-N2-C7	3.03	127.22	122.90
3	N	1	NAG	C2-N2-C7	3.00	127.18	122.90
3	H	1	NAG	C2-N2-C7	3.00	127.17	122.90
3	L	2	NAG	C1-O5-C5	2.86	116.07	112.19
3	H	1	NAG	C1-O5-C5	2.56	115.66	112.19

There are no chirality outliers.

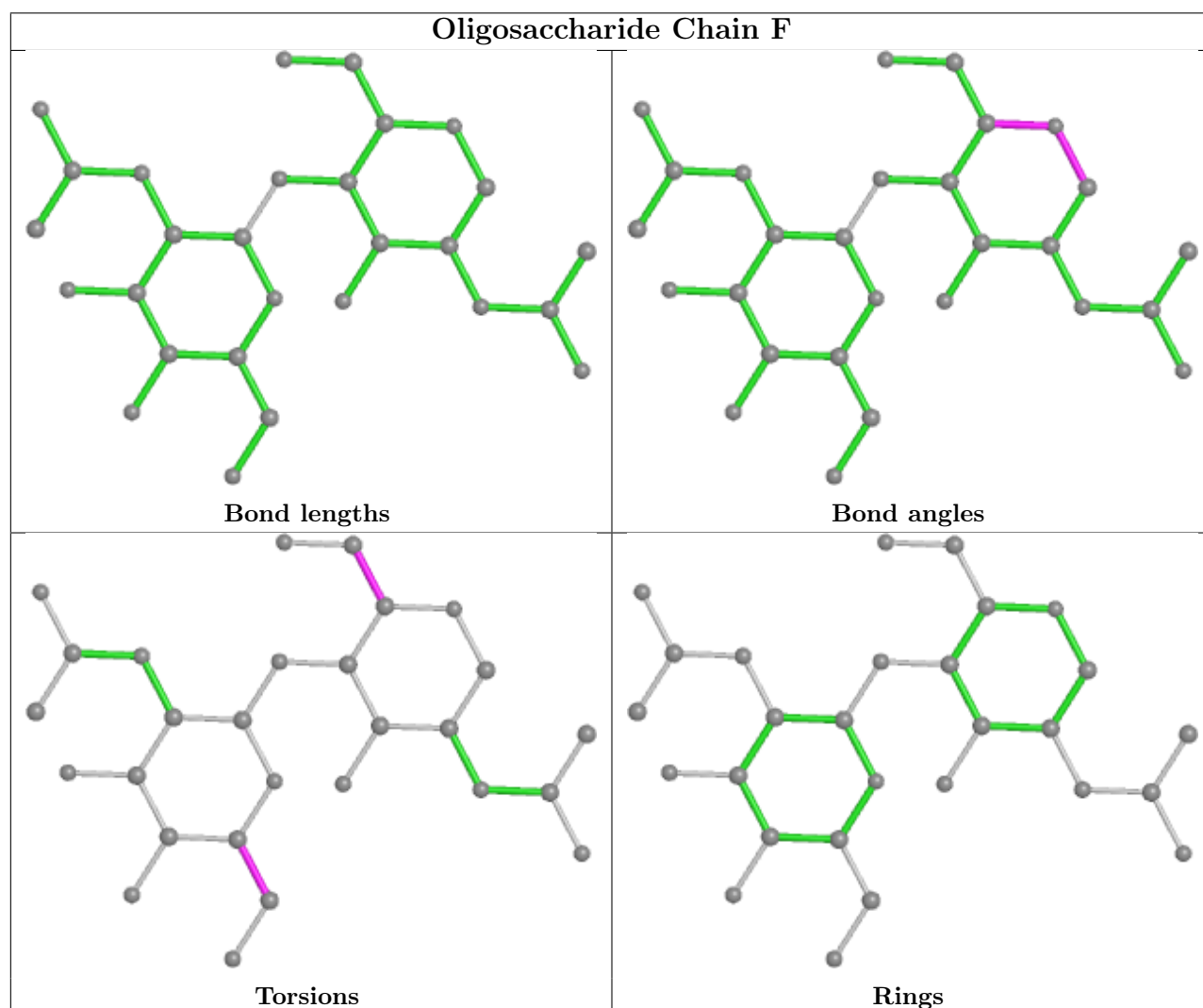
5 of 54 torsion outliers are listed below:

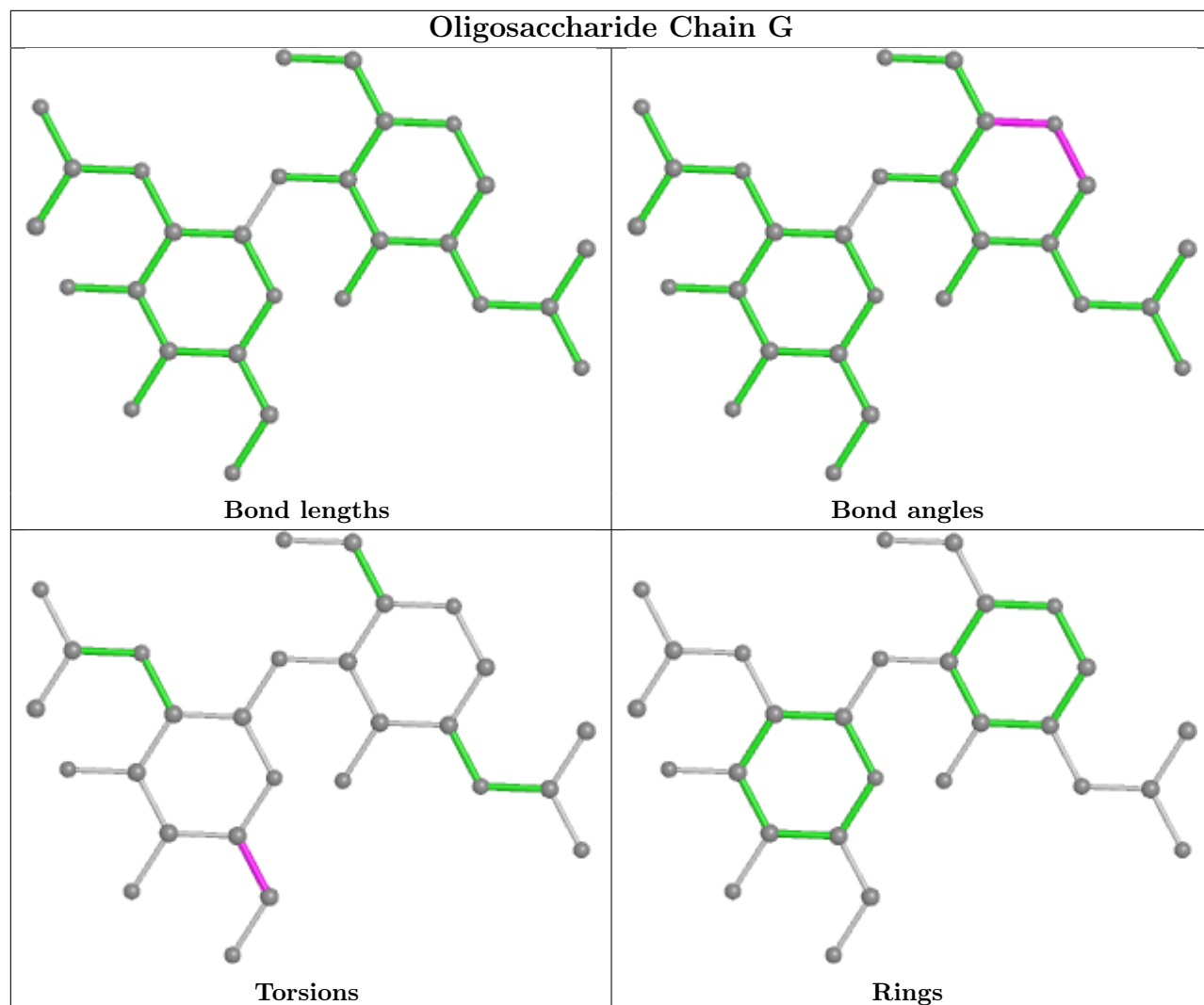
Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

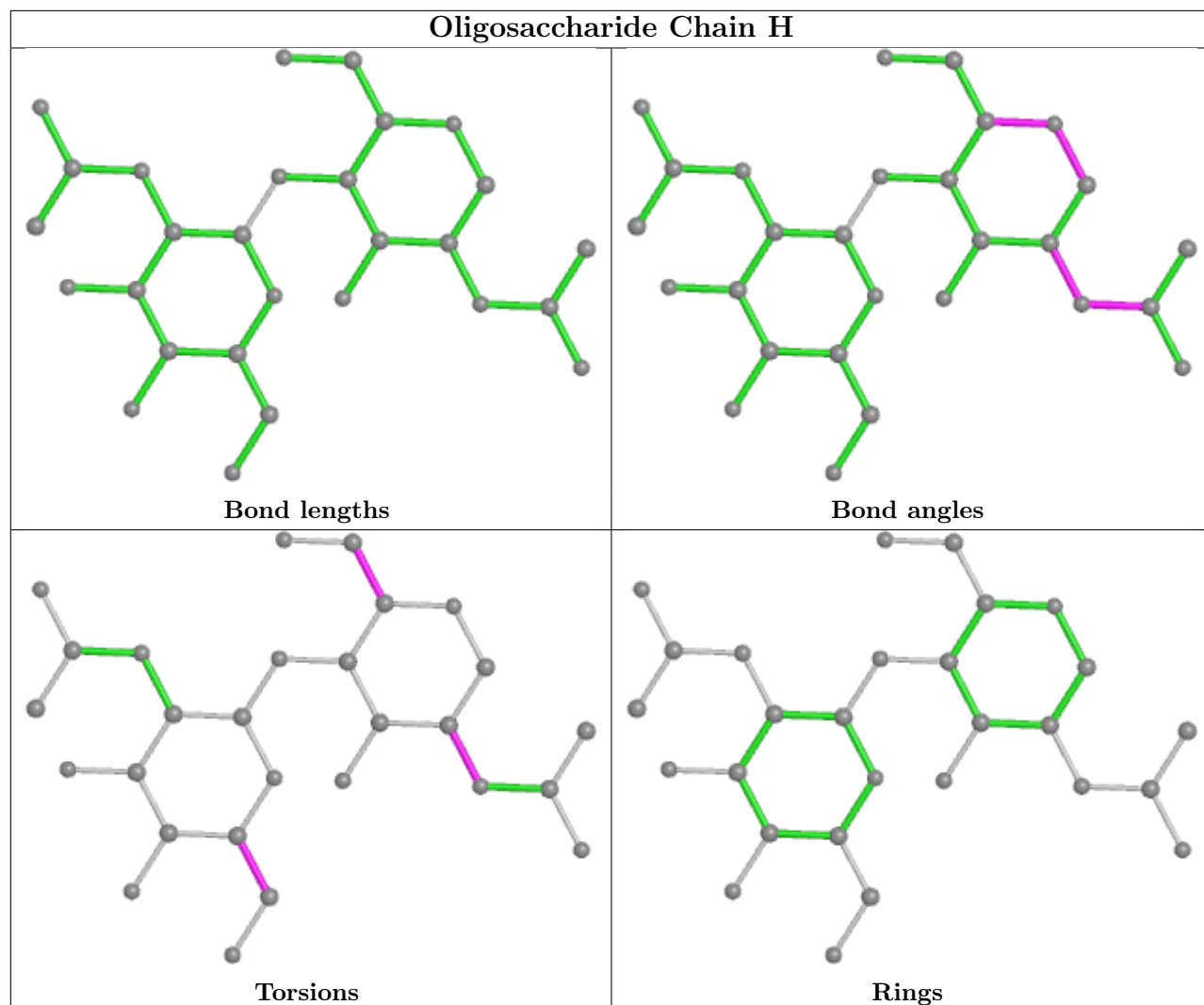
There are no ring outliers.

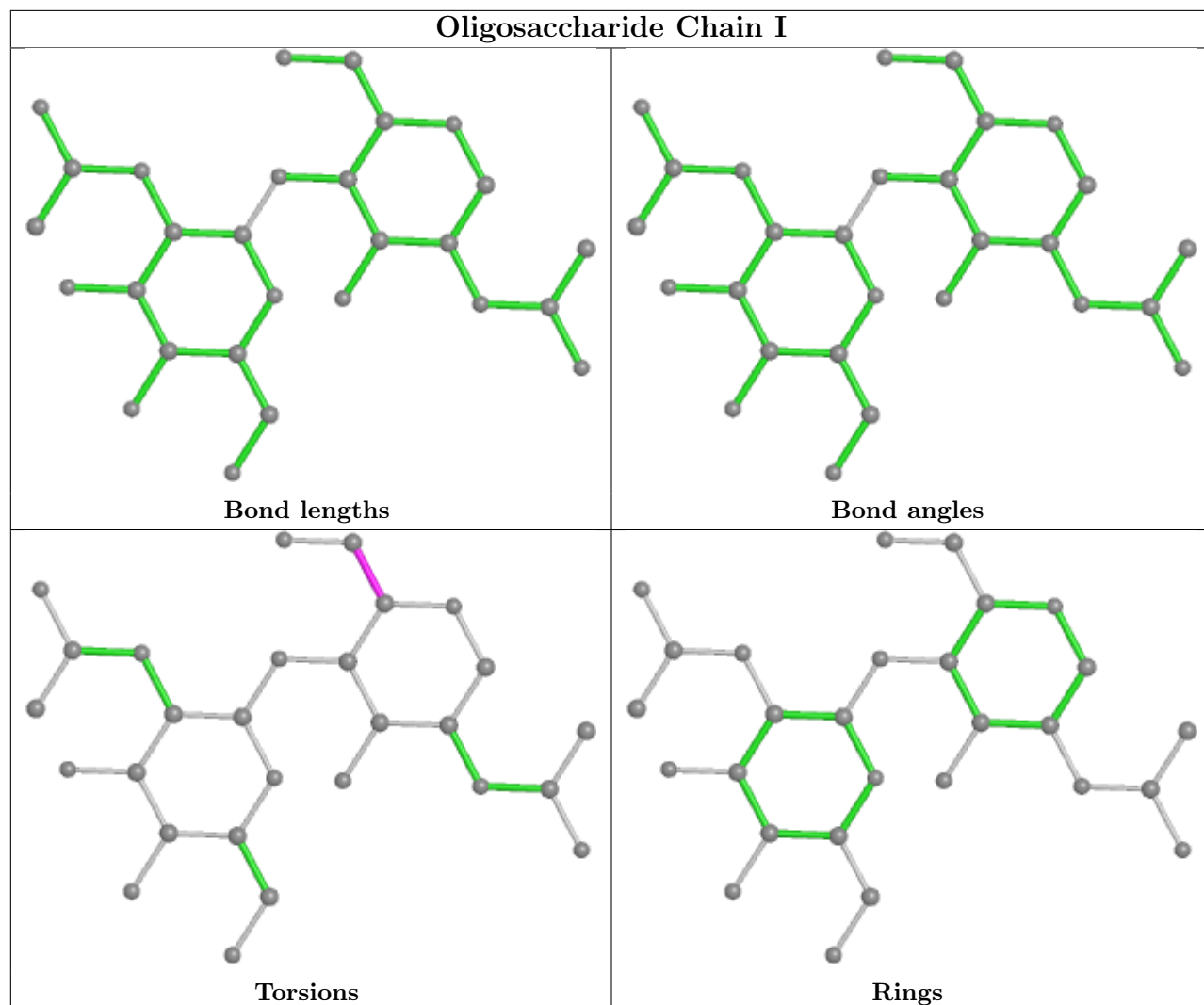
No monomer is involved in short contacts.

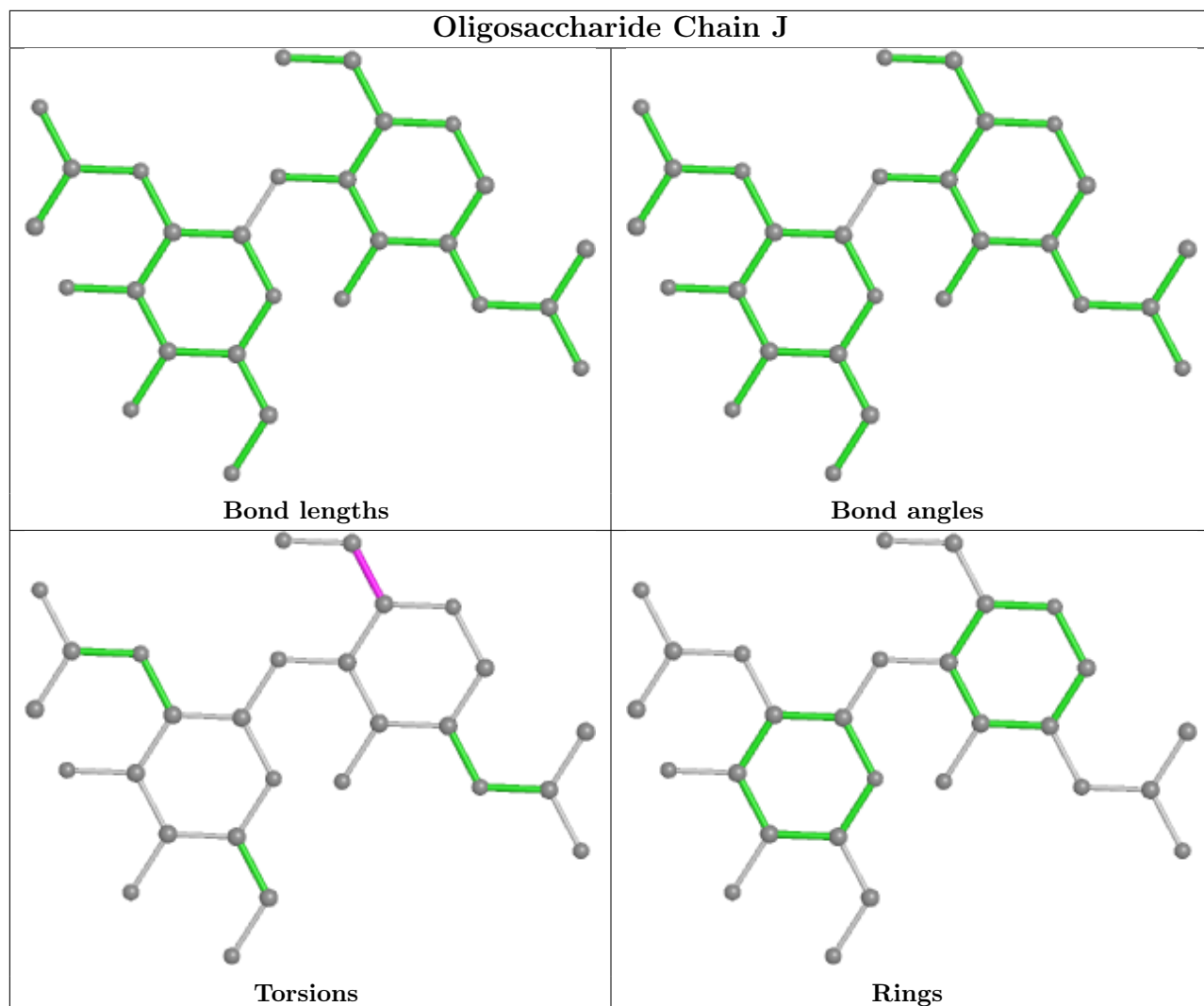
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

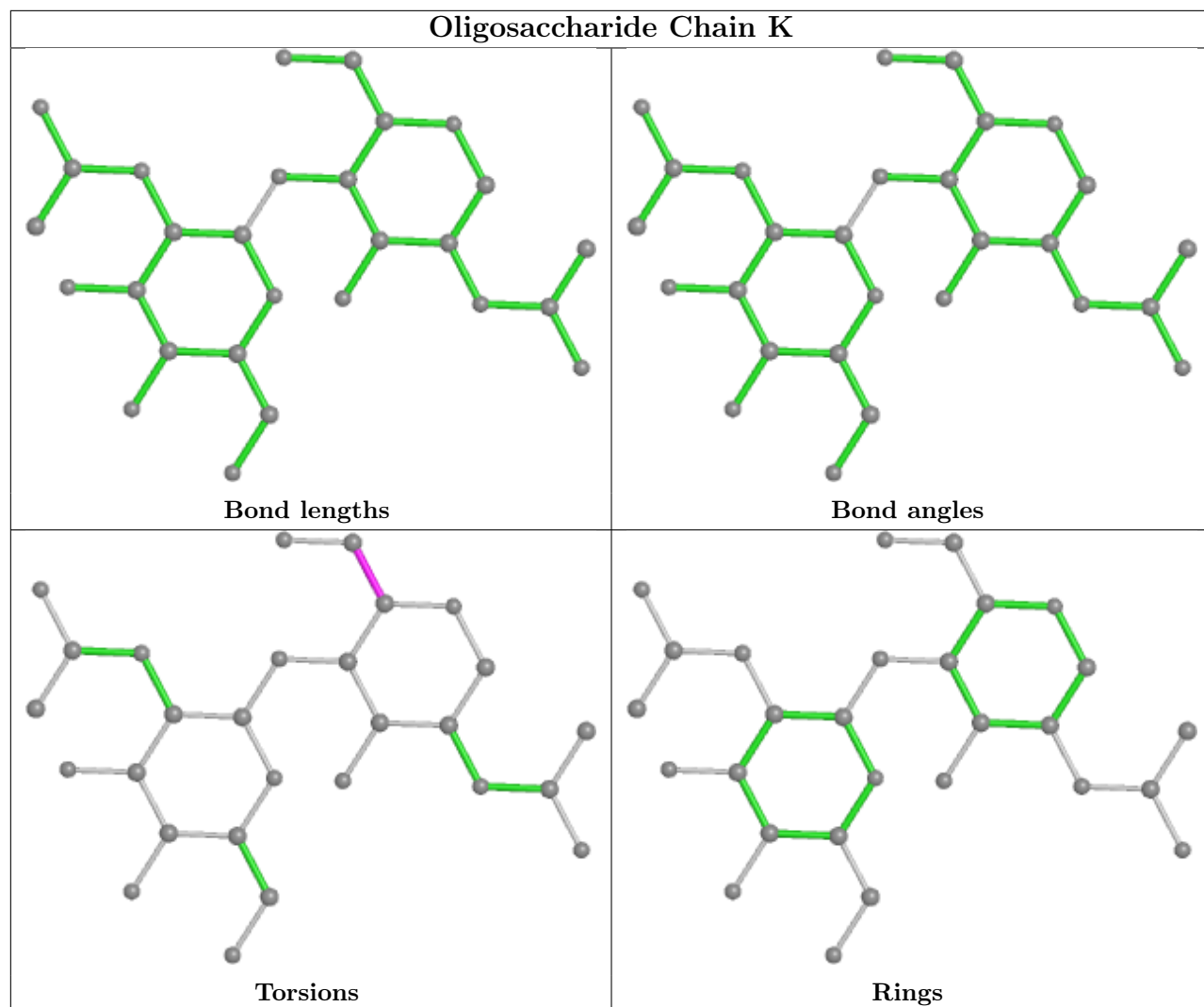


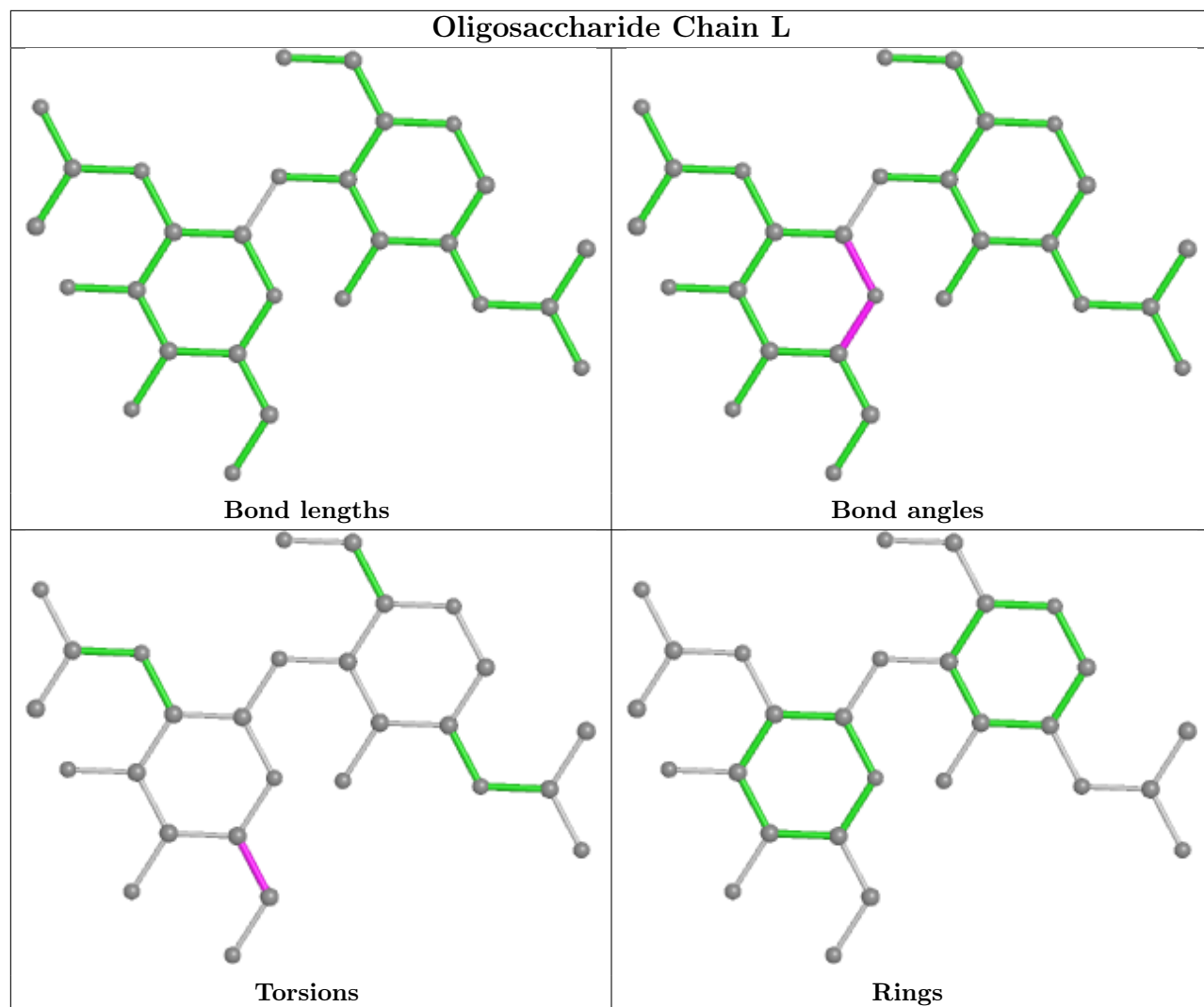


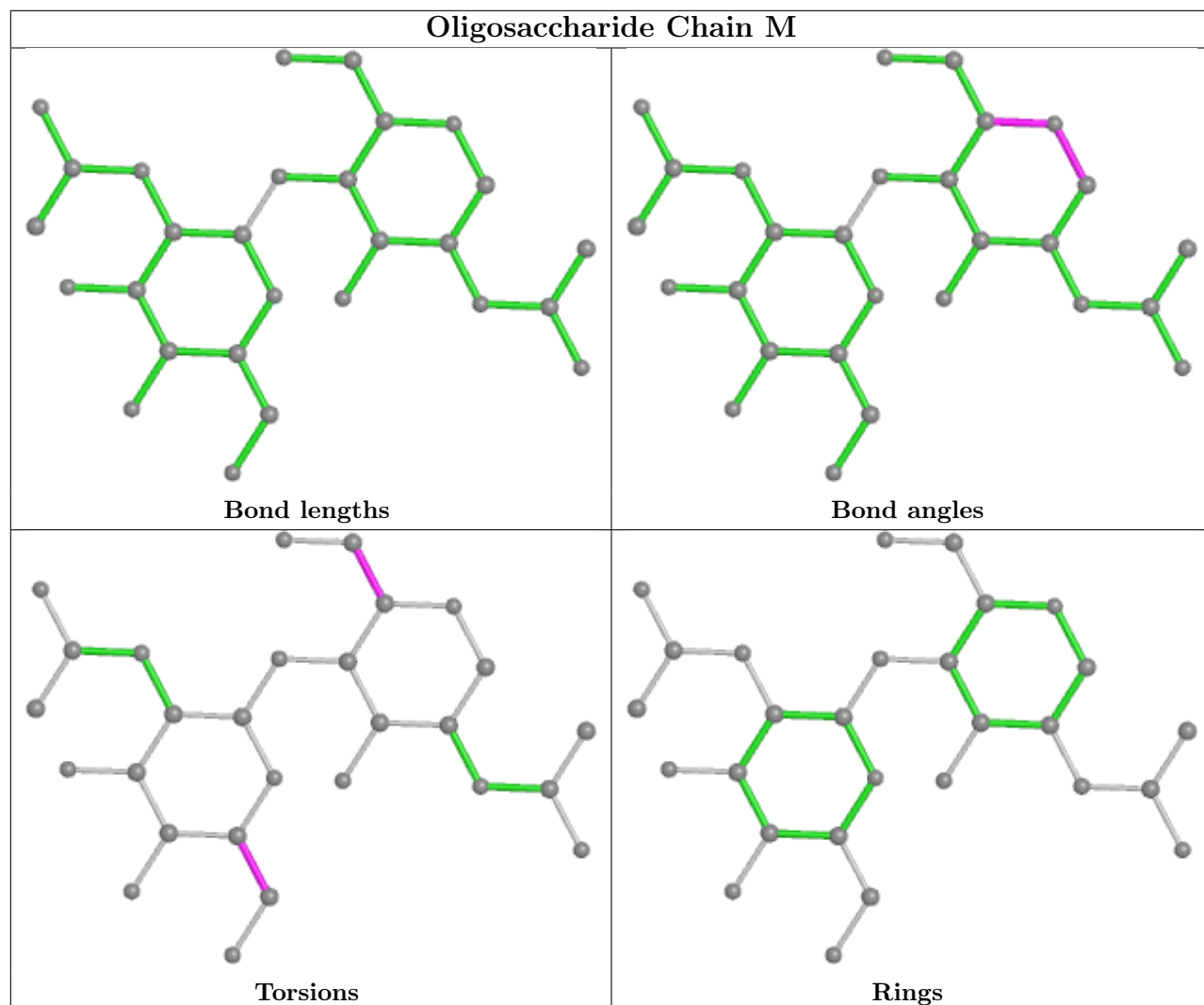


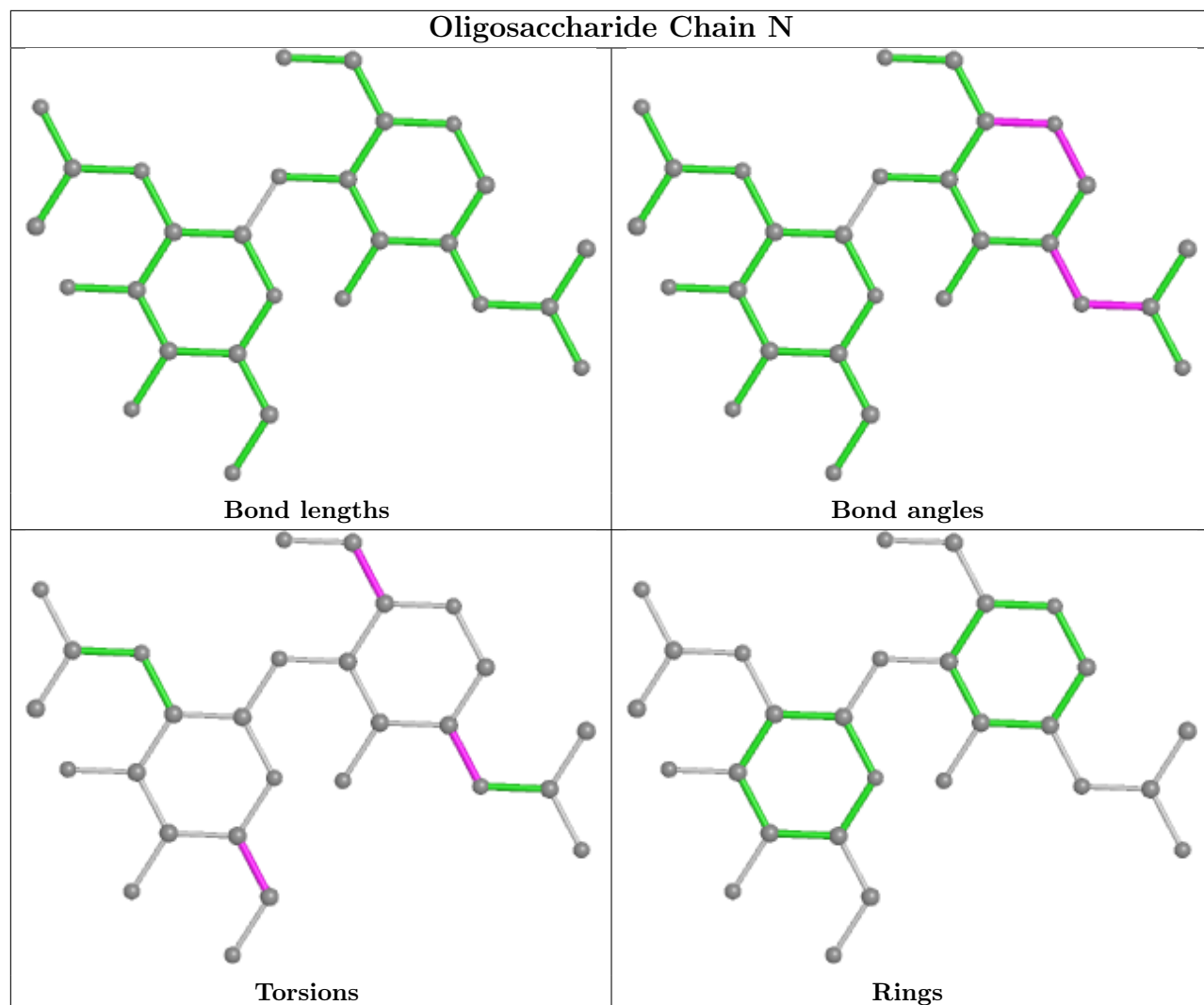


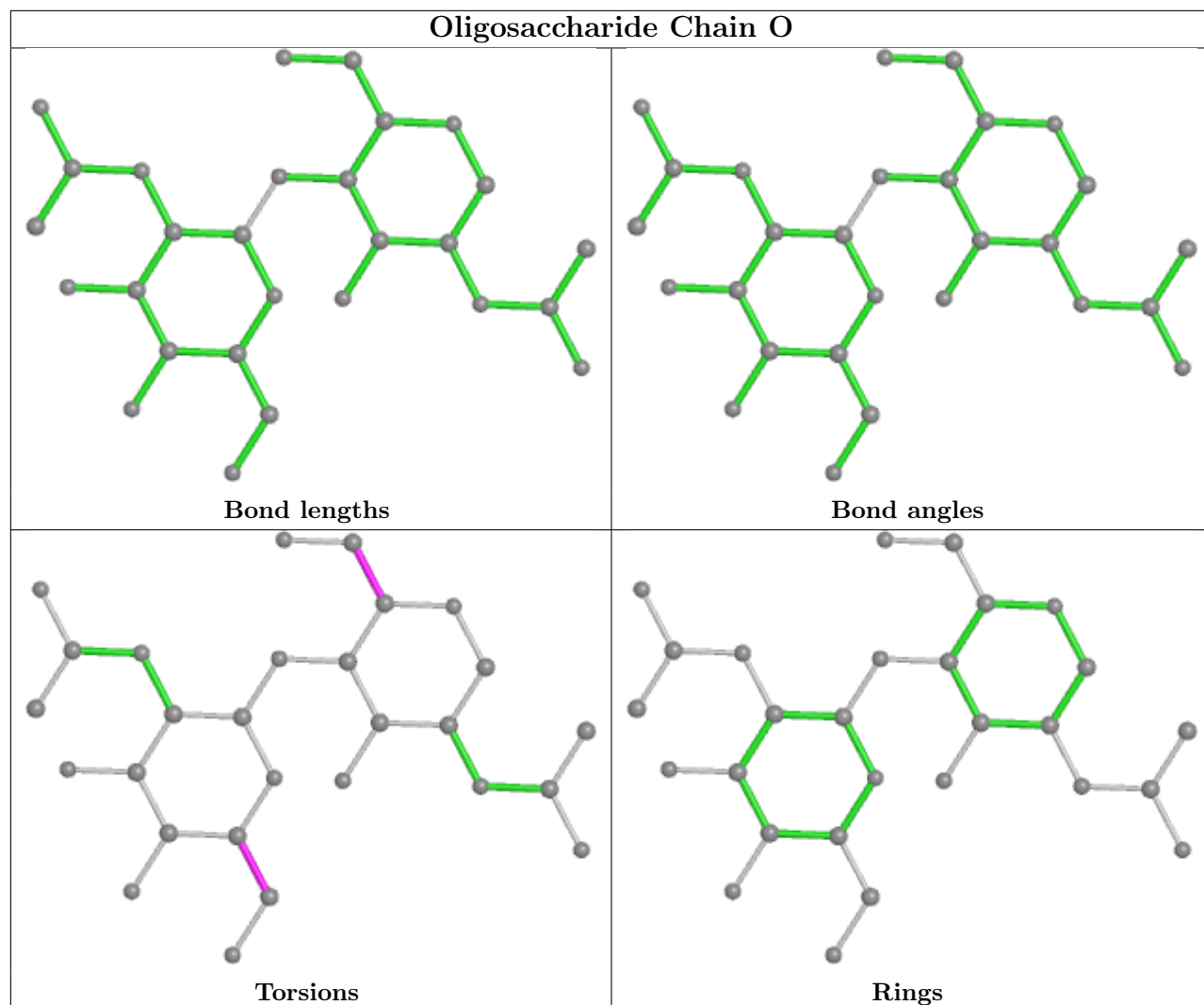


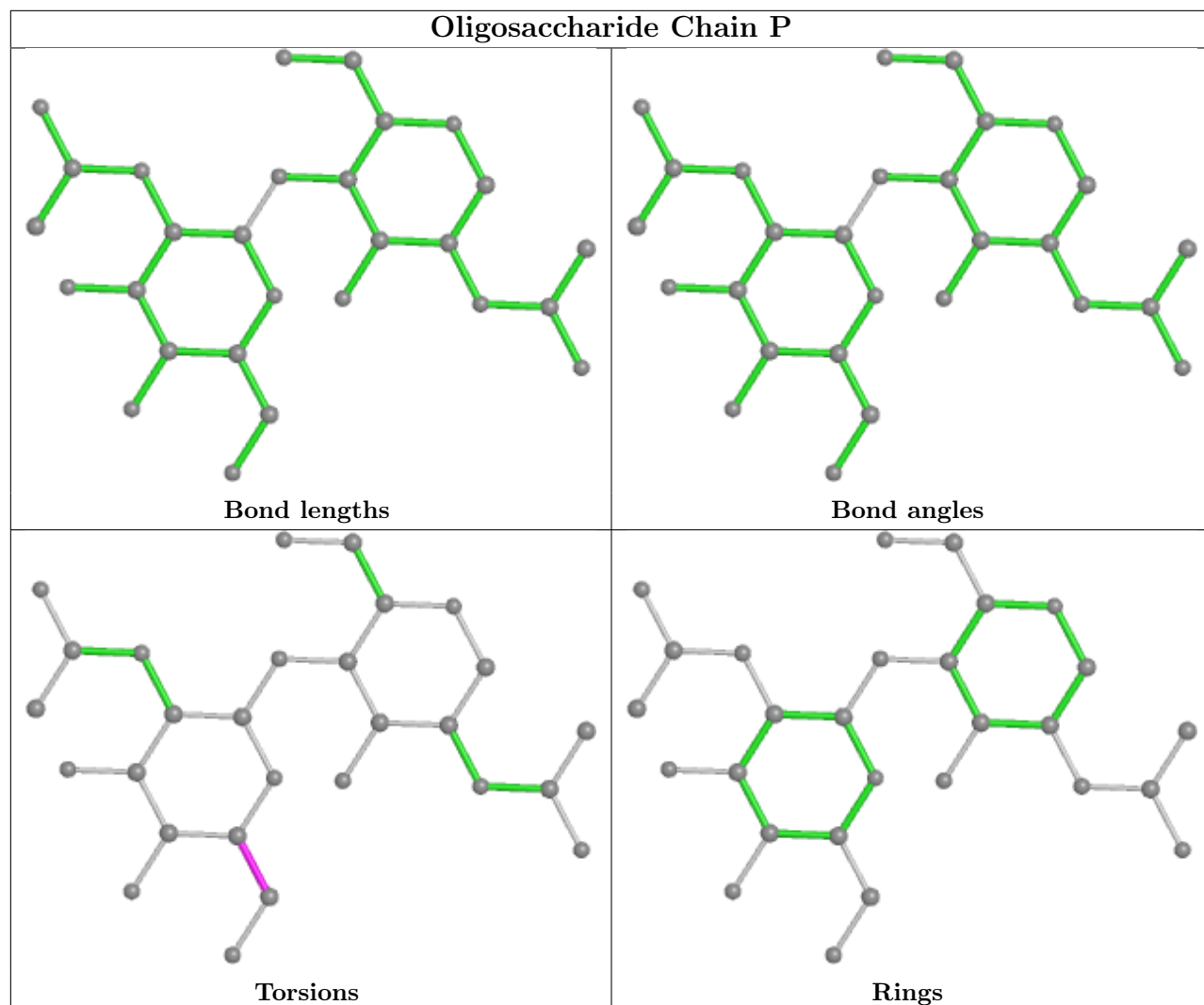


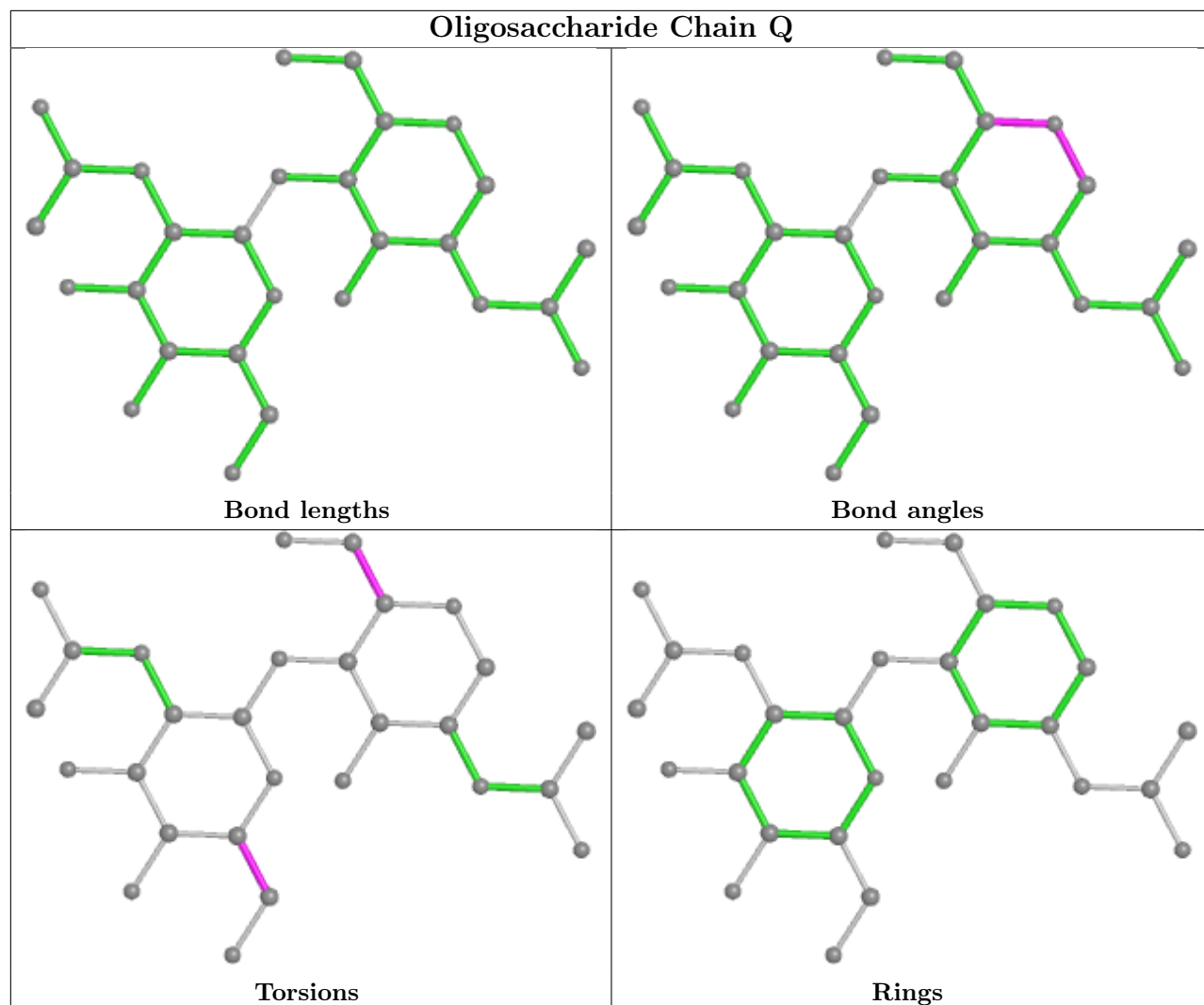


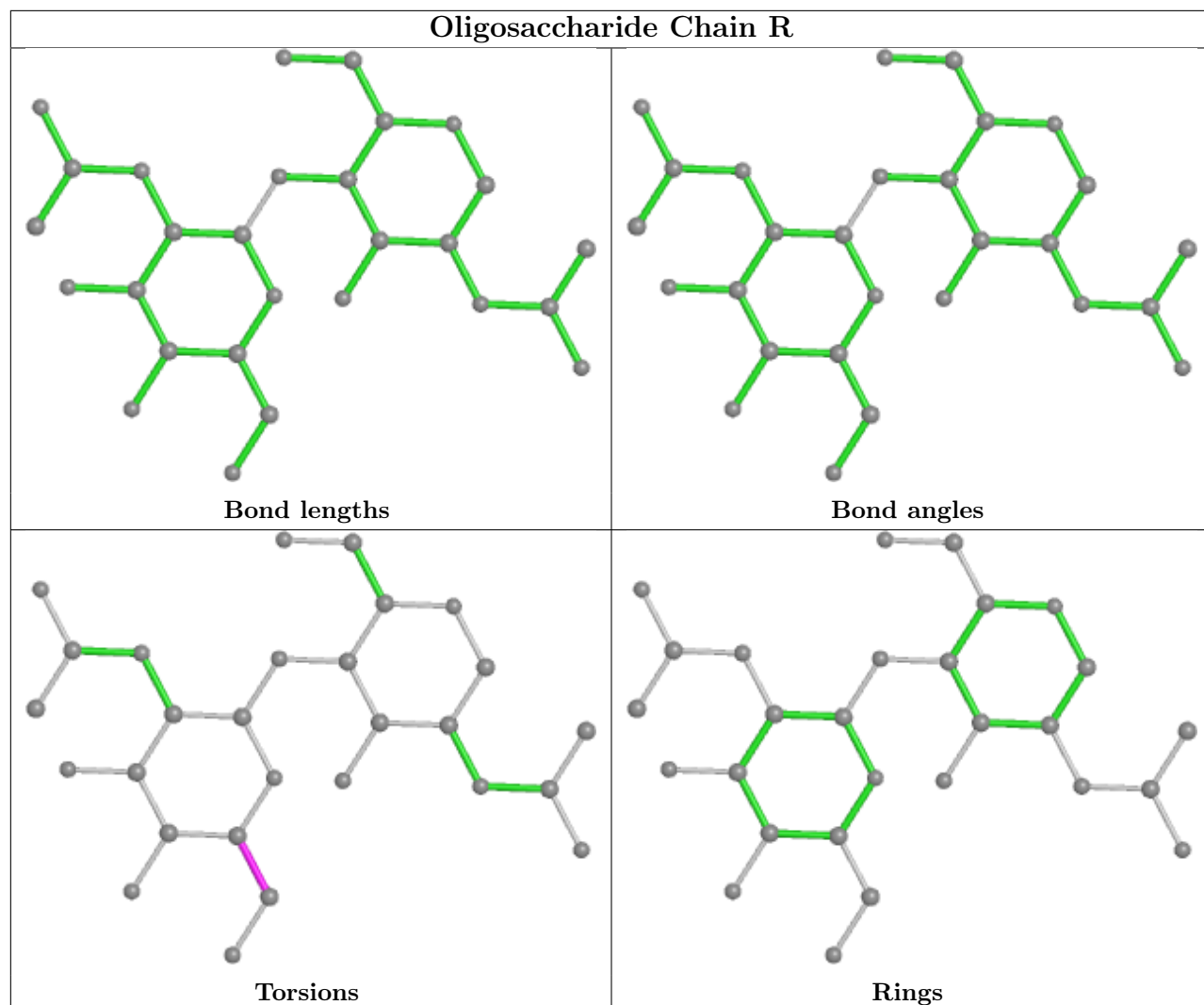


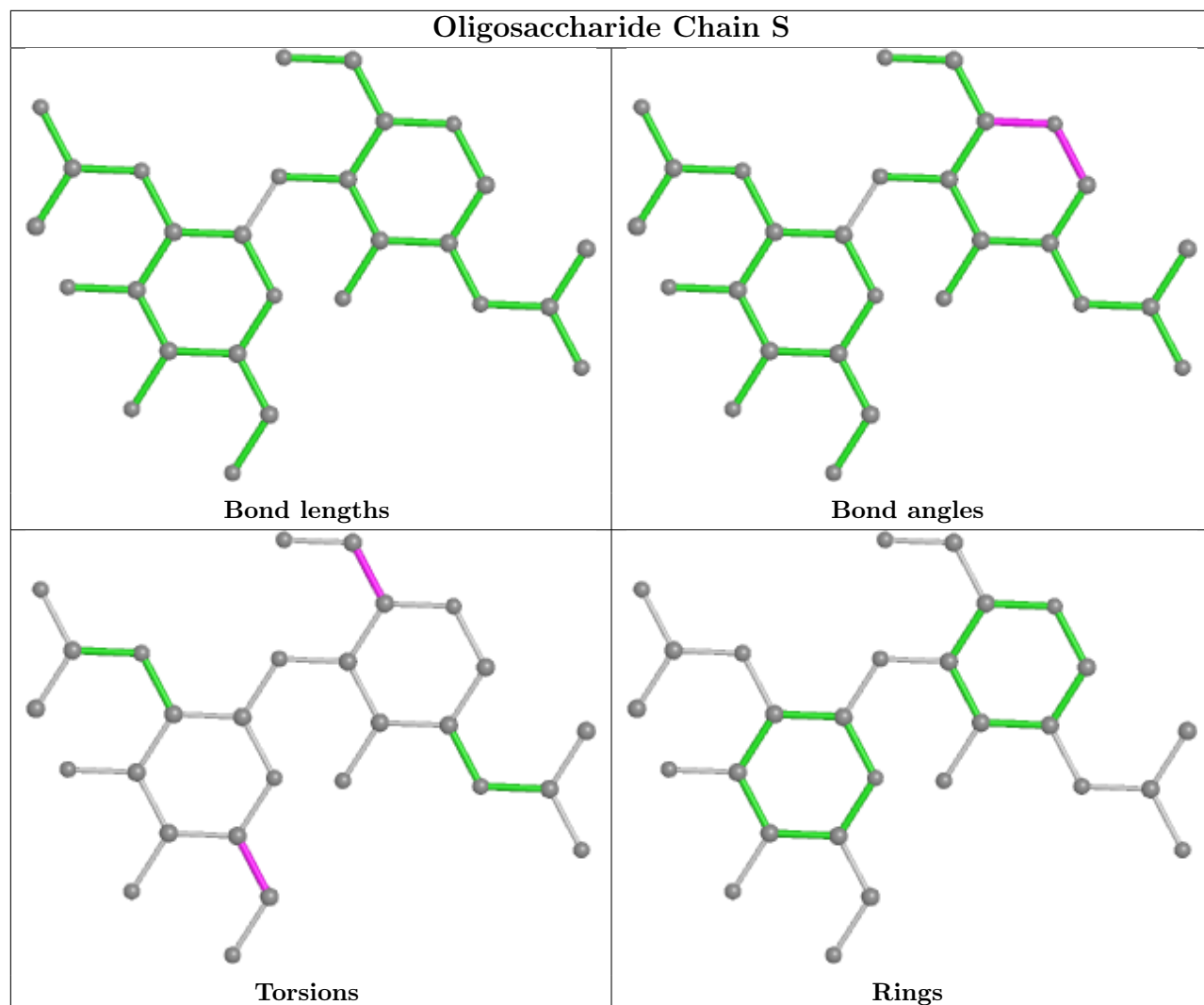


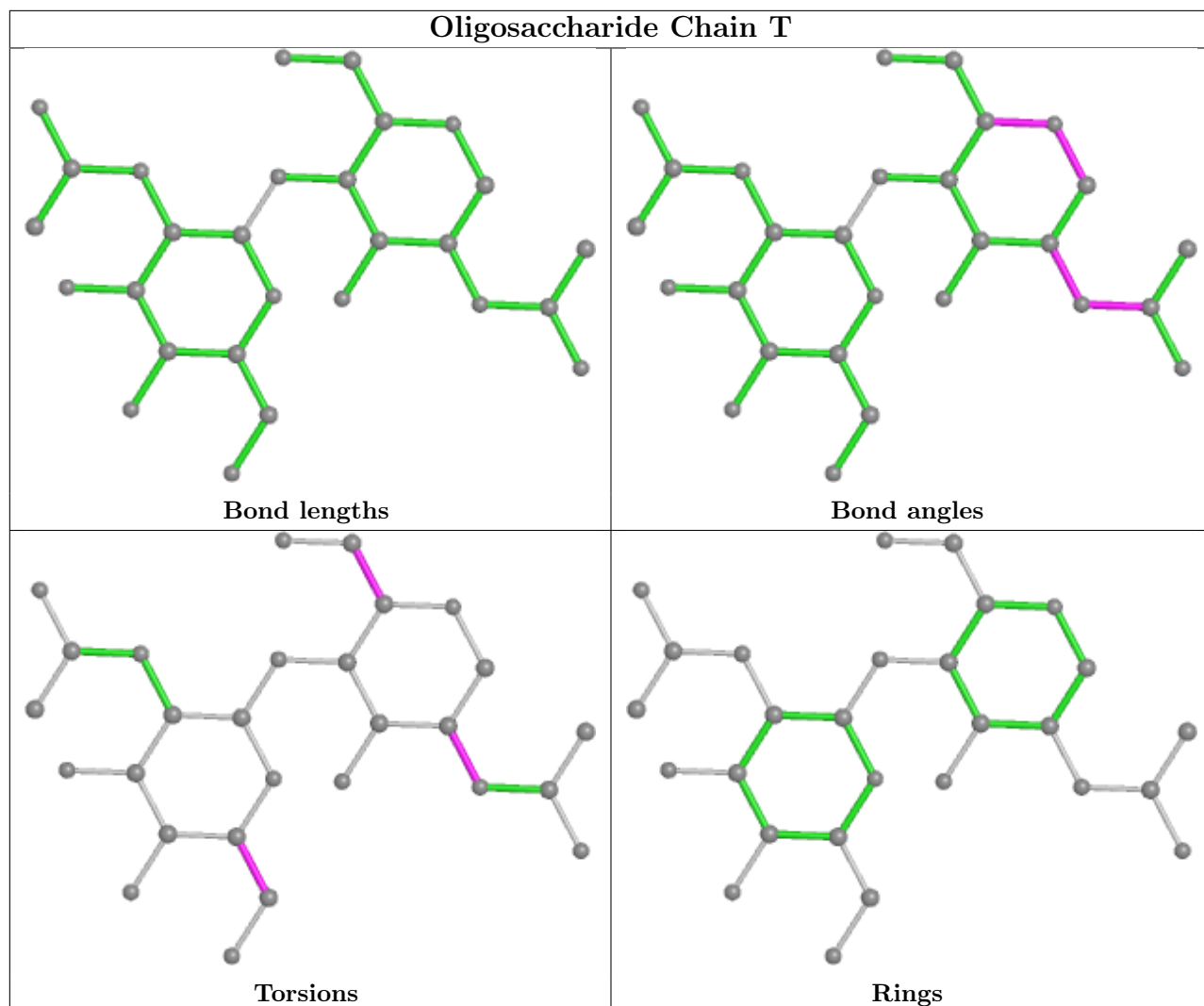


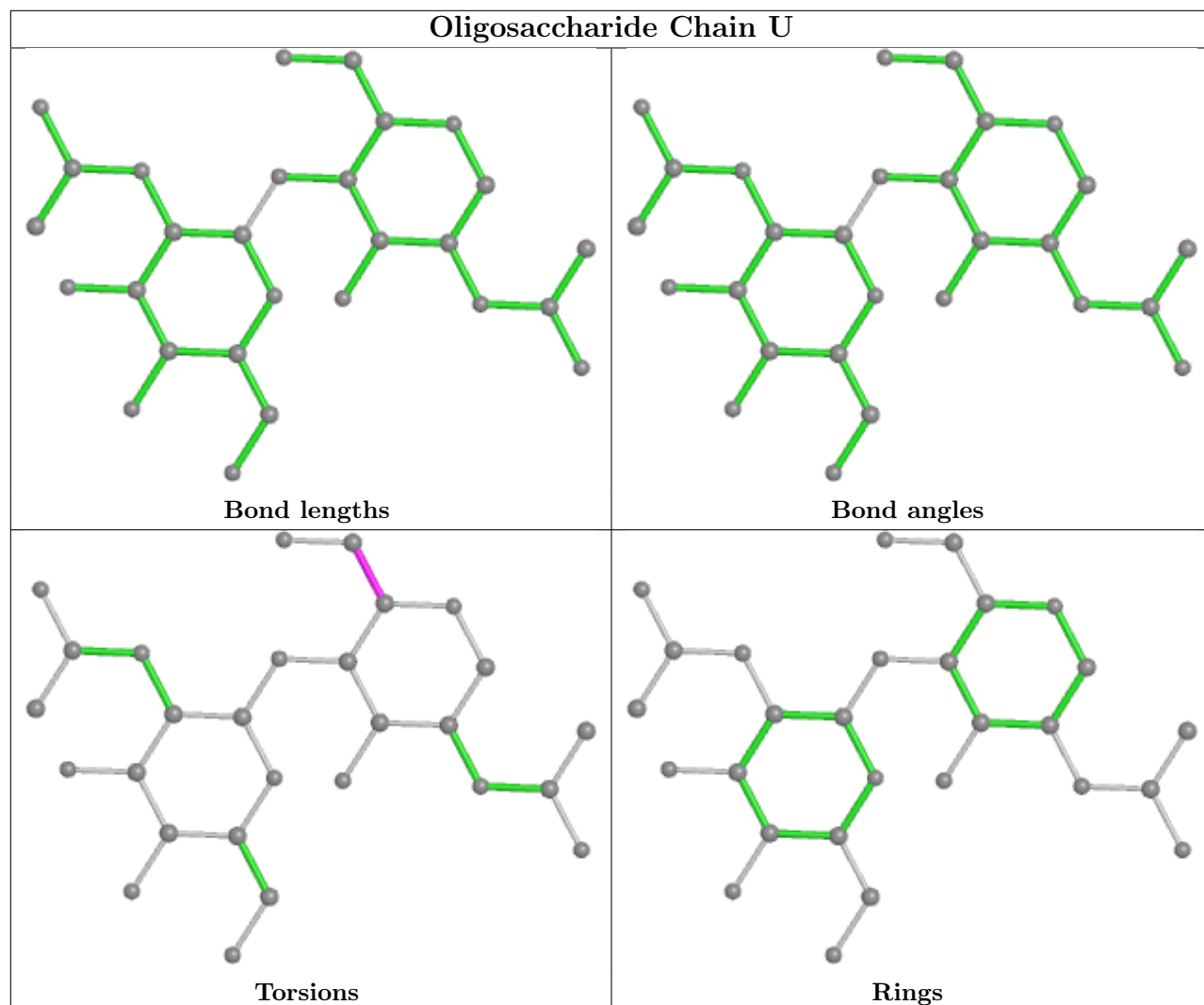


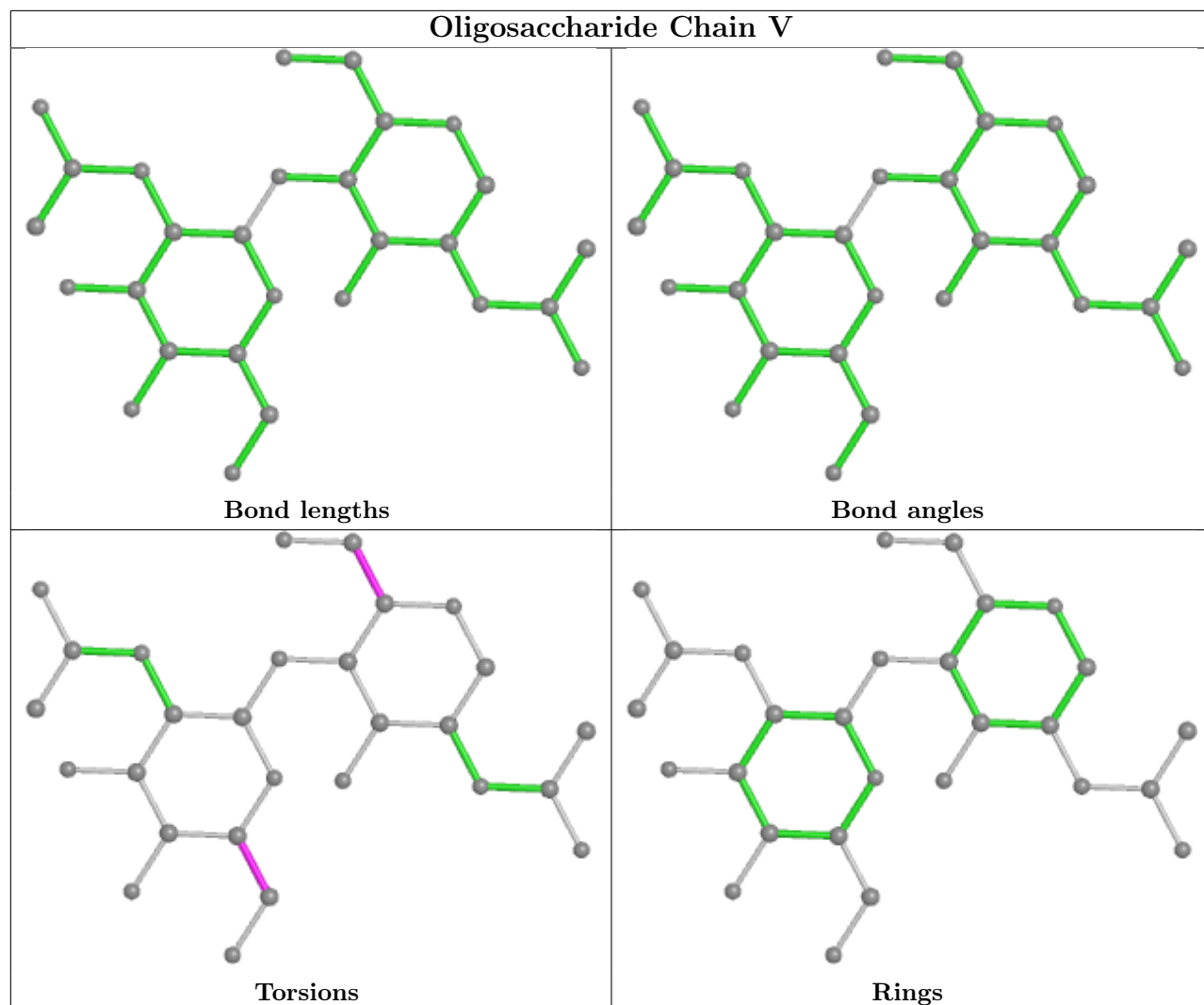


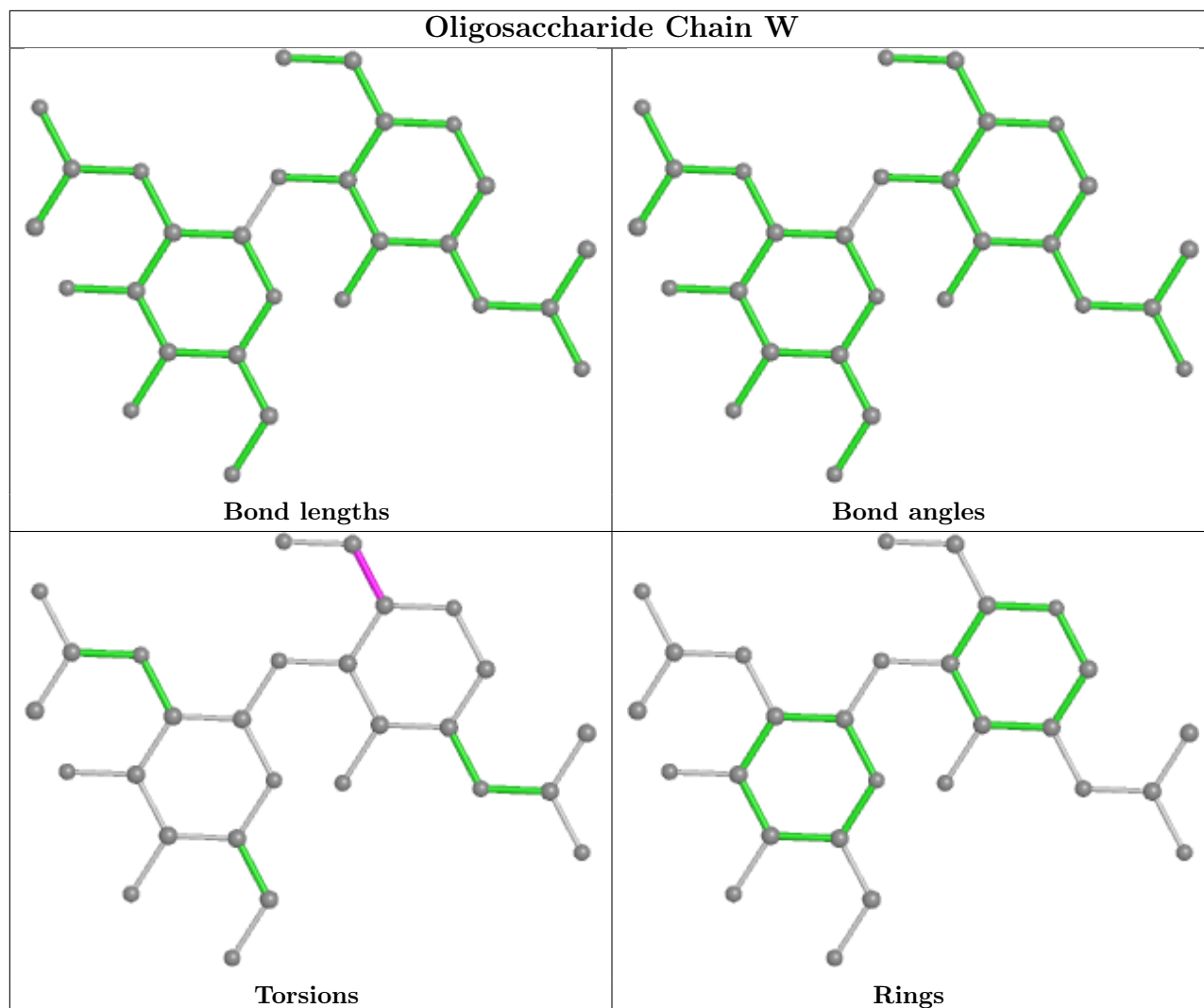












5.6 Ligand geometry [i](#)

34 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	A	1302	1	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	E	706	2	14,14,15	0.60	0	17,19,21	0.61	1 (5%)
4	NAG	A	1308	1	14,14,15	0.32	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	D	706	2	14,14,15	0.56	0	17,19,21	0.62	1 (5%)
4	NAG	E	705	2	14,14,15	0.39	0	17,19,21	0.49	0
4	NAG	B	1306	1	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	E	701	2	14,14,15	0.38	0	17,19,21	0.51	0
4	NAG	B	1308	1	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	E	704	2	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	E	703	2	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	E	702	2	14,14,15	0.45	0	17,19,21	0.53	0
4	NAG	D	704	2	14,14,15	0.35	0	17,19,21	0.52	0
4	NAG	C	1301	1	14,14,15	0.52	0	17,19,21	0.61	1 (5%)
4	NAG	D	702	2	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	C	1306	1	14,14,15	0.37	0	17,19,21	0.51	0
4	NAG	C	1305	1	14,14,15	0.39	0	17,19,21	0.44	0
4	NAG	C	1303	1	14,14,15	0.63	0	17,19,21	0.63	1 (5%)
4	NAG	D	703	2	14,14,15	0.34	0	17,19,21	0.45	0
4	NAG	A	1307	1	14,14,15	0.51	0	17,19,21	0.98	1 (5%)
4	NAG	D	701	2	14,14,15	0.37	0	17,19,21	0.50	0
4	NAG	B	1307	1	14,14,15	0.54	0	17,19,21	0.97	1 (5%)
4	NAG	B	1304	1	14,14,15	0.47	0	17,19,21	0.57	0
4	NAG	B	1302	1	14,14,15	0.34	0	17,19,21	0.54	0
4	NAG	B	1301	1	14,14,15	0.42	0	17,19,21	0.59	1 (5%)
4	NAG	A	1301	1	14,14,15	0.44	0	17,19,21	0.64	1 (5%)
4	NAG	C	1304	1	14,14,15	0.53	0	17,19,21	0.57	1 (5%)
4	NAG	A	1305	1	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	A	1306	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1303	1	14,14,15	0.67	1 (7%)	17,19,21	0.68	1 (5%)
4	NAG	B	1305	1	14,14,15	0.40	0	17,19,21	0.58	1 (5%)
4	NAG	C	1302	1	14,14,15	0.34	0	17,19,21	0.55	0
4	NAG	D	705	2	14,14,15	0.40	0	17,19,21	0.48	0
4	NAG	A	1303	1	14,14,15	0.61	0	17,19,21	0.62	1 (5%)
4	NAG	A	1304	1	14,14,15	1.24	2 (14%)	17,19,21	0.96	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	706	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	D	706	2	-	0/6/23/26	0/1/1/1
4	NAG	E	705	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	E	701	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	E	704	2	-	2/6/23/26	0/1/1/1
4	NAG	E	703	2	-	0/6/23/26	0/1/1/1
4	NAG	E	702	2	-	0/6/23/26	0/1/1/1
4	NAG	D	704	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	D	702	2	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	D	703	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	D	701	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	D	705	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	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	O5-C1	3.59	1.49	1.43
4	A	1304	NAG	C1-C2	2.82	1.56	1.52
4	B	1303	NAG	O5-C1	2.10	1.47	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1304	NAG	C1-O5-C5	3.53	116.97	112.19
4	B	1307	NAG	C2-N2-C7	3.03	127.22	122.90
4	A	1307	NAG	C2-N2-C7	3.01	127.19	122.90
4	B	1303	NAG	C1-O5-C5	2.58	115.69	112.19
4	C	1303	NAG	C1-O5-C5	2.37	115.40	112.19

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	701	NAG	C4-C5-C6-O6
4	E	706	NAG	C4-C5-C6-O6
4	D	704	NAG	O5-C5-C6-O6
4	D	701	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	NAG	1	0
4	C	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.

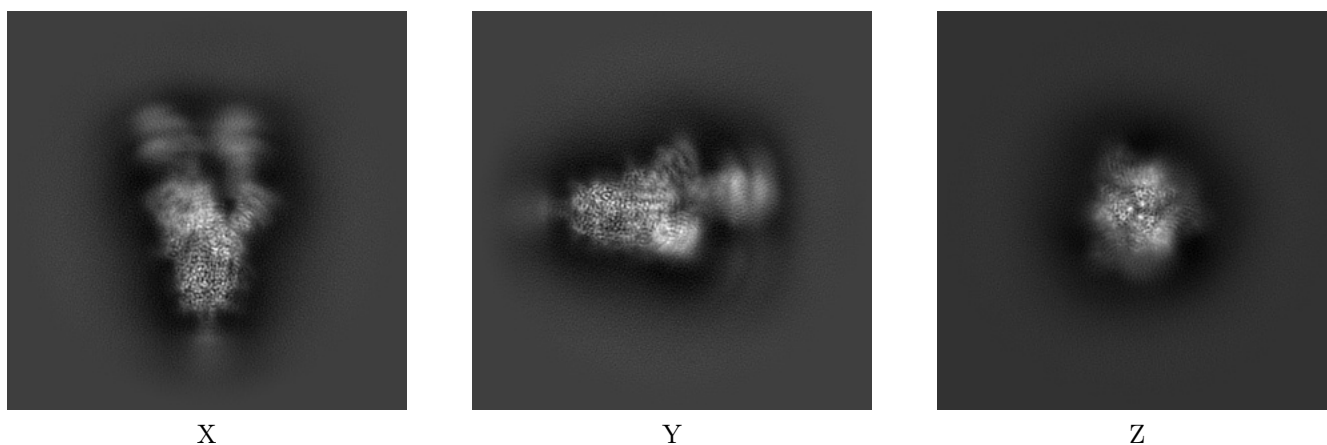
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25760. 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](#)

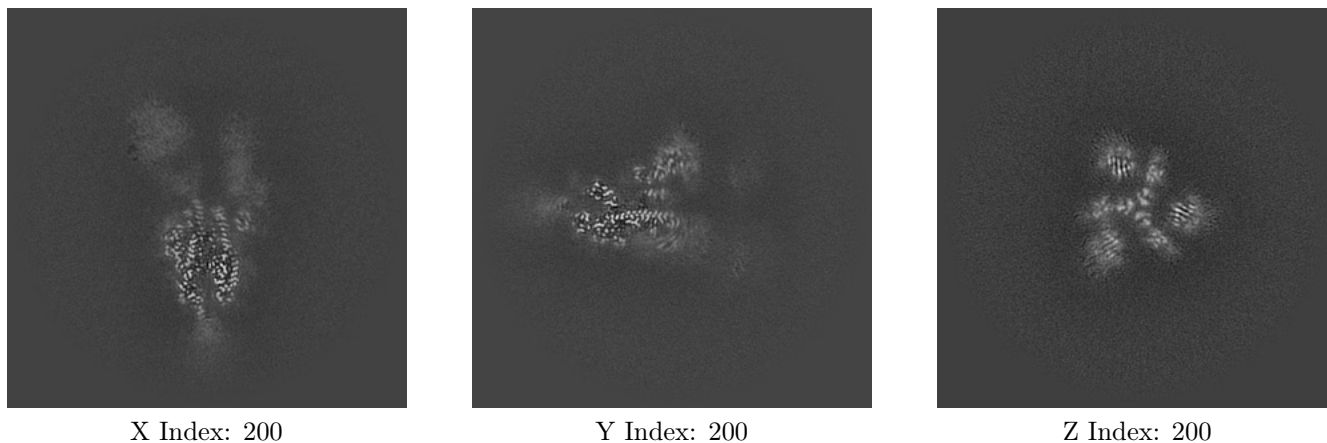
6.1.1 Primary map



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

6.2 Central slices [i](#)

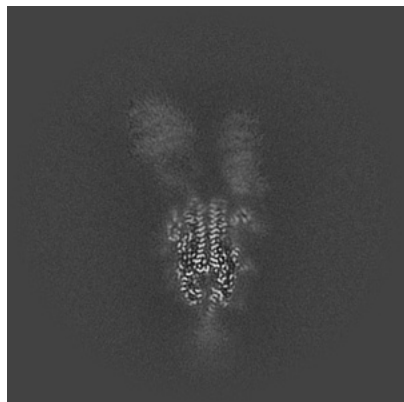
6.2.1 Primary map



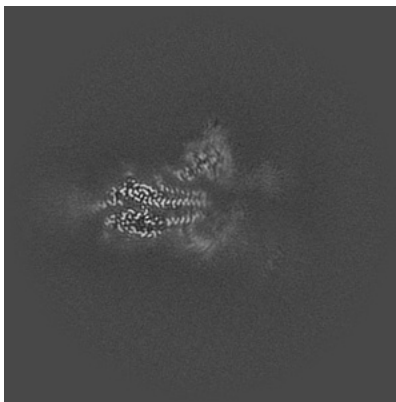
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

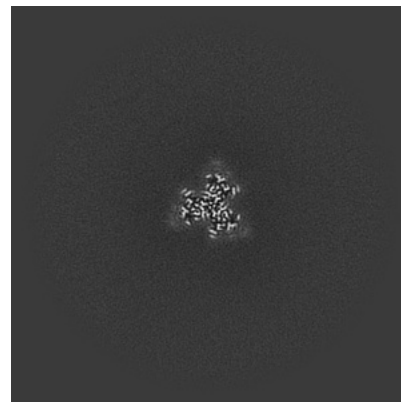
6.3.1 Primary map



X Index: 205



Y Index: 193

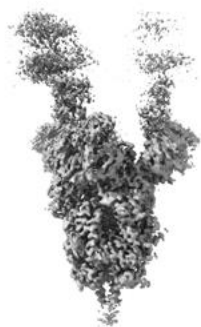


Z Index: 141

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

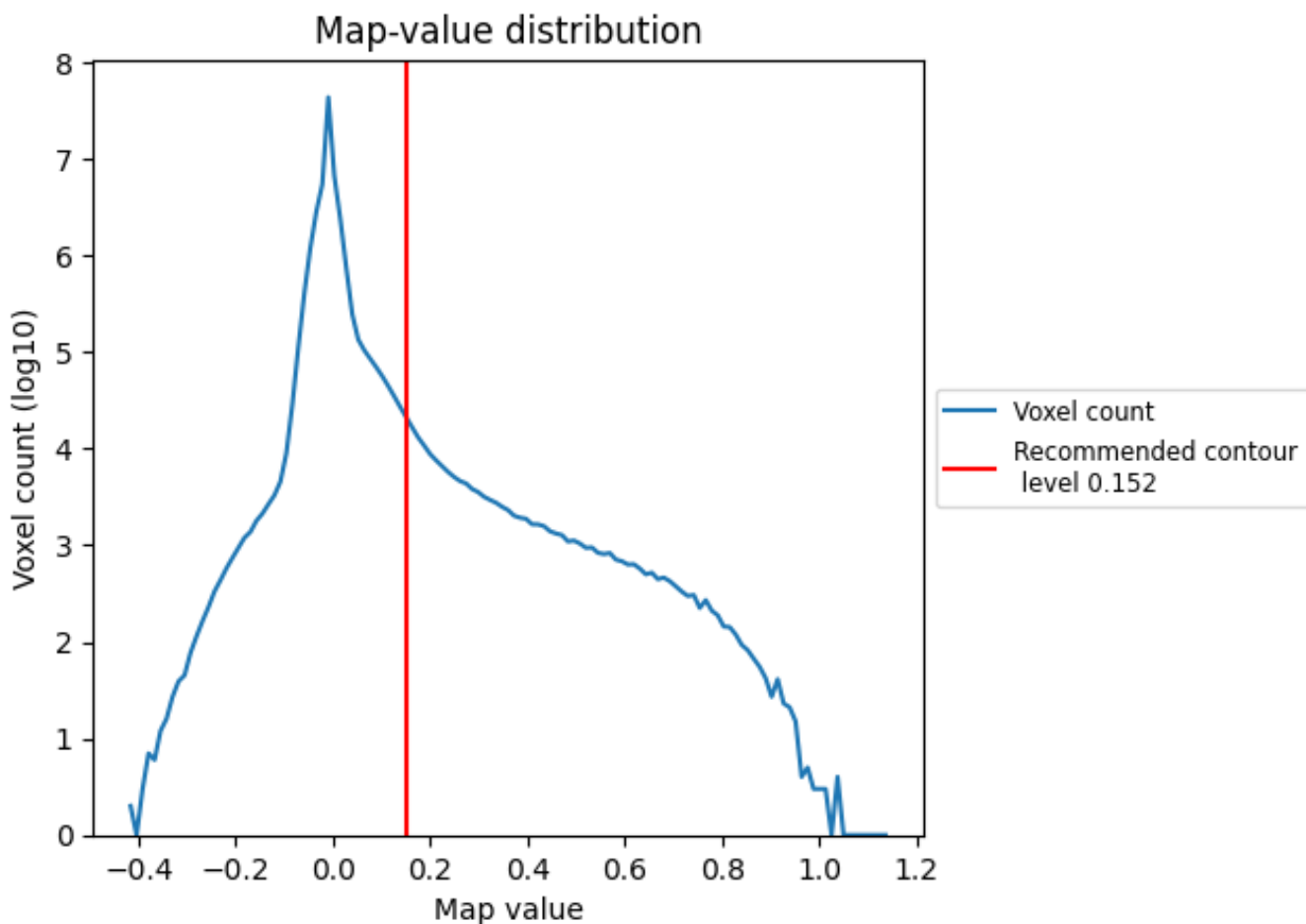
6.5 Mask visualisation

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

7 Map analysis [i](#)

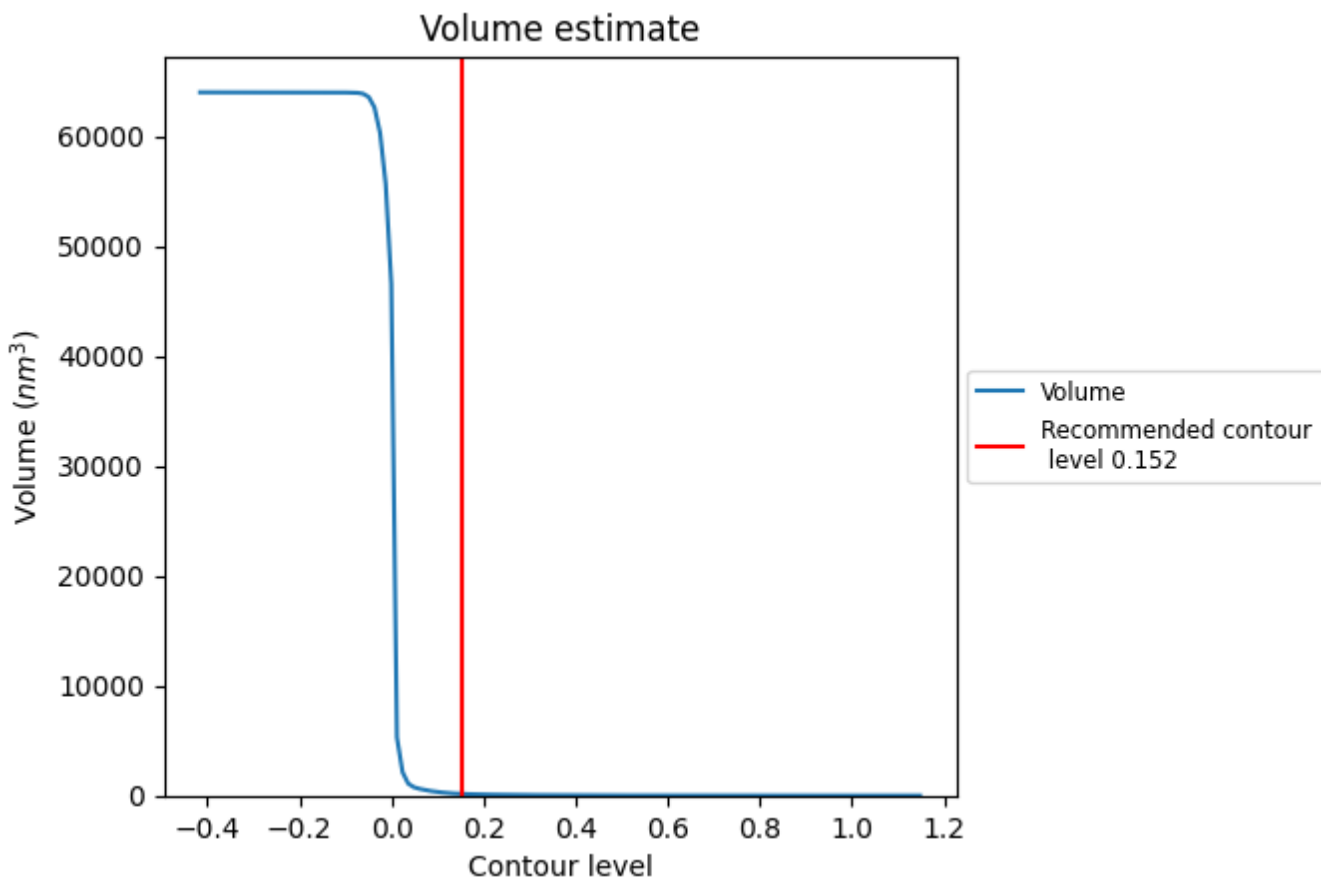
This section contains the results of statistical analysis of the map.

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.

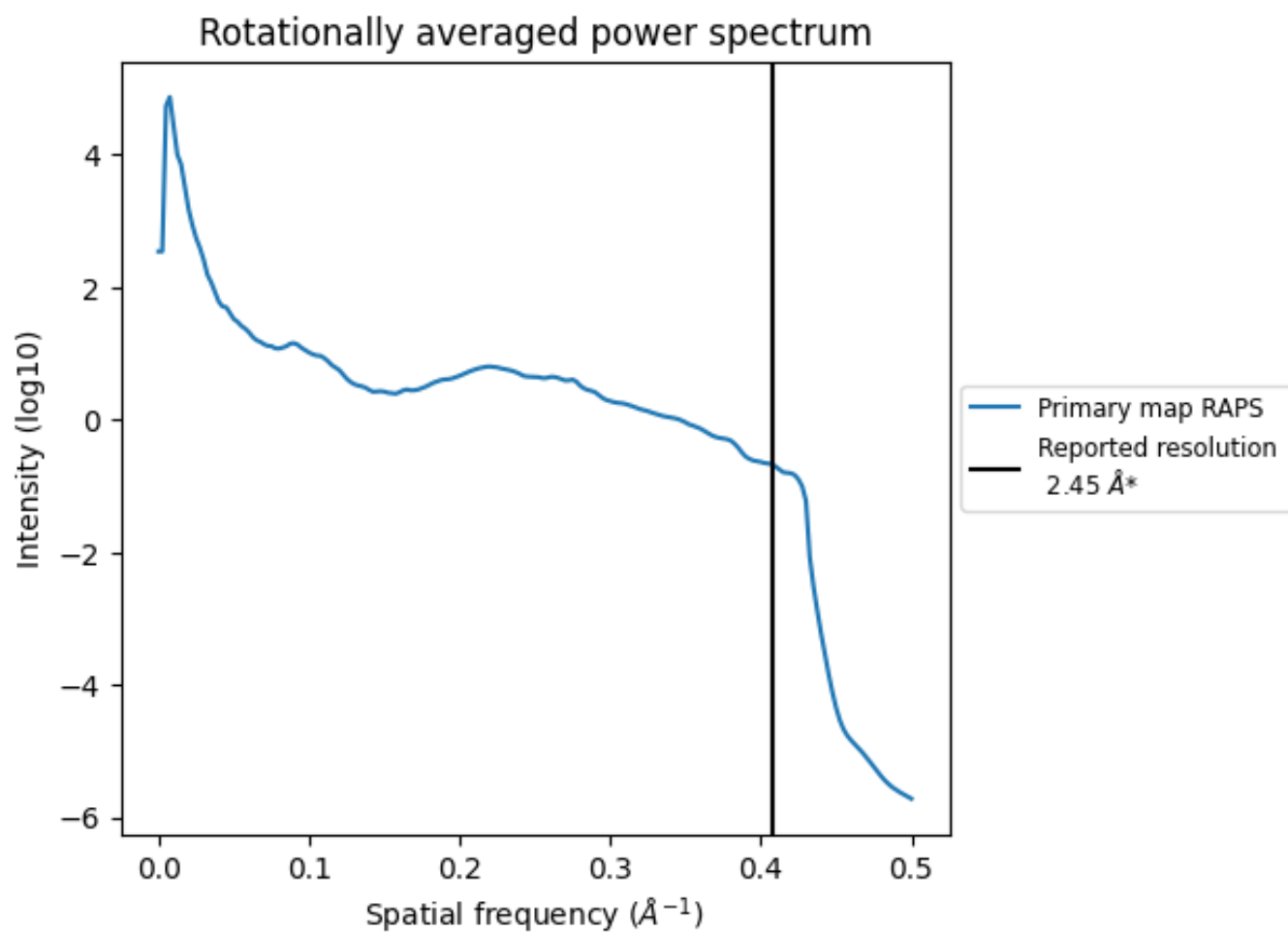
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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

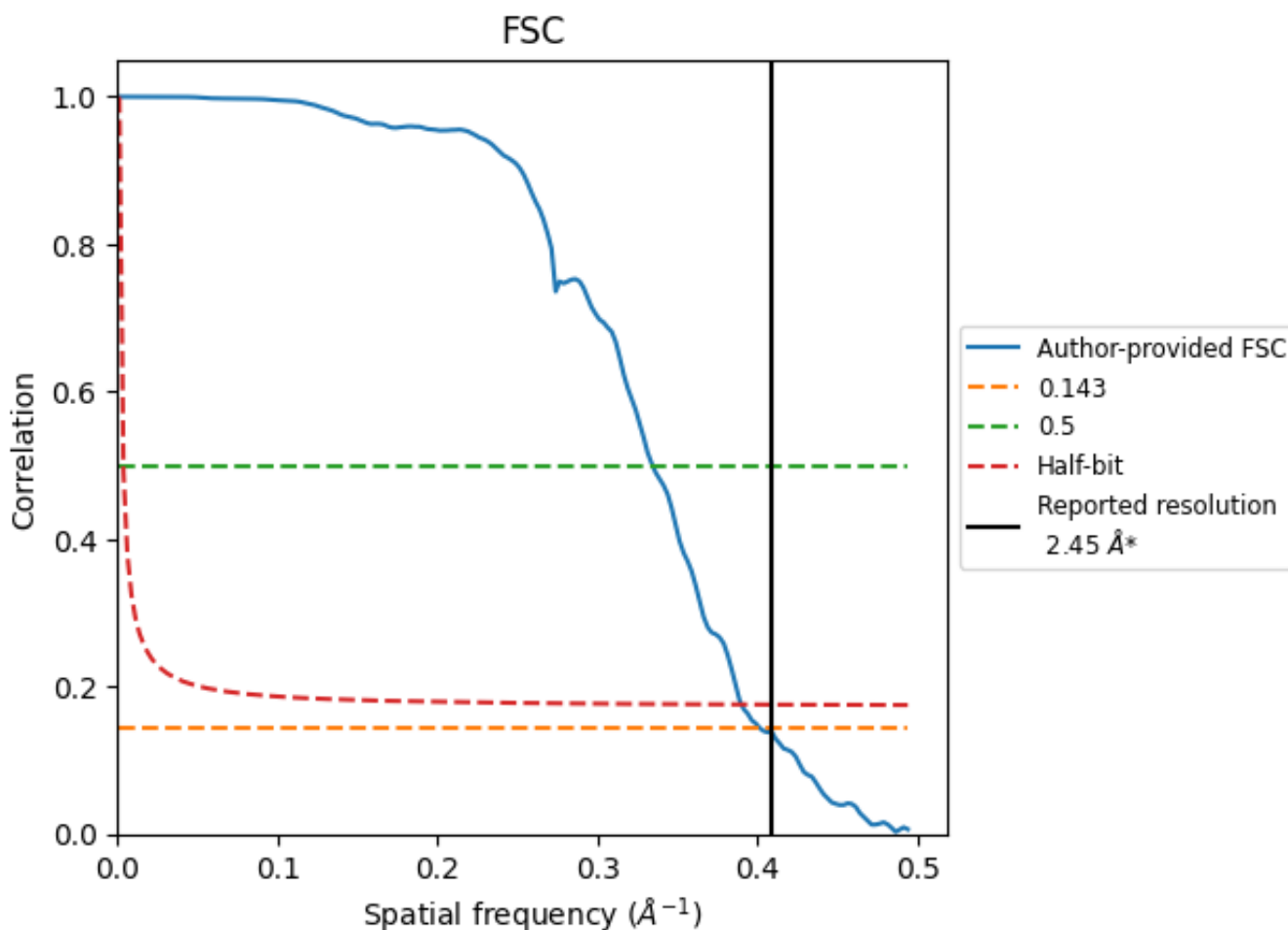


*Reported resolution corresponds to spatial frequency of 0.408 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.408 Å⁻¹

8.2 Resolution estimates [i](#)

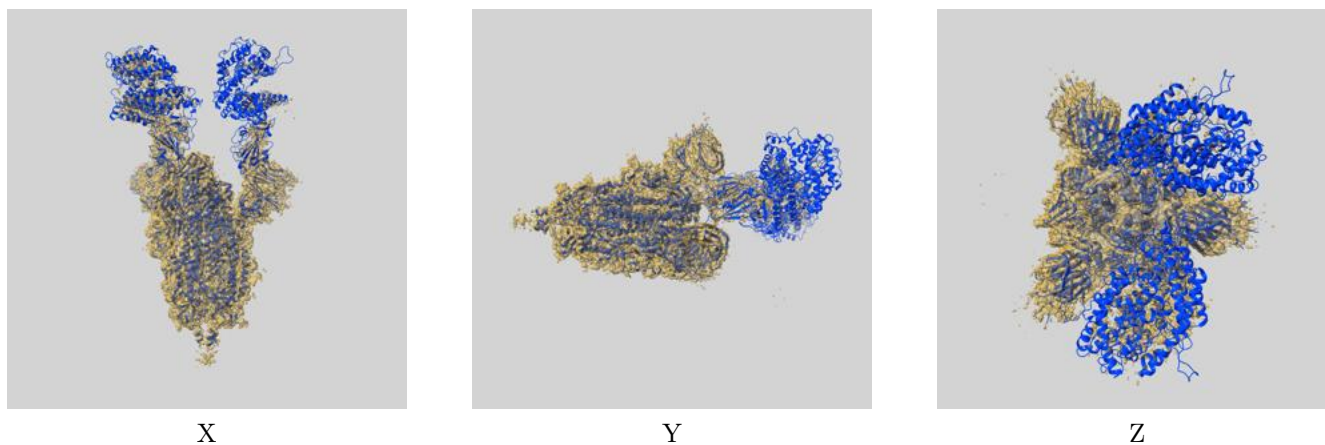
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.49	2.99	2.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

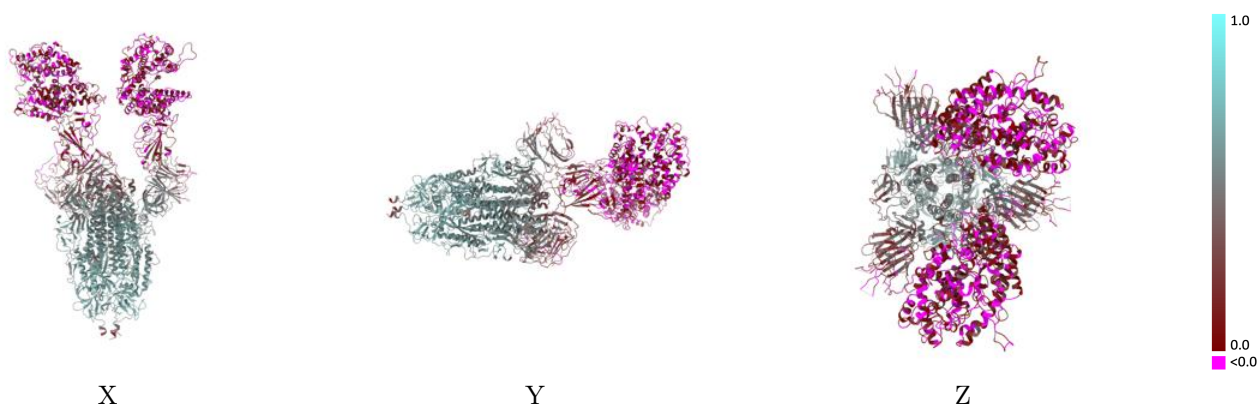
This section contains information regarding the fit between EMDB map EMD-25760 and PDB model 7T9K. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



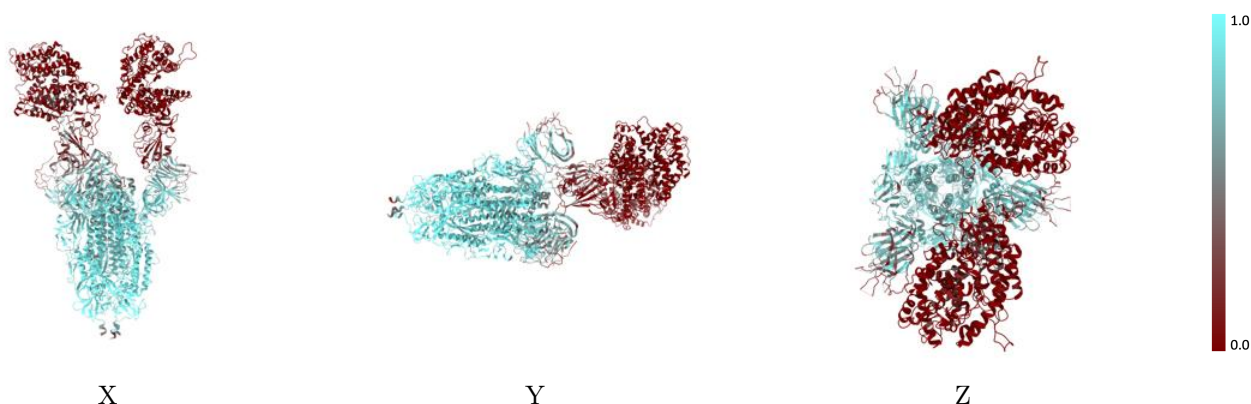
The images above show the 3D surface view of the map at the recommended contour level 0.152 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



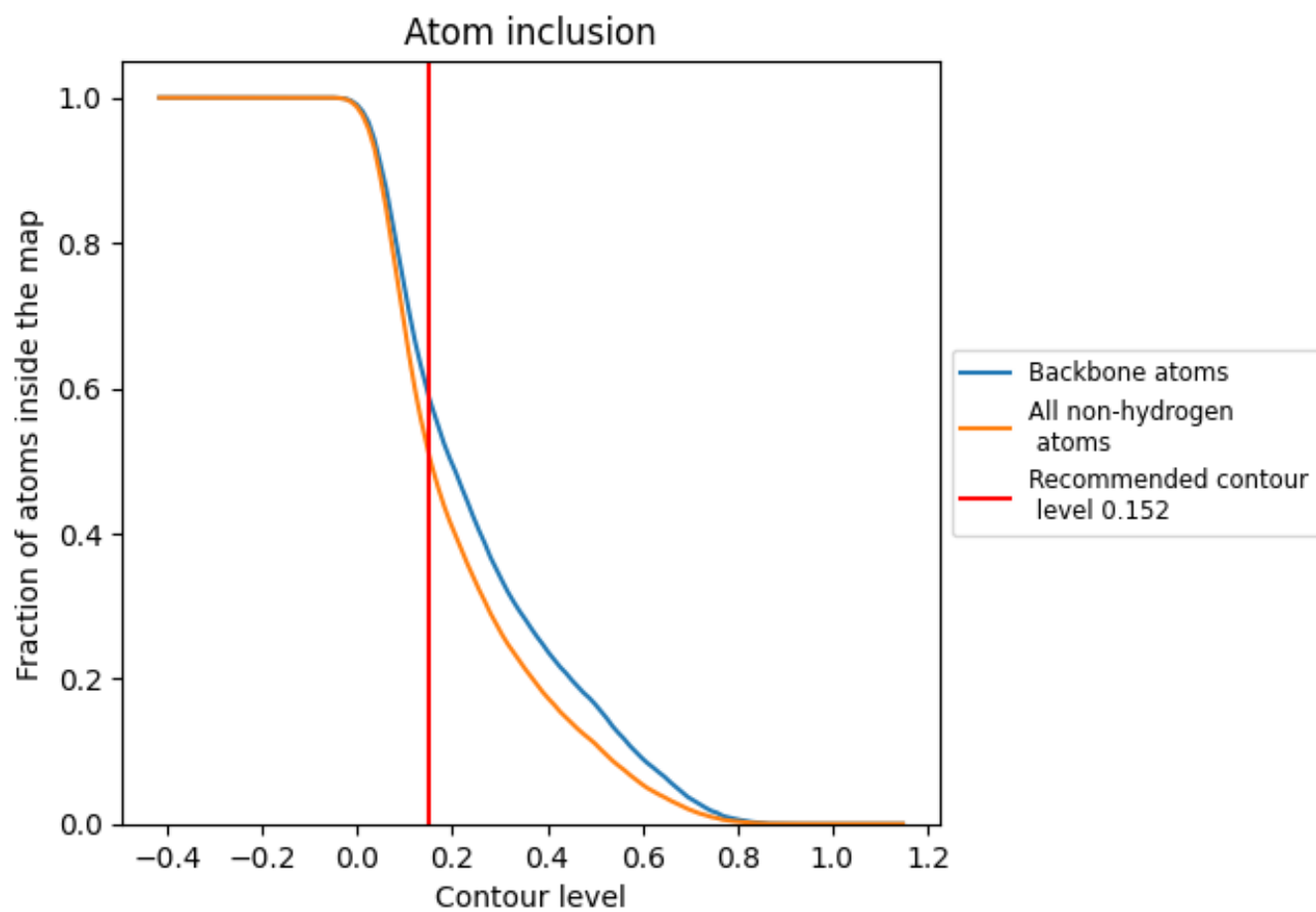
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.152).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 51% 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 (0.152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5056	 0.3230
A	 0.6597	 0.4060
B	 0.6793	 0.4280
C	 0.8198	 0.4970
D	 0.0420	 0.0530
E	 0.0062	 0.0410
F	 0.0357	 0.0850
G	 0.7500	 0.5070
H	 0.7500	 0.4640
I	 0.3571	 0.5200
J	 0.5357	 0.3910
K	 0.4286	 0.3910
L	 0.0357	 0.0900
M	 0.7143	 0.4950
N	 0.7857	 0.5270
O	 0.3571	 0.4480
P	 0.5000	 0.4530
Q	 0.4643	 0.3650
R	 0.0357	 0.0650
S	 0.7143	 0.5110
T	 0.7143	 0.4870
U	 0.3571	 0.4580
V	 0.5357	 0.4350
W	 0.5000	 0.4240

