



## Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 02:28 am BST

PDB ID : 7ND4 / pdb\_00007nd4  
EMDB ID : EMD-12275  
Title : EM structure of SARS-CoV-2 Spike glycoprotein in complex with COVOX-88 Fab  
Authors : Duyvesteyn, H.M.E.; Zhao, Y.; Ren, J.; Stuart, D.  
Deposited on : 2021-01-30  
Resolution : 3.60 Å(reported)  
Based on initial model : 6Z97

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

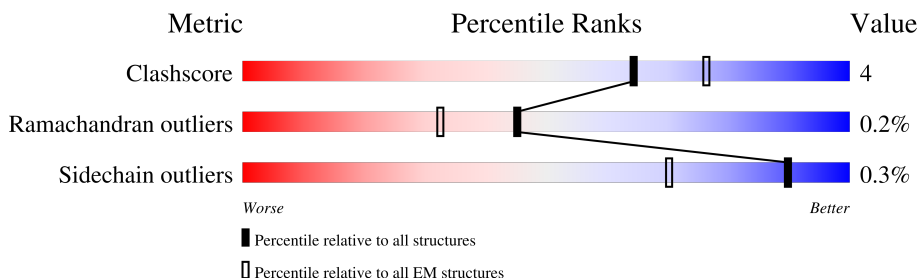
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 Å.

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



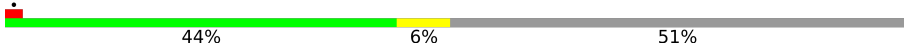
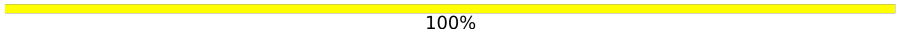
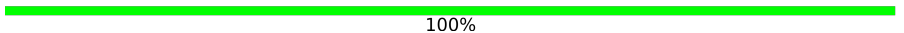
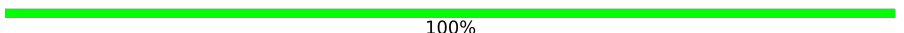

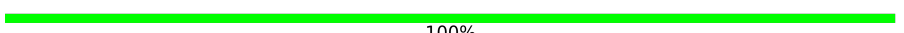
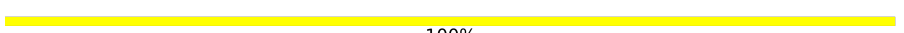








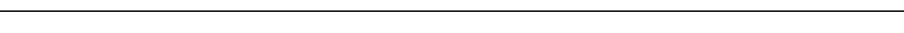
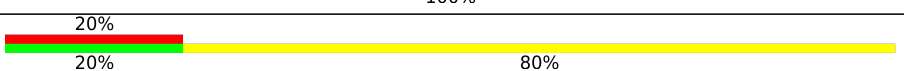
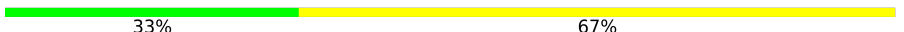

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1288	
1	B	1288	
1	C	1288	
2	D	245	
2	F	245	
2	H	245	
3	E	229	
3	G	229	

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Mol	Chain	Length	Quality of chain
3	L	229	
4	I	2	
4	J	2	
4	K	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
5	Y	5	
6	Z	3	
6	a	3	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		
1	B	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		
1	C	1002	Total	C	N	O	S	0	0
			7823	4996	1300	1492	35		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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	GLY	-	expression tag	UNP P0DTC2
A	1259	SER	-	expression tag	UNP P0DTC2
A	1260	ALA	-	expression tag	UNP P0DTC2
A	1261	TRP	-	expression tag	UNP P0DTC2
A	1262	SER	-	expression tag	UNP P0DTC2
A	1263	HIS	-	expression tag	UNP P0DTC2
A	1264	PRO	-	expression tag	UNP P0DTC2
A	1265	GLN	-	expression tag	UNP P0DTC2
A	1266	PHE	-	expression tag	UNP P0DTC2
A	1267	GLU	-	expression tag	UNP P0DTC2
A	1268	LYS	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	SER	-	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	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	GLY	-	expression tag	UNP P0DTC2
B	1259	SER	-	expression tag	UNP P0DTC2
B	1260	ALA	-	expression tag	UNP P0DTC2
B	1261	TRP	-	expression tag	UNP P0DTC2
B	1262	SER	-	expression tag	UNP P0DTC2
B	1263	HIS	-	expression tag	UNP P0DTC2
B	1264	PRO	-	expression tag	UNP P0DTC2
B	1265	GLN	-	expression tag	UNP P0DTC2
B	1266	PHE	-	expression tag	UNP P0DTC2
B	1267	GLU	-	expression tag	UNP P0DTC2
B	1268	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	SER	-	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	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	GLY	-	expression tag	UNP P0DTC2
C	1259	SER	-	expression tag	UNP P0DTC2
C	1260	ALA	-	expression tag	UNP P0DTC2
C	1261	TRP	-	expression tag	UNP P0DTC2
C	1262	SER	-	expression tag	UNP P0DTC2
C	1263	HIS	-	expression tag	UNP P0DTC2
C	1264	PRO	-	expression tag	UNP P0DTC2
C	1265	GLN	-	expression tag	UNP P0DTC2
C	1266	PHE	-	expression tag	UNP P0DTC2
C	1267	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1268	LYS	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	SER	-	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

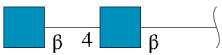
- Molecule 2 is a protein called COVOX-88 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	128	Total	C	N	O	S	0	0
			968	605	167	191	5		
2	D	128	Total	C	N	O	S	0	0
			968	605	167	191	5		
2	F	128	Total	C	N	O	S	0	0
			968	605	167	191	5		

- Molecule 3 is a protein called COVOX-88 Fab light chain.

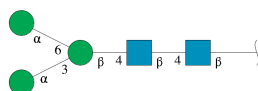
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	113	Total	C	N	O	S	0	0
			832	519	139	172	2		
3	E	113	Total	C	N	O	S	0	0
			832	519	139	172	2		
3	G	113	Total	C	N	O	S	0	0
			832	519	139	172	2		

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



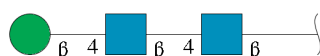
Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16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

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



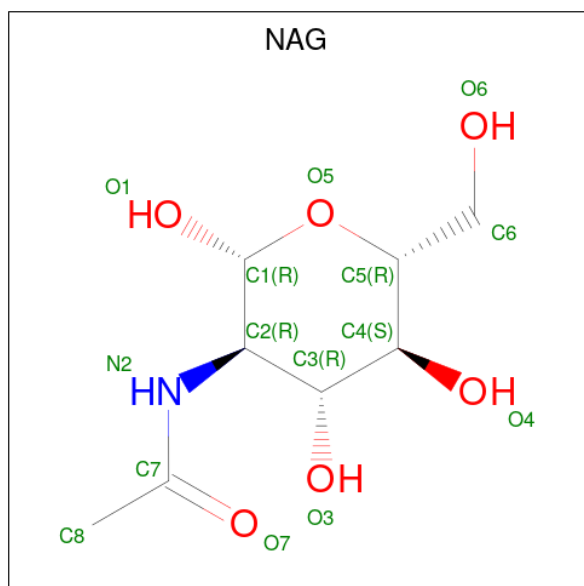
Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	5	Total	C	N	O	0	0
			61	34	2	25		

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

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

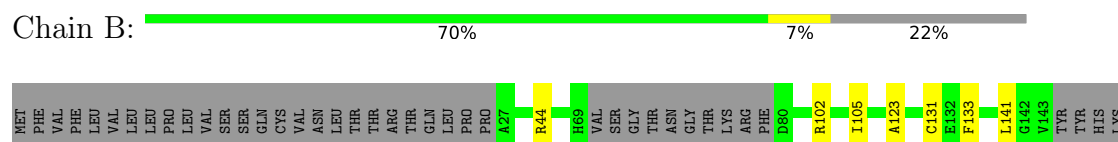
### 3 Residue-property plots [i](#)

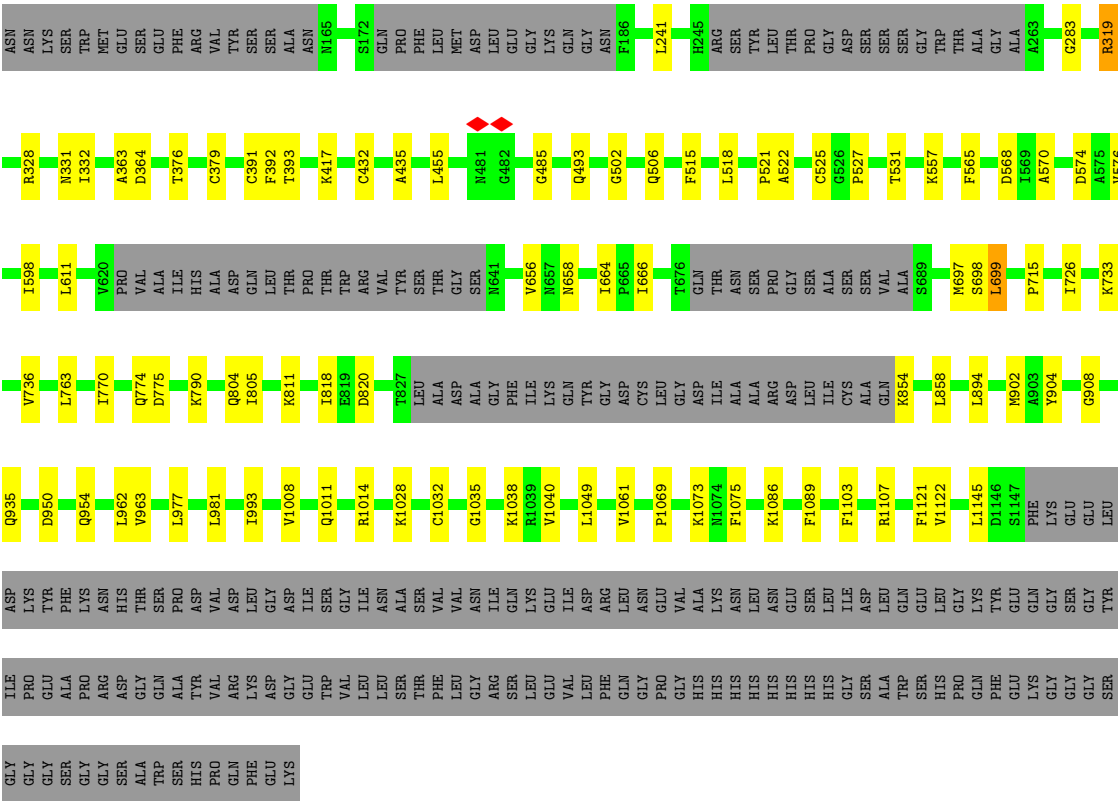
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Spike glycoprotein

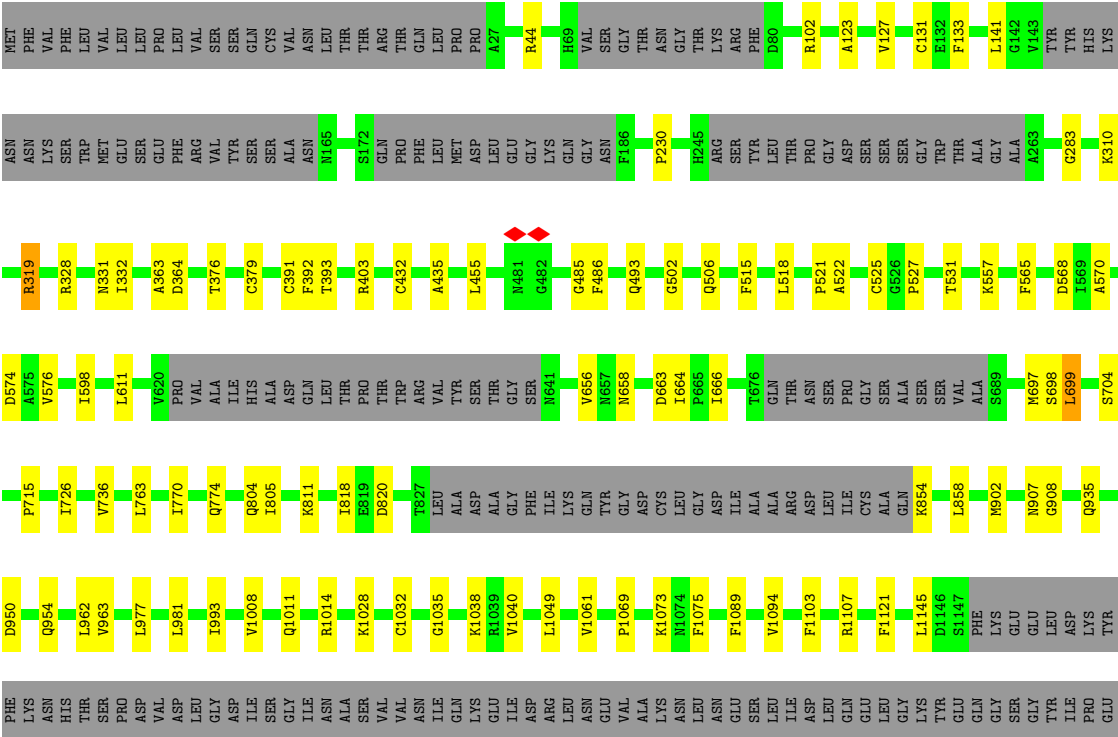


#### • Molecule 1: Spike glycoprotein





● Molecule 1: Spike glycoprotein





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

- Molecule 2: COVOX-88 Fab heavy chain

Chain H: 40% 12% 48%

LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	PRO	ALA	VAL	LEU	GLN	SER	SER	GLY	LEU	TYR	LEU	SER	LEU	SER	VAL	VAL	THR	VAL	PRO	SER	SER	SER	LEU	GLY	THR	GLN	TYR	ILE	CYS	ASN	VAL	ASN	HIS	CYS	LYS	PRO	SER	ASN	VAL	LYS	VAL	GLU	THR	VAL	PRO	LYS	SER	CYS	ASP	LYS
H100	C101	S102	G103		Y111	Y112	G113	M114	D115		Q119		T124		A128	SER	THR	LYS	GLY	PRO	SER	SER	VAL	PHE	PRO	LEU	ALA	PRO	SER	SER	SER	LYS	THR	GLY	GLY	THR	CYS	ALA	ALA	LEU	GLY	CYS	LEU	VAL	LYS	ASP	TYR	PHE	PRO	GLU	VAL	THR	VAL	SER	TRP	ASN	GLY	ALA
ILE	LEU	PHE	LEU	VAL	ALA	THR	ALA	THR	GLY	VAL	HIS	SER	Q1	L4	Q16	T17	C22	G27	S28	N35	W36	W38	T37	I39	R40	Q41	L47	I50	I53	F54	N55	S56	G57	T70	V73	S76	K77	L80	S81	L82	K83	A89	T92	R99														

- Molecule 2: COVOX-88 Fab heavy chain

Chain D: 41% 11% 48%

THR	SER	GLY	VAL	HIS	THR	PHE	PRO	PRO	ALA	VAL	LEU	GLN	SER	SER	GLY	LEU	TYR	SER	LEU	SER	SER	VAL	VAL	THR	VAL	PRO	ALA	PRO	SER	SER	SER	LEU	GLY	THR	GLN	THR	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	ASN	VAL	LYS	THR	VAL	GLU	THR	PRO	PRO	LYS	LYS	SER	CYS	ASP	LYS
C101	S102	Y110	Y111	Y112	G113	M114	D115	Q119	T124	A128	SER	THR	LYS	GLY	PRO	SER	VAL	PHE	PRO	LEU	LEU	ALA	PRO	SER	SER	SER	SER	SER	SER	SER	GLY	THR	SER	GLY	THR	GLY	THR	GLY	CYS	ALA	ALA	LEU	GLY	CYS	VAL	VAL	VAL	VAL	THR	VAL	VAL	VAL	THR	TRP	ASN	GLY	ALA	LEU			
ILE	LEU	PHE	LEU	VAL	ALA	THR	ALA	THR	GLY	VAL	HIS	SER	Q1	S15	Q16	T17	N35	W36	T37	W38	I39	R40	Q41	P42	A43	G44	L47	I53	F54	N55	S56	Y61	K66	T70	V73	S76	K77	L80	S81	K83	A89	A90	D91	T92	R99	H100															

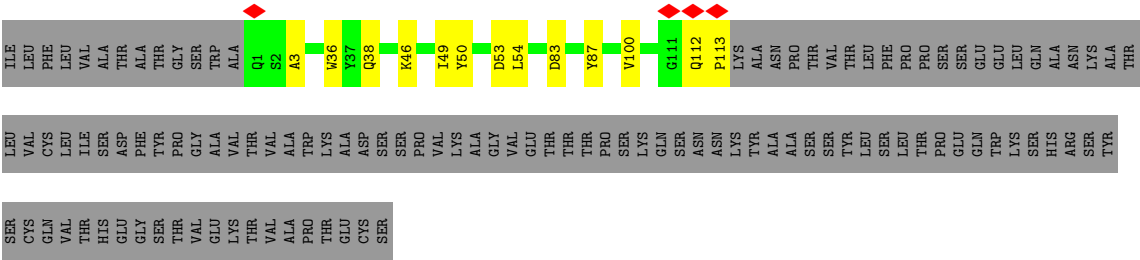
- Molecule 2: COVOX-88 Fab heavy chain

Chain F: 40% 11% 48%

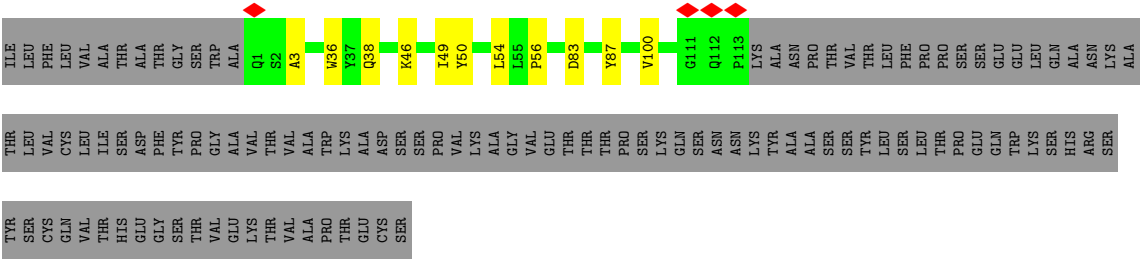
ILE	LEU	PHE	LEU	VAL	ALA	THR	ALA	THR	VAL	SER	THR	GLY	VAL	HIS	SER	Q1	L11	S15	Q16	T17	G27	N35	W36	T37	W38	I39	R40	Q41	P42	A43	L47	I50	I53	Y54	N55	S56	G57	T70	V73	S76	K77	L80	S81	L82	K83	A89	T92	R99				
H100	G101	S102	T106	Y112	G113	D115	Q119	T124	A128	SER	THR	LYS	GLY	PRO	SER	VAL	PHE	PRO	ALA	PRO	SER	SER	LYS	SER	THR	SER	GLY	THR	GLN	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	ASP	VAL	LYS	THR	VAL	GLU	THR	PRO	LYS	SER	CYS	ASP	ALA
LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	PRO	ALA	VAL	GLN	SER	SER	GLY	TYR	LEU	SER	LEU	SER	VAL	VAL	THR	VAL	PRO	SER	GLY	THR	GLN	TYR	ILE	CYS	ASN	VAL	ASN	HIS	LYS	PRO	SER	ASP	VAL	LYS	THR	VAL	GLU	THR	PRO	LYS	SER	CYS	ASP	LYS

- Molecule 3: COVOX-88 Fab light chain

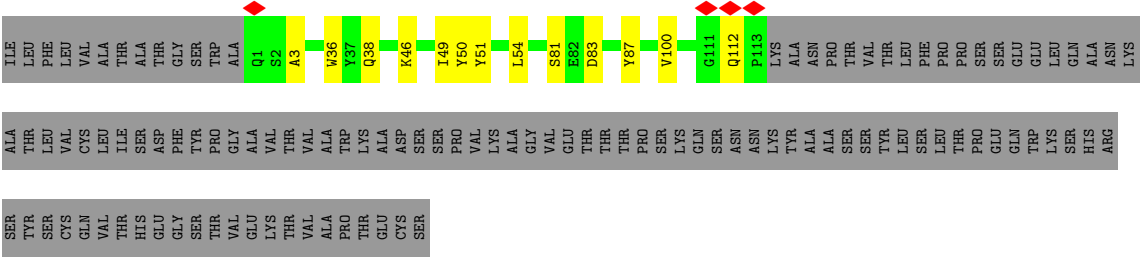
Chain L: 44% 6% 51%



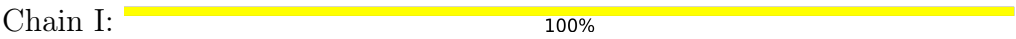
• Molecule 3: COVOX-88 Fab light chain



• Molecule 3: COVOX-88 Fab light chain



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



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



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

Chain K:  100%

MAG1  
MAG2

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

Chain M:  50% 50%

MAG1  
MAG2

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

Chain N:  100%

MAG1  
MAG2

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

Chain O:  100%

MAG1  
MAG2

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

Chain P:  100%

MAG1  
MAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain R:  50% 50%



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

Chain S:  100%



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

Chain T:  100%



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

Chain U:  100%



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

Chain V:  100%



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

Chain W:  50% 50%

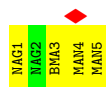


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%



- Molecule 5:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	56686	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; cryoSPARC implementation.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	57.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.101	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.028	Depositor
Map size ( $\text{\AA}$ )	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, 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	0.12	0/7999	0.35	0/10885
1	B	0.12	0/7999	0.35	0/10885
1	C	0.12	0/7999	0.35	0/10885
2	D	0.07	0/990	0.26	0/1348
2	F	0.07	0/990	0.26	0/1348
2	H	0.07	0/990	0.26	0/1348
3	E	0.07	0/850	0.26	0/1159
3	G	0.07	0/850	0.26	0/1159
3	L	0.07	0/850	0.26	0/1159
All	All	0.11	0/29517	0.33	0/40176

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	7823	0	7625	59	0
1	B	7823	0	7625	62	0
1	C	7823	0	7625	65	0
2	D	968	0	944	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	968	0	944	16	0
2	H	968	0	944	17	0
3	E	832	0	795	6	0
3	G	832	0	795	7	0
3	L	832	0	795	7	0
4	I	28	0	25	1	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	1	0
4	N	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
4	W	28	0	25	1	0
4	X	28	0	25	0	0
5	Y	61	0	52	3	0
6	Z	39	0	34	1	0
6	a	39	0	34	1	0
7	A	140	0	130	1	0
7	B	140	0	130	1	0
7	C	140	0	130	2	0
All	All	29848	0	28977	230	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.

All (230) 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:485:GLY:HA2	2:F:105:THR:HG23	1.75	0.67
1:B:1103:PHE:HZ	4:R:1:NAG:H62	1.61	0.65
1:A:1103:PHE:HZ	4:M:1:NAG:H62	1.61	0.65
1:C:1103:PHE:HZ	4:W:1:NAG:H62	1.61	0.64
3:L:3:ALA:HB3	3:L:100:VAL:HG11	1.79	0.63
3:G:3:ALA:HB3	3:G:100:VAL:HG11	1.79	0.63
3:E:3:ALA:HB3	3:E:100:VAL:HG11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:VAL:HG22	1:A:858:LEU:HG	1.80	0.63
1:B:391:CYS:HA	1:B:525:CYS:HA	1.81	0.63
1:C:391:CYS:HA	1:C:525:CYS:HA	1.81	0.63
1:B:736:VAL:HG22	1:B:858:LEU:HG	1.81	0.62
1:A:391:CYS:HA	1:A:525:CYS:HA	1.81	0.62
1:C:736:VAL:HG22	1:C:858:LEU:HG	1.80	0.62
1:A:1040:VAL:HG21	1:B:1035:GLY:HA3	1.81	0.62
1:B:557:LYS:NZ	1:B:574:ASP:OD2	2.34	0.61
1:C:557:LYS:NZ	1:C:574:ASP:OD2	2.34	0.61
1:A:854:LYS:NZ	1:C:568:ASP:OD2	2.33	0.61
1:A:977:LEU:HD11	1:A:993:ILE:HG12	1.84	0.60
1:A:557:LYS:NZ	1:A:574:ASP:OD2	2.34	0.60
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.66	0.60
1:C:319:ARG:HG2	1:C:319:ARG:HH11	1.66	0.60
1:B:319:ARG:HG2	1:B:319:ARG:HH11	1.66	0.59
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.35	0.59
1:C:977:LEU:HD11	1:C:993:ILE:HG12	1.84	0.59
1:B:521:PRO:HB2	1:C:230:PRO:HB2	1.85	0.59
1:A:568:ASP:OD2	1:B:854:LYS:NZ	2.34	0.59
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.85	0.59
1:B:977:LEU:HD11	1:B:993:ILE:HG12	1.83	0.59
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.85	0.59
3:L:36:TRP:HB2	3:L:49:ILE:HB	1.85	0.59
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.35	0.58
3:G:36:TRP:HB2	3:G:49:ILE:HB	1.85	0.58
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.85	0.58
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.35	0.58
3:E:36:TRP:HB2	3:E:49:ILE:HB	1.85	0.58
2:F:70:THR:HB	2:F:83:LYS:HB2	1.87	0.57
2:F:53:ILE:HD13	2:F:73:VAL:HG23	1.86	0.57
2:D:53:ILE:HD13	2:D:73:VAL:HG23	1.86	0.57
2:H:70:THR:HB	2:H:83:LYS:HB2	1.87	0.57
2:D:70:THR:HB	2:D:83:LYS:HB2	1.87	0.57
2:H:53:ILE:HD13	2:H:73:VAL:HG23	1.86	0.56
1:C:1028:LYS:O	1:C:1032:CYS:CB	2.54	0.56
1:A:1028:LYS:O	1:A:1032:CYS:CB	2.54	0.56
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.88	0.56
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.88	0.56
1:C:364:ASP:HA	1:C:527:PRO:HG3	1.88	0.56
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.88	0.55
2:D:41:GLN:HB2	2:D:47:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASP:HA	1:B:527:PRO:HG3	1.88	0.55
1:B:1028:LYS:O	1:B:1032:CYS:CB	2.54	0.55
2:F:41:GLN:HB2	2:F:47:LEU:HD23	1.88	0.54
1:A:364:ASP:HA	1:A:527:PRO:HG3	1.88	0.54
2:H:99:ARG:HE	2:H:115:ASP:HB3	1.73	0.54
2:H:41:GLN:HB2	2:H:47:LEU:HD23	1.88	0.54
2:F:99:ARG:HE	2:F:115:ASP:HB3	1.73	0.54
1:B:568:ASP:OD2	1:C:854:LYS:NZ	2.40	0.53
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.91	0.53
1:B:379:CYS:HA	1:B:432:CYS:HA	1.91	0.53
2:D:100:HIS:NE2	2:D:112:TYR:O	2.38	0.53
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.91	0.53
1:C:379:CYS:HA	1:C:432:CYS:HA	1.91	0.53
2:D:99:ARG:HE	2:D:115:ASP:HB3	1.73	0.52
1:A:1028:LYS:O	1:A:1032:CYS:HB3	2.10	0.52
1:A:379:CYS:HA	1:A:432:CYS:HA	1.90	0.52
3:L:83:ASP:O	3:L:87:TYR:OH	2.28	0.52
1:C:1028:LYS:O	1:C:1032:CYS:HB3	2.10	0.52
1:B:1028:LYS:O	1:B:1032:CYS:HB3	2.10	0.51
2:F:35:ASN:HB2	2:F:100:HIS:HB3	1.93	0.51
1:C:332:ILE:HB	7:C:1304:NAG:H82	1.92	0.51
3:G:83:ASP:O	3:G:87:TYR:OH	2.28	0.51
1:B:332:ILE:HB	7:B:1304:NAG:H82	1.92	0.51
1:B:1107:ARG:HH22	1:C:907:ASN:HD22	1.57	0.51
1:A:328:ARG:NH2	1:A:531:THR:O	2.40	0.50
2:H:35:ASN:HB2	2:H:100:HIS:HB3	1.93	0.50
2:F:102:SER:HB3	6:a:1:NAG:HN2	1.77	0.50
1:A:332:ILE:HB	7:A:1304:NAG:H82	1.92	0.50
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.45	0.50
2:D:102:SER:HB3	6:Z:1:NAG:HN2	1.77	0.50
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.45	0.50
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.45	0.50
3:L:38:GLN:O	3:L:46:LYS:N	2.37	0.50
2:H:102:SER:HB3	5:Y:1:NAG:HN2	1.76	0.49
3:E:38:GLN:O	3:E:46:LYS:N	2.37	0.49
1:C:950:ASP:OD2	1:C:954:GLN:NE2	2.46	0.49
1:A:963:VAL:HG11	1:C:570:ALA:HB1	1.95	0.49
2:D:35:ASN:HB2	2:D:100:HIS:HB3	1.93	0.48
3:G:38:GLN:O	3:G:46:LYS:N	2.37	0.48
1:A:805:ILE:HG22	1:A:818:ILE:HD12	1.96	0.48
1:C:805:ILE:HG22	1:C:818:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LYS:NZ	3:G:51:TYR:OH	2.28	0.48
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.47	0.48
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.47	0.47
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.47	0.47
1:C:486:PHE:HZ	5:Y:1:NAG:H5	1.78	0.47
1:B:715:PRO:HB3	1:B:1069:PRO:HB3	1.97	0.47
1:C:715:PRO:HB3	1:C:1069:PRO:HB3	1.97	0.47
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.96	0.47
1:A:790:LYS:HE2	1:C:704:SER:HB3	1.97	0.47
1:B:805:ILE:HG22	1:B:818:ILE:HD12	1.96	0.47
3:E:83:ASP:O	3:E:87:TYR:OH	2.28	0.47
1:A:715:PRO:HB3	1:A:1069:PRO:HB3	1.97	0.47
1:B:950:ASP:OD2	1:B:954:GLN:NE2	2.46	0.47
1:C:486:PHE:CZ	5:Y:1:NAG:H5	2.49	0.47
2:F:39:ILE:HD11	2:F:114:MET:HE1	1.97	0.47
2:F:100:HIS:NE2	2:F:112:TYR:O	2.38	0.46
1:A:950:ASP:OD2	1:A:954:GLN:NE2	2.46	0.46
1:A:565:PHE:HD1	1:A:576:VAL:HG12	1.81	0.46
1:B:565:PHE:HD1	1:B:576:VAL:HG12	1.81	0.46
1:C:310:LYS:NZ	1:C:663:ASP:OD1	2.45	0.46
2:H:39:ILE:HD11	2:H:114:MET:HE1	1.97	0.46
2:F:38:TRP:CE2	2:F:82:LEU:HB2	2.51	0.46
1:A:393:THR:HA	1:A:522:ALA:HA	1.98	0.46
1:C:328:ARG:NH2	1:C:531:THR:O	2.40	0.46
2:H:100:HIS:NE2	2:H:112:TYR:O	2.38	0.46
2:D:38:TRP:CE2	2:D:82:LEU:HB2	2.51	0.45
1:C:565:PHE:HD1	1:C:576:VAL:HG12	1.81	0.45
2:H:38:TRP:CE2	2:H:82:LEU:HB2	2.51	0.45
1:A:858:LEU:HD21	1:A:962:LEU:HD23	1.98	0.45
1:A:907:ASN:HD22	1:C:1107:ARG:HH22	1.63	0.45
1:B:858:LEU:HD21	1:B:962:LEU:HD23	1.98	0.45
1:B:393:THR:HA	1:B:522:ALA:HA	1.98	0.45
1:B:570:ALA:HB1	1:C:963:VAL:HG11	1.99	0.45
1:C:363:ALA:O	1:C:527:PRO:HD3	2.16	0.45
1:A:363:ALA:O	1:A:527:PRO:HD3	2.16	0.45
1:B:363:ALA:O	1:B:527:PRO:HD3	2.16	0.45
1:A:1073:LYS:HB2	1:A:1075:PHE:CE2	2.53	0.44
1:B:328:ARG:NH2	1:B:531:THR:O	2.40	0.44
1:C:393:THR:HA	1:C:522:ALA:HA	1.98	0.44
1:C:393:THR:HG21	1:C:518:LEU:H	1.82	0.44
1:C:485:GLY:O	2:H:103:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:ILE:HD11	2:D:114:MET:HE1	1.98	0.44
1:B:902:MET:HE1	1:B:1049:LEU:HD13	1.99	0.44
1:B:1073:LYS:HB2	1:B:1075:PHE:CE2	2.53	0.44
1:C:902:MET:HE1	1:C:1049:LEU:HD13	1.99	0.44
1:B:131:CYS:HB2	1:B:133:PHE:CE2	2.52	0.44
1:B:611:LEU:HD22	1:B:666:ILE:HG23	1.99	0.44
1:C:1073:LYS:HB2	1:C:1075:PHE:CE2	2.53	0.44
1:C:131:CYS:HB2	1:C:133:PHE:CE2	2.52	0.44
1:C:858:LEU:HD21	1:C:962:LEU:HD23	1.98	0.44
1:A:131:CYS:HB2	1:A:133:PHE:CE2	2.52	0.43
1:A:393:THR:HG21	1:A:518:LEU:H	1.82	0.43
1:A:502:GLY:O	1:A:506:GLN:HG3	2.18	0.43
1:B:44:ARG:O	1:B:283:GLY:HA2	2.18	0.43
1:B:455:LEU:HD22	1:B:493:GLN:HG3	2.00	0.43
1:A:908:GLY:O	1:A:1038:LYS:HE3	2.18	0.43
1:B:393:THR:HG21	1:B:518:LEU:H	1.82	0.43
1:C:611:LEU:HD22	1:C:666:ILE:HG23	1.99	0.43
3:E:50:TYR:O	3:E:54:LEU:HB2	2.18	0.43
1:A:904:TYR:OH	1:C:1094:VAL:HG11	2.18	0.43
1:B:981:LEU:HD21	1:B:993:ILE:HD11	2.00	0.43
1:C:455:LEU:HD22	1:C:493:GLN:HG3	2.00	0.43
1:C:502:GLY:O	1:C:506:GLN:HG3	2.18	0.43
1:A:704:SER:HB3	1:B:790:LYS:HE2	2.00	0.43
3:L:50:TYR:O	3:L:54:LEU:HB2	2.18	0.43
1:A:455:LEU:HD22	1:A:493:GLN:HG3	2.00	0.43
1:A:698:SER:O	1:A:699:LEU:HG	2.18	0.43
1:C:698:SER:O	1:C:699:LEU:HG	2.19	0.43
1:A:44:ARG:O	1:A:283:GLY:HA2	2.18	0.43
1:B:502:GLY:O	1:B:506:GLN:HG3	2.18	0.43
1:A:902:MET:HE1	1:A:1049:LEU:HD13	1.99	0.43
1:A:1089:PHE:HB2	1:A:1121:PHE:CZ	2.54	0.43
1:B:908:GLY:O	1:B:1038:LYS:HE3	2.18	0.43
4:O:1:NAG:H61	4:O:2:NAG:N2	2.34	0.43
1:C:981:LEU:HD21	1:C:993:ILE:HD11	2.00	0.43
1:B:1107:ARG:HH22	1:C:907:ASN:ND2	2.17	0.43
1:B:1145:LEU:HD21	1:C:1145:LEU:HD12	2.01	0.43
1:C:908:GLY:O	1:C:1038:LYS:HE3	2.18	0.43
1:B:1089:PHE:HB2	1:B:1121:PHE:CZ	2.54	0.42
2:F:92:THR:HG23	2:F:124:THR:HA	2.01	0.42
3:G:50:TYR:O	3:G:54:LEU:HB2	2.18	0.42
1:B:598:ILE:HG23	1:B:664:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:HB3	2:H:80:LEU:HD13	2.02	0.42
4:I:1:NAG:H61	4:I:2:NAG:N2	2.34	0.42
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.02	0.42
1:A:611:LEU:HD22	1:A:666:ILE:HG23	1.99	0.42
1:A:656:VAL:HG12	1:A:658:ASN:H	1.85	0.42
1:C:44:ARG:O	1:C:283:GLY:HA2	2.18	0.42
1:C:392:PHE:CD1	1:C:515:PHE:HB3	2.55	0.42
2:D:110:TYR:CZ	3:E:56:PRO:HB3	2.55	0.42
4:T:1:NAG:H61	4:T:2:NAG:N2	2.34	0.42
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.36	0.42
1:B:102:ARG:HD2	1:B:141:LEU:HD23	2.01	0.42
1:B:1028:LYS:O	1:B:1032:CYS:HB2	2.20	0.42
1:C:102:ARG:HD2	1:C:141:LEU:HD23	2.01	0.42
3:G:81:SER:OG	3:G:112:GLN:OE1	2.30	0.42
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.20	0.42
1:B:392:PHE:CD1	1:B:515:PHE:HB3	2.54	0.42
1:C:770:ILE:O	1:C:774:GLN:HG2	2.20	0.42
2:F:36:TRP:HB3	2:F:80:LEU:HD13	2.01	0.42
1:A:1072:GLU:HG2	1:B:894:LEU:CD2	2.50	0.42
1:B:656:VAL:HG12	1:B:658:ASN:H	1.85	0.42
2:D:16:GLN:HG3	2:D:17:THR:H	1.85	0.42
1:A:392:PHE:CD1	1:A:515:PHE:HB3	2.54	0.42
1:A:981:LEU:HD21	1:A:993:ILE:HD11	2.00	0.42
1:B:698:SER:O	1:B:699:LEU:HG	2.18	0.42
1:C:1028:LYS:O	1:C:1032:CYS:HB2	2.20	0.42
1:A:102:ARG:HD2	1:A:141:LEU:HD23	2.01	0.42
1:B:770:ILE:O	1:B:774:GLN:HG2	2.20	0.42
1:C:656:VAL:HG12	1:C:658:ASN:H	1.85	0.42
1:A:230:PRO:HB2	1:C:521:PRO:HB2	2.02	0.42
1:A:1094:VAL:HG11	1:B:904:TYR:OH	2.20	0.42
1:B:697:MET:HE3	1:B:699:LEU:HD21	2.02	0.42
1:C:598:ILE:HG23	1:C:664:ILE:HG21	2.02	0.42
1:C:1089:PHE:HB2	1:C:1121:PHE:CZ	2.54	0.42
2:F:55:ASN:HB3	2:F:56:SER:H	1.68	0.41
1:A:770:ILE:O	1:A:774:GLN:HG2	2.19	0.41
2:D:36:TRP:HB3	2:D:80:LEU:HD13	2.01	0.41
1:C:403:ARG:HH22	3:L:53:ASP:HB2	1.86	0.41
2:F:40:ARG:HB3	2:F:50:ILE:HD11	2.03	0.41
1:A:440:ASN:OD1	1:A:440:ASN:N	2.53	0.41
1:B:105:ILE:HD11	1:B:241:LEU:HD21	2.03	0.41
2:D:92:THR:HG23	2:D:124:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:GLN:HG3	2:H:17:THR:H	1.85	0.41
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.38	0.41
2:H:92:THR:HG23	2:H:124:THR:HA	2.01	0.41
1:B:376:THR:HB	1:B:435:ALA:HB3	2.03	0.41
1:C:493:GLN:HE21	2:H:111:TYR:HE2	1.69	0.41
2:H:4:LEU:HD23	2:H:22:CYS:SG	2.61	0.41
2:H:40:ARG:HB3	2:H:50:ILE:HD11	2.03	0.41
3:L:112:GLN:HA	3:L:113:PRO:HD3	1.94	0.41
1:A:718:PHE:HE1	1:A:923:ILE:HG12	1.87	0.40
1:A:429:PHE:HE1	1:A:514:SER:HB3	1.87	0.40
1:B:1086:LYS:HD2	1:B:1122:VAL:HG11	2.03	0.40
1:C:376:THR:HB	1:C:435:ALA:HB3	2.03	0.40
2:D:61:TYR:HB2	2:D:66:LYS:HG3	2.03	0.40
1:C:127:VAL:HG21	7:C:1302:NAG:H5	2.04	0.40
1:C:697:MET:HE3	1:C:699:LEU:HD21	2.02	0.40
2:H:119:GLN:HE21	2:H:119:GLN:HB3	1.73	0.40
2:F:11:LEU:HD23	2:F:124:THR:HB	2.04	0.40
2:F:16:GLN:HG3	2:F:17:THR:H	1.85	0.40

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	986/1288 (77%)	947 (96%)	36 (4%)	3 (0%)	37	67
1	B	986/1288 (77%)	947 (96%)	36 (4%)	3 (0%)	37	67
1	C	986/1288 (77%)	946 (96%)	37 (4%)	3 (0%)	37	67
2	D	126/245 (51%)	117 (93%)	9 (7%)	0	100	100
2	F	126/245 (51%)	117 (93%)	9 (7%)	0	100	100
2	H	126/245 (51%)	117 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	111/229 (48%)	106 (96%)	5 (4%)	0	100	100
3	G	111/229 (48%)	106 (96%)	5 (4%)	0	100	100
3	L	111/229 (48%)	106 (96%)	5 (4%)	0	100	100
All	All	3669/5286 (69%)	3509 (96%)	151 (4%)	9 (0%)	45	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	699	LEU
1	B	699	LEU
1	C	699	LEU
1	A	331	ASN
1	B	331	ASN
1	C	331	ASN
1	A	123	ALA
1	B	123	ALA
1	C	123	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	876/1113 (79%)	875 (100%)	1 (0%)	92	97
1	B	876/1113 (79%)	875 (100%)	1 (0%)	92	97
1	C	876/1113 (79%)	875 (100%)	1 (0%)	92	97
2	D	108/209 (52%)	106 (98%)	2 (2%)	52	73
2	F	108/209 (52%)	106 (98%)	2 (2%)	52	73
2	H	108/209 (52%)	106 (98%)	2 (2%)	52	73
3	E	92/192 (48%)	92 (100%)	0	100	100
3	G	92/192 (48%)	92 (100%)	0	100	100
3	L	92/192 (48%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3228/4542 (71%)	3219 (100%)	9 (0%)	90 96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ARG
1	B	319	ARG
1	C	319	ARG
2	H	55	ASN
2	H	119	GLN
2	D	55	ASN
2	D	119	GLN
2	F	55	ASN
2	F	119	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	317	ASN
1	A	804	GLN
1	A	1071	GLN
1	A	1088	HIS
1	A	1135	ASN
1	B	314	GLN
1	B	317	ASN
1	B	804	GLN
1	B	935	GLN
1	B	1071	GLN
1	B	1088	HIS
1	C	314	GLN
1	C	317	ASN
1	C	487	ASN
1	C	804	GLN
1	C	907	ASN
1	C	1071	GLN
1	C	1088	HIS
1	C	1135	ASN
2	H	60	ASN
3	L	16	GLN
3	L	32	ASN

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Mol	Chain	Res	Type
2	D	60	ASN
3	E	16	GLN
3	E	32	ASN
2	F	60	ASN
3	G	16	GLN
3	G	32	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

41 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	I	1	4,1	14,14,15	0.17	0	17,19,21	0.53	0
4	NAG	I	2	4	14,14,15	0.36	0	17,19,21	0.57	0
4	NAG	J	1	4,1	14,14,15	0.20	0	17,19,21	0.54	0
4	NAG	J	2	4	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	K	1	4,1	14,14,15	0.19	0	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	M	1	4,1	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	N	1	4,1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	N	2	4	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	O	1	4,1	14,14,15	0.15	0	17,19,21	0.53	0
4	NAG	O	2	4	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	P	1	4,1	14,14,15	0.20	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	P	2	4	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	Q	1	4,1	14,14,15	0.19	0	17,19,21	0.50	0
4	NAG	Q	2	4	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	R	1	4,1	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	R	2	4	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	S	1	4,1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	S	2	4	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	T	1	4,1	14,14,15	0.16	0	17,19,21	0.54	0
4	NAG	T	2	4	14,14,15	0.35	0	17,19,21	0.57	0
4	NAG	U	1	4,1	14,14,15	0.19	0	17,19,21	0.54	0
4	NAG	U	2	4	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	V	1	4,1	14,14,15	0.18	0	17,19,21	0.51	0
4	NAG	V	2	4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	W	1	4,1	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	W	2	4	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	X	1	4,1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	X	2	4	14,14,15	0.32	0	17,19,21	0.56	0
5	NAG	Y	1	2,5	14,14,15	0.30	0	17,19,21	0.53	0
5	NAG	Y	2	5	14,14,15	0.40	0	17,19,21	0.38	0
5	BMA	Y	3	5	11,11,12	1.31	2 (18%)	15,15,17	2.26	4 (26%)
5	MAN	Y	4	5	11,11,12	0.72	1 (9%)	15,15,17	1.35	3 (20%)
5	MAN	Y	5	5	11,11,12	0.67	0	15,15,17	1.16	2 (13%)
6	NAG	Z	1	2,6	14,14,15	0.31	0	17,19,21	0.53	0
6	NAG	Z	2	6	14,14,15	0.39	0	17,19,21	0.37	0
6	BMA	Z	3	6	11,11,12	1.30	2 (18%)	15,15,17	2.26	4 (26%)
6	NAG	a	1	2,6	14,14,15	0.32	0	17,19,21	0.53	0
6	NAG	a	2	6	14,14,15	0.40	0	17,19,21	0.38	0
6	BMA	a	3	6	11,11,12	1.31	2 (18%)	15,15,17	2.26	4 (26%)

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	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	3	BMA	O5-C5	3.07	1.49	1.43
5	Y	3	BMA	O5-C5	3.07	1.49	1.43
6	Z	3	BMA	O5-C5	3.05	1.49	1.43
5	Y	3	BMA	C4-C5	2.32	1.57	1.53
6	a	3	BMA	C4-C5	2.30	1.57	1.53
6	Z	3	BMA	C4-C5	2.27	1.57	1.53
5	Y	4	MAN	C1-C2	2.05	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	3	BMA	C1-O5-C5	7.12	121.84	112.19
6	a	3	BMA	C1-O5-C5	7.11	121.83	112.19
5	Y	3	BMA	C1-O5-C5	7.10	121.81	112.19
5	Y	4	MAN	C1-O5-C5	3.62	117.09	112.19
5	Y	3	BMA	C1-C2-C3	-3.16	105.78	109.67
6	a	3	BMA	C1-C2-C3	-3.16	105.78	109.67
6	Z	3	BMA	C1-C2-C3	-3.16	105.78	109.67
5	Y	5	MAN	C1-O5-C5	2.60	115.71	112.19
6	a	3	BMA	O3-C3-C2	2.35	114.48	109.99
6	Z	3	BMA	O3-C3-C2	2.34	114.47	109.99
5	Y	3	BMA	O3-C3-C2	2.33	114.46	109.99
5	Y	5	MAN	O2-C2-C3	-2.15	105.83	110.14
5	Y	4	MAN	O2-C2-C3	-2.09	105.95	110.14
5	Y	4	MAN	O5-C1-C2	2.04	113.92	110.77
5	Y	3	BMA	O5-C5-C4	2.02	115.75	110.83
6	Z	3	BMA	O5-C5-C4	2.02	115.74	110.83
6	a	3	BMA	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
6	Z	3	BMA	O5-C5-C6-O6
6	a	3	BMA	O5-C5-C6-O6

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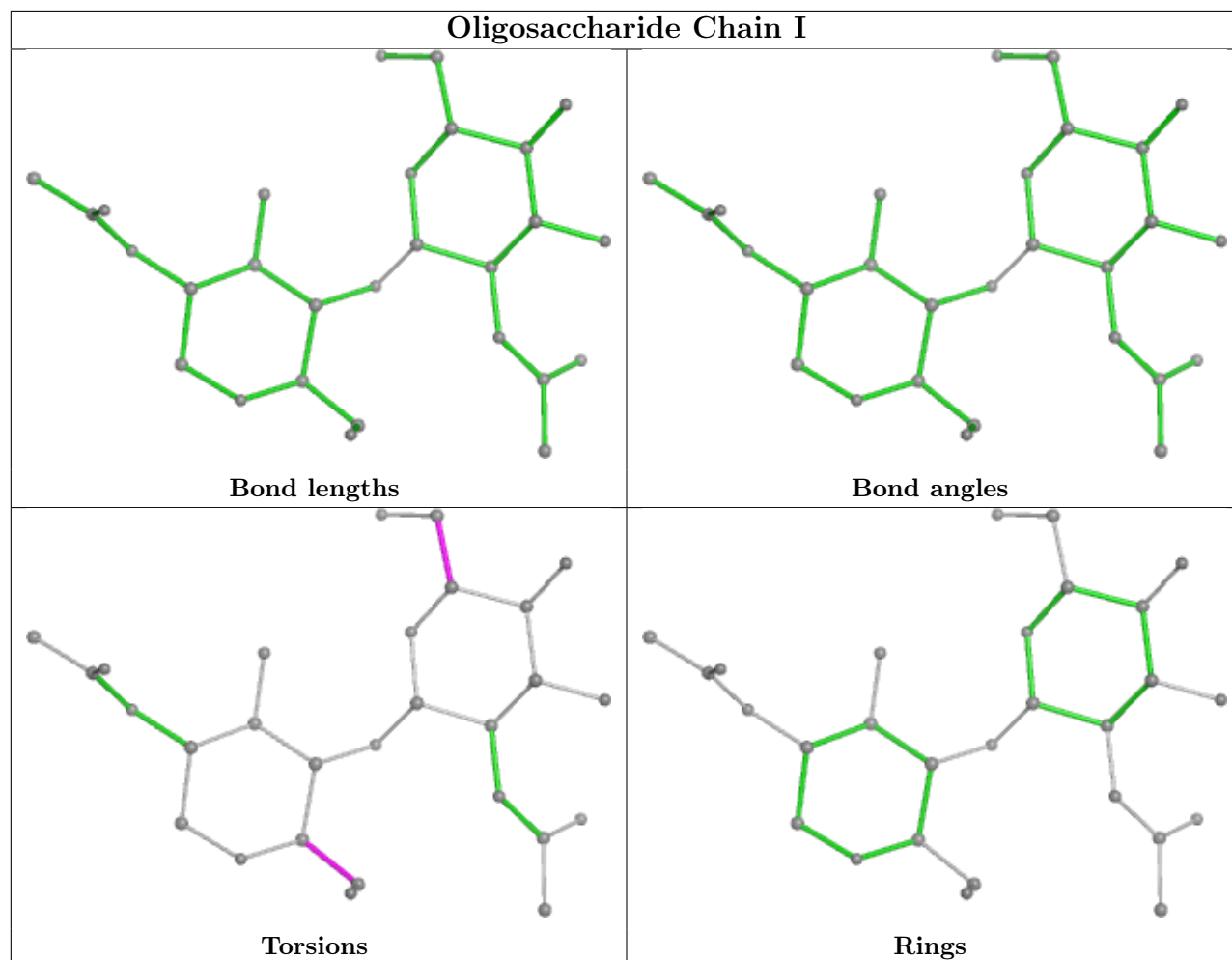
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
6	Z	3	BMA	C4-C5-C6-O6
6	a	3	BMA	C4-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
5	Y	5	MAN	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
5	Y	5	MAN	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6

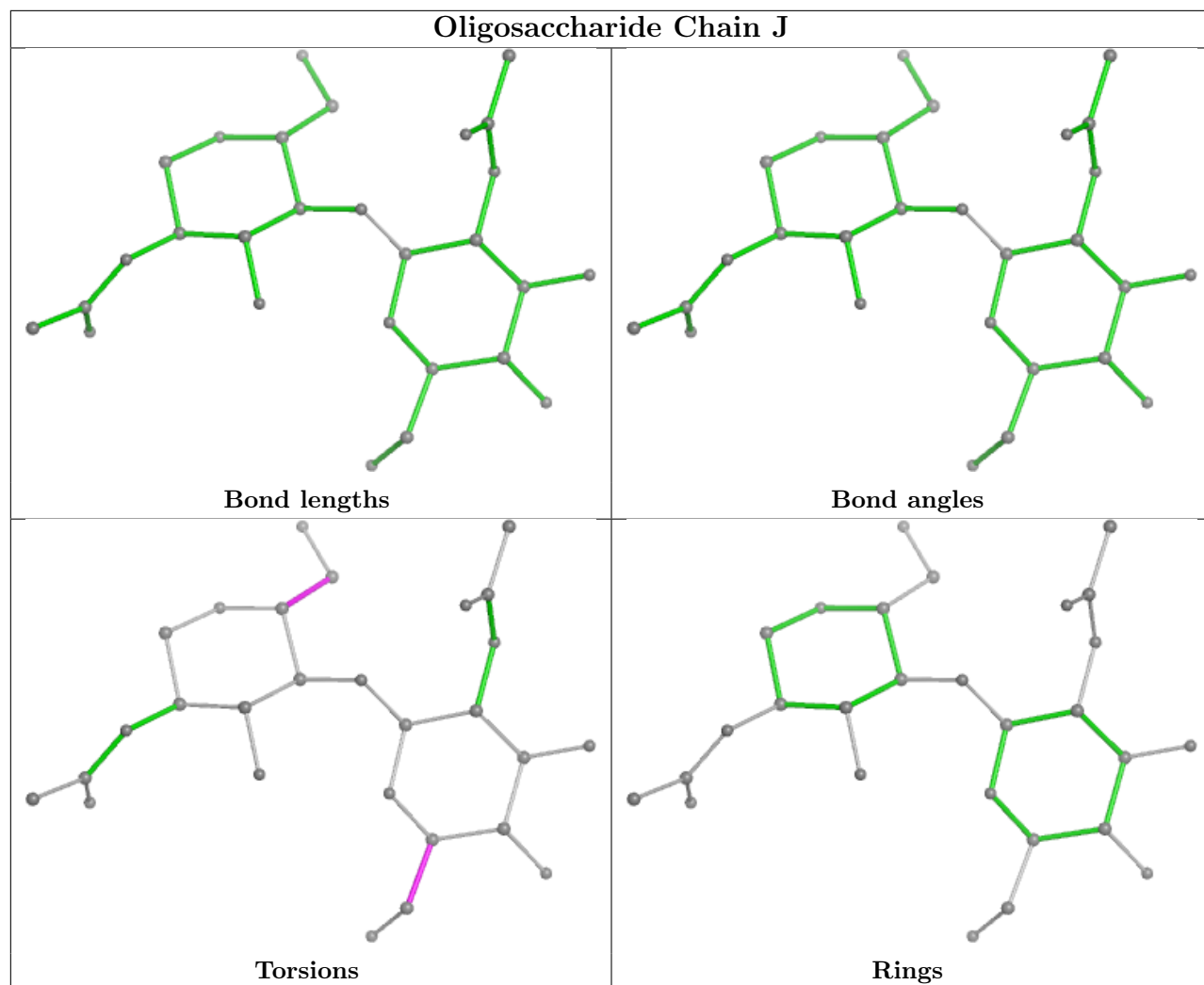
There are no ring outliers.

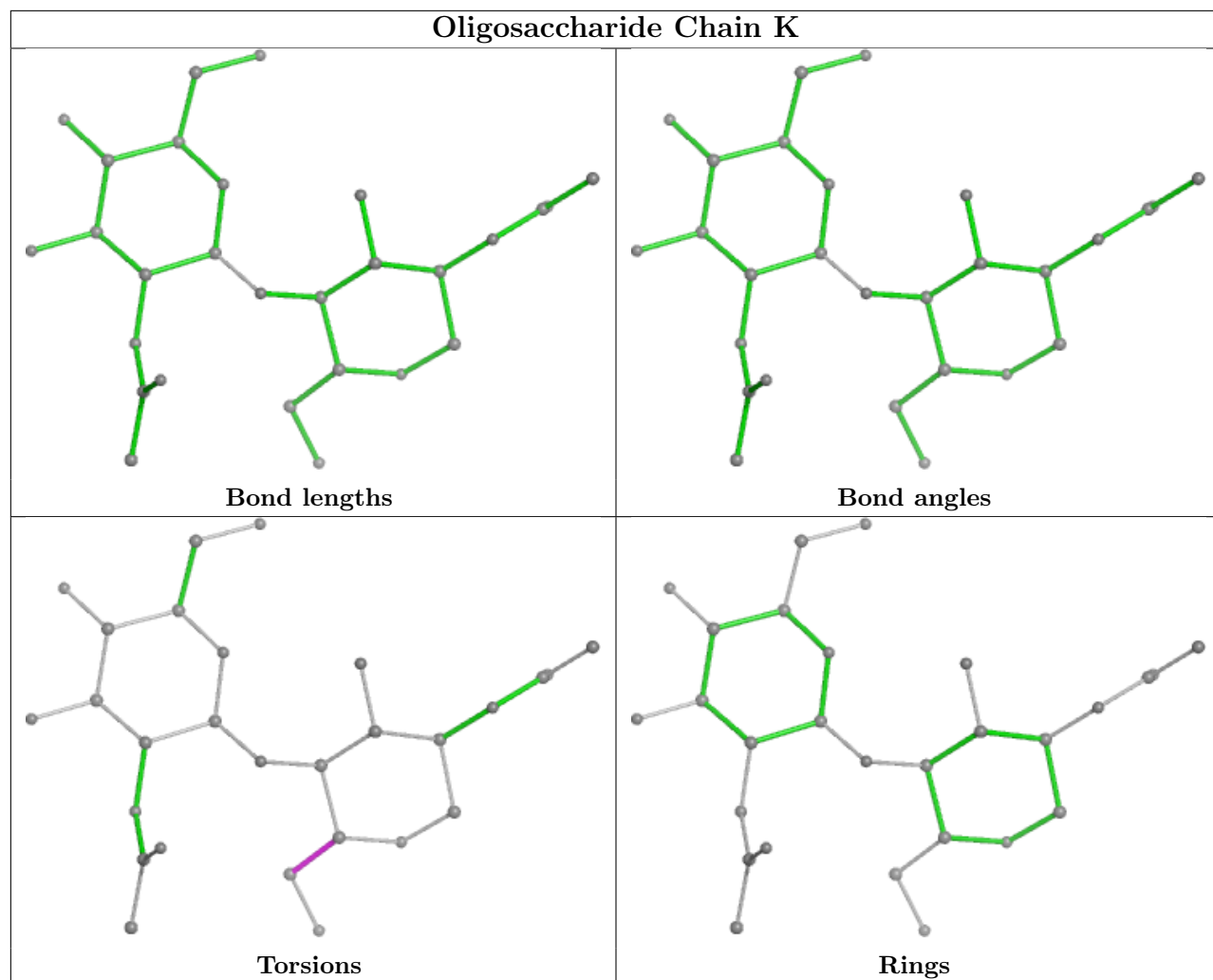
12 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	1	NAG	3	0
6	a	1	NAG	1	0
4	I	1	NAG	1	0
4	I	2	NAG	1	0
4	T	2	NAG	1	0
4	T	1	NAG	1	0
4	W	1	NAG	1	0
4	M	1	NAG	1	0
6	Z	1	NAG	1	0
4	O	1	NAG	1	0
4	R	1	NAG	1	0
4	O	2	NAG	1	0

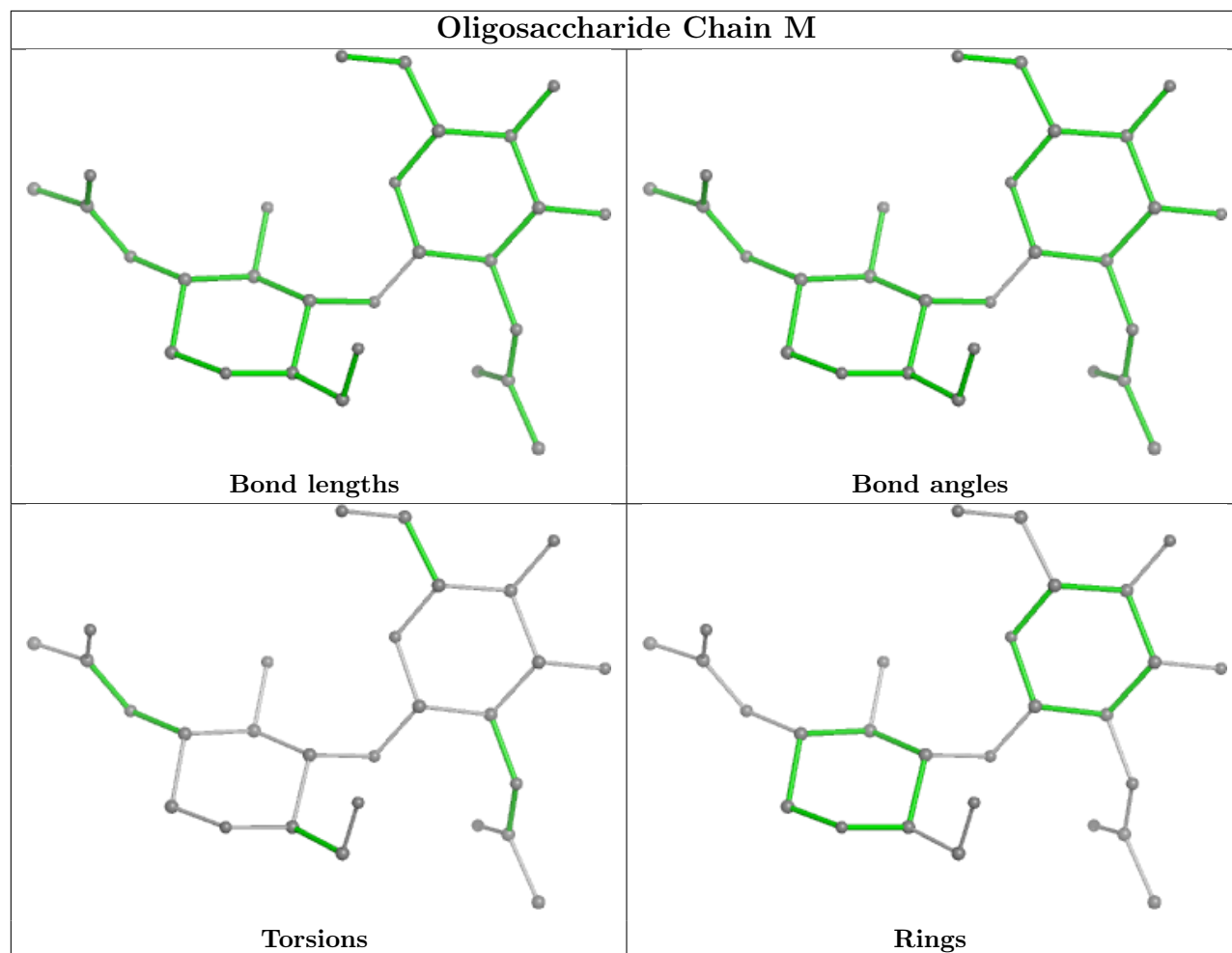
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

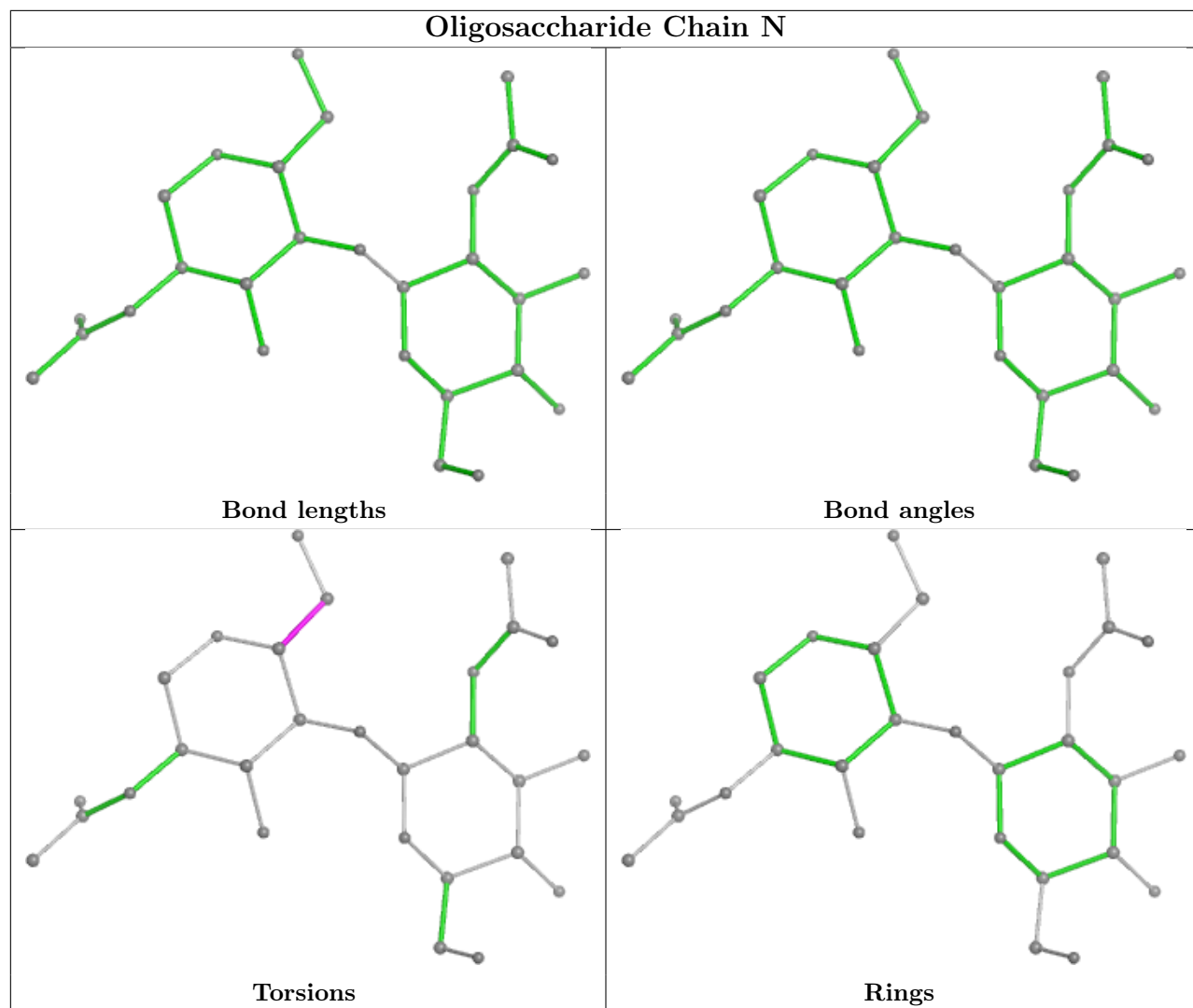


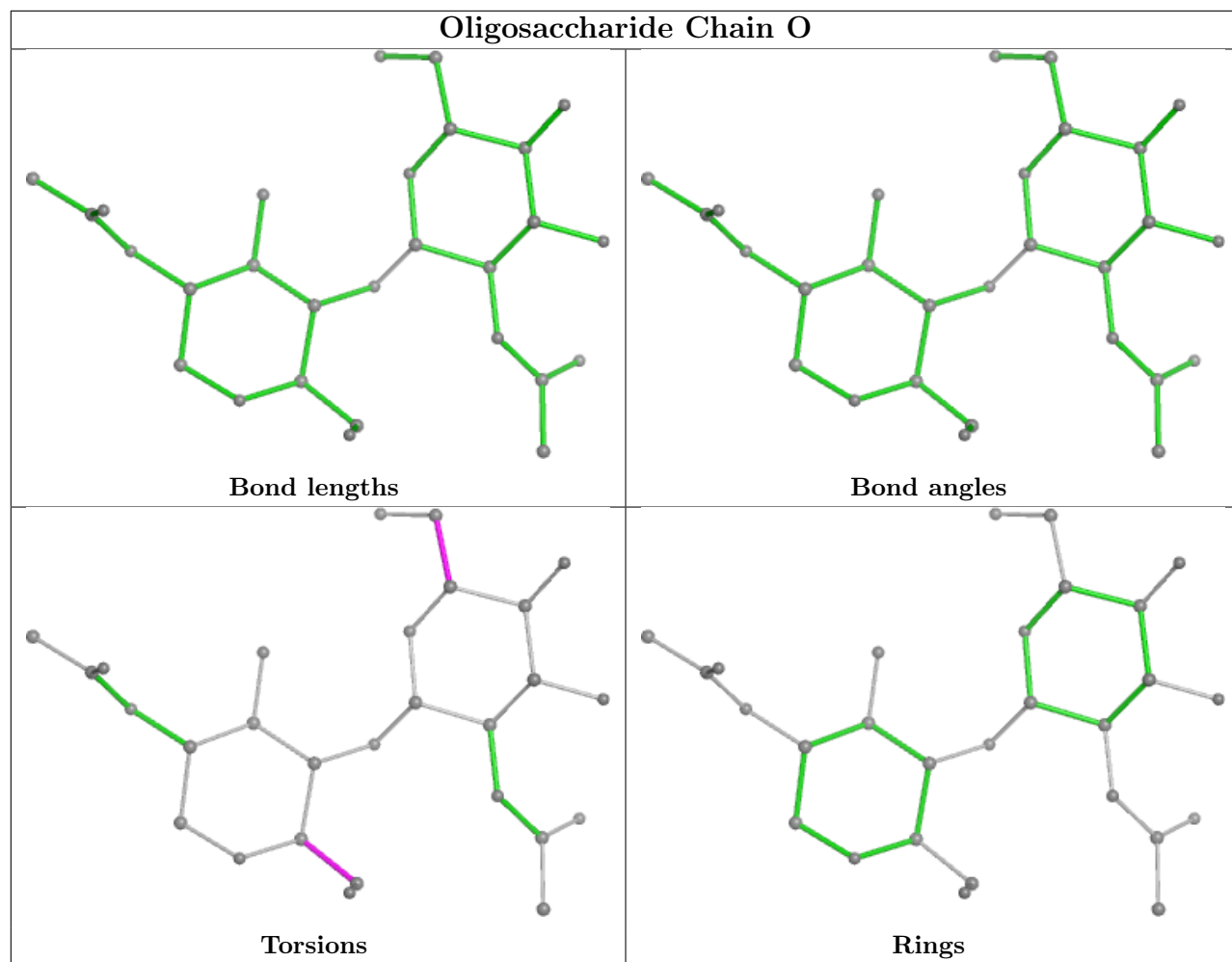


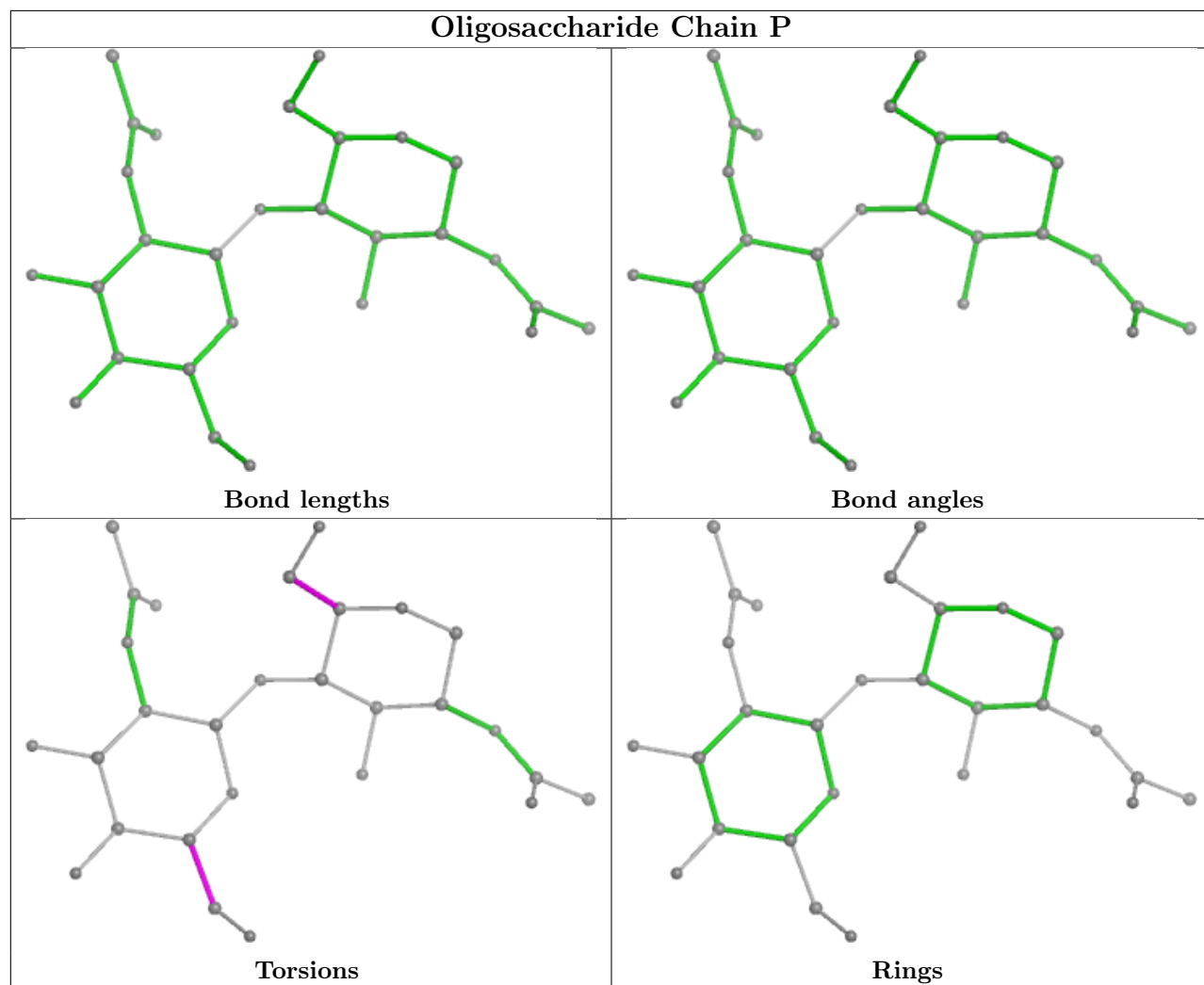


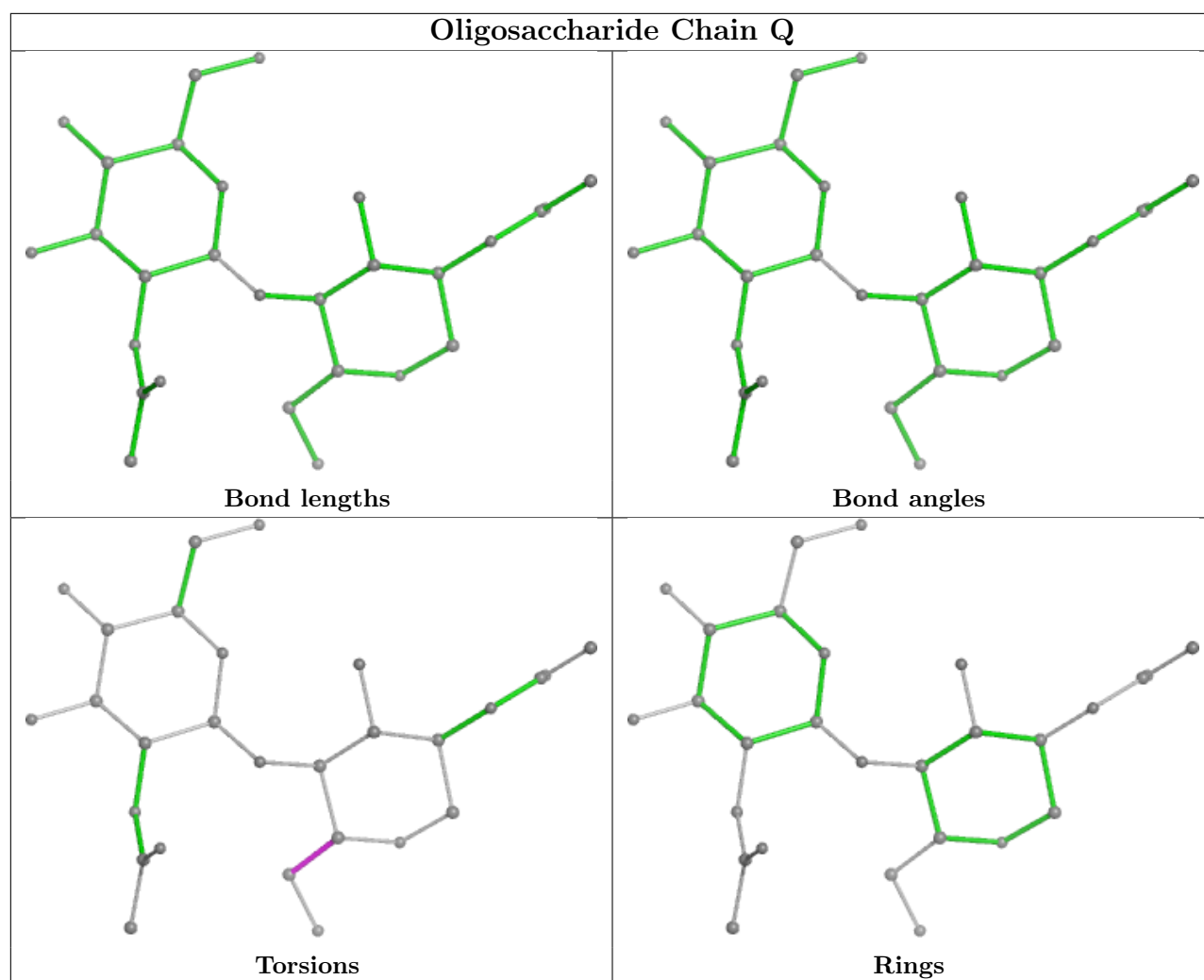


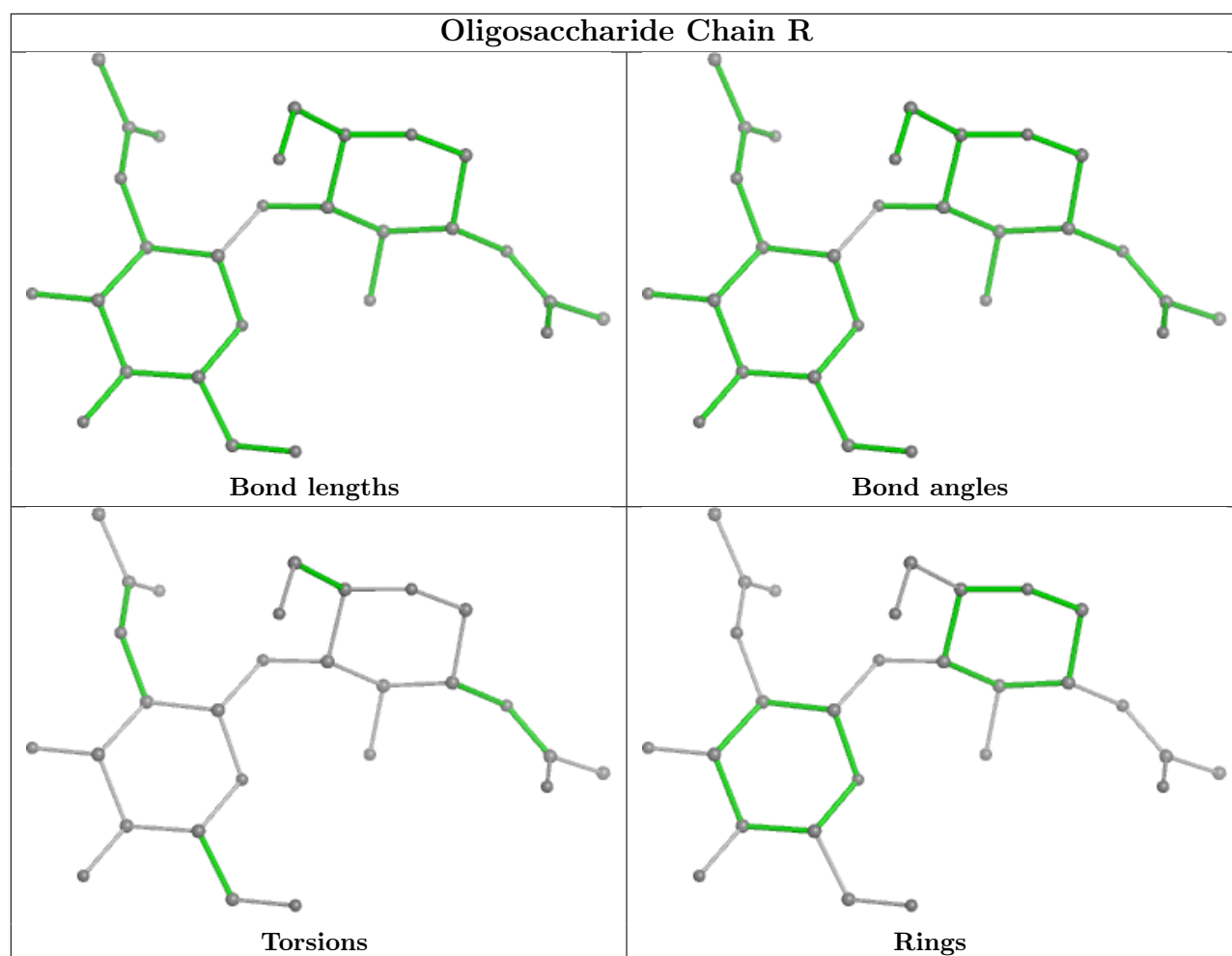


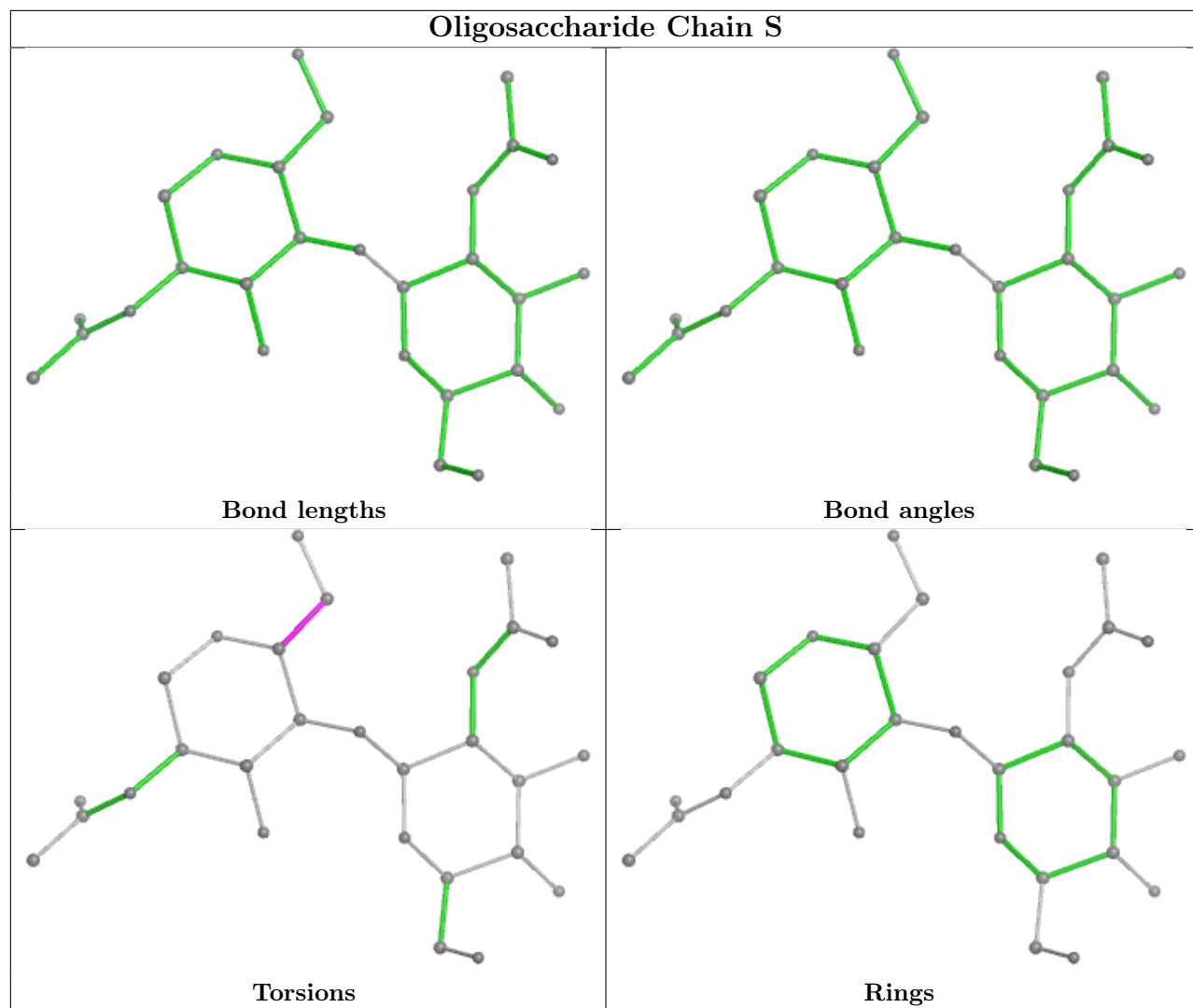


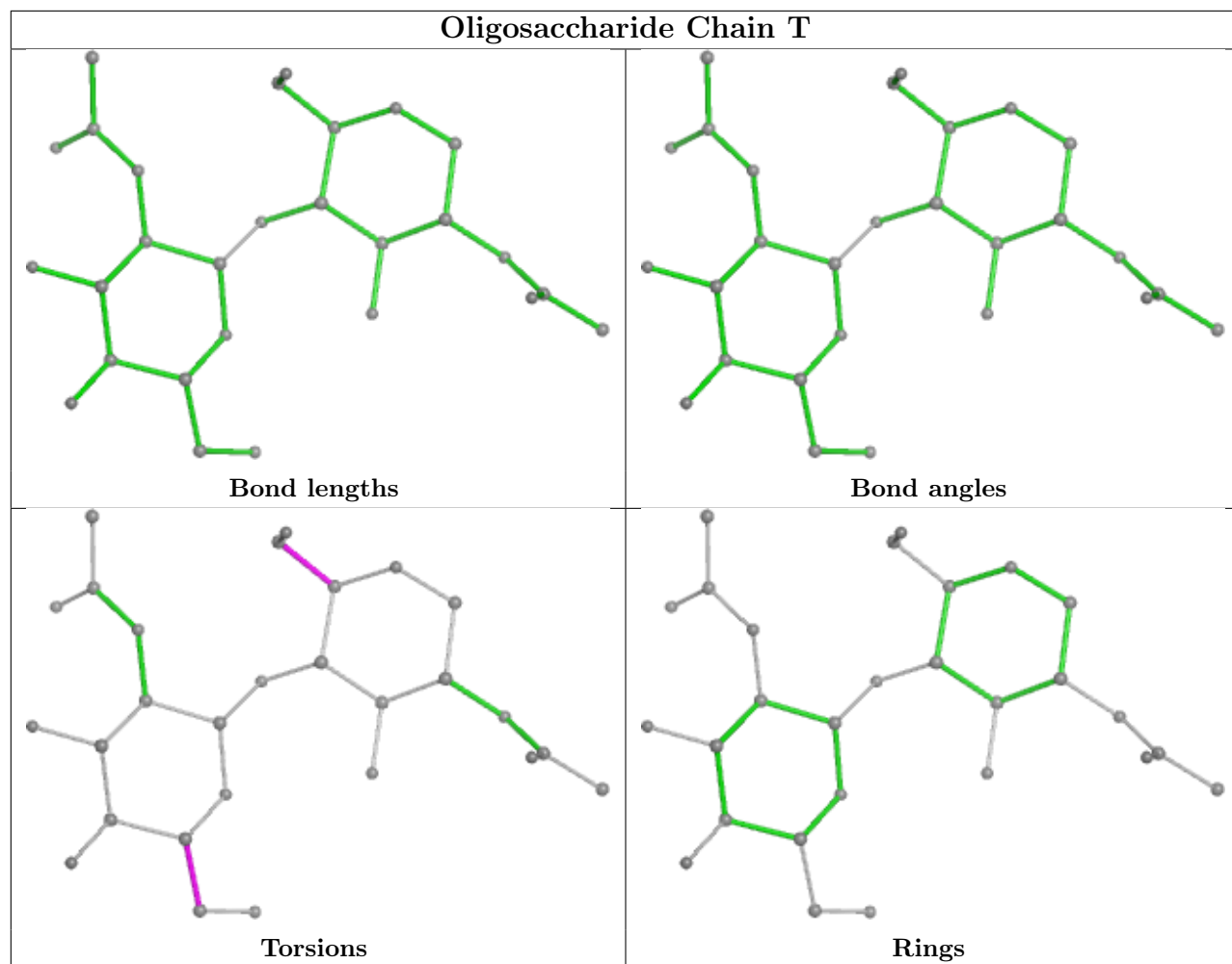




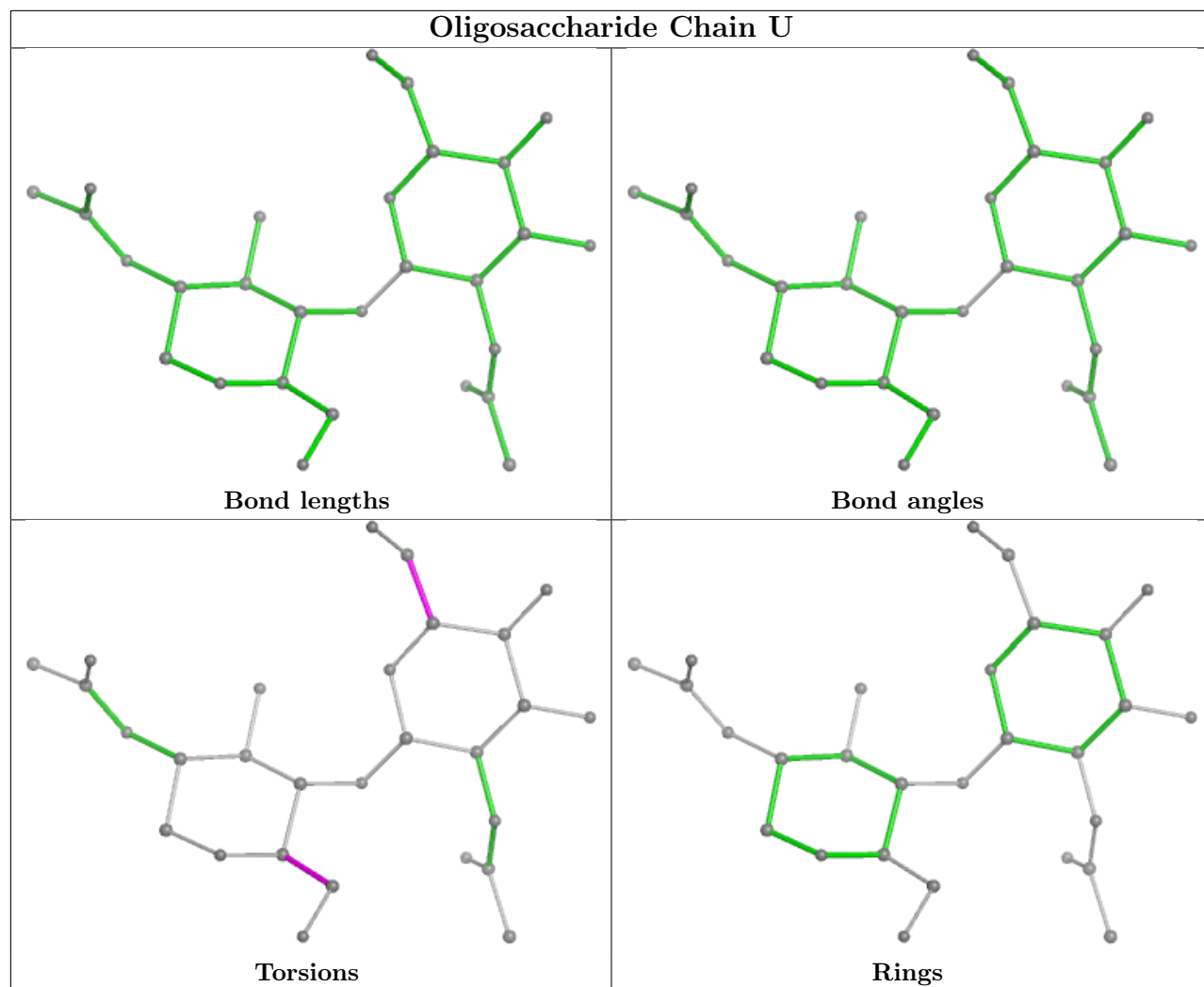


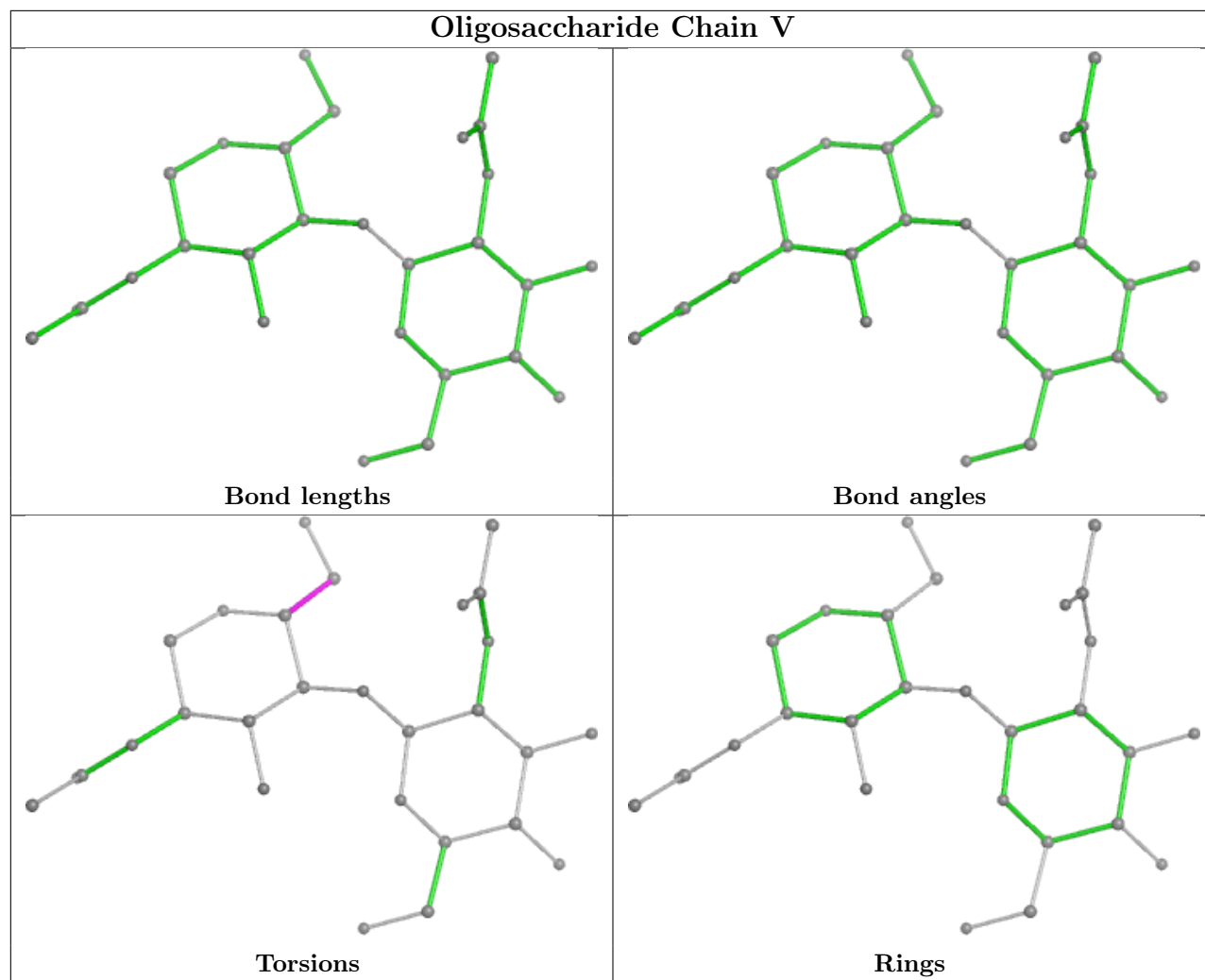


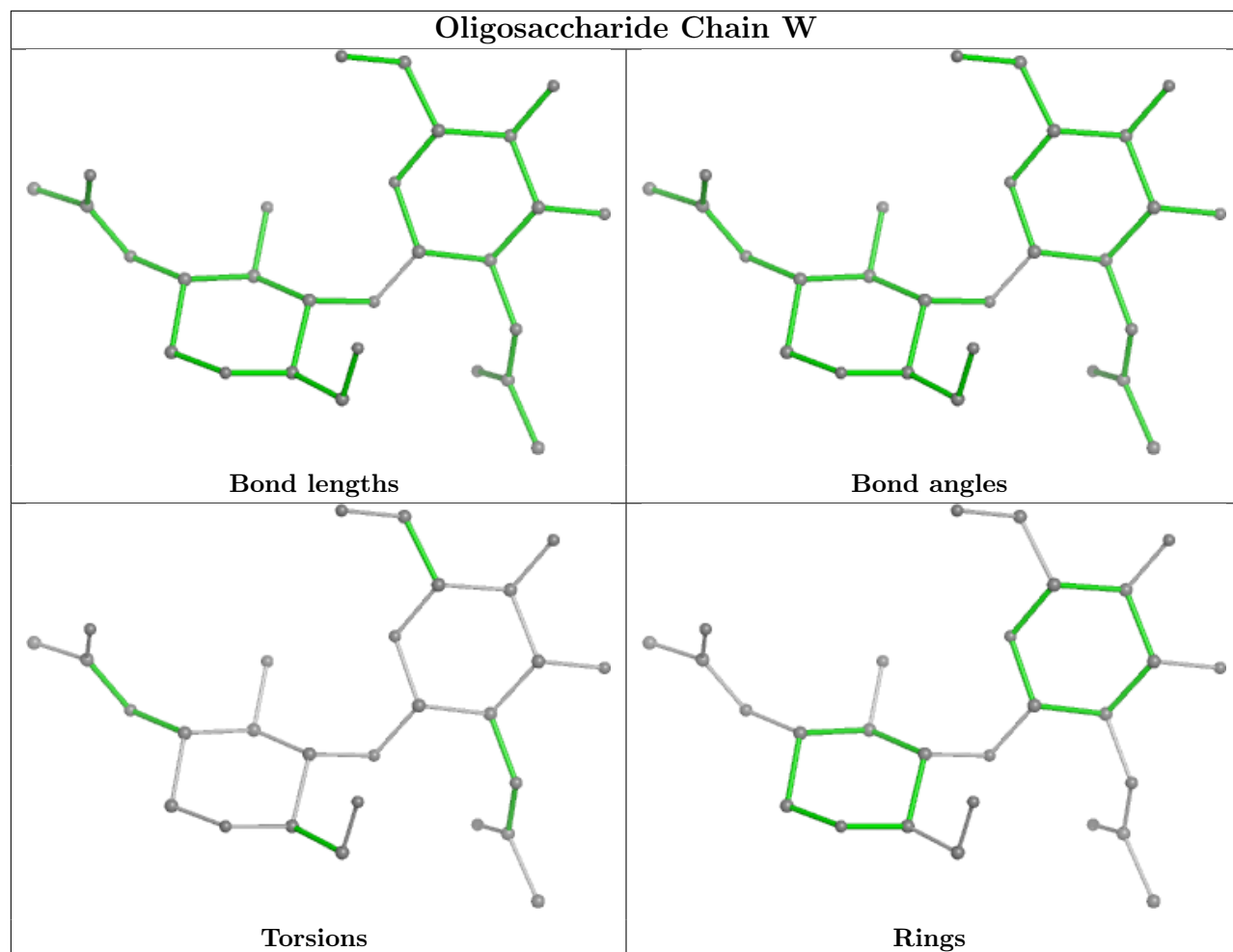


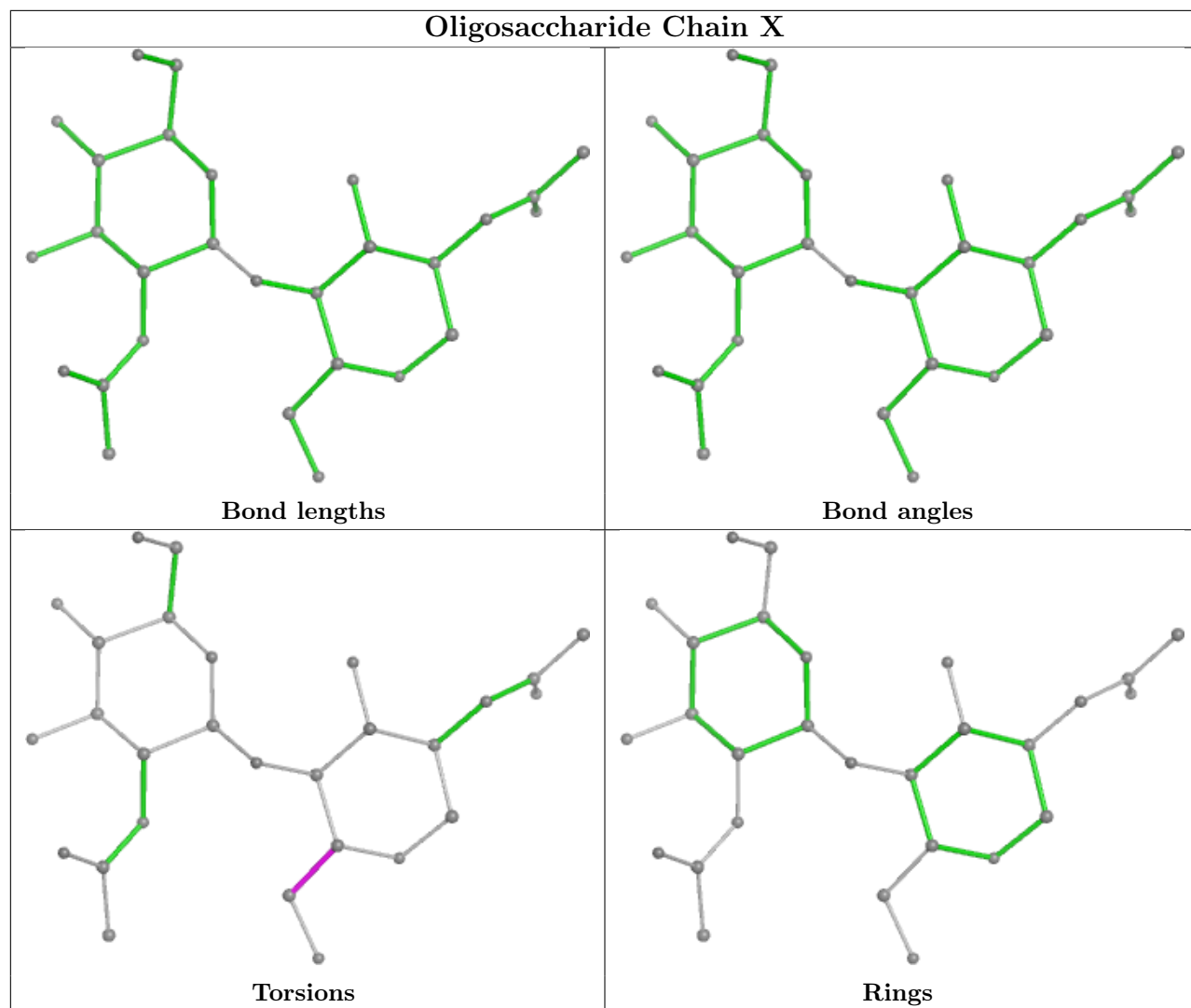


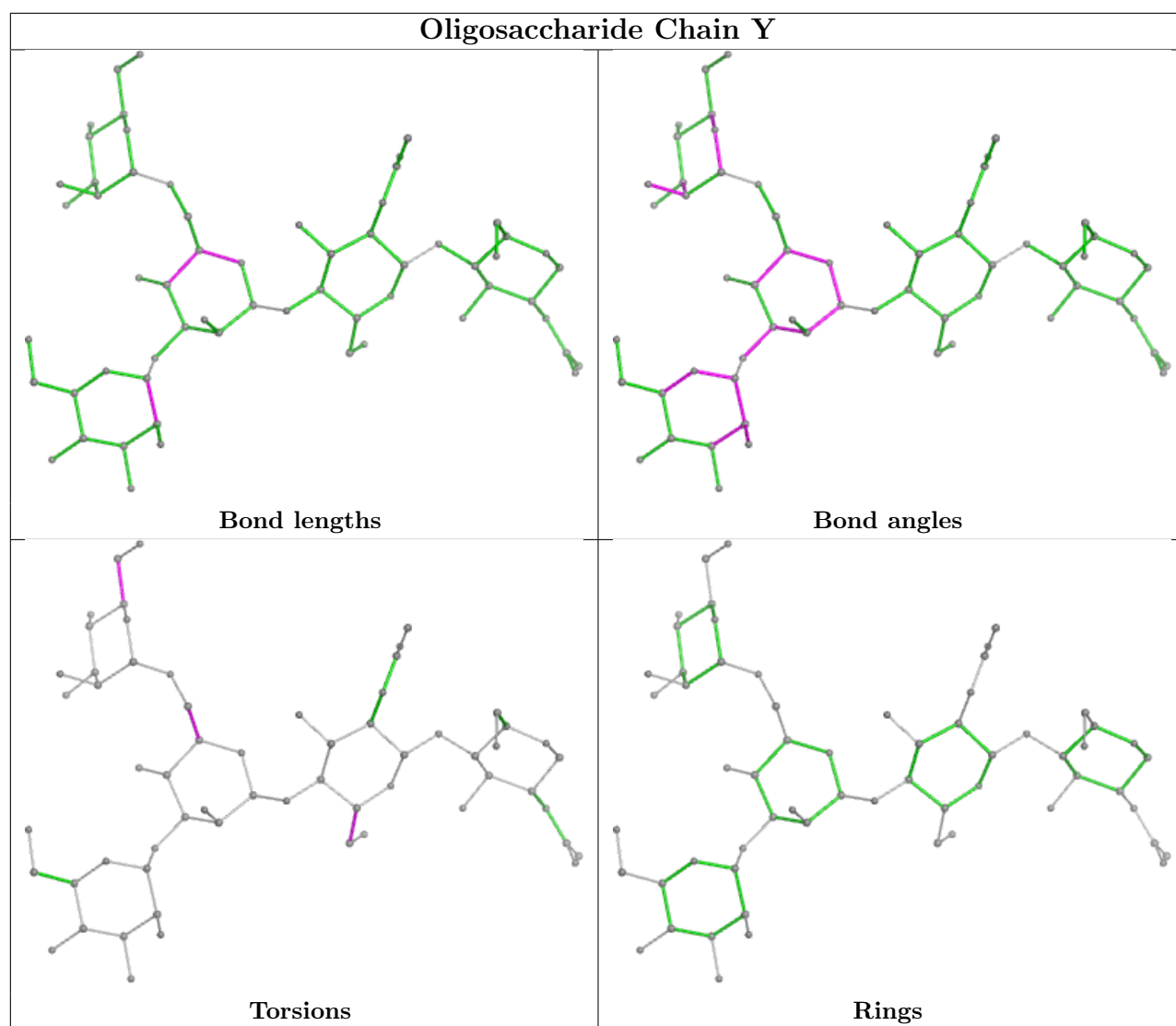


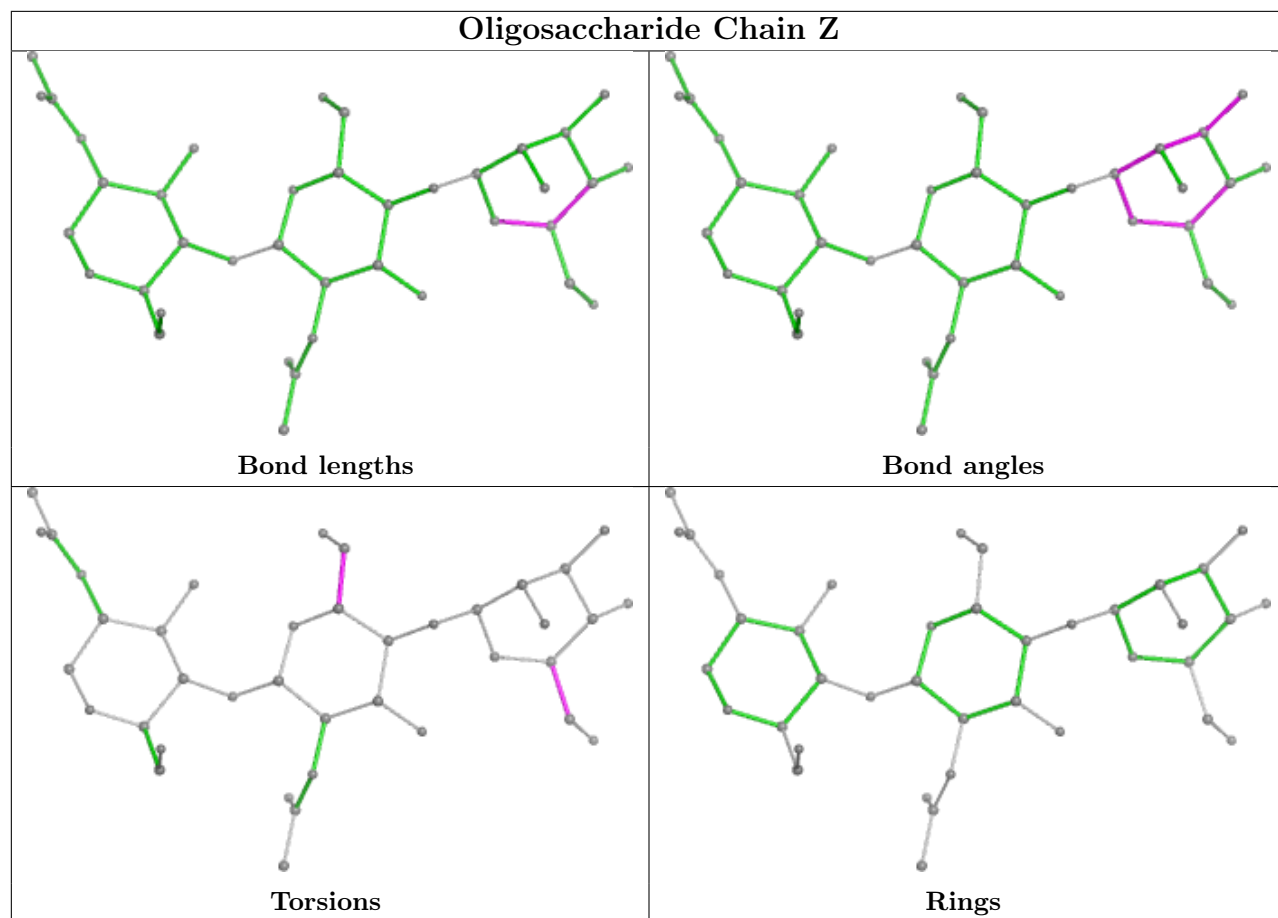


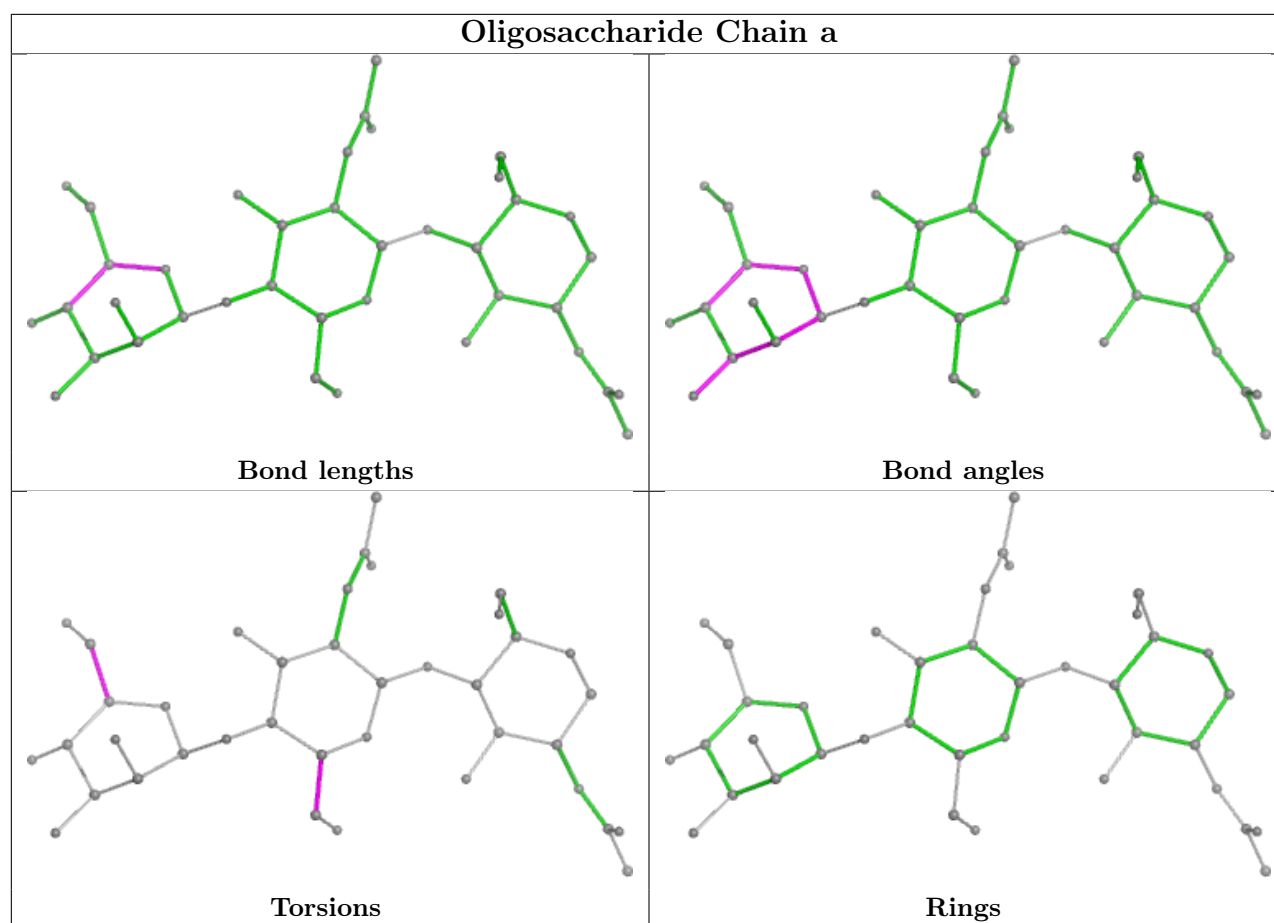












## 5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	C	1310	1	14,14,15	0.30	0	17,19,21	0.51	0
7	NAG	C	1305	1	14,14,15	0.28	0	17,19,21	0.50	0
7	NAG	A	1307	1	14,14,15	0.32	0	17,19,21	0.53	0
7	NAG	A	1309	1	14,14,15	0.31	0	17,19,21	0.53	0
7	NAG	A	1304	1	14,14,15	0.29	0	17,19,21	0.59	0
7	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.49	0
7	NAG	C	1304	1	14,14,15	0.28	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	C	1306	1	14,14,15	0.27	0	17,19,21	0.52	0
7	NAG	B	1301	1	14,14,15	0.32	0	17,19,21	0.47	0
7	NAG	C	1303	1	14,14,15	0.26	0	17,19,21	0.49	0
7	NAG	B	1302	1	14,14,15	0.34	0	17,19,21	0.64	0
7	NAG	B	1308	1	14,14,15	0.25	0	17,19,21	0.52	0
7	NAG	B	1305	1	14,14,15	0.28	0	17,19,21	0.49	0
7	NAG	A	1302	1	14,14,15	0.34	0	17,19,21	0.63	0
7	NAG	B	1306	1	14,14,15	0.28	0	17,19,21	0.52	0
7	NAG	C	1301	1	14,14,15	0.31	0	17,19,21	0.47	0
7	NAG	C	1308	1	14,14,15	0.25	0	17,19,21	0.53	0
7	NAG	B	1310	1	14,14,15	0.30	0	17,19,21	0.50	0
7	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.53	0
7	NAG	C	1309	1	14,14,15	0.30	0	17,19,21	0.53	0
7	NAG	A	1310	1	14,14,15	0.31	0	17,19,21	0.50	0
7	NAG	C	1307	1	14,14,15	0.31	0	17,19,21	0.52	0
7	NAG	A	1301	1	14,14,15	0.32	0	17,19,21	0.47	0
7	NAG	B	1304	1	14,14,15	0.29	0	17,19,21	0.60	0
7	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.49	0
7	NAG	C	1302	1	14,14,15	0.35	0	17,19,21	0.63	0
7	NAG	A	1306	1	14,14,15	0.27	0	17,19,21	0.52	0
7	NAG	A	1303	1	14,14,15	0.27	0	17,19,21	0.50	0
7	NAG	B	1307	1	14,14,15	0.32	0	17,19,21	0.52	0
7	NAG	B	1309	1	14,14,15	0.30	0	17,19,21	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1309	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1306	NAG	O5-C5-C6-O6
7	B	1306	NAG	O5-C5-C6-O6
7	C	1306	NAG	O5-C5-C6-O6
7	A	1305	NAG	O5-C5-C6-O6
7	B	1305	NAG	O5-C5-C6-O6
7	C	1305	NAG	O5-C5-C6-O6
7	A	1306	NAG	C4-C5-C6-O6
7	B	1306	NAG	C4-C5-C6-O6
7	C	1306	NAG	C4-C5-C6-O6
7	A	1310	NAG	O5-C5-C6-O6
7	B	1310	NAG	O5-C5-C6-O6
7	C	1310	NAG	O5-C5-C6-O6
7	A	1310	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	B	1310	NAG	C4-C5-C6-O6
7	C	1310	NAG	C4-C5-C6-O6
7	A	1305	NAG	C4-C5-C6-O6
7	B	1305	NAG	C4-C5-C6-O6
7	C	1305	NAG	C4-C5-C6-O6
7	A	1301	NAG	O5-C5-C6-O6
7	B	1301	NAG	O5-C5-C6-O6
7	C	1301	NAG	O5-C5-C6-O6
7	A	1309	NAG	O5-C5-C6-O6
7	B	1309	NAG	O5-C5-C6-O6
7	C	1309	NAG	O5-C5-C6-O6
7	A	1301	NAG	C4-C5-C6-O6
7	B	1301	NAG	C4-C5-C6-O6
7	C	1301	NAG	C4-C5-C6-O6
7	B	1304	NAG	C4-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6
7	A	1302	NAG	C3-C2-N2-C7
7	B	1302	NAG	C3-C2-N2-C7
7	C	1302	NAG	C3-C2-N2-C7
7	A	1304	NAG	C4-C5-C6-O6
7	C	1303	NAG	O5-C5-C6-O6
7	B	1303	NAG	O5-C5-C6-O6
7	A	1303	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1304	NAG	1	0
7	C	1304	NAG	1	0
7	B	1304	NAG	1	0
7	C	1302	NAG	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

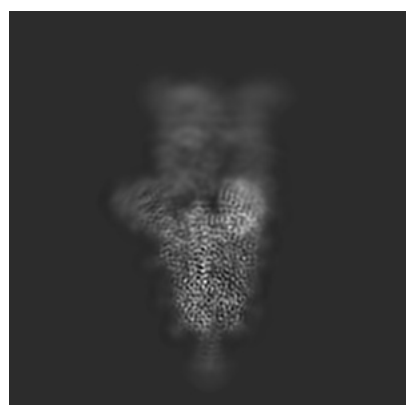
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12275. These allow visual inspection of the internal detail of the map and identification of artifacts.

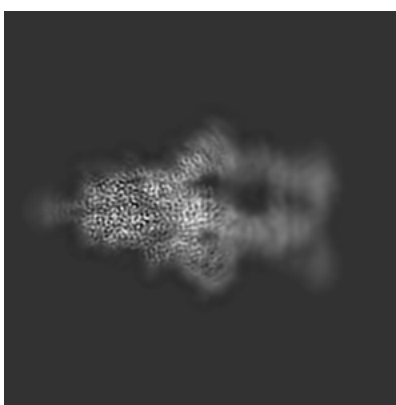
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

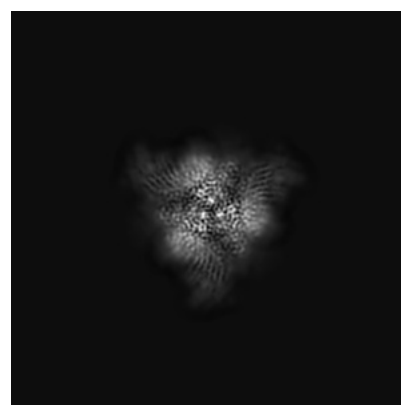
#### 6.1.1 Primary map



X



Y



Z

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

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

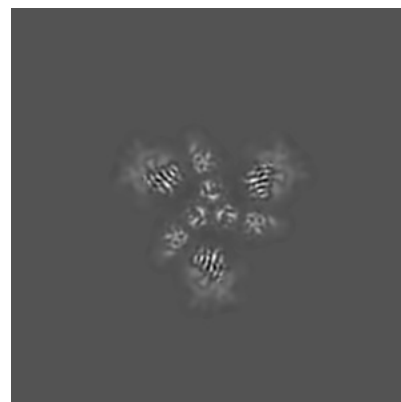
#### 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

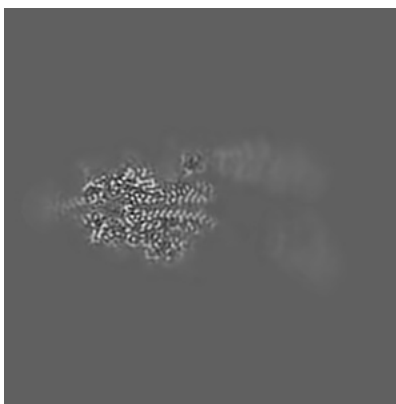
The images above show central slices of the map in three orthogonal directions.

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

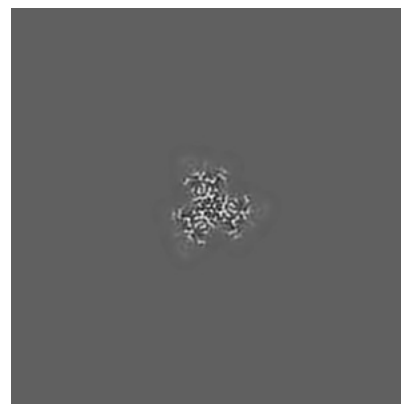
### 6.3.1 Primary map



X Index: 191



Y Index: 194

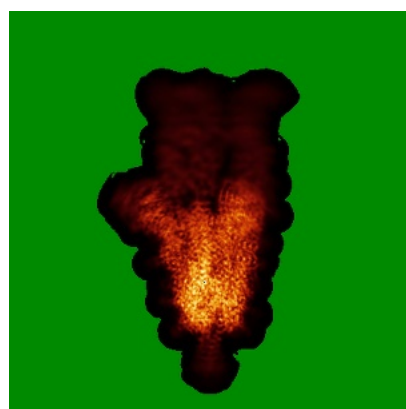


Z Index: 128

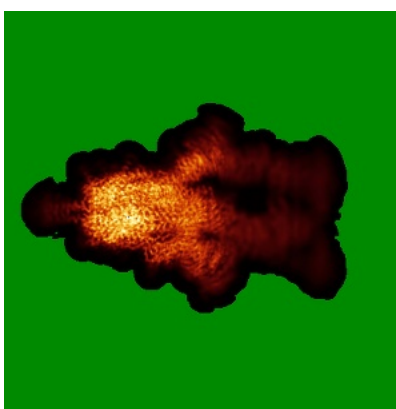
The images above show the largest variance slices of the map in three orthogonal directions.

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

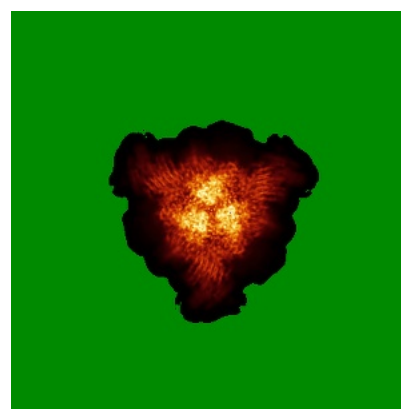
### 6.4.1 Primary map



X



Y



Z

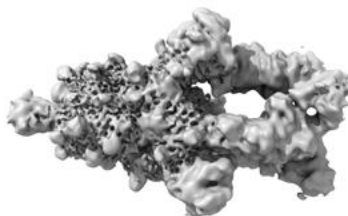
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

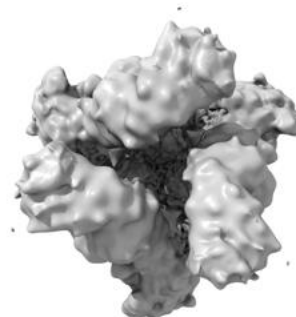
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

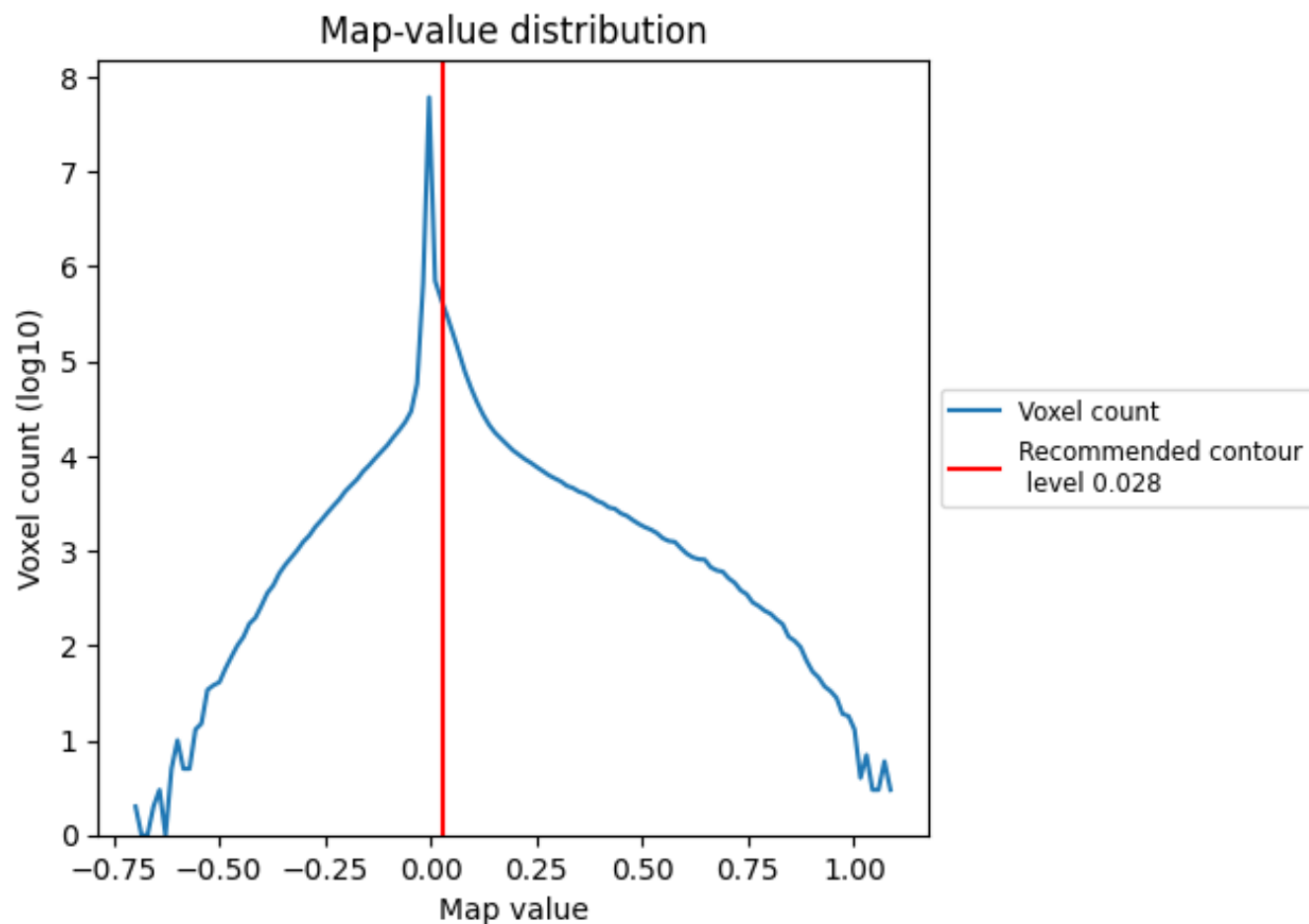
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

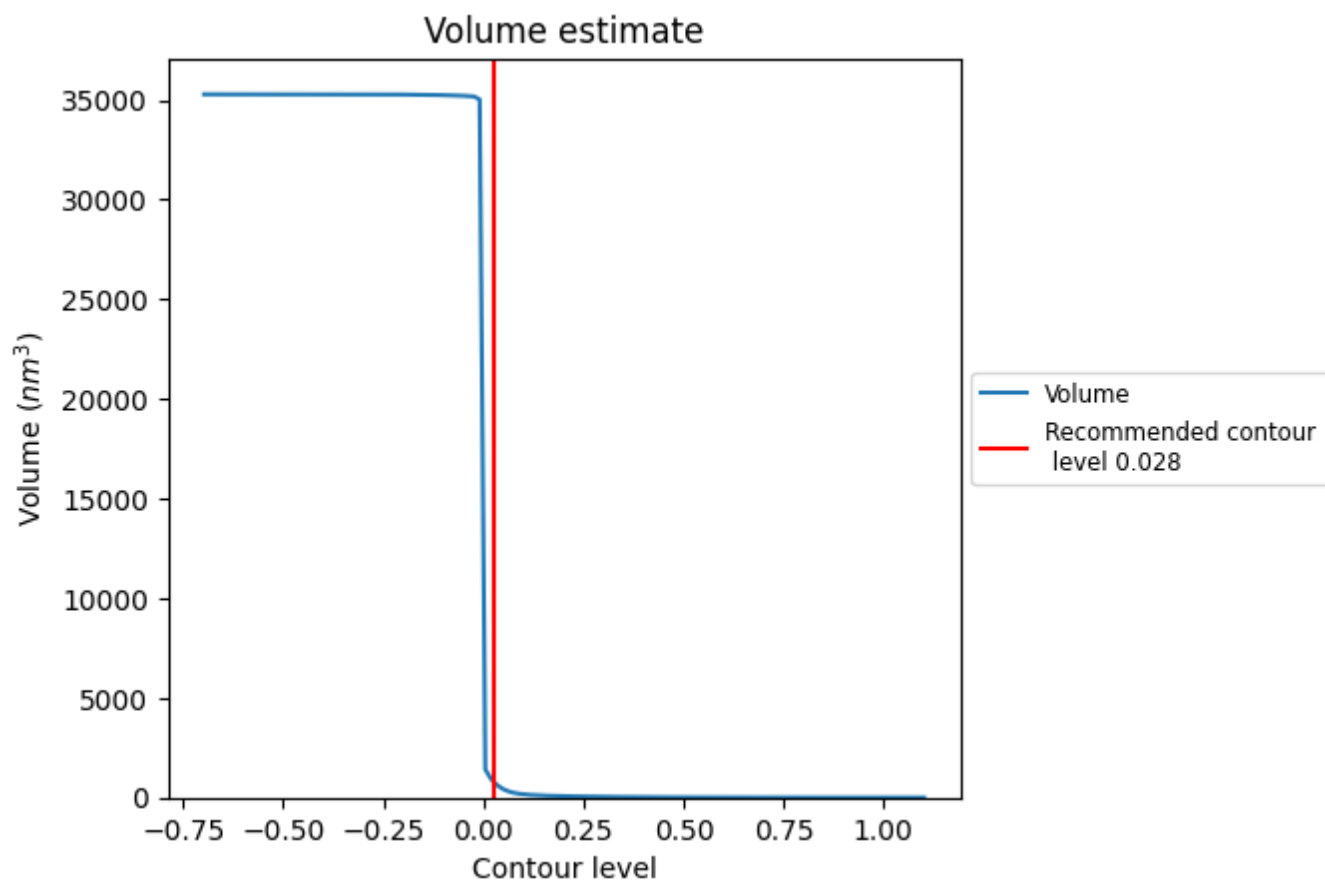
This section contains the results of statistical analysis of the map.

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



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

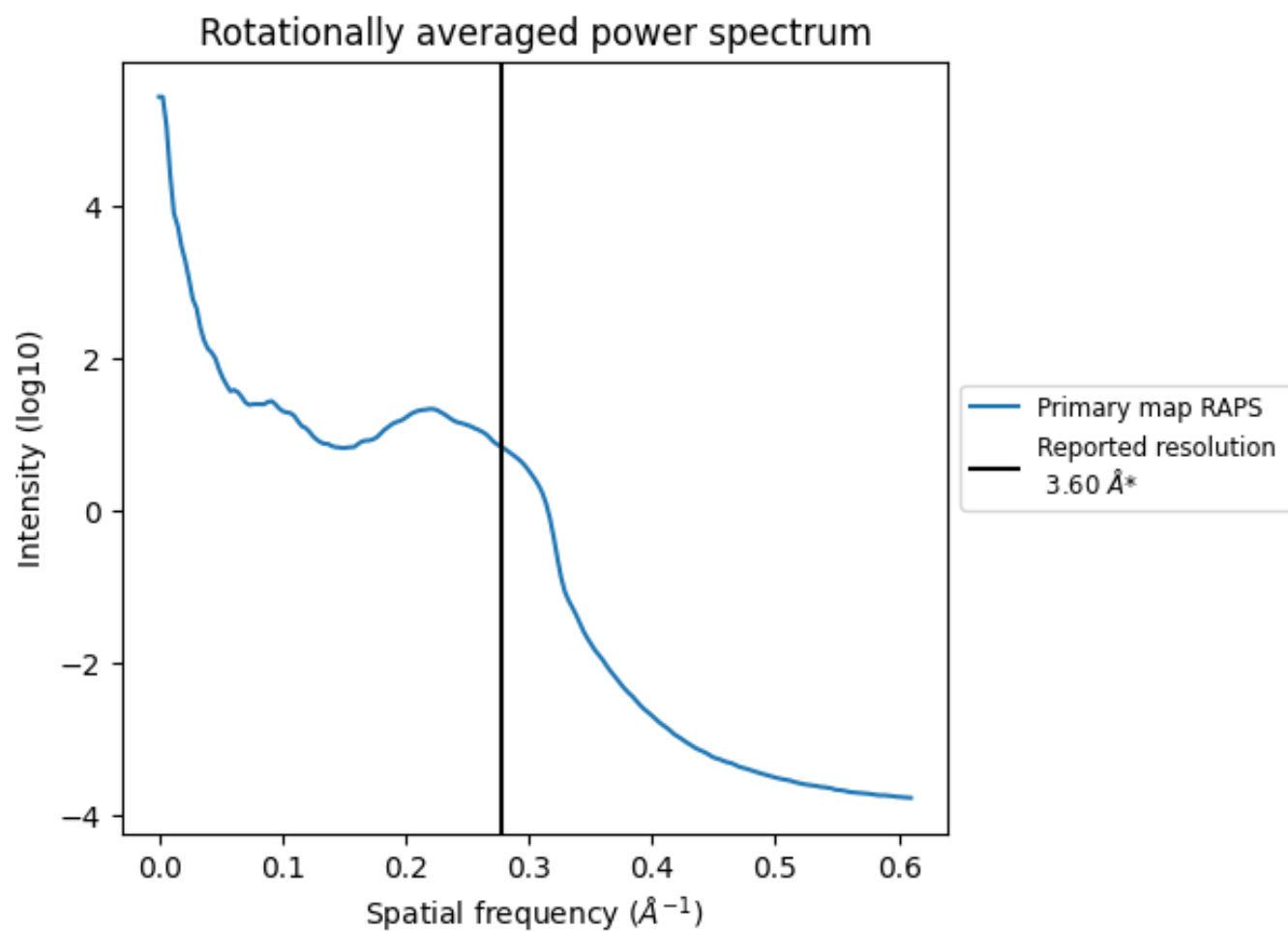
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753  $\text{nm}^3$ ; this corresponds to an approximate mass of 680 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>



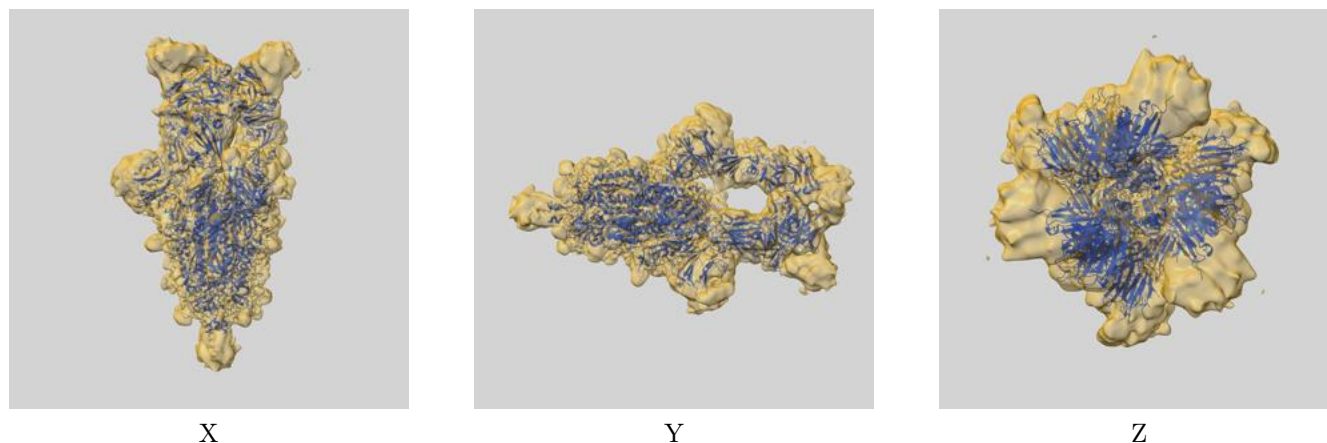
## 8 Fourier-Shell correlation

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

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

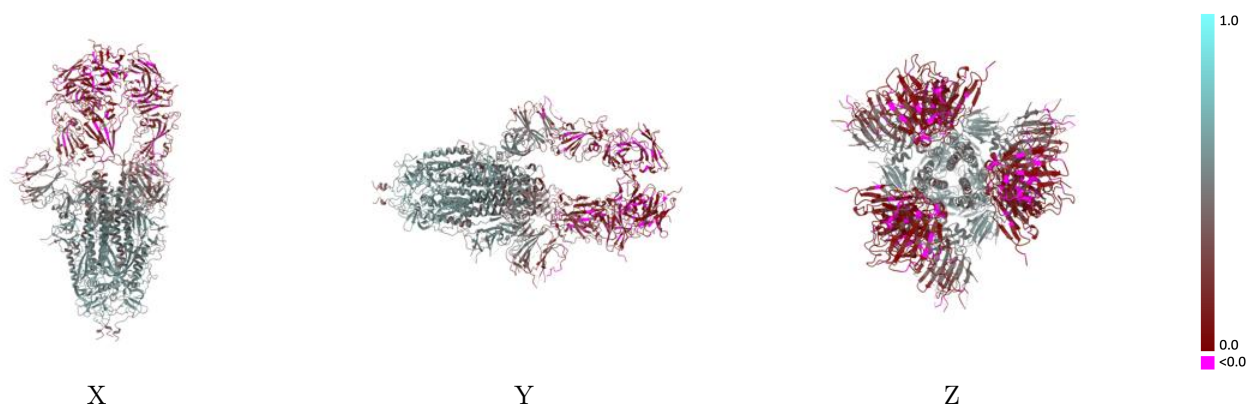
This section contains information regarding the fit between EMDB map EMD-12275 and PDB model 7ND4. Per-residue inclusion information can be found in section [3](#) on page [15](#).

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



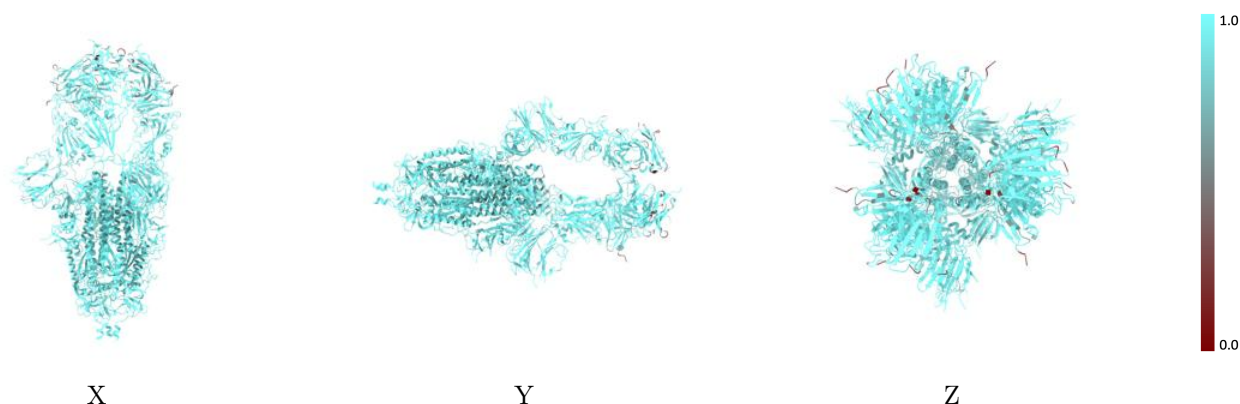
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



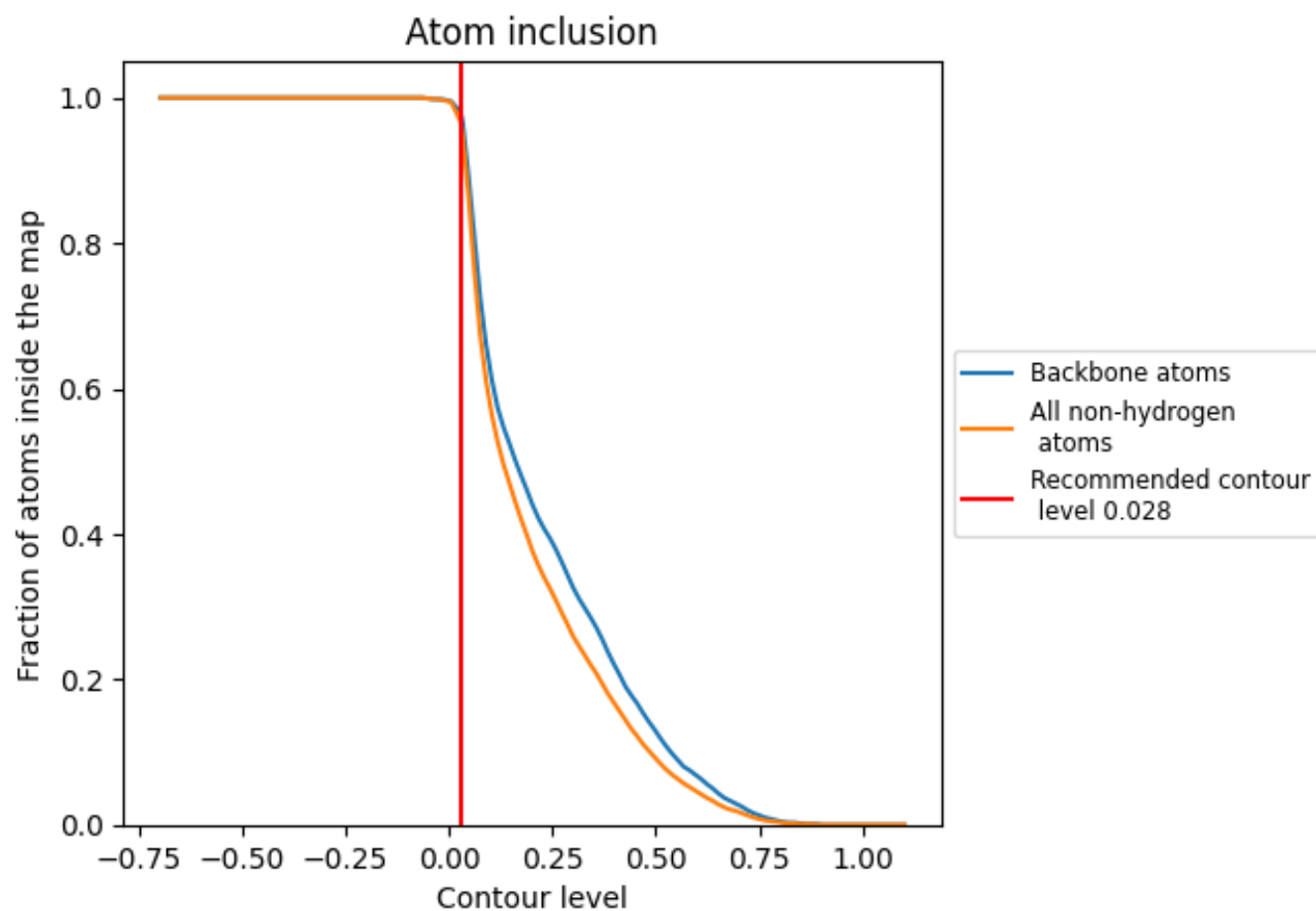
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9670	 0.3550
A	 0.9780	 0.4140
B	 0.9770	 0.4150
C	 0.9780	 0.4160
D	 0.9060	 0.0940
E	 0.9290	 0.1000
F	 0.9100	 0.0940
G	 0.9380	 0.0980
H	 0.9130	 0.0930
I	 0.8930	 0.2510
J	 0.9640	 0.4170
K	 1.0000	 0.4210
L	 0.9430	 0.0880
M	 1.0000	 0.4070
N	 0.9640	 0.3980
O	 0.9290	 0.2480
P	 0.9640	 0.4100
Q	 0.9640	 0.4200
R	 1.0000	 0.4070
S	 0.9640	 0.4110
T	 0.8570	 0.2450
U	 0.9640	 0.4070
V	 0.9640	 0.3980
W	 1.0000	 0.4170
X	 0.9640	 0.4160
Y	 0.8850	 0.1530
Z	 1.0000	 0.1780
a	 1.0000	 0.1760

