



wwPDB EM Validation Summary Report ⓘ

Dec 1, 2025 – 10:34 AM EST

PDB ID : 9OG4 / pdb_00009og4
EMDB ID : EMD-70451
Title : SARS-COV-2-6P-MUT7 S PROTEIN-DY-III-281 complex closed conformation
Authors : Chandravanshi, M.; Niu, L.; Tolbert, W.D.; Pazgier, M.
Deposited on : 2025-04-30
Resolution : 3.56 Å(reported)
Based on initial model : 7RU1

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

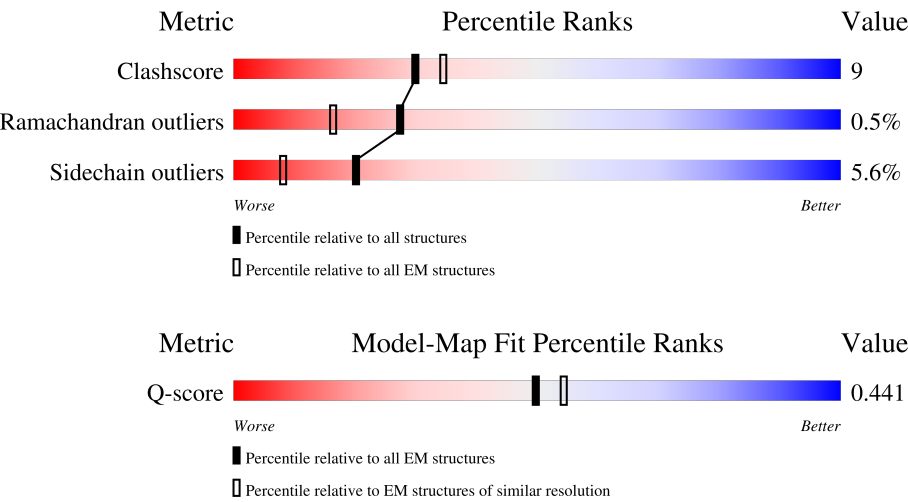
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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.




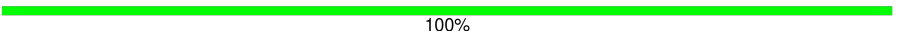

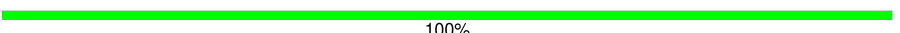
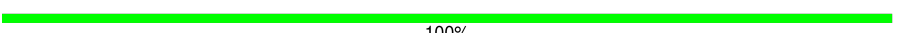
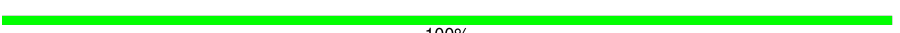







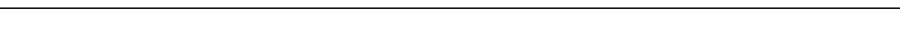



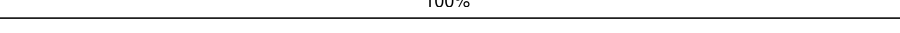

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12750 (3.06 - 4.06)

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	1280	<div><div></div><div>61%19%18%</div></div>
1	B	1280	<div><div></div><div>65%18%16%</div></div>
1	C	1280	<div><div></div><div>60%18%20%</div></div>
2	D	2	<div><div></div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
2	E	2	 50% 50%
2	G	2	 100%
2	H	2	 50% 50%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 50% 50%
2	N	2	 50% 50%
2	O	2	 50% 50%
2	P	2	 100%
2	Q	2	 50% 50%
2	T	2	 50% 50%
3	F	3	 33% 100%
3	I	3	 33% 67%
3	R	3	 67% 33%
3	S	3	 33% 67%
3	U	3	 100%
3	V	3	 33% 67%
3	W	3	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25594 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	1053	Total	C	N	O	S	0	0
			8217	5240	1368	1569	40		
1	C	1025	Total	C	N	O	S	0	0
			7998	5105	1325	1529	39		
1	B	1079	Total	C	N	O	S	0	0
			8434	5379	1407	1606	42		

There are 249 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	705	CYS	VAL	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	883	CYS	THR	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	SER	-	expression tag	UNP P0DTC2
A	1251	ALA	-	expression tag	UNP P0DTC2
A	1252	TRP	-	expression tag	UNP P0DTC2
A	1253	SER	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	PRO	-	expression tag	UNP P0DTC2
A	1256	GLN	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	LYS	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	GLY	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	GLY	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	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	ALA	-	expression tag	UNP P0DTC2
A	1273	TRP	-	expression tag	UNP P0DTC2
A	1274	SER	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	PRO	-	expression tag	UNP P0DTC2
A	1277	GLN	-	expression tag	UNP P0DTC2
A	1278	PHE	-	expression tag	UNP P0DTC2
A	1279	GLU	-	expression tag	UNP P0DTC2
A	1280	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	705	CYS	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	883	CYS	THR	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	GLY	-	expression tag	UNP P0DTC2
C	1239	ARG	-	expression tag	UNP P0DTC2
C	1240	SER	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	VAL	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	PHE	-	expression tag	UNP P0DTC2
C	1246	GLN	-	expression tag	UNP P0DTC2
C	1247	GLY	-	expression tag	UNP P0DTC2
C	1248	PRO	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	ALA	-	expression tag	UNP P0DTC2
C	1252	TRP	-	expression tag	UNP P0DTC2
C	1253	SER	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	PRO	-	expression tag	UNP P0DTC2
C	1256	GLN	-	expression tag	UNP P0DTC2
C	1257	PHE	-	expression tag	UNP P0DTC2
C	1258	GLU	-	expression tag	UNP P0DTC2
C	1259	LYS	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	GLY	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	SER	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1265	GLY	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	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	ALA	-	expression tag	UNP P0DTC2
C	1273	TRP	-	expression tag	UNP P0DTC2
C	1274	SER	-	expression tag	UNP P0DTC2
C	1275	HIS	-	expression tag	UNP P0DTC2
C	1276	PRO	-	expression tag	UNP P0DTC2
C	1277	GLN	-	expression tag	UNP P0DTC2
C	1278	PHE	-	expression tag	UNP P0DTC2
C	1279	GLU	-	expression tag	UNP P0DTC2
C	1280	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	705	CYS	VAL	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	883	CYS	THR	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	SER	-	expression tag	UNP P0DTC2
B	1251	ALA	-	expression tag	UNP P0DTC2
B	1252	TRP	-	expression tag	UNP P0DTC2
B	1253	SER	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	PRO	-	expression tag	UNP P0DTC2
B	1256	GLN	-	expression tag	UNP P0DTC2
B	1257	PHE	-	expression tag	UNP P0DTC2
B	1258	GLU	-	expression tag	UNP P0DTC2
B	1259	LYS	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	GLY	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	SER	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	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	ALA	-	expression tag	UNP P0DTC2
B	1273	TRP	-	expression tag	UNP P0DTC2
B	1274	SER	-	expression tag	UNP P0DTC2
B	1275	HIS	-	expression tag	UNP P0DTC2
B	1276	PRO	-	expression tag	UNP P0DTC2
B	1277	GLN	-	expression tag	UNP P0DTC2
B	1278	PHE	-	expression tag	UNP P0DTC2
B	1279	GLU	-	expression tag	UNP P0DTC2
B	1280	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.



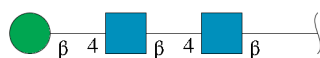
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16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

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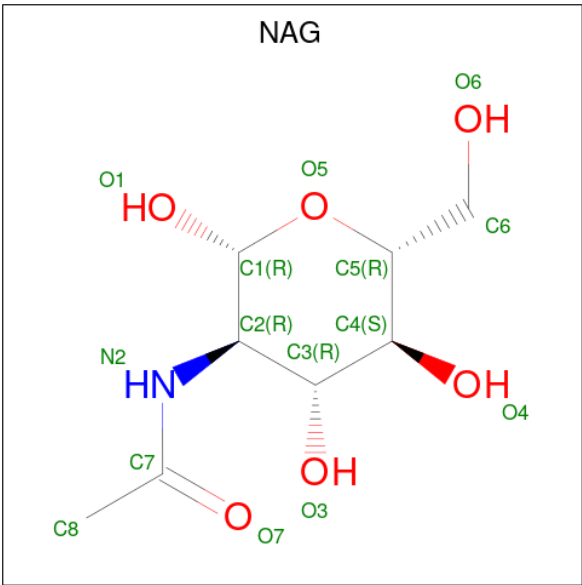
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	R	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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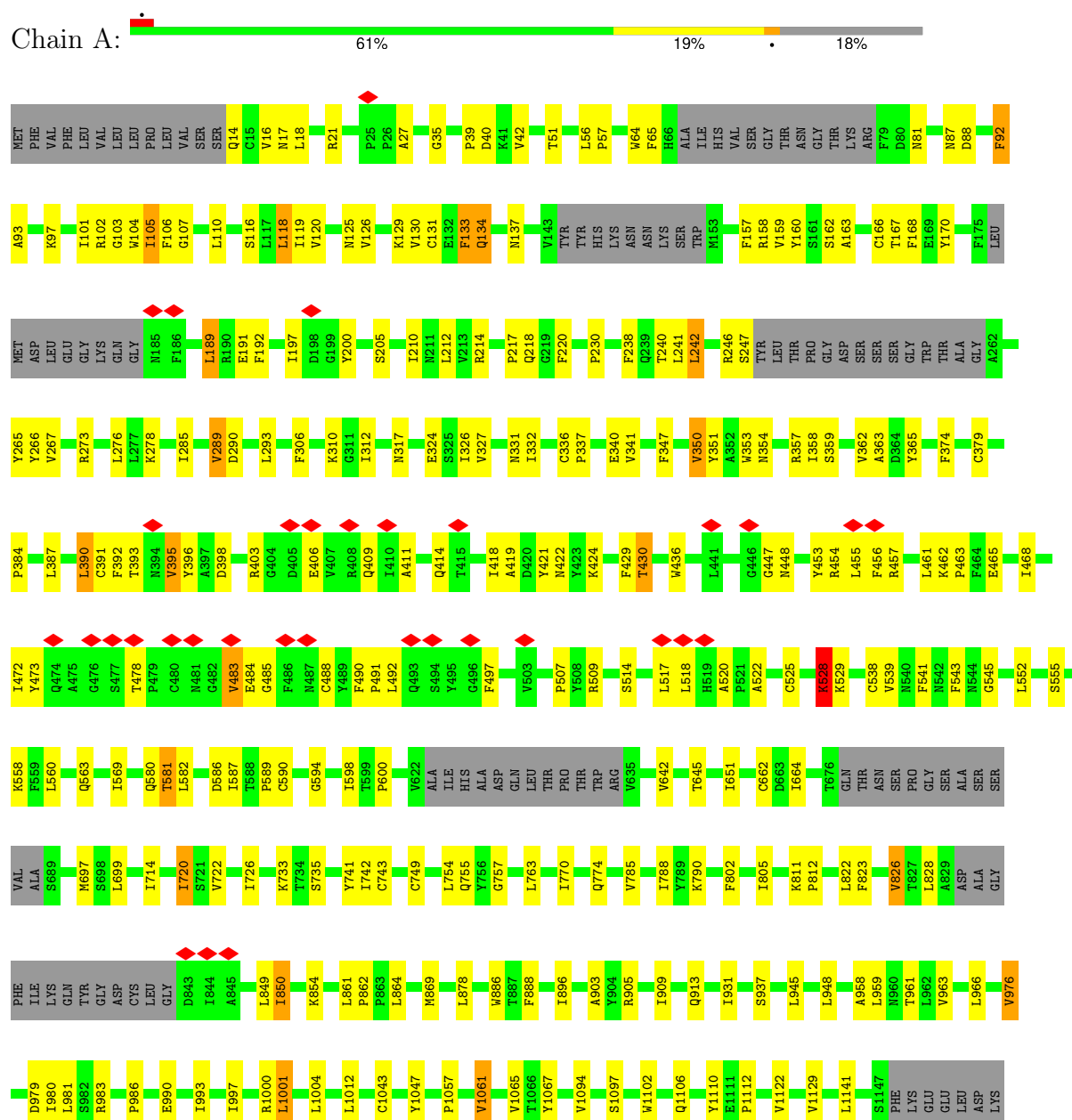
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C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

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



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

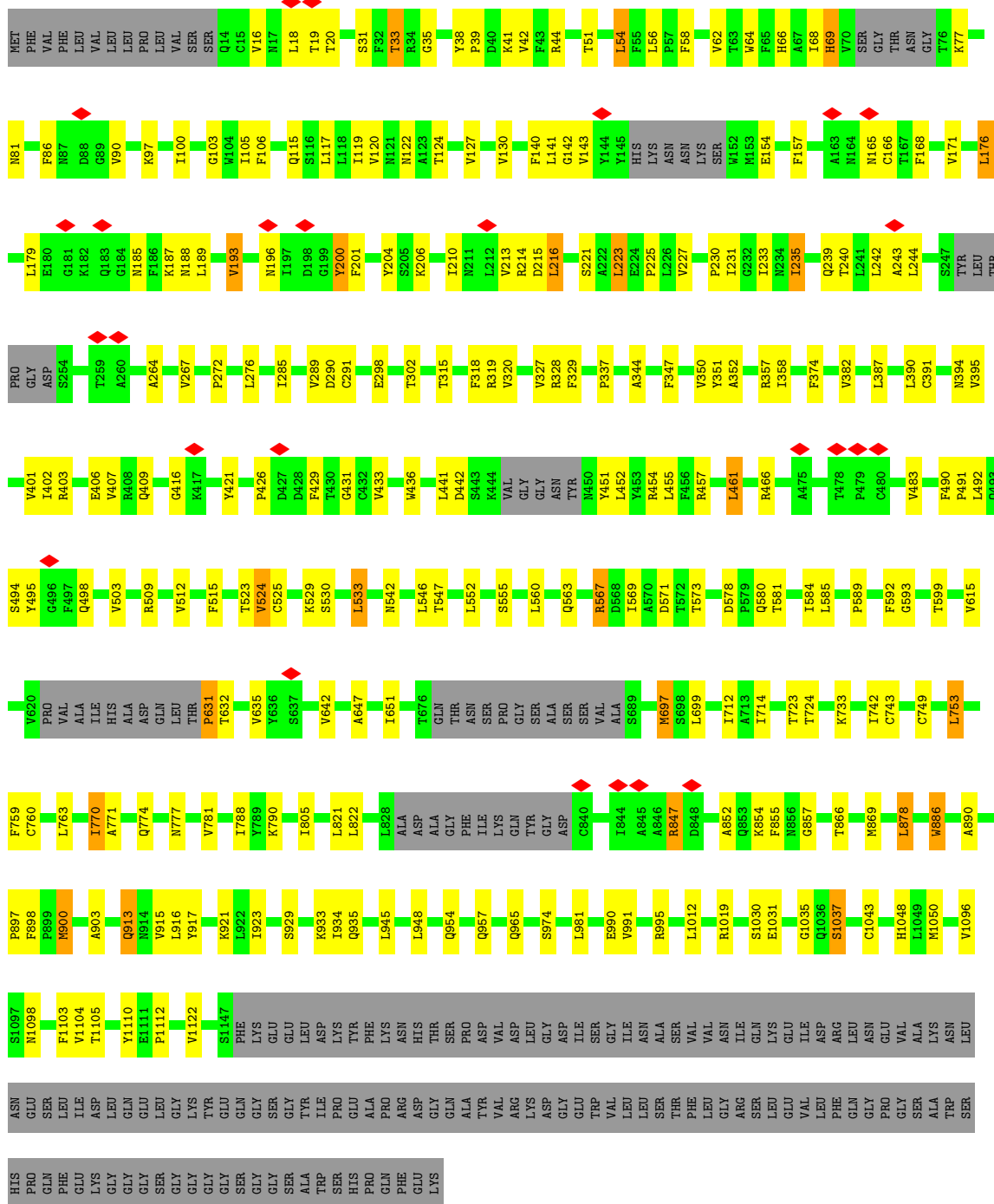
• Molecule 1: Spike glycoprotein

Chain C: 

ASN	HIS	THR	SER	PRO	ASP	VAL	ASP	GLY	ASP	ILE	SER	GLY	ASN	ASN	ALA	SER	VAL	SER	ASN	ILE	GLN	GLY	ILE	ASP	GLU	ASP	ARG	LEU	ASN	GLU	SER	LEU	ILE	LYS	TYR	GLY	ASN	PRO	GLY	ALA	GLU	PRO										
R1000	L1001	Q1002	S1003	L1004	L1012	R1019	F1019	L1024	K1028	M1029	S1030	V1040	D1041	G1046	M1050	V1061	V1065	F1075	T1076	L1084	G1085	K1086	S1097	F1103	V1104	Y1110	E1111	P1112	V1122	V1128	V1129	S1147	PHE	LYS	GLU	GLU	LEU	ASP	LYS	PRO	GLU	ALA	PRO									
ALA	ALA	ARG	ASP	LEU	ILE	C851	K854	F855	L864	W869	L878	I882	F898	M902	A903	Y904	N907	L916	Y917	L922	I923	Q926	I931	I934	S937	L945	L948	V952	Q957	A958	L959	V963	V976	L984	A989	E990	Y991															
ALA	SER	SER	VAL	ALA	S689	M697	S698	Y707	V722	I726	T734	C738	Y741	I742	C743	C749	F759	C760	L763	I770	Q774	N777	L806	S810	L822	L828	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE										
R577	D578	P579	Q580	T581	D586	S591	F592	G593	I598	D614	V615	P621	V622	A623	R624	H625	A626	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	G636	S637	T638	N641	V642	L650	I651	G652	A653	V656	S659	C662	D663	I664	T676	GLN	THR	ASN	SER	PRO	GLY	SER					
F456	P463	I468	S469	T470	Y473	Q474	A475	C480	Y481	G482	E484	C488	P491	L492	C496	N501	G502	V503	G504	Y505	V512	F515	A520	P521	A522	K528	V534	K537	C538	V539	T547	T553	E554	S555	L560	P561	F562	Q563	V576													
Y351	A352	W353	W354	R355	N360	C361	D364	V367	K378	C379	Y380	T385	C391	F392	T393	Y396	F400	G404	D405	E406	G407	R408	T415	G416	K417	I418	Y421	N422	Y423	K424	L425	D428	G431	C432	V433	I434	S443	VAL	GLY	GLY	W448	Y449	L452									
TYR	LEU	THR	PRO	ASP	GLY	SER	SER	SER	THR	ALA	G261	A262	A263	A264	Y265	Y266	L276	L277	N282	I285	P295	T299	K300	C301	T302	L303	T307	V308	I312	T315	F318	R319	V320	I326	V327	R328	F329	I332	C336	F342	T345	V350										
P174	F175	L176	MET	LEU	GLU	GLY	GLN	GLY	ASN	PHE	LYS	N188	L189	R190	E191	V193	F194	K195	F201	K202	S205	K206	L212	V213	R214	C301	D215	L216	P217	L223	L226	V227	D228	L229	P230	I231	G232	I233	N234	I235	T236	R237	Q238	Q239	T240	L241	L242	ALA	LEU	HIS	ARG	SER
F86	V90	Y91	F92	A93	S94	I100	G103	W104	I105	F106	L110	L117	L118	L119	N122	N123	N124	V126	V130	C131	E132	F135	L141	G142	V143	TYR	HIS	LYS	ASN	ASN	LYS	SER	TRP	M153	F157	R158	Y159	Y160	N164	N165	F168	V169	Y170									
MET	PHE	PHE	LEU	VAL	LEU	LEU	PRO	LEU	VAL	SER	GLN	CYS	VAL	ASN	LEU	THR	THR	ARG	THR	GLN	PRO	LEU	PRO	P26	A27	R34	P39	V47	T51	N61	W64	F65	H66	ALA	ILE	HIS	VAL	SER	GLY	THR	LYS	ARG	F79	D80	N81	P82	V83	L84	P85			

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

- Molecule 1: Spike glycoprotein



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

Chain D:  100%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%



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

Chain M:  50% 50%



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

Chain N:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain T:  50% 50%



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

Chain F:  33% 100%



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

Chain I:  33% 67%



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

Chain R:  67% 67% 33%



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

Chain S:  33% 33% 67%



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

Chain U:  100%



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

Chain V:  33% 67%



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

Chain W:

100%

MAG1
MAG2
EMJ3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.798	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.079	Depositor
Map size (Å)	331.13602, 331.13602, 331.13602	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.16	0/8404	0.34	0/11441
1	B	0.14	0/8629	0.32	0/11744
1	C	0.14	0/8182	0.31	0/11138
All	All	0.14	0/25215	0.32	0/34323

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8217	0	8011	171	0
1	B	8434	0	8212	151	0
1	C	7998	0	7773	149	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	H	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	28	0	25	1	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	T	28	0	25	0	0
3	F	39	0	34	0	0
3	I	39	0	34	0	0
3	R	39	0	34	0	0
3	S	39	0	34	0	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
3	W	39	0	34	0	0
4	A	56	0	52	0	0
4	B	126	0	117	2	0
4	C	126	0	117	3	0
All	All	25594	0	24845	447	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 9.

The worst 5 of 447 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:318:PHE:HB3	1:B:593:GLY:HA3	1.58	0.86
1:C:406:GLU:HG2	1:C:418:ILE:HG13	1.60	0.84
1:C:106:PHE:HB2	1:C:117:LEU:HB2	1.61	0.82
1:C:201:PHE:HB3	1:C:229:LEU:HB3	1.66	0.78
1:C:105:ILE:HB	1:C:239:GLN:HB2	1.67	0.76

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	1037/1280 (81%)	939 (90%)	94 (9%)	4 (0%)	30	62
1	B	1063/1280 (83%)	963 (91%)	96 (9%)	4 (0%)	30	62
1	C	1007/1280 (79%)	900 (89%)	101 (10%)	6 (1%)	22	56
All	All	3107/3840 (81%)	2802 (90%)	291 (9%)	14 (0%)	27	59

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	615	VAL
1	A	483	VAL
1	C	126	VAL
1	C	624	ILE
1	B	503	VAL

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	924/1108 (83%)	878 (95%)	46 (5%)	20	49
1	B	946/1108 (85%)	896 (95%)	50 (5%)	19	48
1	C	899/1108 (81%)	840 (93%)	59 (7%)	14	42
All	All	2769/3324 (83%)	2614 (94%)	155 (6%)	20	46

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	200	TYR
1	B	847	ARG
1	B	240	THR
1	B	547	THR
1	B	990	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	957	GLN
1	B	1011	GLN
1	C	506	GLN
1	C	437	ASN
1	B	1058	HIS

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 ⓘ

47 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	0.73	0	17,19,21	1.07	2 (11%)
2	NAG	D	2	2	14,14,15	0.69	0	17,19,21	1.22	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.69	0	17,19,21	0.98	1 (5%)
2	NAG	E	2	2	14,14,15	0.73	0	17,19,21	0.85	0
3	NAG	F	1	1,3	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
3	NAG	F	2	3	14,14,15	0.74	0	17,19,21	0.94	1 (5%)
3	BMA	F	3	3	11,11,12	0.84	0	15,15,17	2.06	4 (26%)
2	NAG	G	1	1,2	14,14,15	0.74	0	17,19,21	0.86	0
2	NAG	G	2	2	14,14,15	0.71	0	17,19,21	0.84	0
2	NAG	H	1	1,2	14,14,15	0.69	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	2	2	14,14,15	0.73	0	17,19,21	0.86	0
3	NAG	I	1	1,3	14,14,15	0.76	0	17,19,21	1.14	1 (5%)
3	NAG	I	2	3	14,14,15	0.73	0	17,19,21	0.86	0
3	BMA	I	3	3	11,11,12	0.85	0	15,15,17	2.13	3 (20%)
2	NAG	J	1	1,2	14,14,15	0.74	0	17,19,21	0.92	0
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.86	0
2	NAG	K	1	1,2	14,14,15	0.72	0	17,19,21	0.88	0
2	NAG	K	2	2	14,14,15	0.71	0	17,19,21	0.83	0
2	NAG	L	1	1,2	14,14,15	0.71	0	17,19,21	0.91	0
2	NAG	L	2	2	14,14,15	0.74	0	17,19,21	0.82	0
2	NAG	M	1	1,2	14,14,15	0.71	0	17,19,21	0.81	1 (5%)
2	NAG	M	2	2	14,14,15	0.74	0	17,19,21	0.84	0
2	NAG	N	1	1,2	14,14,15	0.78	0	17,19,21	2.06	3 (17%)
2	NAG	N	2	2	14,14,15	0.71	0	17,19,21	1.03	1 (5%)
2	NAG	O	1	1,2	14,14,15	0.73	0	17,19,21	1.12	1 (5%)
2	NAG	O	2	2	14,14,15	0.75	0	17,19,21	0.90	0
2	NAG	P	1	1,2	14,14,15	0.76	0	17,19,21	0.83	0
2	NAG	P	2	2	14,14,15	0.71	0	17,19,21	0.87	0
2	NAG	Q	1	1,2	14,14,15	0.72	0	17,19,21	0.90	0
2	NAG	Q	2	2	14,14,15	0.73	0	17,19,21	0.89	1 (5%)
3	NAG	R	1	1,3	14,14,15	0.74	0	17,19,21	0.82	0
3	NAG	R	2	3	14,14,15	0.70	0	17,19,21	0.89	0
3	BMA	R	3	3	11,11,12	0.85	0	15,15,17	2.19	4 (26%)
3	NAG	S	1	1,3	14,14,15	0.73	0	17,19,21	0.81	0
3	NAG	S	2	3	14,14,15	0.70	0	17,19,21	0.90	1 (5%)
3	BMA	S	3	3	11,11,12	0.84	0	15,15,17	2.14	4 (26%)
2	NAG	T	1	1,2	14,14,15	0.72	0	17,19,21	1.10	1 (5%)
2	NAG	T	2	2	14,14,15	0.73	0	17,19,21	0.95	0
3	NAG	U	1	1,3	14,14,15	0.74	0	17,19,21	1.35	2 (11%)
3	NAG	U	2	3	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
3	BMA	U	3	3	11,11,12	0.87	0	15,15,17	2.15	3 (20%)
3	NAG	V	1	1,3	14,14,15	0.74	0	17,19,21	0.84	0
3	NAG	V	2	3	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
3	BMA	V	3	3	11,11,12	0.83	0	15,15,17	2.05	3 (20%)
3	NAG	W	1	1,3	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
3	NAG	W	2	3	14,14,15	0.70	0	17,19,21	0.96	1 (5%)
3	BMA	W	3	3	11,11,12	0.86	0	15,15,17	2.10	3 (20%)

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	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	1/6/23/26	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
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	BMA	R	3	3	-	0/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	BMA	S	3	3	-	0/2/19/22	0/1/1/1
2	NAG	T	1	1,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	1/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	3	BMA	C1-O5-C5	6.61	121.05	112.19
3	I	3	BMA	C1-O5-C5	6.60	121.03	112.19
3	U	3	BMA	C1-O5-C5	6.46	120.84	112.19
3	S	3	BMA	C1-O5-C5	6.41	120.77	112.19
3	V	3	BMA	C1-O5-C5	6.32	120.65	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

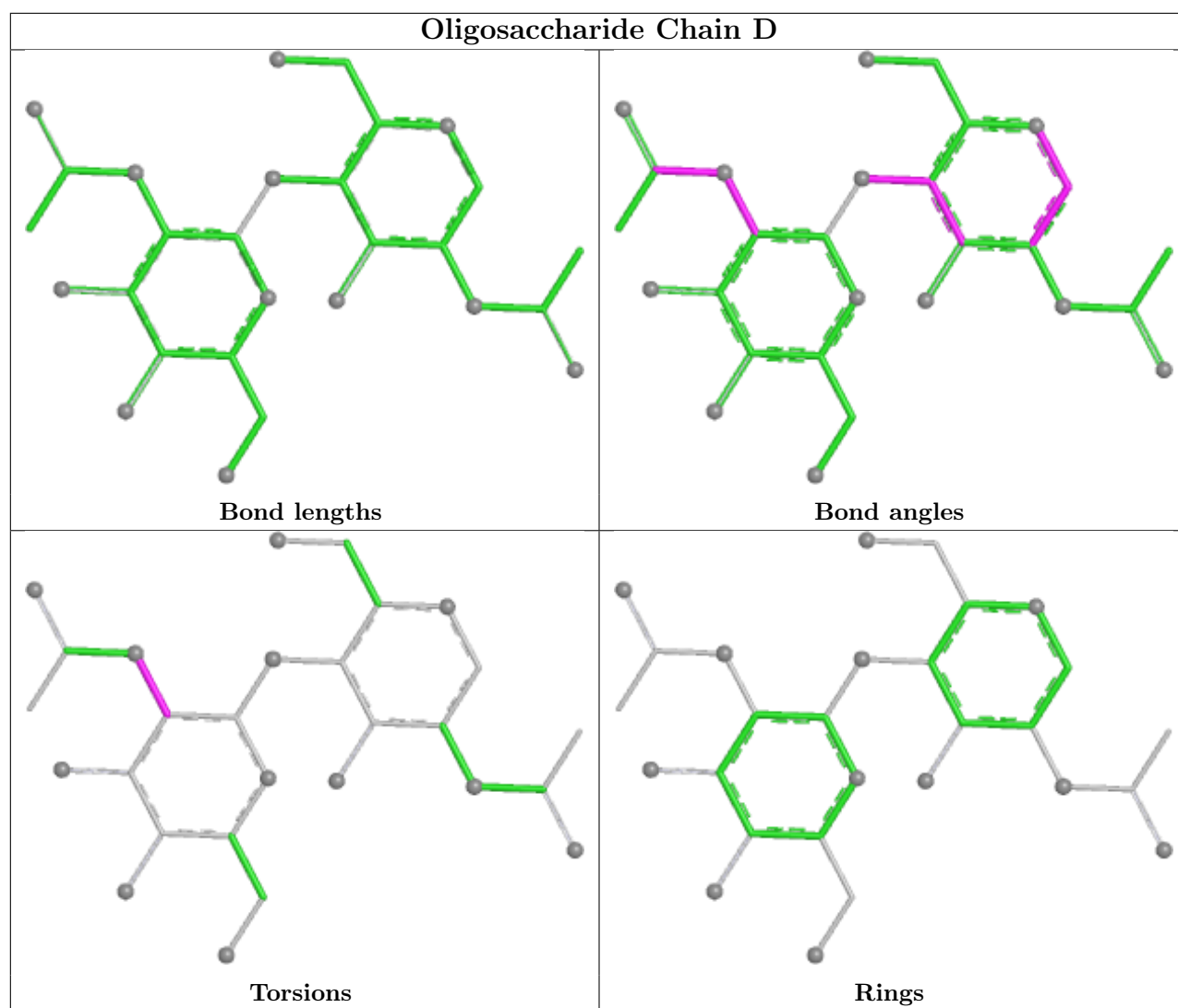
Mol	Chain	Res	Type	Atoms
3	I	3	BMA	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2

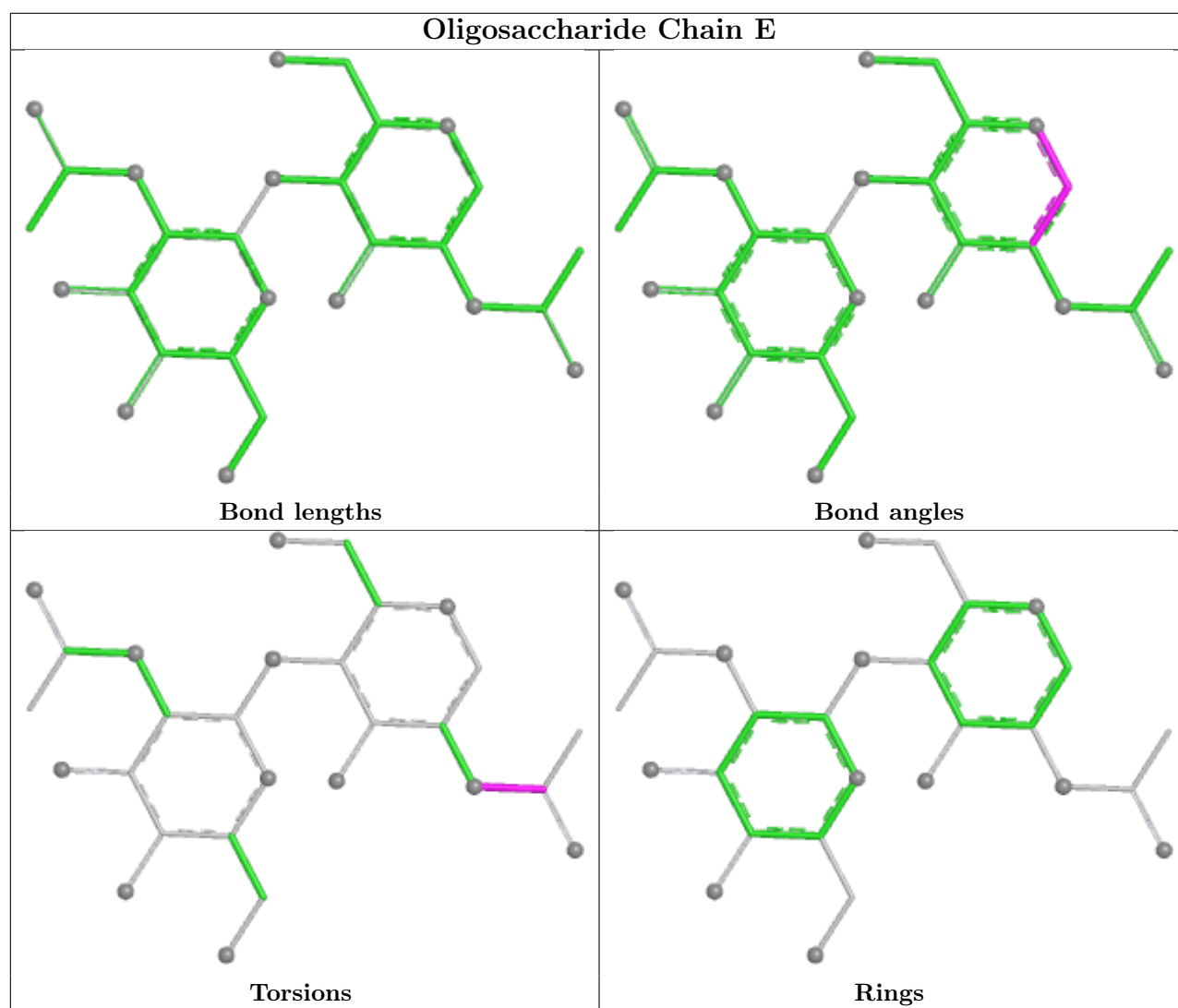
There are no ring outliers.

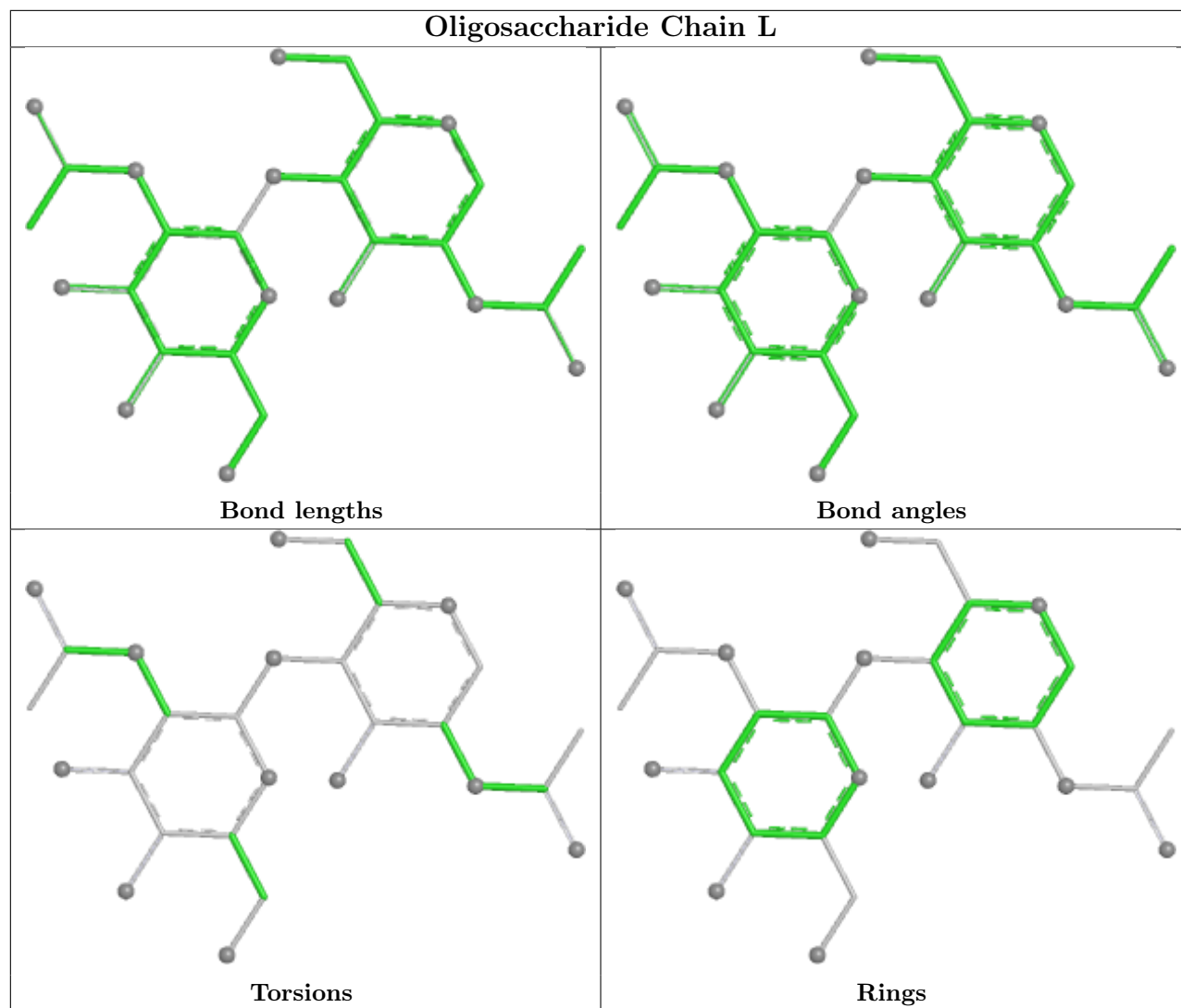
2 monomers are involved in 2 short contacts:

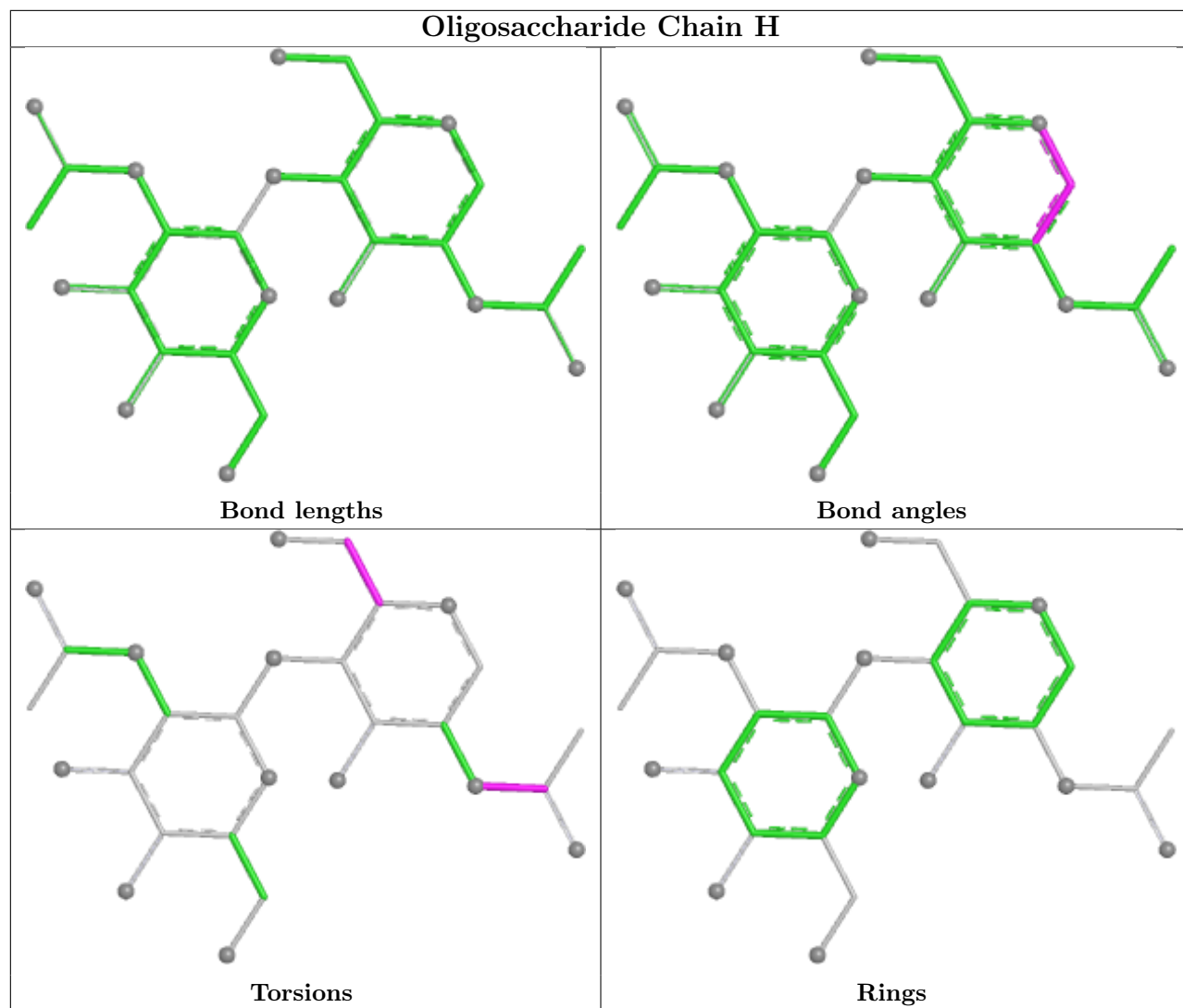
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	NAG	1	0
2	N	1	NAG	1	0

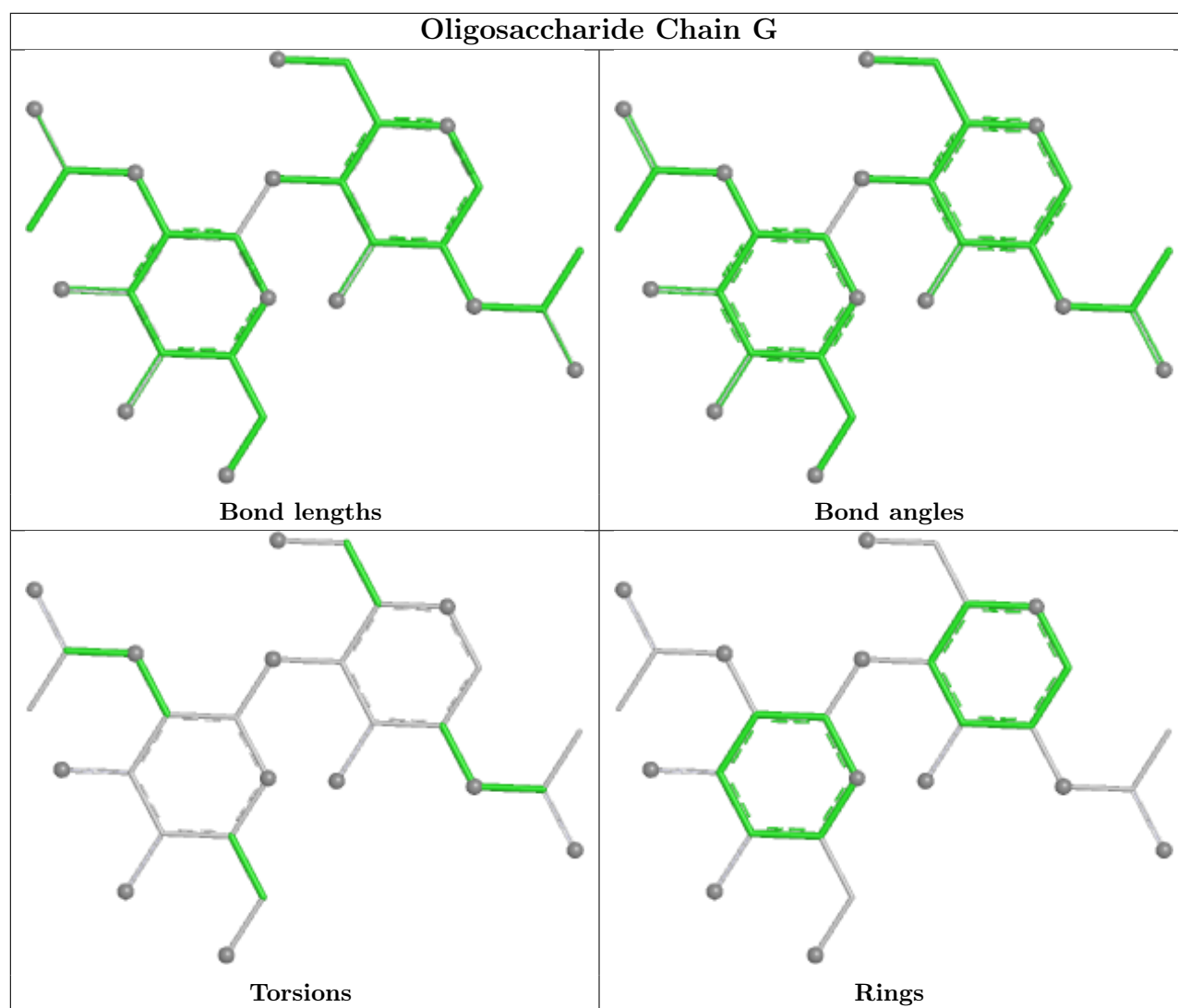
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

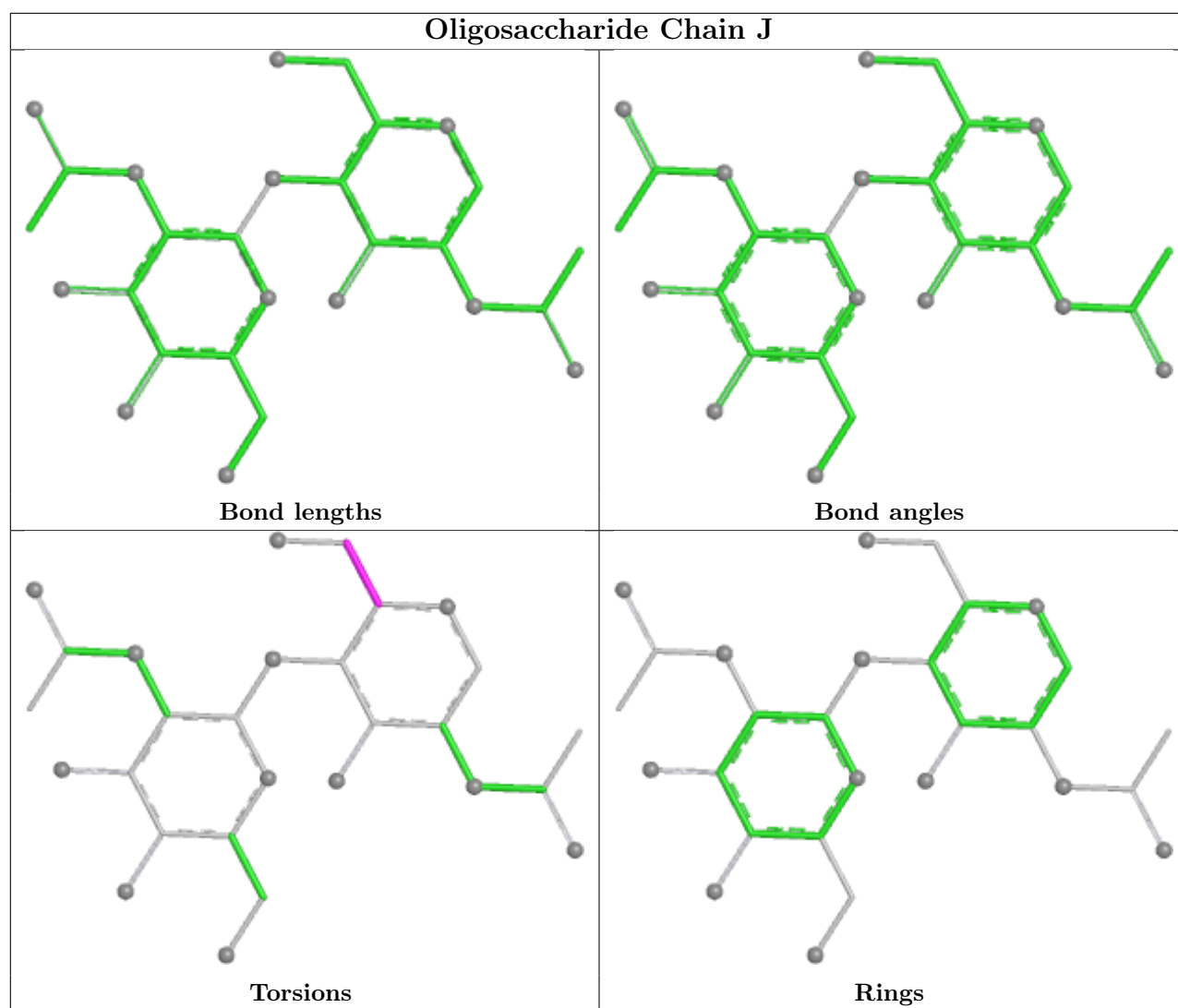


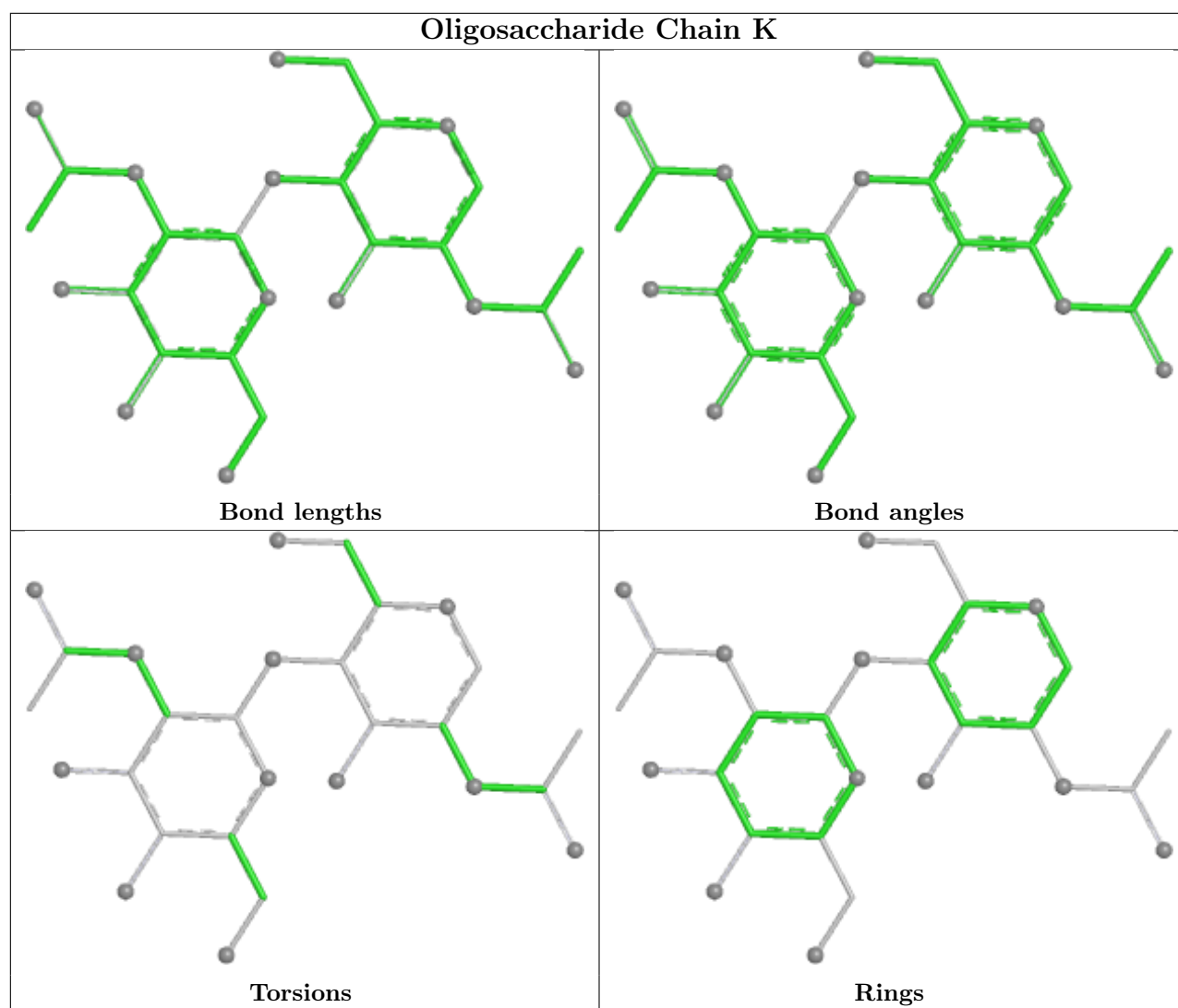


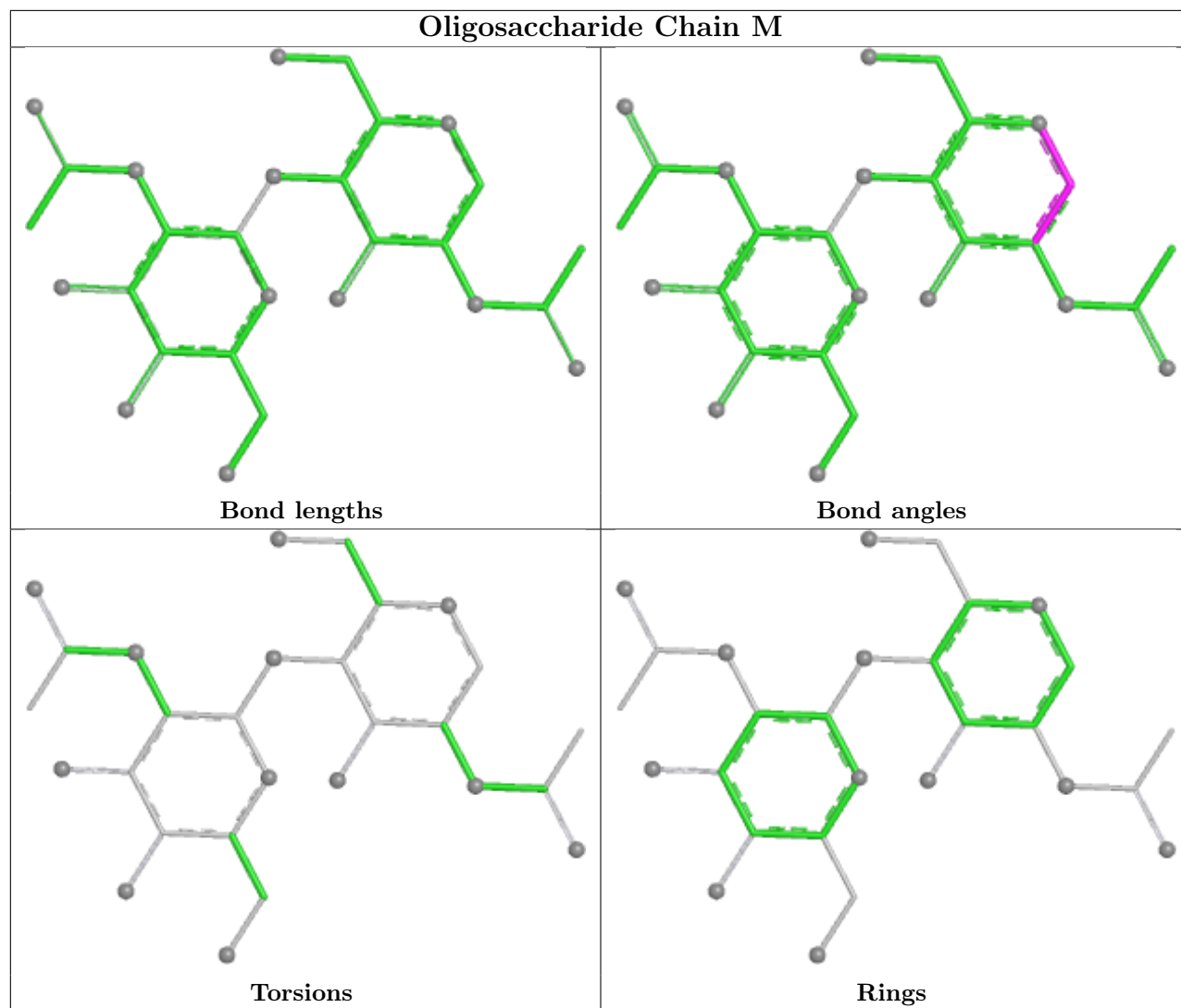


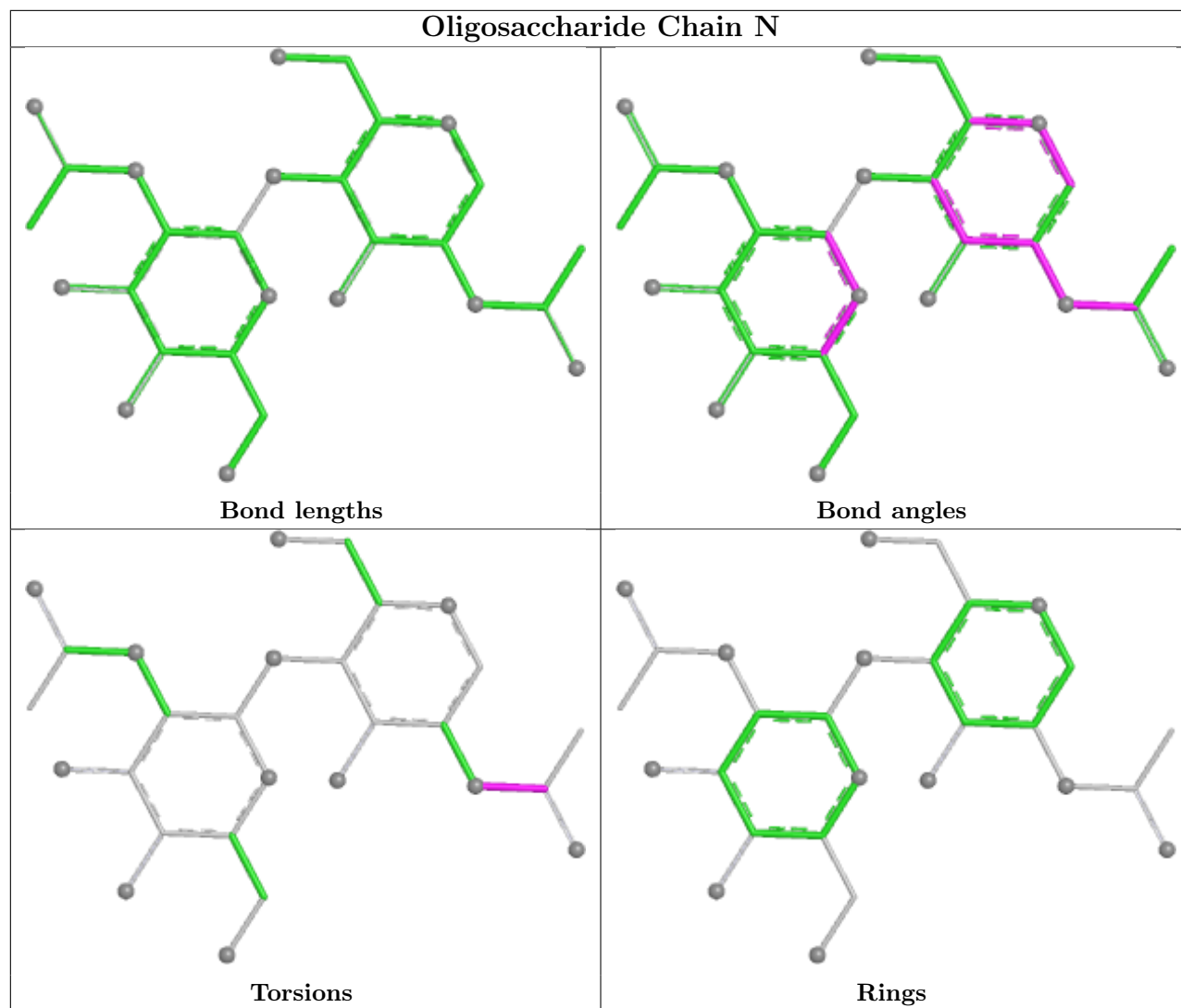


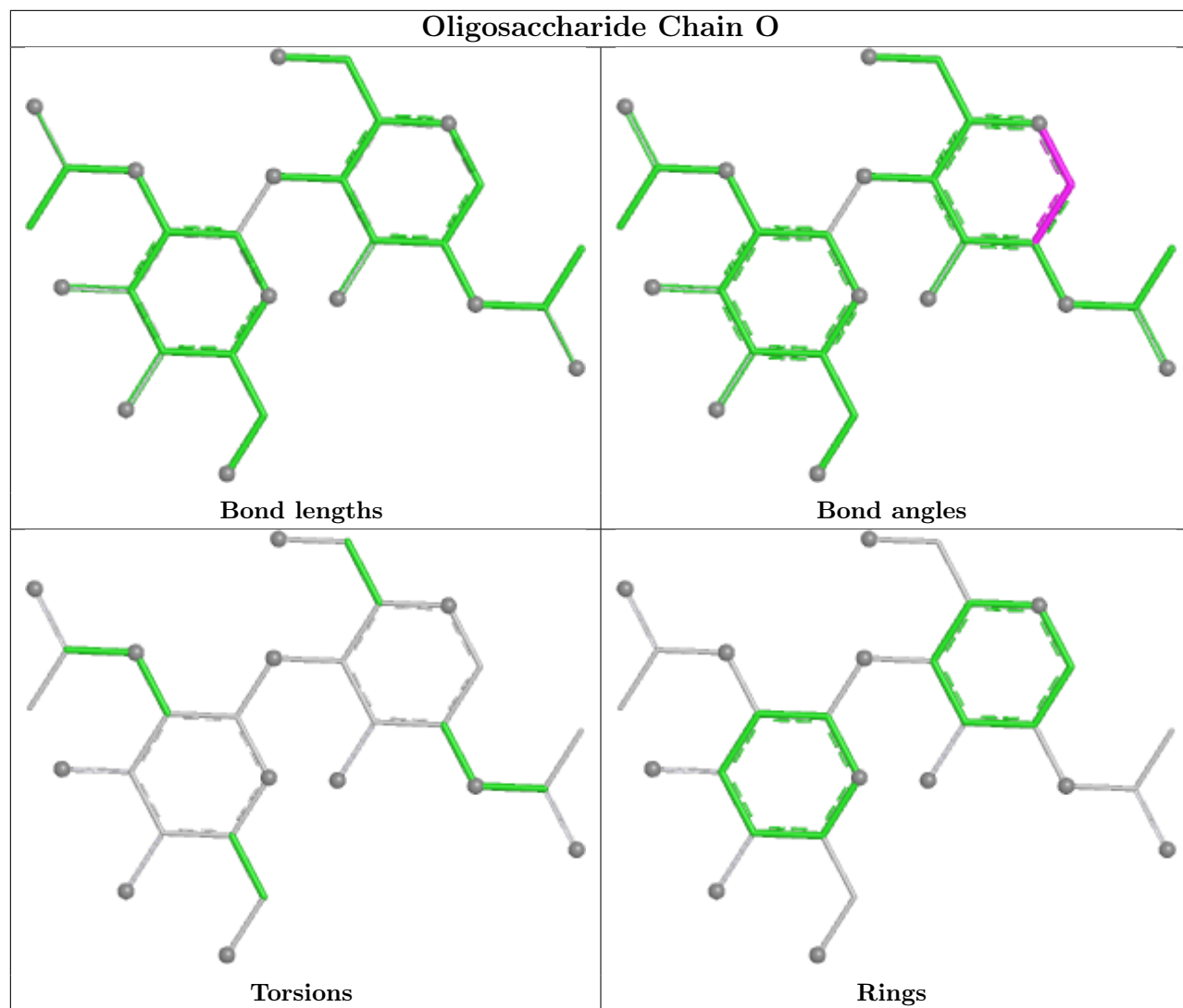


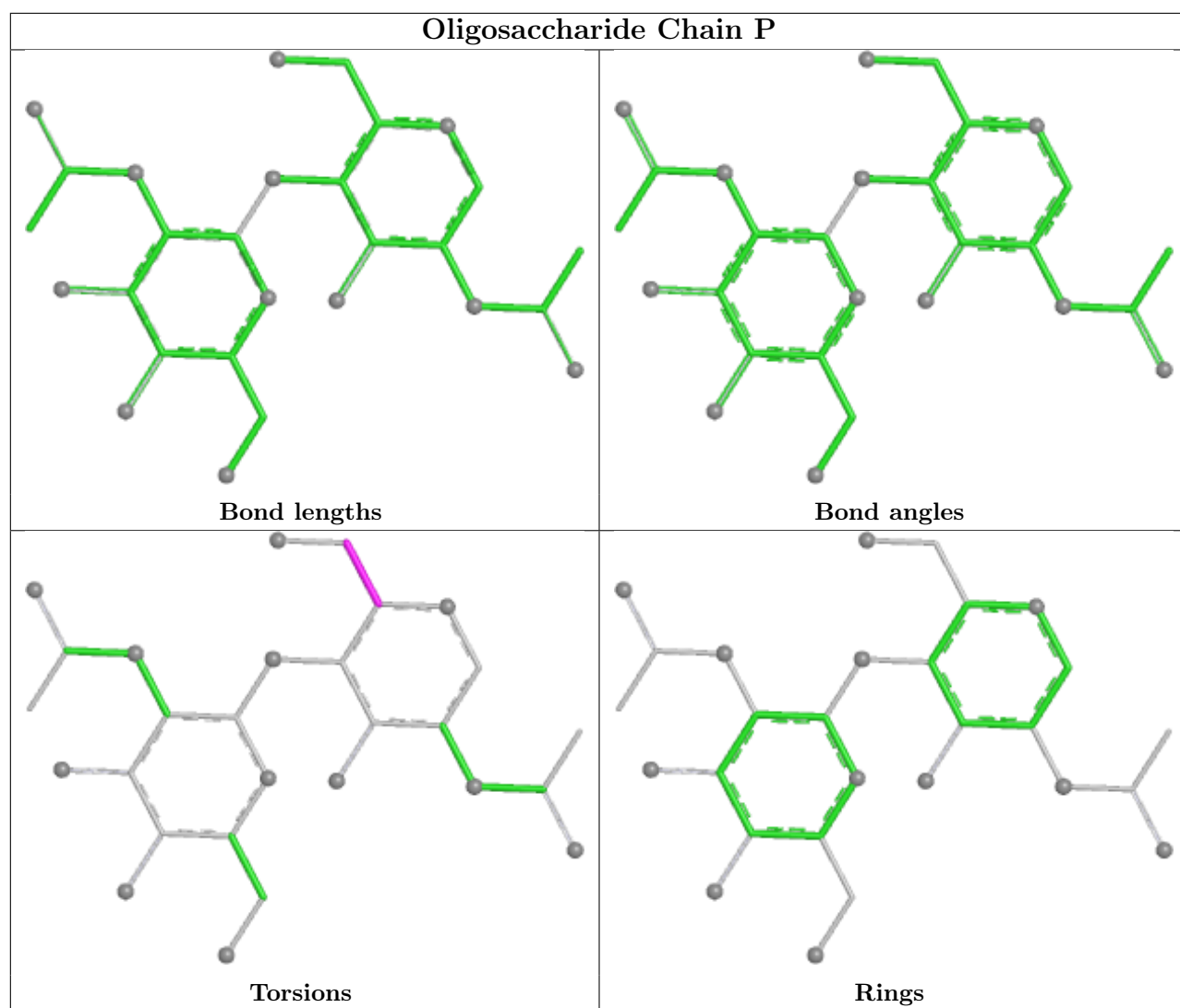


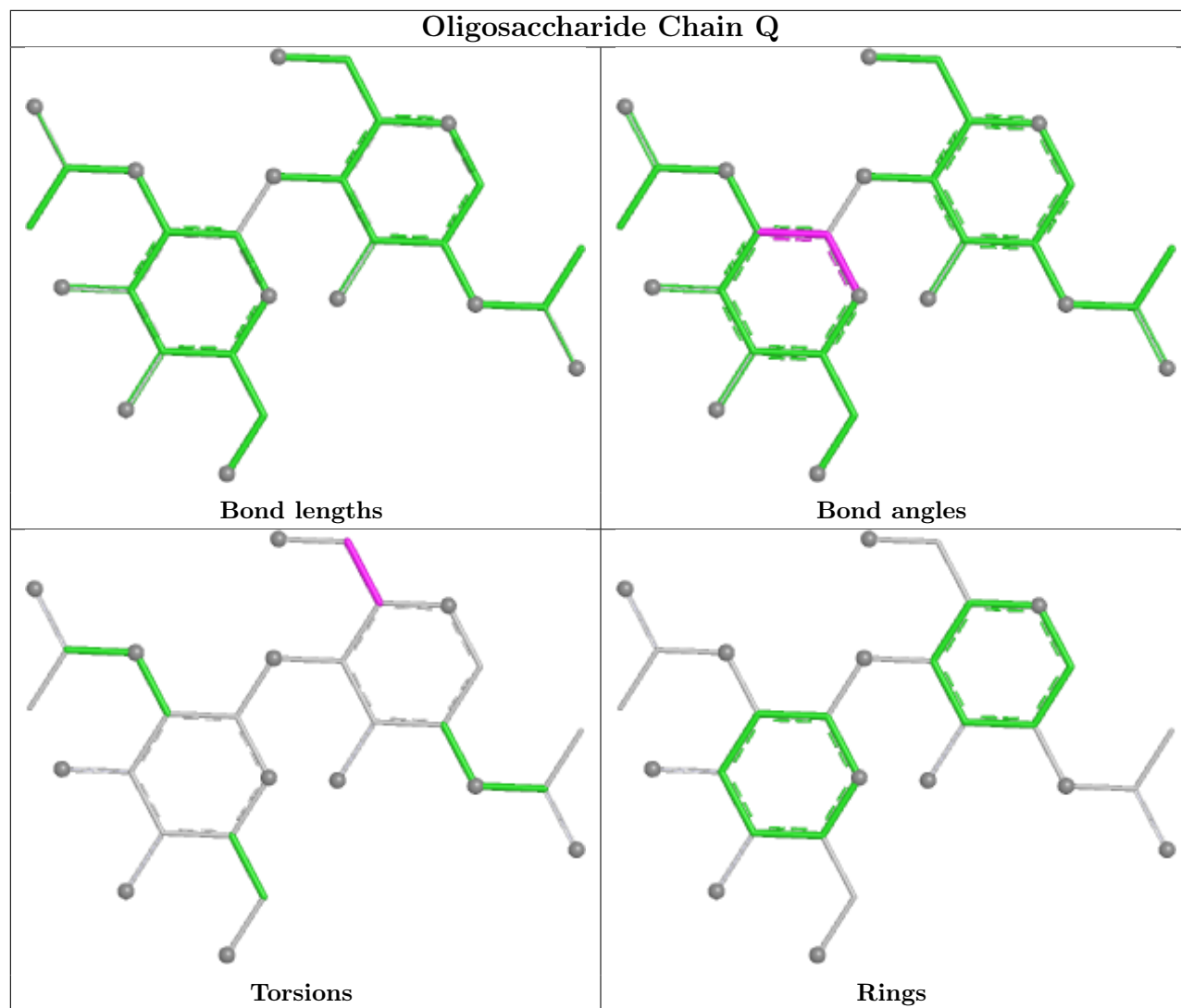


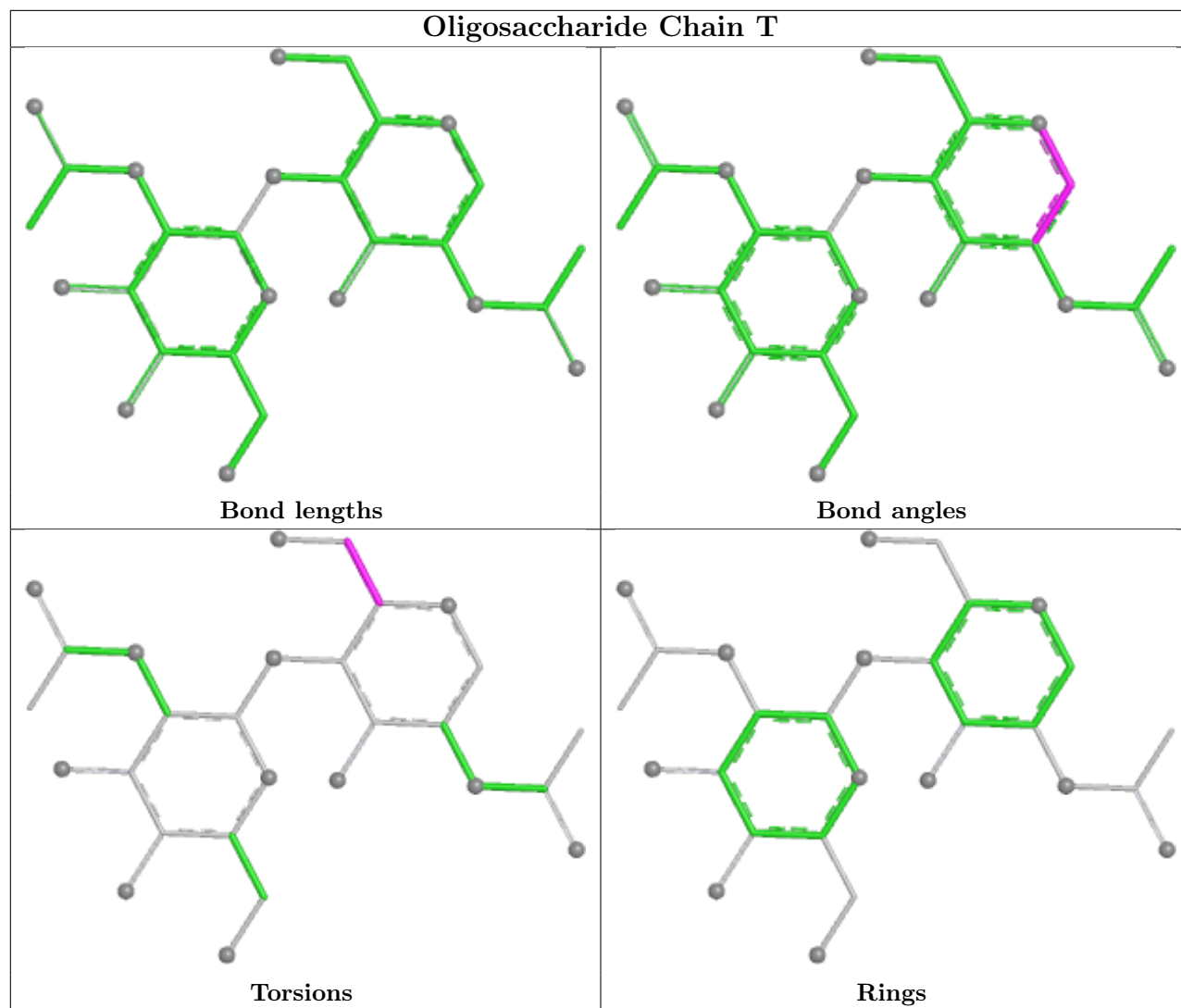


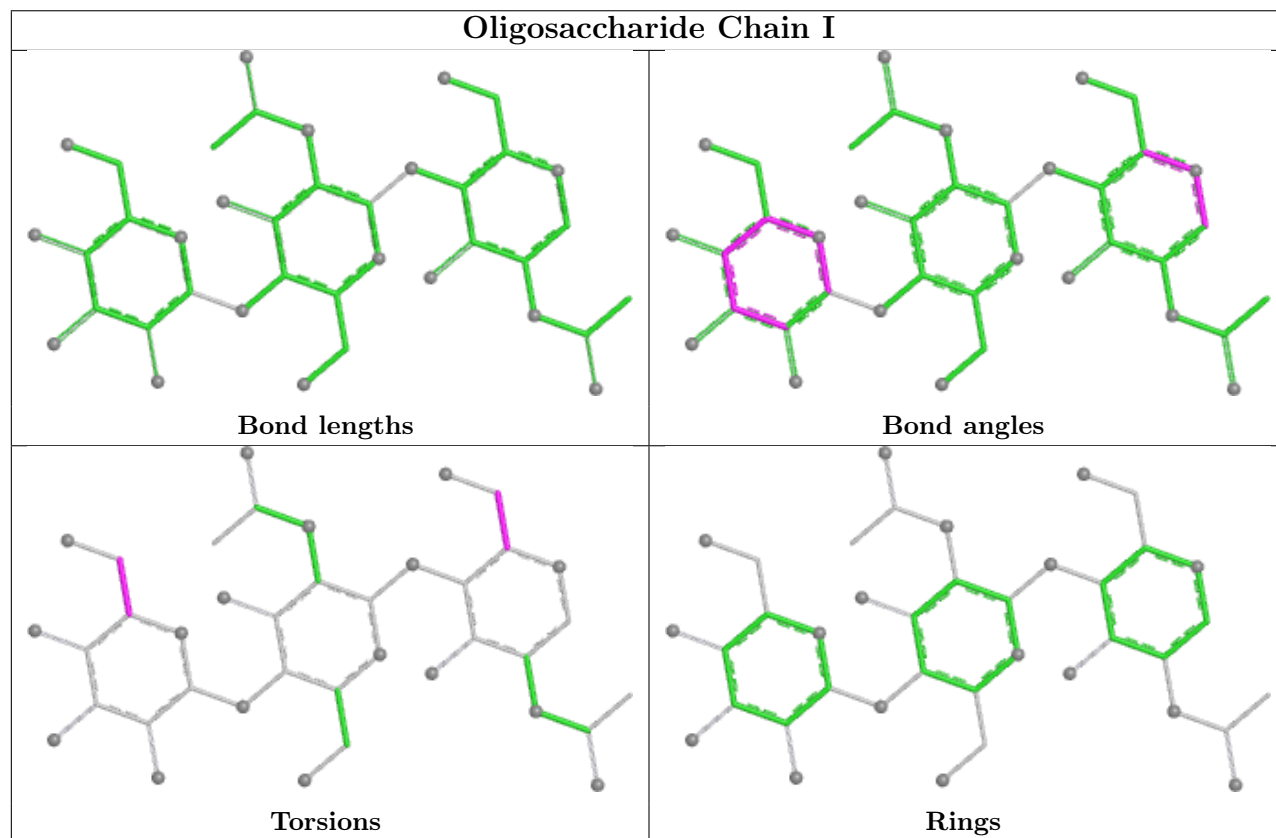
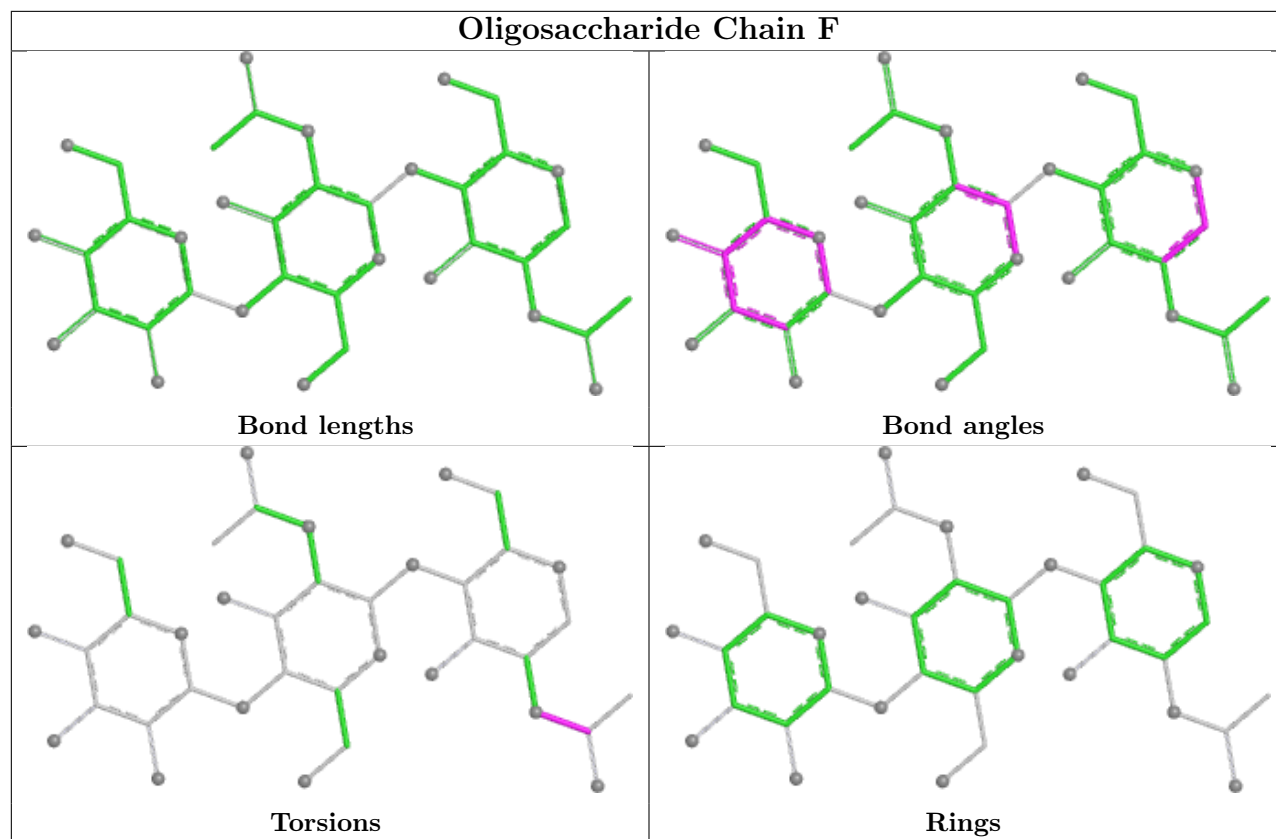


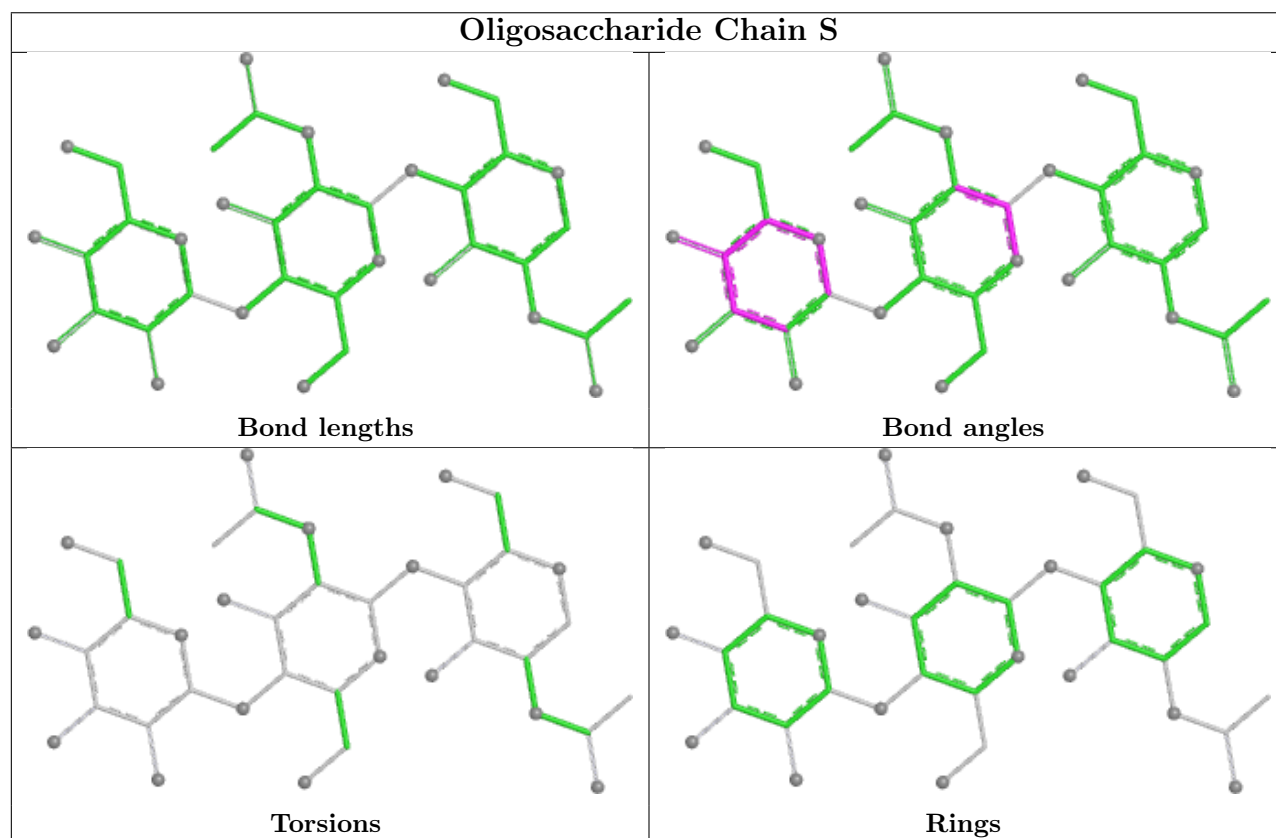
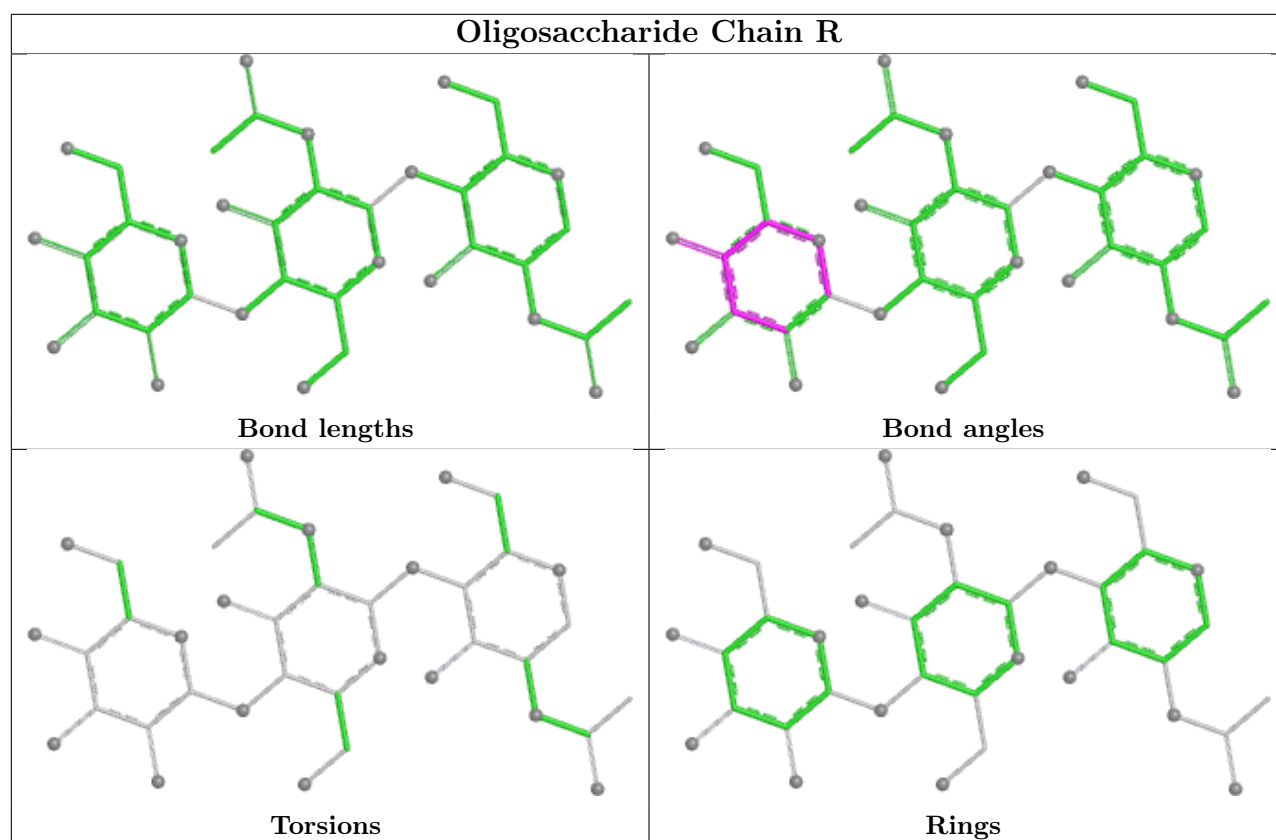


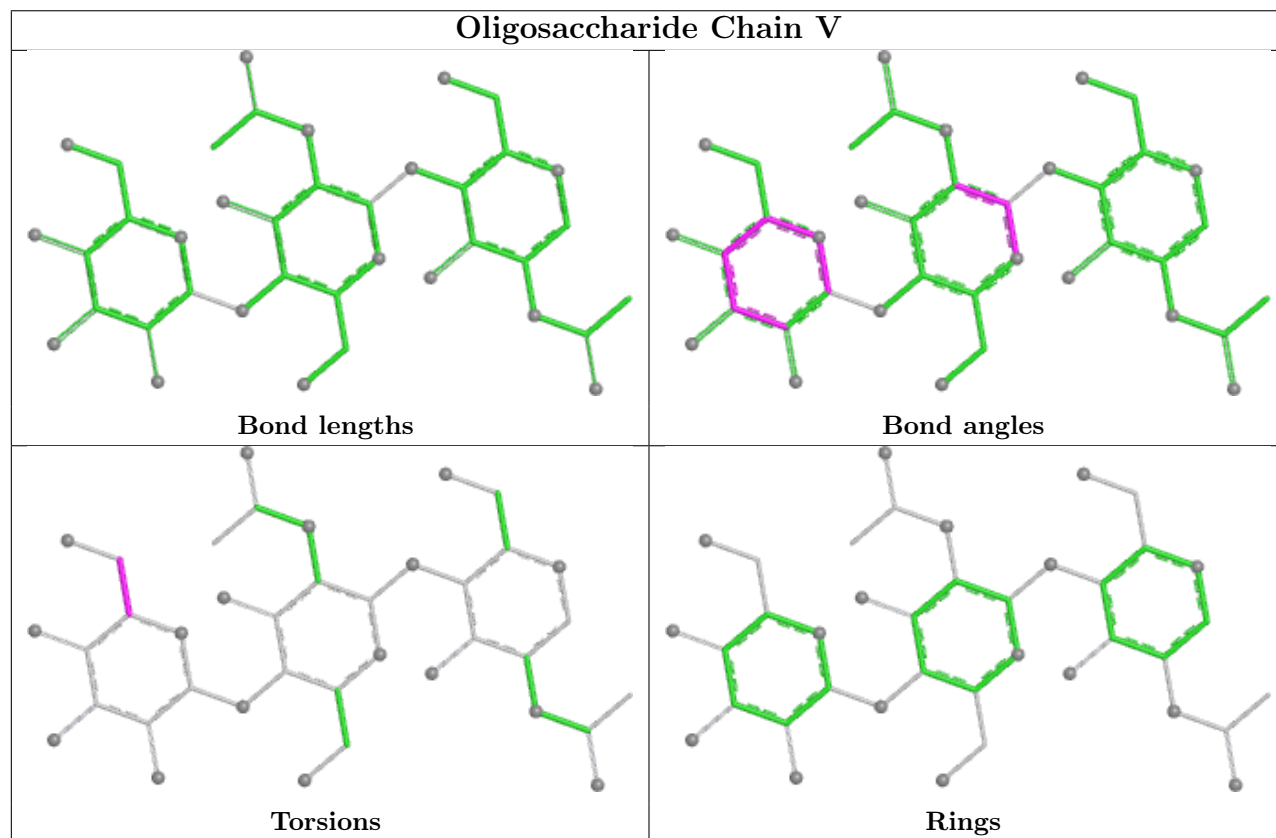
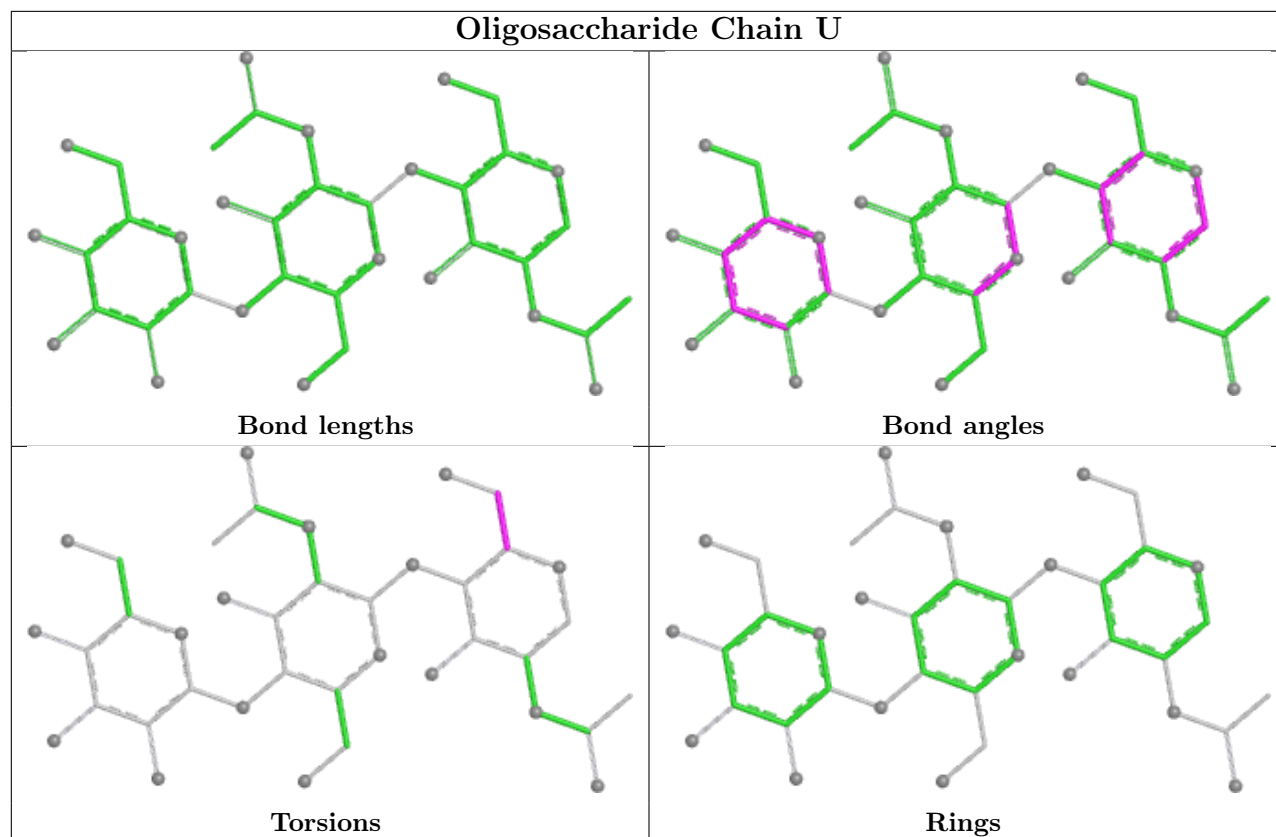


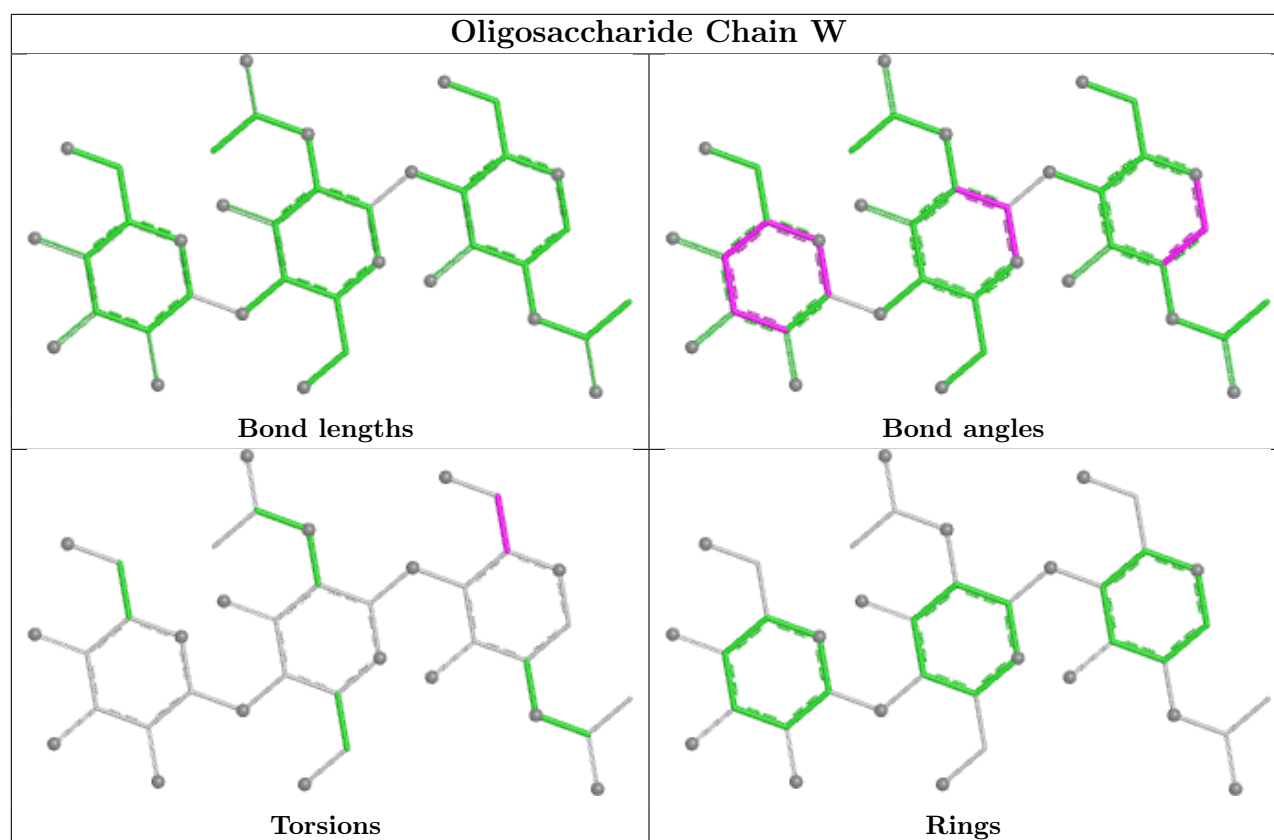












5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1301	1	14,14,15	0.72	0	17,19,21	0.79	0
4	NAG	B	1303	1	14,14,15	0.73	0	17,19,21	0.89	0
4	NAG	B	1309	1	14,14,15	0.71	0	17,19,21	0.81	0
4	NAG	A	1304	1	14,14,15	0.70	0	17,19,21	0.88	1 (5%)
4	NAG	C	1307	1	14,14,15	0.72	0	17,19,21	0.97	1 (5%)
4	NAG	C	1302	1	14,14,15	0.73	0	17,19,21	0.80	0
4	NAG	B	1304	1	14,14,15	0.75	0	17,19,21	0.74	0
4	NAG	A	1302	1	14,14,15	0.74	0	17,19,21	0.80	0
4	NAG	C	1309	1	14,14,15	0.69	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1302	1	14,14,15	0.74	0	17,19,21	0.86	0
4	NAG	C	1303	1	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
4	NAG	C	1304	1	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
4	NAG	B	1301	1	14,14,15	0.70	0	17,19,21	0.85	0
4	NAG	A	1303	1	14,14,15	0.74	0	17,19,21	0.89	0
4	NAG	B	1307	1	14,14,15	0.71	0	17,19,21	0.83	0
4	NAG	B	1306	1	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	C	1305	1	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
4	NAG	B	1308	1	14,14,15	0.72	0	17,19,21	0.87	1 (5%)
4	NAG	B	1305	1	14,14,15	0.72	0	17,19,21	0.83	0
4	NAG	C	1306	1	14,14,15	0.69	0	17,19,21	1.04	1 (5%)
4	NAG	C	1301	1	14,14,15	0.71	0	17,19,21	0.79	0
4	NAG	C	1308	1	14,14,15	0.72	0	17,19,21	0.80	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	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1304	NAG	C2-N2-C7	3.21	127.20	122.90
4	C	1306	NAG	O5-C1-C2	-3.18	106.37	111.29
4	C	1305	NAG	O5-C1-C2	-2.77	107.00	111.29
4	C	1307	NAG	O5-C1-C2	-2.46	107.48	111.29
4	A	1304	NAG	O5-C1-C2	-2.41	107.57	111.29

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1303	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1307	NAG	1	0
4	B	1304	NAG	1	0
4	C	1309	NAG	1	0
4	C	1304	NAG	1	0
4	B	1301	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

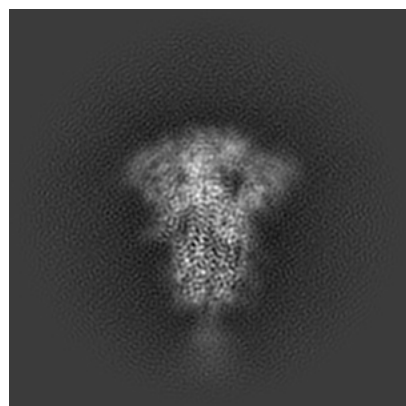
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70451. These allow visual inspection of the internal detail of the map and identification of artifacts.

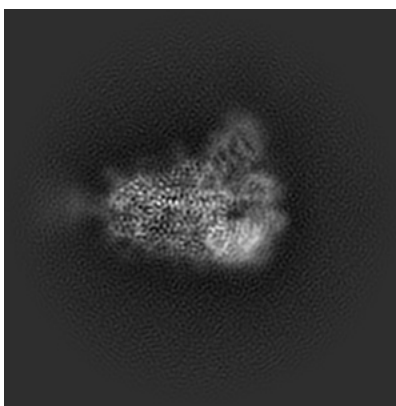
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

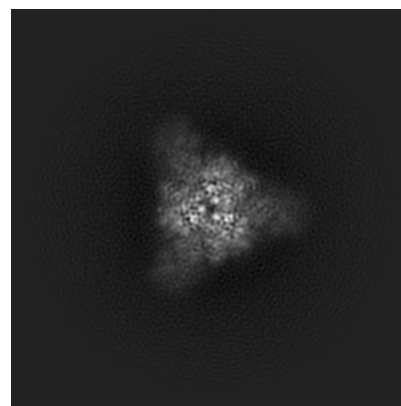
6.1.1 Primary map



X

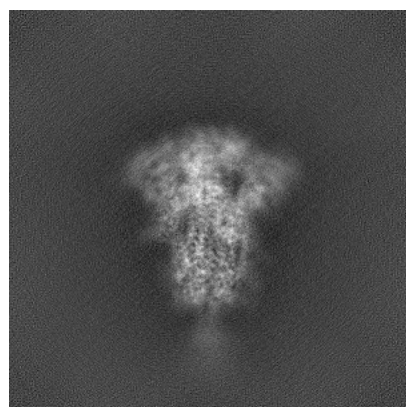


Y

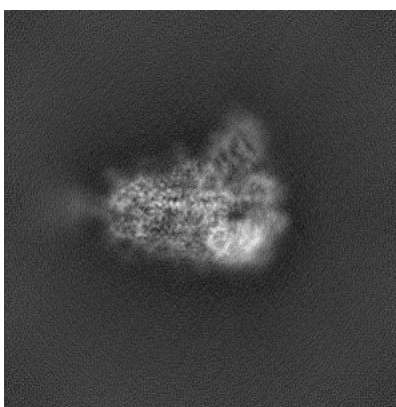


Z

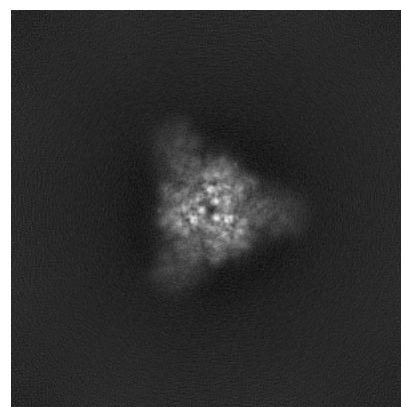
6.1.2 Raw map



X



Y

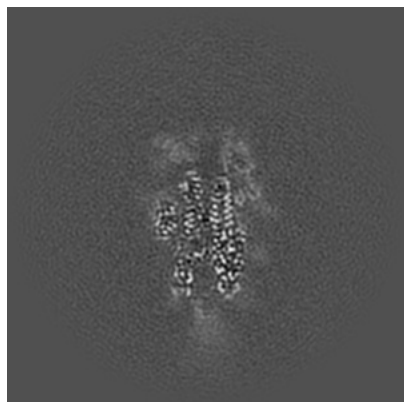


Z

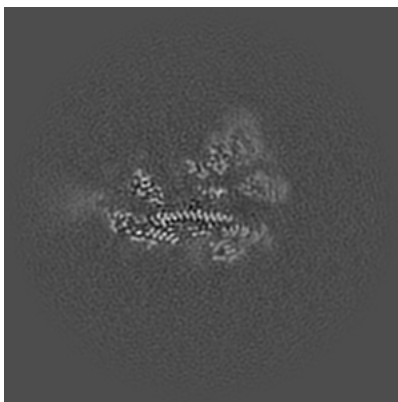
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

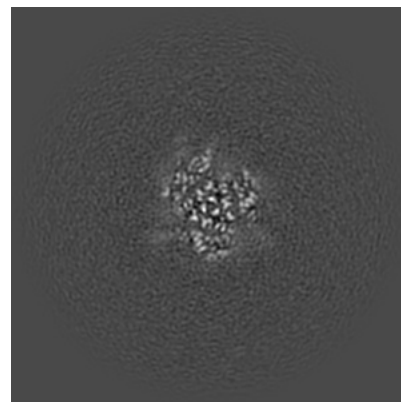
6.2.1 Primary map



X Index: 199

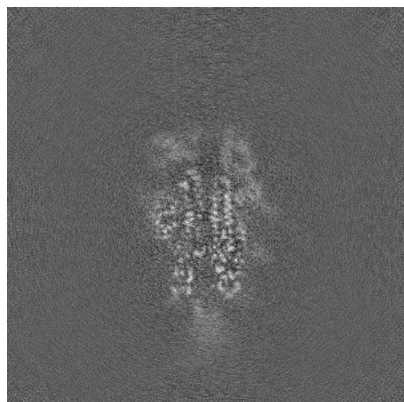


Y Index: 199

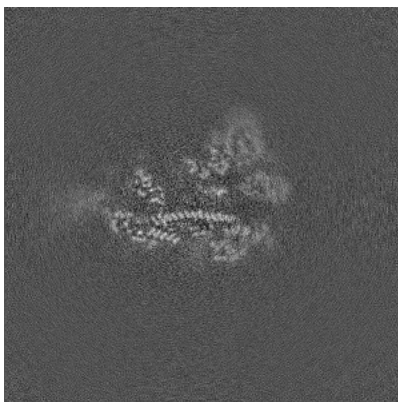


Z Index: 199

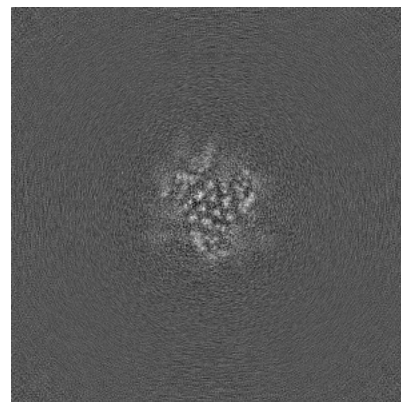
6.2.2 Raw map



X Index: 199



Y Index: 199

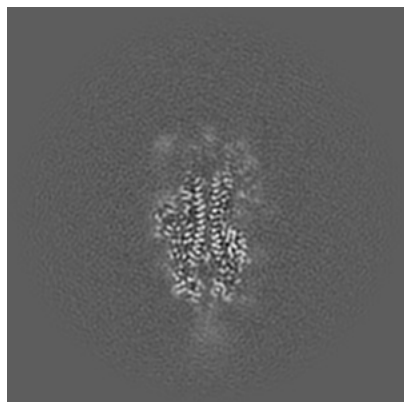


Z Index: 199

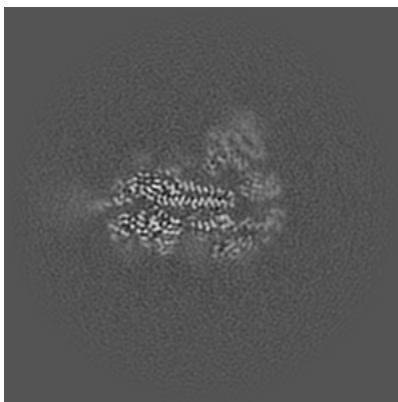
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

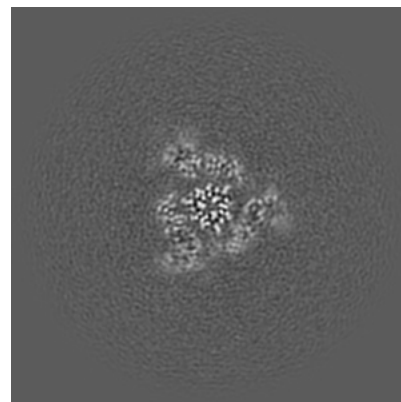
6.3.1 Primary map



X Index: 205

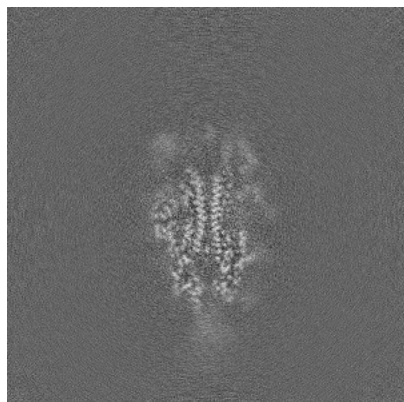


Y Index: 191

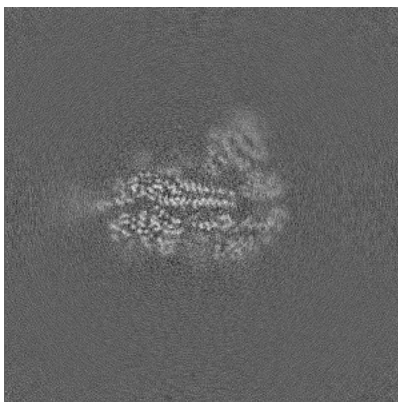


Z Index: 213

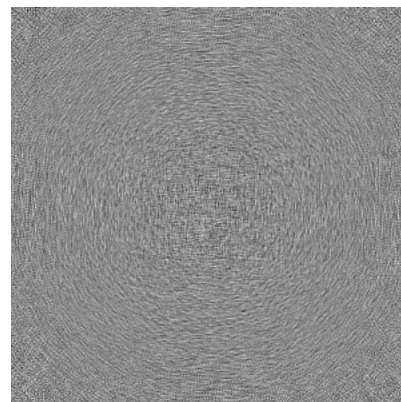
6.3.2 Raw map



X Index: 203



Y Index: 191

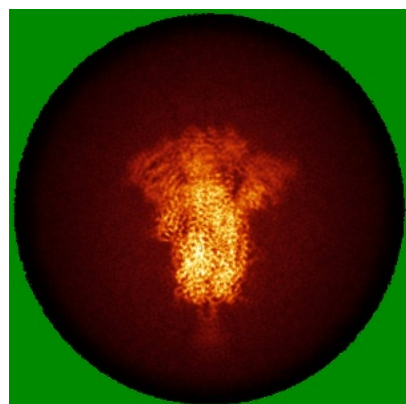


Z Index: 1

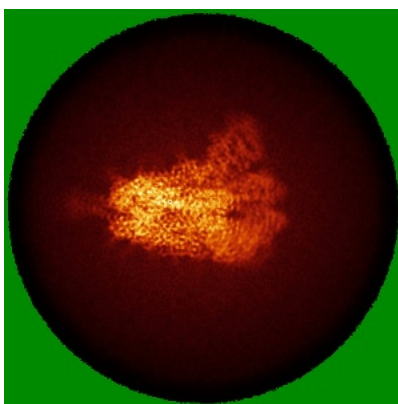
The images above show the largest variance slices of the map in three orthogonal directions.

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

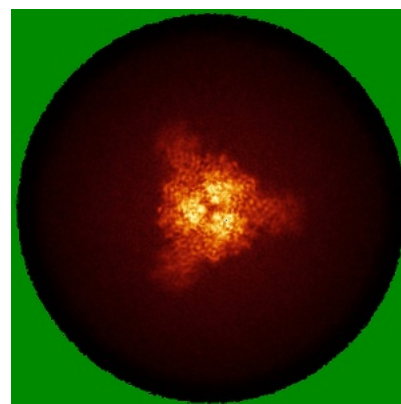
6.4.1 Primary map



X

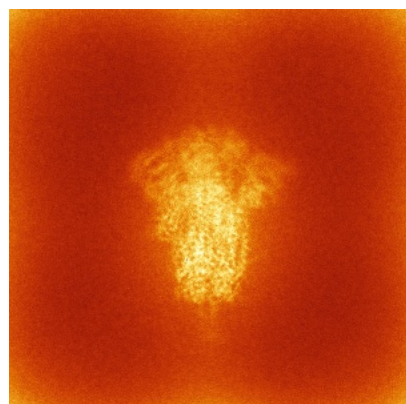


Y

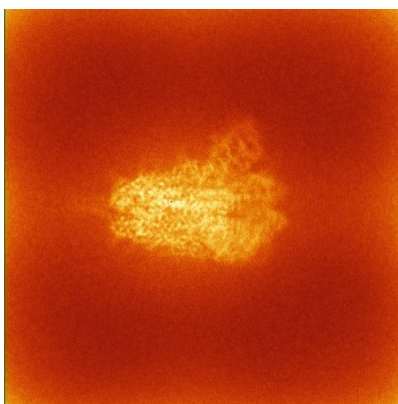


Z

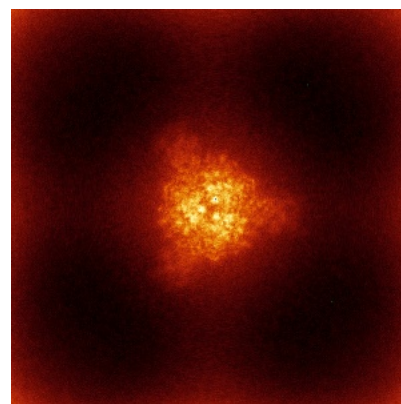
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



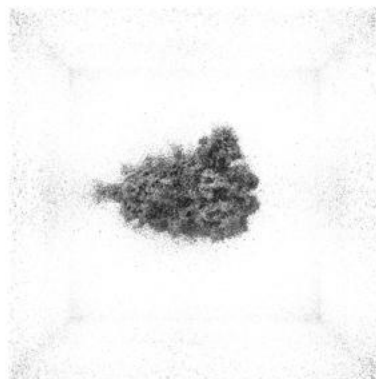
Z

The images above show the 3D surface view of the map at the recommended contour level 0.079. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

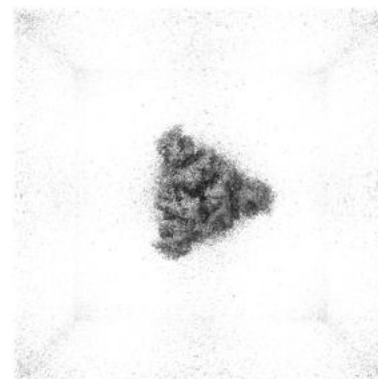
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

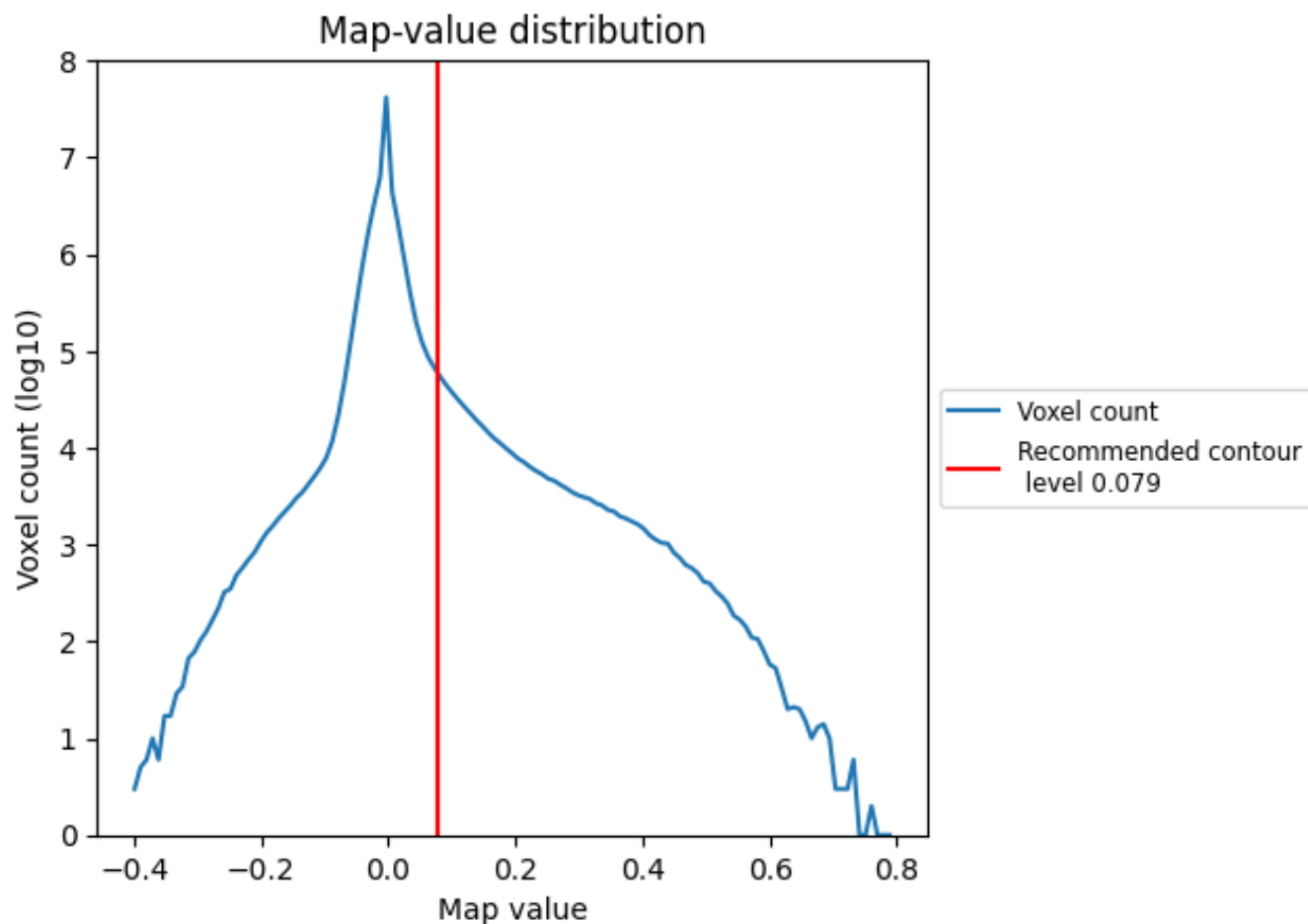
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

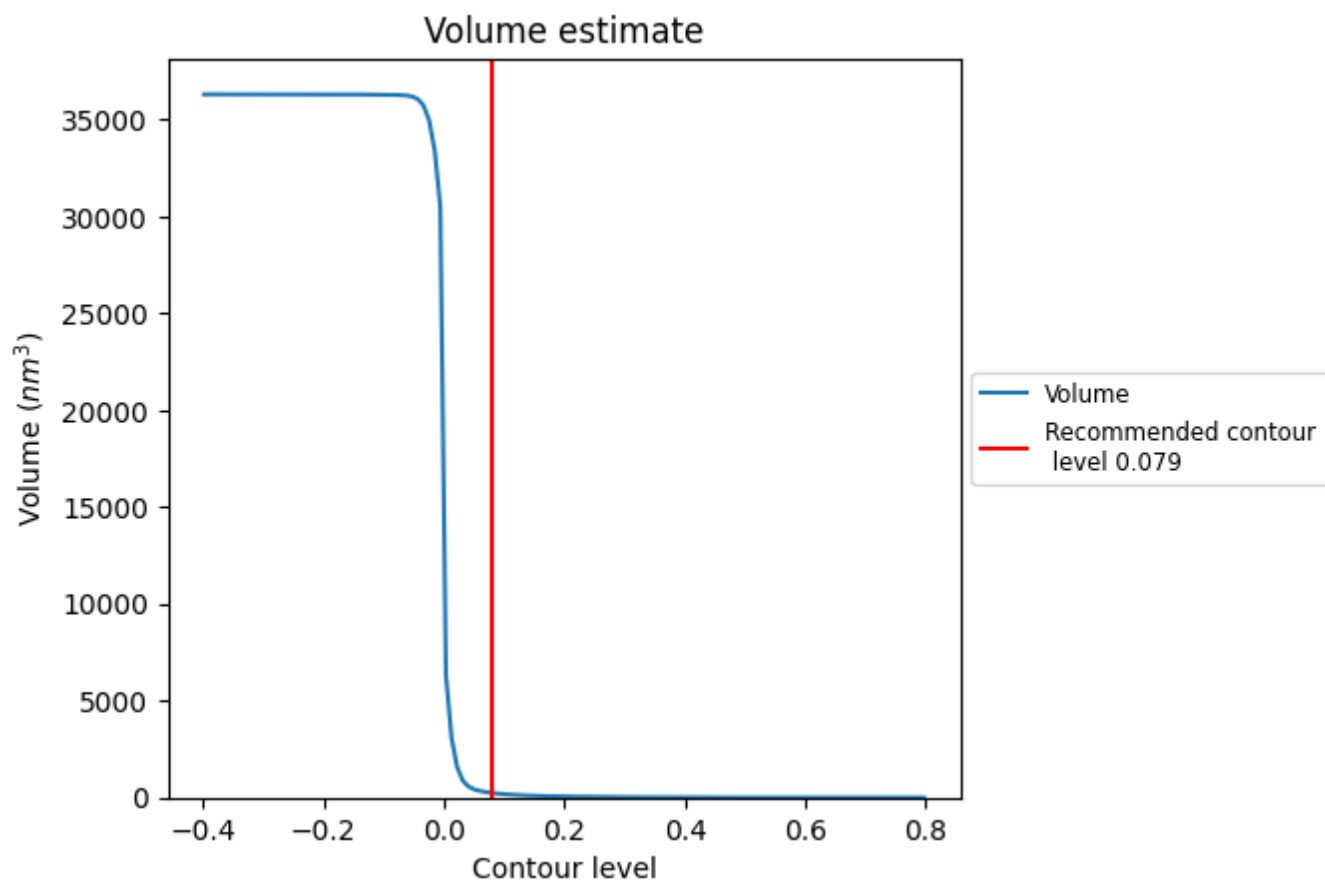
This section contains the results of statistical analysis of the map.

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.

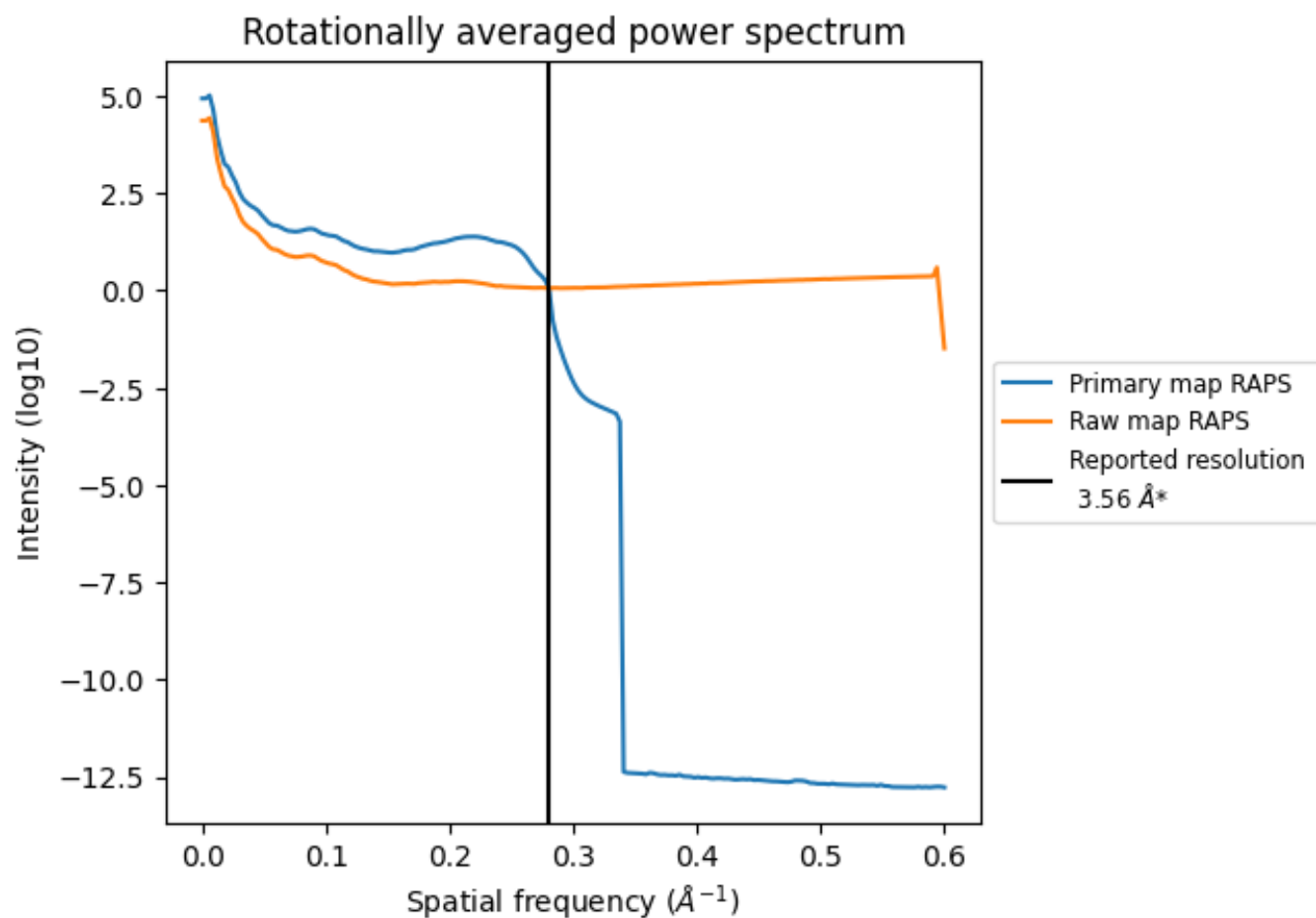
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm³; this corresponds to an approximate mass of 219 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 ⓘ

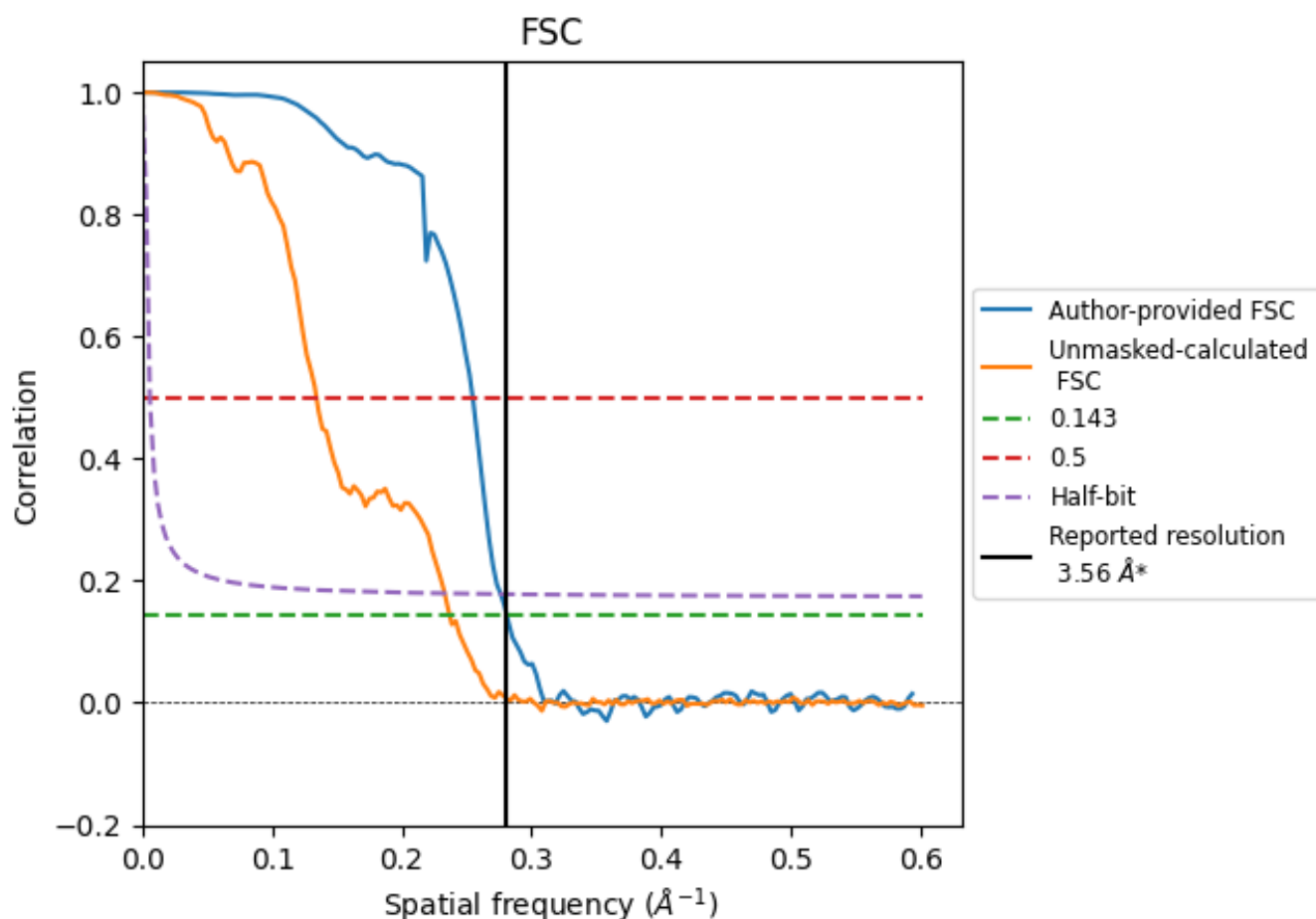


*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

8.2 Resolution estimates [i](#)

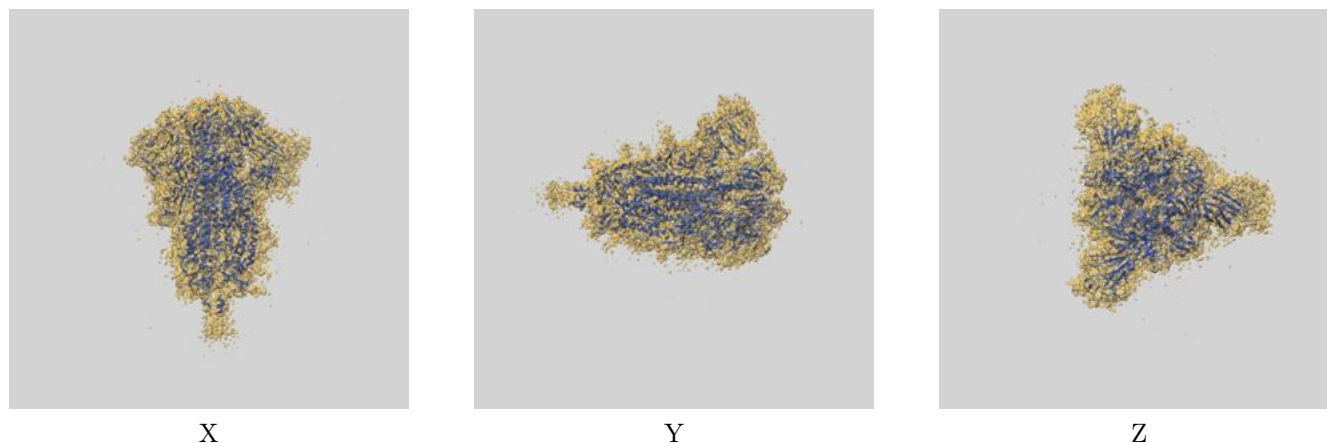
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.56	3.93	3.62
Unmasked-calculated*	4.22	7.45	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.56 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70451 and PDB model 9OG4. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



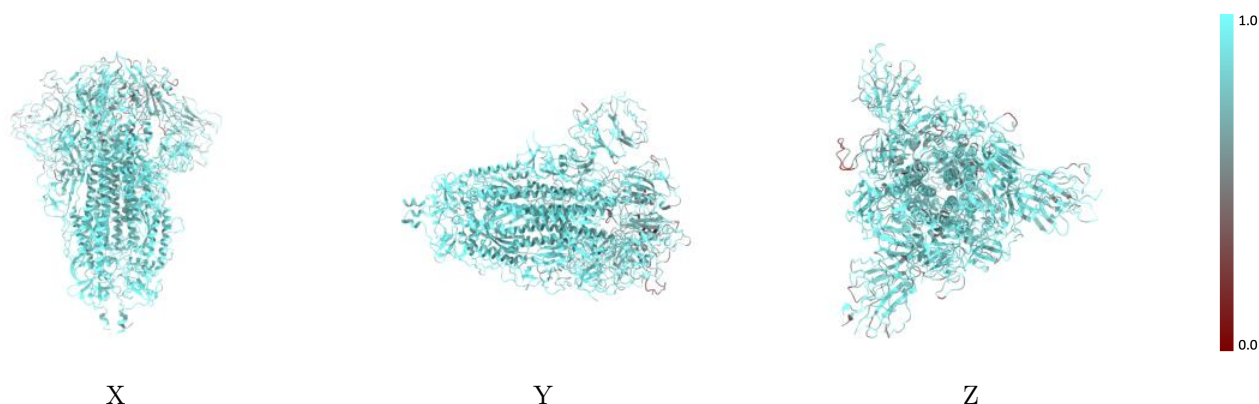
The images above show the 3D surface view of the map at the recommended contour level 0.079 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



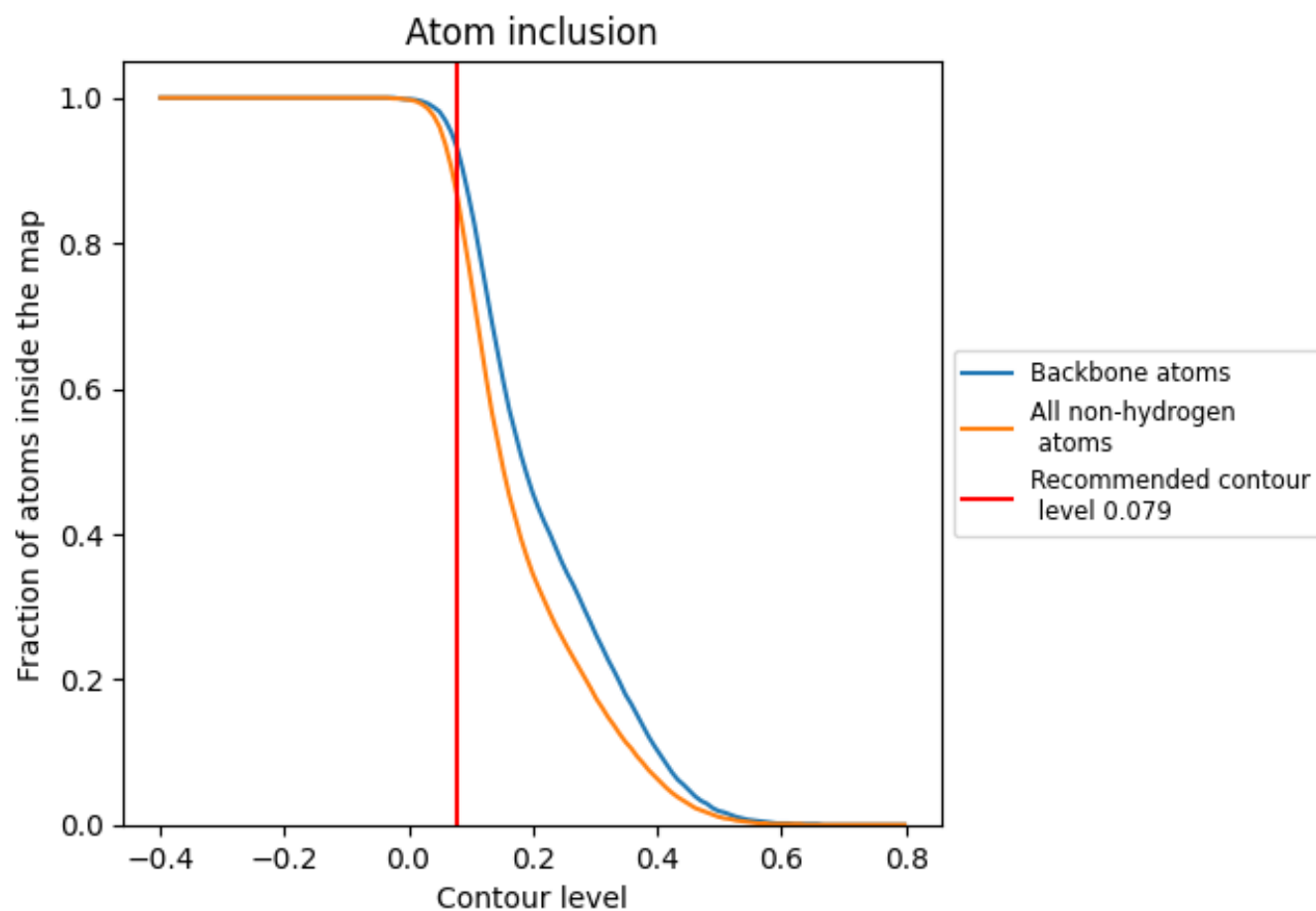
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.079).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.079) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.4410
A	 0.8550	 0.4400
B	 0.8630	 0.4370
C	 0.8790	 0.4520
D	 0.4640	 0.3220
E	 0.7140	 0.4420
F	 0.6670	 0.3810
G	 0.8930	 0.4380
H	 0.5710	 0.4030
I	 0.8210	 0.3890
J	 0.9290	 0.5160
K	 0.7860	 0.4240
L	 0.7140	 0.4500
M	 0.7860	 0.3790
N	 0.7140	 0.2540
O	 0.6790	 0.3890
P	 0.7500	 0.3910
Q	 0.7860	 0.4130
R	 0.4870	 0.3490
S	 0.6150	 0.3180
T	 0.6790	 0.3640
U	 0.6920	 0.3570
V	 0.7440	 0.3640
W	 0.6670	 0.3570

