



# wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 07:00 am GMT

PDB ID : 7NDD  
EMDB ID : EMD-12284  
Title : EM structure of SARS-CoV-2 Spike glycoprotein (one RBD up) in complex with COVOX-159  
Authors : Duyvesteyn, H.M.E.; Zhao, Y.; Ren, J.; Stuart, D.  
Deposited on : 2021-01-30  
Resolution : 4.20 Å(reported)  
Based on initial model : 6Z97

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

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

A user guide is available at

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

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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

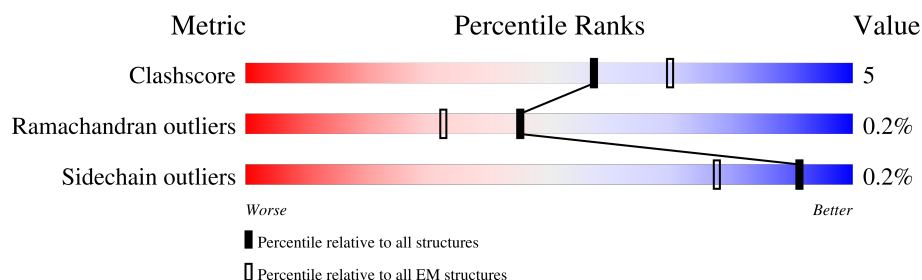
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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.




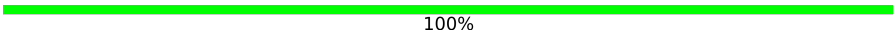
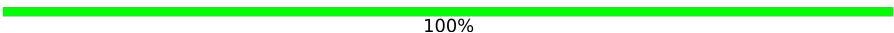
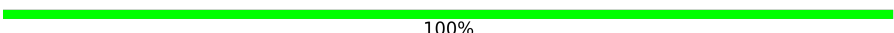
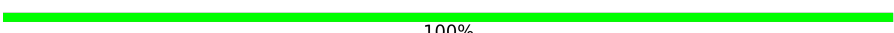
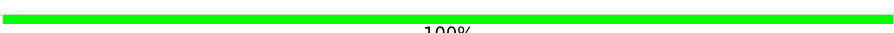
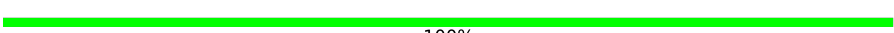






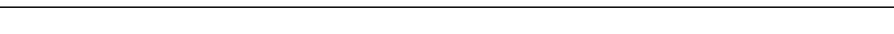
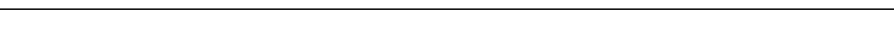
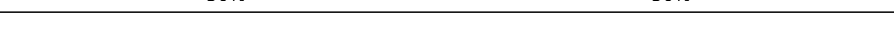
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	241	
2	F	241	
2	H	241	
3	E	227	
3	G	227	

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Mol	Chain	Length	Quality of chain
3	L	227	 43% 53%
4	I	2	 100%
4	J	2	 100%
4	K	2	 100%
4	M	2	 100%
4	N	2	 100%
4	O	2	 100%
4	P	2	 100%
4	Q	2	 100%
4	R	2	 50% 50%
4	S	2	 100%
4	T	2	 100%
4	U	2	 100%
4	V	2	 100%
4	W	2	 50% 50%
4	X	2	 100%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30645 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	1063	Total	C	N	O	S	0	0
			8314	5306	1387	1583	38		
1	B	1063	Total	C	N	O	S	0	0
			8314	5306	1387	1583	38		
1	C	1063	Total	C	N	O	S	0	0
			8314	5306	1387	1583	38		

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-159 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	115	Total	C	N	O	S	0	0
			856	534	153	164	5		
2	F	115	Total	C	N	O	S	0	0
			856	534	153	164	5		
2	H	115	Total	C	N	O	S	0	0
			856	534	153	164	5		

- Molecule 3 is a protein called COVOX-159 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	106	Total	C	N	O	S	0	0
			793	499	135	157	2		
3	G	106	Total	C	N	O	S	0	0
			793	499	135	157	2		
3	L	106	Total	C	N	O	S	0	0
			793	499	135	157	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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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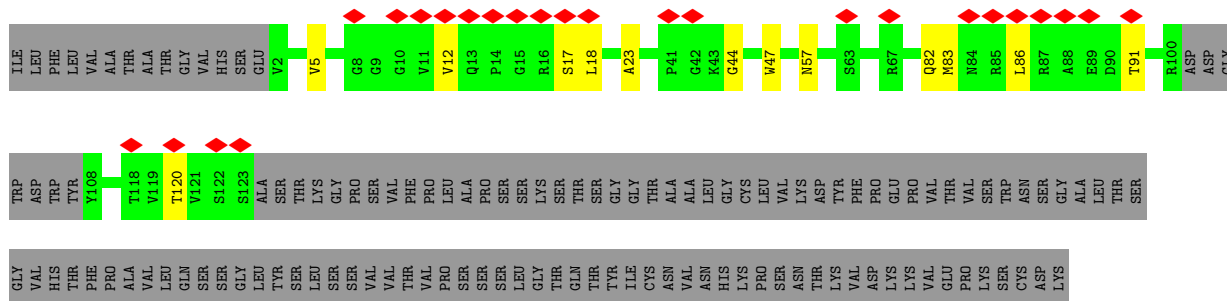
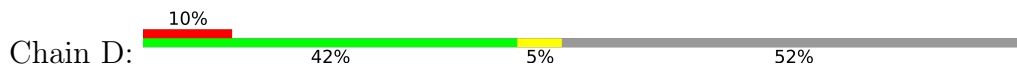
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C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



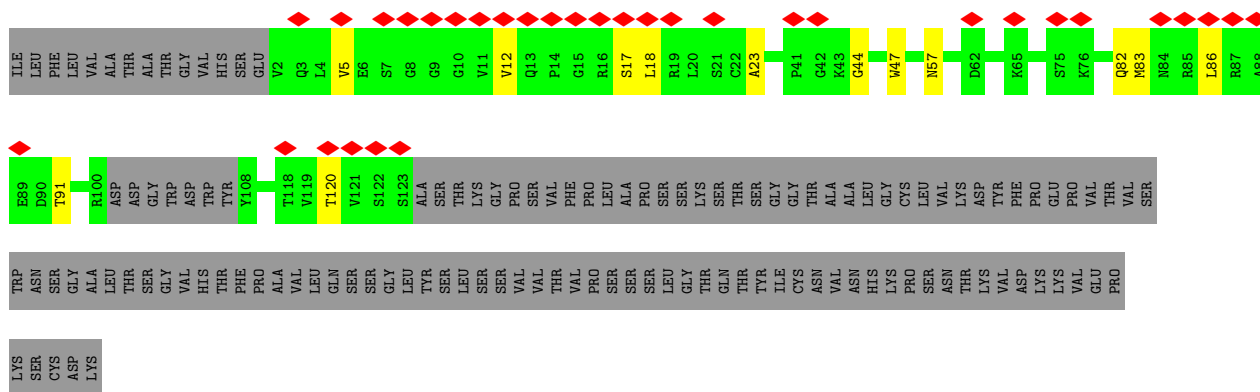
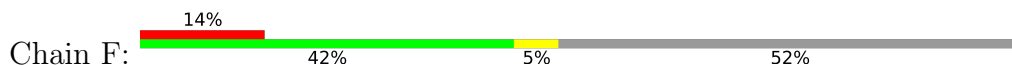


LYS	ASN	L859	SER	T523	V320	M149	MET
ASN	THR	Y873	VAL	G526	V327	W152	PHE
SER	SER		ALA	K529	R328		VAL
PRO	ASP	S884	S689	K529		F157	LEU
ASP	ASP		P715	S530	N331	R158	VAL
ASP	ASP	T887		T531	I332		LEU
LEU	ASP	N914	V722	S532	I333	T167	LEU
GLY	ASP		I726	L533	C336	S172	PRO
ASP	GLY	D950		K557		Q173	VAL
ILE	SER	Q954	V736	Q564	Y351		SER
GLY	GLY	Y976	L763	D574	A352	D176	Q14
ASN	ASN	D979	I770	R577	I358	LEU	
ALA	SER	I980	Q774	D578	R359	GLY	L18
SER	VAL			T581	N360	GLN	T19
VAL	VAL	L984	K790		A363	GLY	A27
ASN	ASN	V1008	D796	V608		N185	T33
GLN	ILE				F374	N188	V42
LYS	GLN	K1028	I805	E619	S375	L189	
GLU	ILE	E1031	K811	V620	T376	R190	P87
ASP	ASP	C1032	D820	VAL	F377	E191	
ARG	ARG	R1039	I818	ILE	R378	F192	S60
LEU	LEU		S319	HIS	F194	K195	W64
ASN	ASN	V1061	D820	ASP	N394	N196	
VAL	VAL	H1064	T827	GLN	V395	I197	H69
LYS	ALA		LEU	LEU	Y421	D198	VAL
ASN	ASP	P1069	ALA	THR	D427	G199	GLY
LEU	ALA		ASP	PRO		Y200	THR
ASN	GLY	K1086	GLY	THR	G431	Y204	ASN
GLU	PHE	R1091	ARG	TRP	C432	T208	GLY
SER	ILE		VAL	ARG	P209	P209	THR
LEU	LYS		THR	VAL	A435		K77
ILE	GLN	S1097	SER	TYR	W436	D215	Y91
ASP	TYR		THR	SER			
LEU	GLY	W1102	GLY	THR	L452	G219	R102
GLN	ASP	F1103	ASP	GLY	R457	L223	F106
GLU	CYS		GLN	H641			
LEU	LEU	T1120	LEU		L461	D228	T109
GLY	GLY	F1121	GLY	V656	R466	L223	L110
LYS	ASP	V1122	ASP	H657	D467	P230	D111
THR	ILE		ALA	N658			
GLU	ALA	S1147	ALA	T676	G502	S255	L117
GLN	ARG		ARG	GLN			
LYS	LYS		ASP	THR	Q506	V258	F140
SER	GLU		LEU	ASN			L141
GLY	LEU		ILE	SER	F515	R273	G142
ILE	ASP		CYS	PRO		D290	V143
PRO	LYS		ALA	GLY	A520		H146
GLU	TYR		GLN	SER	P521	L296	H147
ALA	PHE		S654	ALA	S523		N149

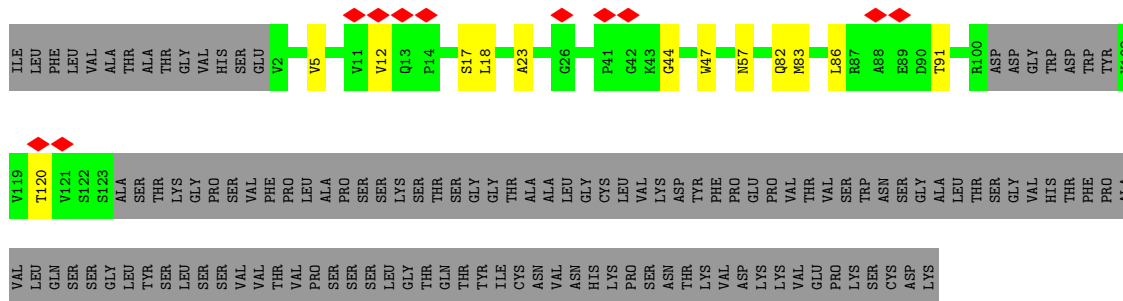
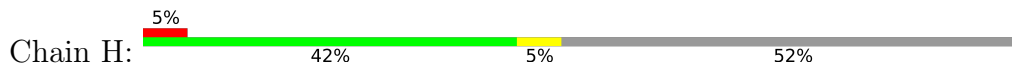
- Molecule 2: COVOX-159 Fab heavy chain



- Molecule 2: COVOX-159 Fab heavy chain

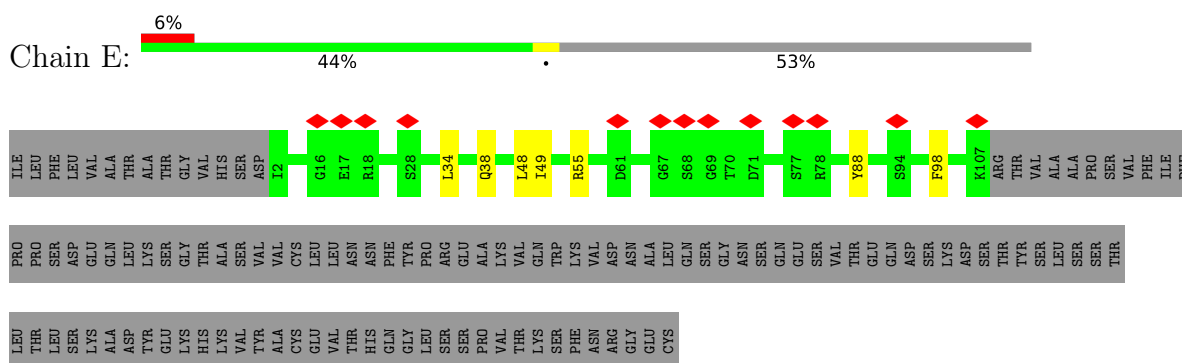


- Molecule 2: COVOX-159 Fab heavy chain

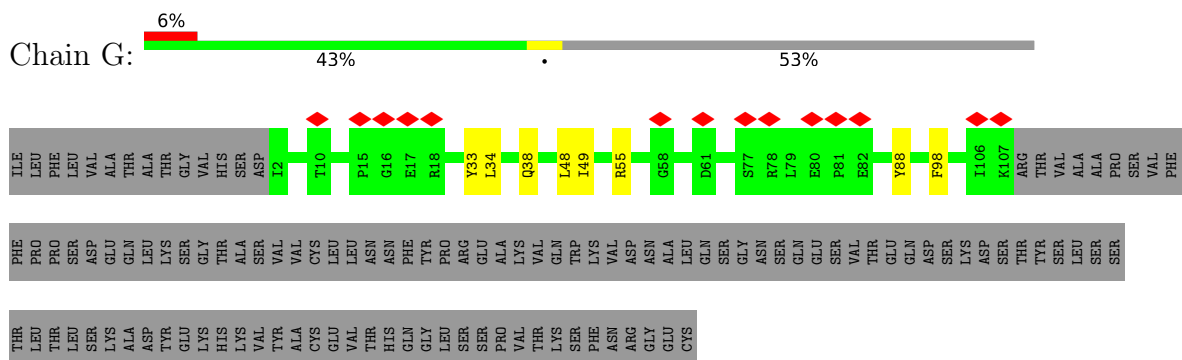


- Molecule 3: COVOX-159 Fab light chain

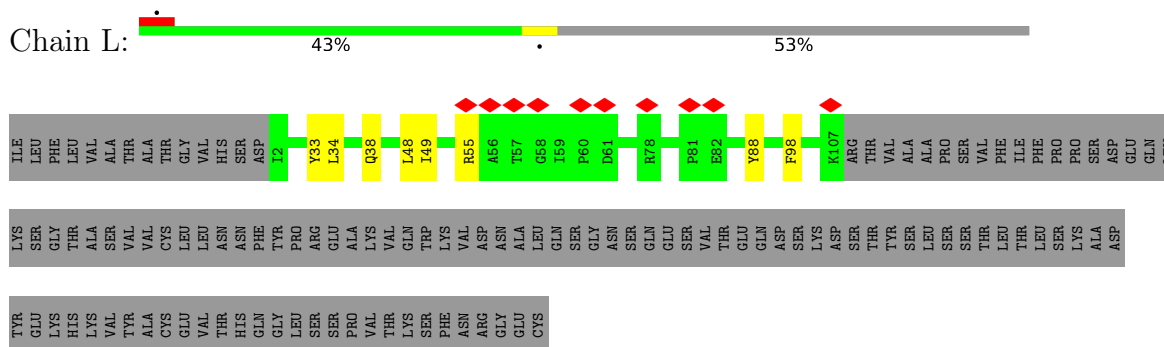




- Molecule 3: COVOX-159 Fab light chain



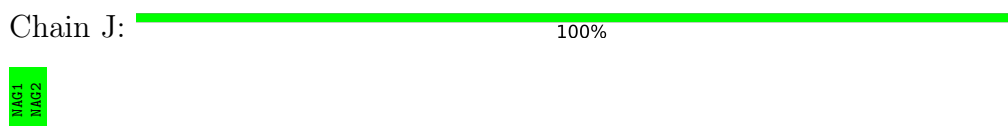
- Molecule 3: COVOX-159 Fab light chain



- 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%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  100%



- 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%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27880	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 ( $e^-/\text{\AA}^2$ )	50.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.441	Depositor
Minimum map value	-0.821	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.046	Depositor
Map size ( $\text{\AA}$ )	459.19998, 459.19998, 459.19998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.64, 1.64, 1.64	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.26	0/8508	0.48	0/11580
1	B	0.27	0/8508	0.51	2/11580 (0.0%)
1	C	0.27	0/8508	0.49	1/11580 (0.0%)
2	D	0.25	0/873	0.50	0/1180
2	F	0.25	0/873	0.50	0/1180
2	H	0.25	0/873	0.50	0/1180
3	E	0.25	0/811	0.52	0/1100
3	G	0.25	0/811	0.51	0/1100
3	L	0.25	0/811	0.52	0/1100
All	All	0.26	0/30576	0.50	3/41580 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
1	C	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	GLY	C-N-CD	-10.37	97.80	120.60
1	C	526	GLY	C-N-CD	-5.54	108.41	120.60
1	B	321	GLN	C-N-CD	-5.17	109.22	120.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	526	GLY	Peptide
1	B	331	ASN	Peptide
1	B	333	THR	Peptide
1	B	527	PRO	Peptide
1	B	528	LYS	Peptide

## 5.2 Too-close contacts

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	8314	0	8088	74	0
1	B	8314	0	8088	98	0
1	C	8314	0	8088	84	0
2	D	856	0	782	9	0
2	F	856	0	782	9	0
2	H	856	0	782	9	0
3	E	793	0	753	4	0
3	G	793	0	753	5	0
3	L	793	0	753	5	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	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	0	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	A	112	0	104	0	0
5	B	112	0	104	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	112	0	104	1	0
All	All	30645	0	29556	274	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 5.

The worst 5 of 274 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:335:LEU:O	1:B:361:CYS:HB2	1.84	0.78
1:A:147:LYS:NZ	2:F:57:ASN:OD1	2.24	0.70
1:C:147:LYS:NZ	2:D:57:ASN:OD1	2.25	0.69
1:A:394:ASN:ND2	1:B:200:TYR:OH	2.27	0.68
1:A:564:GLN:NE2	1:A:577:ARG:O	2.28	0.67

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	1051/1288 (82%)	1006 (96%)	44 (4%)	1 (0%)	48	82
1	B	1051/1288 (82%)	998 (95%)	46 (4%)	7 (1%)	19	56
1	C	1051/1288 (82%)	1002 (95%)	48 (5%)	1 (0%)	48	82
2	D	111/241 (46%)	109 (98%)	2 (2%)	0	100	100
2	F	111/241 (46%)	109 (98%)	2 (2%)	0	100	100
2	H	111/241 (46%)	109 (98%)	2 (2%)	0	100	100
3	E	104/227 (46%)	100 (96%)	4 (4%)	0	100	100
3	G	104/227 (46%)	100 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	104/227 (46%)	100 (96%)	4 (4%)	0	100	100
All	All	3798/5268 (72%)	3633 (96%)	156 (4%)	9 (0%)	45	77

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	PRO
1	B	332	ILE
1	B	334	ASN
1	B	528	LYS
1	C	529	LYS

### 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	929/1113 (84%)	928 (100%)	1 (0%)	92	94
1	B	929/1113 (84%)	927 (100%)	2 (0%)	92	94
1	C	929/1113 (84%)	927 (100%)	2 (0%)	92	94
2	D	83/202 (41%)	83 (100%)	0	100	100
2	F	83/202 (41%)	83 (100%)	0	100	100
2	H	83/202 (41%)	83 (100%)	0	100	100
3	E	82/194 (42%)	81 (99%)	1 (1%)	67	78
3	G	82/194 (42%)	81 (99%)	1 (1%)	67	78
3	L	82/194 (42%)	81 (99%)	1 (1%)	67	78
All	All	3282/4527 (72%)	3274 (100%)	8 (0%)	91	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	34	LEU
3	G	34	LEU

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Mol	Chain	Res	Type
1	C	914	ASN
1	C	377	PHE
3	E	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	613	GLN
2	F	82	GLN

### 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 ⓘ

30 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	0.22	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.34	0	17,19,21	0.52	0
4	NAG	J	1	4,1	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	J	2	4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	K	1	4,1	14,14,15	0.16	0	17,19,21	0.47	0
4	NAG	K	2	4	14,14,15	0.30	0	17,19,21	0.50	0
4	NAG	M	1	4,1	14,14,15	0.18	0	17,19,21	0.48	0
4	NAG	M	2	4	14,14,15	0.28	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	N	1	4,1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	N	2	4	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	O	1	4,1	14,14,15	0.18	0	17,19,21	0.52	0
4	NAG	O	2	4	14,14,15	0.37	0	17,19,21	0.51	0
4	NAG	P	1	4,1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	P	2	4	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	Q	1	4,1	14,14,15	0.15	0	17,19,21	0.49	0
4	NAG	Q	2	4	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	R	1	4,1	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	R	2	4	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	S	1	4,1	14,14,15	0.24	0	17,19,21	0.48	0
4	NAG	S	2	4	14,14,15	0.27	0	17,19,21	0.54	0
4	NAG	T	1	4,1	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	T	2	4	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	U	1	4,1	14,14,15	0.18	0	17,19,21	0.53	0
4	NAG	U	2	4	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	V	1	4,1	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	V	2	4	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	W	1	4,1	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	W	2	4	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	X	1	4,1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	X	2	4	14,14,15	0.27	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	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
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	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
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	-	2/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

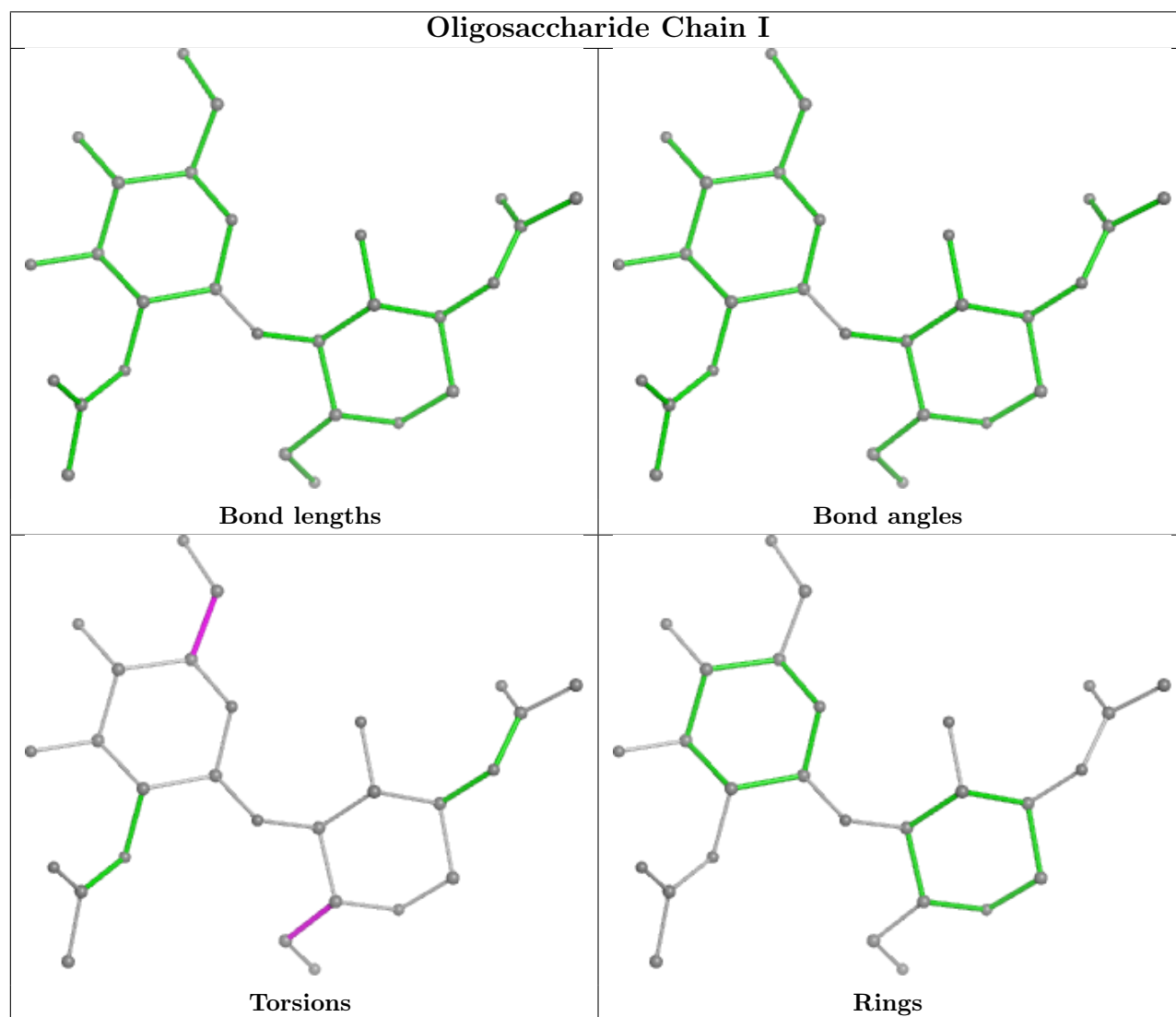
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6

There are no ring outliers.

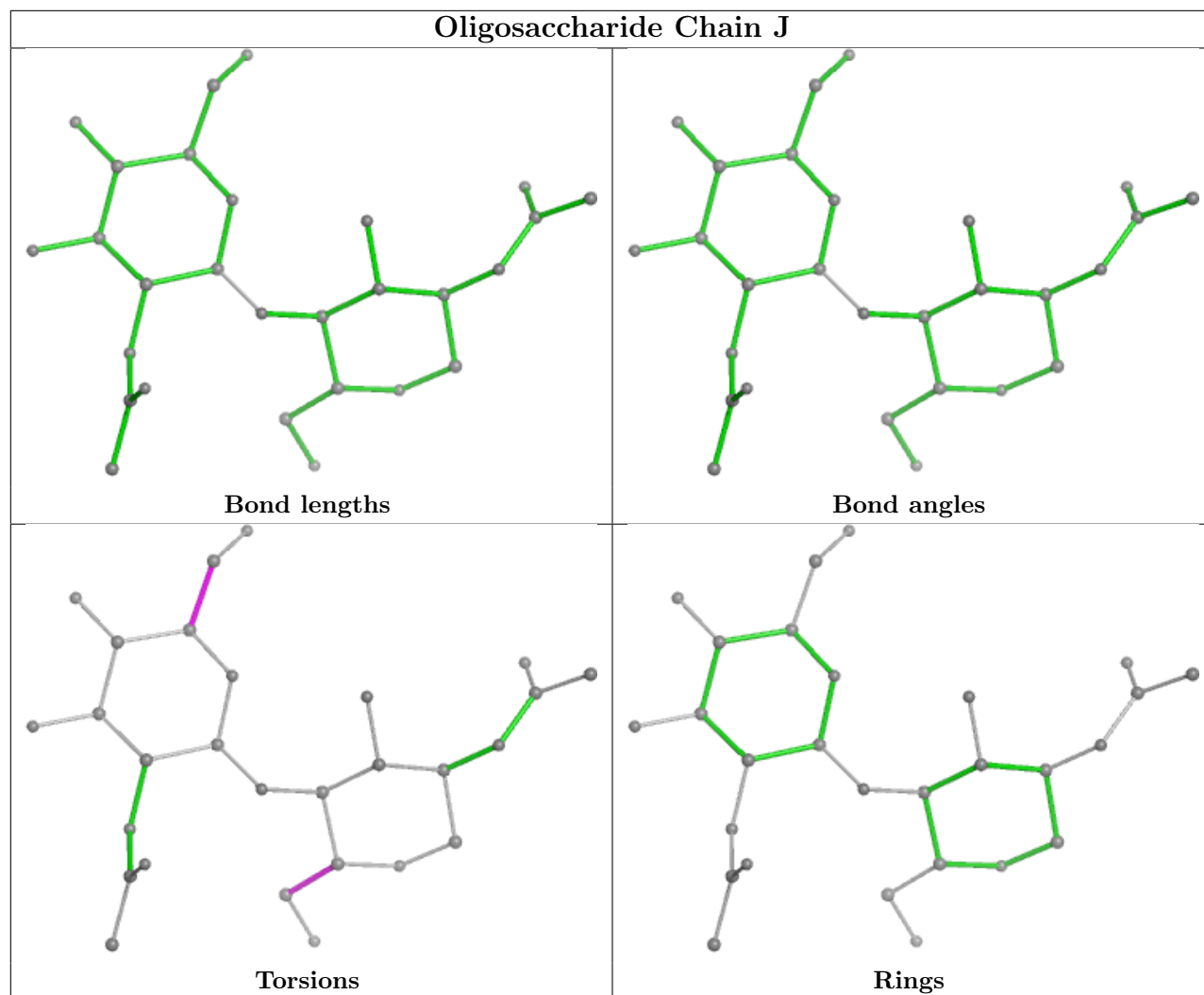
2 monomers are involved in 2 short contacts:

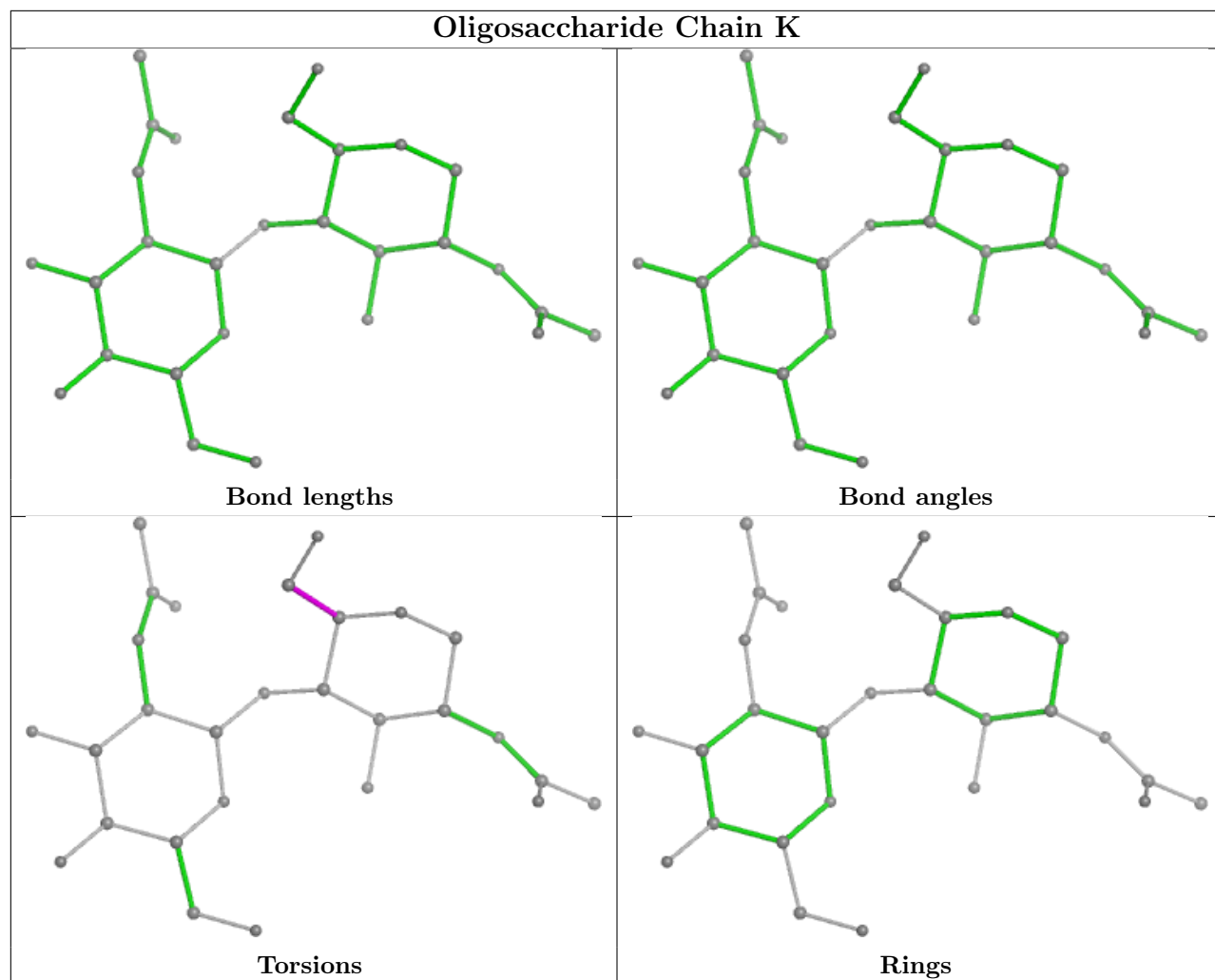
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	W	1	NAG	1	0
4	R	1	NAG	1	0

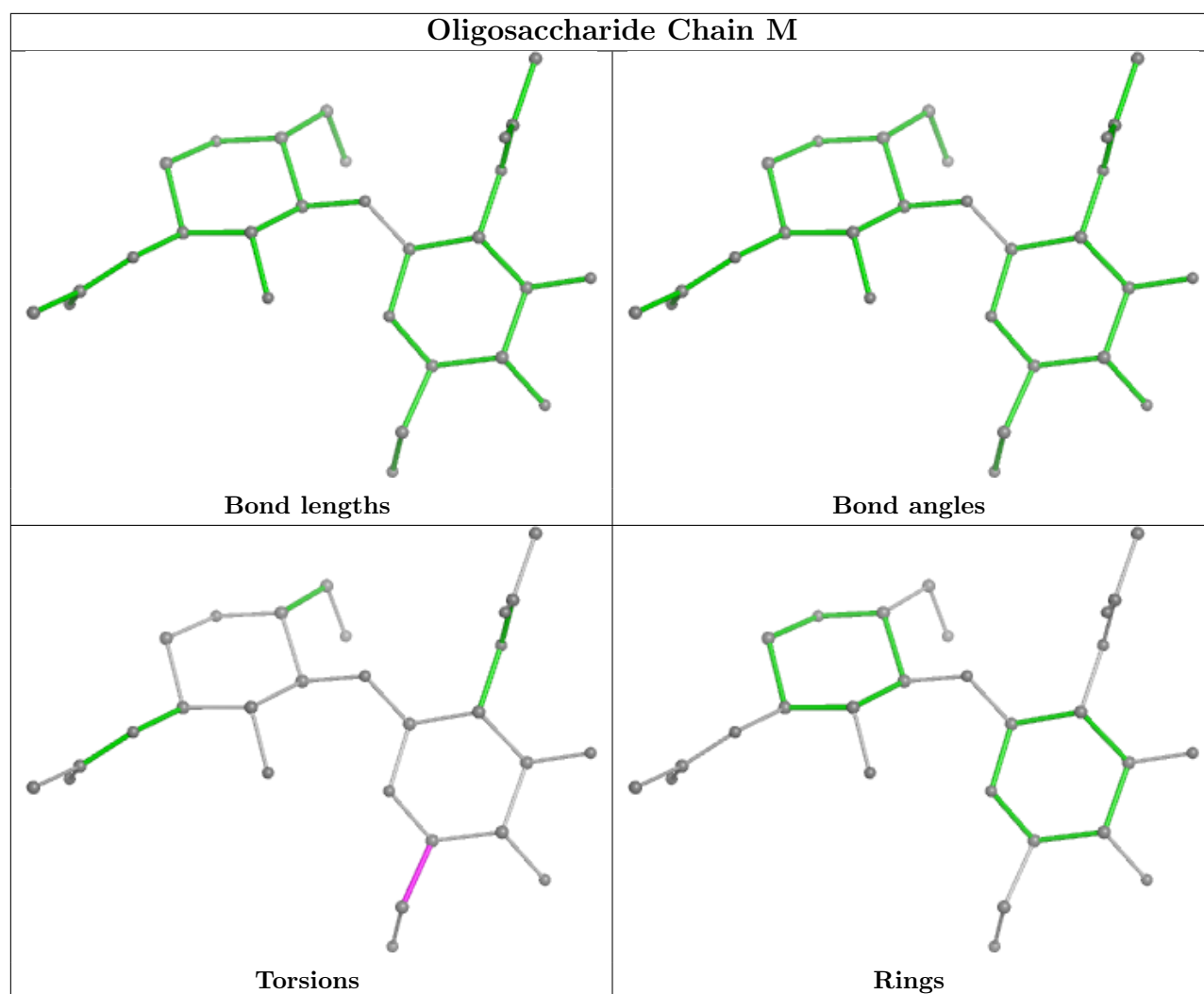
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

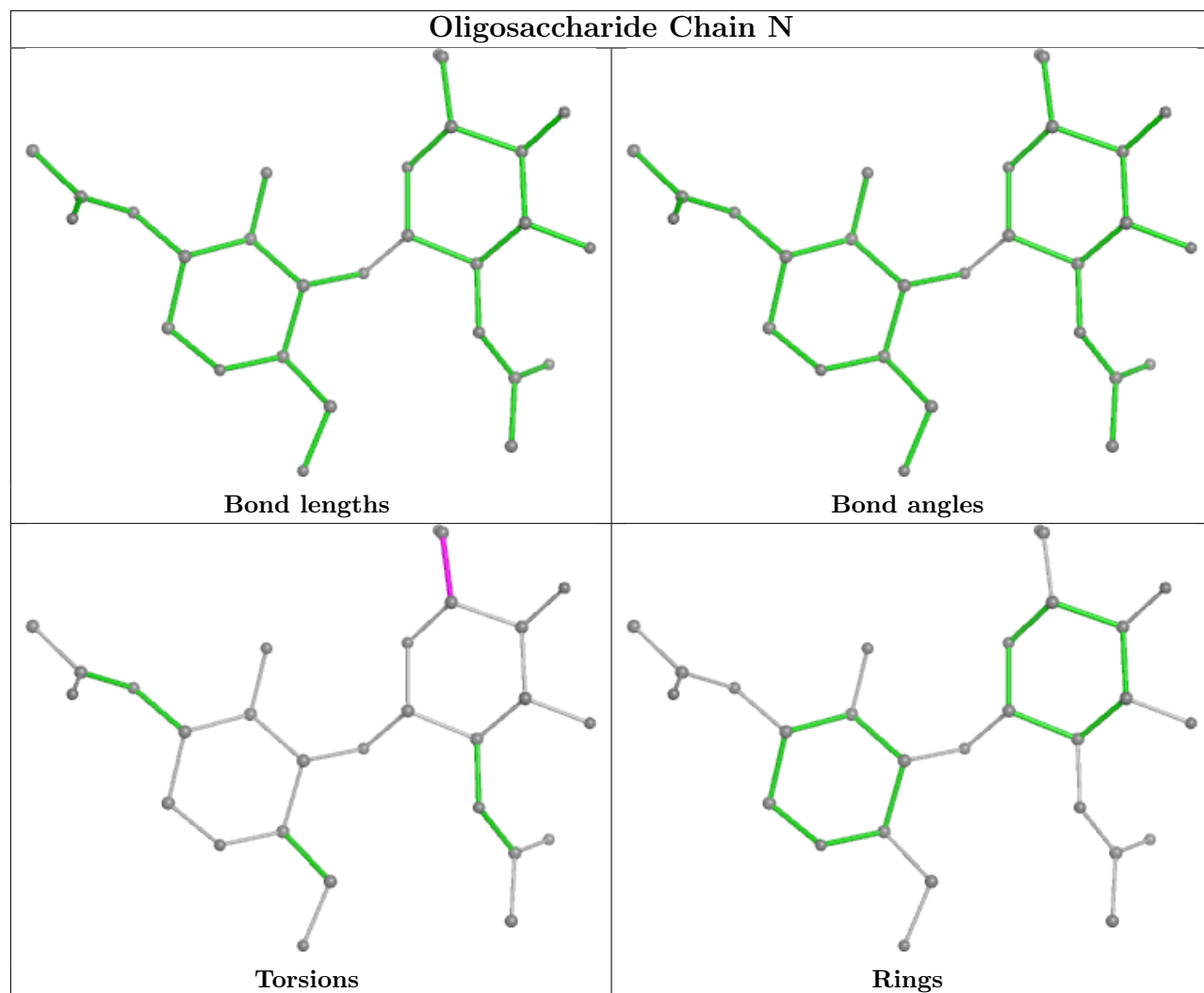


## Oligosaccharide Chain J

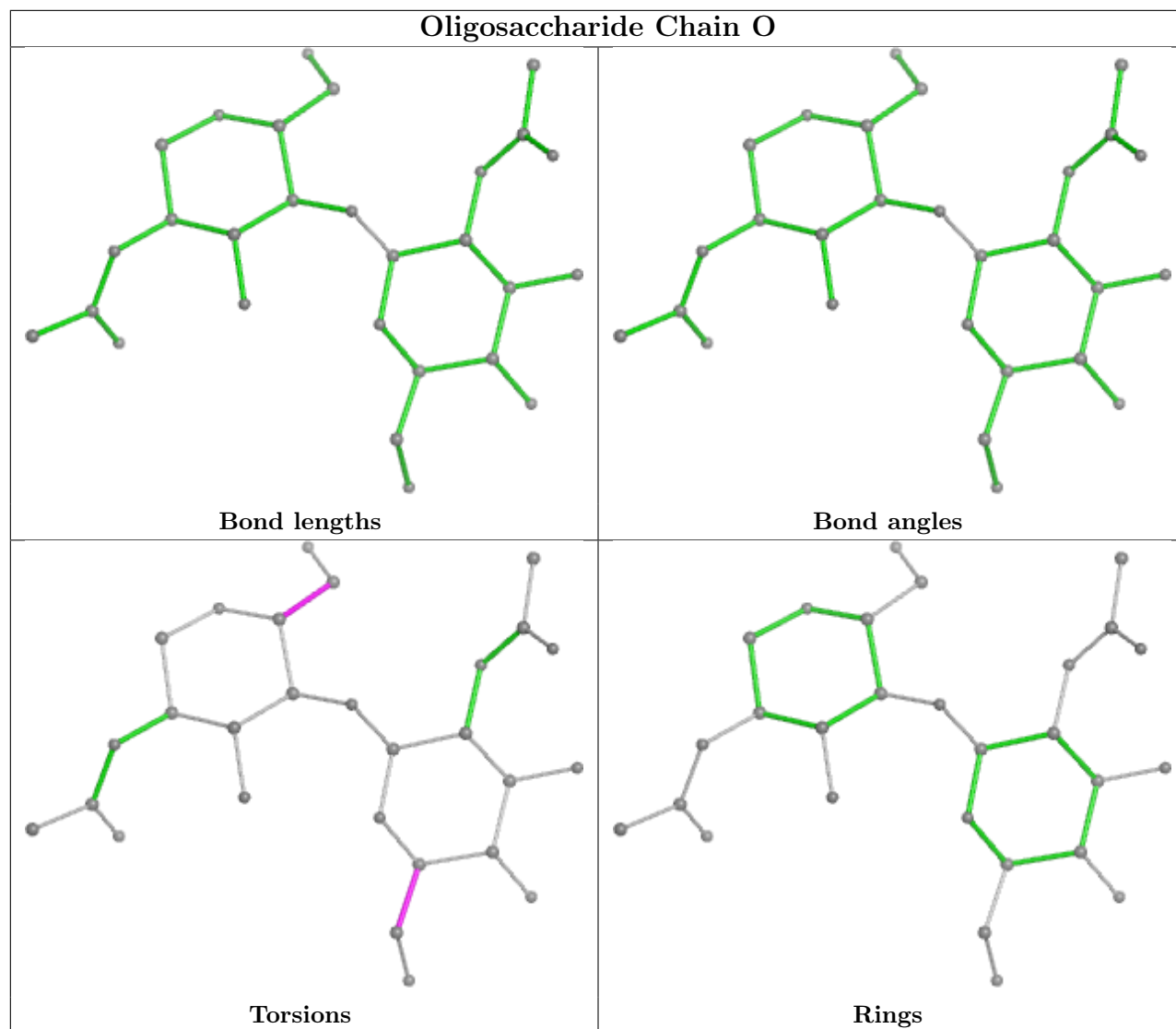




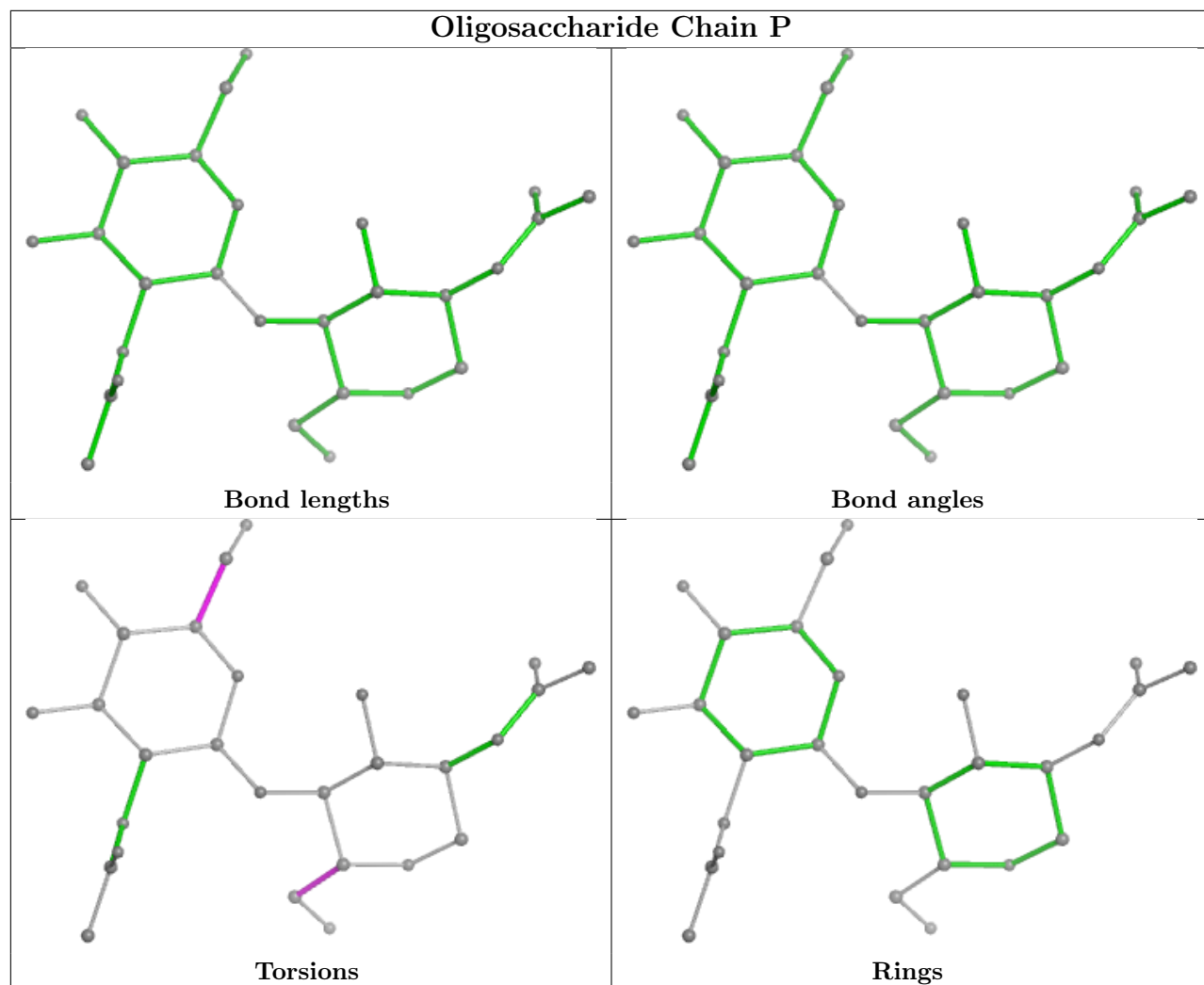


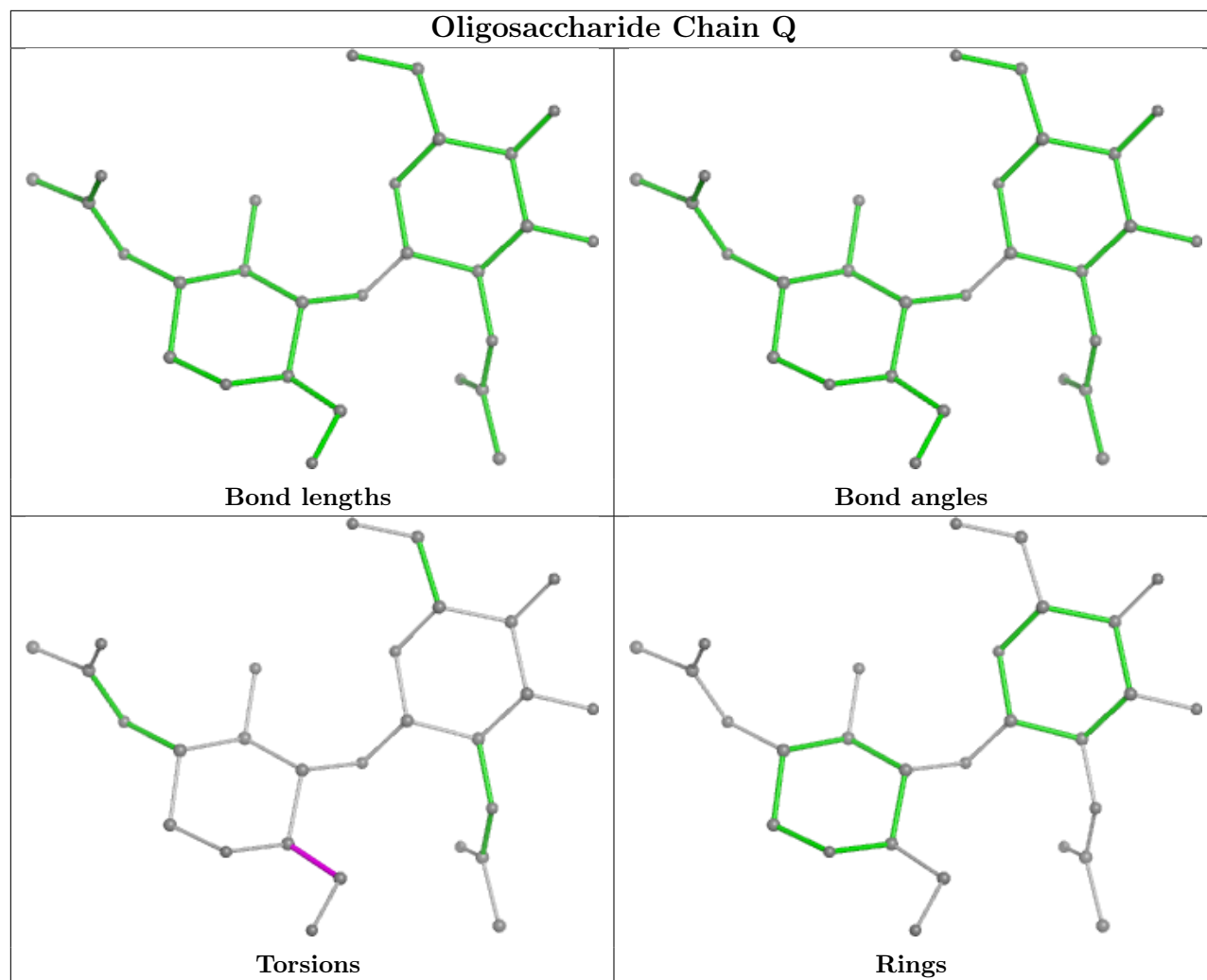


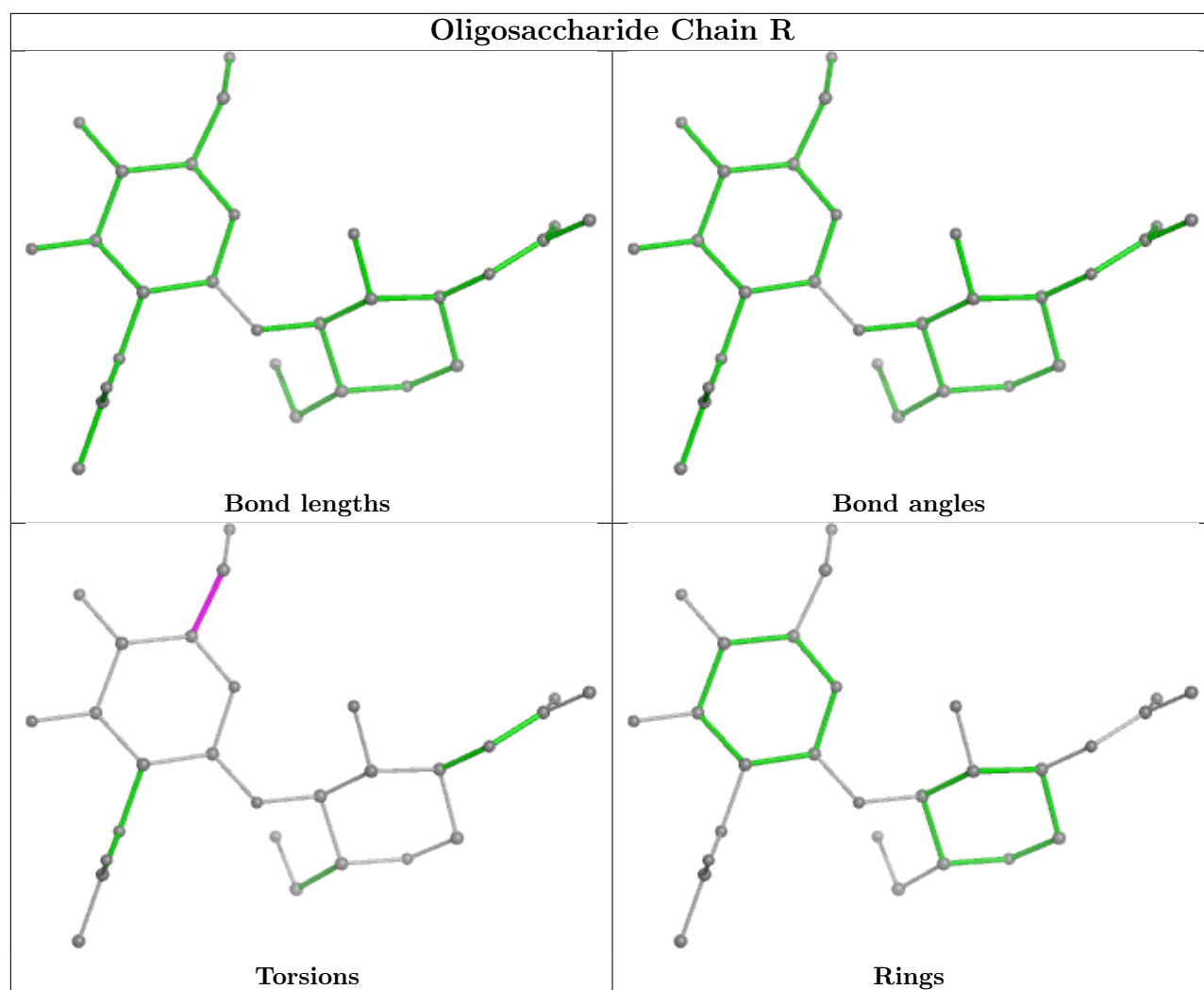


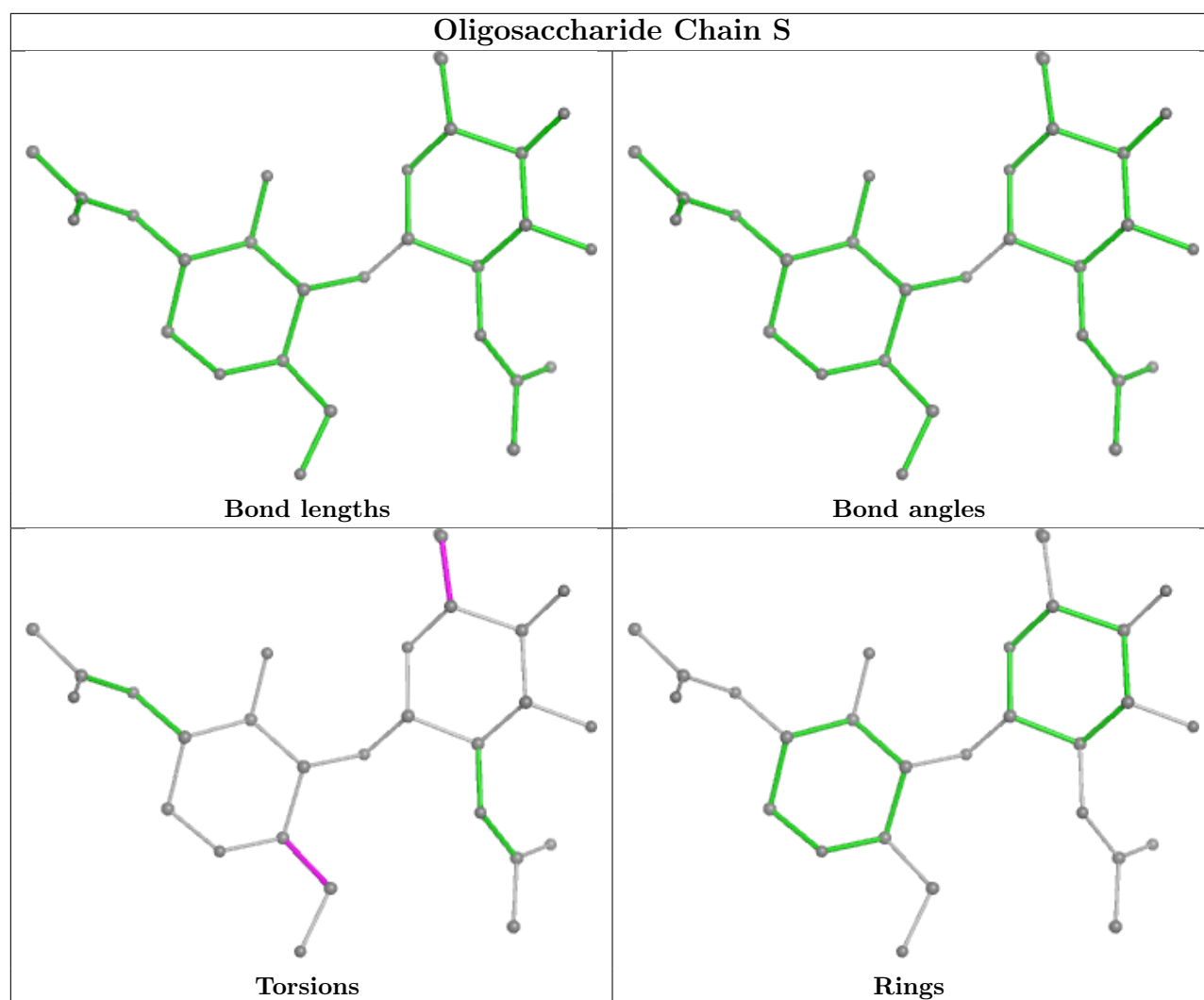


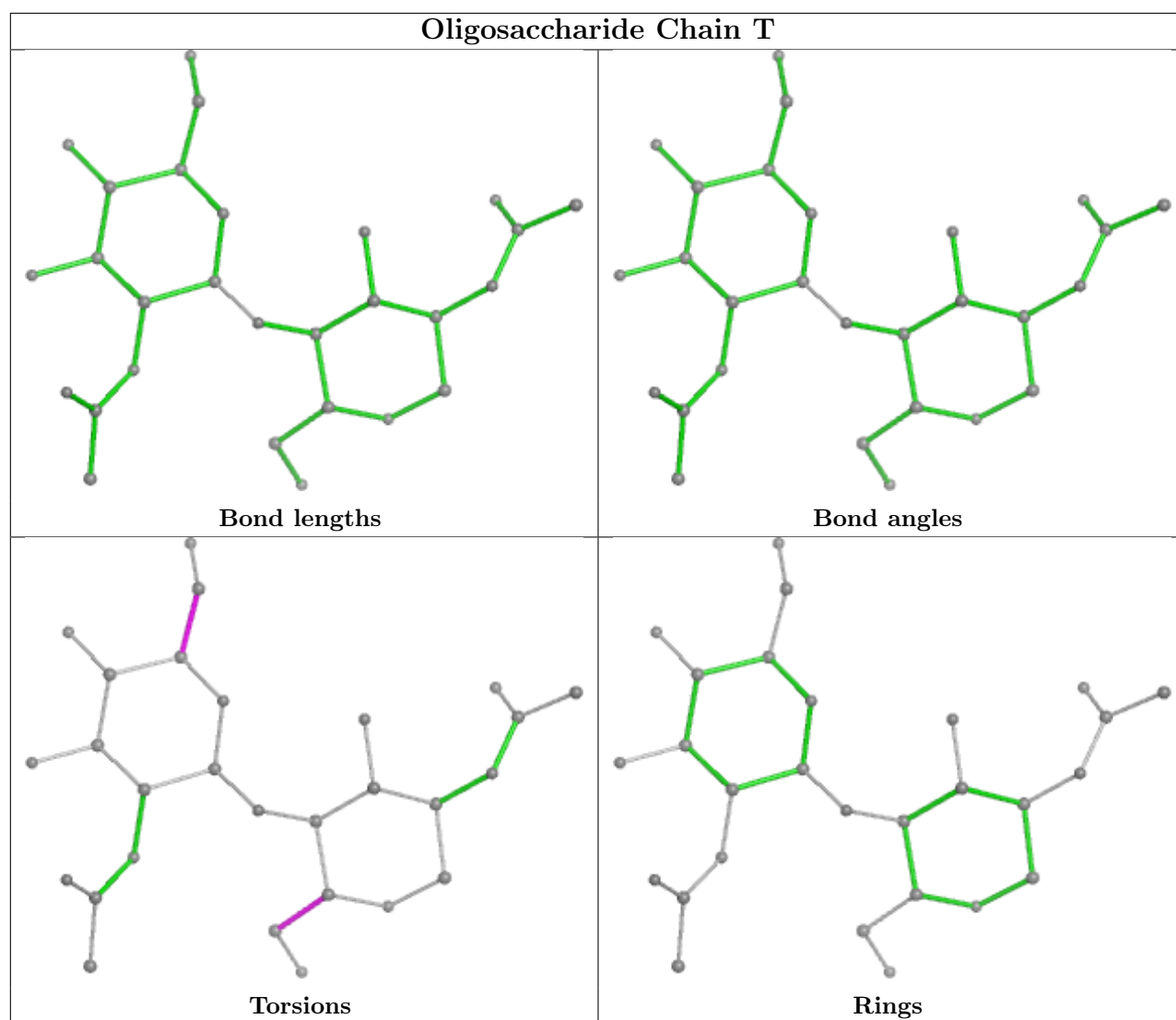
## Oligosaccharide Chain P

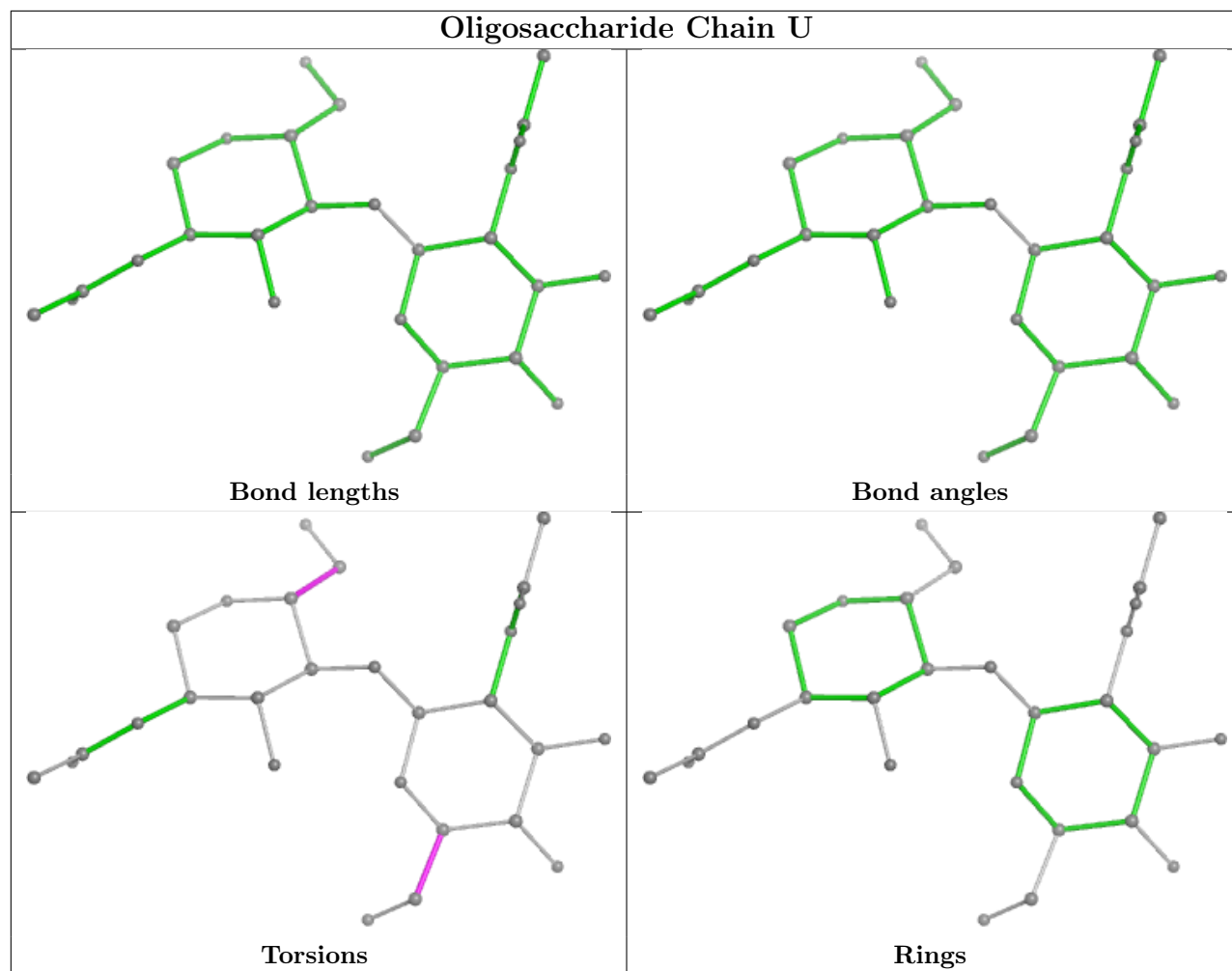


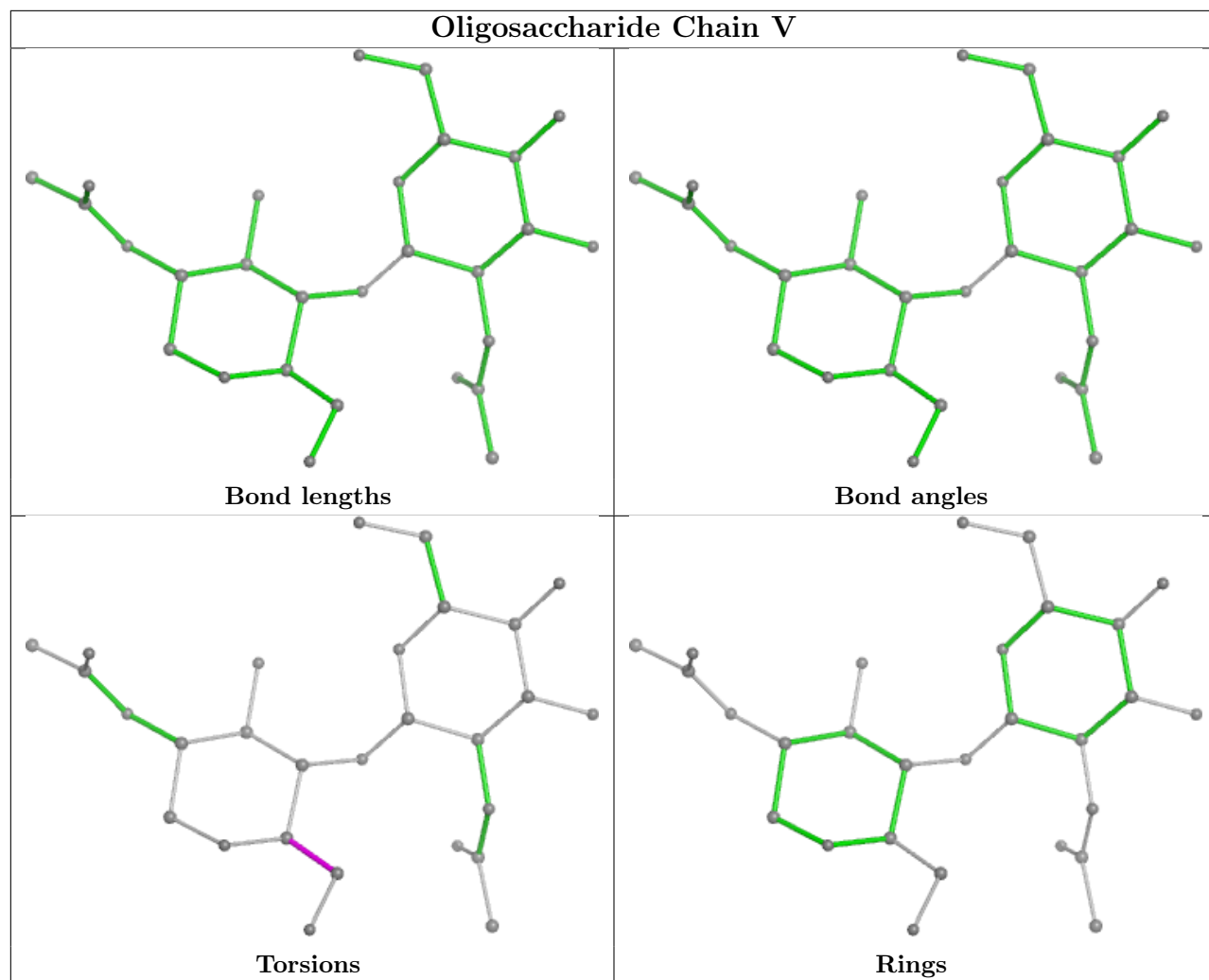




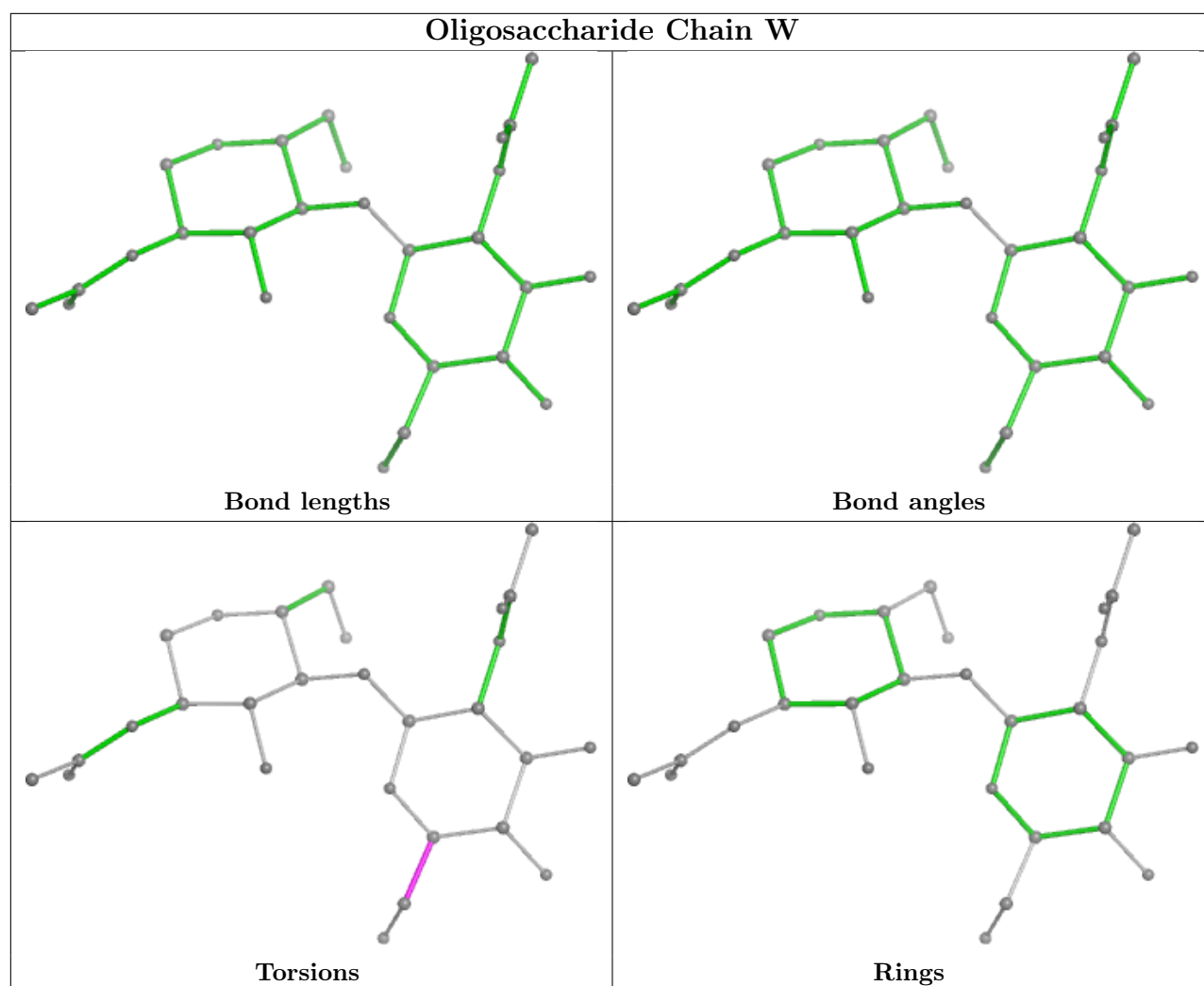


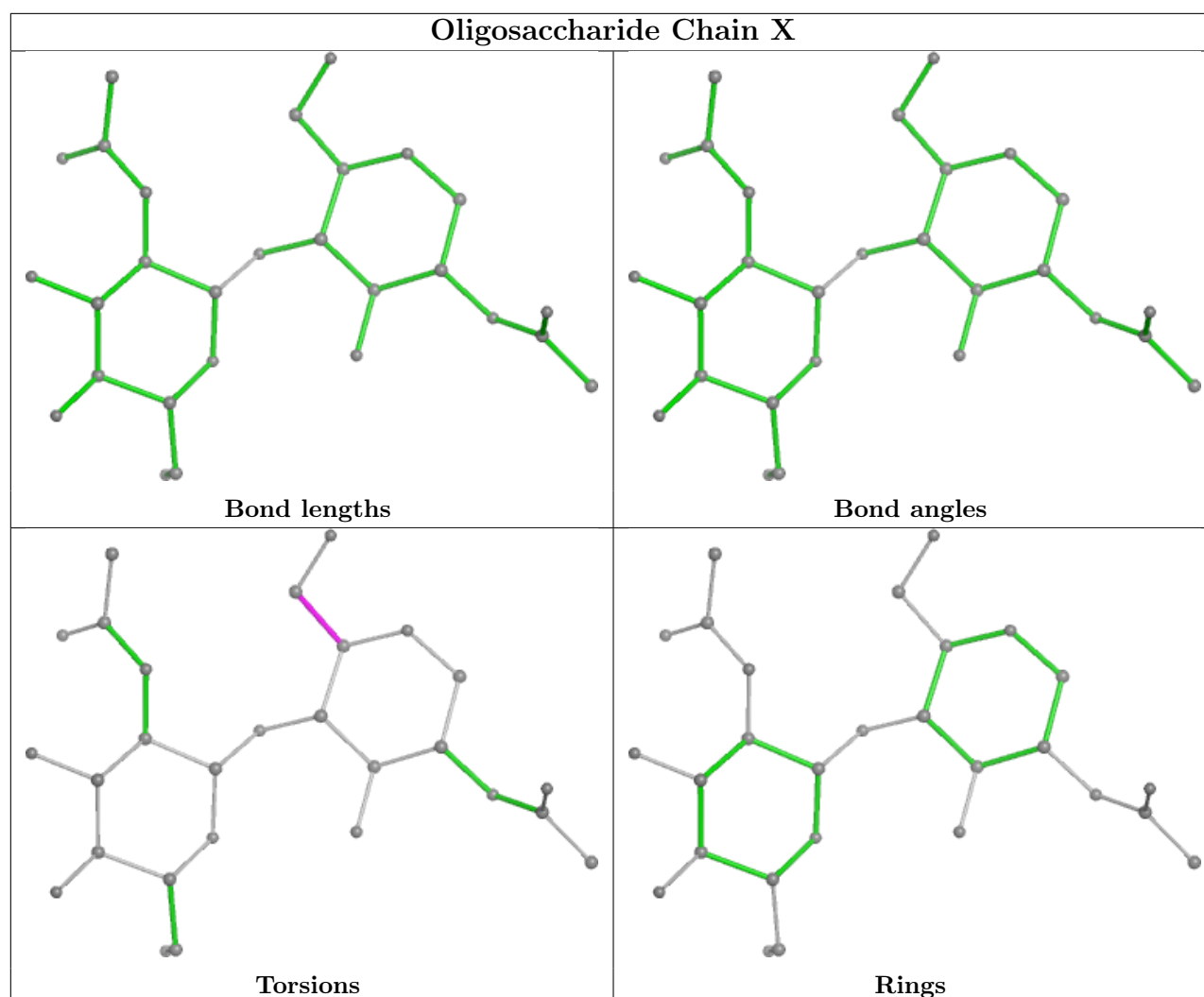












## 5.6 Ligand geometry [i](#)

24 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	$\# Z  > 2$
5	NAG	A	1308	1	14,14,15	0.32	0	17,19,21	0.44	0
5	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	0.50	0
5	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.47	0
5	NAG	C	1302	1	14,14,15	0.30	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	1304	1	14,14,15	0.27	0	17,19,21	0.50	0
5	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.51	0
5	NAG	B	1306	1	14,14,15	0.24	0	17,19,21	0.49	0
5	NAG	B	1303	1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	B	1308	1	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	A	1307	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	C	1304	1	14,14,15	0.23	0	17,19,21	0.50	0
5	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.48	0
5	NAG	C	1301	1	14,14,15	0.20	0	17,19,21	0.48	0
5	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.49	0
5	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.51	0
5	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.52	0
5	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	B	1302	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	A	1302	1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	C	1308	1	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	C	1305	1	14,14,15	0.32	0	17,19,21	0.48	0
5	NAG	C	1307	1	14,14,15	0.27	0	17,19,21	0.53	0
5	NAG	C	1303	1	14,14,15	0.23	0	17,19,21	0.50	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
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1305	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1308	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.

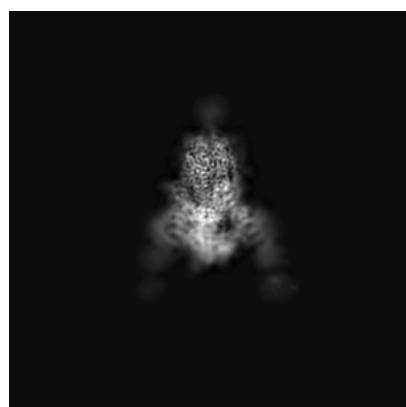
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12284. These allow visual inspection of the internal detail of the map and identification of artifacts.

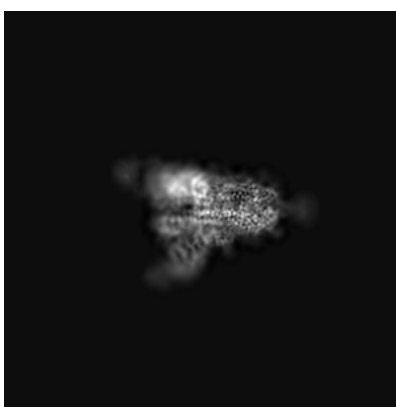
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

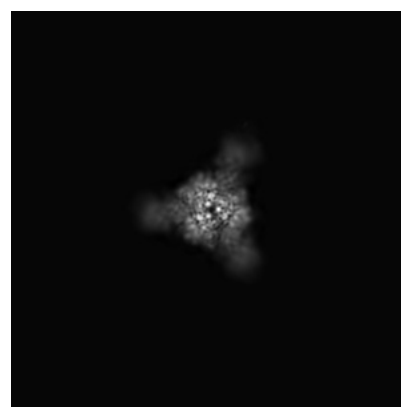
#### 6.1.1 Primary map



X



Y

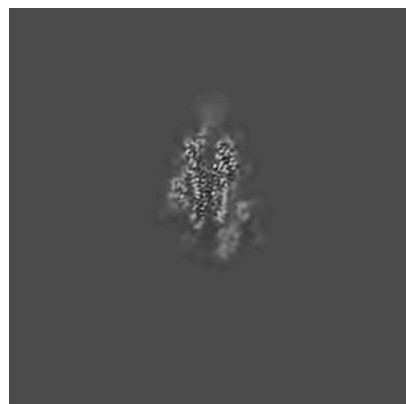


Z

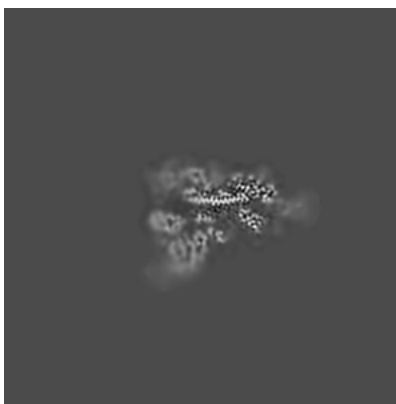
The images above show the map projected in three orthogonal directions.

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

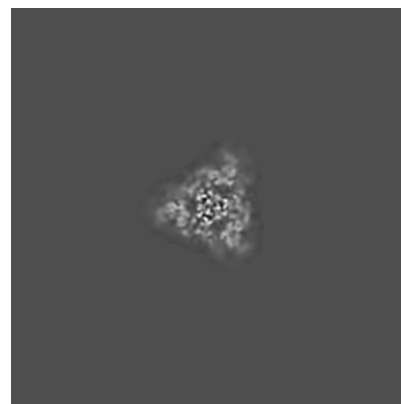
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

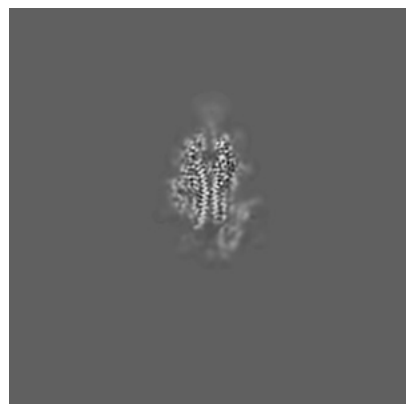


Z Index: 140

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

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

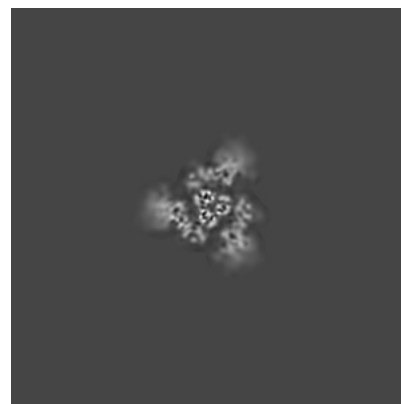
### 6.3.1 Primary map



X Index: 138



Y Index: 135

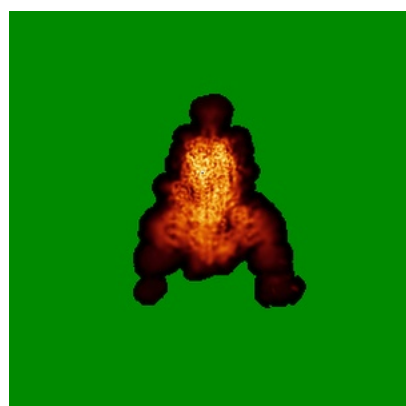


Z Index: 133

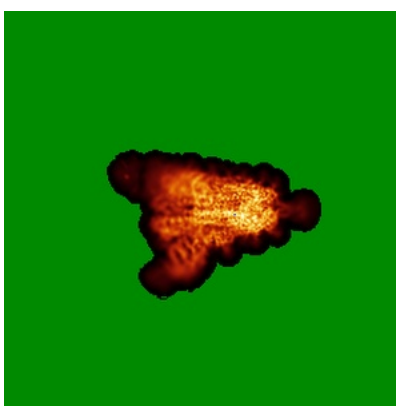
The images above show the largest variance slices of the map in three orthogonal directions.

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

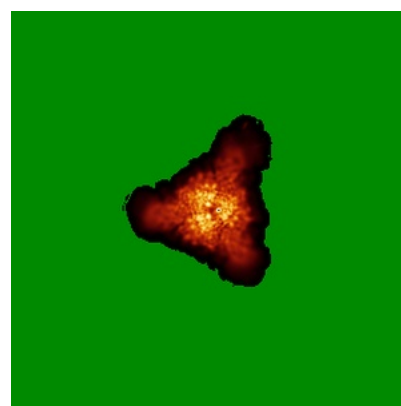
### 6.4.1 Primary map



X



Y

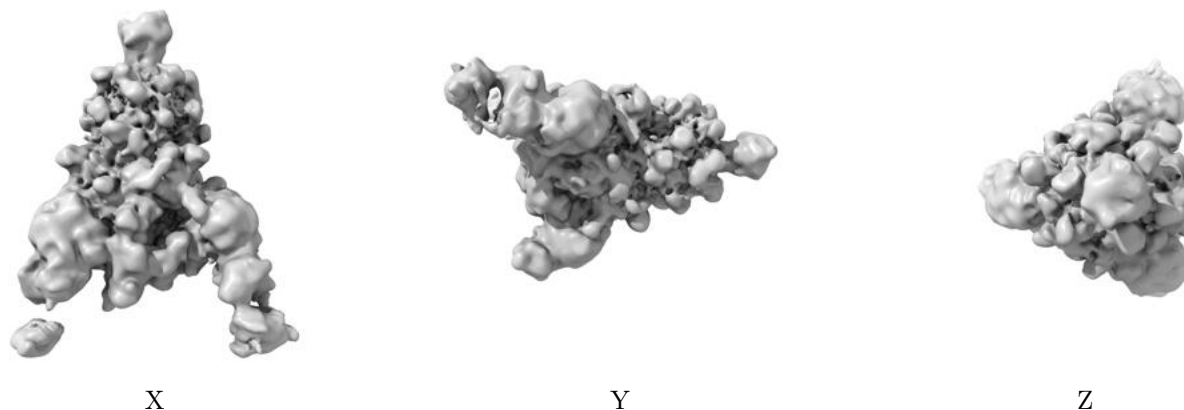


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.046. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

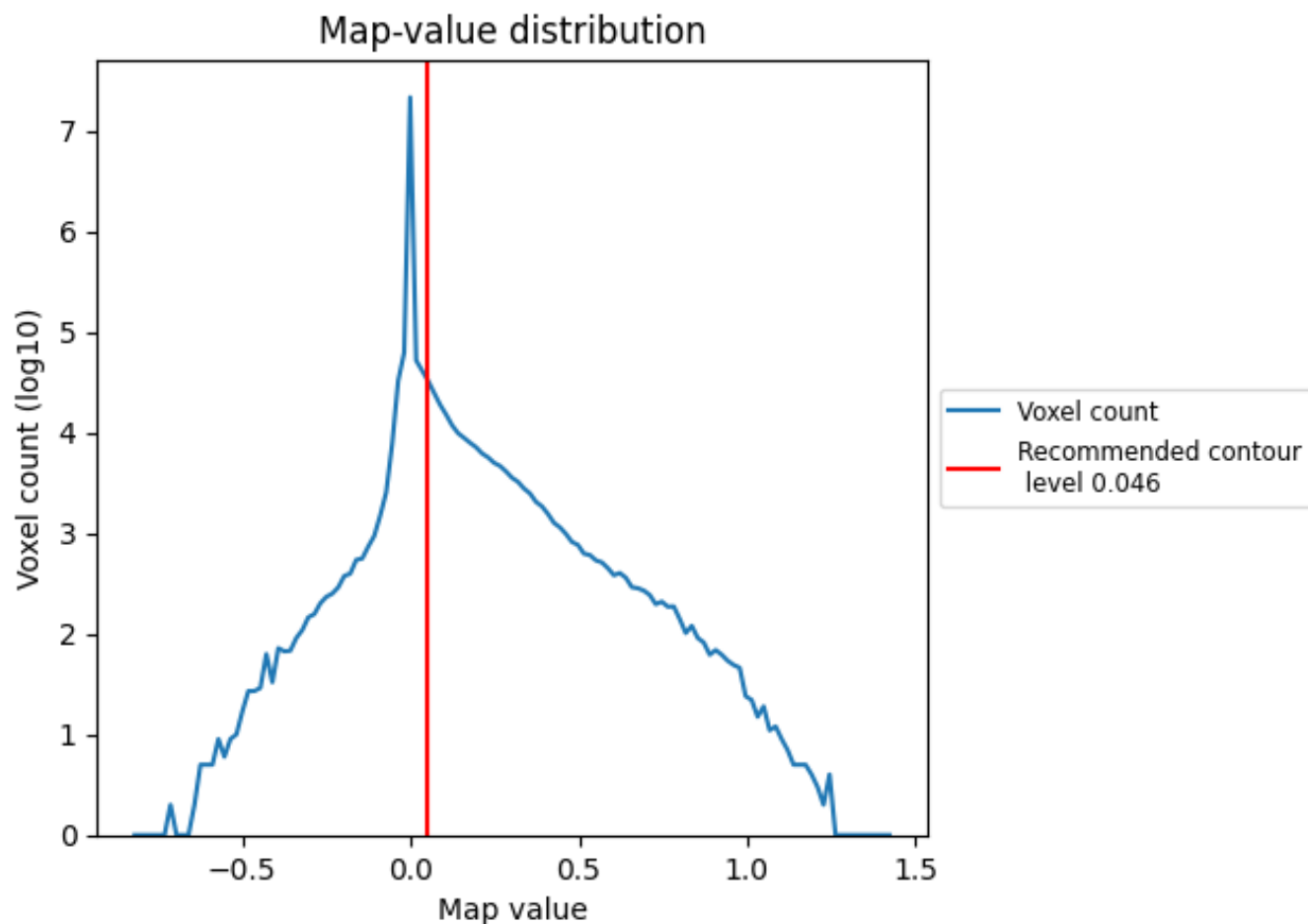
## 6.6 Mask visualisation [i](#)

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.

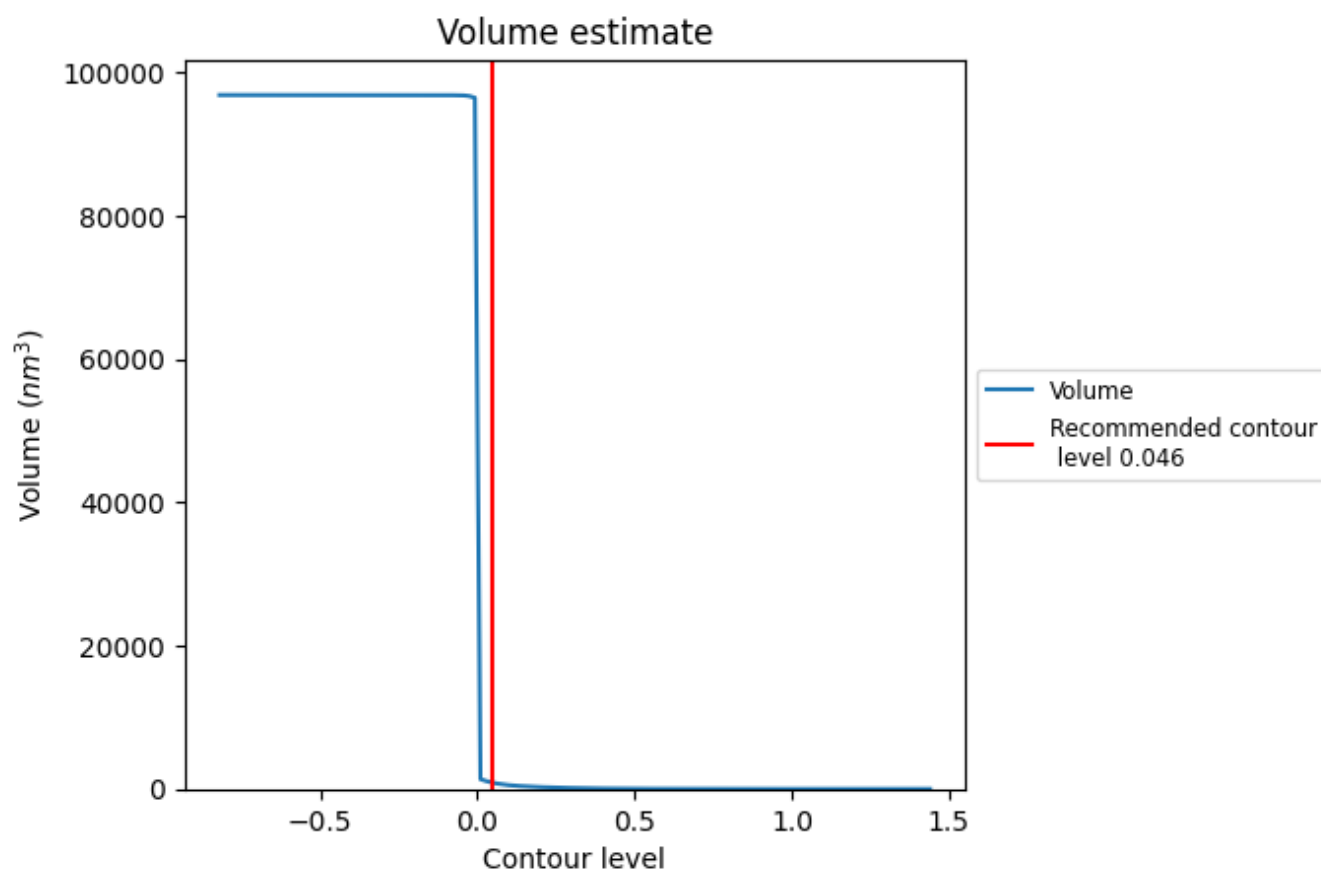
### 7.1 Map-value distribution [i](#)



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.



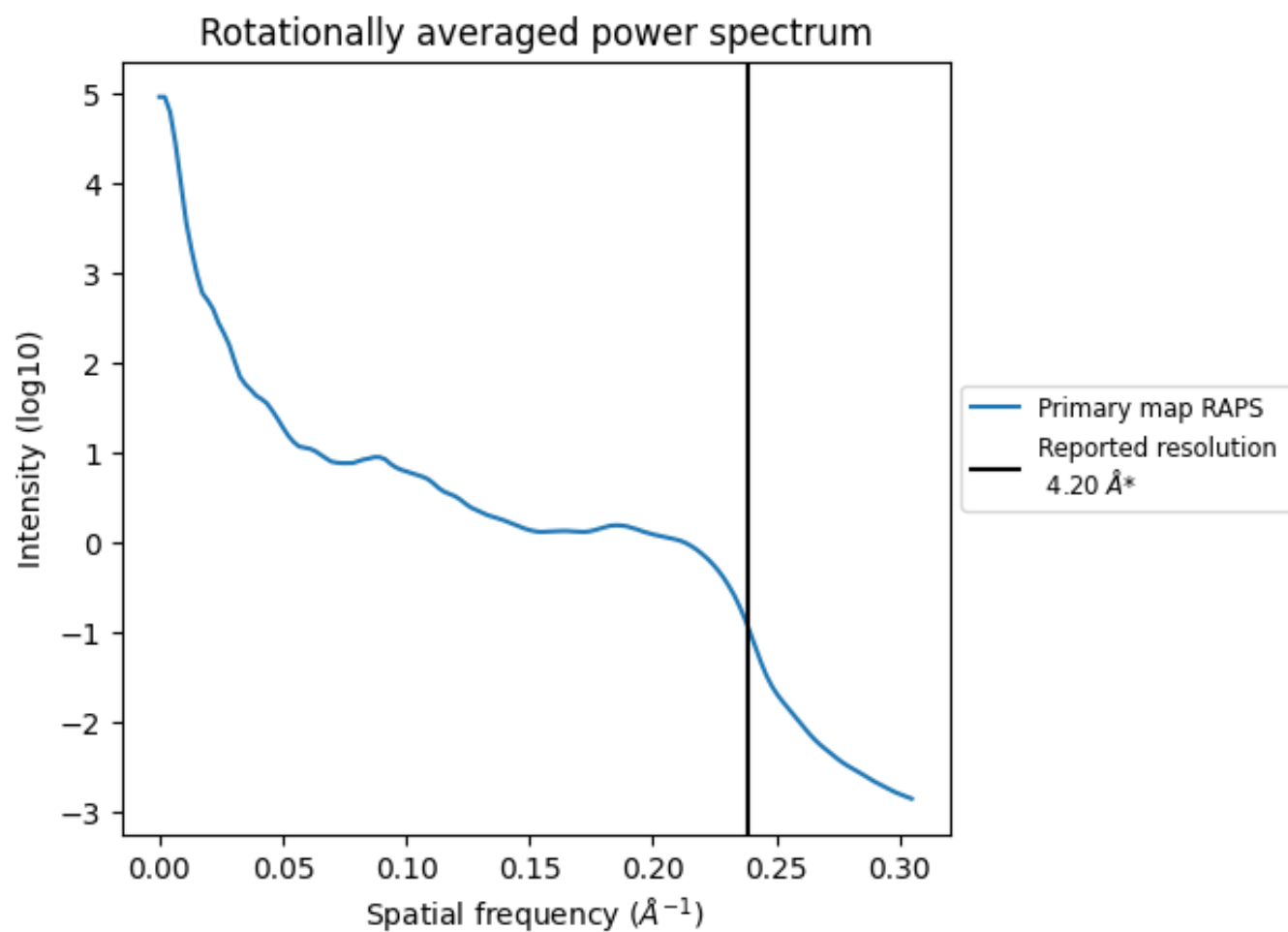
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 904 nm<sup>3</sup>; this corresponds to an approximate mass of 817 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 0.238 Å<sup>-1</sup>

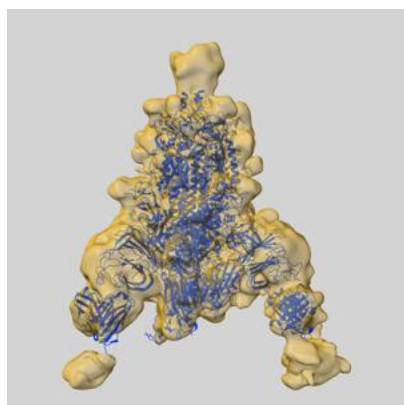
## 8 Fourier-Shell correlation

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

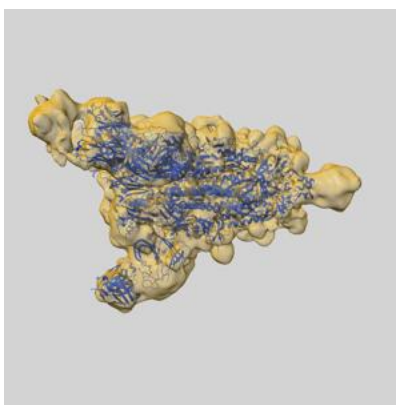
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12284 and PDB model 7NDD. Per-residue inclusion information can be found in section [3](#) on page [14](#).

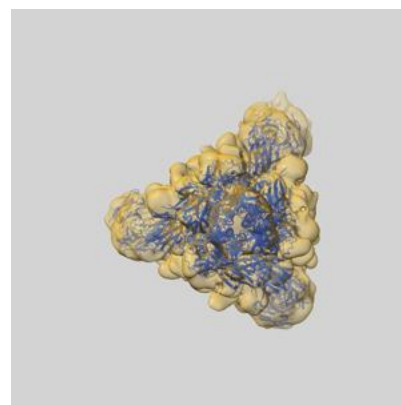
### 9.1 Map-model overlay [i](#)



X



Y



Z

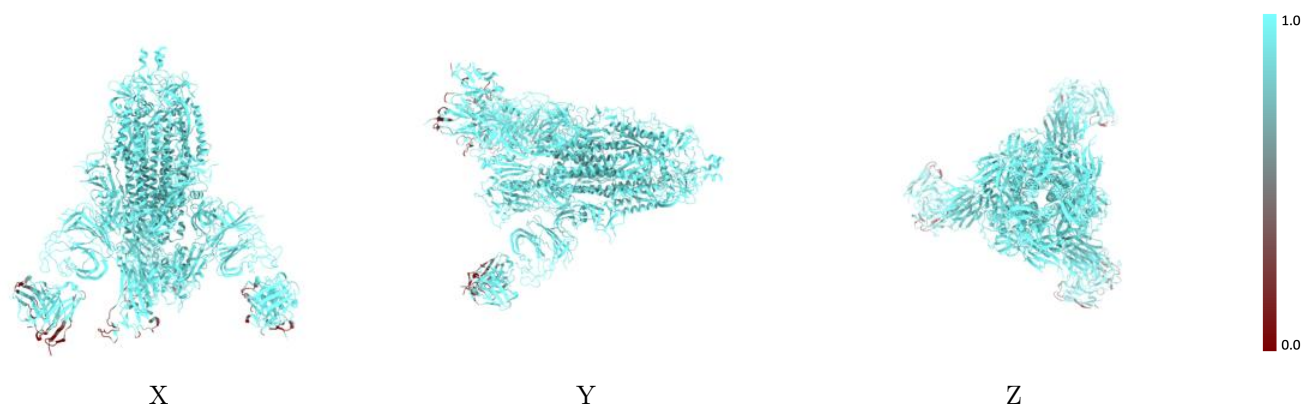
The images above show the 3D surface view of the map at the recommended contour level 0.046 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



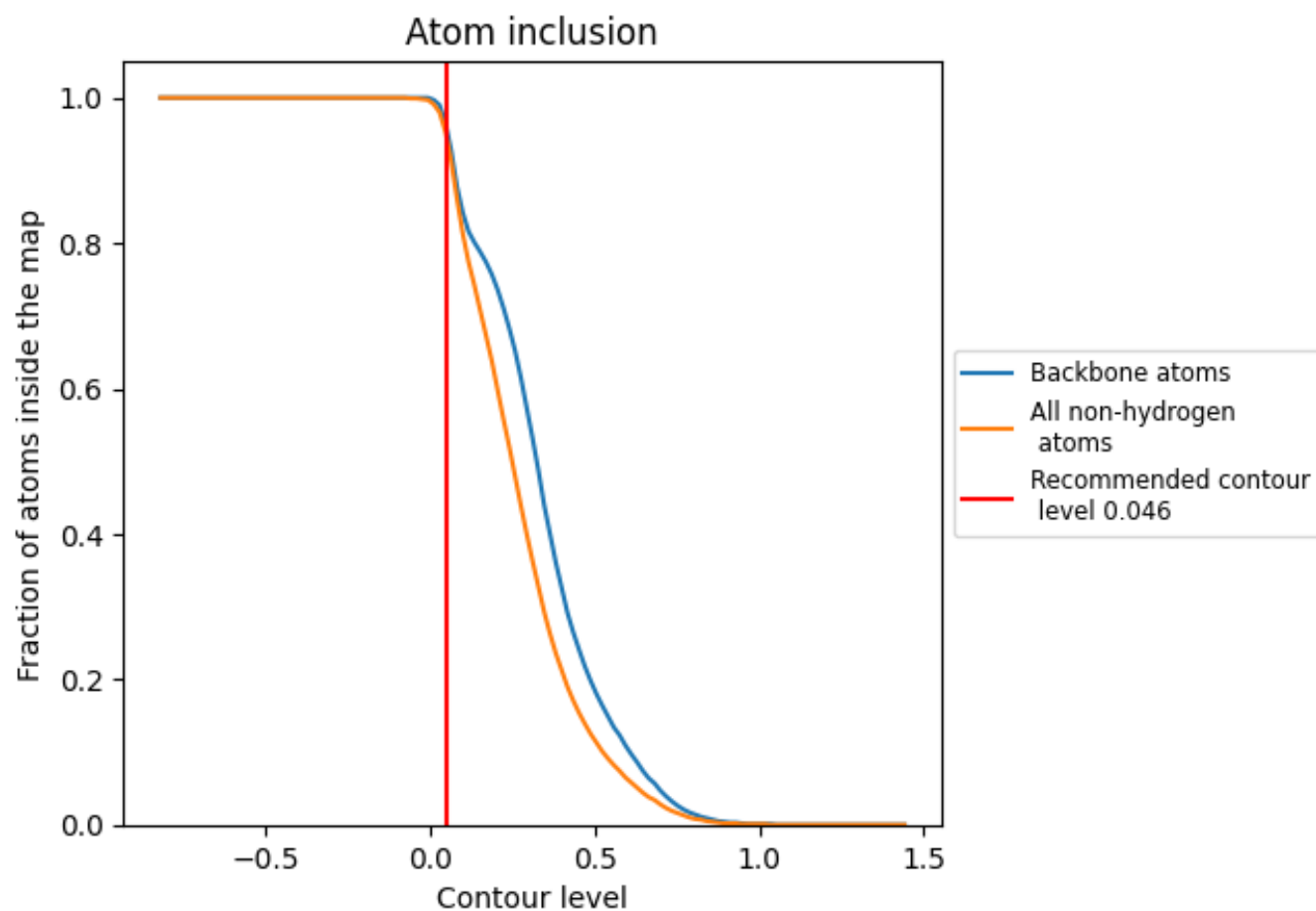
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.046).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.046) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9520	 0.2180
A	 0.9870	 0.2530
B	 0.9650	 0.2380
C	 0.9880	 0.2550
D	 0.7500	 0.0370
E	 0.8190	 0.0600
F	 0.6920	 0.0360
G	 0.8310	 0.0530
H	 0.8730	 0.0480
I	 1.0000	 0.2970
J	 1.0000	 0.3900
K	 1.0000	 0.3590
L	 0.8770	 0.0600
M	 1.0000	 0.3590
N	 1.0000	 0.3310
O	 1.0000	 0.2690
P	 1.0000	 0.3860
Q	 1.0000	 0.2930
R	 1.0000	 0.2590
S	 1.0000	 0.3370
T	 0.7500	 0.2320
U	 1.0000	 0.3940
V	 1.0000	 0.3470
W	 1.0000	 0.3070
X	 0.9640	 0.3090

