



wwPDB EM Validation Summary Report ⓘ

Apr 18, 2024 – 12:33 PM JST

PDB ID : 8XI6
EMDB ID : EMD-38372
Title : SARS-CoV-2 Omicron BQ.1.1 Variant Spike Protein Complexed with MO11 Fab
Authors : Ishimaru, H.; Nishimura, M.; Shigematsu, H.; Marini, M.I.; Hasegawa, N.; Takamiya, R.; Iwata, S.; Mori, Y.
Deposited on : 2023-12-19
Resolution : 2.30 Å (reported)
Based on initial models : 8H3N, .

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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

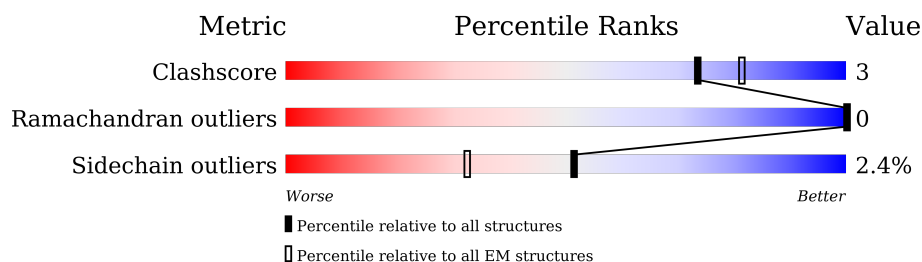
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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.





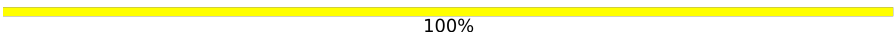


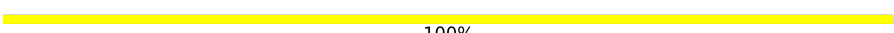










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1247	72% 9% 19%
1	B	1247	72% 9% 19%
1	C	1247	71% 9% 19%
2	D	232	5% 47% 6% 47%
2	F	232	5% 47% 6% 47%
2	H	232	5% 47% 6% 47%
3	E	214	45% 52%
3	G	214	45% 52%

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Mol	Chain	Length	Quality of chain
3	I	214	
4	J	2	
4	K	2	
4	L	2	
4	O	2	
4	P	2	
4	Q	2	
4	T	2	
4	U	2	
4	V	2	
5	M	4	
5	R	4	
5	W	4	
6	N	3	
6	S	3	
6	X	3	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29262 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	1006	Total	C	N	O	S	0	0
			7813	5009	1297	1472	35		
1	B	1006	Total	C	N	O	S	0	0
			7813	5009	1297	1472	35		
1	C	1006	Total	C	N	O	S	0	0
			7813	5009	1297	1472	35		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	444	THR	LYS	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	682	LYS	ASN	variant	UNP P0DTC2
A	684	HIS	PRO	variant	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	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	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	VAL	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	PHE	-	expression tag	UNP P0DTC2
A	1219	GLN	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	ILE	-	expression tag	UNP P0DTC2
A	1225	PRO	-	expression tag	UNP P0DTC2
A	1226	GLU	-	expression tag	UNP P0DTC2
A	1227	ALA	-	expression tag	UNP P0DTC2
A	1228	PRO	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	ASP	-	expression tag	UNP P0DTC2
A	1231	GLY	-	expression tag	UNP P0DTC2
A	1232	GLN	-	expression tag	UNP P0DTC2
A	1233	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1234	TYR	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	ARG	-	expression tag	UNP P0DTC2
A	1237	LYS	-	expression tag	UNP P0DTC2
A	1238	ASP	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	GLU	-	expression tag	UNP P0DTC2
A	1241	TRP	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	PHE	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	SER	-	expression tag	UNP P0DTC2
A	1246	THR	-	expression tag	UNP P0DTC2
A	1247	PHE	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	444	THR	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	ARG	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	682	LYS	ASN	variant	UNP P0DTC2
B	684	HIS	PRO	variant	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	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	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1214	LEU	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	VAL	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	PHE	-	expression tag	UNP P0DTC2
B	1219	GLN	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	ILE	-	expression tag	UNP P0DTC2
B	1225	PRO	-	expression tag	UNP P0DTC2
B	1226	GLU	-	expression tag	UNP P0DTC2
B	1227	ALA	-	expression tag	UNP P0DTC2
B	1228	PRO	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1230	ASP	-	expression tag	UNP P0DTC2
B	1231	GLY	-	expression tag	UNP P0DTC2
B	1232	GLN	-	expression tag	UNP P0DTC2
B	1233	ALA	-	expression tag	UNP P0DTC2
B	1234	TYR	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	ARG	-	expression tag	UNP P0DTC2
B	1237	LYS	-	expression tag	UNP P0DTC2
B	1238	ASP	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	GLU	-	expression tag	UNP P0DTC2
B	1241	TRP	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	PHE	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	SER	-	expression tag	UNP P0DTC2
B	1246	THR	-	expression tag	UNP P0DTC2
B	1247	PHE	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	444	THR	LYS	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	682	LYS	ASN	variant	UNP P0DTC2
C	684	HIS	PRO	variant	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	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	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1214	LEU	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	VAL	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	PHE	-	expression tag	UNP P0DTC2
C	1219	GLN	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	ILE	-	expression tag	UNP P0DTC2
C	1225	PRO	-	expression tag	UNP P0DTC2

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

- Molecule 2 is a protein called MO11 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	123	Total	C	N	O	S	0	0
			923	590	152	178	3		
2	F	123	Total	C	N	O	S	0	0
			923	590	152	178	3		
2	H	123	Total	C	N	O	S	0	0
			923	590	152	178	3		

- Molecule 3 is a protein called MO11 light chain.

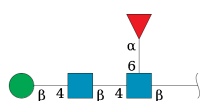
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	103	Total	C	N	O	S	0	0
			749	468	132	147	2		
3	G	103	Total	C	N	O	S	0	0
			749	468	132	147	2		
3	I	103	Total	C	N	O	S	0	0
			749	468	132	147	2		

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



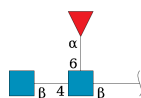
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		

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



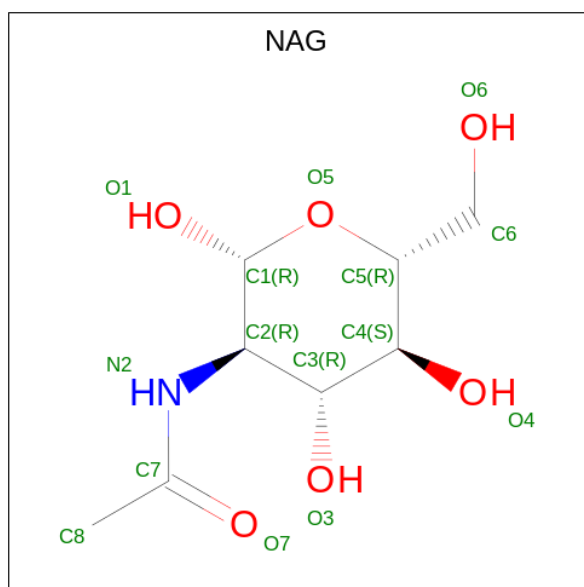
Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	4	Total	C	N	O	0	0
			49	28	2	19		
5	R	4	Total	C	N	O	0	0
			49	28	2	19		
5	W	4	Total	C	N	O	0	0
			49	28	2	19		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	3	Total	C	N	O	0	0
			38	22	2	14		
6	S	3	Total	C	N	O	0	0
			38	22	2	14		
6	X	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

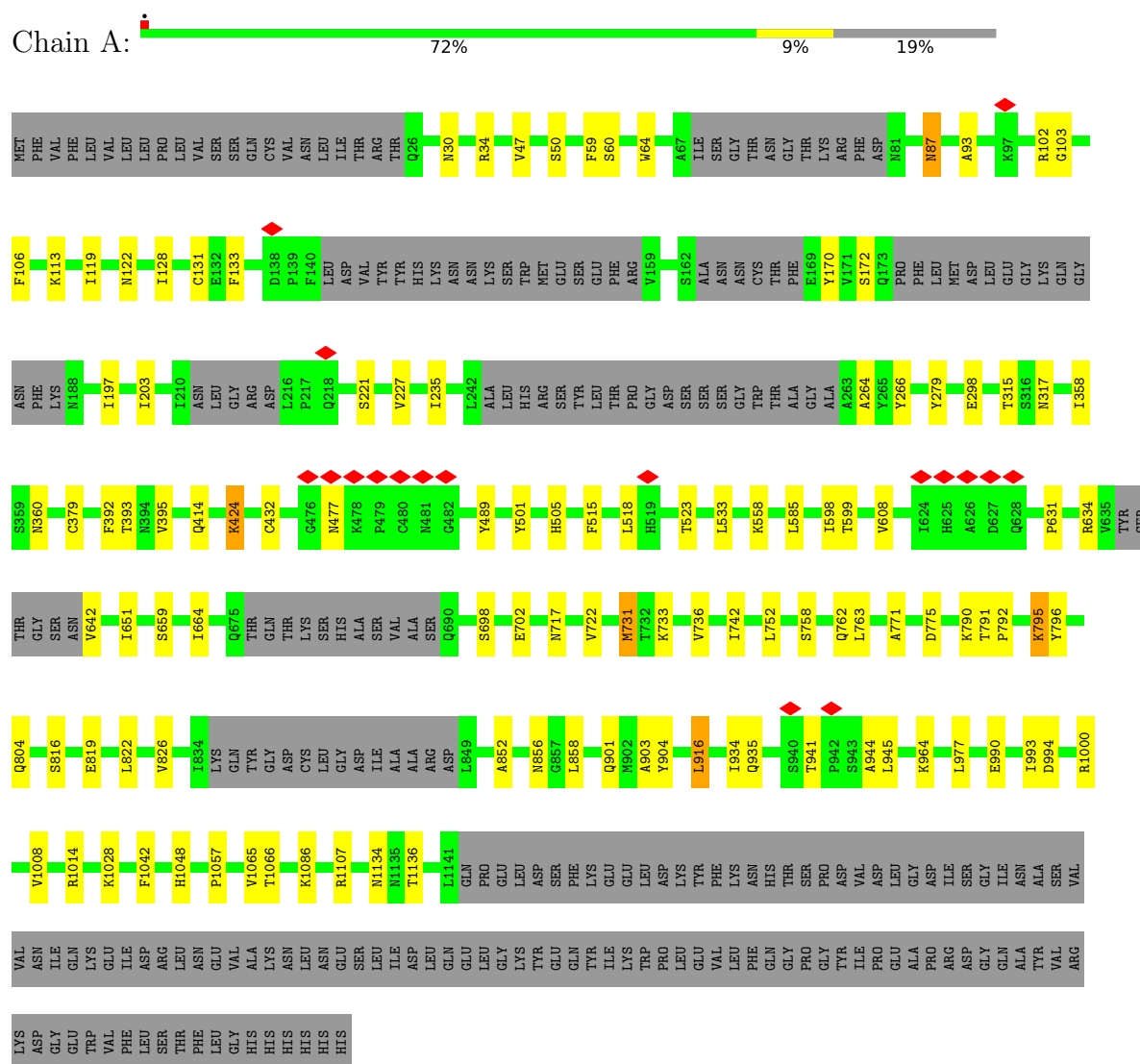


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	B	1	Total	C	N	O	0
			14	8	1	5	
7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

3 Residue-property plots

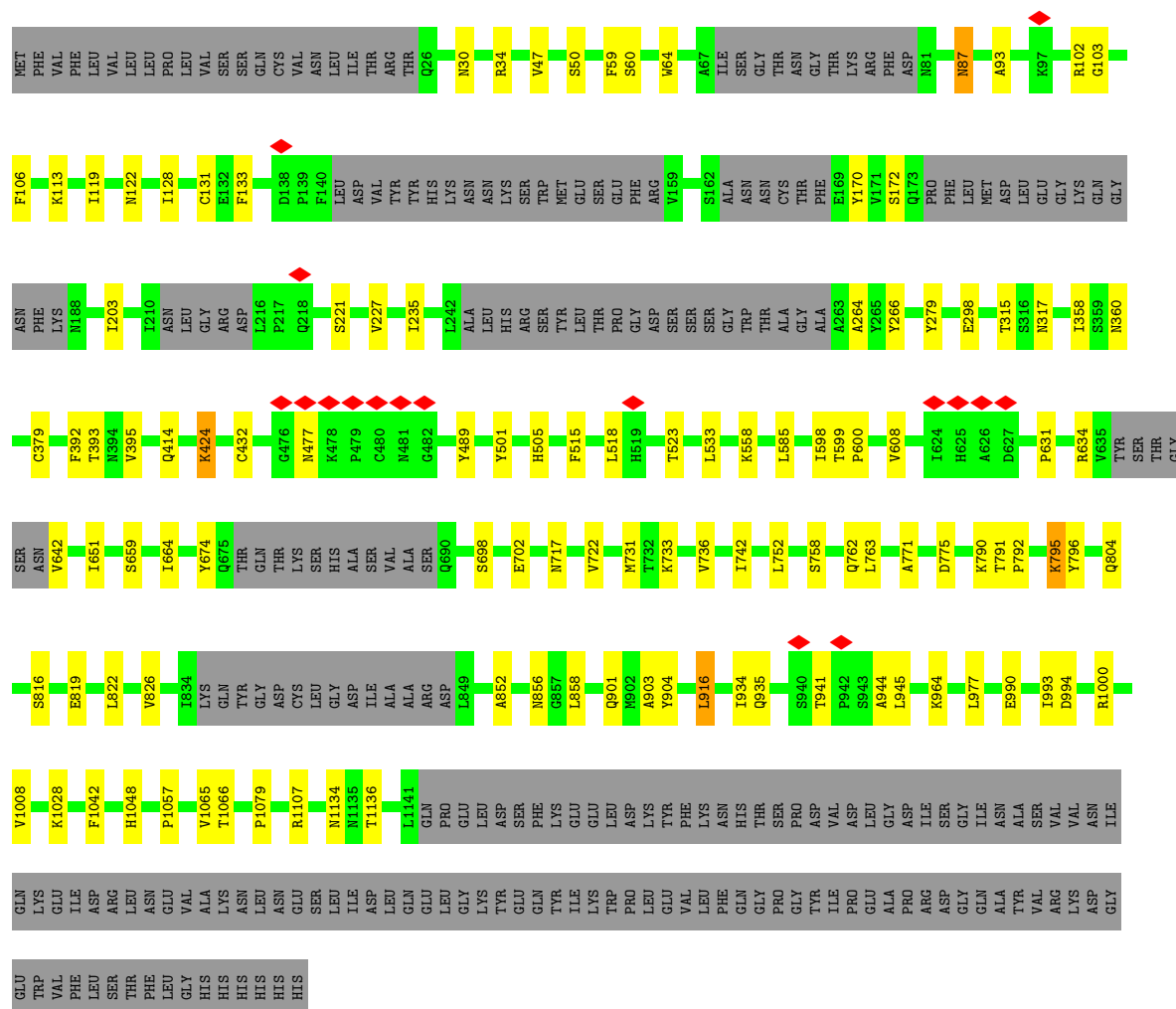
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein



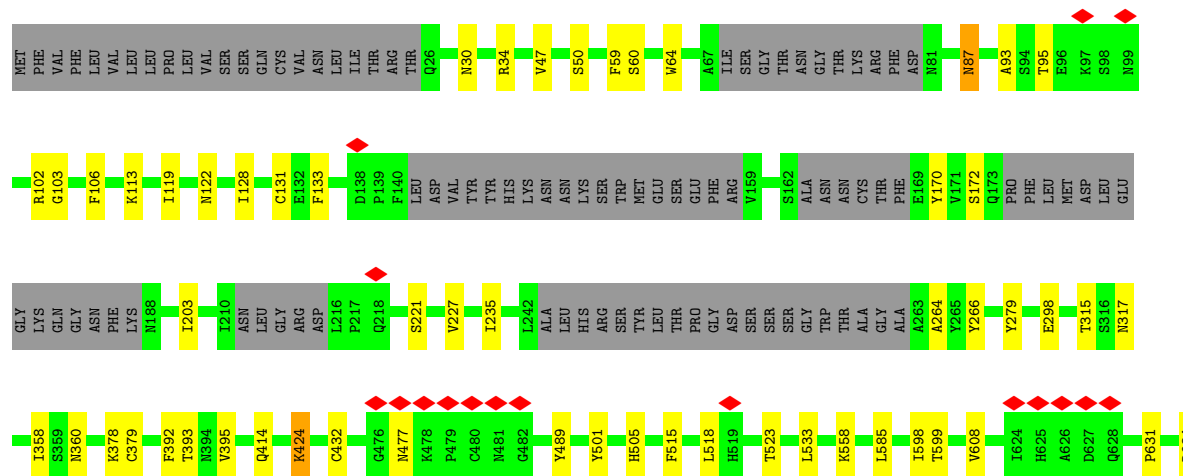
• Molecule 1: Spike glycoprotein





- Molecule 1: Spike glycoprotein

Chain C:



GLY
THR
GLN
THR
TYR
ILE
CYS
ASN
VAL
ASN
HIS
LYS
LYS
PRO
SER
ASN
THR
LYS
VAL
ASP
LYS
LYS
VAL
GLU
PRO
LYS
SER
CYS
ASP
LYS
THR
HIS

• Molecule 3: MO11 light chain

Chain E:  45% 52%

SER
Y3
G16
LYS
T18
N26
W35
A40
G41
I48
S63
A80
G81
C88
V96
G99
L104
ILE
VAL
GLY
GLN
ASN
PRO
LYS
ALA
ALA
PRO
SER
SER
VAL
THR
LEU
PHE
PRO
PRO
SER
SER
GLU
GLU
TRP
LYS
GLN
HIS
ALA
ASN
LYS
TYR
SER
THR
CYS
VAL
LEU

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

THR
HIS
GLU
GLY
SER
THR
VAL
GLU
LYS
THR
VAL
VAL
PRO
THR
GLU
CYS
SER

• Molecule 3: MO11 light chain

Chain G:  45% 52%

SER
Y3
G16
LYS
T18
N26
W35
G41
I48
S63
A80
G81
C88
V96
G99
L104
ILE
VAL
LEU
GLY
GLN
SER
PRO
LYS
ALA
ALA
PRO
SER
SER
VAL
THR
LEU
PHE
PRO
PRO
SER
SER
GLU
GLU
LEU
GLN
SER
HIS
ARG
LYS
ALA
THR
SER
CYS
GLN
VAL
THR
ILE

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

HIS
GLU
GLY
SER
THR
VAL
GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

• Molecule 3: MO11 light chain

Chain I:  46% 52%

SER
Y3
G16
LYS
T18
N26
W35
G41
I48
S63
A80
G81
C88
G99
L104
ILE
VAL
LEU
GLY
GLN
PRO
LYS
LYS
ALA
ALA
PRO
SER
SER
VAL
THR
PHE
PRO
PRO
SER
SER
GLU
GLN
TRP
LYS
HIS
ARG
LYS
ALA
THR
CYS
VAL
CYS
THR
HIS
ILE
SER
ASP

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

GLY
SER
THR
VAL
GLY
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

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

Chain J:  50% 50%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain L:  50%  50%

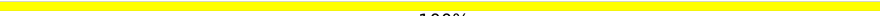
MAG1
MAG2

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

Chain O:  50%  50%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  50%  50%

MAG1
MAG2

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

Chain T:  50%  50%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain V: 



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	246238	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	360.96, 360.96, 360.96	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	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: FUC, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/7997	0.47	0/10897
1	B	0.26	0/7997	0.47	0/10897
1	C	0.26	0/7997	0.47	0/10897
2	D	0.25	0/947	0.48	0/1286
2	F	0.25	0/947	0.48	0/1286
2	H	0.25	0/947	0.48	0/1286
3	E	0.24	0/767	0.47	0/1048
3	G	0.24	0/767	0.48	0/1048
3	I	0.24	0/767	0.48	0/1048
All	All	0.26	0/29133	0.47	0/39693

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	7813	0	7597	57	0
1	B	7813	0	7597	55	0
1	C	7813	0	7597	58	0
2	D	923	0	878	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	923	0	878	6	0
2	H	923	0	878	5	0
3	E	749	0	684	3	0
3	G	749	0	684	3	0
3	I	749	0	684	2	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
4	V	28	0	25	0	0
5	M	49	0	43	1	0
5	R	49	0	43	1	0
5	W	49	0	43	1	0
6	N	38	0	34	0	0
6	S	38	0	34	0	0
6	X	38	0	34	0	0
7	A	98	0	91	1	0
7	B	98	0	91	1	0
7	C	98	0	91	1	0
All	All	29262	0	28206	188	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 3.

The worst 5 of 188 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:87:ASN:OD1	1:A:87:ASN:N	2.24	0.68
3:E:35:TRP:HB2	3:E:48:ILE:HB	1.76	0.68
3:I:35:TRP:HB2	3:I:48:ILE:HB	1.76	0.67
1:A:360:ASN:H	1:A:523:THR:HB	1.60	0.67
1:C:360:ASN:H	1:C:523:THR:HB	1.60	0.66

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	986/1247 (79%)	966 (98%)	20 (2%)	0	100	100
1	B	986/1247 (79%)	966 (98%)	20 (2%)	0	100	100
1	C	986/1247 (79%)	966 (98%)	20 (2%)	0	100	100
2	D	121/232 (52%)	118 (98%)	3 (2%)	0	100	100
2	F	121/232 (52%)	118 (98%)	3 (2%)	0	100	100
2	H	121/232 (52%)	118 (98%)	3 (2%)	0	100	100
3	E	99/214 (46%)	96 (97%)	3 (3%)	0	100	100
3	G	99/214 (46%)	96 (97%)	3 (3%)	0	100	100
3	I	99/214 (46%)	96 (97%)	3 (3%)	0	100	100
All	All	3618/5079 (71%)	3540 (98%)	78 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	864/1088 (79%)	844 (98%)	20 (2%)	50	67
1	B	864/1088 (79%)	844 (98%)	20 (2%)	50	67
1	C	864/1088 (79%)	844 (98%)	20 (2%)	50	67
2	D	96/194 (50%)	92 (96%)	4 (4%)	30	42
2	F	96/194 (50%)	92 (96%)	4 (4%)	30	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	96/194 (50%)	92 (96%)	4 (4%)	30	42
3	E	75/179 (42%)	74 (99%)	1 (1%)	69	82
3	G	75/179 (42%)	74 (99%)	1 (1%)	69	82
3	I	75/179 (42%)	74 (99%)	1 (1%)	69	82
All	All	3105/4383 (71%)	3030 (98%)	75 (2%)	51	66

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1107	ARG
2	H	35	SER
1	C	1136	THR
2	F	21	SER
1	B	317	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	1	4,1	14,14,15	0.65	0	17,19,21	1.40	2 (11%)
4	NAG	J	2	4	14,14,15	0.73	0	17,19,21	0.93	0
4	NAG	K	1	4,1	14,14,15	0.71	0	17,19,21	1.01	2 (11%)
4	NAG	K	2	4	14,14,15	0.70	0	17,19,21	0.87	1 (5%)
4	NAG	L	1	4,1	14,14,15	0.72	0	17,19,21	1.41	1 (5%)
4	NAG	L	2	4	14,14,15	0.74	0	17,19,21	0.83	0
5	NAG	M	1	5,1	14,14,15	1.13	1 (7%)	17,19,21	1.17	1 (5%)
5	NAG	M	2	5	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
5	BMA	M	3	5	11,11,12	0.83	0	15,15,17	1.78	1 (6%)
5	FUC	M	4	5	10,10,11	0.80	0	14,14,16	1.00	0
6	NAG	N	1	6,1	14,14,15	0.73	0	17,19,21	1.34	2 (11%)
6	NAG	N	2	6	14,14,15	0.74	0	17,19,21	0.88	0
6	FUC	N	3	6	10,10,11	0.82	0	14,14,16	0.95	0
4	NAG	O	1	4,1	14,14,15	0.65	0	17,19,21	1.40	2 (11%)
4	NAG	O	2	4	14,14,15	0.73	0	17,19,21	0.93	0
4	NAG	P	1	4,1	14,14,15	0.71	0	17,19,21	1.01	2 (11%)
4	NAG	P	2	4	14,14,15	0.70	0	17,19,21	0.87	1 (5%)
4	NAG	Q	1	4,1	14,14,15	0.72	0	17,19,21	1.41	1 (5%)
4	NAG	Q	2	4	14,14,15	0.75	0	17,19,21	0.83	0
5	NAG	R	1	5,1	14,14,15	1.13	1 (7%)	17,19,21	1.17	1 (5%)
5	NAG	R	2	5	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
5	BMA	R	3	5	11,11,12	0.83	0	15,15,17	1.78	1 (6%)
5	FUC	R	4	5	10,10,11	0.80	0	14,14,16	1.01	0
6	NAG	S	1	6,1	14,14,15	0.73	0	17,19,21	1.34	2 (11%)
6	NAG	S	2	6	14,14,15	0.74	0	17,19,21	0.88	0
6	FUC	S	3	6	10,10,11	0.82	0	14,14,16	0.95	0
4	NAG	T	1	4,1	14,14,15	0.65	0	17,19,21	1.40	2 (11%)
4	NAG	T	2	4	14,14,15	0.73	0	17,19,21	0.93	0
4	NAG	U	1	4,1	14,14,15	0.71	0	17,19,21	1.01	2 (11%)
4	NAG	U	2	4	14,14,15	0.70	0	17,19,21	0.87	1 (5%)
4	NAG	V	1	4,1	14,14,15	0.72	0	17,19,21	1.41	1 (5%)
4	NAG	V	2	4	14,14,15	0.75	0	17,19,21	0.83	0
5	NAG	W	1	5,1	14,14,15	1.13	1 (7%)	17,19,21	1.17	1 (5%)
5	NAG	W	2	5	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
5	BMA	W	3	5	11,11,12	0.83	0	15,15,17	1.78	1 (6%)
5	FUC	W	4	5	10,10,11	0.80	0	14,14,16	1.00	0
6	NAG	X	1	6,1	14,14,15	0.73	0	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	X	2	6	14,14,15	0.74	0	17,19,21	0.88	0
6	FUC	X	3	6	10,10,11	0.82	0	14,14,16	0.95	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	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	BMA	M	3	5	-	1/2/19/22	0/1/1/1
5	FUC	M	4	5	-	-	0/1/1/1
6	NAG	N	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	FUC	N	3	6	-	-	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	1/6/23/26	0/1/1/1
5	BMA	R	3	5	-	1/2/19/22	0/1/1/1
5	FUC	R	4	5	-	-	0/1/1/1
6	NAG	S	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	FUC	S	3	6	-	-	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	1/6/23/26	0/1/1/1
5	BMA	W	3	5	-	1/2/19/22	0/1/1/1
5	FUC	W	4	5	-	-	0/1/1/1
6	NAG	X	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	FUC	X	3	6	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	C1-C2	3.01	1.56	1.52
5	R	1	NAG	C1-C2	3.01	1.56	1.52
5	W	1	NAG	C1-C2	3.01	1.56	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	3	BMA	C1-O5-C5	5.30	119.37	112.19
5	M	3	BMA	C1-O5-C5	5.30	119.37	112.19
5	W	3	BMA	C1-O5-C5	5.29	119.36	112.19
4	L	1	NAG	C1-O5-C5	5.19	119.23	112.19
4	Q	1	NAG	C1-O5-C5	5.19	119.23	112.19

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

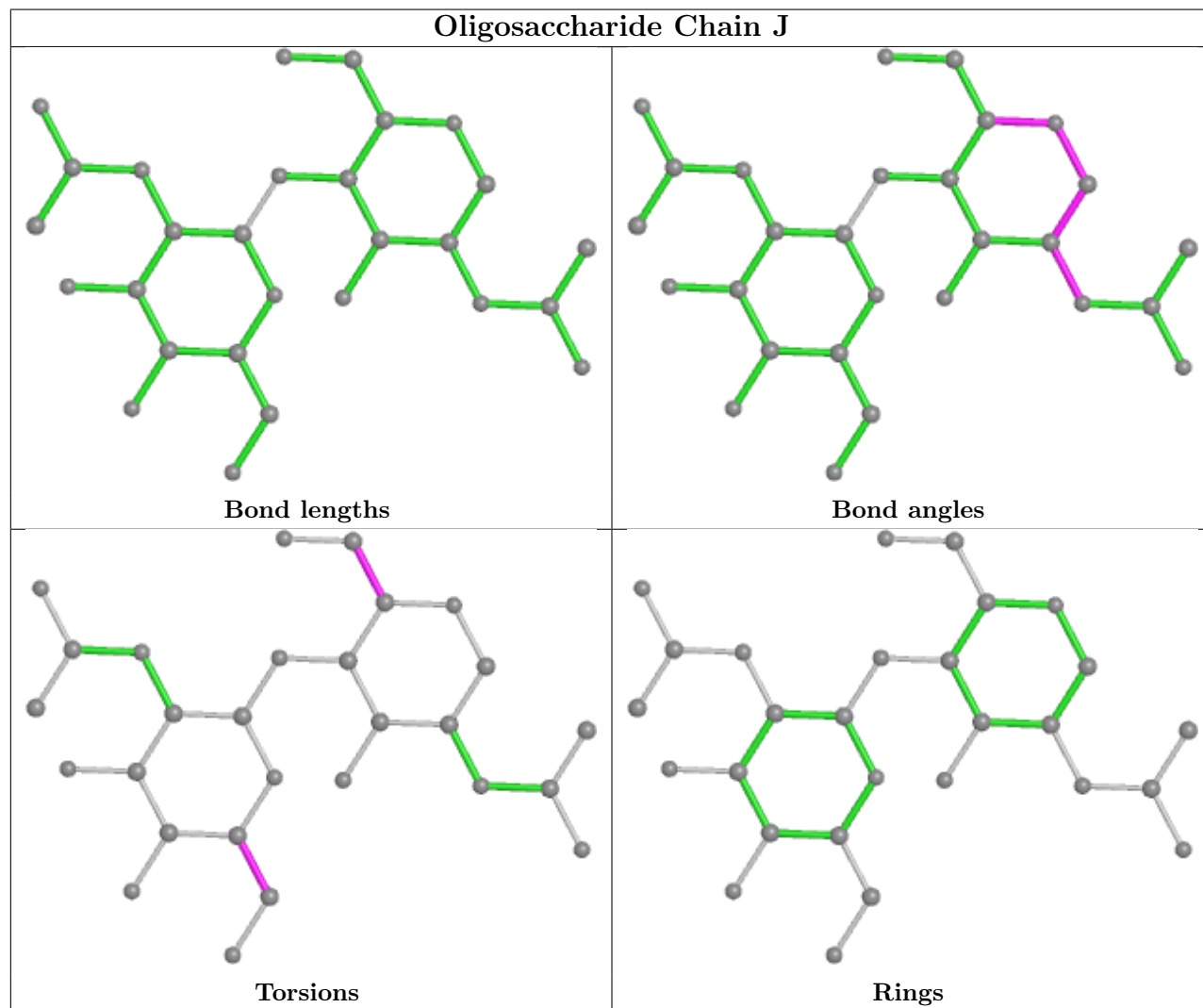
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	W	1	NAG	1	0

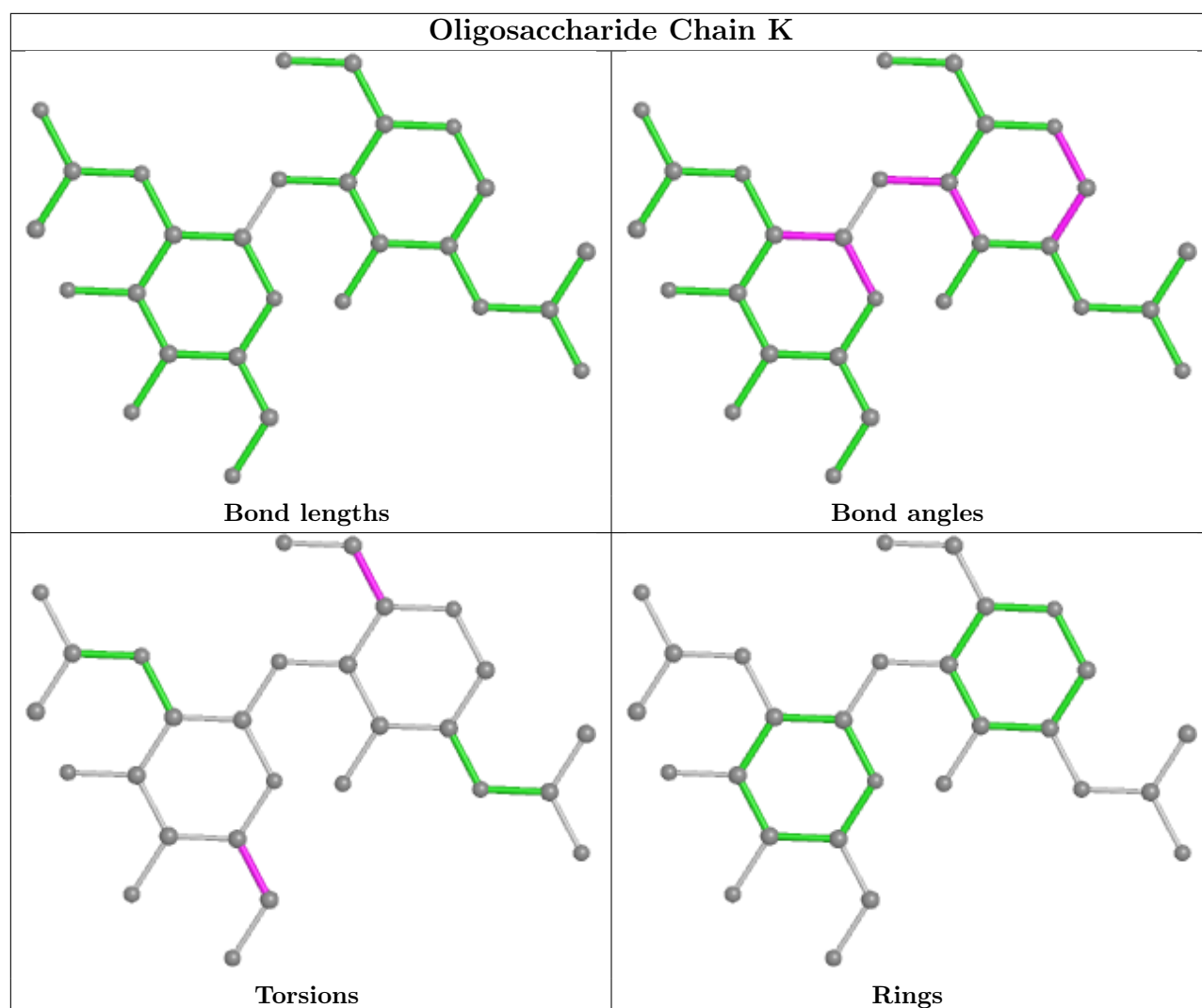
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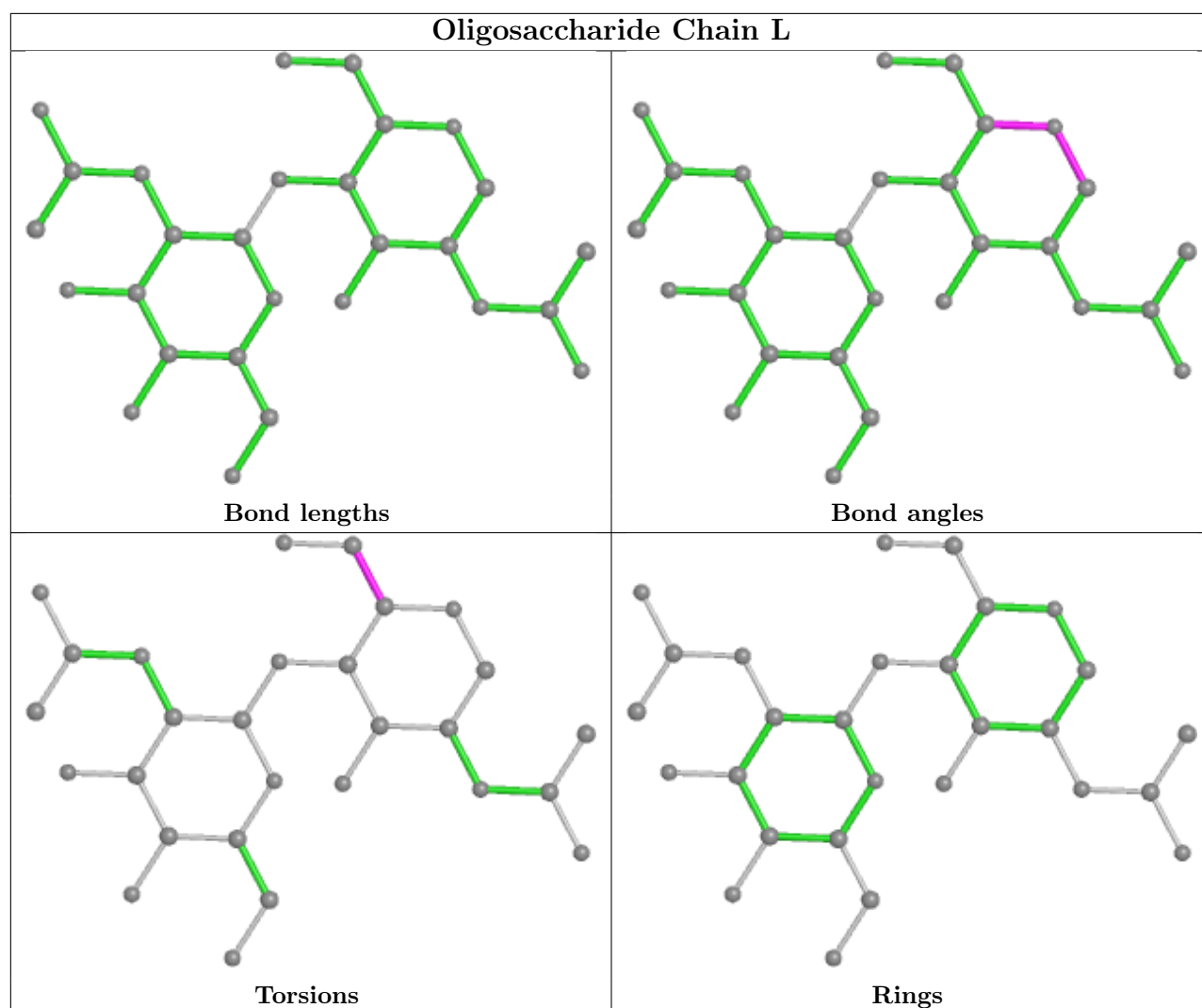
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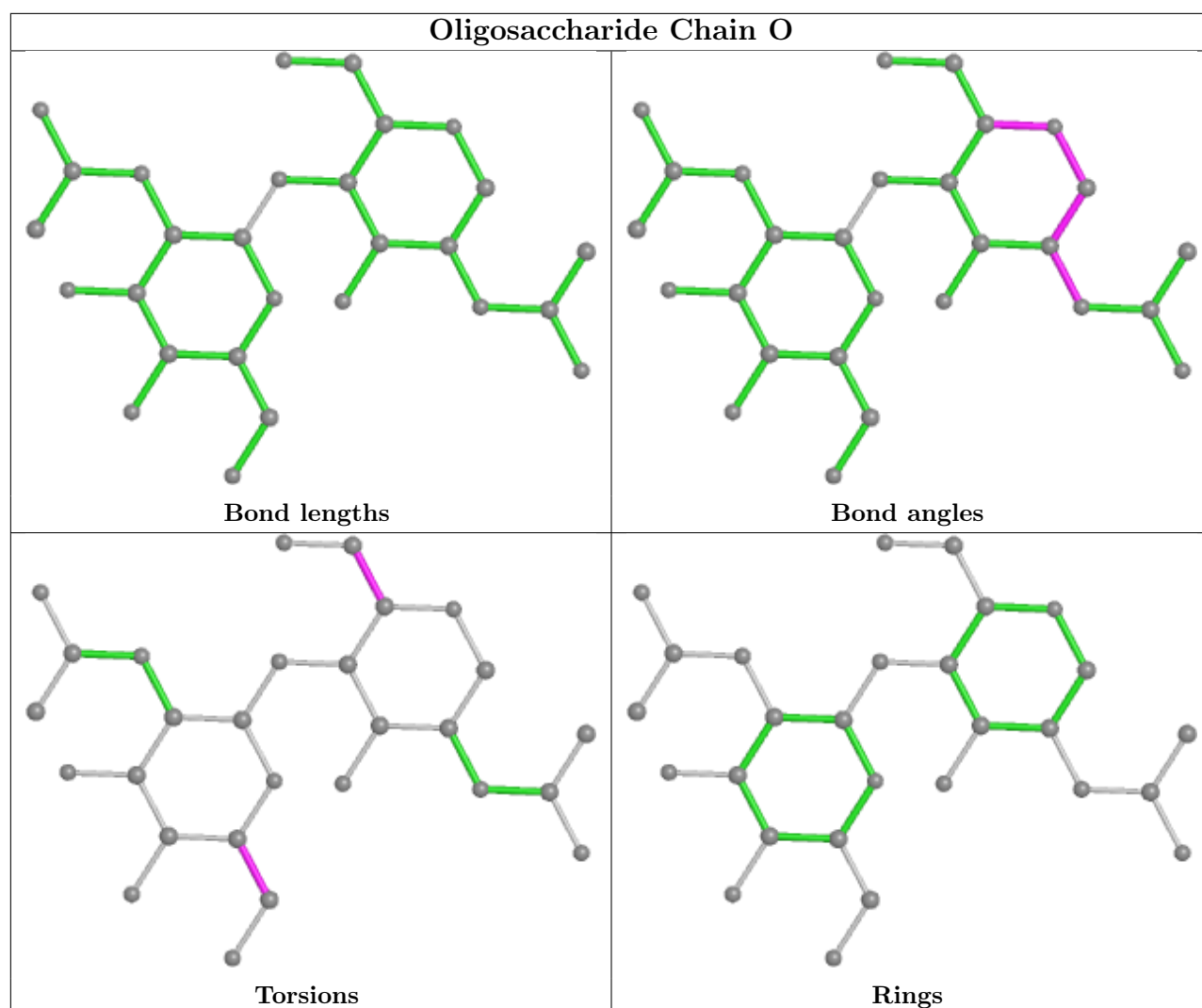
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1	NAG	1	0
5	R	1	NAG	1	0

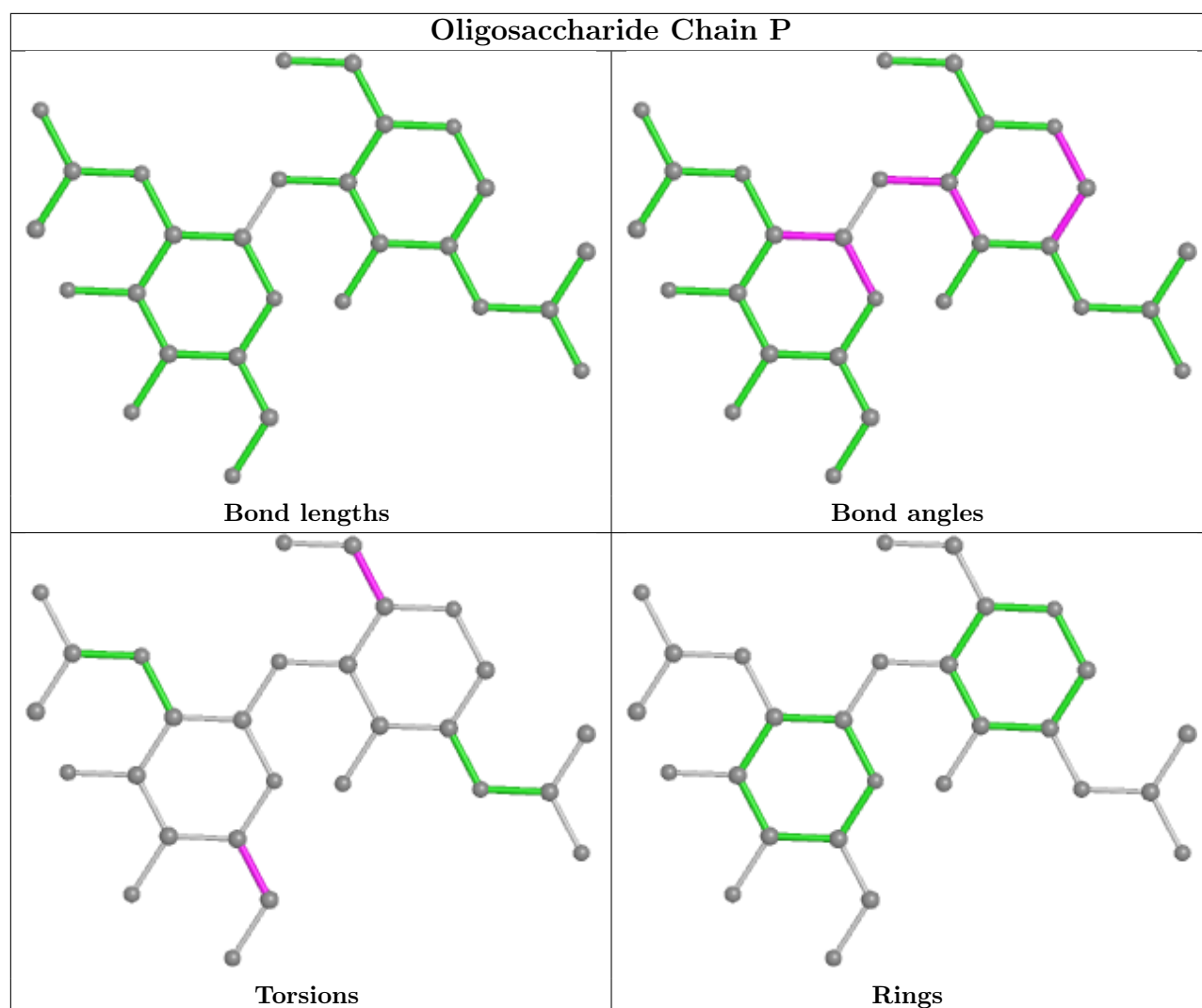
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

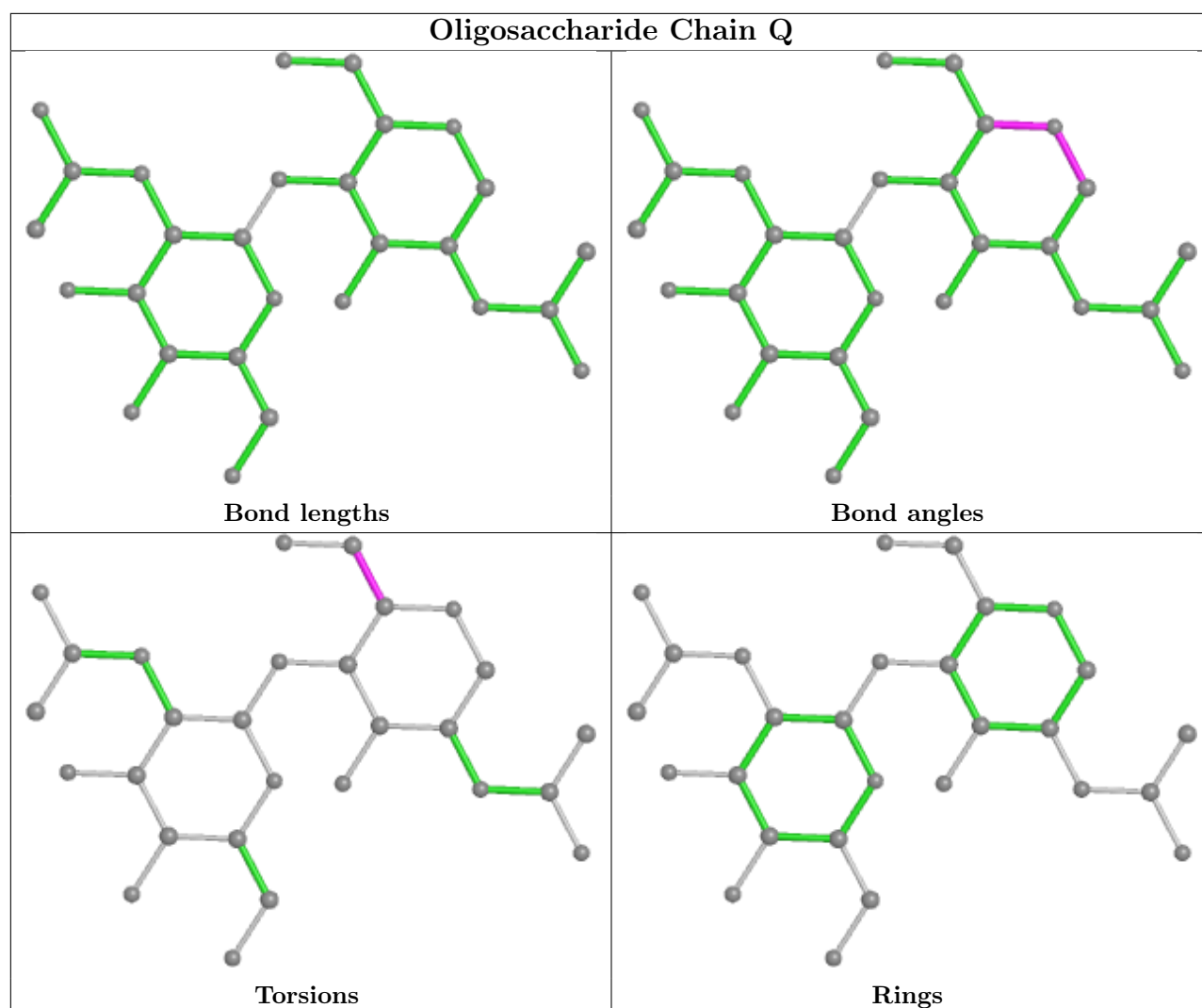


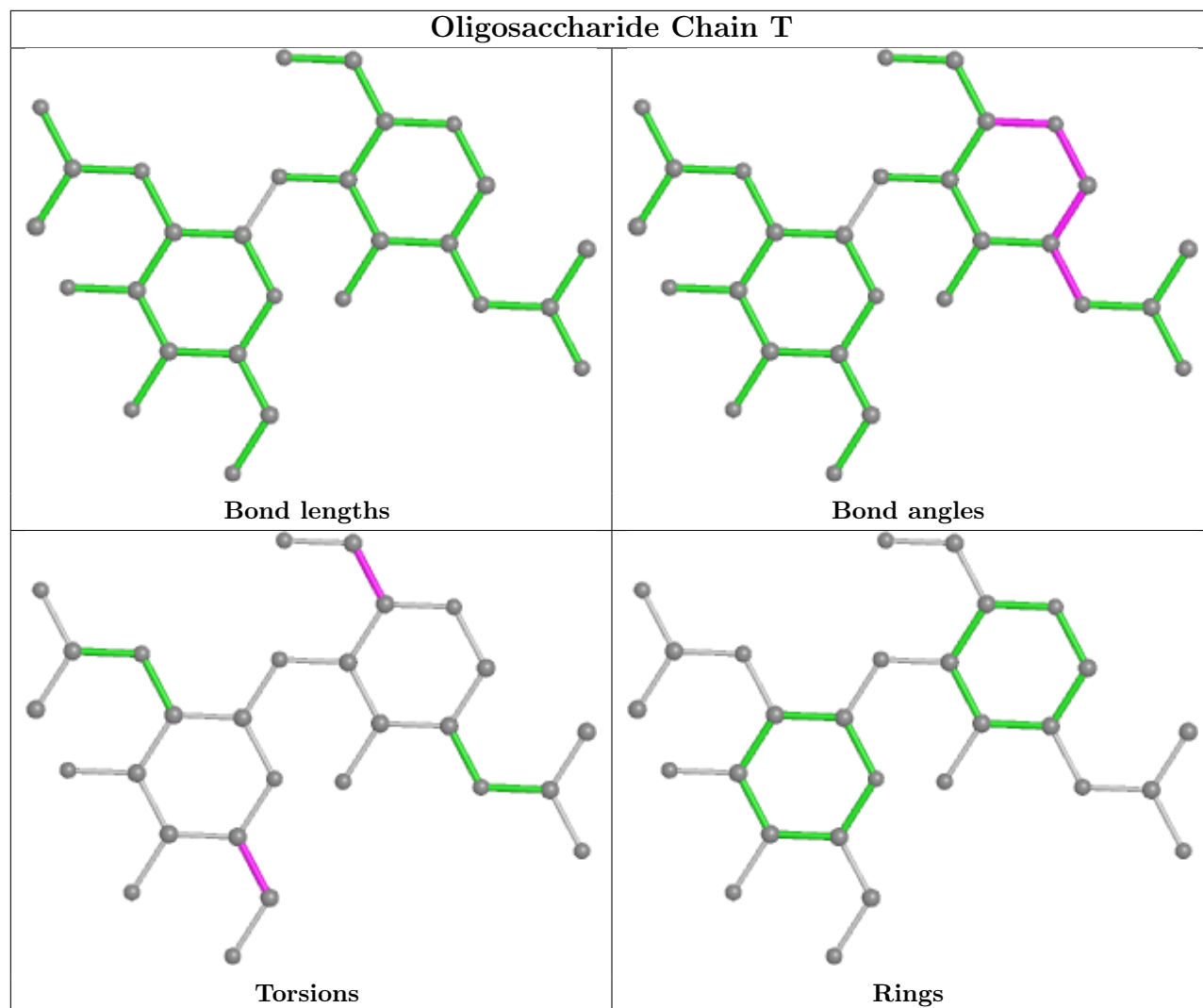


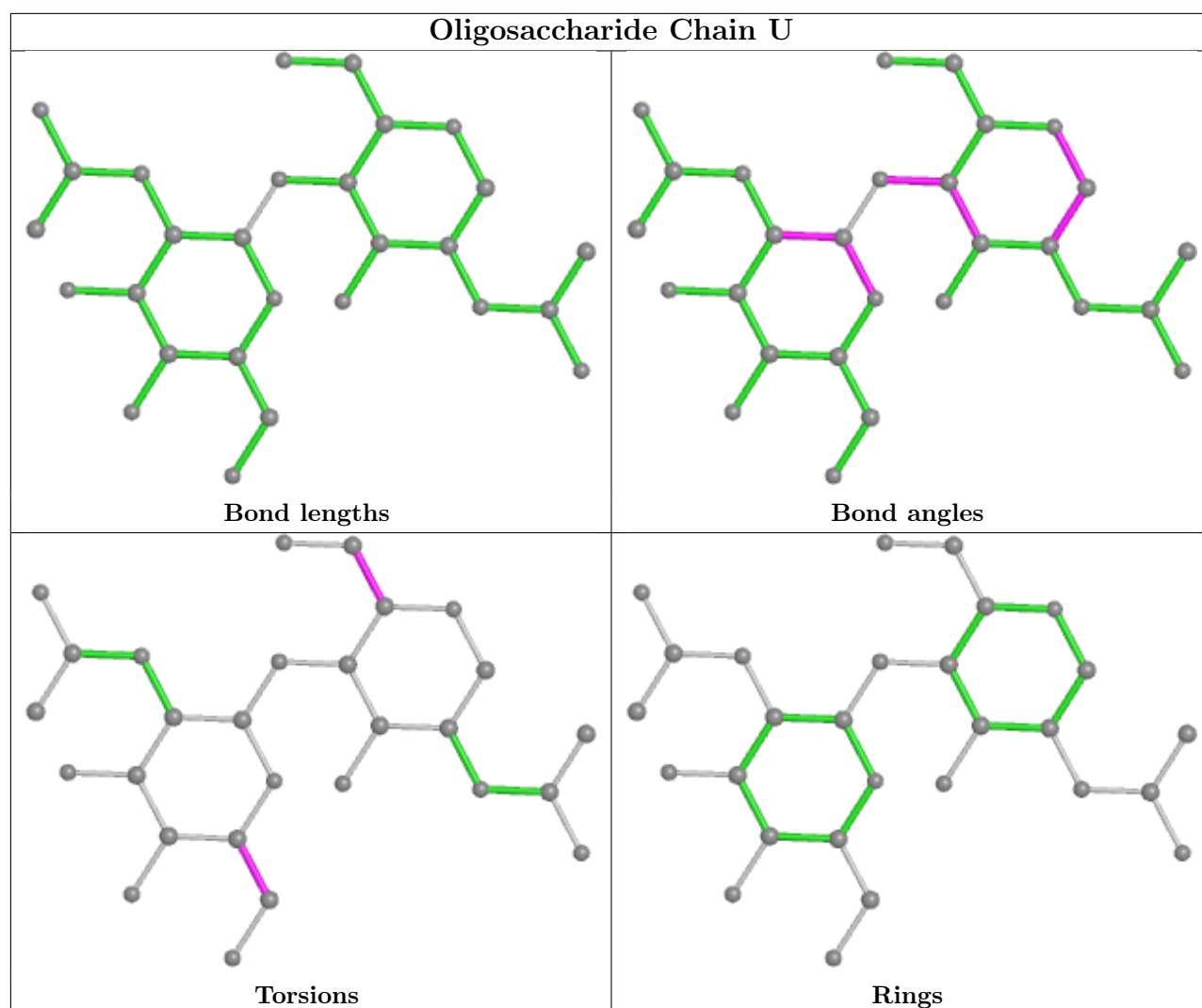


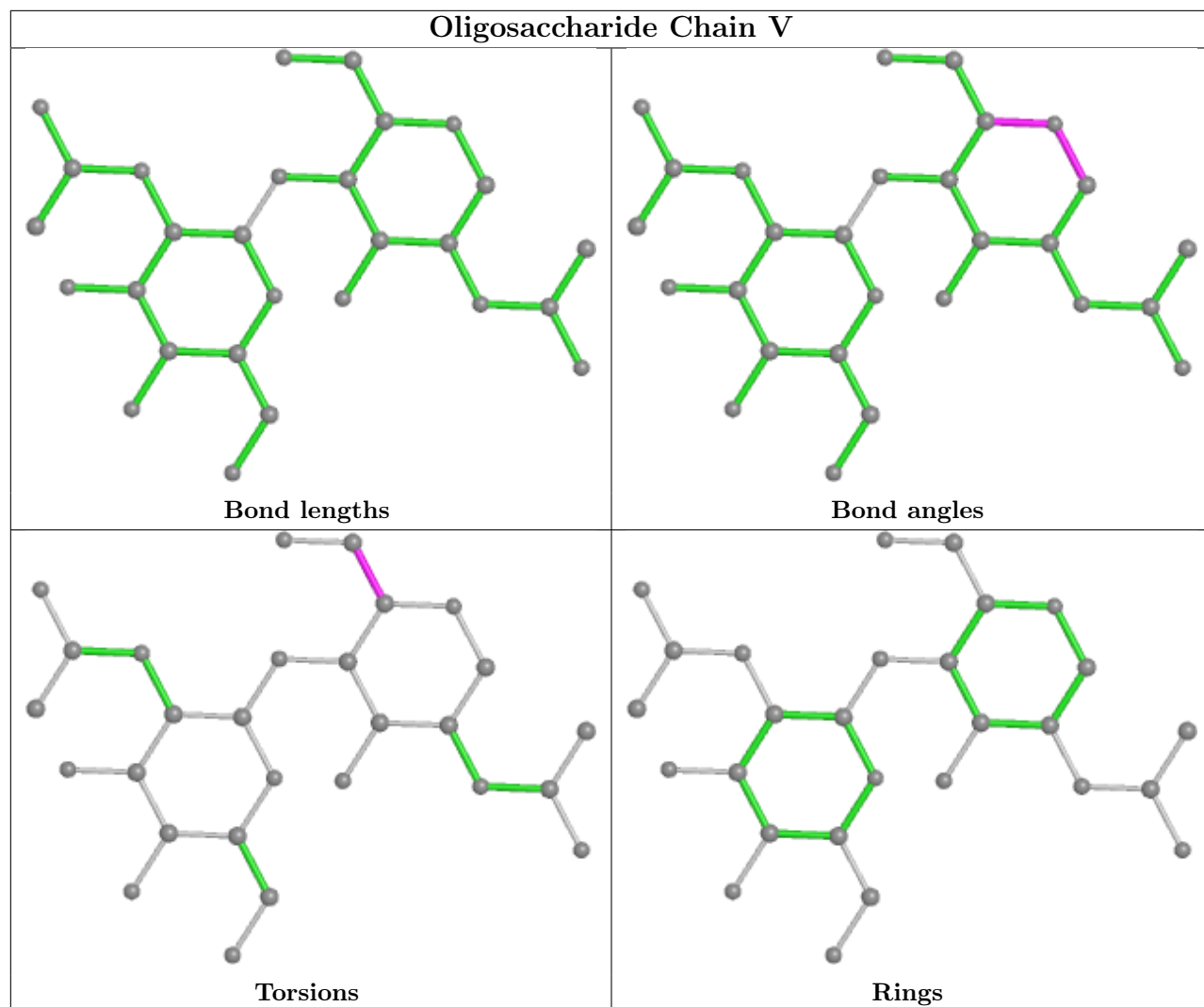


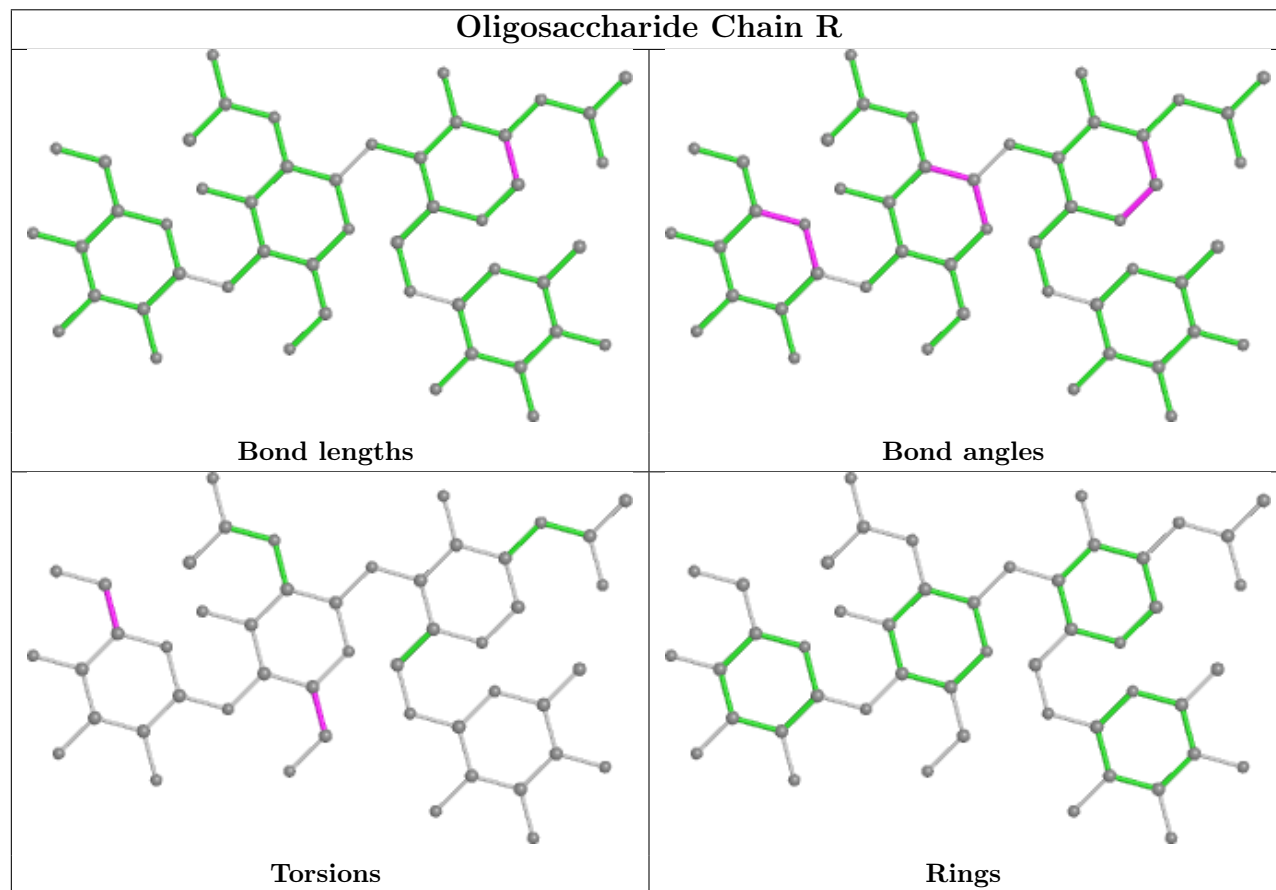
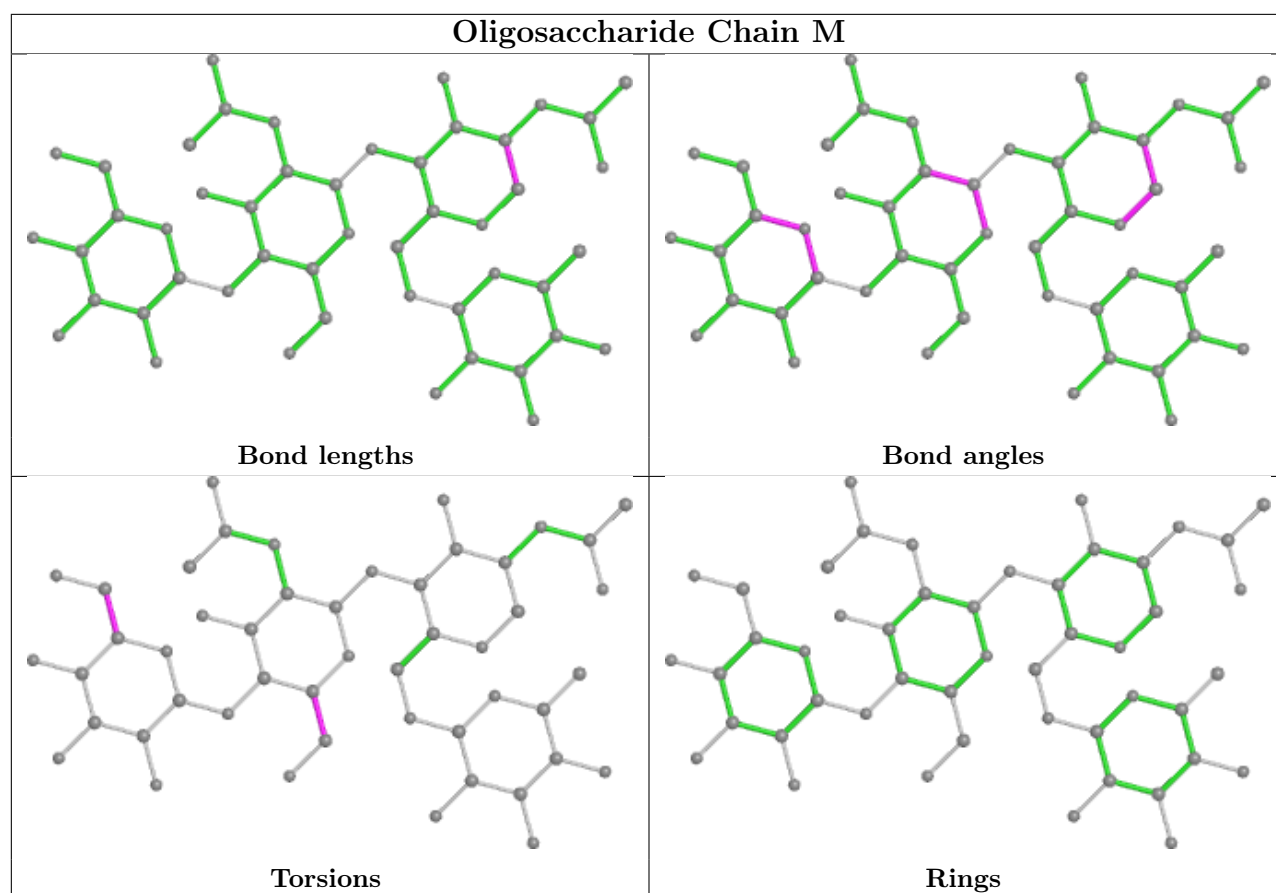


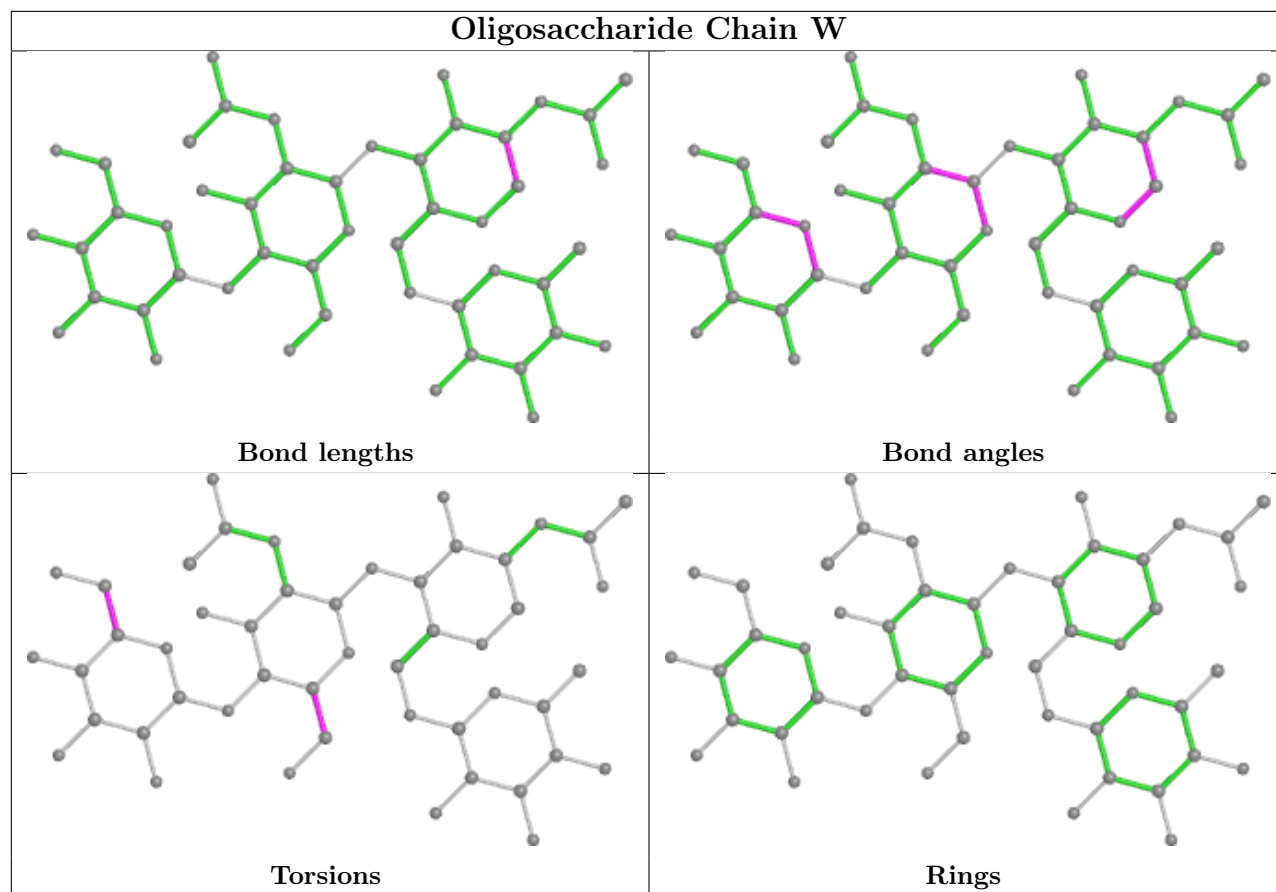


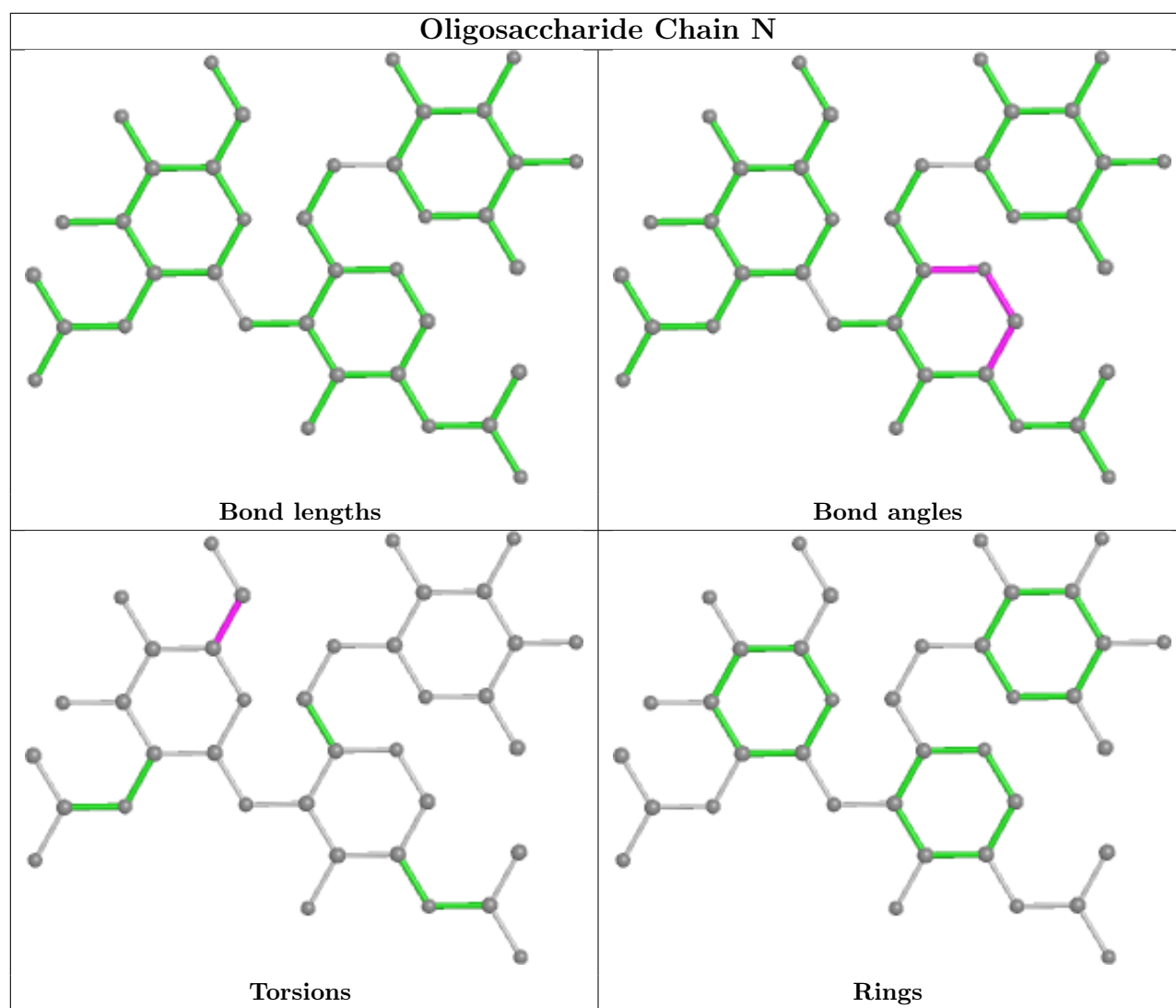


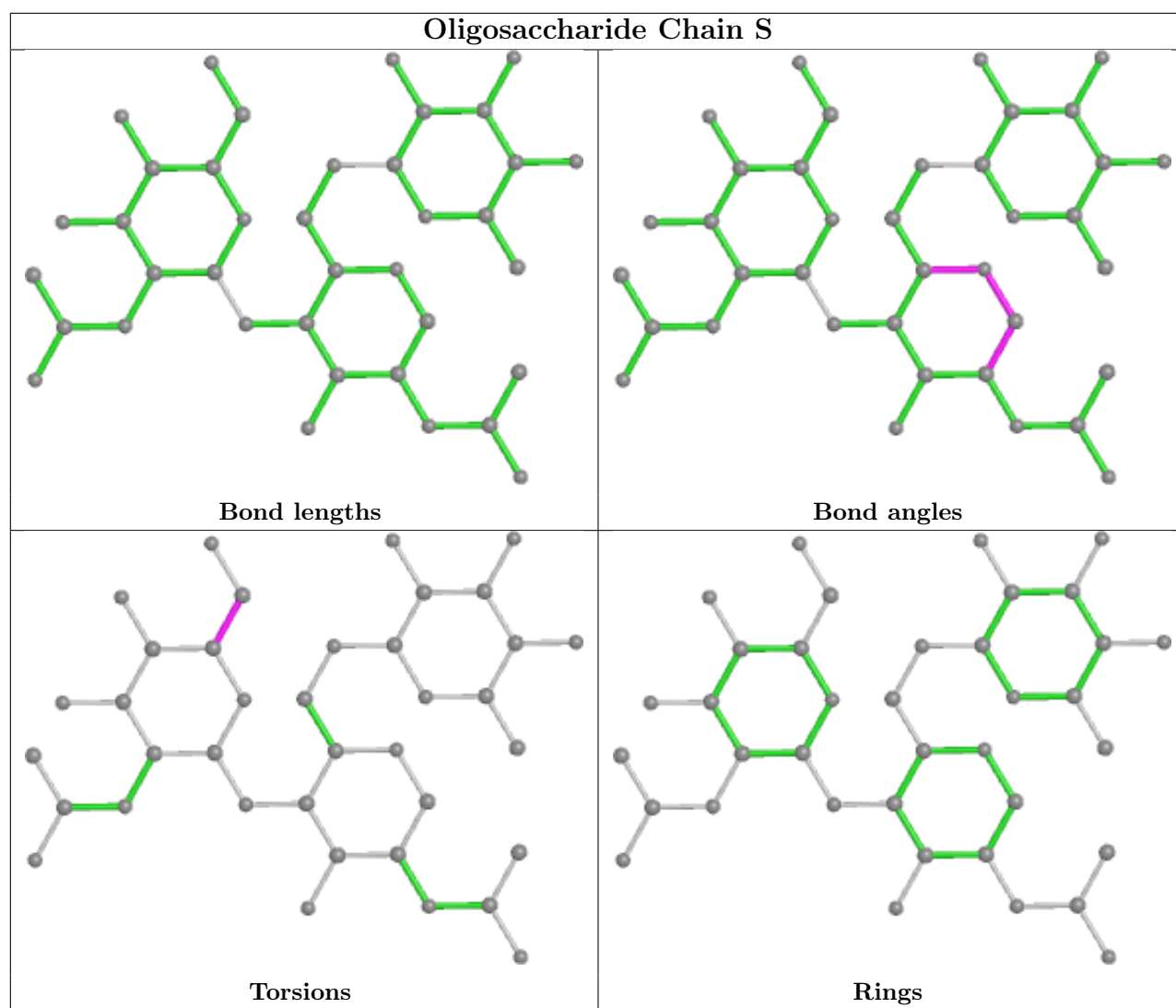


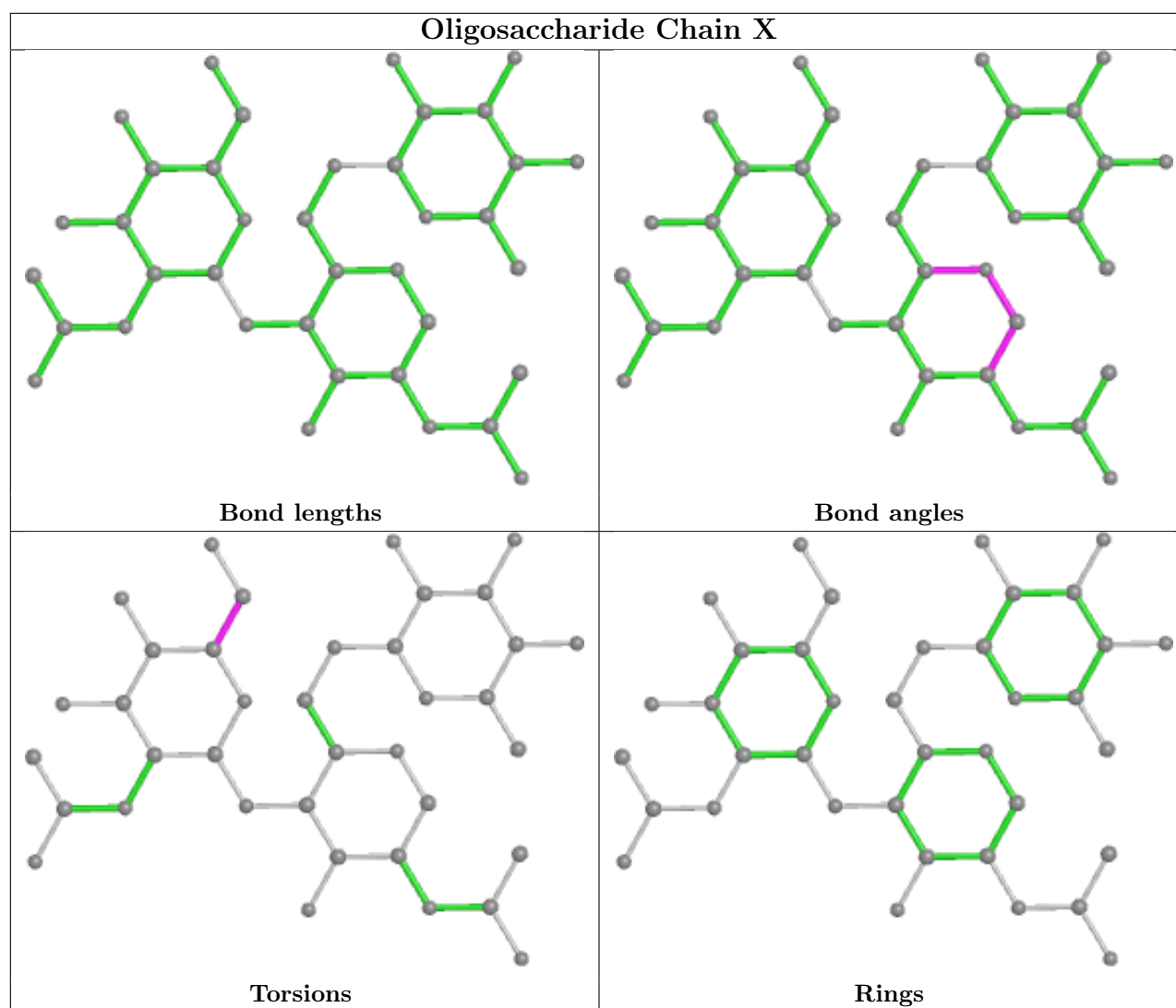












5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	C	1306	1	14,14,15	0.73	0	17,19,21	0.84	0
7	NAG	B	1303	1	14,14,15	0.68	0	17,19,21	1.21	1 (5%)
7	NAG	C	1307	1	14,14,15	0.67	0	17,19,21	1.49	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1302	1	14,14,15	0.69	0	17,19,21	0.84	0
7	NAG	B	1304	1	14,14,15	0.69	0	17,19,21	1.29	2 (11%)
7	NAG	B	1301	1	14,14,15	0.69	0	17,19,21	1.22	1 (5%)
7	NAG	C	1303	1	14,14,15	0.68	0	17,19,21	1.21	1 (5%)
7	NAG	A	1302	1	14,14,15	0.69	0	17,19,21	0.84	0
7	NAG	B	1306	1	14,14,15	0.72	0	17,19,21	0.84	0
7	NAG	A	1301	1	14,14,15	0.68	0	17,19,21	1.22	1 (5%)
7	NAG	C	1305	1	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	A	1306	1	14,14,15	0.72	0	17,19,21	0.84	0
7	NAG	C	1302	1	14,14,15	0.69	0	17,19,21	0.84	0
7	NAG	B	1307	1	14,14,15	0.67	0	17,19,21	1.49	2 (11%)
7	NAG	B	1305	1	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	C	1301	1	14,14,15	0.68	0	17,19,21	1.22	1 (5%)
7	NAG	A	1303	1	14,14,15	0.68	0	17,19,21	1.21	1 (5%)
7	NAG	C	1304	1	14,14,15	0.69	0	17,19,21	1.29	2 (11%)
7	NAG	A	1307	1	14,14,15	0.67	0	17,19,21	1.49	2 (11%)
7	NAG	A	1305	1	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	A	1304	1	14,14,15	0.69	0	17,19,21	1.29	2 (11%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1301	NAG	C1-O5-C5	4.08	117.73	112.19
7	A	1301	NAG	C1-O5-C5	4.08	117.72	112.19
7	C	1301	NAG	C1-O5-C5	4.08	117.72	112.19
7	A	1303	NAG	C1-O5-C5	3.95	117.54	112.19
7	C	1303	NAG	C1-O5-C5	3.95	117.54	112.19

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1303	NAG	O5-C5-C6-O6
7	B	1303	NAG	O5-C5-C6-O6
7	C	1303	NAG	O5-C5-C6-O6
7	A	1301	NAG	O5-C5-C6-O6
7	B	1301	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1307	NAG	1	0
7	B	1307	NAG	1	0
7	A	1307	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.

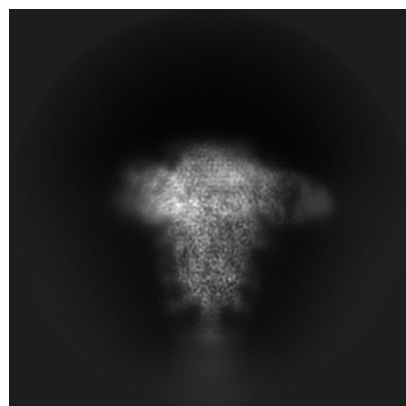
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38372. These allow visual inspection of the internal detail of the map and identification of artifacts.

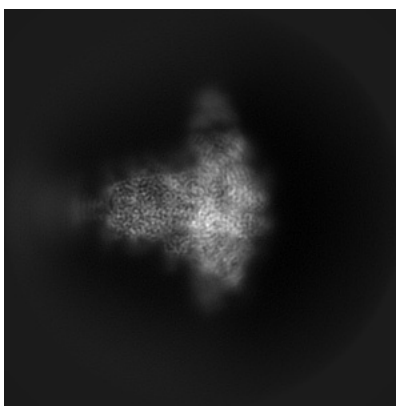
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

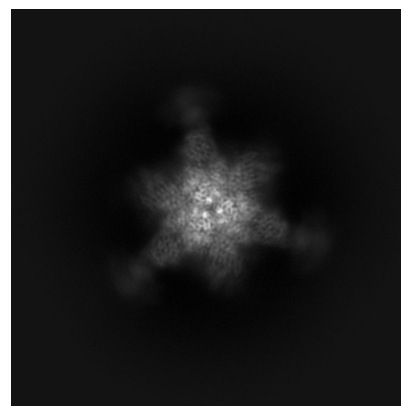
6.1.1 Primary map



X

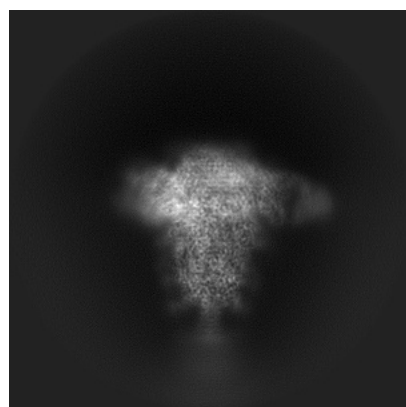


Y

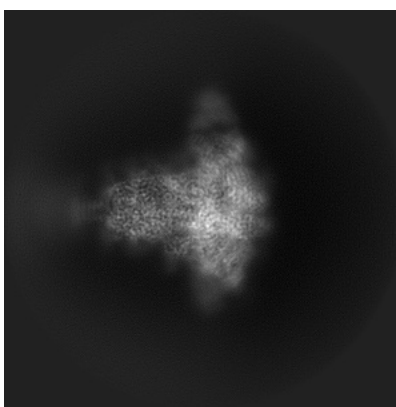


Z

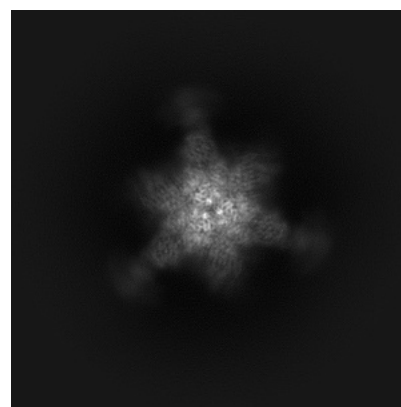
6.1.2 Raw map



X



Y

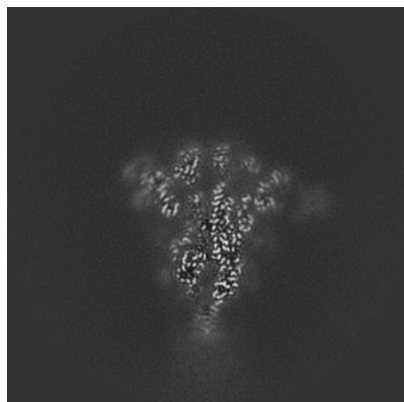


Z

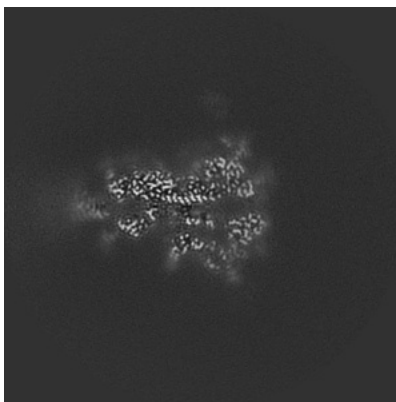
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

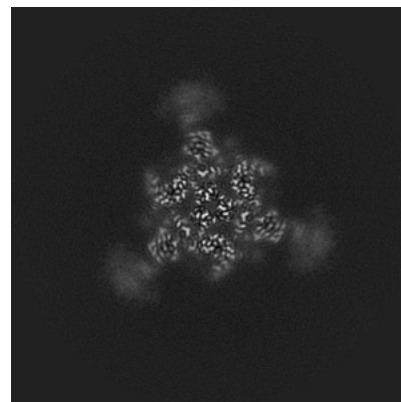
6.2.1 Primary map



X Index: 240

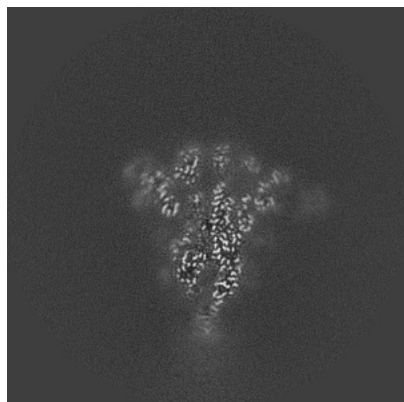


Y Index: 240

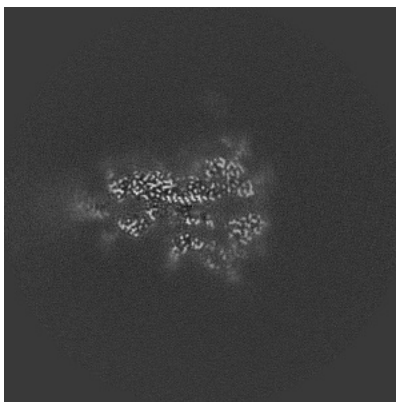


Z Index: 240

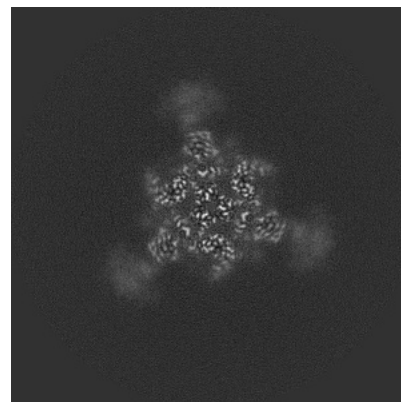
6.2.2 Raw map



X Index: 240



Y Index: 240

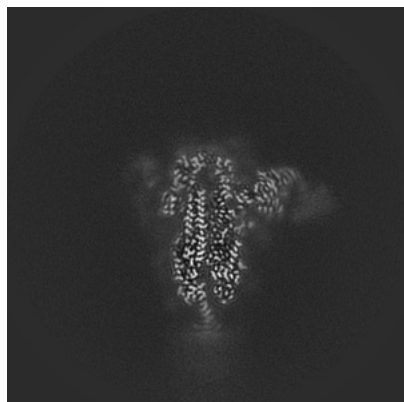


Z Index: 240

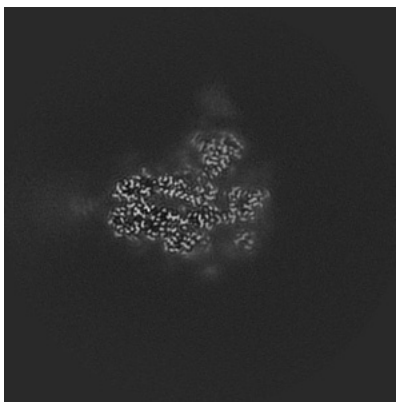
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

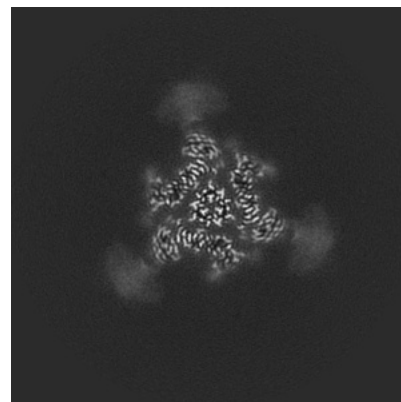
6.3.1 Primary map



X Index: 232

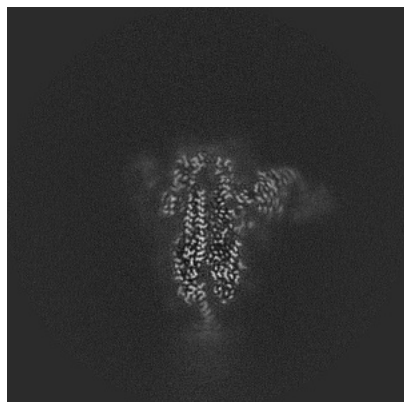


Y Index: 225

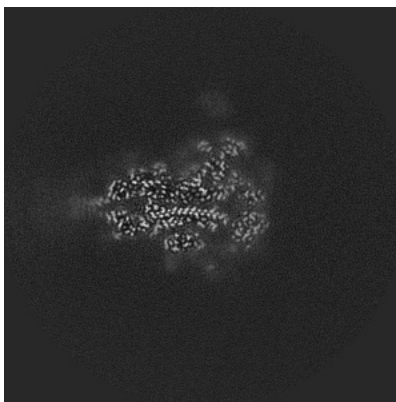


Z Index: 244

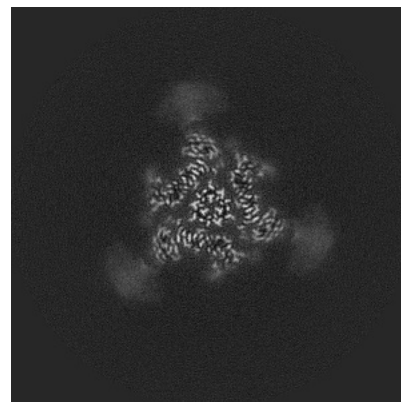
6.3.2 Raw map



X Index: 232



Y Index: 232

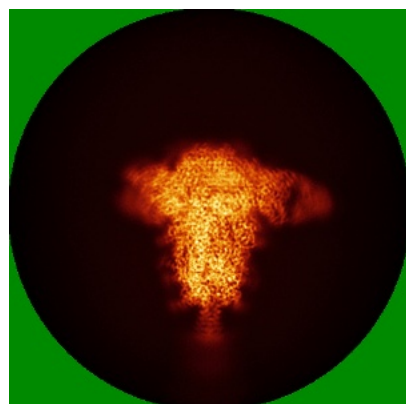


Z Index: 244

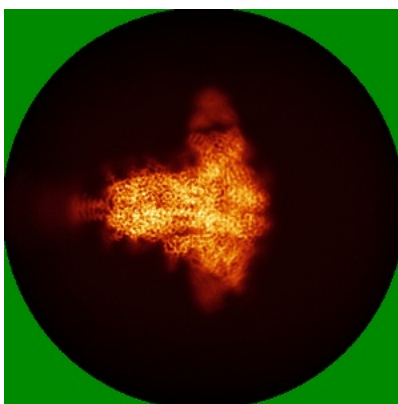
The images above show the largest variance slices of the map in three orthogonal directions.

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

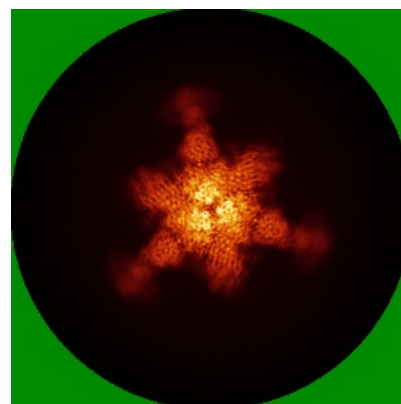
6.4.1 Primary map



X

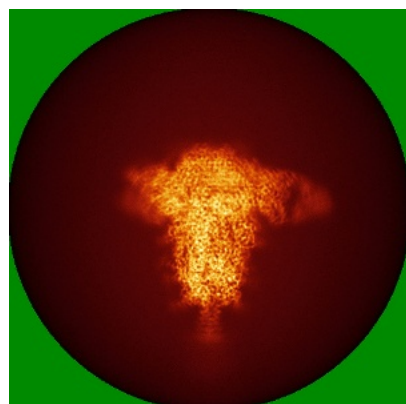


Y

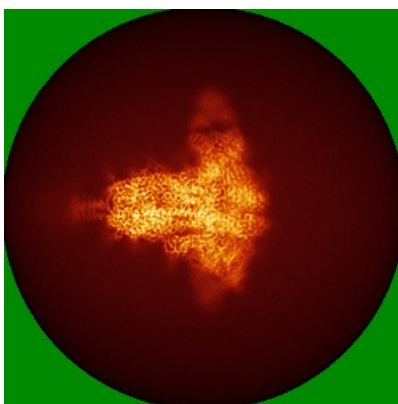


Z

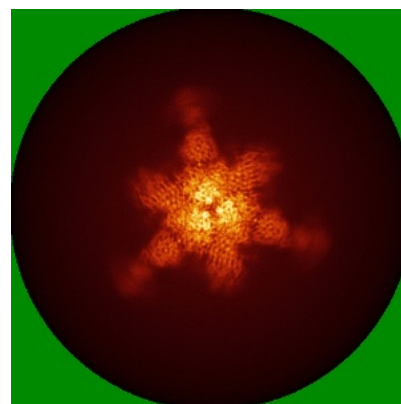
6.4.2 Raw map



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



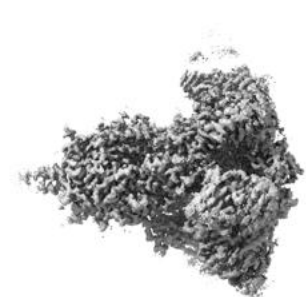
Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

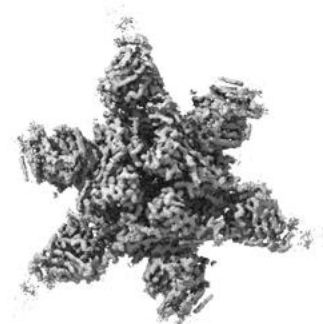
6.5.2 Raw map



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.

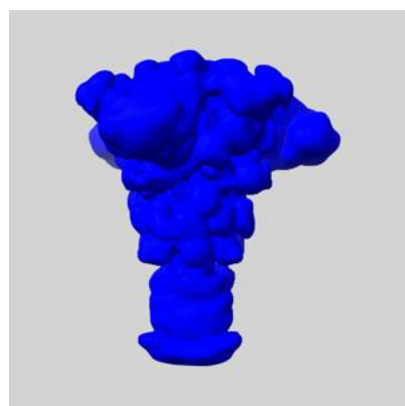
6.6 Mask visualisation [i](#)

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

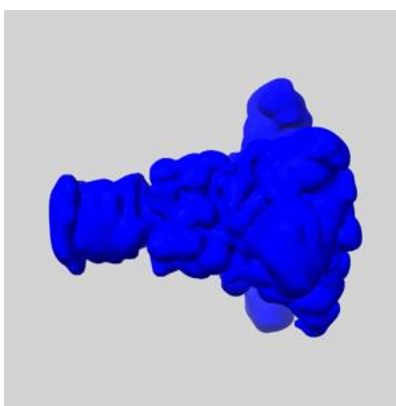
A mask typically either:

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

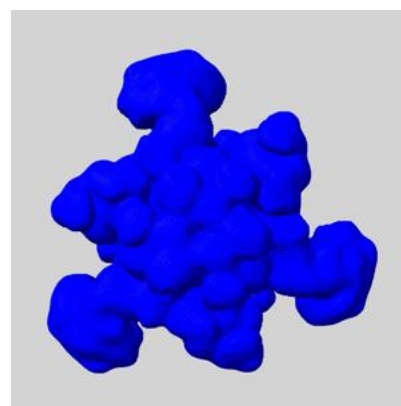
6.6.1 emd_38372_msk_1.map [i](#)



X



Y

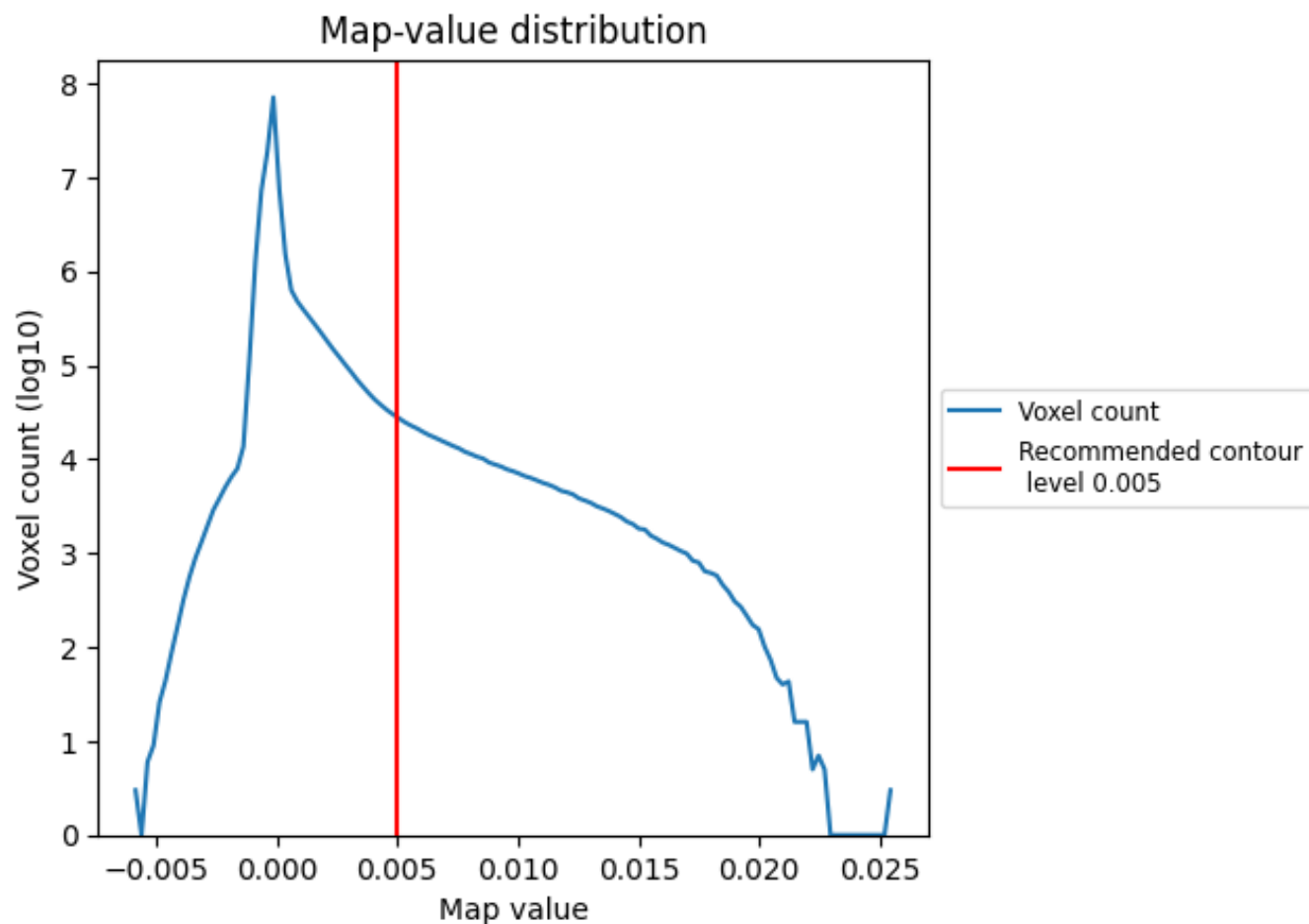


Z

7 Map analysis [i](#)

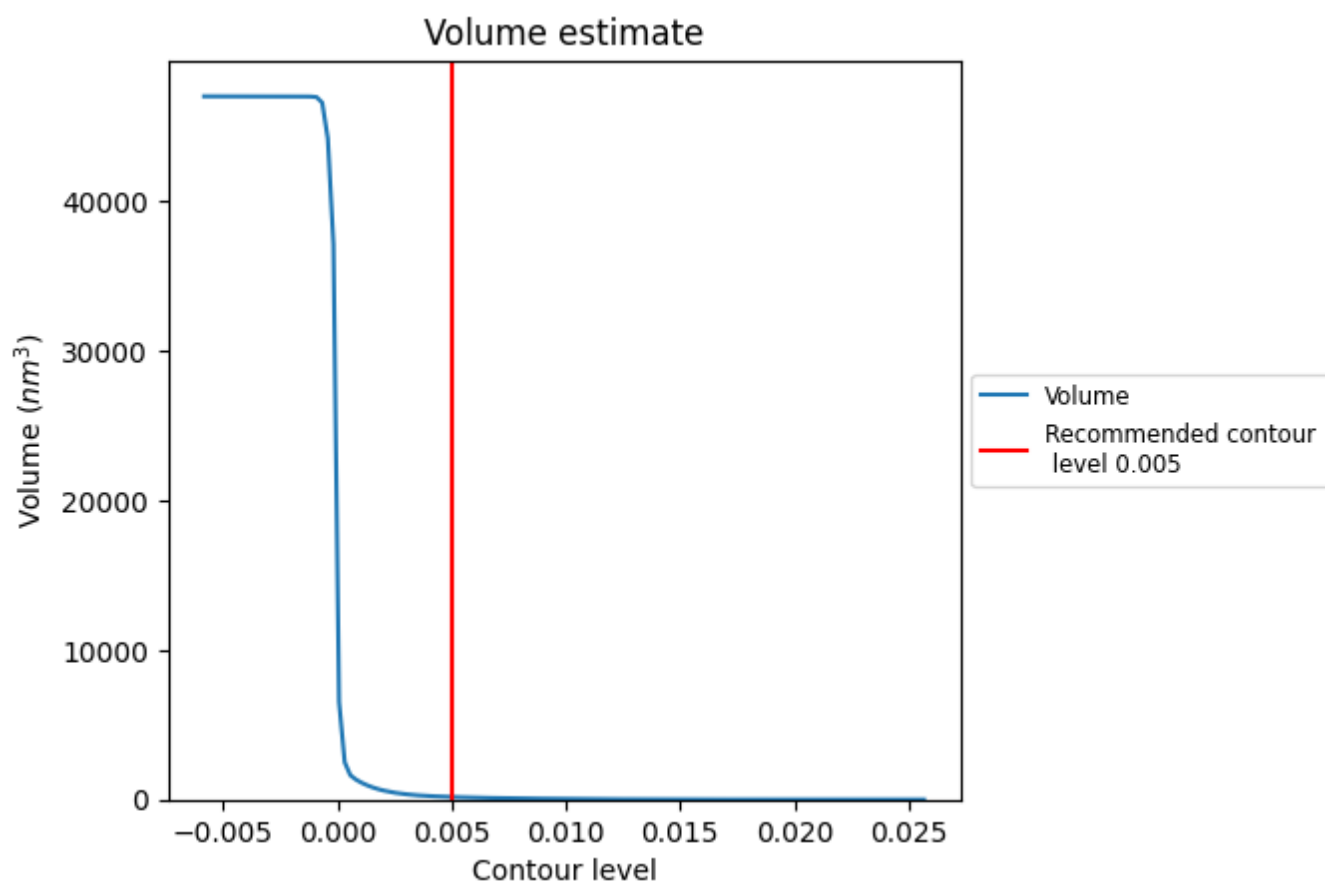
This section contains the results of statistical analysis of the map.

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.

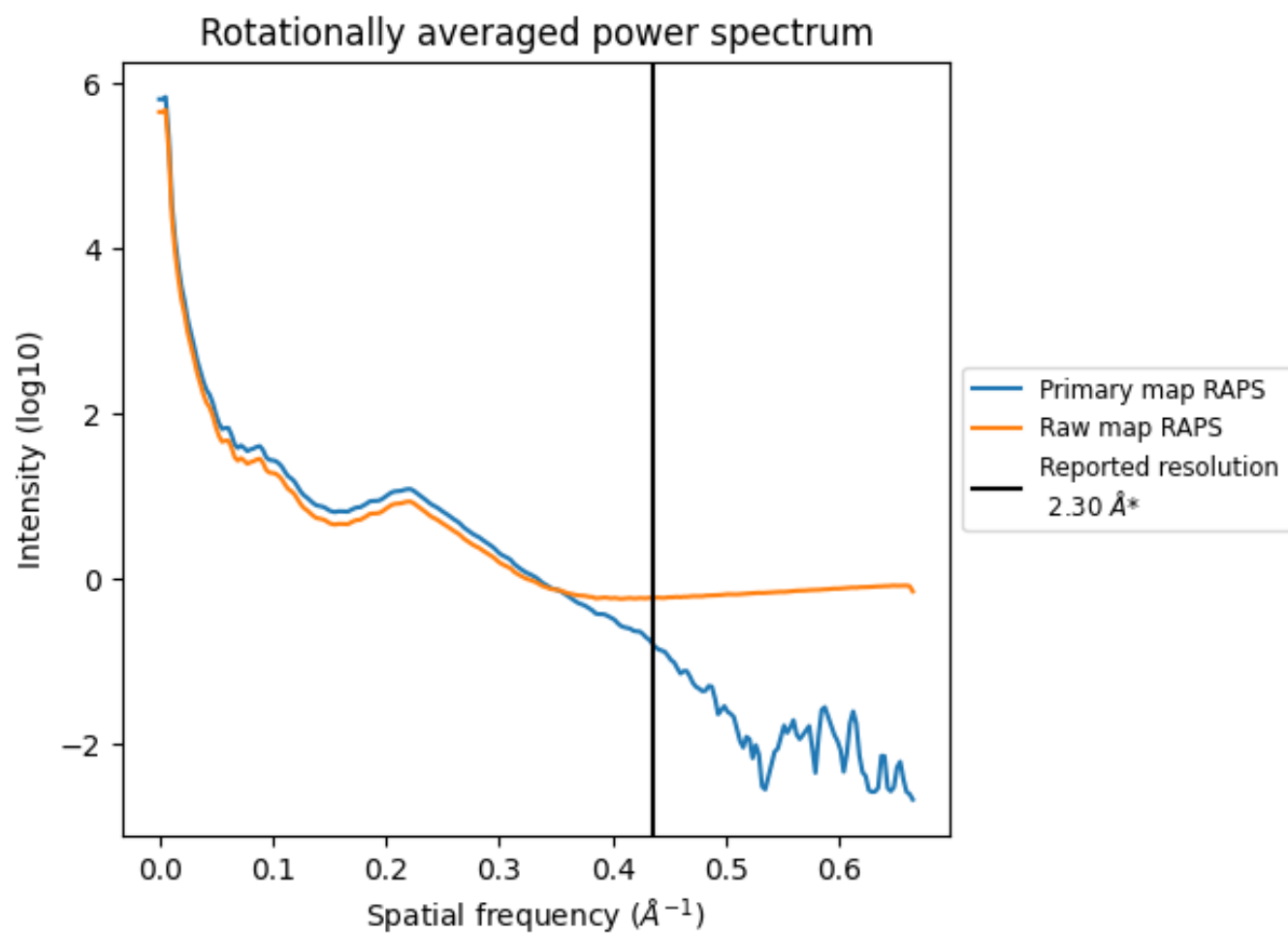
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm^3 ; this corresponds to an approximate mass of 155 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 ⓘ

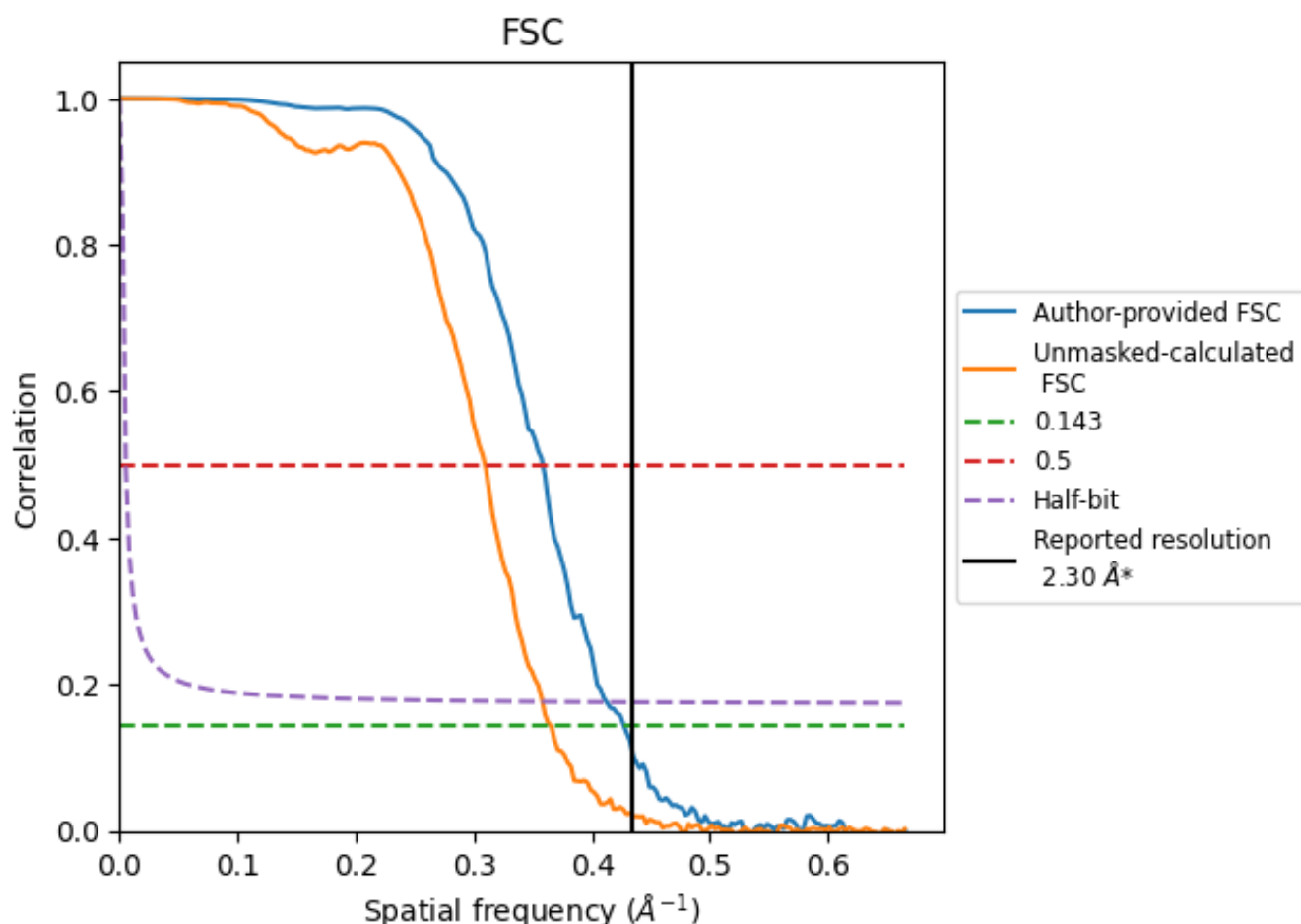


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

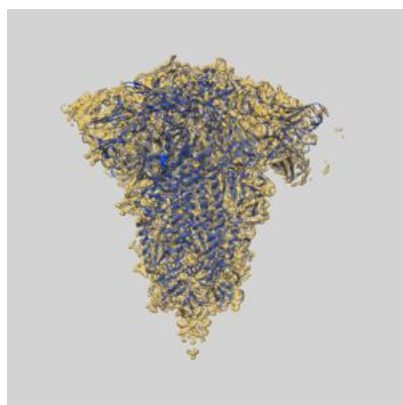
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.34	2.79	2.42
Unmasked-calculated*	2.74	3.23	2.79

*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 2.74 differs from the reported value 2.3 by more than 10 %

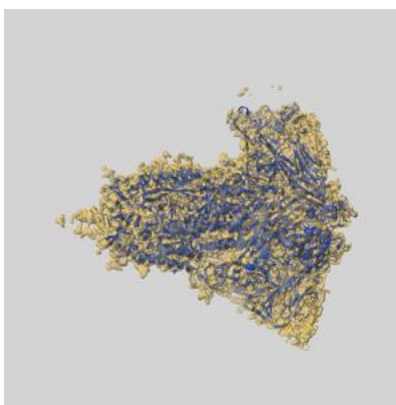
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38372 and PDB model 8XI6. Per-residue inclusion information can be found in section 3 on page 14.

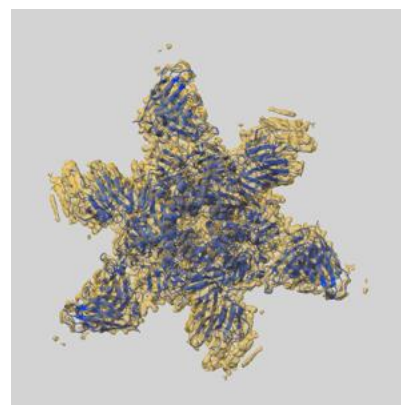
9.1 Map-model overlay [i](#)



X



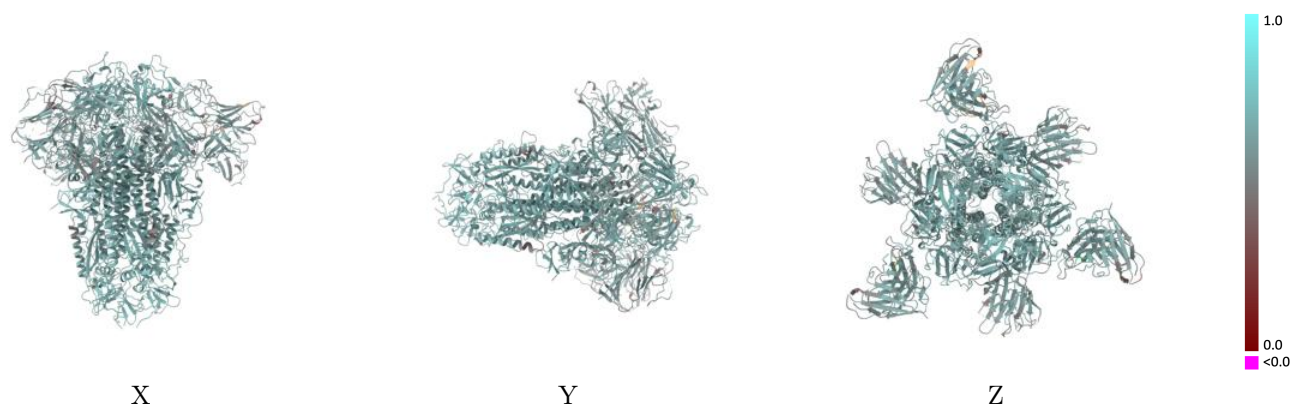
Y



Z

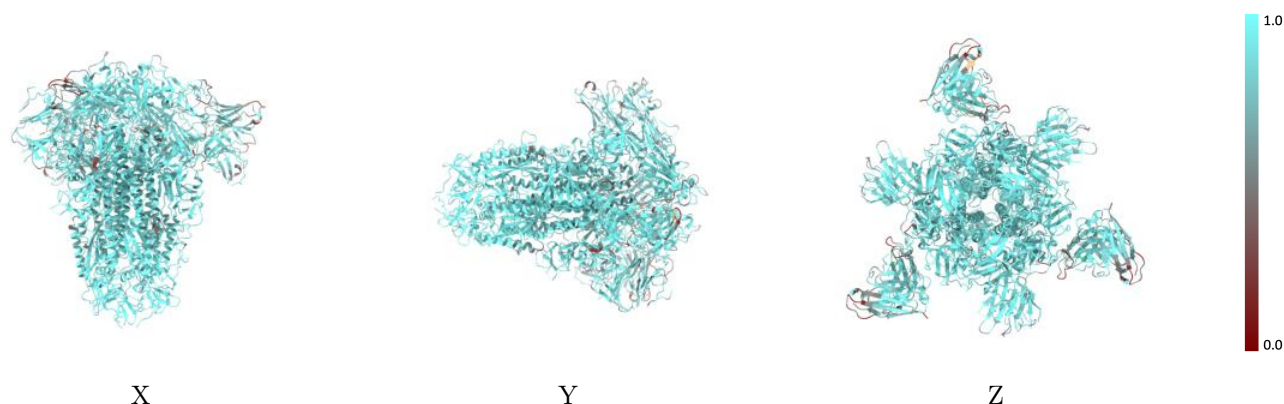
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



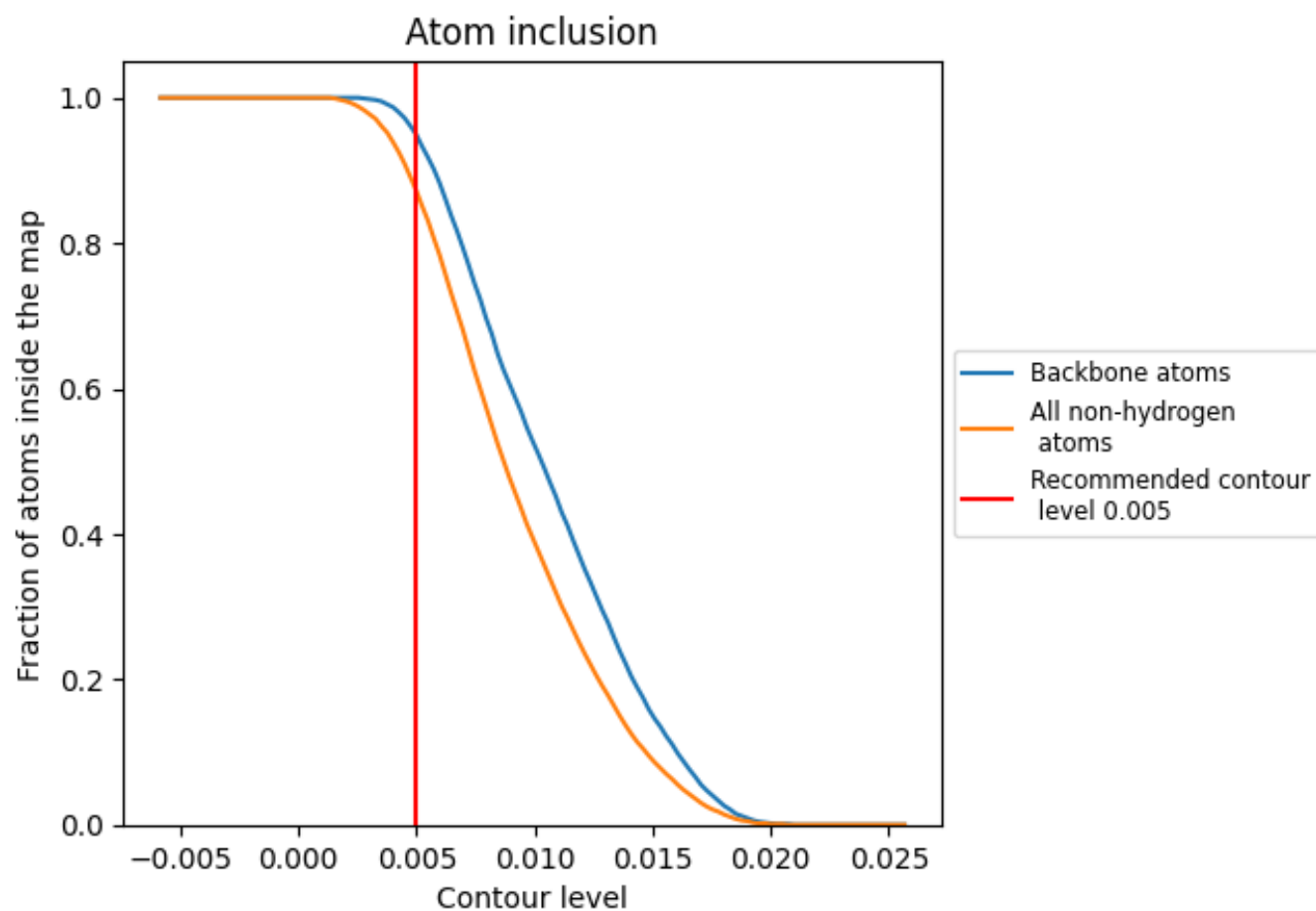
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8720	 0.6120
A	 0.8970	 0.6220
B	 0.8980	 0.6220
C	 0.8970	 0.6220
D	 0.7590	 0.5740
E	 0.8120	 0.5750
F	 0.7590	 0.5750
G	 0.8120	 0.5760
H	 0.7610	 0.5790
I	 0.8130	 0.5760
J	 0.6070	 0.4850
K	 0.6790	 0.5610
L	 0.6790	 0.5660
M	 0.5710	 0.5450
N	 0.3420	 0.4390
O	 0.6070	 0.4790
P	 0.6790	 0.5660
Q	 0.6790	 0.5660
R	 0.5710	 0.5360
S	 0.3420	 0.4310
T	 0.6070	 0.4960
U	 0.6790	 0.5580
V	 0.6790	 0.5630
W	 0.5920	 0.5370
X	 0.3420	 0.4400

