



Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 04:48 PM EDT

PDB ID : 7TPC / pdb_00007tpc
EMDB ID : EMD-26051
Title : Delta (B.1.617.2) SARS-CoV-2 variant spike protein (S-GSAS-Delta) in the 1-RBD-up conformation; Subclassification D15 state
Authors : Gobeil, S.; Acharya, P.
Deposited on : 2022-01-25
Resolution : 3.91 Å(reported)
Based on initial model : 7KDL

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.43.1

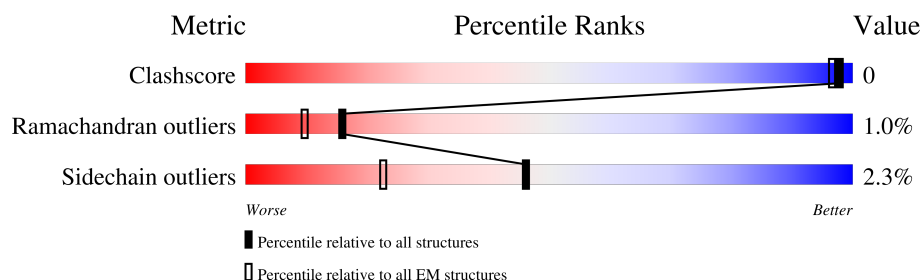
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 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 ≥ 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	1286	
1	B	1286	
1	C	1286	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
2	I	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	J	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	K	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	L	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	M	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	N	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>
2	O	2	<div><div></div><div>50%</div><div></div><div>100%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23199 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	1005	Total	C	N	O	S	0	0
			7700	4932	1291	1443	34		
1	B	975	Total	C	N	O	S	0	0
			7070	4495	1204	1339	32		
1	C	1003	Total	C	N	O	S	0	0
			7617	4879	1281	1423	34		

There are 279 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ARG	THR	engineered mutation	UNP P0DTC2
A	142	ASP	GLY	engineered mutation	UNP P0DTC2
A	?	-	GLU	deletion	UNP P0DTC2
A	?	-	PHE	deletion	UNP P0DTC2
A	158	GLY	ARG	engineered mutation	UNP P0DTC2
A	452	ARG	LEU	engineered mutation	UNP P0DTC2
A	478	LYS	THR	engineered mutation	UNP P0DTC2
A	614	GLY	ASP	engineered mutation	UNP P0DTC2
A	681	ARG	PRO	engineered mutation	UNP P0DTC2
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	950	ASN	ASP	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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	19	ARG	THR	engineered mutation	UNP P0DTC2
B	142	ASP	GLY	engineered mutation	UNP P0DTC2
B	?	-	GLU	deletion	UNP P0DTC2
B	?	-	PHE	deletion	UNP P0DTC2
B	158	GLY	ARG	engineered mutation	UNP P0DTC2
B	452	ARG	LEU	engineered mutation	UNP P0DTC2
B	478	LYS	THR	engineered mutation	UNP P0DTC2
B	614	GLY	ASP	engineered mutation	UNP P0DTC2
B	681	ARG	PRO	engineered mutation	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	950	ASN	ASP	engineered mutation	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2
C	19	ARG	THR	engineered mutation	UNP P0DTC2
C	142	ASP	GLY	engineered mutation	UNP P0DTC2
C	?	-	GLU	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	158	GLY	ARG	engineered mutation	UNP P0DTC2
C	452	ARG	LEU	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	478	LYS	THR	engineered mutation	UNP P0DTC2
C	614	GLY	ASP	engineered mutation	UNP P0DTC2
C	681	ARG	PRO	engineered mutation	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	950	ASN	ASP	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	ALA	-	expression tag	UNP P0DTC2
C	1260	TRP	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	PRO	-	expression tag	UNP P0DTC2
C	1264	GLN	-	expression tag	UNP P0DTC2
C	1265	PHE	-	expression tag	UNP P0DTC2
C	1266	GLU	-	expression tag	UNP P0DTC2
C	1267	LYS	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	GLY	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	GLY	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	GLY	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	ALA	-	expression tag	UNP P0DTC2
C	1281	TRP	-	expression tag	UNP P0DTC2
C	1282	SER	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	PRO	-	expression tag	UNP P0DTC2
C	1285	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1286	PHE	-	expression tag	UNP P0DTC2
C	1287	GLU	-	expression tag	UNP P0DTC2
C	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

[illegible]

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



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



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



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



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



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



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



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



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



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



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





- Molecule 2: 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, Not provided	
Number of particles used	70958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.890	Depositor
Minimum map value	-0.723	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.131	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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	0.73	0/7871	1.27	11/10725 (0.1%)
1	B	0.72	0/7210	1.29	8/9846 (0.1%)
1	C	0.73	0/7789	1.27	12/10624 (0.1%)
All	All	0.73	0/22870	1.28	31/31195 (0.1%)

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	8
1	B	0	3
1	C	0	5
All	All	0	16

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	592	PHE	CA-CB-CG	8.60	122.40	113.80
1	B	212	LEU	CB-CG-CD1	7.87	134.29	110.70
1	A	620	VAL	CA-C-N	6.04	127.39	119.84
1	A	620	VAL	C-N-CA	6.04	127.39	119.84
1	C	643	PHE	CA-CB-CG	5.96	119.77	113.80
1	B	643	PHE	CA-CB-CG	5.93	119.73	113.80
1	C	633	TRP	CA-C-N	5.86	132.74	121.54
1	C	633	TRP	C-N-CA	5.86	132.74	121.54
1	C	565	PHE	CA-CB-CG	5.83	119.63	113.80
1	C	1064	HIS	CB-CG-CD2	-5.81	123.64	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	ASN	CA-CB-CG	5.77	118.37	112.60
1	C	1110	TYR	CA-C-N	5.67	127.27	122.28
1	C	1110	TYR	C-N-CA	5.67	127.27	122.28
1	A	633	TRP	CA-CB-CG	5.66	124.36	113.60
1	B	638	THR	CA-C-N	5.54	126.42	122.16
1	B	638	THR	C-N-CA	5.54	126.42	122.16
1	C	294	ASP	N-CA-C	5.50	112.97	108.07
1	A	1064	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	A	632	THR	CA-C-N	5.46	128.14	120.28
1	A	632	THR	C-N-CA	5.46	128.14	120.28
1	B	559	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	955	ASN	CA-CB-CG	-5.32	107.28	112.60
1	C	655	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	A	965	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	275	PHE	CA-CB-CG	5.23	119.03	113.80
1	B	197	ILE	CA-C-N	5.17	131.42	121.54
1	B	197	ILE	C-N-CA	5.17	131.42	121.54
1	A	207	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	A	1106	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	820	ASP	CA-CB-CG	-5.08	107.52	112.60
1	C	507	PRO	N-CA-CB	5.02	107.77	103.31

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1138	TYR	Sidechain
1	A	269	TYR	Sidechain
1	A	421	TYR	Sidechain
1	A	44	ARG	Sidechain
1	A	466	ARG	Sidechain
1	A	695	TYR	Sidechain
1	A	707	TYR	Sidechain
1	A	789	TYR	Sidechain
1	B	342	PHE	Sidechain
1	B	707	TYR	Sidechain
1	B	917	TYR	Sidechain
1	C	466	ARG	Sidechain
1	C	473	TYR	Sidechain
1	C	495	TYR	Sidechain
1	C	707	TYR	Sidechain
1	C	917	TYR	Sidechain

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	7700	0	7423	4	0
1	B	7070	0	6516	7	0
1	C	7617	0	7276	10	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
3	A	140	0	130	0	0
3	B	168	0	156	0	0
3	C	168	0	156	3	0
All	All	23199	0	21957	20	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 0.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:PHE:CG	3:C:1305:NAG:H82	2.39	0.56
1:C:326:ILE:HD12	1:C:539:VAL:HG21	1.92	0.51
1:A:64:TRP:CD1	1:A:214:ARG:HH12	2.30	0.50
1:B:342:PHE:CZ	1:B:436:TRP:CB	2.95	0.50
1:C:1043:CYS:HB2	1:C:1048:HIS:CG	2.49	0.48
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.50	0.47
1:C:233:ILE:HG23	3:C:1301:NAG:H82	1.96	0.47
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.50	0.47
1:B:980:ILE:H	1:B:980:ILE:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.54	0.46
1:B:198:ASP:C	1:B:200:TYR:H	2.25	0.45
1:B:351:TYR:HA	1:B:422:ASN:CB	2.48	0.44
1:B:715:PRO:HD3	1:C:894:LEU:HD11	2.00	0.44
1:C:980:ILE:H	1:C:980:ILE:HD12	1.84	0.43
1:B:349:SER:CB	1:B:452:ARG:H	2.31	0.43
1:A:104:TRP:HB2	1:A:106:PHE:CE1	2.54	0.43
1:A:712:ILE:HB	1:A:1077:THR:HG21	2.00	0.42
1:C:559:PHE:CD2	1:C:584:ILE:HD12	2.55	0.41
1:C:342:PHE:CB	3:C:1305:NAG:H82	2.50	0.41
1:C:1078:ALA:CB	1:C:1133:VAL:HG22	2.52	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	983/1286 (76%)	882 (90%)	96 (10%)	5 (0%)	25 60
1	B	953/1286 (74%)	867 (91%)	71 (8%)	15 (2%)	8 37
1	C	985/1286 (77%)	884 (90%)	91 (9%)	10 (1%)	13 46
All	All	2921/3858 (76%)	2633 (90%)	258 (9%)	30 (1%)	16 46

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	621	PRO
1	B	198	ASP
1	C	634	ARG
1	A	110	LEU
1	A	481	ASN
1	B	97	LYS

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Mol	Chain	Res	Type
1	B	334	ASN
1	B	350	VAL
1	C	213	VAL
1	C	418	ILE
1	C	640	SER
1	B	434	ILE
1	C	626	ALA
1	A	449	TYR
1	B	110	LEU
1	B	165	ASN
1	B	385	THR
1	B	448	ASN
1	C	347	PHE
1	C	447	GLY
1	C	663	ASP
1	B	32	PHE
1	B	709	ASN
1	B	814	LYS
1	C	706	ALA
1	C	187	LYS
1	B	631	PRO
1	A	720	ILE
1	B	630	THR
1	B	496	GLY

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	834/1110 (75%)	819 (98%)	15 (2%)	54	71
1	B	704/1110 (63%)	692 (98%)	12 (2%)	56	72
1	C	811/1110 (73%)	785 (97%)	26 (3%)	34	56
All	All	2349/3330 (70%)	2296 (98%)	53 (2%)	46	64

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	VAL
1	A	294	ASP
1	A	350	VAL
1	A	437	ASN
1	A	461	LEU
1	A	493	GLN
1	A	539	VAL
1	A	544	ASN
1	A	547	THR
1	A	588	THR
1	A	608	VAL
1	A	621	PRO
1	A	739	THR
1	A	760	CYS
1	A	996	LEU
1	B	29	THR
1	B	116	SER
1	B	122	ASN
1	B	212	LEU
1	B	286	THR
1	B	628	GLN
1	B	632	THR
1	B	634	ARG
1	B	773	GLU
1	B	907	ASN
1	B	950	ASN
1	B	1127	ASP
1	C	102	ARG
1	C	130	VAL
1	C	210	ILE
1	C	226	LEU
1	C	227	VAL
1	C	234	ASN
1	C	294	ASP
1	C	328	ARG
1	C	408	ARG
1	C	523	THR
1	C	544	ASN
1	C	565	PHE
1	C	592	PHE
1	C	603	ASN
1	C	608	VAL
1	C	615	VAL

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Mol	Chain	Res	Type
1	C	622	VAL
1	C	628	GLN
1	C	634	ARG
1	C	702	GLU
1	C	752	LEU
1	C	873	TYR
1	C	935	GLN
1	C	996	LEU
1	C	1082	CYS
1	C	1106	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	334	ASN
1	A	450	ASN
1	A	487	ASN
1	A	536	ASN
1	A	606	ASN
1	A	690	GLN
1	A	1002	GLN
1	A	1058	HIS
1	A	1142	GLN
1	B	188	ASN
1	B	536	ASN
1	B	606	ASN
1	B	777	ASN
1	B	978	ASN
1	B	1002	GLN
1	B	1088	HIS
1	C	188	ASN
1	C	360	ASN
1	C	450	ASN
1	C	506	GLN
1	C	536	ASN
1	C	540	ASN
1	C	564	GLN
1	C	606	ASN
1	C	690	GLN
1	C	762	GLN
1	C	764	ASN

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Mol	Chain	Res	Type
1	C	784	GLN
1	C	804	GLN
1	C	907	ASN
1	C	913	GLN
1	C	935	GLN
1	C	1005	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 ⓘ

24 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
2	NAG	D	1	1,2	14,14,15	1.53	4 (28%)	17,19,21	1.00	2 (11%)
2	NAG	D	2	2	14,14,15	1.34	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	E	1	1,2	14,14,15	1.18	1 (7%)	17,19,21	0.62	0
2	NAG	E	2	2	14,14,15	1.26	2 (14%)	17,19,21	0.72	0
2	NAG	F	1	1,2	14,14,15	1.18	2 (14%)	17,19,21	0.74	1 (5%)
2	NAG	F	2	2	14,14,15	1.16	1 (7%)	17,19,21	0.91	1 (5%)
2	NAG	G	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	1.14	2 (11%)
2	NAG	G	2	2	14,14,15	1.13	1 (7%)	17,19,21	0.86	1 (5%)
2	NAG	H	1	1,2	14,14,15	1.10	1 (7%)	17,19,21	1.20	3 (17%)
2	NAG	H	2	2	14,14,15	1.25	2 (14%)	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	1	1,2	14,14,15	1.12	1 (7%)	17,19,21	1.13	2 (11%)
2	NAG	I	2	2	14,14,15	1.11	1 (7%)	17,19,21	0.70	0
2	NAG	J	1	1,2	14,14,15	1.14	1 (7%)	17,19,21	0.86	1 (5%)
2	NAG	J	2	2	14,14,15	1.20	1 (7%)	17,19,21	1.00	2 (11%)
2	NAG	K	1	1,2	14,14,15	1.18	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	K	2	2	14,14,15	1.25	2 (14%)	17,19,21	0.93	1 (5%)
2	NAG	L	1	1,2	14,14,15	1.28	2 (14%)	17,19,21	0.69	0
2	NAG	L	2	2	14,14,15	1.24	1 (7%)	17,19,21	0.83	1 (5%)
2	NAG	M	1	1,2	14,14,15	1.19	2 (14%)	17,19,21	0.79	0
2	NAG	M	2	2	14,14,15	1.15	1 (7%)	17,19,21	1.11	2 (11%)
2	NAG	N	1	1,2	14,14,15	1.15	2 (14%)	17,19,21	1.10	1 (5%)
2	NAG	N	2	2	14,14,15	1.23	1 (7%)	17,19,21	0.62	0
2	NAG	O	1	1,2	14,14,15	1.09	1 (7%)	17,19,21	0.90	1 (5%)
2	NAG	O	2	2	14,14,15	1.18	1 (7%)	17,19,21	1.07	1 (5%)

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

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

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

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C5	3.02	1.49	1.43
2	N	2	NAG	O5-C5	2.88	1.49	1.43
2	J	2	NAG	O5-C5	2.85	1.49	1.43
2	K	2	NAG	O5-C5	2.84	1.49	1.43
2	L	2	NAG	O5-C5	2.82	1.48	1.43
2	H	2	NAG	O5-C5	2.81	1.48	1.43
2	E	2	NAG	O5-C5	2.79	1.48	1.43
2	O	2	NAG	O5-C5	2.65	1.48	1.43
2	M	2	NAG	O5-C5	2.64	1.48	1.43
2	F	2	NAG	O5-C5	2.63	1.48	1.43
2	G	2	NAG	O5-C5	2.60	1.48	1.43
2	D	2	NAG	C1-C2	2.59	1.55	1.52
2	G	1	NAG	O5-C5	2.57	1.48	1.43
2	D	1	NAG	O4-C4	2.50	1.49	1.43
2	L	1	NAG	C1-C2	2.49	1.55	1.52
2	D	2	NAG	O5-C5	2.48	1.48	1.43
2	I	1	NAG	O5-C5	2.43	1.48	1.43
2	N	1	NAG	O5-C5	2.37	1.48	1.43
2	I	2	NAG	O5-C5	2.37	1.48	1.43
2	O	1	NAG	O5-C5	2.31	1.47	1.43
2	E	1	NAG	O5-C5	2.29	1.47	1.43
2	D	1	NAG	C1-C2	2.29	1.55	1.52
2	K	1	NAG	O5-C5	2.26	1.47	1.43
2	M	1	NAG	O4-C4	2.24	1.48	1.43
2	M	1	NAG	O5-C5	2.21	1.47	1.43
2	J	1	NAG	O5-C5	2.14	1.47	1.43
2	F	1	NAG	O5-C5	2.13	1.47	1.43
2	E	2	NAG	O5-C1	2.11	1.47	1.43
2	D	2	NAG	O5-C1	2.09	1.47	1.43
2	K	2	NAG	O5-C1	2.08	1.47	1.43
2	F	1	NAG	O4-C4	2.06	1.48	1.43
2	H	1	NAG	C1-C2	2.04	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	O5-C1	2.03	1.47	1.43
2	N	1	NAG	C1-C2	2.02	1.55	1.52
2	L	1	NAG	O5-C5	2.01	1.47	1.43
2	D	1	NAG	O5-C1	2.01	1.47	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	NAG	C1-O5-C5	3.86	117.36	112.19
2	H	2	NAG	C1-O5-C5	3.74	117.19	112.19
2	M	2	NAG	O5-C1-C2	-2.84	106.89	111.29
2	K	1	NAG	C4-C3-C2	2.80	115.12	111.02
2	H	1	NAG	O4-C4-C5	-2.75	102.54	109.32
2	I	1	NAG	C1-O5-C5	2.71	115.81	112.19
2	K	2	NAG	C1-O5-C5	2.67	115.77	112.19
2	O	1	NAG	C1-O5-C5	2.62	115.69	112.19
2	G	1	NAG	C3-C4-C5	2.58	114.91	110.23
2	N	1	NAG	C3-C4-C5	2.51	114.77	110.23
2	L	2	NAG	C1-O5-C5	2.50	115.53	112.19
2	I	1	NAG	C3-C4-C5	2.48	114.74	110.23
2	F	2	NAG	C1-O5-C5	2.48	115.52	112.19
2	D	2	NAG	C1-O5-C5	2.41	115.42	112.19
2	G	2	NAG	C1-O5-C5	2.38	115.37	112.19
2	J	2	NAG	C1-O5-C5	2.37	115.37	112.19
2	D	1	NAG	O5-C1-C2	-2.35	107.66	111.29
2	M	2	NAG	C1-O5-C5	2.26	115.22	112.19
2	H	1	NAG	C3-C4-C5	2.24	114.29	110.23
2	D	1	NAG	C4-C3-C2	2.23	114.29	111.02
2	J	2	NAG	O5-C1-C2	-2.16	107.95	111.29
2	F	1	NAG	C1-O5-C5	2.15	115.06	112.19
2	J	1	NAG	C1-O5-C5	2.12	115.03	112.19
2	G	1	NAG	C4-C3-C2	-2.10	107.94	111.02
2	H	1	NAG	O5-C1-C2	-2.05	108.12	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C1-C2-N2-C7

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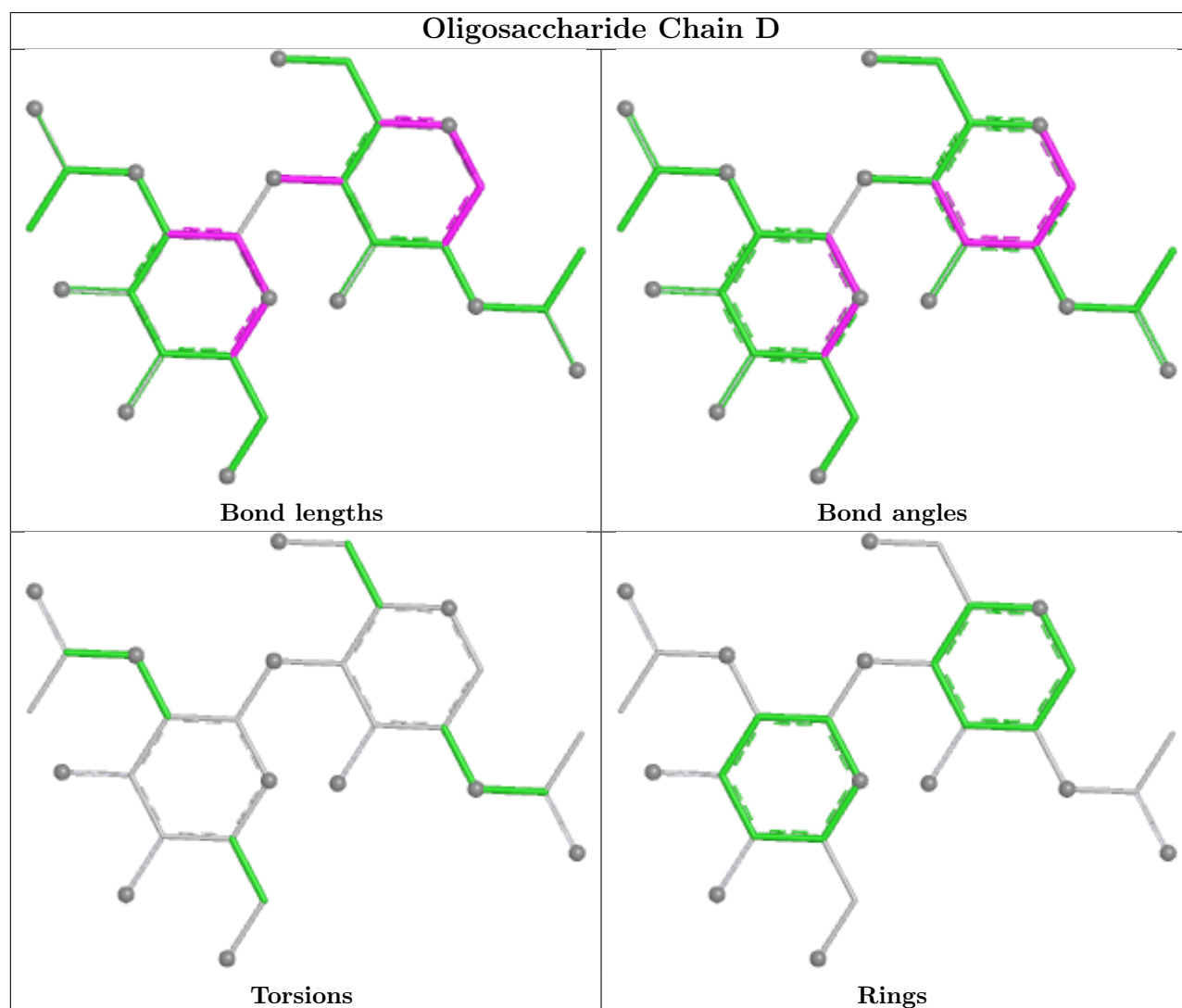
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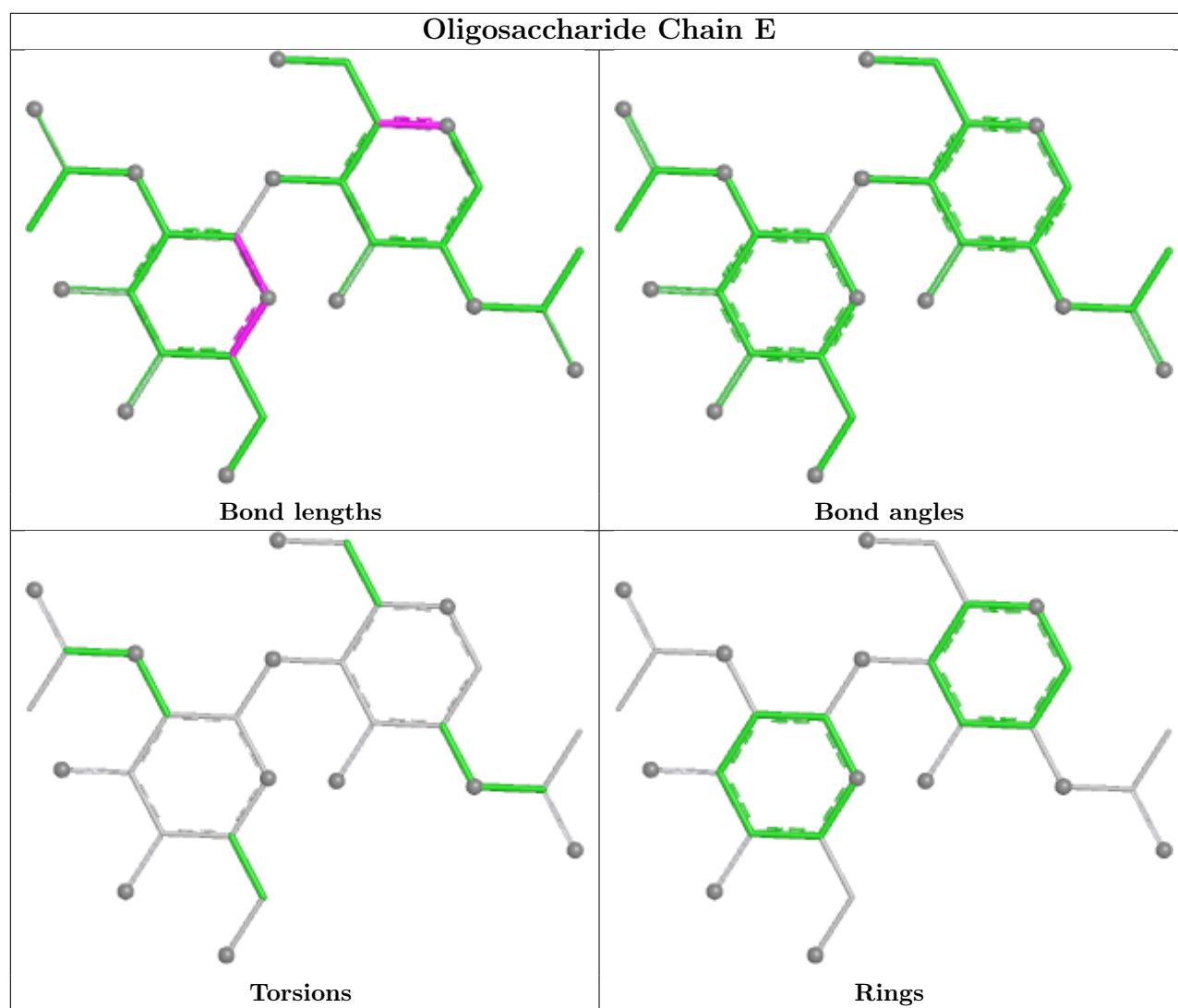
Mol	Chain	Res	Type	Atoms
2	M	1	NAG	C1-C2-N2-C7
2	N	1	NAG	C1-C2-N2-C7

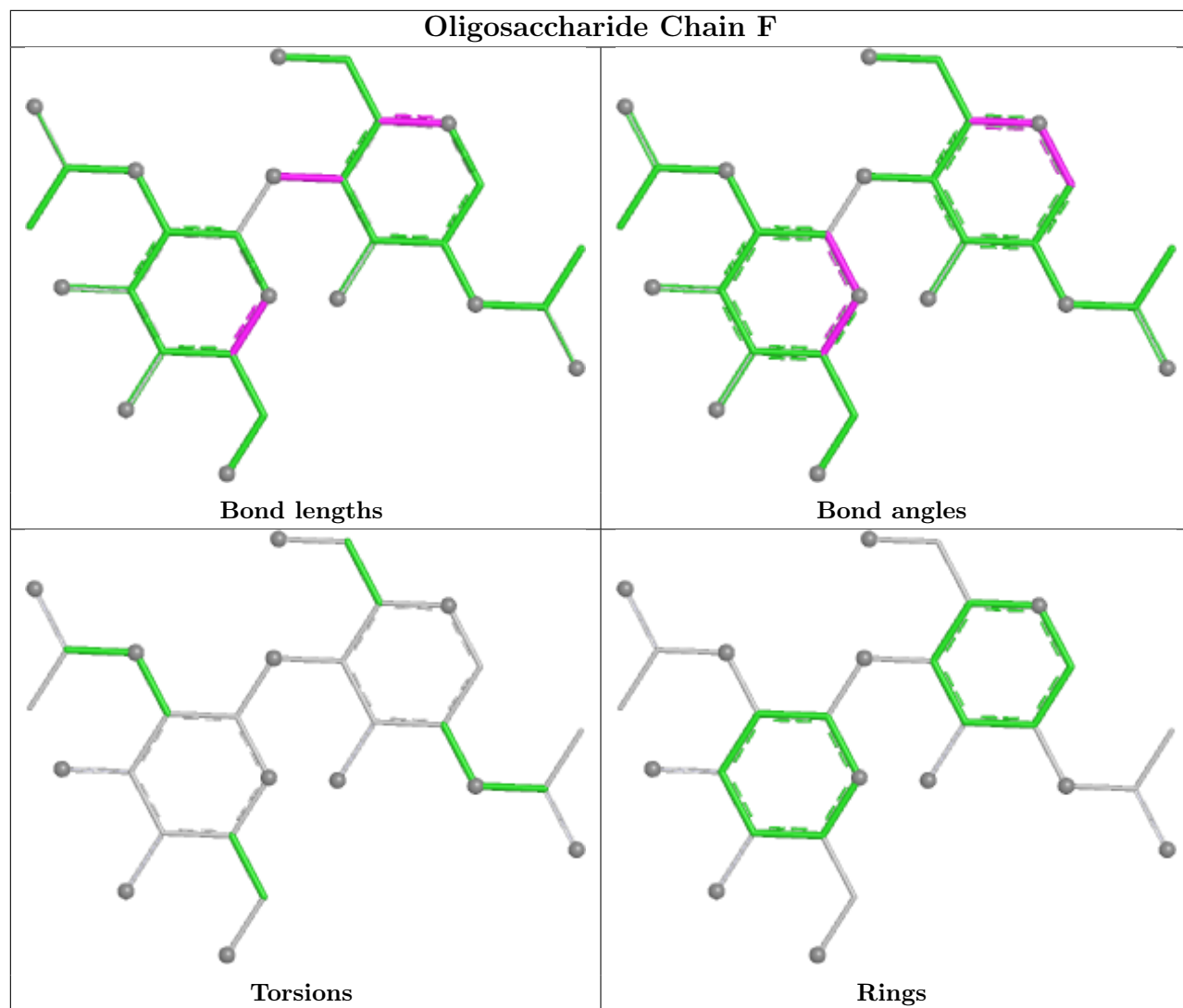
There are no ring outliers.

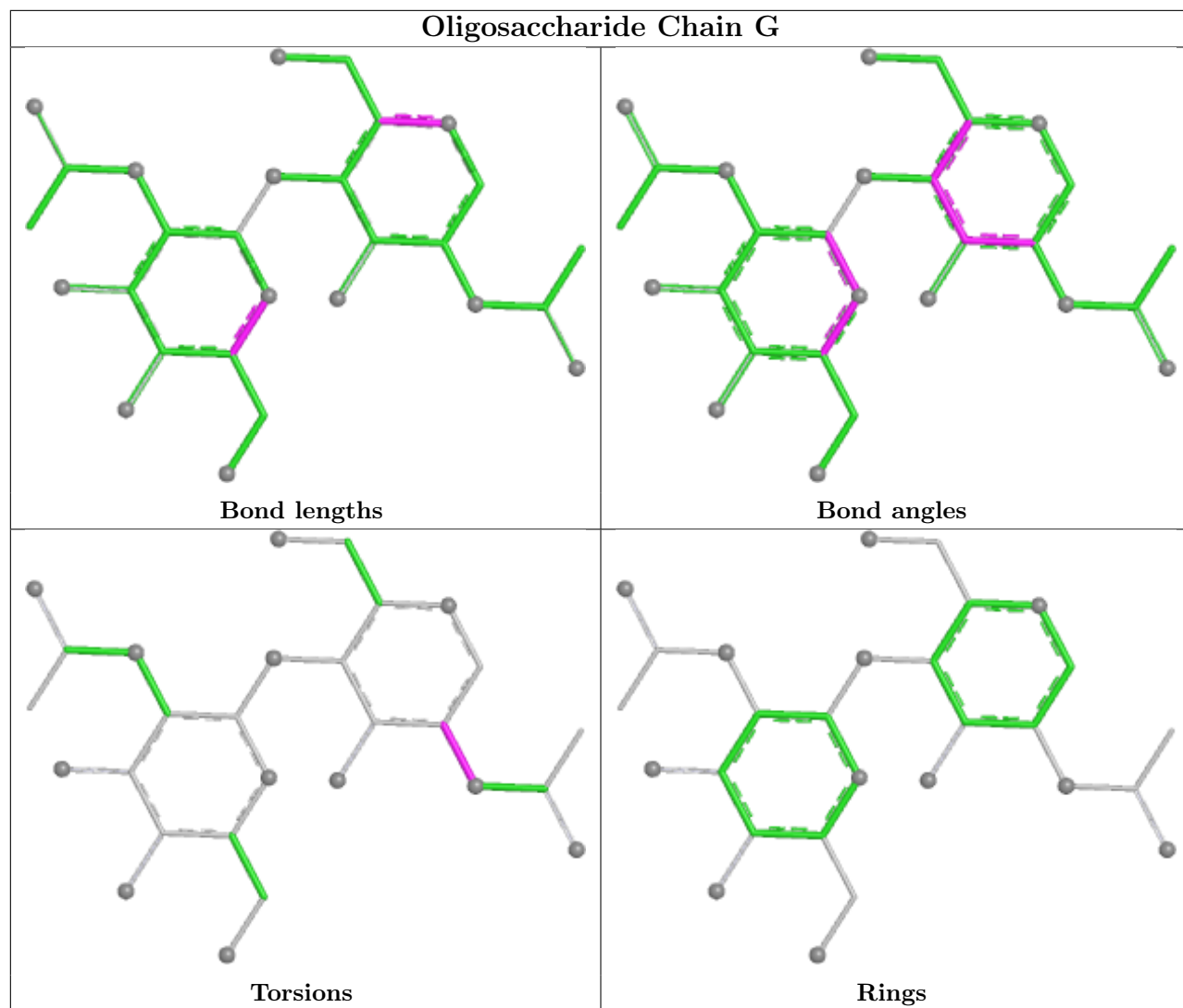
No monomer is involved in short contacts.

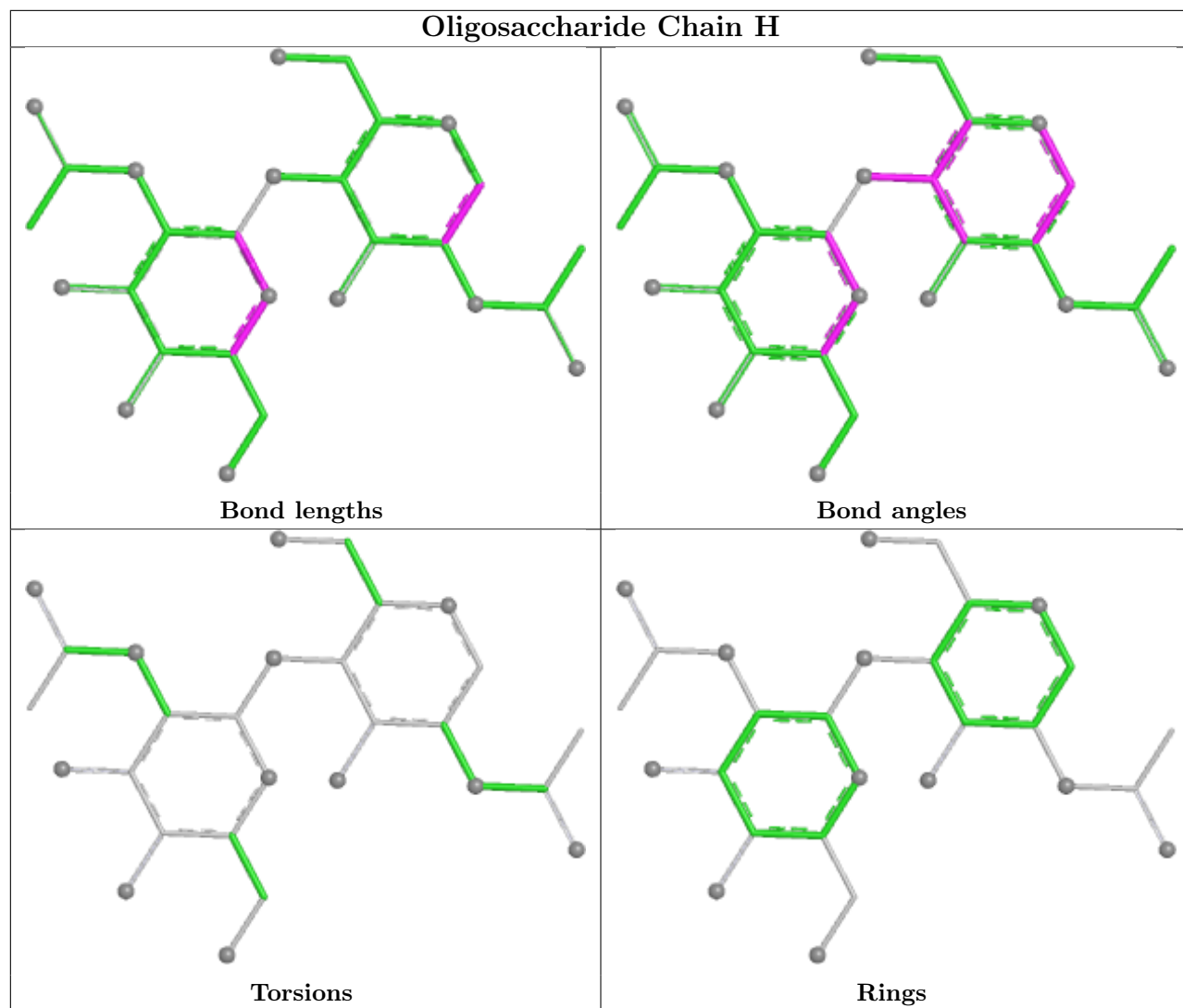
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

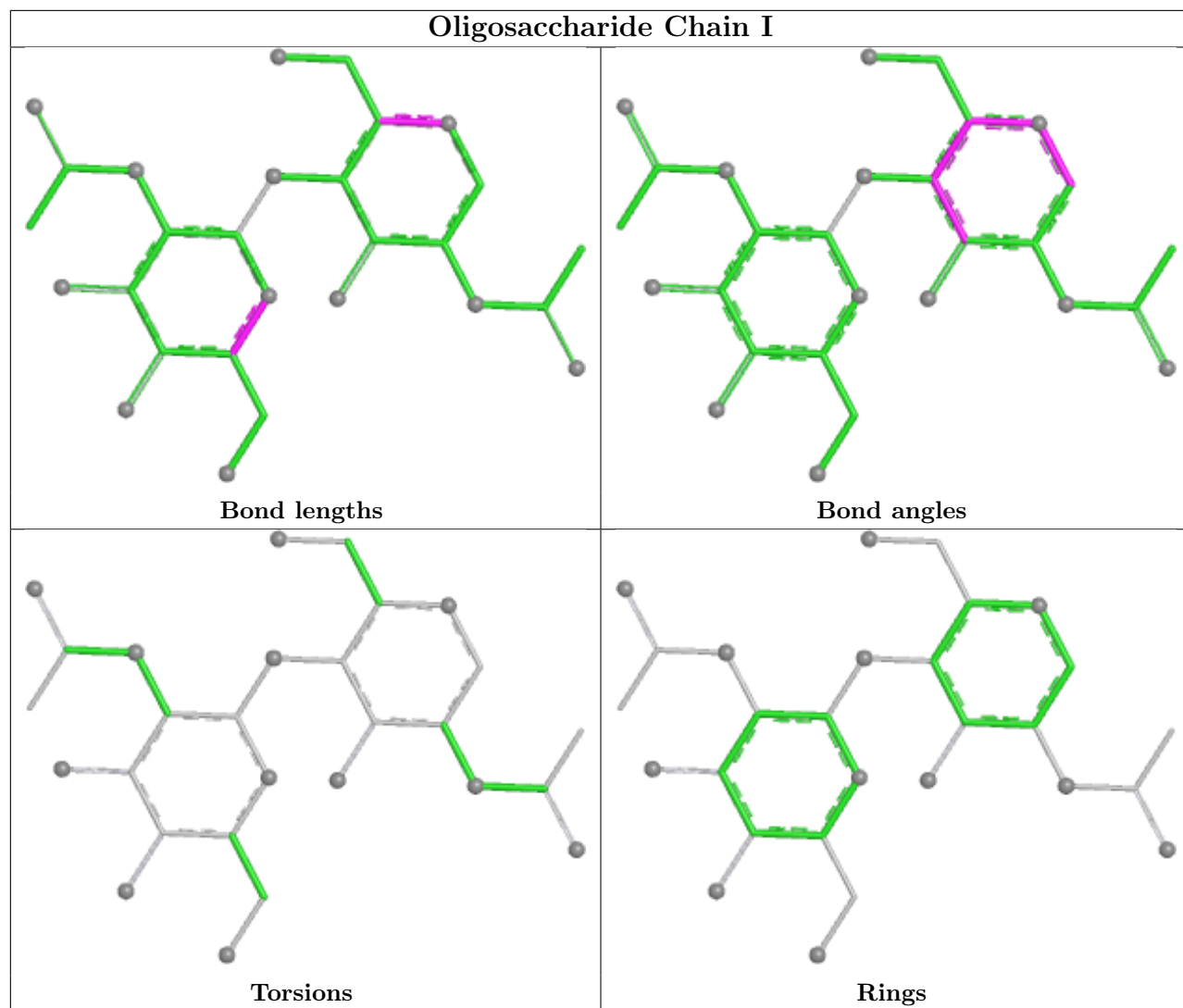


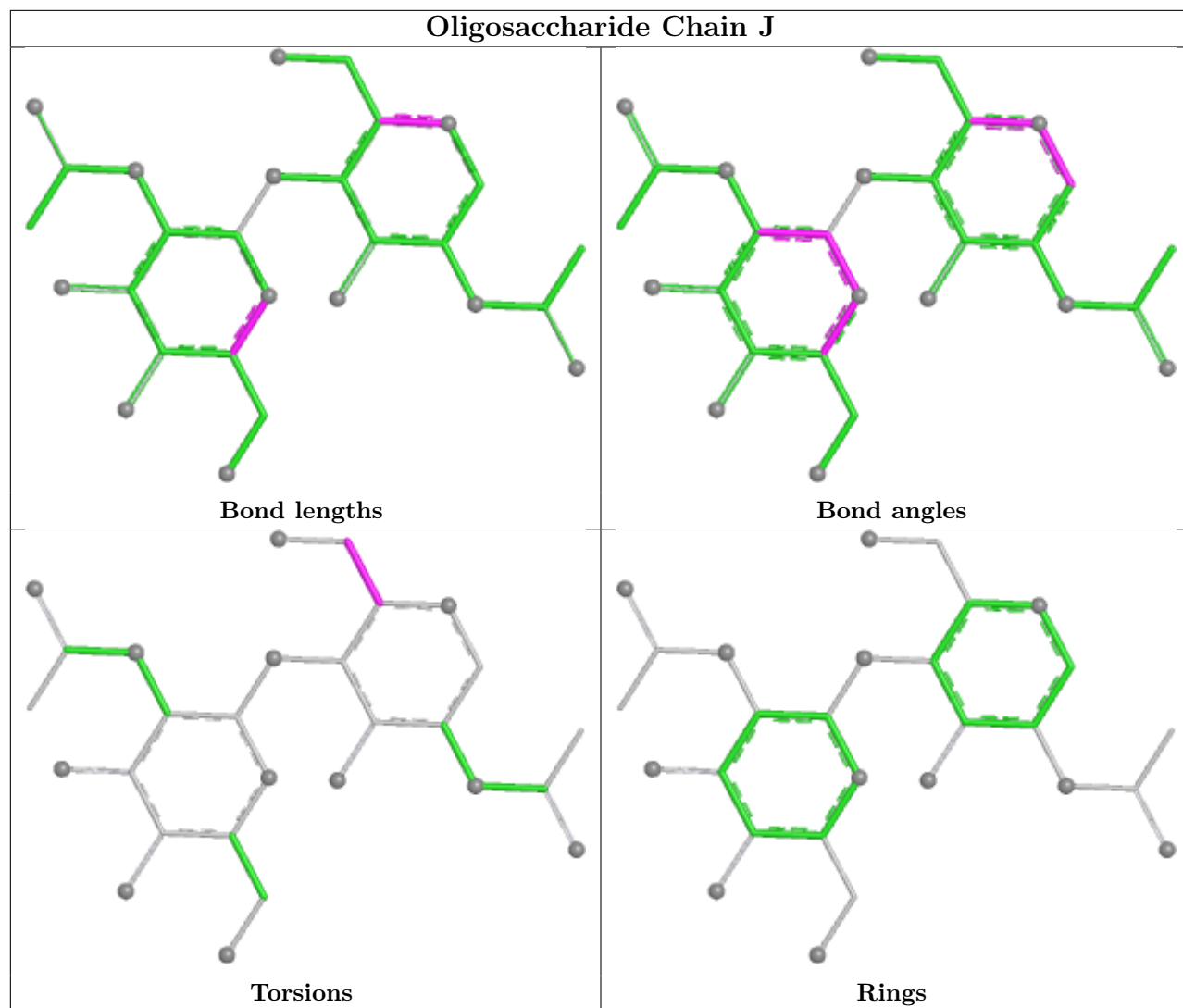


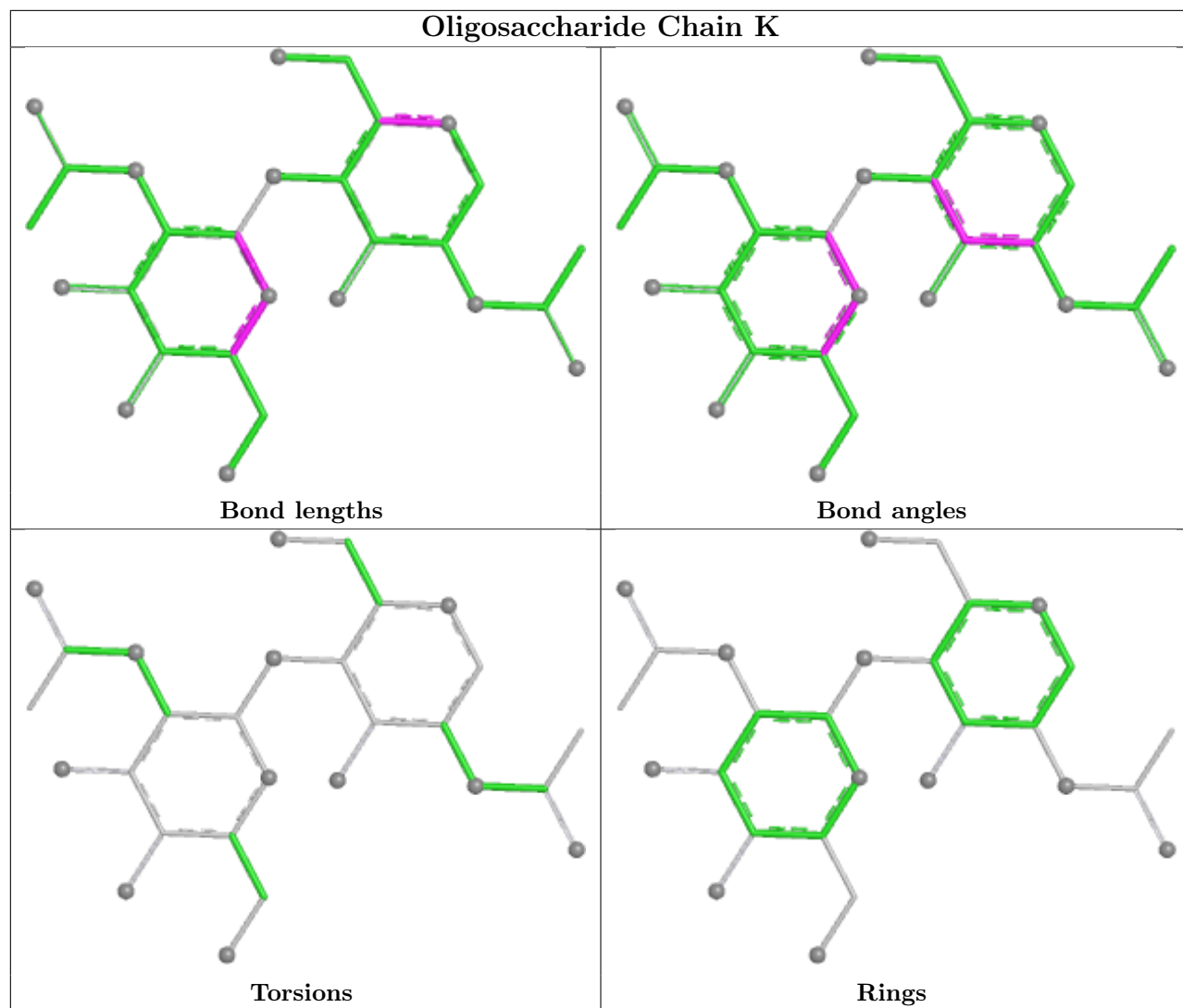


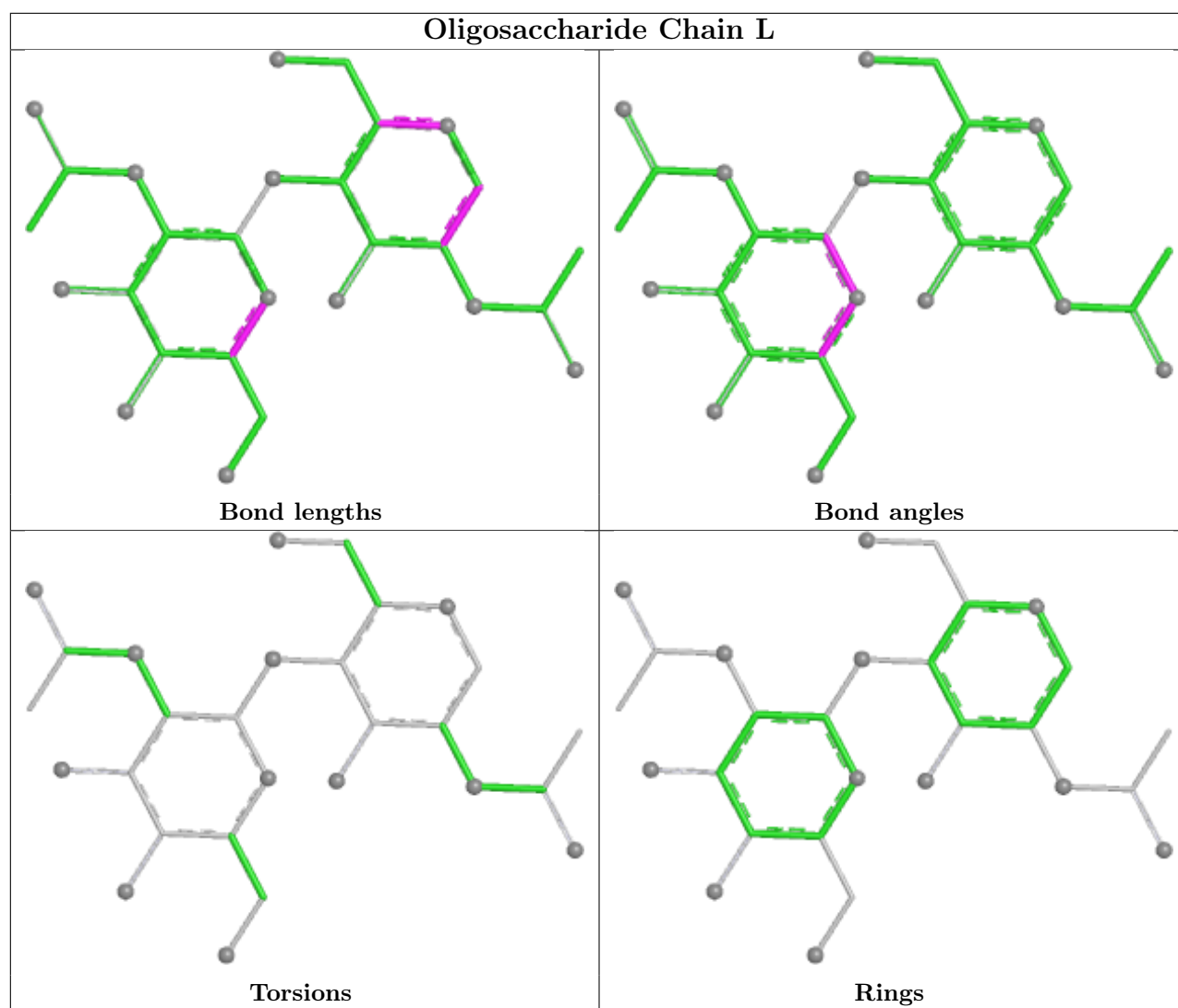


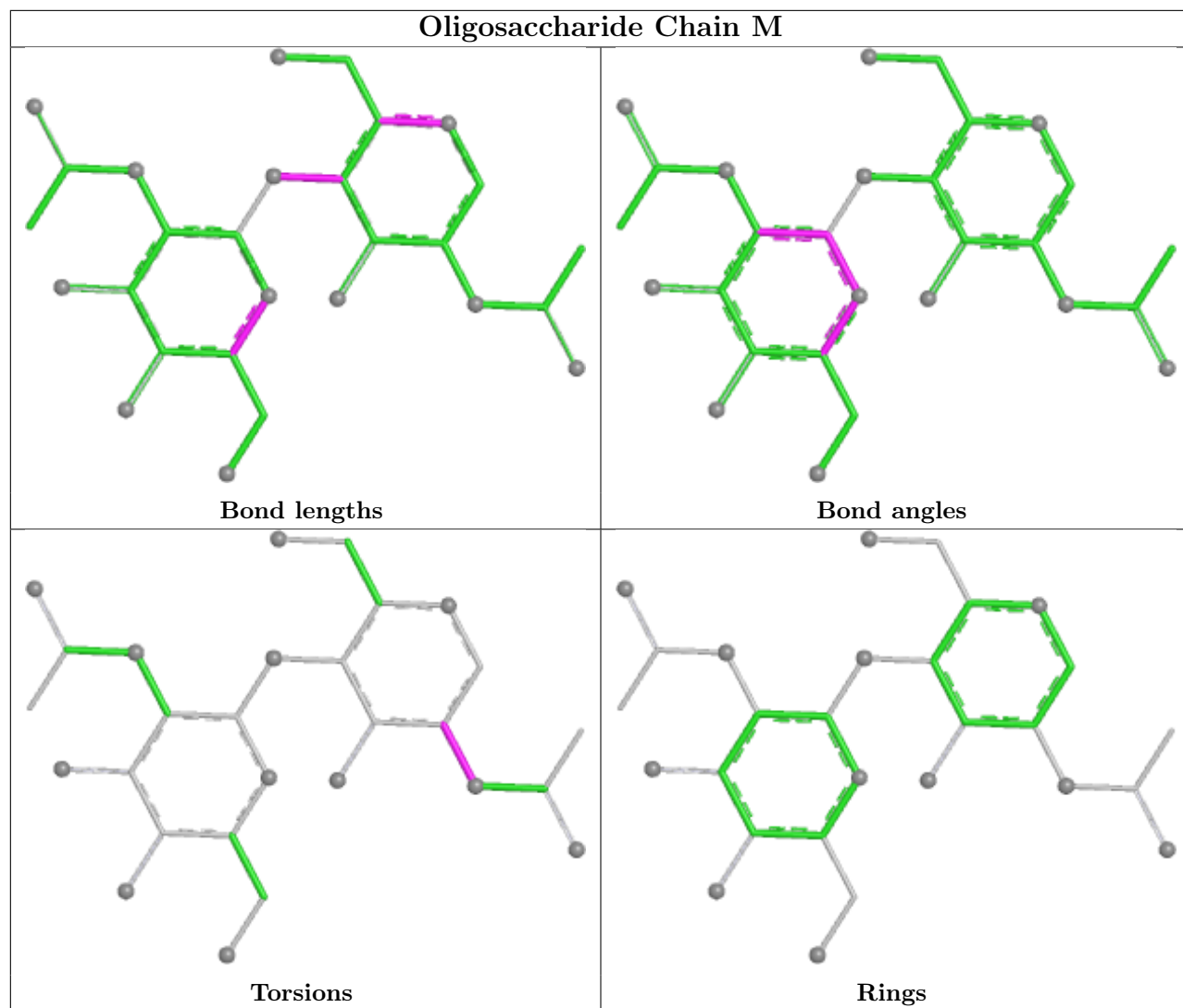


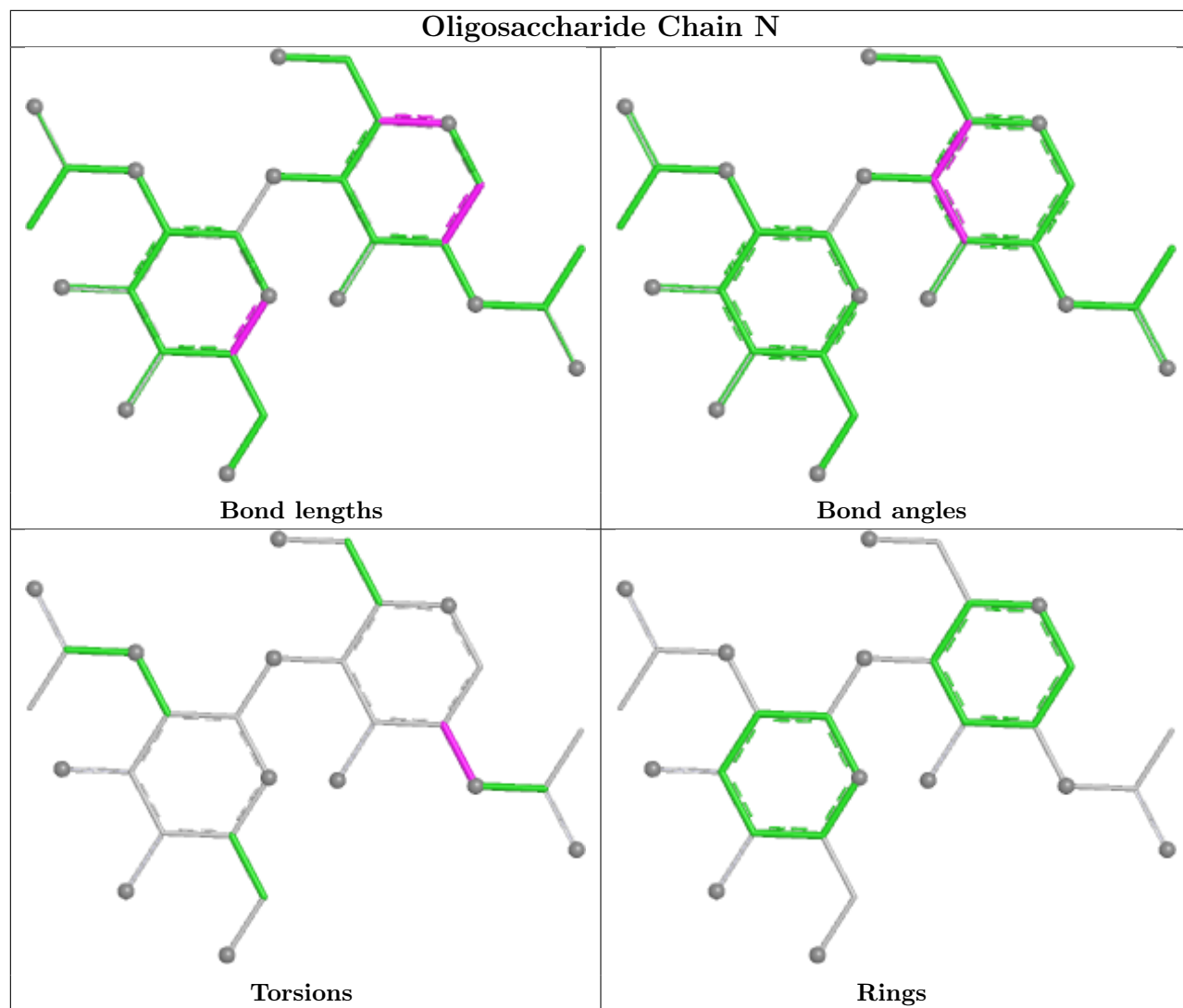


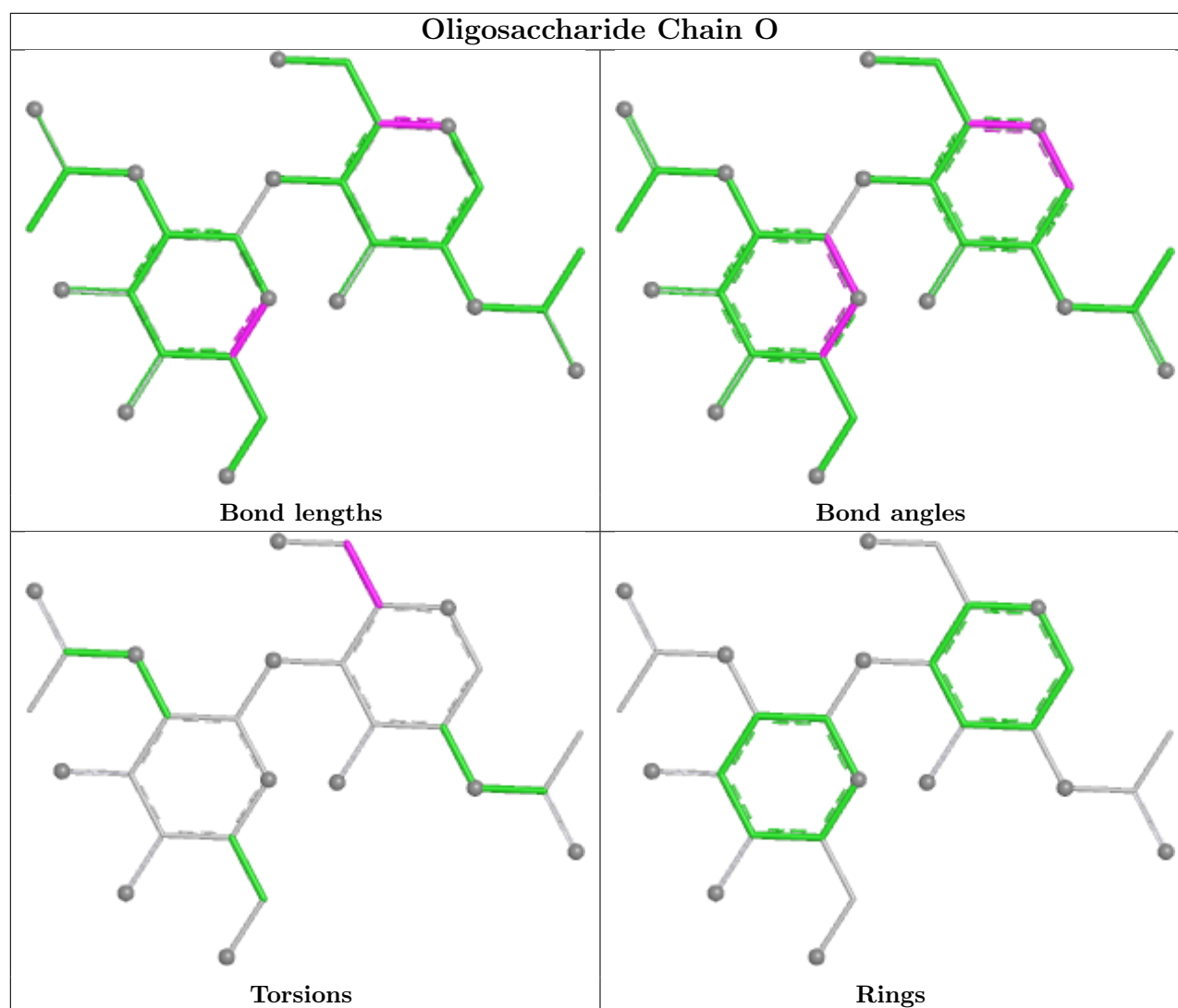












5.6 Ligand geometry [i](#)

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1303	1	14,14,15	1.25	2 (14%)	17,19,21	0.74	0
3	NAG	A	1305	1	14,14,15	1.32	2 (14%)	17,19,21	0.93	1 (5%)
3	NAG	C	1303	1	14,14,15	1.22	1 (7%)	17,19,21	1.01	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1301	1	14,14,15	1.27	1 (7%)	17,19,21	1.15	2 (11%)
3	NAG	B	1305	1	14,14,15	1.23	2 (14%)	17,19,21	0.66	0
3	NAG	C	1310	1	14,14,15	1.23	2 (14%)	17,19,21	0.89	1 (5%)
3	NAG	C	1305	1	14,14,15	1.29	2 (14%)	17,19,21	0.83	0
3	NAG	B	1302	1	14,14,15	1.29	2 (14%)	17,19,21	1.11	1 (5%)
3	NAG	A	1304	1	14,14,15	1.30	3 (21%)	17,19,21	0.99	1 (5%)
3	NAG	B	1312	1	14,14,15	1.20	2 (14%)	17,19,21	0.71	0
3	NAG	C	1312	1	14,14,15	1.26	2 (14%)	17,19,21	0.82	1 (5%)
3	NAG	B	1311	1	14,14,15	1.32	3 (21%)	17,19,21	0.93	1 (5%)
3	NAG	B	1303	1	14,14,15	1.20	2 (14%)	17,19,21	0.77	1 (5%)
3	NAG	B	1308	1	14,14,15	1.14	1 (7%)	17,19,21	0.73	0
3	NAG	C	1302	1	14,14,15	1.28	2 (14%)	17,19,21	0.88	1 (5%)
3	NAG	C	1311	1	14,14,15	1.34	3 (21%)	17,19,21	1.09	1 (5%)
3	NAG	A	1310	1	14,14,15	1.25	2 (14%)	17,19,21	0.97	1 (5%)
3	NAG	C	1308	1	14,14,15	1.05	0	17,19,21	1.43	1 (5%)
3	NAG	C	1306	1	14,14,15	1.23	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	C	1309	1	14,14,15	1.22	2 (14%)	17,19,21	0.59	0
3	NAG	A	1308	1	14,14,15	1.25	1 (7%)	17,19,21	0.67	0
3	NAG	A	1302	1	14,14,15	1.15	1 (7%)	17,19,21	0.56	0
3	NAG	B	1306	1	14,14,15	1.16	2 (14%)	17,19,21	0.79	0
3	NAG	A	1306	1	14,14,15	1.35	3 (21%)	17,19,21	0.58	0
3	NAG	A	1309	1	14,14,15	1.19	2 (14%)	17,19,21	0.81	0
3	NAG	B	1301	1	14,14,15	1.25	3 (21%)	17,19,21	1.02	1 (5%)
3	NAG	A	1307	1	14,14,15	1.25	2 (14%)	17,19,21	1.08	1 (5%)
3	NAG	B	1304	1	14,14,15	1.28	2 (14%)	17,19,21	0.66	0
3	NAG	B	1309	1	14,14,15	1.29	3 (21%)	17,19,21	0.72	1 (5%)
3	NAG	A	1301	1	14,14,15	1.29	2 (14%)	17,19,21	1.04	1 (5%)
3	NAG	B	1307	1	14,14,15	1.19	2 (14%)	17,19,21	0.77	1 (5%)
3	NAG	C	1304	1	14,14,15	1.32	3 (21%)	17,19,21	0.64	0
3	NAG	B	1310	1	14,14,15	1.23	2 (14%)	17,19,21	0.81	1 (5%)
3	NAG	C	1307	1	14,14,15	1.30	3 (21%)	17,19,21	1.00	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1312	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	1/6/23/26	0/1/1/1

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1311	NAG	O5-C5	3.10	1.49	1.43
3	A	1306	NAG	O5-C5	3.03	1.49	1.43
3	C	1301	NAG	O5-C5	3.02	1.49	1.43
3	B	1302	NAG	O5-C5	2.94	1.49	1.43
3	A	1307	NAG	O5-C5	2.93	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1303	NAG	O5-C5	2.89	1.49	1.43
3	A	1301	NAG	O5-C5	2.88	1.49	1.43
3	C	1312	NAG	O5-C5	2.88	1.49	1.43
3	A	1308	NAG	O5-C5	2.85	1.49	1.43
3	A	1303	NAG	O5-C5	2.85	1.49	1.43
3	B	1311	NAG	O5-C5	2.80	1.48	1.43
3	C	1304	NAG	O5-C5	2.78	1.48	1.43
3	B	1304	NAG	O5-C5	2.77	1.48	1.43
3	C	1310	NAG	O5-C5	2.74	1.48	1.43
3	B	1309	NAG	O5-C5	2.74	1.48	1.43
3	A	1304	NAG	O5-C5	2.73	1.48	1.43
3	C	1305	NAG	O5-C5	2.72	1.48	1.43
3	B	1312	NAG	O5-C5	2.68	1.48	1.43
3	C	1302	NAG	O5-C5	2.66	1.48	1.43
3	C	1306	NAG	O5-C5	2.66	1.48	1.43
3	B	1310	NAG	O5-C5	2.65	1.48	1.43
3	C	1307	NAG	O5-C5	2.63	1.48	1.43
3	B	1305	NAG	O5-C5	2.62	1.48	1.43
3	A	1305	NAG	O5-C5	2.62	1.48	1.43
3	A	1310	NAG	O5-C5	2.61	1.48	1.43
3	A	1302	NAG	O5-C5	2.59	1.48	1.43
3	B	1303	NAG	O5-C5	2.57	1.48	1.43
3	B	1301	NAG	O5-C5	2.54	1.48	1.43
3	B	1306	NAG	O5-C5	2.53	1.48	1.43
3	C	1309	NAG	O5-C5	2.50	1.48	1.43
3	B	1307	NAG	O5-C5	2.43	1.48	1.43
3	C	1307	NAG	C1-C2	2.43	1.55	1.52
3	B	1304	NAG	C1-C2	2.39	1.55	1.52
3	B	1311	NAG	C1-C2	2.39	1.55	1.52
3	B	1301	NAG	C1-C2	2.36	1.55	1.52
3	C	1304	NAG	C1-C2	2.35	1.55	1.52
3	A	1305	NAG	C1-C2	2.34	1.55	1.52
3	A	1309	NAG	C1-C2	2.33	1.55	1.52
3	B	1308	NAG	C1-C2	2.33	1.55	1.52
3	A	1309	NAG	O5-C5	2.32	1.48	1.43
3	B	1307	NAG	C1-C2	2.31	1.55	1.52
3	C	1305	NAG	C1-C2	2.31	1.55	1.52
3	A	1304	NAG	C1-C2	2.30	1.55	1.52
3	C	1302	NAG	C1-C2	2.29	1.55	1.52
3	C	1309	NAG	C1-C2	2.28	1.55	1.52
3	B	1309	NAG	C1-C2	2.27	1.55	1.52
3	A	1301	NAG	C1-C2	2.25	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1306	NAG	C1-C2	2.23	1.55	1.52
3	C	1311	NAG	O5-C1	2.19	1.47	1.43
3	B	1312	NAG	C1-C2	2.18	1.55	1.52
3	B	1305	NAG	C1-C2	2.17	1.55	1.52
3	A	1310	NAG	C1-C2	2.15	1.55	1.52
3	B	1310	NAG	C1-C2	2.15	1.55	1.52
3	B	1301	NAG	O5-C1	2.11	1.47	1.43
3	A	1306	NAG	O5-C1	2.10	1.47	1.43
3	A	1306	NAG	C1-C2	2.09	1.55	1.52
3	C	1304	NAG	O5-C1	2.09	1.47	1.43
3	B	1311	NAG	O5-C1	2.06	1.47	1.43
3	C	1307	NAG	O5-C1	2.06	1.47	1.43
3	B	1303	NAG	C1-C2	2.06	1.55	1.52
3	B	1306	NAG	C1-C2	2.06	1.55	1.52
3	C	1312	NAG	C1-C2	2.06	1.55	1.52
3	A	1307	NAG	O5-C1	2.04	1.47	1.43
3	A	1303	NAG	C1-C2	2.04	1.55	1.52
3	B	1302	NAG	C1-C2	2.03	1.55	1.52
3	A	1304	NAG	O5-C1	2.02	1.47	1.43
3	C	1310	NAG	C1-C2	2.01	1.55	1.52
3	C	1311	NAG	C1-C2	2.01	1.55	1.52
3	B	1309	NAG	O5-C1	2.00	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1308	NAG	C1-O5-C5	5.33	119.33	112.19
3	B	1302	NAG	C1-O5-C5	3.67	117.11	112.19
3	A	1307	NAG	C1-O5-C5	3.58	116.98	112.19
3	B	1301	NAG	C1-O5-C5	3.55	116.95	112.19
3	C	1306	NAG	C1-O5-C5	3.51	116.89	112.19
3	A	1304	NAG	C1-O5-C5	3.50	116.88	112.19
3	A	1301	NAG	C1-O5-C5	3.44	116.80	112.19
3	B	1311	NAG	C1-O5-C5	3.35	116.68	112.19
3	C	1307	NAG	C1-O5-C5	3.19	116.46	112.19
3	C	1310	NAG	C1-O5-C5	3.15	116.40	112.19
3	C	1311	NAG	C1-O5-C5	3.07	116.30	112.19
3	A	1310	NAG	C1-O5-C5	3.04	116.26	112.19
3	C	1302	NAG	C1-O5-C5	2.96	116.15	112.19
3	C	1301	NAG	C1-C2-N2	2.84	114.91	110.43
3	B	1310	NAG	C1-O5-C5	2.62	115.69	112.19
3	C	1312	NAG	C1-O5-C5	2.48	115.51	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1303	NAG	C1-O5-C5	2.43	115.44	112.19
3	C	1301	NAG	O5-C1-C2	-2.43	107.54	111.29
3	B	1307	NAG	C1-O5-C5	2.38	115.38	112.19
3	A	1305	NAG	C1-O5-C5	2.13	115.04	112.19
3	B	1309	NAG	C1-O5-C5	2.13	115.03	112.19
3	C	1303	NAG	C1-O5-C5	2.10	115.00	112.19
3	C	1303	NAG	O5-C1-C2	-2.07	108.09	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1307	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	C	1307	NAG	C1-C2-N2-C7
3	C	1312	NAG	C1-C2-N2-C7
3	C	1301	NAG	O7-C7-N2-C2
3	B	1303	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	NAG	1	0
3	C	1305	NAG	2	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.

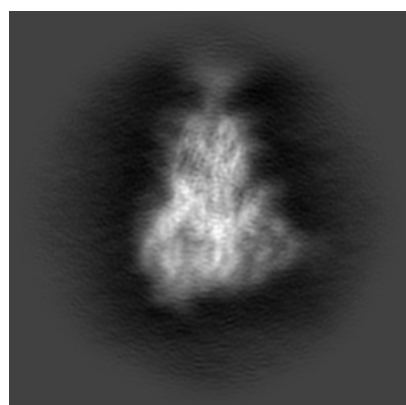
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26051. These allow visual inspection of the internal detail of the map and identification of artifacts.

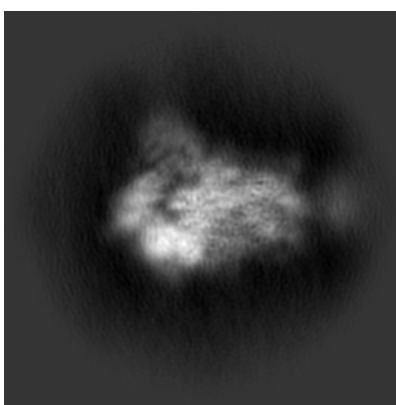
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

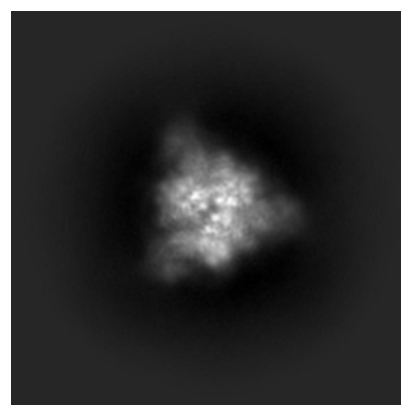
6.1.1 Primary map



X



Y

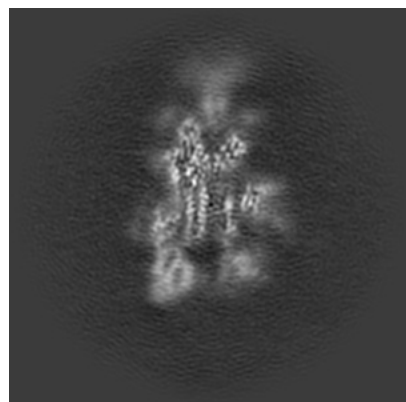


Z

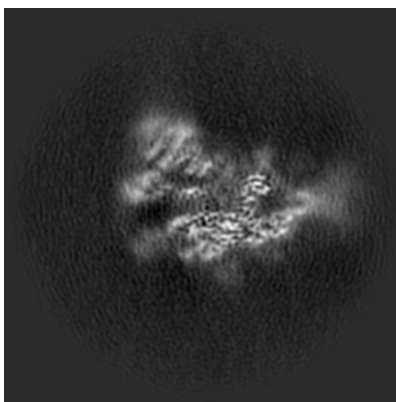
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

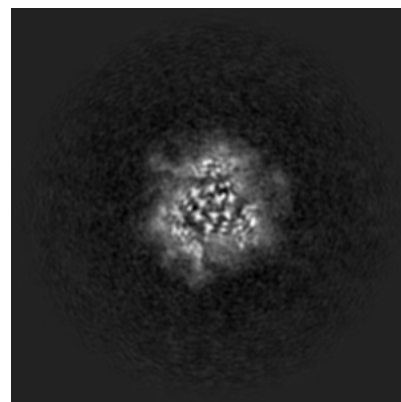
6.2.1 Primary map



X Index: 150



Y Index: 150

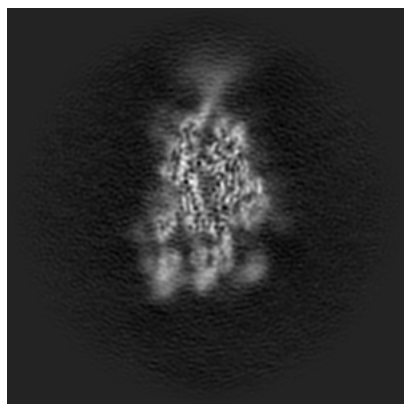


Z Index: 150

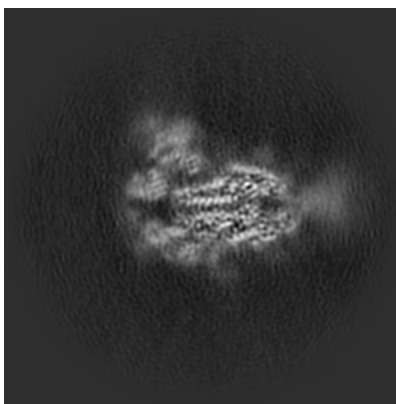
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

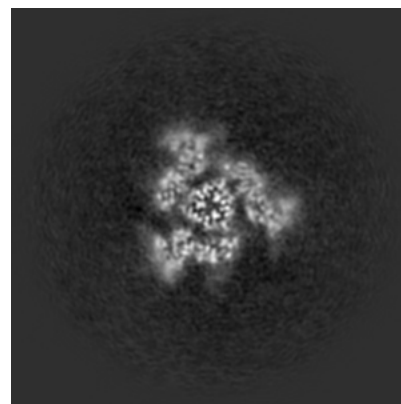
6.3.1 Primary map



X Index: 160



Y Index: 155

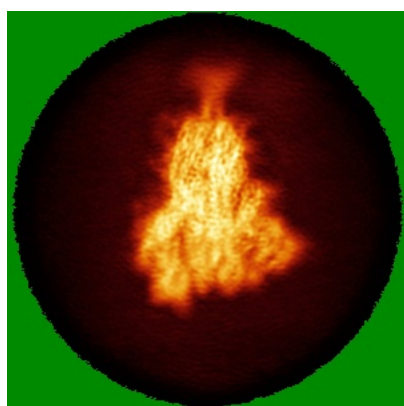


Z Index: 138

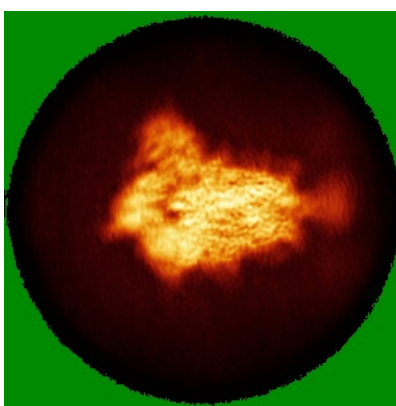
The images above show the largest variance slices of the map in three orthogonal directions.

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

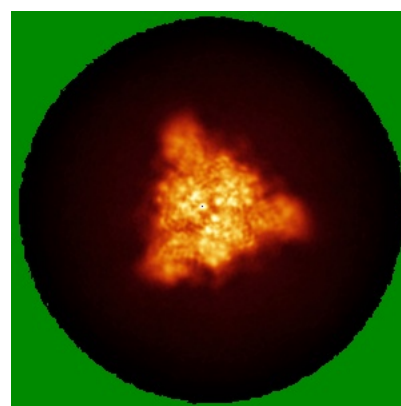
6.4.1 Primary map



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

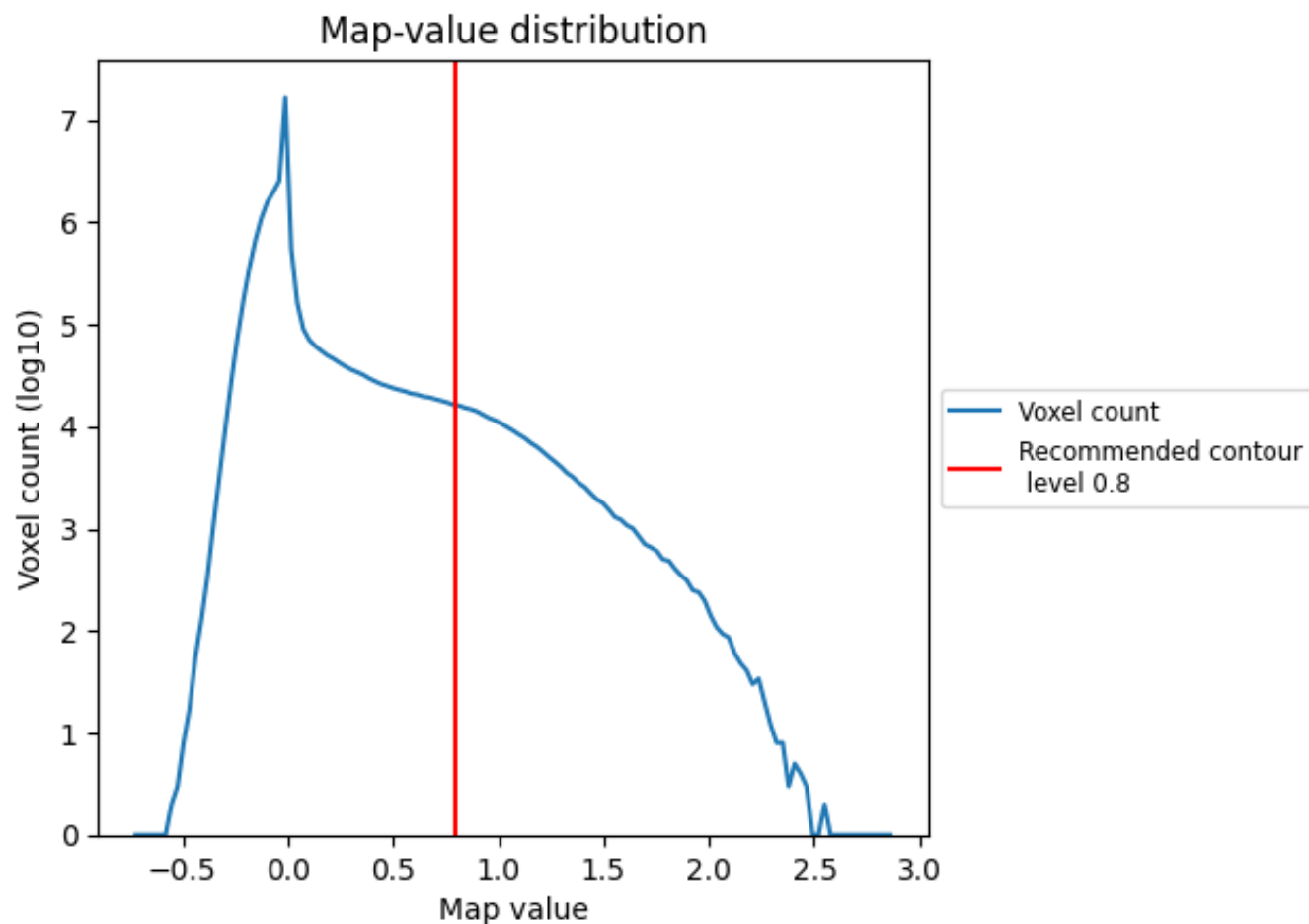
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

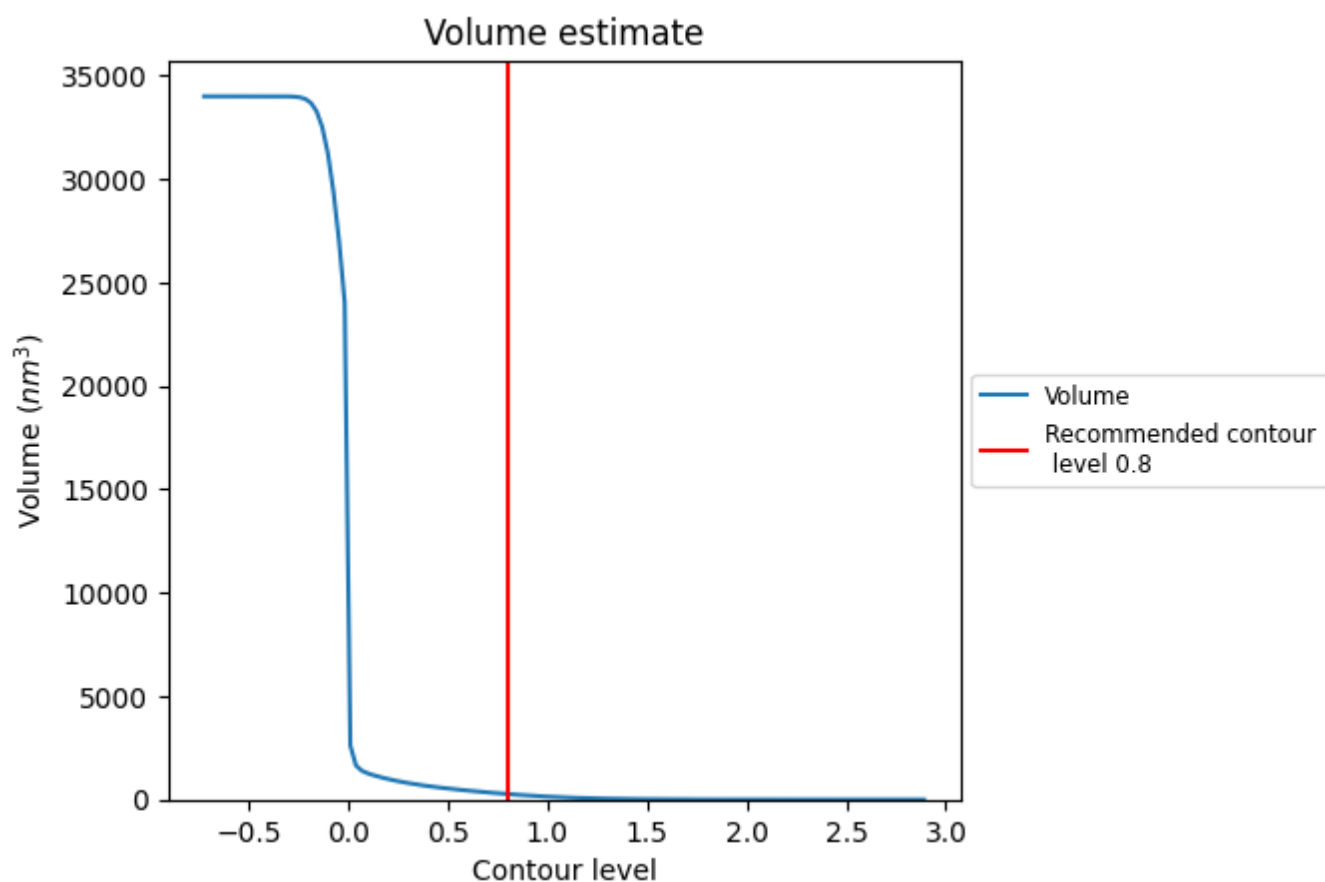
This section contains the results of statistical analysis of the map.

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.

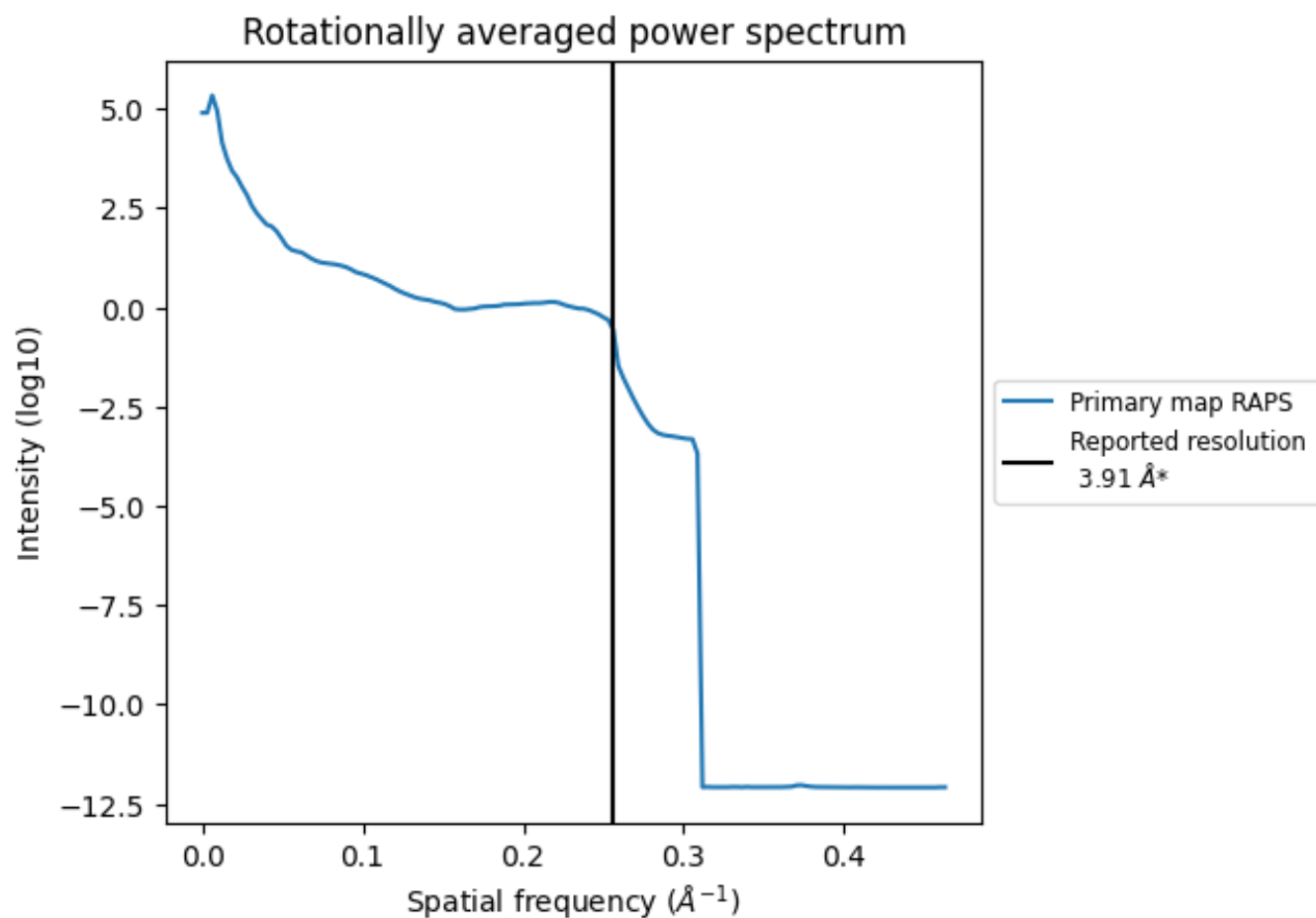
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 268 nm³; this corresponds to an approximate mass of 242 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 0.256 Å⁻¹

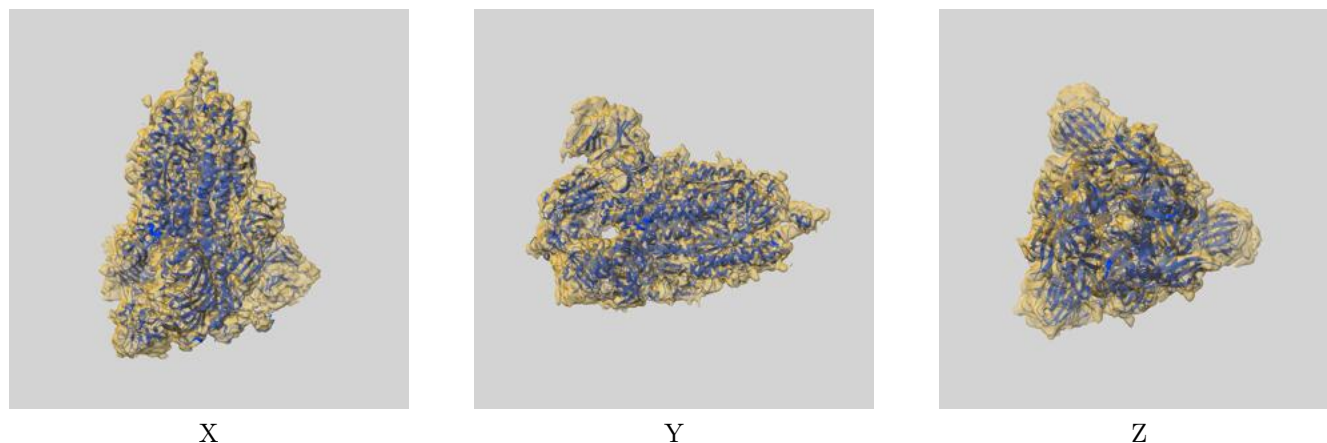
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

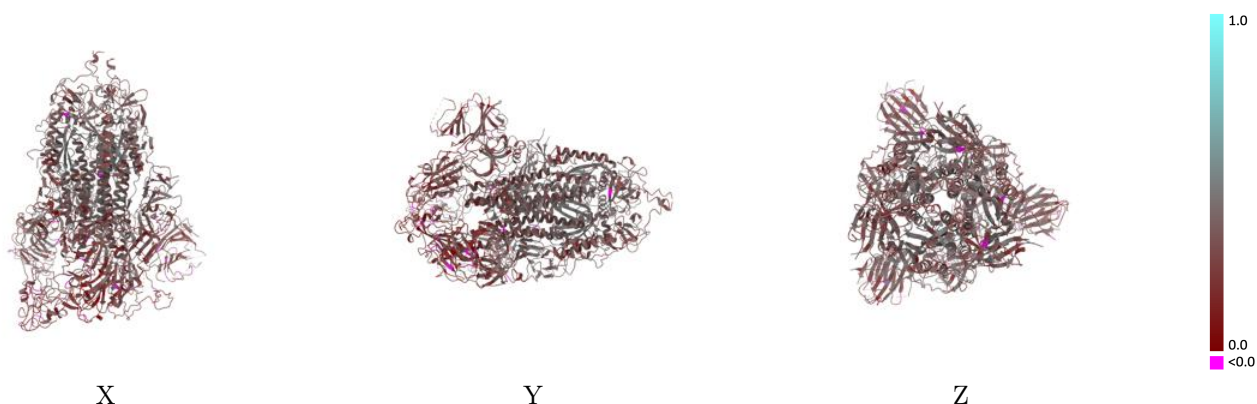
This section contains information regarding the fit between EMDB map EMD-26051 and PDB model 7TPC. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



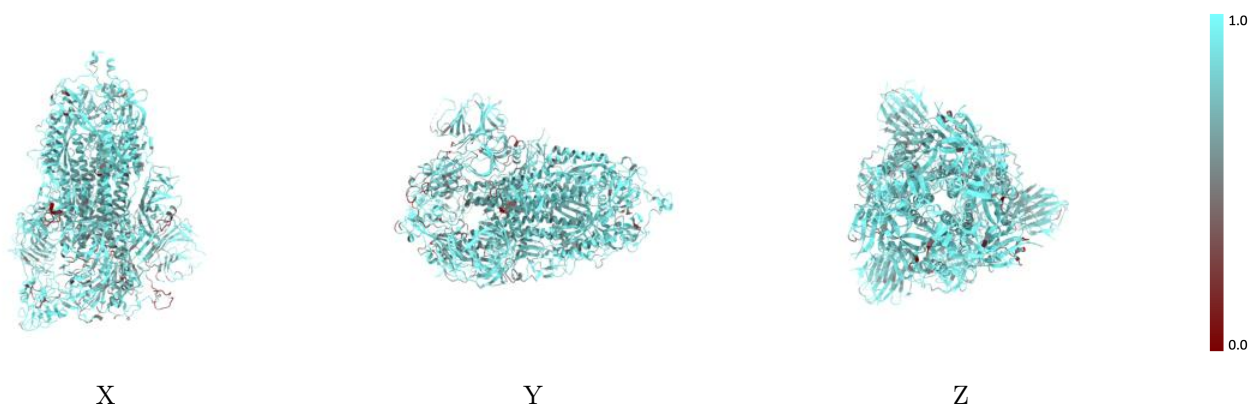
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



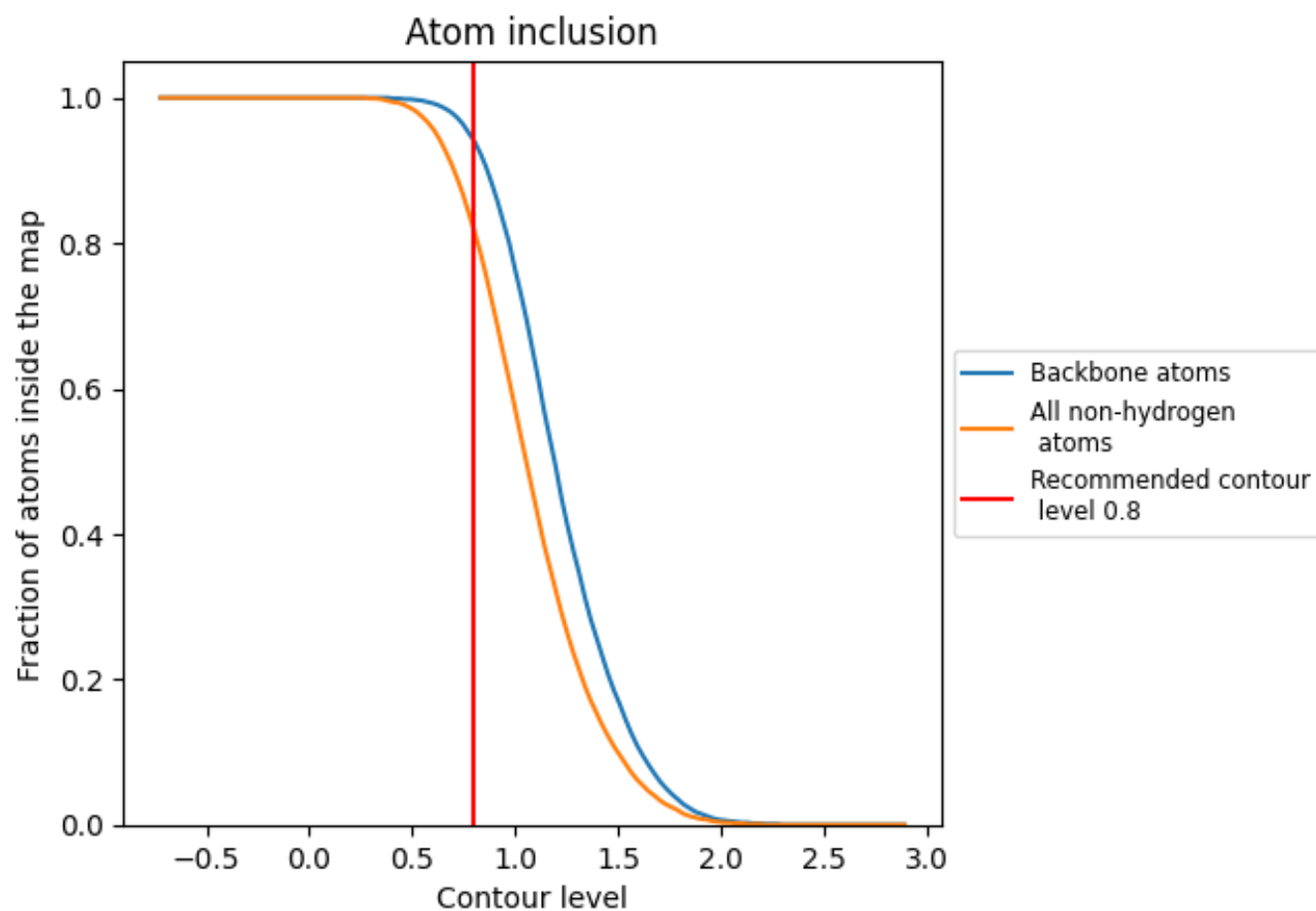
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 82% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8180	<div></div> 0.3210
A	<div></div> 0.8080	<div></div> 0.3130
B	<div></div> 0.8390	<div></div> 0.3250
C	<div></div> 0.8230	<div></div> 0.3240
D	<div></div> 0.4290	<div></div> 0.2310
E	<div></div> 0.4640	<div></div> 0.4490
F	<div></div> 0.4640	<div></div> 0.4090
G	<div></div> 0.6070	<div></div> 0.3700
H	<div></div> 0.3210	<div></div> 0.3830
I	<div></div> 0.6070	<div></div> 0.3650
J	<div></div> 0.5000	<div></div> 0.3830
K	<div></div> 0.3930	<div></div> 0.3700
L	<div></div> 0.3930	<div></div> 0.4160
M	<div></div> 0.5000	<div></div> 0.4250
N	<div></div> 0.5000	<div></div> 0.2420
O	<div></div> 0.5710	<div></div> 0.3740

1.0

0.0

<0.0