



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 02:01 AM EDT

PDB ID : 7MTD
EMDB ID : EMD-23983
Title : Structure of aged SARS-CoV-2 S2P spike at pH 7.4
Authors : Tsybovsky, Y.; Olia, A.S.; Kwong, P.D.
Deposited on : 2021-05-13
Resolution : 3.50 Å(reported)

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

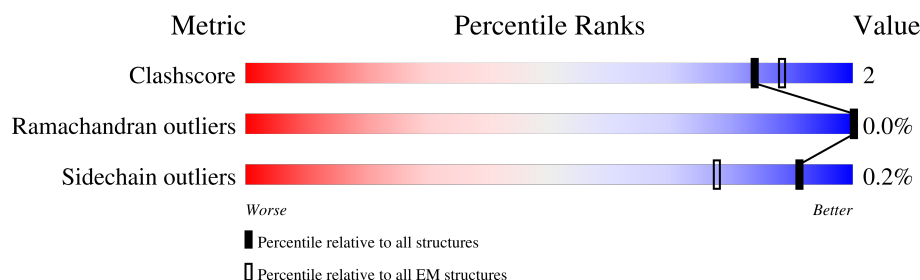
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	1281	<div> <div>9%</div> <div>59%</div> <div>37%</div> </div>
1	B	1281	<div> <div>5%</div> <div>56%</div> <div>41%</div> </div>
1	C	1281	<div> <div>7%</div> <div>56%</div> <div>5%</div> <div>39%</div> </div>
2	D	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>50%</div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>100%</div> </div>
2	G	2	<div> <div>50%</div> <div>100%</div> </div>
2	H	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	2	<div><div></div><div></div></div>
2	J	2	<div><div></div><div></div></div>
2	K	2	<div><div></div><div></div></div>
2	L	2	<div><div></div><div></div></div>
2	M	2	<div><div></div><div></div></div>
2	N	2	<div><div></div><div></div></div>
2	O	2	<div><div></div><div></div></div>
2	P	2	<div><div></div><div></div></div>
2	Q	2	<div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18833 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	806	Total	C	N	O	S	0	0
			6271	4014	1032	1198	27		
1	B	759	Total	C	N	O	S	0	0
			5900	3771	980	1125	24		
1	C	783	Total	C	N	O	S	0	0
			6088	3893	1005	1162	28		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P0DTC2
A	-17	GLY	-	expression tag	UNP P0DTC2
A	-16	ILE	-	expression tag	UNP P0DTC2
A	-15	LEU	-	expression tag	UNP P0DTC2
A	-14	PRO	-	expression tag	UNP P0DTC2
A	-13	SER	-	expression tag	UNP P0DTC2
A	-12	PRO	-	expression tag	UNP P0DTC2
A	-11	GLY	-	expression tag	UNP P0DTC2
A	-10	MET	-	expression tag	UNP P0DTC2
A	-9	PRO	-	expression tag	UNP P0DTC2
A	-8	ALA	-	expression tag	UNP P0DTC2
A	-7	LEU	-	expression tag	UNP P0DTC2
A	-6	LEU	-	expression tag	UNP P0DTC2
A	-5	SER	-	expression tag	UNP P0DTC2
A	-4	LEU	-	expression tag	UNP P0DTC2
A	-3	VAL	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	LEU	-	expression tag	UNP P0DTC2
A	1	SER	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	LEU	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	MET	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP P0DTC2
A	7	CYS	-	expression tag	UNP P0DTC2
A	8	VAL	-	expression tag	UNP P0DTC2
A	9	ALA	-	expression tag	UNP P0DTC2
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	683	GLY	ARG	conflict	UNP P0DTC2
A	685	GLY	ARG	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
B	-18	MET	-	expression tag	UNP P0DTC2
B	-17	GLY	-	expression tag	UNP P0DTC2
B	-16	ILE	-	expression tag	UNP P0DTC2
B	-15	LEU	-	expression tag	UNP P0DTC2
B	-14	PRO	-	expression tag	UNP P0DTC2
B	-13	SER	-	expression tag	UNP P0DTC2
B	-12	PRO	-	expression tag	UNP P0DTC2
B	-11	GLY	-	expression tag	UNP P0DTC2
B	-10	MET	-	expression tag	UNP P0DTC2
B	-9	PRO	-	expression tag	UNP P0DTC2
B	-8	ALA	-	expression tag	UNP P0DTC2
B	-7	LEU	-	expression tag	UNP P0DTC2
B	-6	LEU	-	expression tag	UNP P0DTC2
B	-5	SER	-	expression tag	UNP P0DTC2
B	-4	LEU	-	expression tag	UNP P0DTC2
B	-3	VAL	-	expression tag	UNP P0DTC2
B	-2	SER	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2
B	0	LEU	-	expression tag	UNP P0DTC2
B	1	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	LEU	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	MET	-	expression tag	UNP P0DTC2
B	6	GLY	-	expression tag	UNP P0DTC2
B	7	CYS	-	expression tag	UNP P0DTC2
B	8	VAL	-	expression tag	UNP P0DTC2
B	9	ALA	-	expression tag	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	683	GLY	ARG	conflict	UNP P0DTC2
B	685	GLY	ARG	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
C	-18	MET	-	expression tag	UNP P0DTC2
C	-17	GLY	-	expression tag	UNP P0DTC2
C	-16	ILE	-	expression tag	UNP P0DTC2
C	-15	LEU	-	expression tag	UNP P0DTC2
C	-14	PRO	-	expression tag	UNP P0DTC2
C	-13	SER	-	expression tag	UNP P0DTC2
C	-12	PRO	-	expression tag	UNP P0DTC2
C	-11	GLY	-	expression tag	UNP P0DTC2
C	-10	MET	-	expression tag	UNP P0DTC2
C	-9	PRO	-	expression tag	UNP P0DTC2
C	-8	ALA	-	expression tag	UNP P0DTC2
C	-7	LEU	-	expression tag	UNP P0DTC2
C	-6	LEU	-	expression tag	UNP P0DTC2
C	-5	SER	-	expression tag	UNP P0DTC2
C	-4	LEU	-	expression tag	UNP P0DTC2
C	-3	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	SER	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	LEU	-	expression tag	UNP P0DTC2
C	1	SER	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	LEU	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	MET	-	expression tag	UNP P0DTC2
C	6	GLY	-	expression tag	UNP P0DTC2
C	7	CYS	-	expression tag	UNP P0DTC2
C	8	VAL	-	expression tag	UNP P0DTC2
C	9	ALA	-	expression tag	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	683	GLY	ARG	conflict	UNP P0DTC2
C	685	GLY	ARG	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	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		

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Mol	Chain	Residues	Atoms				AltConf	Trace
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		
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		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

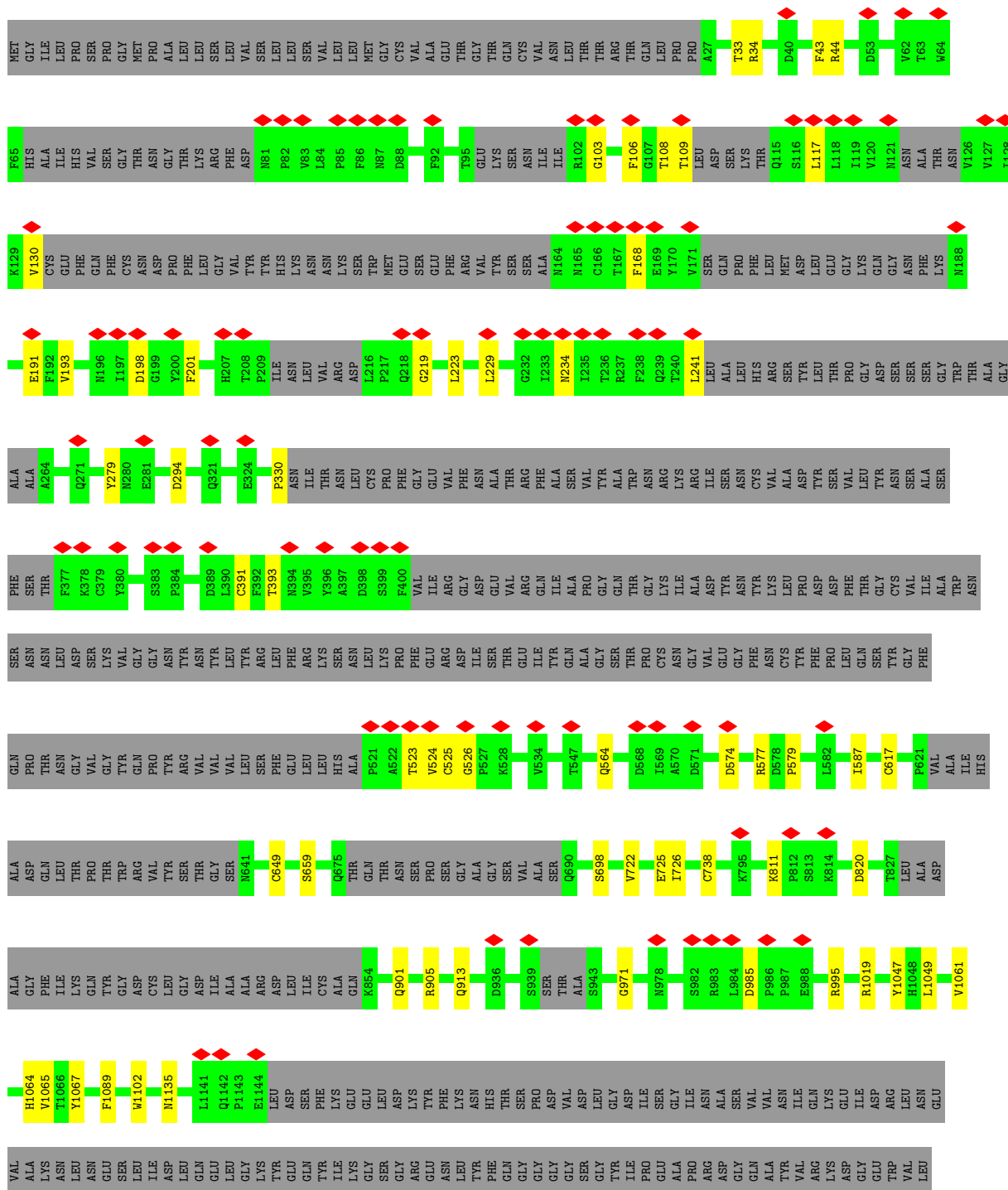


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3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



PHE	GLN	GLY	GLY	GLY	SER	GLY	Tyr	ASP	ARG	ASP	ALA	ASN	VAL	Lys	ASP	GLY	GLU	TRP	LEU	Ser	THR	Thr	His	HIS	HIS	HIS	HIS	HIS	HIS
THR	SER	PRO	VAL	ASP	LEU	GLY	ASP	Ile	Gly	Gly	AlA	SER	Val	Lys	Asn	Leu	GLU	Arg	LEU	Val	Glu	lys	lys	TrR	GLU	GLU	LEU	GLy	Leu

- Molecule 1: Spike glycoprotein



LEU	SER	THR	PHE	LEU	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

Chain D:  100%

NAG1	NAG2
------	------

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

Chain E:  50%
100%

NAG1	NAG2
------	------

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

Chain F:  50%
100%

NAG1	NAG2
------	------

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

Chain G:  50%
100%

NAG1	NAG2
------	------

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

Chain H:  50%
50% 50%

NAG1	NAG2
------	------

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

Chain I:  50%
100%



- 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, C1	Depositor
Number of particles used	95641	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.078	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	376.2, 376.2, 376.2	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	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	0.34	0/6397	0.56	5/8695 (0.1%)
1	B	0.34	0/6024	0.53	0/8196
1	C	0.35	0/6213	0.55	1/8444 (0.0%)
All	All	0.34	0/18634	0.55	6/25335 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	984	LEU	C-N-CA	6.59	138.19	121.70
1	A	1141	LEU	CA-CB-CG	6.46	130.16	115.30
1	A	745	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	546	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	118	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	198	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	904	TYR	Peptide
1	C	524	VAL	Peptide

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	6271	0	6153	30	0
1	B	5900	0	5806	26	0
1	C	6088	0	5974	32	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
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
3	A	56	0	52	1	0
3	B	70	0	65	0	0
3	C	56	0	52	0	0
All	All	18833	0	18452	83	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 2.

All (83) 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:A:106:PHE:HB2	1:A:117:LEU:HB3	1.79	0.63
1:C:103:GLY:H	1:C:241:LEU:HB2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:PHE:HB2	1:B:577:ARG:HH21	1.67	0.59
1:C:201:PHE:HB3	1:C:229:LEU:HB2	1.84	0.59
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.37	0.57
1:C:564:GLN:HG2	1:C:577:ARG:HB3	1.85	0.57
1:B:620:VAL:HG13	1:B:621:PRO:HD3	1.86	0.56
1:A:820:ASP:O	1:A:824:ASN:ND2	2.40	0.55
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.41	0.53
1:B:323:THR:OG1	1:B:537:LYS:NZ	2.41	0.53
1:A:127:VAL:HG11	1:A:170:TYR:H	1.72	0.52
1:B:330:PRO:HG3	1:B:579:PRO:HB2	1.90	0.52
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.43	0.52
1:A:57:PRO:HG3	1:A:273:ARG:HE	1.74	0.52
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.44	0.51
1:A:659:SER:HB3	1:A:698:SER:HB3	1.91	0.51
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.92	0.50
1:C:108:THR:HG23	1:C:109:THR:HG23	1.92	0.50
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.92	0.50
1:C:1102:TRP:HB2	1:C:1135:ASN:HD22	1.77	0.50
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.93	0.49
1:B:1017:GLU:OE1	1:C:1019:ARG:NH1	2.41	0.49
1:C:971:GLY:HA3	1:C:995:ARG:HH21	1.78	0.49
1:A:552:LEU:HD12	1:A:585:LEU:HD13	1.94	0.49
1:A:578:ASP:OD2	1:A:581:THR:OG1	2.31	0.49
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.44	0.49
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.46	0.49
1:C:391:CYS:SG	1:C:526:GLY:N	2.83	0.48
1:B:971:GLY:O	1:B:995:ARG:NH1	2.39	0.48
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.39	0.47
1:C:393:THR:HA	1:C:523:THR:HB	1.96	0.47
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.97	0.47
1:C:659:SER:HB3	1:C:698:SER:HB3	1.95	0.47
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.97	0.47
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.96	0.47
1:A:961:THR:HG21	1:B:762:GLN:HE21	1.79	0.47
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.63	0.46
1:A:298:GLU:OE2	1:A:316:SER:OG	2.31	0.46
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.97	0.46
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.48	0.46
1:C:294:ASP:OD1	1:C:294:ASP:N	2.49	0.46
1:C:725:GLU:OE1	1:C:1064:HIS:NE2	2.44	0.46
1:A:281:GLU:HB2	3:A:1301:NAG:H82	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:N	1:B:208:THR:O	2.50	0.45
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.99	0.45
1:A:81:ASN:ND2	1:A:265:TYR:OH	2.49	0.45
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.76	0.45
1:C:985:ASP:N	1:C:985:ASP:OD1	2.50	0.45
1:C:44:ARG:HB2	1:C:279:TYR:HD2	1.82	0.45
1:C:574:ASP:HA	1:C:587:ILE:HB	1.98	0.45
1:A:985:ASP:OD1	1:A:985:ASP:N	2.47	0.45
1:B:659:SER:HB3	1:B:698:SER:HB3	1.98	0.45
1:A:32:PHE:HD2	1:A:218:GLN:HG2	1.82	0.44
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.98	0.44
1:B:1089:PHE:HB3	1:C:913:GLN:HE21	1.82	0.44
1:A:392:PHE:HA	1:A:517:LEU:HD21	1.99	0.44
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	2.00	0.44
1:A:106:PHE:HD2	1:A:117:LEU:HD23	1.82	0.44
1:C:617:CYS:HB3	1:C:649:CYS:HB3	1.90	0.44
1:A:913:GLN:HE21	1:C:1089:PHE:HB3	1.83	0.44
1:A:294:ASP:N	1:A:294:ASP:OD1	2.51	0.44
1:C:44:ARG:HB2	1:C:279:TYR:CD2	2.52	0.44
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.66	0.43
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.65	0.43
1:B:577:ARG:HD3	1:B:582:LEU:HD22	2.00	0.43
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.48	0.43
1:B:294:ASP:N	1:B:294:ASP:OD1	2.52	0.43
1:C:33:THR:OG1	1:C:219:GLY:O	2.34	0.42
1:C:330:PRO:HB3	1:C:579:PRO:HB2	2.00	0.42
1:C:193:VAL:HG23	1:C:223:LEU:HD22	2.00	0.42
1:A:83:VAL:O	1:A:237:ARG:NH2	2.53	0.42
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.85	0.42
1:B:105:ILE:HG13	1:B:241:LEU:HD23	2.02	0.42
1:B:605:SER:OG	1:B:606:ASN:N	2.53	0.42
1:B:198:ASP:N	1:B:198:ASP:OD1	2.52	0.41
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	2.01	0.41
1:A:105:ILE:HG12	1:A:118:LEU:HD13	2.03	0.41
1:A:825:LYS:HD2	1:A:945:LEU:HD13	2.03	0.41
1:B:566:GLY:HA2	1:C:43:PHE:HB3	2.03	0.41
1:B:825:LYS:HB2	1:B:945:LEU:HD12	2.02	0.41
1:A:83:VAL:HB	1:A:237:ARG:HH21	1.86	0.40
1:A:656:VAL:HG23	1:A:658:ASN:H	1.86	0.40
1:B:617:CYS:HB2	1:B:649:CYS:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	772/1281 (60%)	717 (93%)	55 (7%)	0	100	100
1	B	739/1281 (58%)	697 (94%)	42 (6%)	0	100	100
1	C	753/1281 (59%)	702 (93%)	50 (7%)	1 (0%)	48	79
All	All	2264/3843 (59%)	2116 (94%)	147 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	525	CYS

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	707/1107 (64%)	707 (100%)	0	100	100
1	B	663/1107 (60%)	660 (100%)	3 (0%)	86	93
1	C	686/1107 (62%)	684 (100%)	2 (0%)	91	96
All	All	2056/3321 (62%)	2051 (100%)	5 (0%)	91	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	617	CYS
1	B	620	VAL

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Mol	Chain	Res	Type
1	B	1135	ASN
1	C	234	ASN
1	C	738	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	606	ASN
1	A	824	ASN
1	A	901	GLN
1	A	913	GLN
1	A	953	ASN
1	B	282	ASN
1	B	762	GLN
1	B	804	GLN
1	B	901	GLN
1	B	1135	ASN
1	C	234	ASN
1	C	901	GLN
1	C	1119	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

28 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	2,1	14,14,15	0.21	0	17,19,21	0.62	0
2	NAG	D	2	2	14,14,15	0.37	0	17,19,21	0.49	0
2	NAG	E	1	2,1	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	0.56	0
2	NAG	F	1	2,1	14,14,15	0.22	0	17,19,21	0.59	0
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	0.53	0
2	NAG	G	1	2,1	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	G	2	2	14,14,15	0.46	0	17,19,21	0.46	0
2	NAG	H	1	2,1	14,14,15	0.23	0	17,19,21	0.78	1 (5%)
2	NAG	H	2	2	14,14,15	0.34	0	17,19,21	0.55	0
2	NAG	I	1	2,1	14,14,15	0.25	0	17,19,21	0.86	1 (5%)
2	NAG	I	2	2	14,14,15	0.72	1 (7%)	17,19,21	1.05	1 (5%)
2	NAG	J	1	2,1	14,14,15	0.17	0	17,19,21	0.57	0
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.52	0
2	NAG	K	1	2,1	14,14,15	0.27	0	17,19,21	0.53	0
2	NAG	K	2	2	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	L	1	2,1	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	L	2	2	14,14,15	0.34	0	17,19,21	0.53	0
2	NAG	M	1	2,1	14,14,15	0.27	0	17,19,21	0.58	0
2	NAG	M	2	2	14,14,15	0.39	0	17,19,21	0.59	0
2	NAG	N	1	2,1	14,14,15	0.21	0	17,19,21	0.56	0
2	NAG	N	2	2	14,14,15	0.33	0	17,19,21	0.48	0
2	NAG	O	1	2,1	14,14,15	0.24	0	17,19,21	0.49	0
2	NAG	O	2	2	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
2	NAG	P	1	2,1	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	P	2	2	14,14,15	0.42	0	17,19,21	0.44	0
2	NAG	Q	1	2,1	14,14,15	0.33	0	17,19,21	0.56	0
2	NAG	Q	2	2	14,14,15	0.43	0	17,19,21	0.42	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
2	NAG	D	1	2,1	-	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	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	1	2,1	-	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	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	NAG	C1-C2	2.22	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C2-N2-C7	3.30	127.33	122.90
2	H	1	NAG	C1-O5-C5	2.87	116.03	112.19
2	I	1	NAG	C1-O5-C5	2.85	116.01	112.19
2	O	2	NAG	C1-O5-C5	2.19	115.12	112.19

There are no chirality outliers.

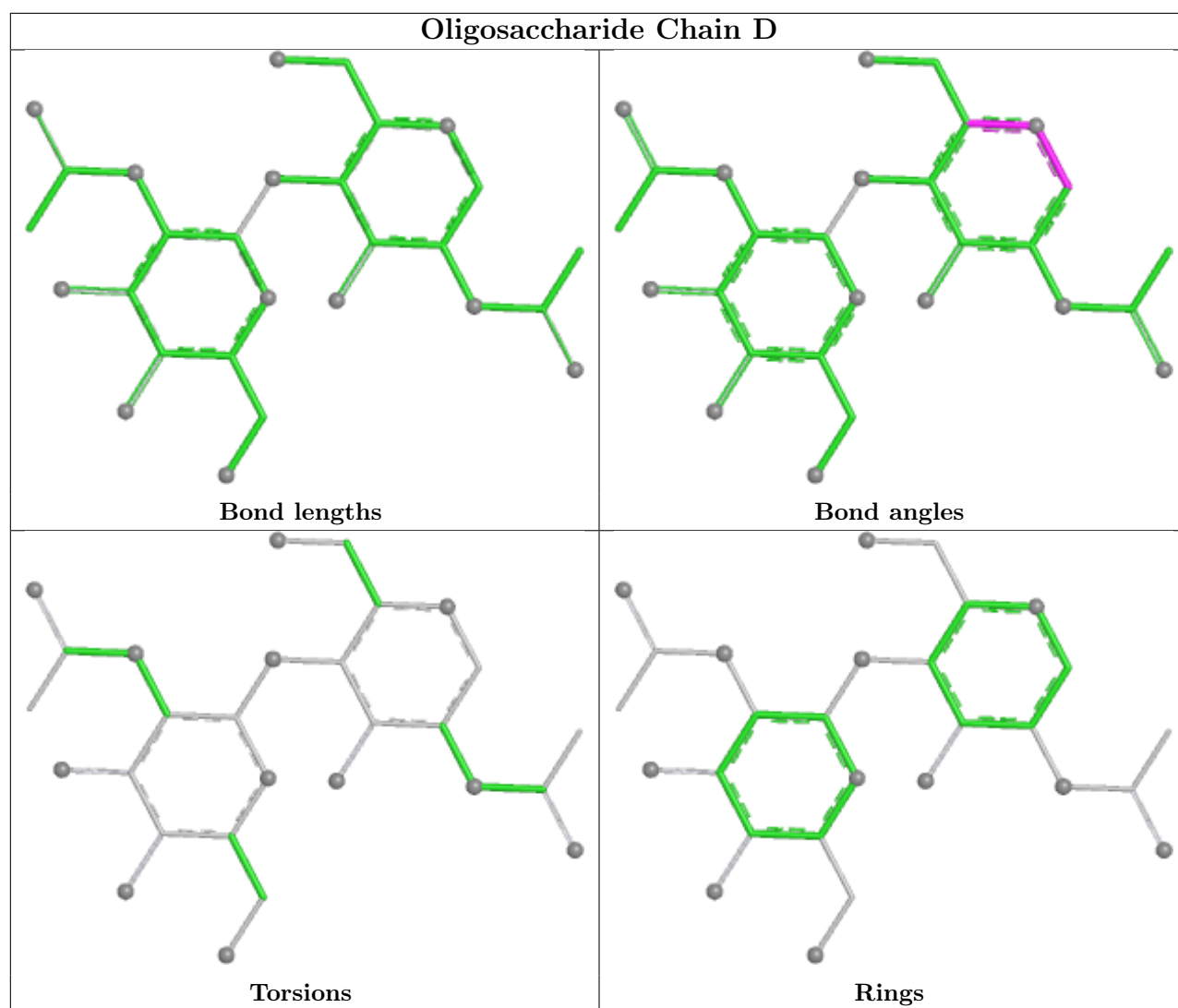
All (27) torsion outliers are listed below:

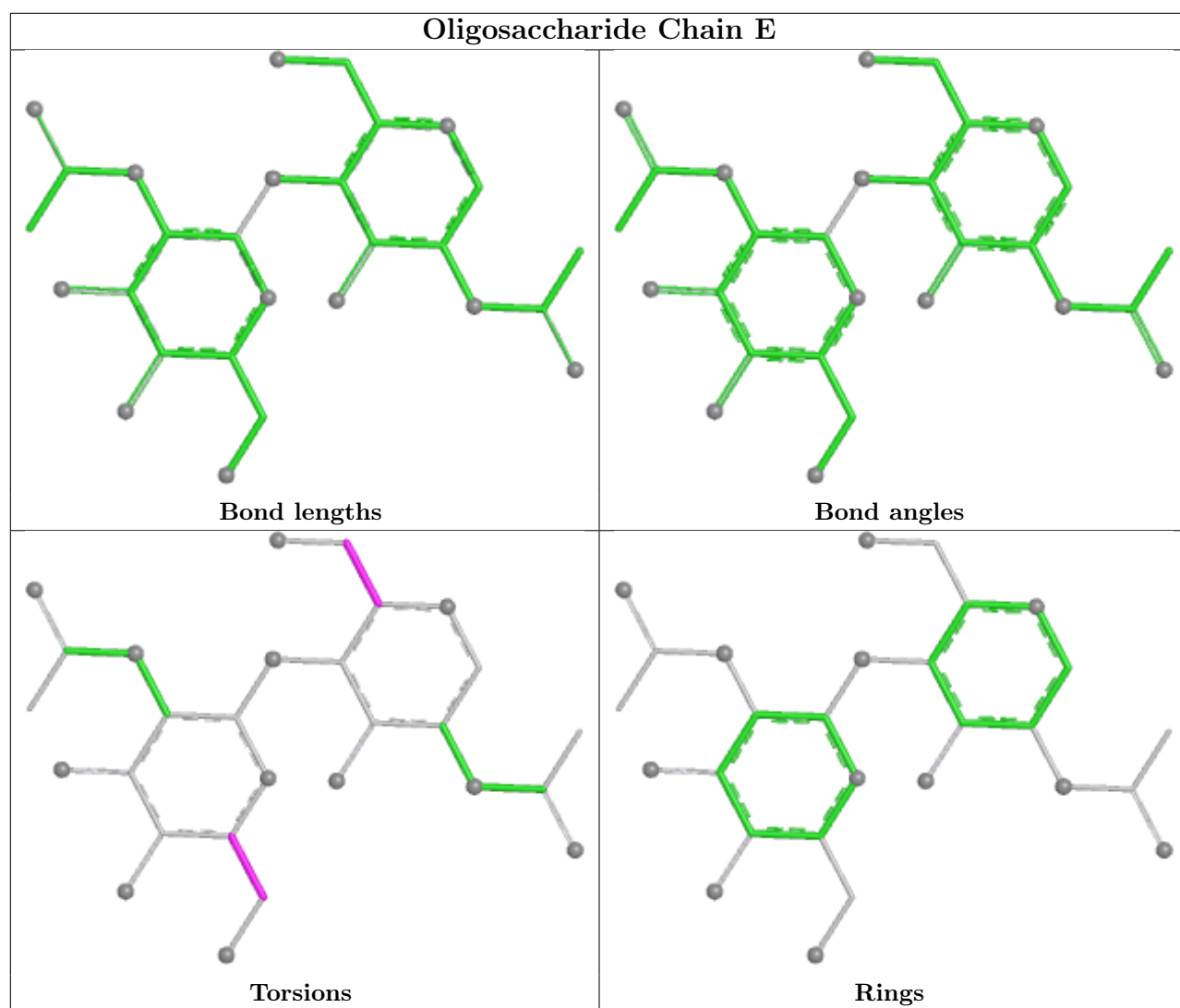
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	H	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C1-C2-N2-C7
2	I	2	NAG	C3-C2-N2-C7
2	P	1	NAG	O5-C5-C6-O6

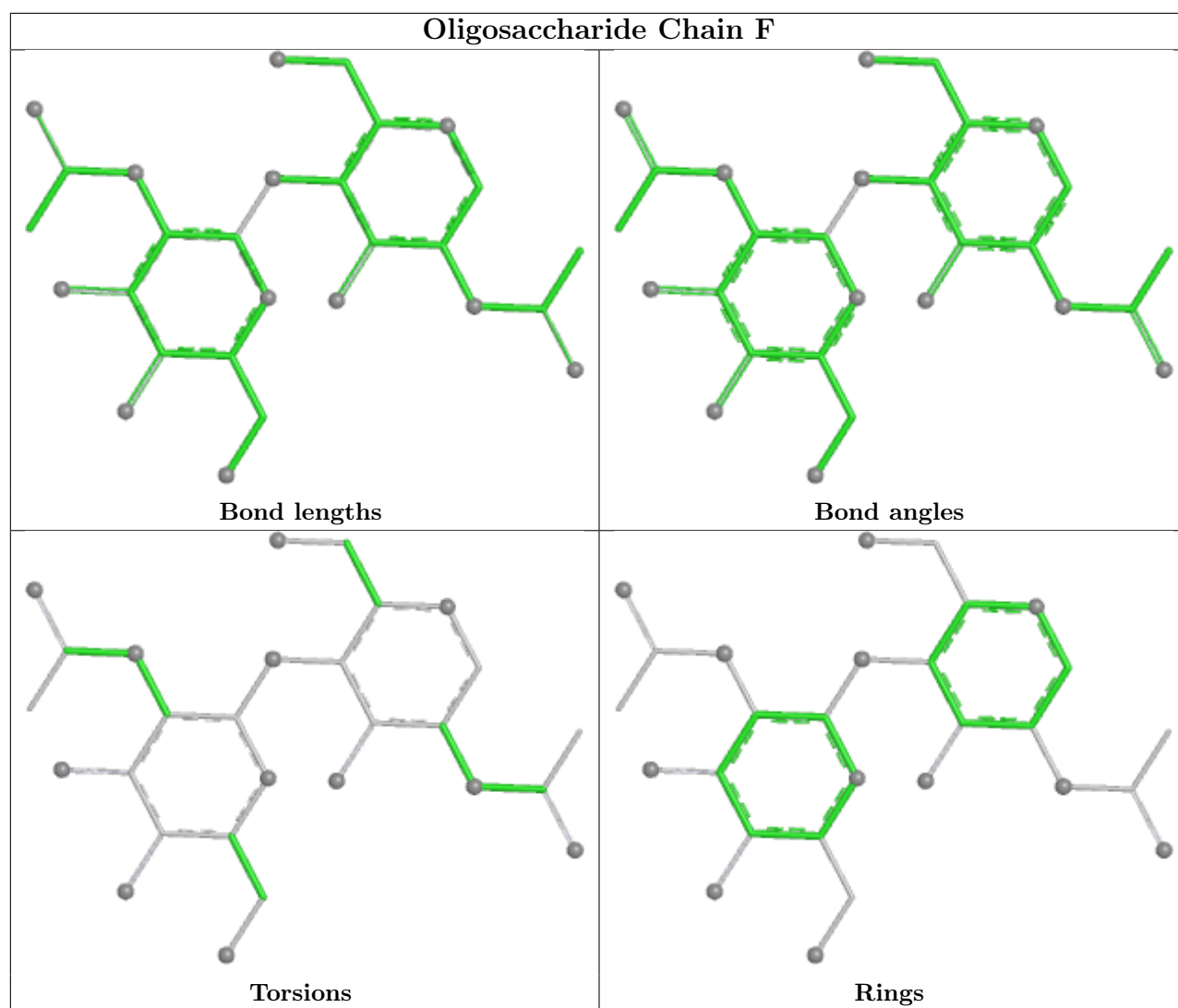
There are no ring outliers.

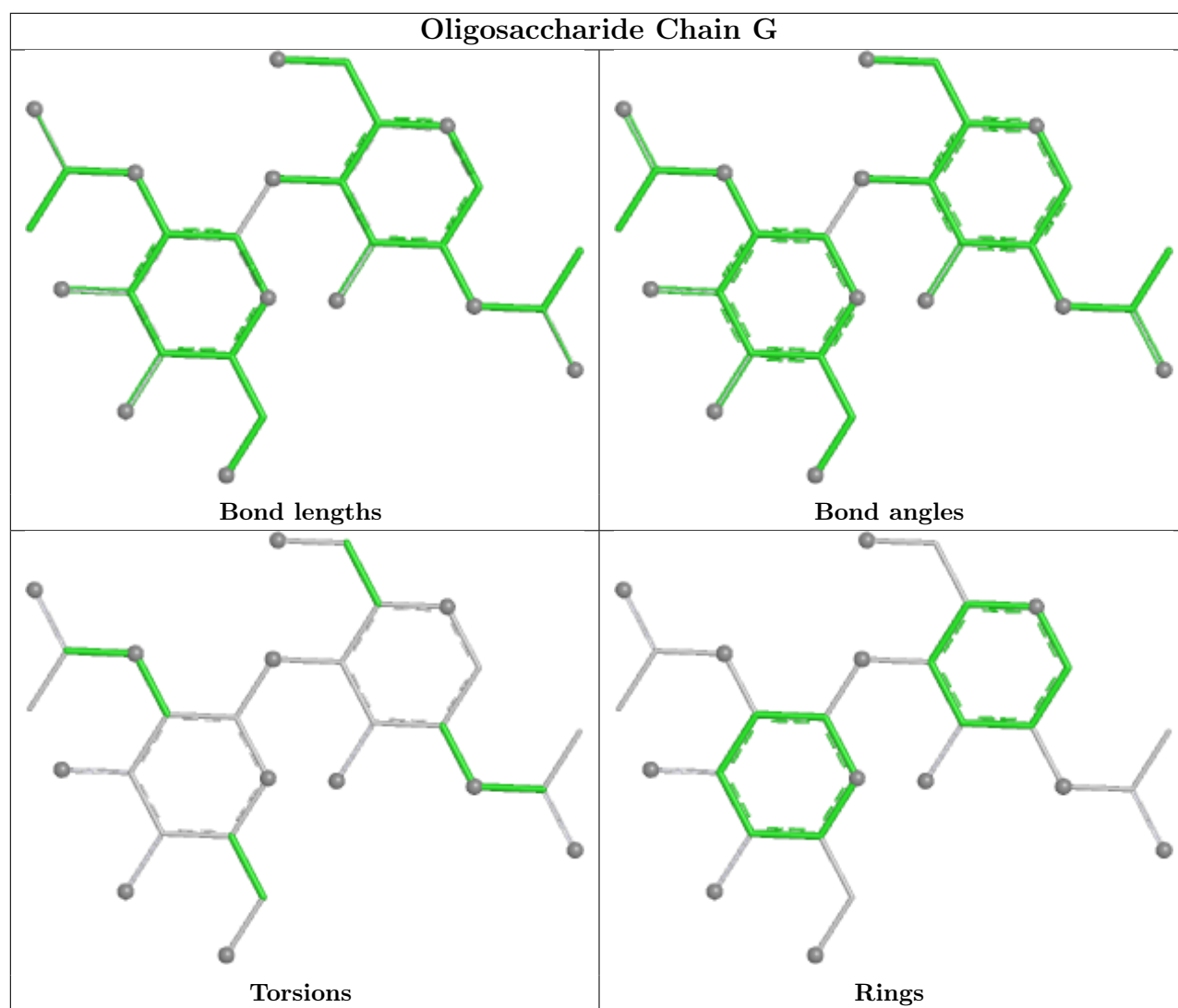
No monomer is involved in short contacts.

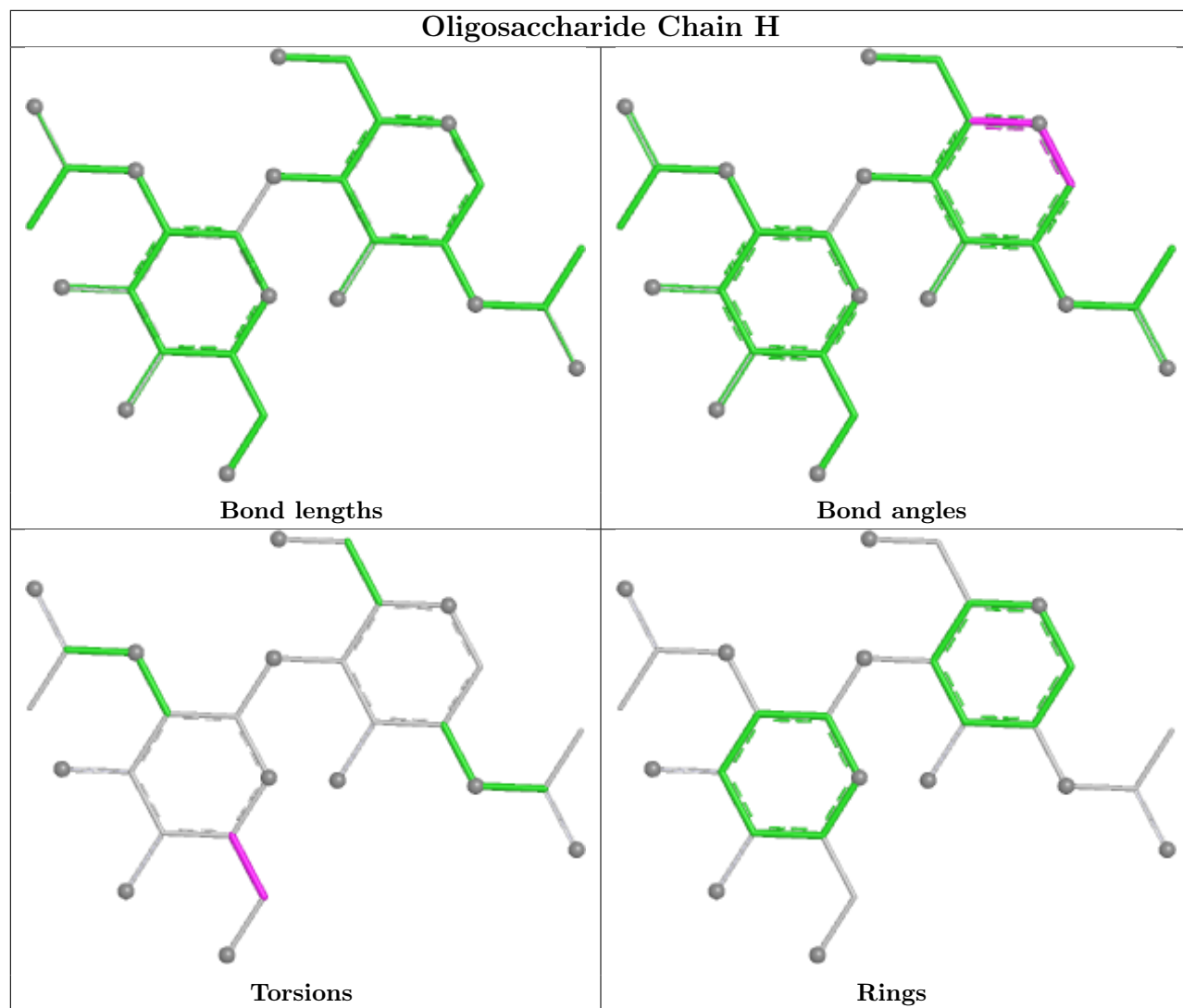
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

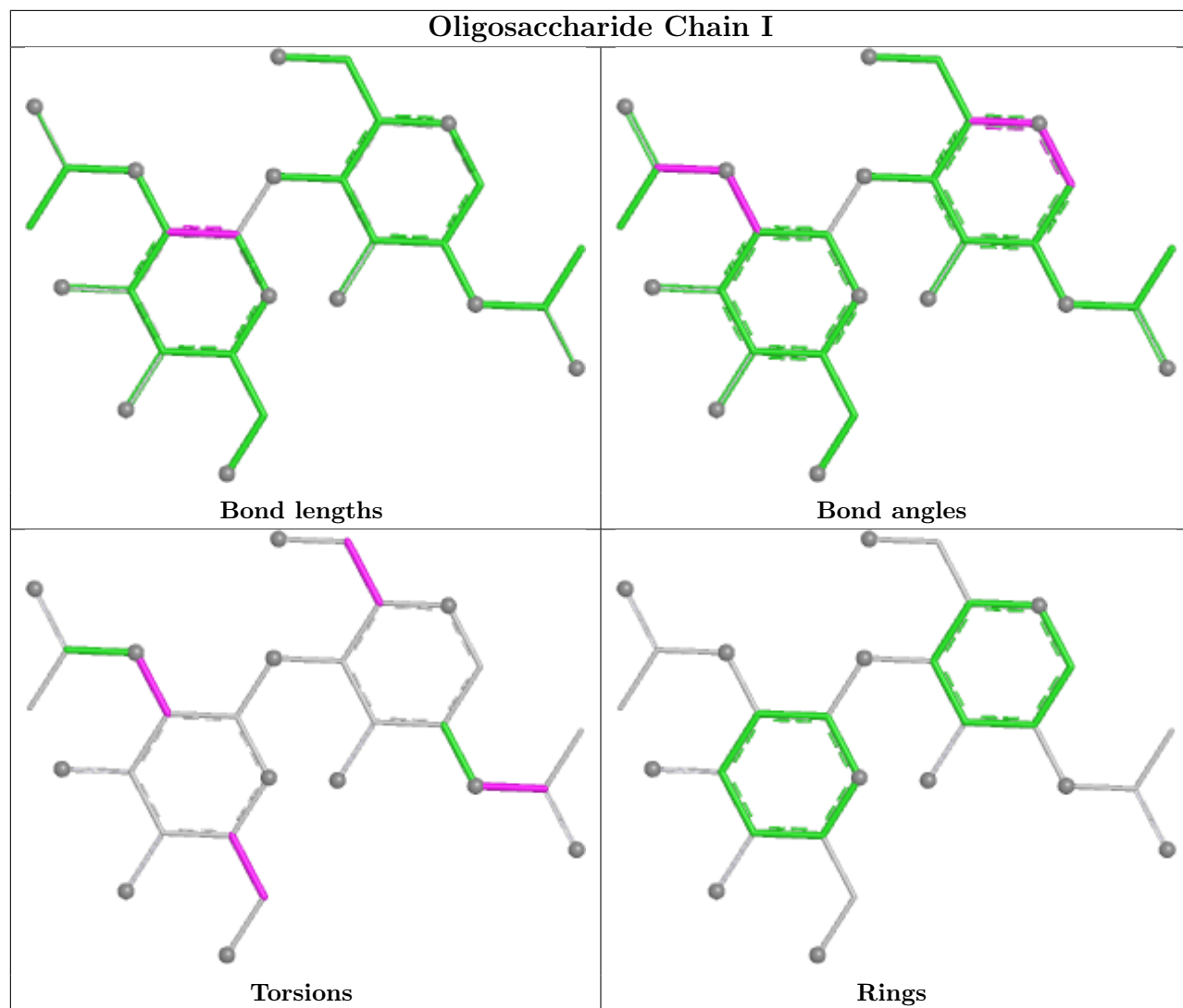


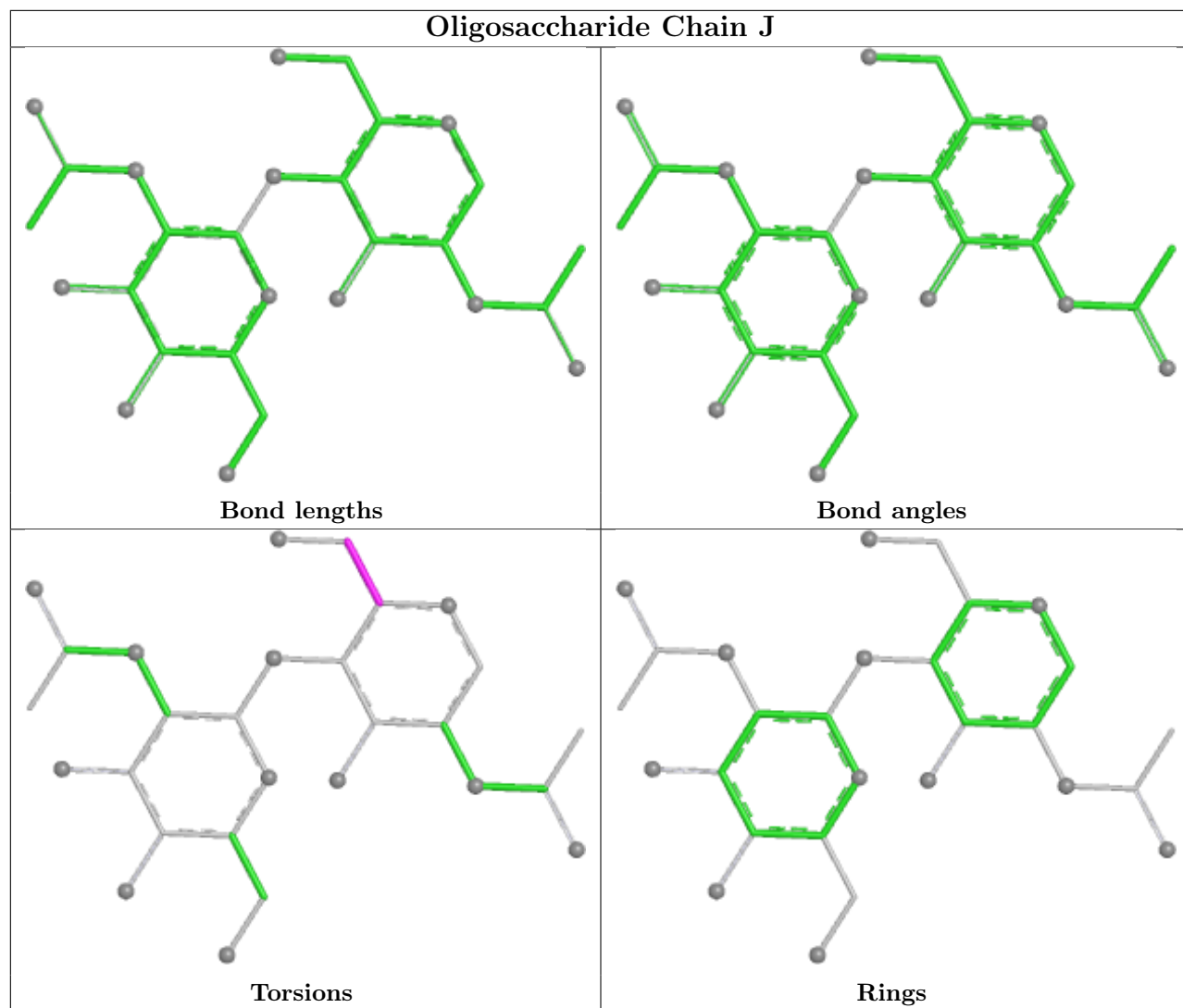


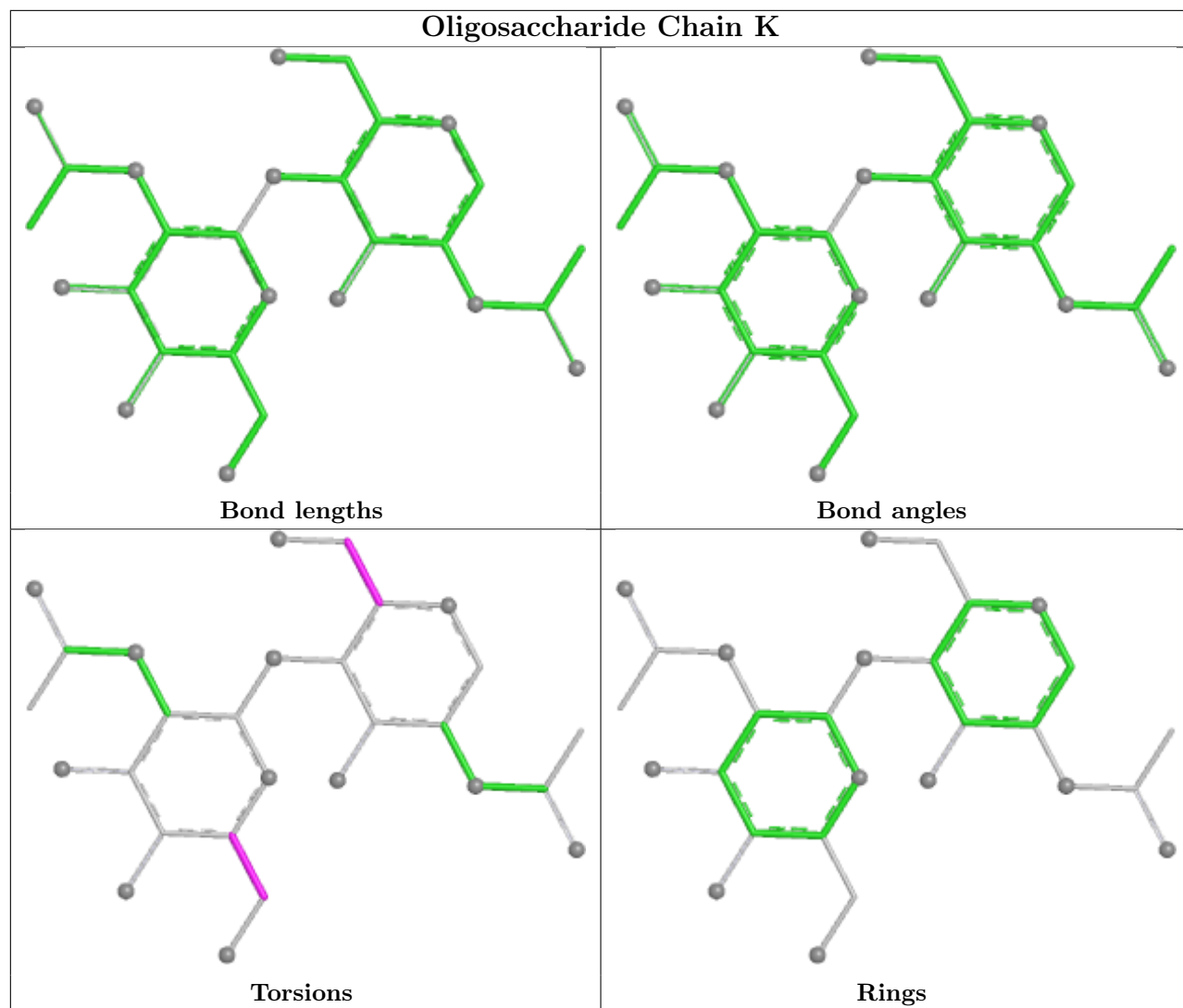


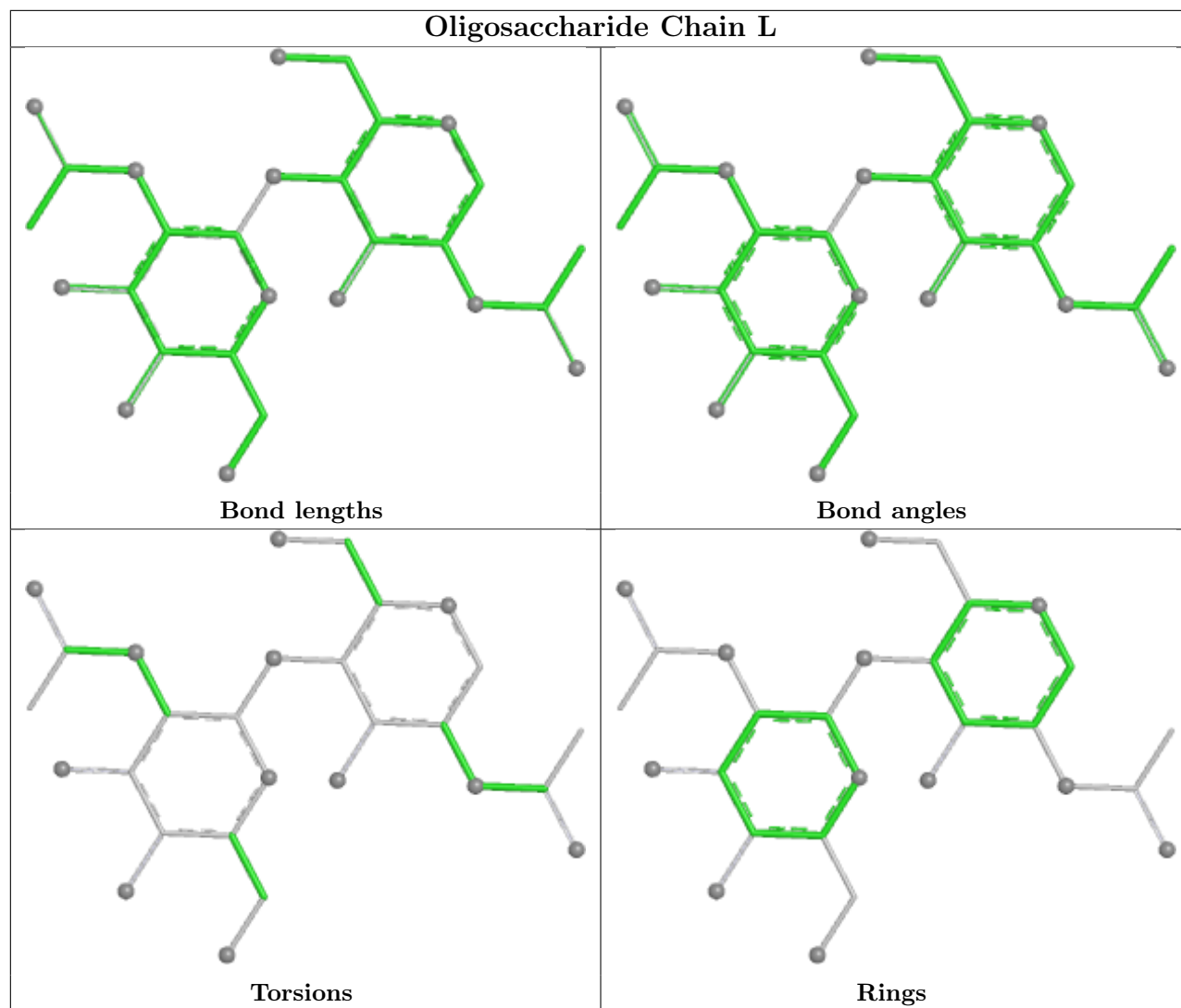


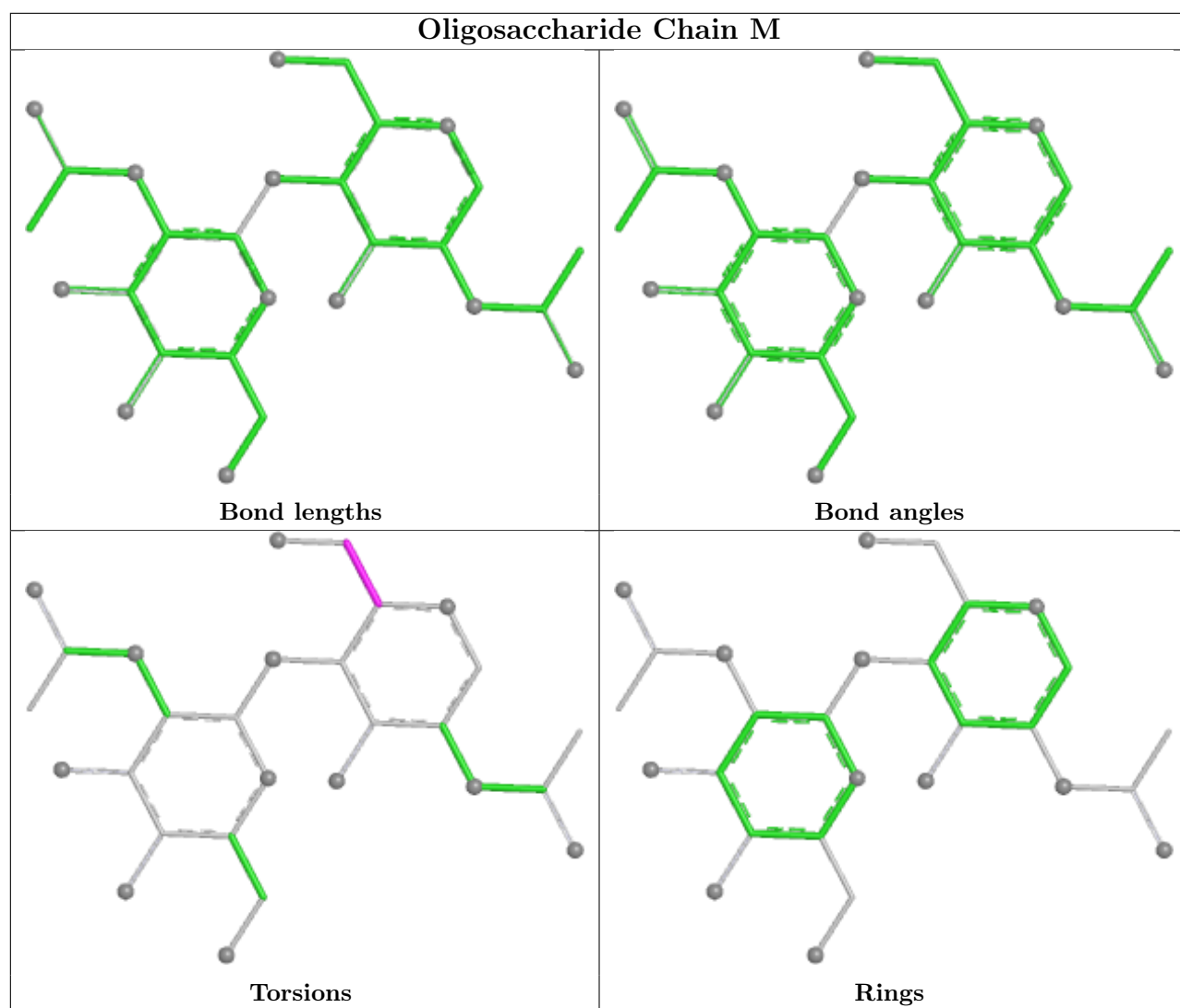


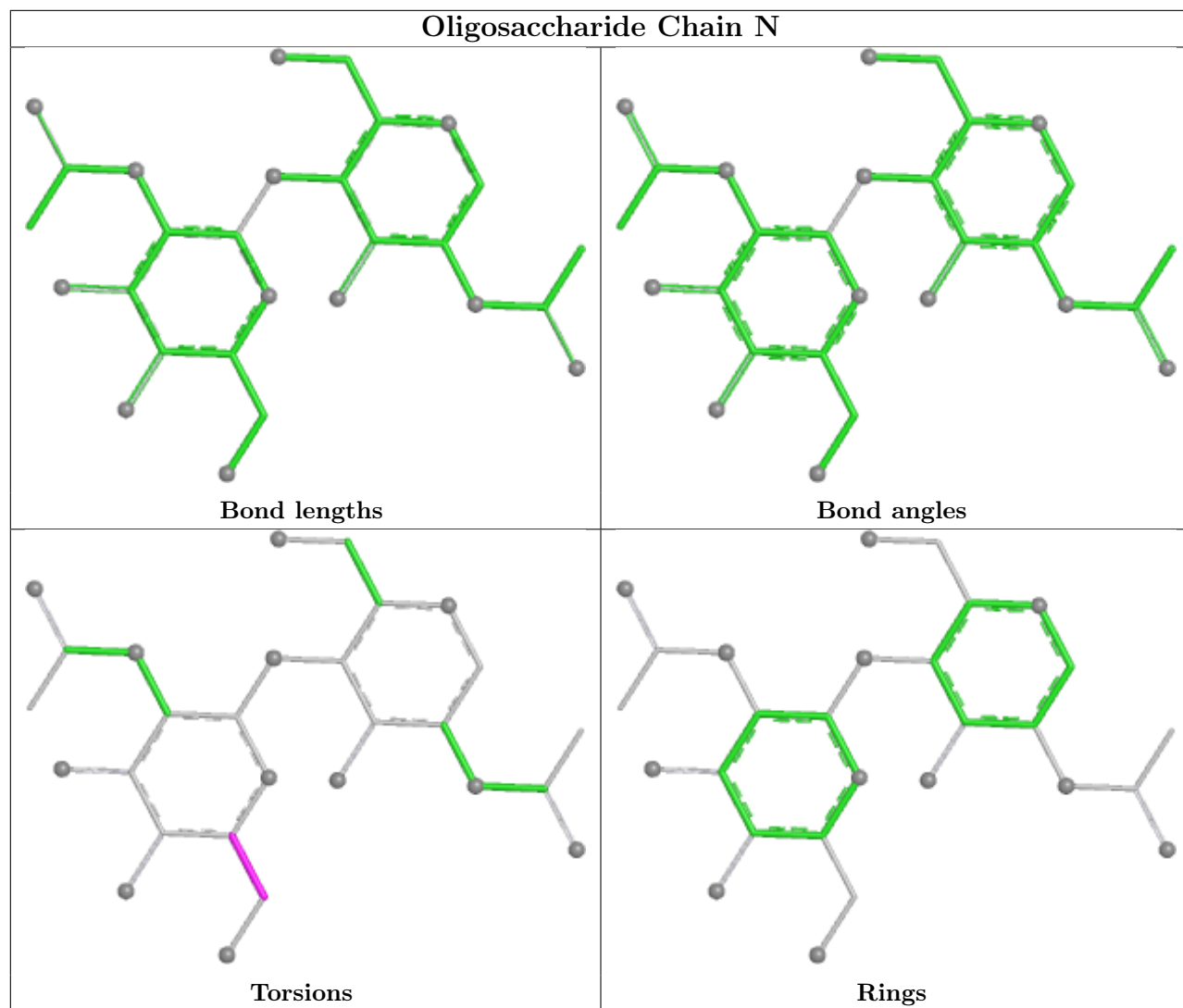


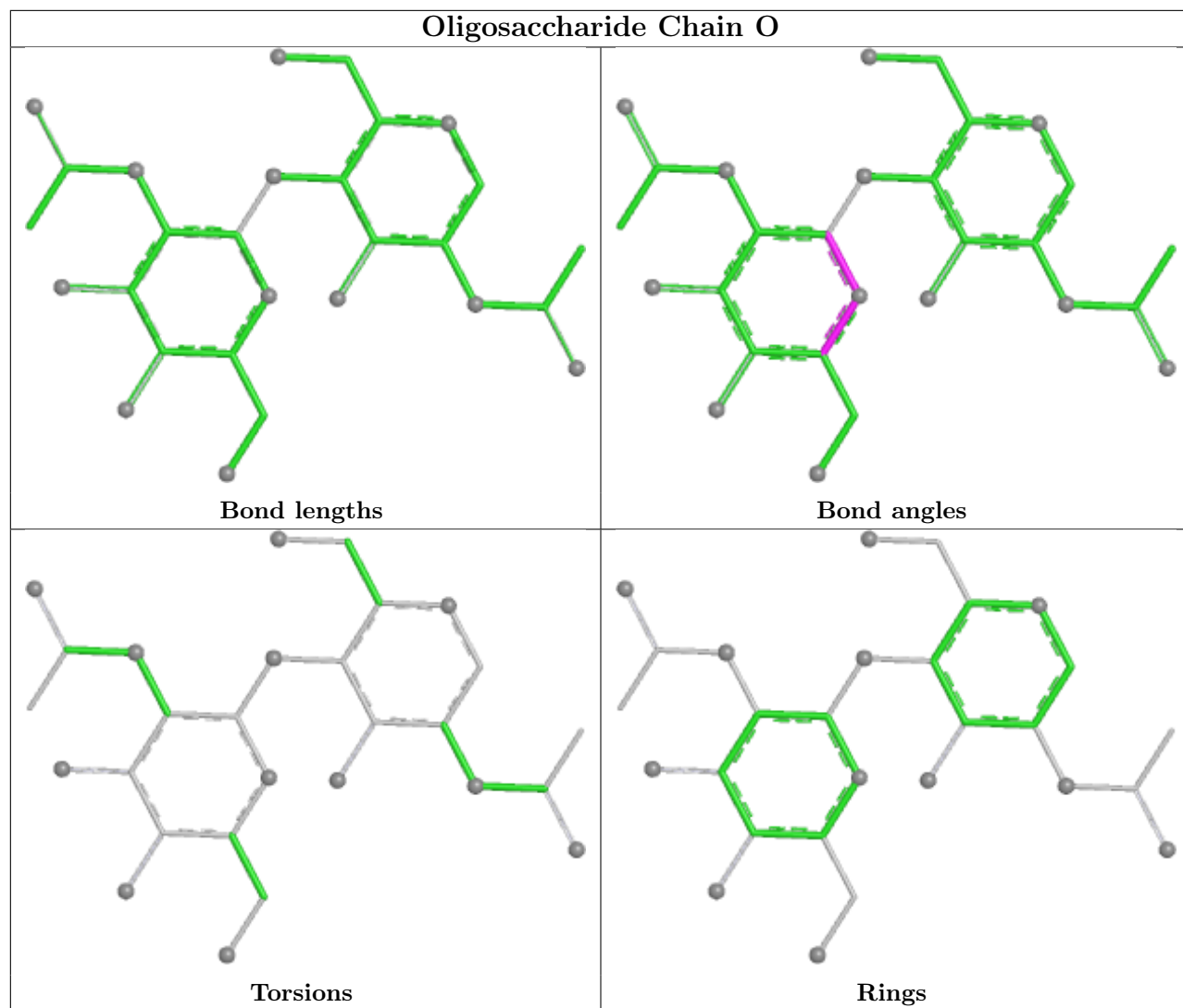


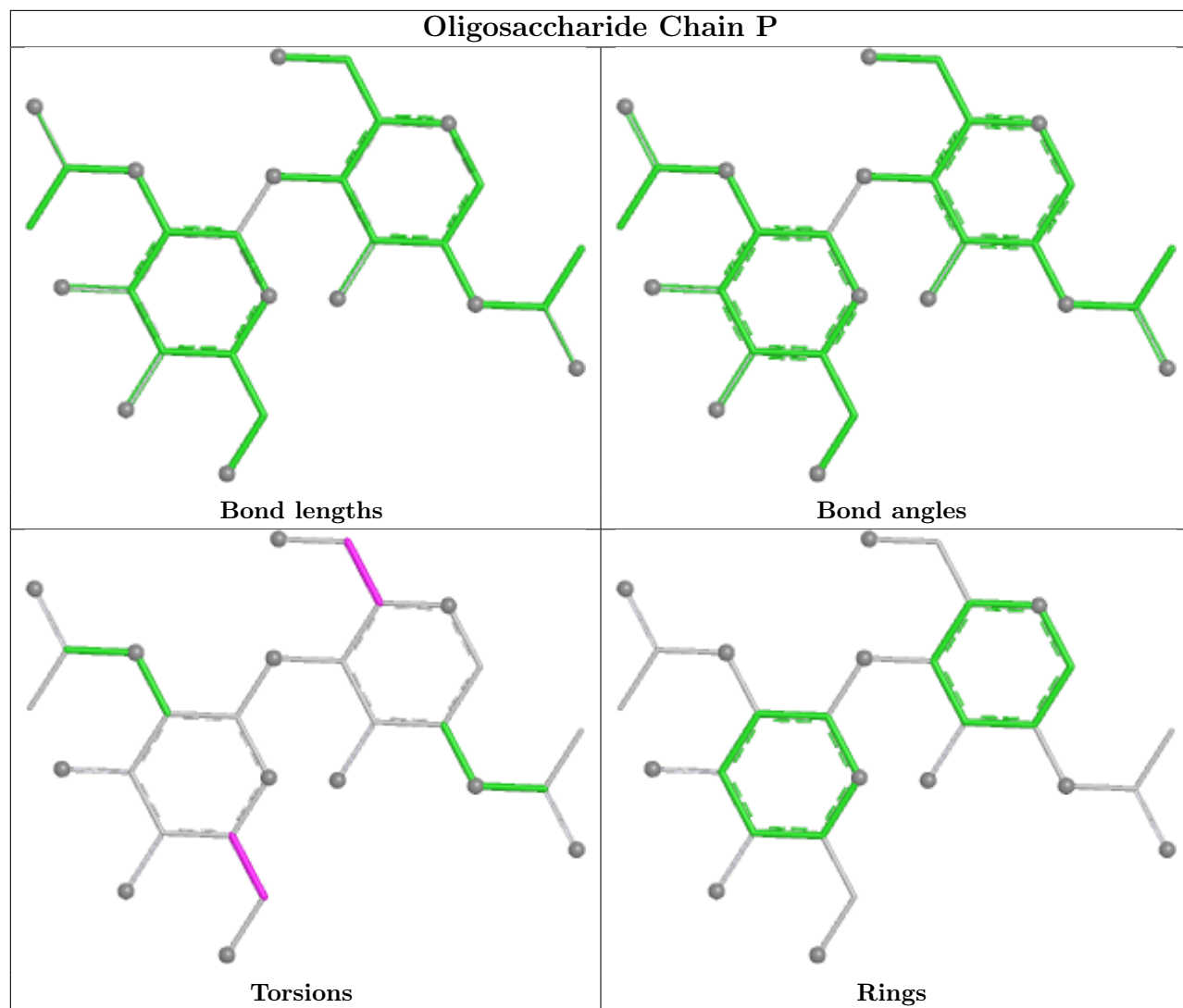


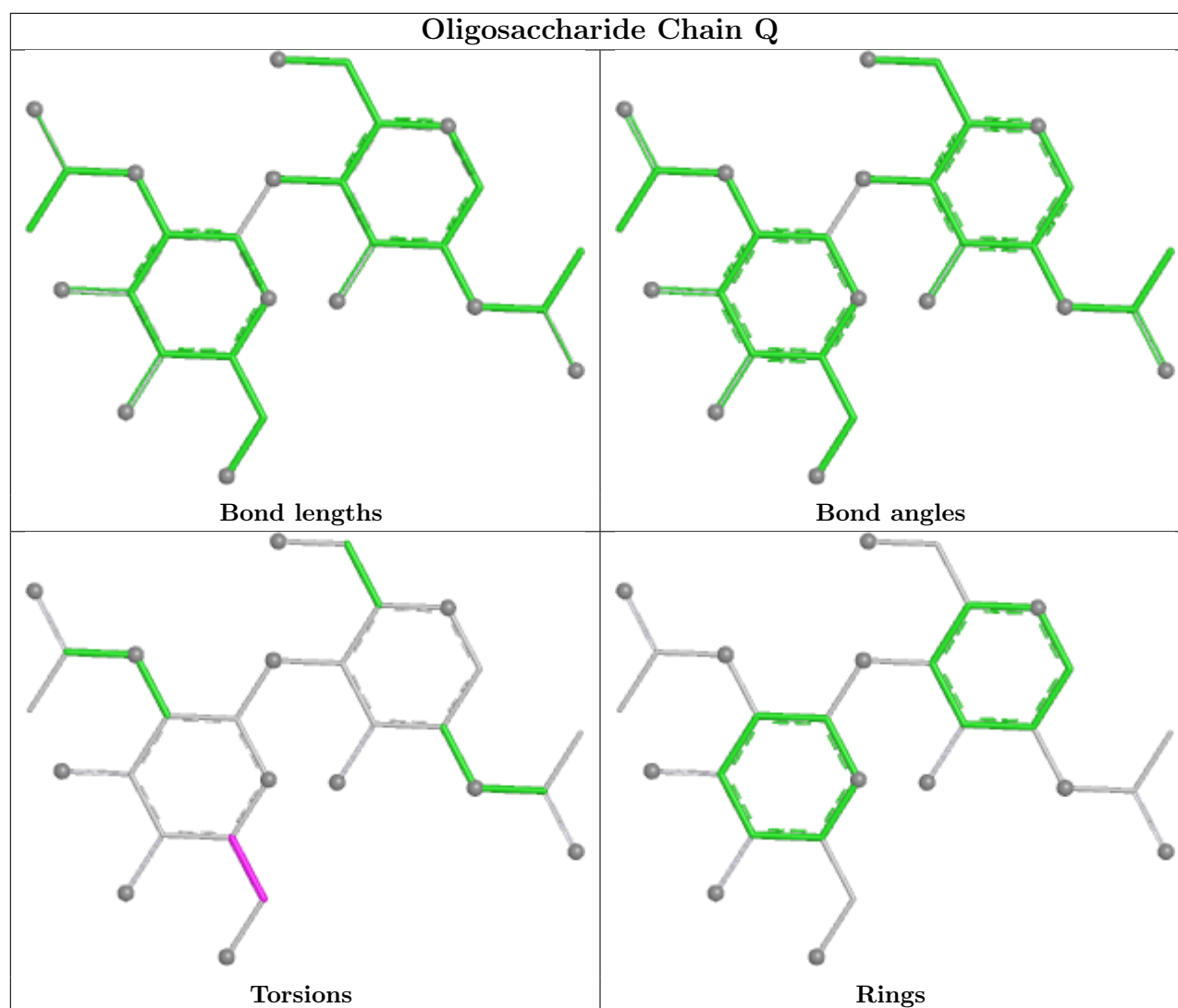












5.6 Ligand geometry [i](#)

13 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	B	1303	1	14,14,15	0.46	0	17,19,21	0.72	1 (5%)
3	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	C	1301	1	14,14,15	0.80	1 (7%)	17,19,21	2.38	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	1304	1	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	B	1305	1	14,14,15	0.35	0	17,19,21	0.65	1 (5%)
3	NAG	C	1303	1	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	B	1302	1	14,14,15	0.17	0	17,19,21	0.59	0
3	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.51	0
3	NAG	A	1302	1	14,14,15	0.42	0	17,19,21	0.50	0
3	NAG	A	1303	1	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	A	1301	1	14,14,15	0.38	0	17,19,21	0.53	0
3	NAG	B	1301	1	14,14,15	0.76	1 (7%)	17,19,21	2.41	3 (17%)
3	NAG	C	1304	1	14,14,15	0.31	0	17,19,21	0.70	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	B	1303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1301	NAG	C1-C2	2.39	1.55	1.52
3	B	1301	NAG	C1-C2	2.17	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1301	NAG	C2-N2-C7	8.39	134.15	122.90
3	C	1301	NAG	C2-N2-C7	8.30	134.03	122.90
3	B	1301	NAG	C1-C2-N2	4.31	117.23	110.43
3	C	1301	NAG	C1-C2-N2	4.06	116.83	110.43
3	C	1304	NAG	C1-O5-C5	2.47	115.50	112.19
3	B	1303	NAG	C1-O5-C5	2.39	115.39	112.19
3	B	1305	NAG	C1-O5-C5	2.31	115.29	112.19
3	C	1301	NAG	C8-C7-N2	2.15	119.69	116.12
3	B	1301	NAG	C8-C7-N2	2.11	119.61	116.12

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1302	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	A	1304	NAG	O5-C5-C6-O6
3	C	1304	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1301	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	C	1301	NAG	C1-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

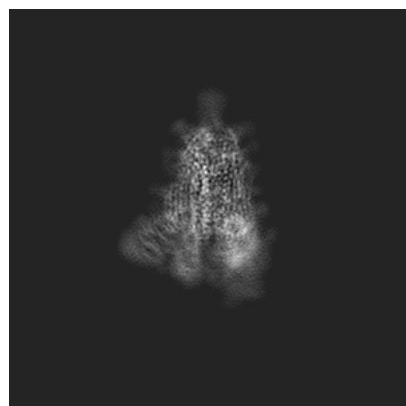
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23983. These allow visual inspection of the internal detail of the map and identification of artifacts.

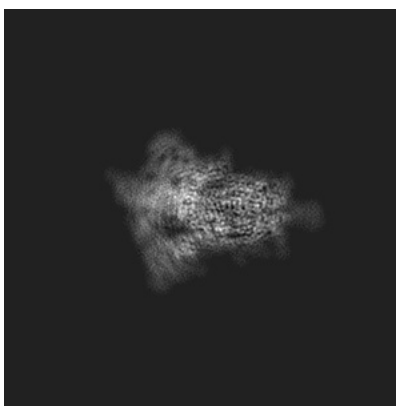
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

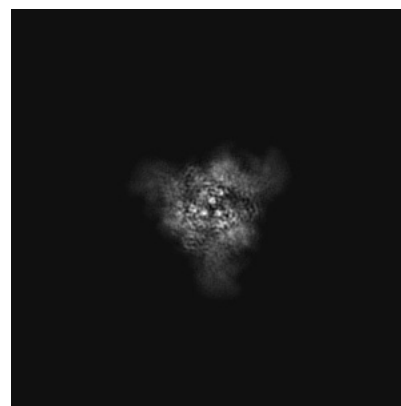
6.1.1 Primary map



X

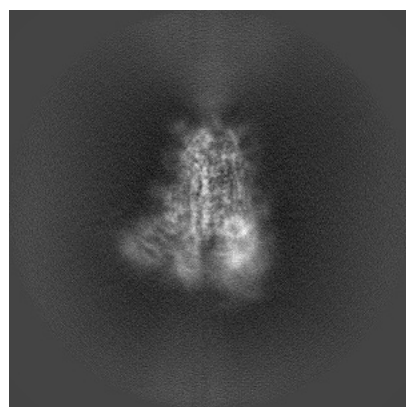


Y

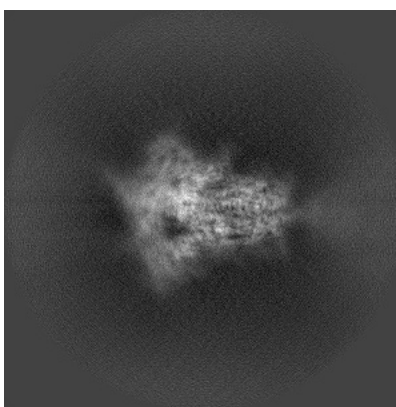


Z

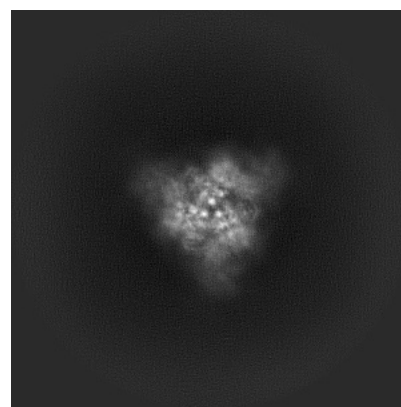
6.1.2 Raw map



X



Y



Z

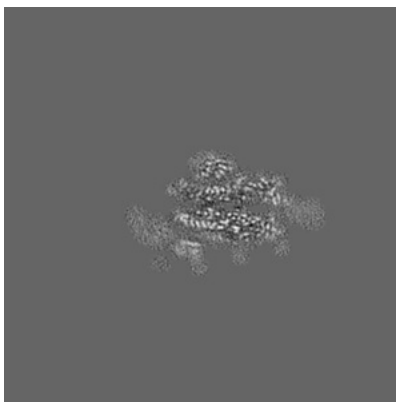
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

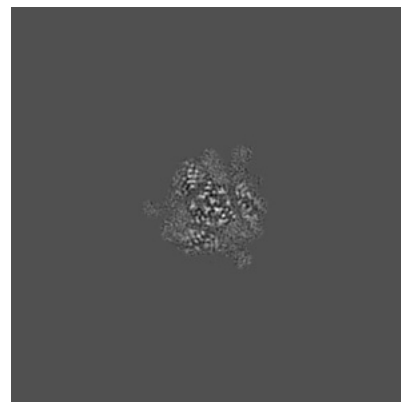
6.2.1 Primary map



X Index: 220

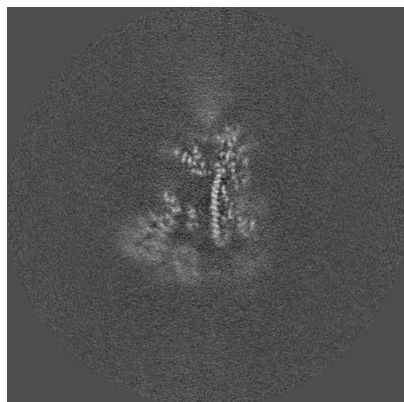


Y Index: 220

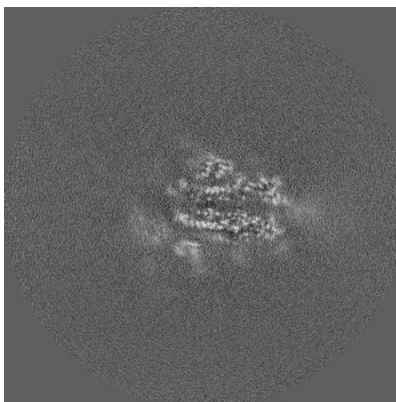


Z Index: 220

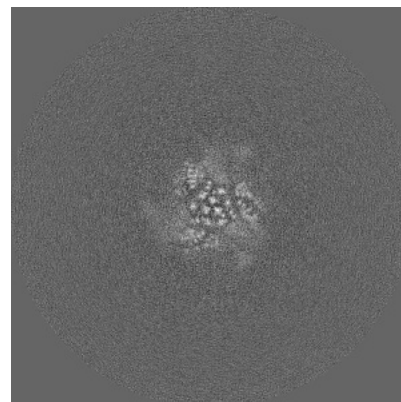
6.2.2 Raw map



X Index: 220



Y Index: 220

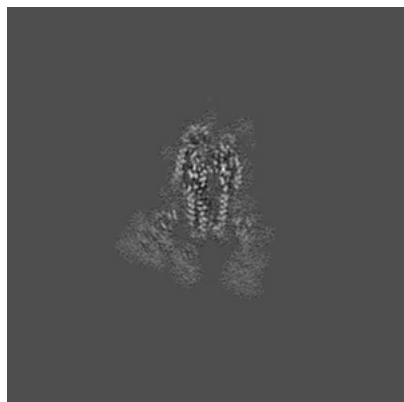


Z Index: 220

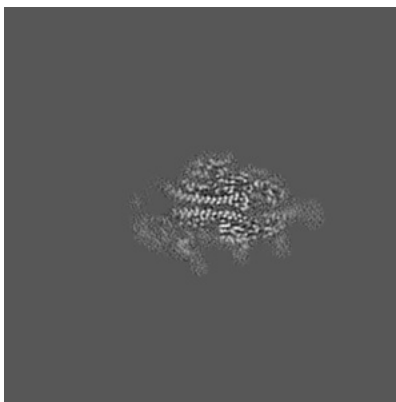
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

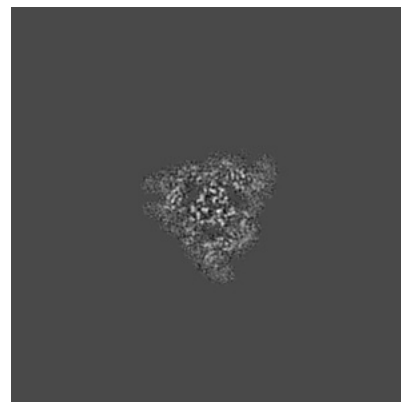
6.3.1 Primary map



X Index: 231

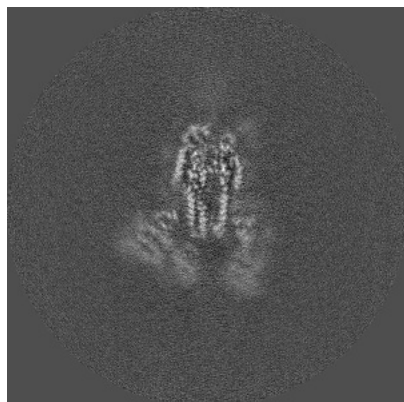


Y Index: 214

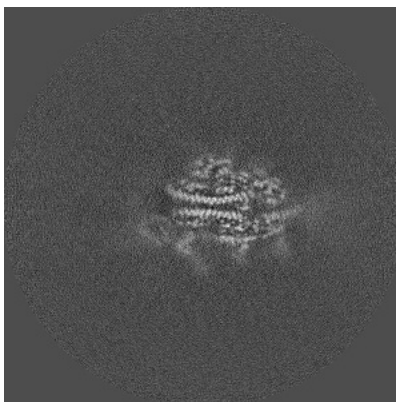


Z Index: 208

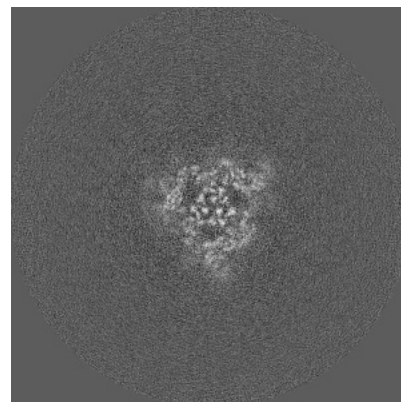
6.3.2 Raw map



X Index: 231



Y Index: 215

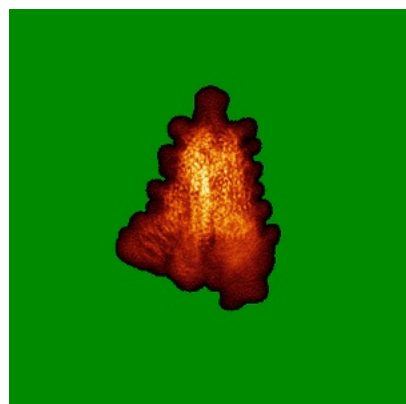


Z Index: 208

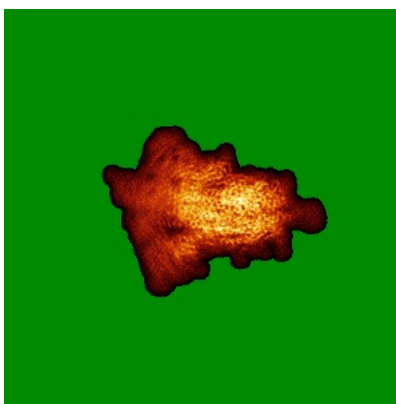
The images above show the largest variance slices of the map in three orthogonal directions.

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

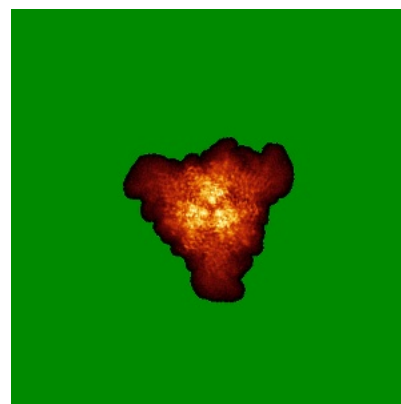
6.4.1 Primary map



X

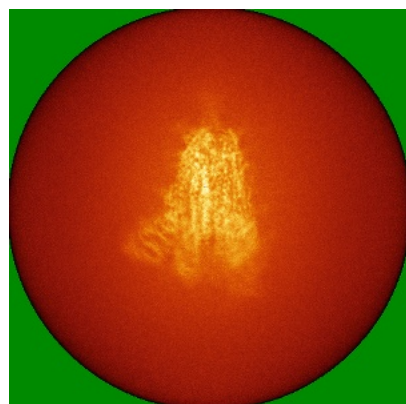


Y

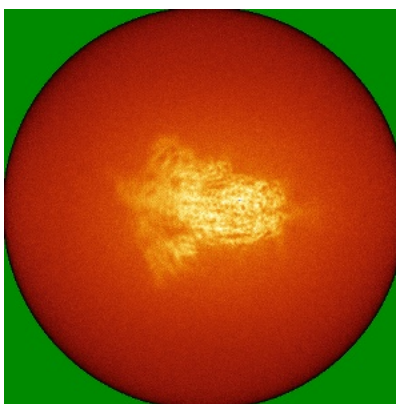


Z

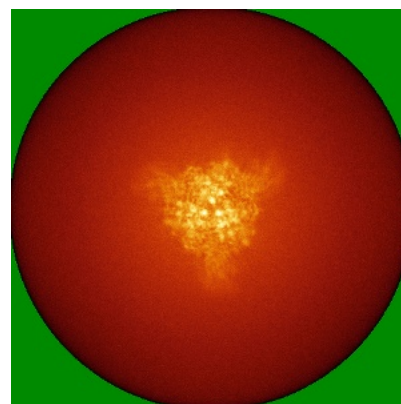
6.4.2 Raw map



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.

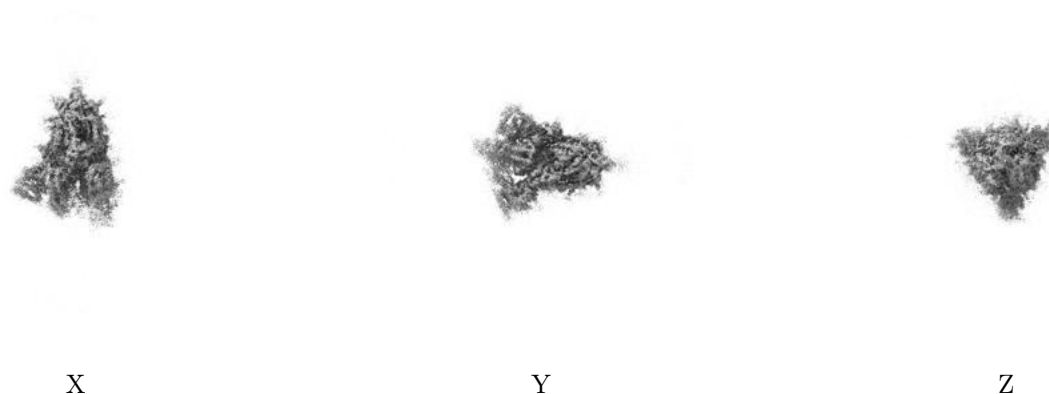
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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



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.

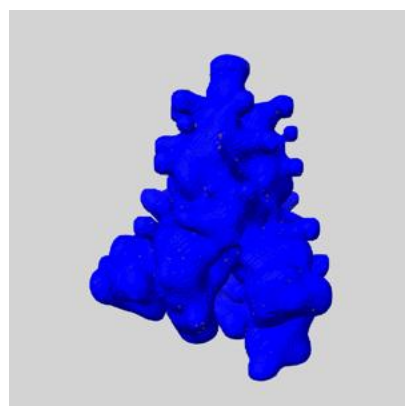
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

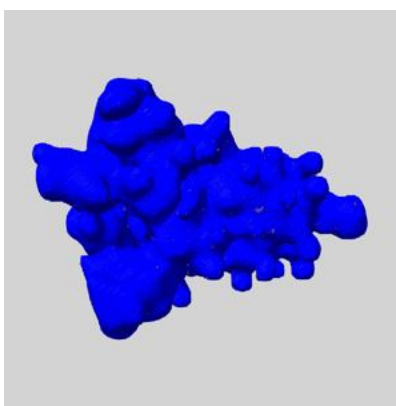
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

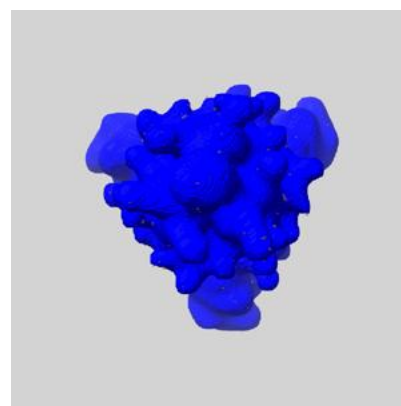
6.6.1 emd_23983_msk_1.map [i](#)



X



Y

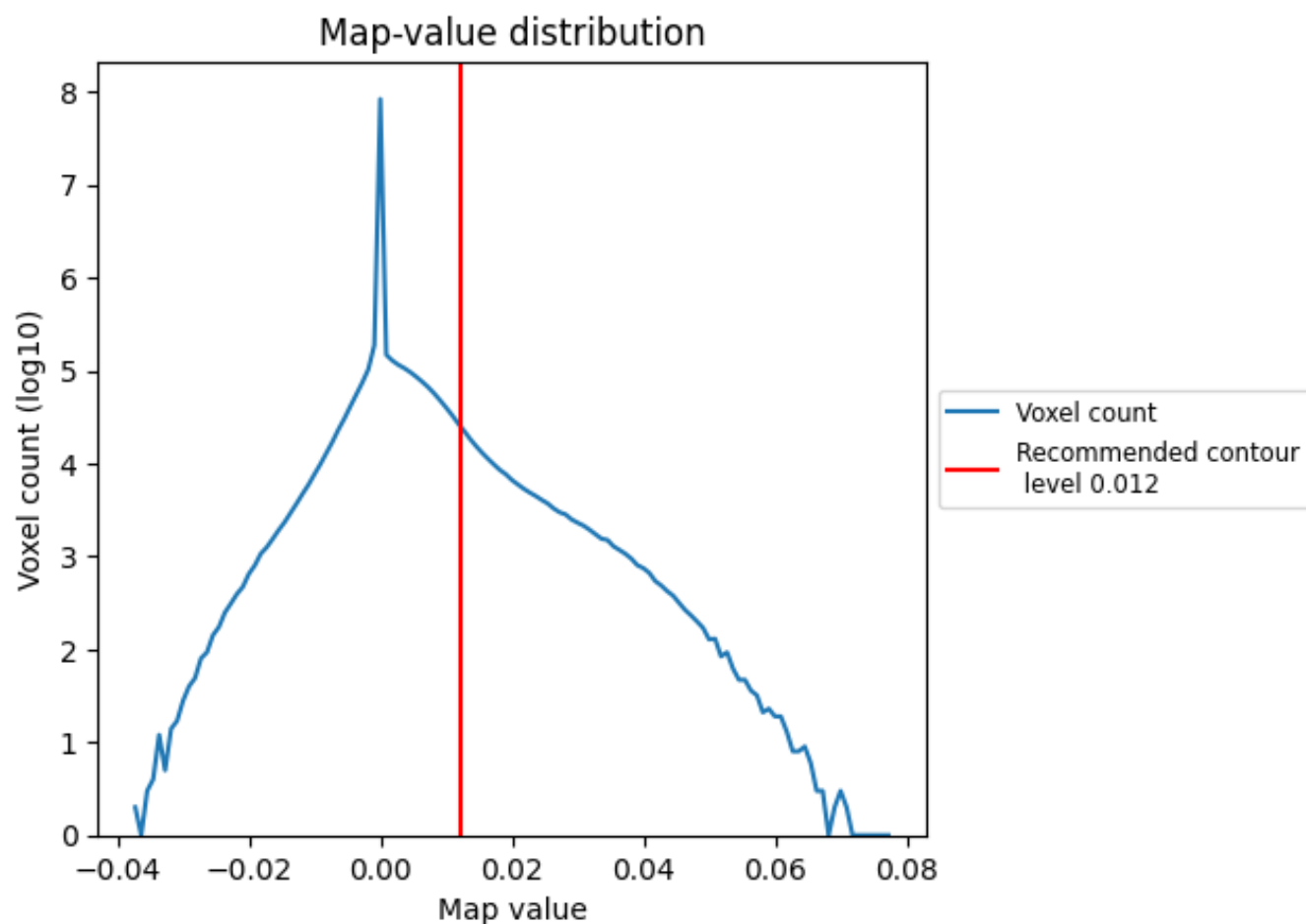


Z

7 Map analysis [i](#)

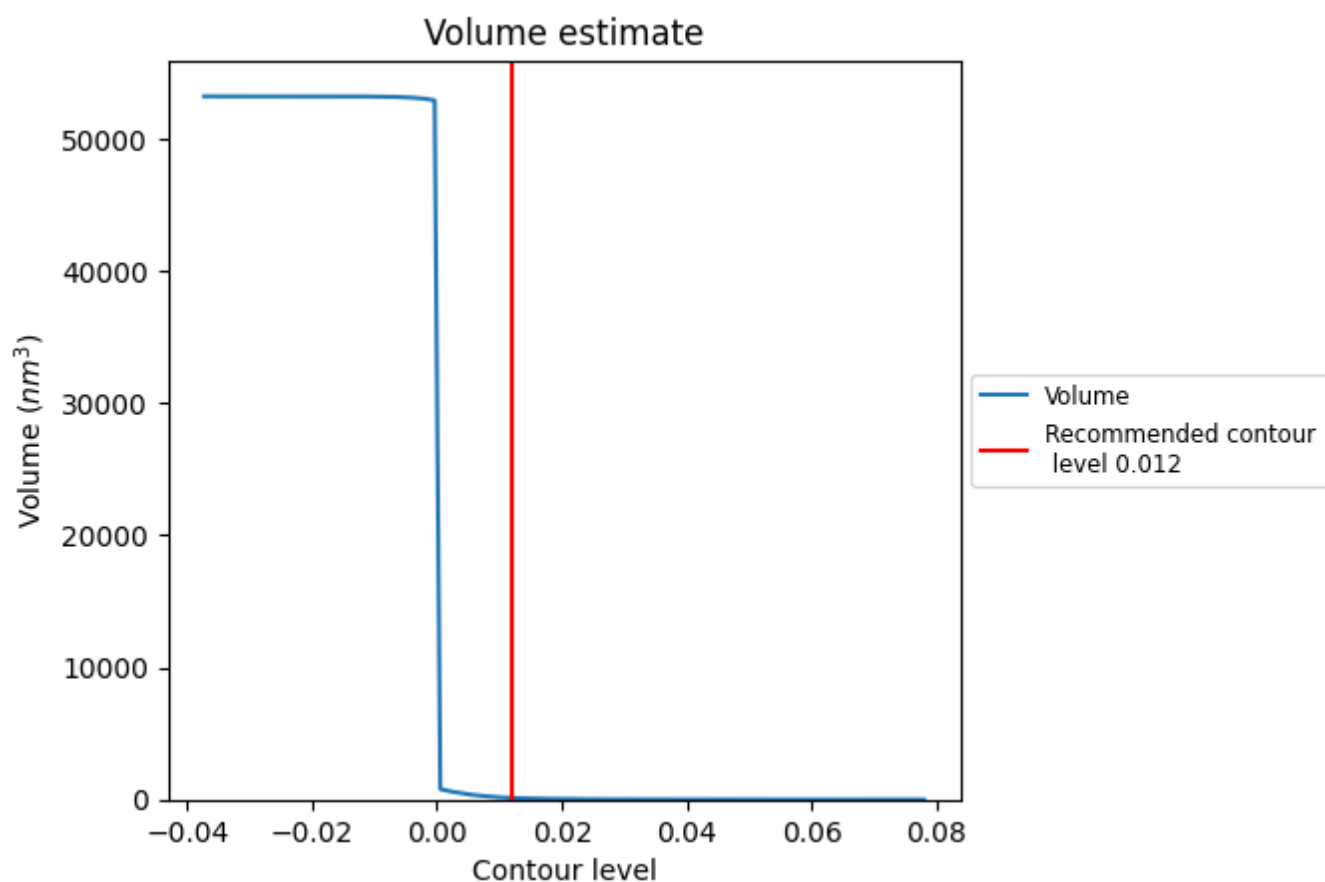
This section contains the results of statistical analysis of the map.

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.

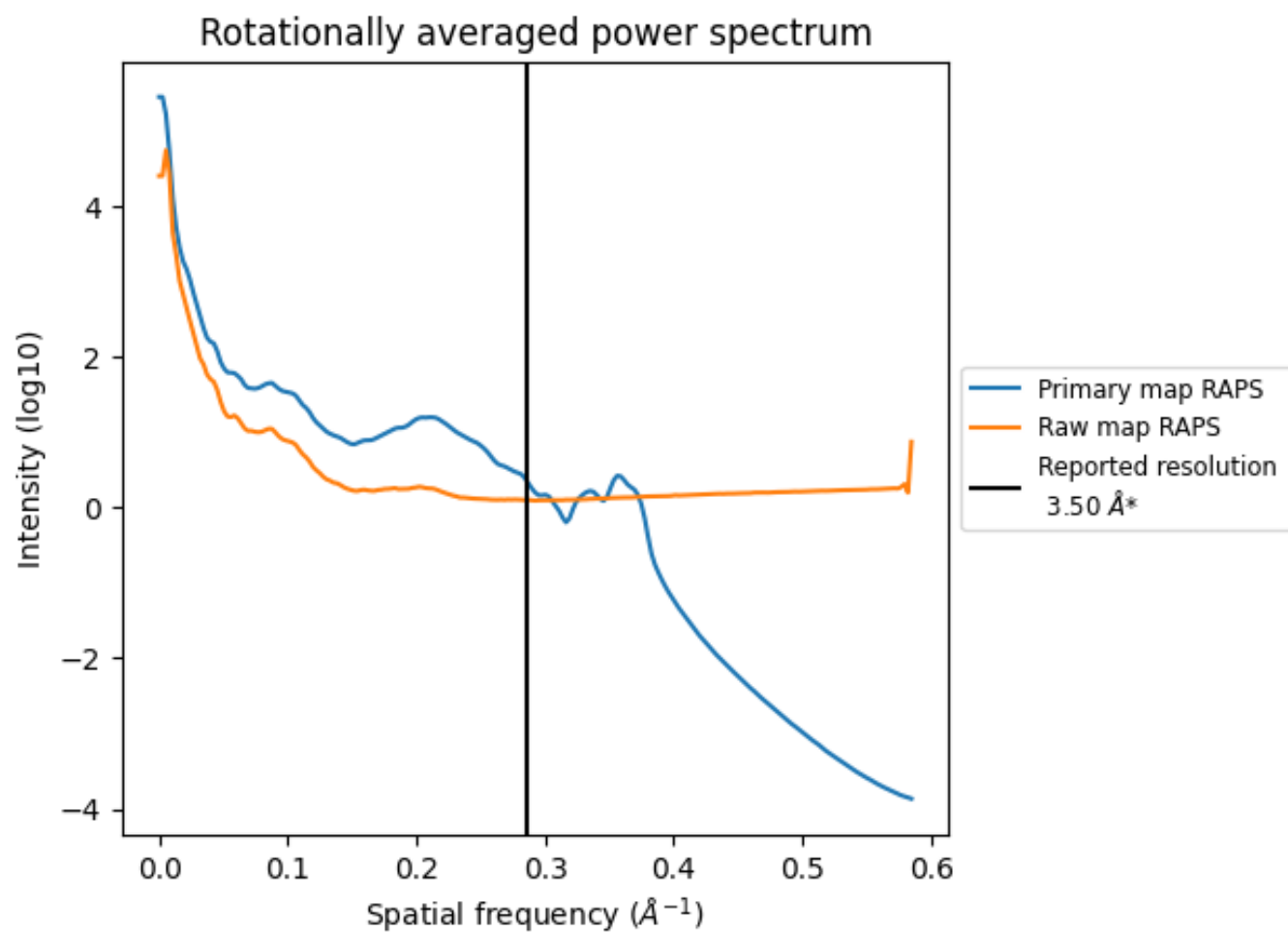
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm^3 ; this corresponds to an approximate mass of 110 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 ⓘ

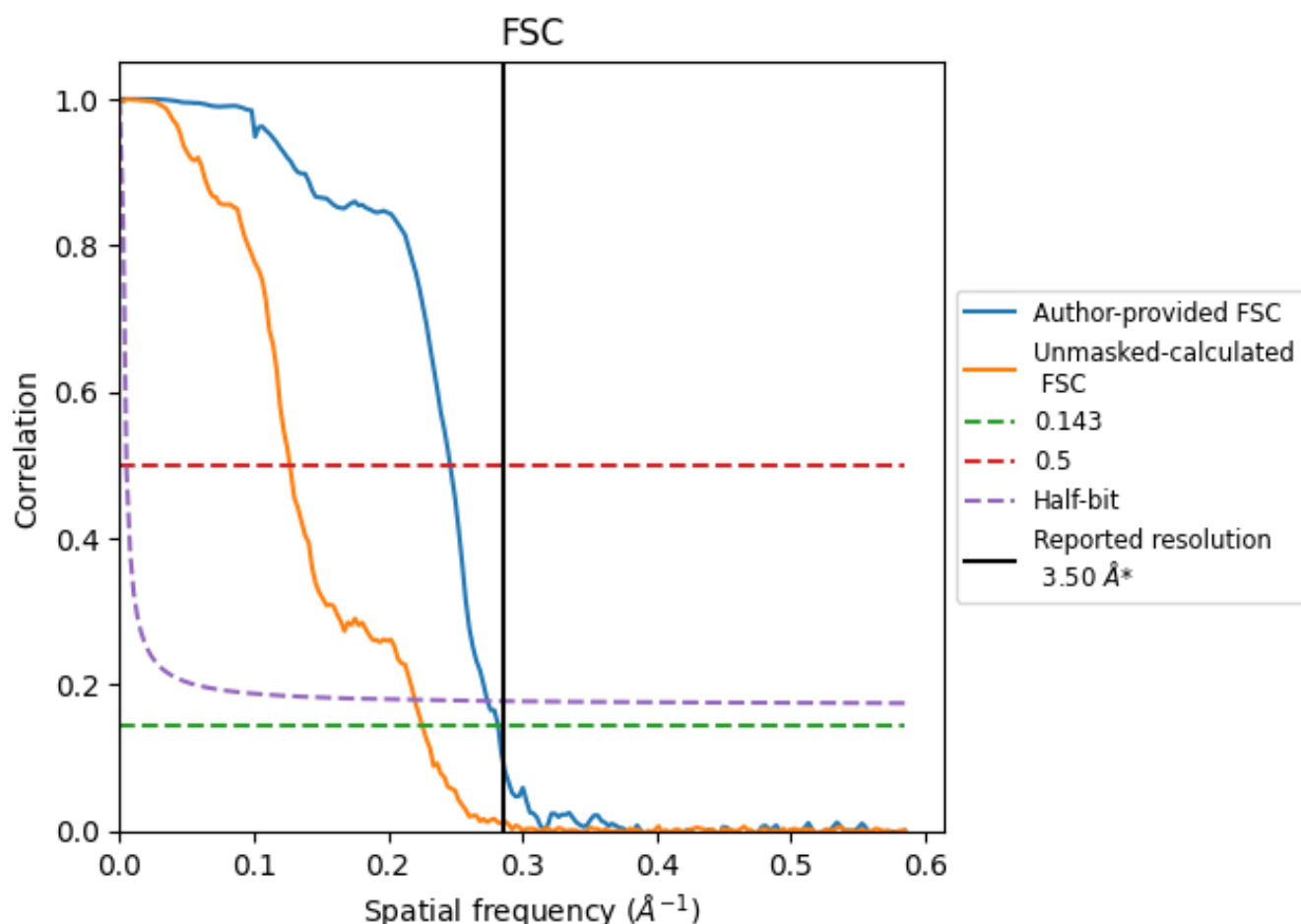


*Reported resolution corresponds to spatial frequency of 0.286 \AA^{-1}

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

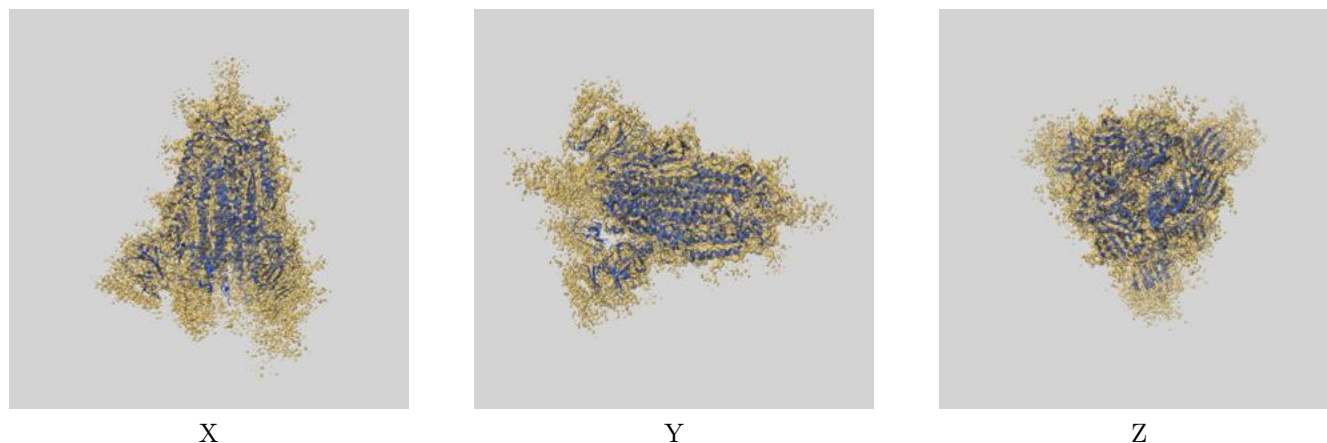
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.55	4.06	3.65
Unmasked-calculated*	4.43	7.89	4.55

*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 4.43 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

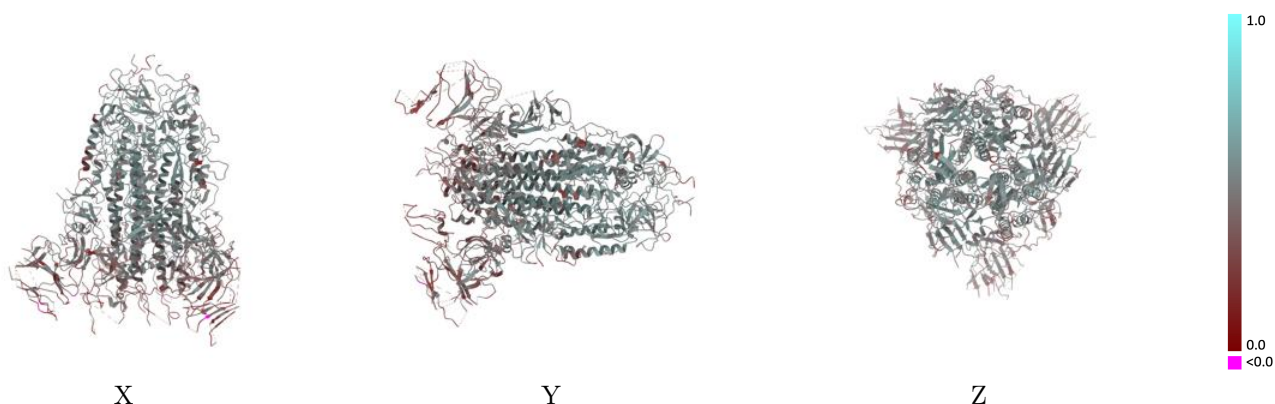
This section contains information regarding the fit between EMDB map EMD-23983 and PDB model 7MTD. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



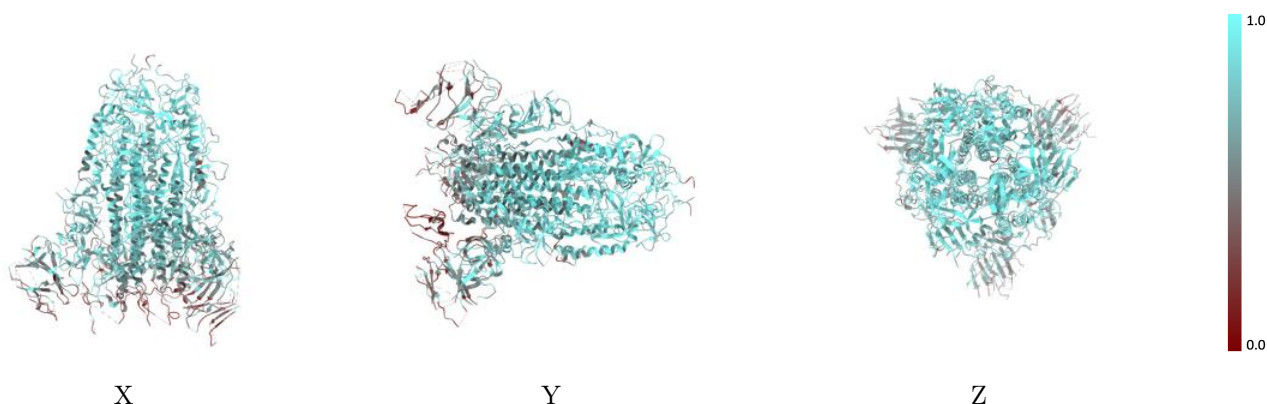
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



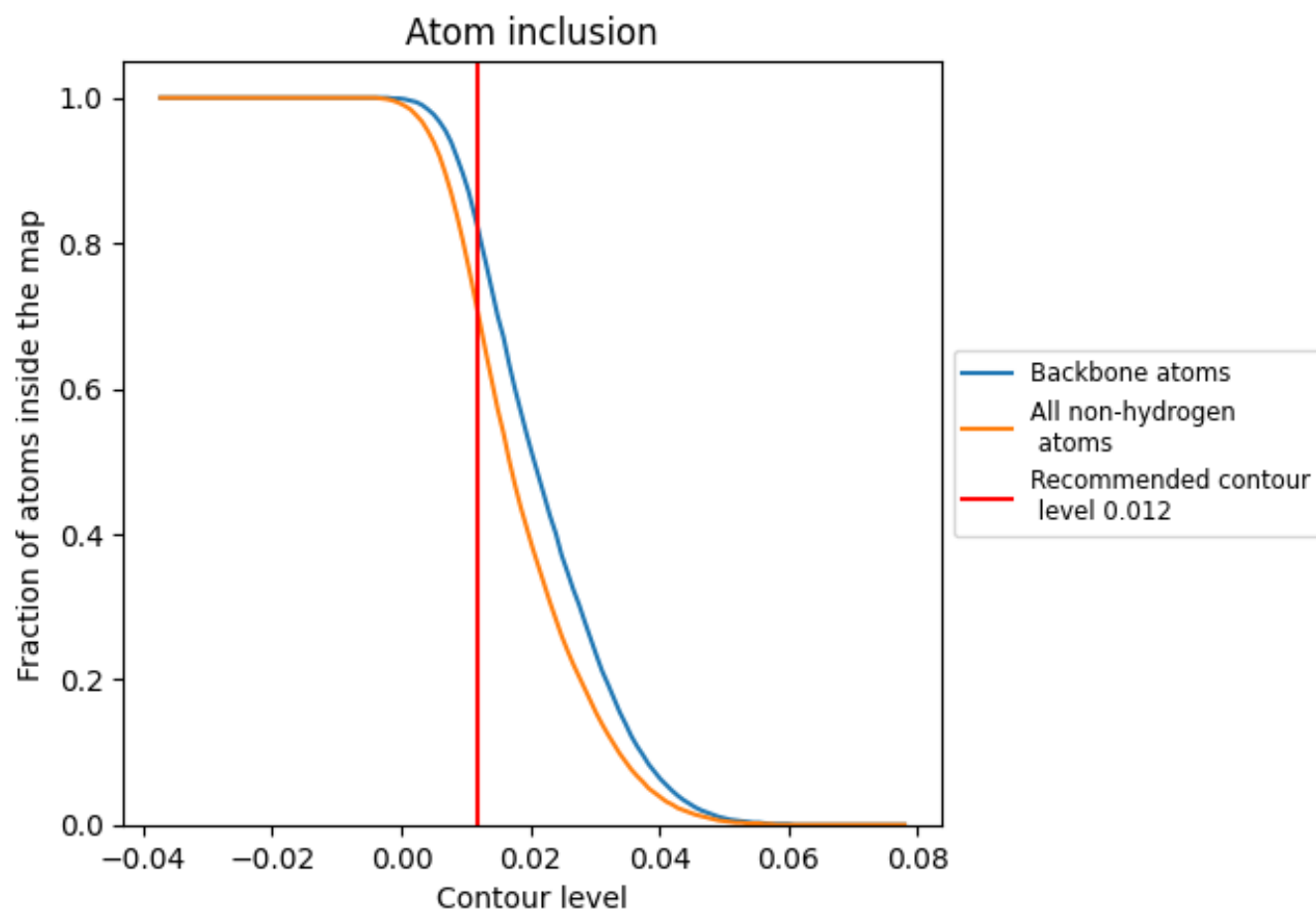
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7010	<div></div> 0.4430
A	<div></div> 0.6880	<div></div> 0.4350
B	<div></div> 0.7250	<div></div> 0.4570
C	<div></div> 0.7060	<div></div> 0.4440
D	<div></div> 0.5710	<div></div> 0.4150
E	<div></div> 0.5360	<div></div> 0.3000
F	<div></div> 0.3210	<div></div> 0.3180
G	<div></div> 0.5360	<div></div> 0.3220
H	<div></div> 0.3570	<div></div> 0.3290
I	<div></div> 0.4640	<div></div> 0.3160
J	<div></div> 0.5710	<div></div> 0.4540
K	<div></div> 0.5000	<div></div> 0.3430
L	<div></div> 0.4640	<div></div> 0.3540
M	<div></div> 0.3570	<div></div> 0.2550
N	<div></div> 0.6070	<div></div> 0.3630
O	<div></div> 0.5000	<div></div> 0.4010
P	<div></div> 0.3930	<div></div> 0.2530
Q	<div></div> 0.5000	<div></div> 0.3440

1.0

0.0

<0.0